Part II: Principles of Quantum Mechanics
Examples Sheet 1 Solutions

Please send all comments and corrections to jmm232@cam.ac.uk.

1. Let $|\mathbf{x}\rangle$ and $|\mathbf{p}\rangle$ be eigenstates of the three-dimensional position and momentum operators respectively.

   (i) Given that $\langle \mathbf{x}|\mathbf{p}\rangle = e^{i\mathbf{x}\cdot\mathbf{p}/\hbar}/(2\pi\hbar)^{3/2}$, show that

   $$\langle \mathbf{x}|L_z|\psi\rangle = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\psi(\mathbf{x}), \qquad \langle \mathbf{p}|L_z|\psi\rangle = -i\hbar\left(p_x\frac{\partial}{\partial p_y} - p_y\frac{\partial}{\partial p_x}\right)\tilde{\psi}(\mathbf{p}),$$

   where $L_z = XP_y - YP_x$, and $|\psi\rangle$ is a generic state with position and momentum wavefunctions $\psi(\mathbf{x}) = \langle \mathbf{x}|\psi\rangle$ and $\tilde{\psi}(\mathbf{p}) = \langle \mathbf{p}|\psi\rangle$.

   (ii) Find the position space wavefunction of $e^{-i\mathbf{a}\cdot\mathbf{P}/\hbar}\,|\psi\rangle$ and the momentum space wavefunction of $e^{i\mathbf{k}\cdot\mathbf{X}}\,|\psi\rangle$, where **a** and **k** are constants.

Solution: (i) Recall that in Part II Principles of Quantum Mechanics, we work with *states in Hilbert space*, rather than with wavefunctions (which you worked with in Part IB Quantum Mechanics). Wavefunctions are now interpreted as the *components of state vectors* in a *continuum basis of Hilbert space*. In mathematical notation, a state $|\psi\rangle$ in Hilbert space may be expressed in terms of the continuum basis of position eigenstates $|\mathbf{x}\rangle$ as:

$$|\psi\rangle = \int d^3\mathbf{x}\ \langle \mathbf{x}|\psi\rangle\,|\mathbf{x}\rangle = \int d^3\mathbf{x}\,\psi(\mathbf{x})\,|\mathbf{x}\rangle\,.$$

Here, $\psi(\mathbf{x}) = \langle \mathbf{x}|\psi\rangle$ is the *position wavefunction* of the state $|\psi\rangle$. Similarly, we can write the state $|\psi\rangle$ in terms of the continuum basis of momentum eigenstates $|\mathbf{p}\rangle$:

$$|\psi\rangle = \int d^3\mathbf{p}\ \langle \mathbf{p}|\psi\rangle\,|\mathbf{p}\rangle = \int d^3\mathbf{p}\,\psi(\mathbf{p})\,|\mathbf{p}\rangle\,.$$

Here, $\psi(\mathbf{p}) = \langle \mathbf{p}|\psi\rangle$ is the *momentum wavefunction* of the state $|\psi\rangle$.

This question is asking us: 'what happens to the position wavefunction, and the momentum wavefunction, of the state $|\psi\rangle$ when we act on it with the operator L_z?'. This is exactly the sort of question you asked (in less formal language) when you discussed angular momentum in Part IB Quantum Mechanics - here, we will just formalise the argument.

For the first equality, we can calculate:

$$\begin{aligned}\langle \mathbf{x}|L_z|\psi\rangle &= \langle \mathbf{x}|XP_y - YP_x|\psi\rangle && \text{(definition of } L_z\text{)}\\ &= \langle \mathbf{x}|XP_y|\psi\rangle - \langle \mathbf{x}|YP_x|\psi\rangle\,.\end{aligned}$$

We now see that X and Y are close to a bra $\langle \mathbf{x}|$. We notice that we can convert the operators X and Y to eigenvalues through the following manipulation:

$$\begin{aligned}\langle \mathbf{x}|XP_y|\psi\rangle &= (X\,|\mathbf{x}\rangle)^\dagger P_y\,|\psi\rangle && \text{(since } X \text{ is Hermitian, and } |\mathbf{x}\rangle^\dagger = \langle \mathbf{x}|\text{)}\\ &= (x\,|\mathbf{x}\rangle)^\dagger P_y\,|\psi\rangle && (|\mathbf{x}\rangle \text{ is an eigenstate of } X)\\ &= x\,\langle \mathbf{x}|P_y|\psi\rangle\,.\end{aligned}$$

In the final step, we note that $x \in \mathbb{R}$ so $x^\dagger = x$. We also note that since x is just a number, we can take it out of the bra-ket expression. Similarly, we have $\langle \mathbf{x}|YP_x|\psi\rangle = y\,\langle \mathbf{x}|P_x|\psi\rangle$. Therefore, we have

$$\langle \mathbf{x}|L_z|\psi\rangle = x\,\langle \mathbf{x}|P_y|\psi\rangle - y\,\langle \mathbf{x}|P_x|\psi\rangle\,.$$

It remains to evaluate two expressions of the form $\langle \mathbf{x}|P_i|\psi\rangle$. To do so, we use the property of *resolution of identity*.

Resolution of identity: The position and momentum bases for Hilbert space satisfy the property of *resolution of identity*:

$$\int d^3\mathbf{x}\ |\mathbf{x}\rangle\langle\mathbf{x}| = 1, \qquad \int d^3\mathbf{p}\,|\mathbf{p}\rangle\langle\mathbf{p}| = 1,$$

where 1 denotes the identity operator.

These results are a special case of a more general theorem for spanning sets in Hilbert spaces:

Theorem: The (discrete or continuous) orthonormal set $\{|a\rangle\}$ spans Hilbert space if and only if $\int da\ |a\rangle\langle a| = 1$.

Proof: Suppose that the identity holds. Then for any state $|\psi\rangle$ in Hilbert space, we have

$$|\psi\rangle = 1\,|\psi\rangle = \left(\int da\ |a\rangle\langle a|\right)|\psi\rangle = \int da\ \langle a|\psi\rangle\,|a\rangle\,.$$

Hence we can express $|\psi\rangle$ as a linear combination of the $\{|a\rangle\}$, and so $\{|a\rangle\}$ spans. Conversely, suppose that $\{|a\rangle\}$ spans. Then given any state $|\psi\rangle$, we can write:

$$|\psi\rangle = \int da\,\psi(a)\,|a\rangle$$

for some set of coefficients $\psi(a)$ (which we usually call a *wavefunction* with respect to the spanning set $\{|a\rangle\}$). Contracting with the bra $\langle a'|$ and using orthonormality, we find $\psi(a) = \langle a|\psi\rangle$, and hence we have:

$$|\psi\rangle = \int da\ |a\rangle\langle a|\psi\rangle = \left(\int da\ |a\rangle\langle a|\right)|\psi\rangle \qquad \Rightarrow \qquad \int da\ |a\rangle\langle a| = 1. \qquad \square$$

Now we know a little more about resolution of identity, we can evaluate the expression $\langle\mathbf{x}|P_i|\psi\rangle$. We have:

$$\begin{aligned}
\langle\mathbf{x}|P_i|\psi\rangle &= \int d^3\mathbf{p}\ \langle\mathbf{x}|P_i|\mathbf{p}\rangle\langle\mathbf{p}|\psi\rangle && \text{(resolution of identity)}\\
&= \int d^3\mathbf{p}\,p_i\,\langle\mathbf{x}|\mathbf{p}\rangle\langle\mathbf{p}|\psi\rangle && \text{(since } P_i\,|\mathbf{p}\rangle = p_i\,|\mathbf{p}\rangle\text{)}\\
&= \int d^3\mathbf{p}\,p_i(2\pi\hbar)^{-3/2}e^{i\mathbf{x}\cdot\mathbf{p}/\hbar}\langle\mathbf{p}|\psi\rangle && \text{(}\langle\mathbf{x}|\mathbf{p}\rangle\text{ given in question)}\\
&= -i\hbar\frac{\partial}{\partial x_i}\int d^3\mathbf{p}\,(2\pi\hbar)^{-3/2}e^{i\mathbf{x}\cdot\mathbf{p}/\hbar}\langle\mathbf{p}|\psi\rangle && \text{(since } \partial(e^{i\mathbf{x}\cdot\mathbf{p}/\hbar})/\partial x_i = ip_ie^{i\mathbf{x}\cdot\mathbf{p}/\hbar}/\hbar\text{)}\\
&= -i\hbar\frac{\partial}{\partial x_i}\int d^3\mathbf{p}\,\langle\mathbf{x}|\mathbf{p}\rangle\langle\mathbf{p}|\psi\rangle\\
&= -i\hbar\frac{\partial}{\partial x_i}\langle\mathbf{x}|\psi\rangle && \text{(resolution of identity again).}
\end{aligned}$$

We now have everything we need. Putting all our results together, we get the required result:

$$\langle\mathbf{x}|L_z|\psi\rangle = x\,\langle\mathbf{x}|P_y|\psi\rangle - y\,\langle\mathbf{x}|P_x|\psi\rangle = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\langle\mathbf{x}|\psi\rangle\,.$$

We now do the analogous calculation in momentum space in order to compute $\langle \mathbf{p}|L_z|\psi\rangle$. The methods used are exactly the same as for $\langle \mathbf{x}|L_z|\psi\rangle$. First, we note:

$$L_z = XP_y - YP_x = P_yX - P_xY,$$

since the canonical commutation relation $[X_i, P_j] = i\hbar\delta_{ij}$ tells us that different components of $\mathbf{X}$ and $\mathbf{P}$ commute with one another (as $\delta_{ij} = 0$ for $i \neq j$). Therefore, we have:

$$\langle \mathbf{p}|L_z|\psi\rangle = \langle \mathbf{p}|P_yX - P_xY|\psi\rangle = p_y \langle \mathbf{p}|X|\psi\rangle - p_x \langle \mathbf{p}|Y|\psi\rangle ,$$

just as in the position space calculation. We must now evaluate two expressions of the form $\langle \mathbf{p}|X_i|\psi\rangle$; again we use resolution of identity:

$$\langle \mathbf{p}|X_i|\psi\rangle = \int d^3\mathbf{x}\ \langle \mathbf{p}|X_i|\mathbf{x}\rangle \langle \mathbf{x}|\psi\rangle = \int d^3\mathbf{x}\, x_i \langle \mathbf{p}|\mathbf{x}\rangle \langle \mathbf{x}|\psi\rangle = \int d^3\mathbf{x}\, x_i (2\pi\hbar)^{-3/2} e^{-i\mathbf{x}\cdot\mathbf{p}/\hbar} \langle \mathbf{x}|\psi\rangle$$

$$= i\hbar\frac{\partial}{\partial p_i}\int d^3\mathbf{x}\,(2\pi\hbar)^{-3/2} e^{-i\mathbf{x}\cdot\mathbf{p}/\hbar} \langle \mathbf{x}|\psi\rangle = i\hbar\frac{\partial}{\partial p_i}\int d^3\mathbf{x}\,\langle \mathbf{p}|\mathbf{x}\rangle \langle \mathbf{x}|\psi\rangle = i\hbar\frac{\partial}{\partial p_i}\langle \mathbf{p}|\psi\rangle .$$

Thus, putting all the pieces together, we see that:

$$\langle \mathbf{p}|L_z|\psi\rangle = p_y \langle \mathbf{p}|X|\psi\rangle - p_x \langle \mathbf{p}|Y|\psi\rangle = i\hbar\left(p_y\frac{\partial}{\partial p_x} - p_x\frac{\partial}{\partial p_y}\right)\langle \mathbf{p}|\psi\rangle = -i\hbar\left(p_x\frac{\partial}{\partial p_y} - p_y\frac{\partial}{\partial p_x}\right)\langle \mathbf{p}|\psi\rangle ,$$

as required.

(ii) In the second part of this question, we must first find the position state wavefunction of $e^{-i\mathbf{a}\cdot\mathbf{P}/\hbar}|\psi\rangle$. We can do this directly using the results on how momentum operators act on position wavefunctions from part (i):

$$\langle \mathbf{x}|e^{-i\mathbf{a}\cdot\mathbf{P}/\hbar}|\psi\rangle = \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n a_{j_1}...a_{j_n}\langle \mathbf{x}|P_{j_1}...P_{j_n}|\psi\rangle \qquad \text{(expanding exponential, and using index notation)}$$

$$= \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n (-i\hbar)^n a_{j_1}...a_{j_n}\frac{\partial}{\partial x_{j_1}}...\frac{\partial}{\partial x_{j_n}}\langle \mathbf{x}|\psi\rangle \qquad \text{(repeatedly using part (i))}$$

$$= \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\mathbf{a}\cdot\nabla_{\mathbf{x}}\right)^n \psi(\mathbf{x}) \qquad \text{(restoring vector notation)}$$

$$= \psi(\mathbf{x}-\mathbf{a}) \qquad \text{(Taylor's theorem)}.$$

Hence we see that the operator $e^{-i\mathbf{a}\cdot\mathbf{P}/\hbar}$ results in a *translation* of the states $|\psi\rangle$ by $\mathbf{a}$. Similarly, we can compute the momentum space wavefunction of the state $e^{i\mathbf{k}\cdot\mathbf{X}}|\psi\rangle$ using the results from part (i):

$$\langle \mathbf{p}|e^{i\mathbf{k}\cdot\mathbf{X}}|\psi\rangle = \sum_{n=0}^{\infty}\frac{i^n}{n!}k_{j_1}...k_{j_n}\langle \mathbf{p}|X_{j_1}...X_{j_n}|\psi\rangle \qquad \text{(expanding exponential, and using index notation)}$$

$$= \sum_{n=0}^{\infty}\frac{i^n}{n!}(i\hbar)^n k_{j_1}...k_{j_n}\frac{\partial}{\partial p_{j_1}}...\frac{\partial}{\partial p_{j_n}}\langle \mathbf{p}|\psi\rangle \qquad \text{(repeatedly using part (i))}$$

$$= \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\hbar\mathbf{k}\cdot\nabla_{\mathbf{p}}\right)^n \tilde{\psi}(\mathbf{p}) \qquad \text{(restoring vector notation)}$$

$$= \tilde{\psi}(\mathbf{p}-\hbar\mathbf{k}) \qquad \text{(Taylor's theorem)}.$$

Hence we see that the operator $e^{i\mathbf{k}\cdot\mathbf{X}}$ results in a translation of the state in *momentum* space by $\hbar\mathbf{k}$. That is, the operator $e^{i\mathbf{k}\cdot\mathbf{X}}$ is the 'momentum boost operator' in quantum mechanics.

⁕ **Comments:** The main result that we used in this question was *resolution of identity* (or *completeness*):

$$\int d^3\mathbf{x}\ |\mathbf{x}\rangle\ \langle\mathbf{x}| = 1, \qquad \int d^3\mathbf{p}\ |\mathbf{p}\rangle\ \langle\mathbf{p}| = 1.$$

As we proved, this holds for a set of orthonormal states $\{|a\rangle\}$ if and only if they span Hilbert space. Using this identity, we are able to derive the standard actions of the operators that we saw in Part IB Quantum Mechanics.

The results of this question can be freely generalised. In particular, we have the Theorem:

Theorem: Let $f(\mathbf{X}, \mathbf{P})$ be a function of the position and momentum operators. Let $|\psi\rangle$ be a state in Hilbert space with position-space expansion:

$$|\psi\rangle = \int d^3\mathbf{x}\, \psi(\mathbf{x})\, |\mathbf{x}\rangle\ ,$$

where $\psi(\mathbf{x}) = \langle\mathbf{x}|\psi\rangle$ is the wavefunction. Assuming that f is *normal ordered*, that is, all momentum operators are to the right of all position operators in some expansion of f, then $f(\mathbf{X}, \mathbf{P})\ |\psi\rangle$ has the position-space expansion:

$$f(\mathbf{X}, \mathbf{P})\ |\psi\rangle = \int d^3\mathbf{x}\, f(\mathbf{x}, -i\hbar\nabla)\psi(\mathbf{x})\ |\mathbf{x}\rangle\ ,$$

i.e. the position-space wavefunction of $f(\mathbf{X}, \mathbf{P})\ |\psi\rangle$ is $f(\mathbf{x}, -i\hbar\nabla)\psi(\mathbf{x})$.

Proof: We use the same techniques as we used in this question. The required wavefunction is:

$$\langle\mathbf{x}|f(\mathbf{X}, \mathbf{P})|\psi\rangle\ .$$

Since f is normal ordered, **X** can act to the left without having to commute past any **P**'s. Therefore we have:

$$\langle\mathbf{x}|f(\mathbf{X}, \mathbf{P})|\psi\rangle = \langle\mathbf{x}|f(\mathbf{x}, \mathbf{P})|\psi\rangle\ .$$

Inserting a resolution of identity, we have

$$\langle\mathbf{x}|f(\mathbf{x}, \mathbf{P})|\psi\rangle = \int d^3\mathbf{x}\ \langle\mathbf{x}|f(\mathbf{x}, \mathbf{P})|\mathbf{p}\rangle\ \langle\mathbf{p}|\psi\rangle = \int d^3\mathbf{x}\, f(\mathbf{x}, \mathbf{p})\ \langle\mathbf{x}|\mathbf{p}\rangle\ \langle\mathbf{p}|\psi\rangle$$

Recalling the expression for $\langle\mathbf{x}|\mathbf{p}\rangle$, we have

$$\int d^3\mathbf{x}\, f(\mathbf{x}, \mathbf{p})(2\pi\hbar)^{-3/2} e^{i\mathbf{x}\cdot\mathbf{p}/\hbar}\ \langle\mathbf{p}|\psi\rangle\ .$$

Given a little thought (consider perhaps expanding f in a Taylor series in **p**), we have

$$\int d^3\mathbf{x}\, f(\mathbf{x}, \mathbf{p})(2\pi\hbar)^{-3/2} e^{i\mathbf{x}\cdot\mathbf{p}/\hbar}\ \langle\mathbf{p}|\psi\rangle = \int d^3\mathbf{x}\, f(\mathbf{x}, -i\hbar\nabla)(2\pi\hbar)^{-3/2} e^{i\mathbf{x}\cdot\mathbf{p}/\hbar}\ \langle\mathbf{p}|\psi\rangle\ .$$

Restoring $(2\pi\hbar)^{-3/2} e^{i\mathbf{x}\cdot\mathbf{p}/\hbar} = \langle\mathbf{x}|\mathbf{p}\rangle$, and applying resolution of identity again, we have the result. □

Note that whilst normal ordering is not strictly necessary, it *is* necessary to specify some ordering of the function $f(\mathbf{X}, \mathbf{P})$. Whilst the functions

$$f_1(\mathbf{x}, \mathbf{p}) = \mathbf{x} \cdot \mathbf{p}, \qquad f_2(\mathbf{x}, \mathbf{p}) = \mathbf{p} \cdot \mathbf{x},$$

are the same in the classical sense, they are *not* the same in the quantum sense. The actions on wavefunctions of these two operators, namely

$$-i\hbar\mathbf{x} \cdot \nabla\psi, \qquad -i\hbar\nabla \cdot (\mathbf{x}\psi).$$

are very different!

2. Let A and B be any operators which each commute with $[A, B]$, and let $\lambda \in \mathbb{C}$.

(i) Prove that $[A, B^n] = nB^{n-1}[A, B]$ for all $n \in \mathbb{N}_0$, and that $[A, e^B] = e^B[A, B]$.

(ii) Define an operator-valued function $F(\lambda) = e^{\lambda A}e^{\lambda B}e^{-\lambda(A+B)}$. Show that $F'(\lambda) = \lambda[A, B]F(\lambda)$. Hence deduce that

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]} = e^B e^A e^{[A,B]}.$$

Now let A and B be any operators (not necessarily commuting with $[A, B]$):

(iii) Prove that $d(e^{\lambda A}Be^{-\lambda A})/d\lambda = e^{\lambda A}[A, B]e^{-\lambda A}$. Hence deduce that:

$$e^A Be^{-A} = B + [A, B] + \frac{1}{2}[A, [A, B]] + \cdots .$$

Solution: (i) We use induction. The base case is $n = 1$, for which we have $[A, B] = 1 \cdot B^{1-1}[A, B] = [A, B]$, and hence the result holds trivially. Assume the result holds for $n = k$, and consider the case $n = k + 1$. We have:

$$[A, B^{k+1}] = [A, B^k]B + B^k[A, B], \tag{$*$}$$

by the *Leibniz rule*, which you should recall from Part IB Quantum Mechanics:

$$[A, BC] = [A, B]C + B[A, C].$$

Evaluating $(*)$ using the induction hypothesis for $n = k$, we have:

$$[A, B^{k+1}] = kB^{k-1}[A, B]B + B^k[A, B] = (k + 1)B^k[A, B],$$

which is the required result. In the last step, we used the fact that B commutes with $[A, B]$.

For the next part, we simply recall the definition of the exponential of an operator, and apply (i). We have:

$$[A, e^B] = \sum_{n=1}^{\infty} \frac{1}{n!}[A, B^n] = \sum_{n=1}^{\infty} \frac{1}{n!} nB^{n-1}[A, B] = \left(\sum_{n=1}^{\infty} \frac{B^{n-1}}{(n-1)!}\right)[A, B] = e^B[A, B],$$

which is the required result. Note in the first step that our sum starts at $n = 1$ rather than $n = 0$; this is allowed because $[A, B^0] = [A, I] = 0$, trivially.

(ii) To find the derivative of $F(\lambda)$, we need to be able to differentiate $e^{\lambda A}$. We have:

$$\frac{d}{d\lambda}(e^{\lambda A}) = \frac{d}{d\lambda}\left(\sum_{n=0}^{\infty} \frac{(\lambda A)^n}{n!}\right) = A\sum_{n=1}^{\infty} \frac{\lambda^{n-1}A^{n-1}}{(n-1)!} = Ae^{\lambda A}.$$

In the third step, we factored out A to the left; we could also have factored out A to the right, so

$$\frac{d}{d\lambda}(e^{\lambda A}) = Ae^{\lambda A} = e^{\lambda A}A.$$

We are now ready to differentiate $F(\lambda)$. We have:

$$F'(\lambda) = Ae^{\lambda A}e^{\lambda B}e^{-\lambda(A+B)} + e^{\lambda A}Be^{\lambda B}e^{-\lambda(A+B)} - e^{\lambda A}e^{\lambda B}(A + B)e^{-\lambda(A+B)}.$$

Begin by noting that the terms where we brought down a B cancel, since B commutes with $e^{\lambda B}$. To get the required form, commute A past $e^{\lambda B}$ and $e^{\lambda A}$ (note A commutes with $e^{\lambda A}$) in the final term to give:

$$F'(\lambda) = Ae^{\lambda A}e^{\lambda B}e^{-\lambda(A+B)} - Ae^{\lambda A}e^{\lambda B}e^{-\lambda(A+B)} + e^{\lambda A}[e^{\lambda B}, A]e^{-\lambda(A+B)}.$$

The first two terms cancel. The remaining term can be evaluated using (i) above to give:

$$F'(\lambda) = \lambda[A, B]e^{\lambda A}e^{\lambda B}e^{-\lambda(A+B)} = \lambda[A, B]F(\lambda),$$

as required.

We have derived an ordinary differential equation, which we now solve:

$$\frac{dF}{d\lambda} = \lambda[A,B]F \qquad \Rightarrow \qquad \int \frac{1}{F}\, dF = \int \lambda[A,B]\, d\lambda \qquad \Rightarrow \qquad F(\lambda) = Ce^{\frac{1}{2}\lambda^2[A,B]},$$

where C is some constant operator. Comparing with the original form of $F(\lambda)$, we see that:

$$e^{\lambda A}e^{\lambda B}e^{-\lambda(A+B)} = Ce^{\frac{1}{2}\lambda^2[A,B]}.$$

Setting $\lambda = 0$ on both sides, we see that $C = I$, the identity operator. Setting $\lambda = 1$ on both sides, we're left with:

$$e^A e^B e^{-(A+B)} = e^{\frac{1}{2}[A,B]}.$$

We've almost derived the equations in the question. There are two facts that we need to use to finish:

- **Fact 1:** If the matrices C and D commute, then we have $e^C e^D = e^{C+D}$. This has a simple proof. Consider:

  $$e^{tC}e^{tD} = \sum_{m,n=0}^{\infty} \frac{t^{m+n}}{m!n!} C^m D^n.$$

  Setting $s = m + n$ in the sum, we can rewrite this as:

  $$e^{tC}e^{tD} = \sum_{s=0}^{\infty} \frac{t^s}{s!} \sum_{m=0}^{s} \frac{s!}{m!(s-m)!} C^m D^{s-m} = \sum_{s=0}^{\infty} \frac{t^s (C+D)^s}{s!} = e^{t(C+D)}.$$

  Setting $t = 1$, we have the result. □

- **Fact 2:** The inverse of the exponential is the exponential of the negative, i.e. $(e^C)^{-1} = e^{-C}$. This also has a simple proof, and follows immediately from Fact 1. Since C and $-C$ trivially commute for any C, we have from Fact 1:

  $$e^C e^{-C} = e^{C+(-C)} = I,$$

  where I is the identity matrix. The result follows. □

Returning to the equation $e^A e^B e^{-(A+B)} = e^{\frac{1}{2}[A,B]}$, we can multiply through by e^{A+B} and use Fact 2 to obtain:

$$e^A e^B = e^{\frac{1}{2}[A,B]} e^{A+B}.$$

Now since A and B both commute with $[A, B]$, it follows that $A + B$ must commute with $\frac{1}{2}[A, B]$. So by Fact 1, we have

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]}.$$

Hence we have derived the first equality in the question.

We can use this equality to establish the second equality. Since $-A$ and $-B$ both commute with $[-A, -B]$, we have:

$$e^{-A}e^{-B}e^A e^B = e^{-A-B}e^{\frac{1}{2}[A,B]}e^{A+B}e^{\frac{1}{2}[A,B]} = e^{[A,B]},$$

where we can cancel e^{A+B} and e^{-A-B} by Facts 1 and 2. Now multiplying through by e^A and e^B, we finally have the result:

$$e^A e^B = e^B e^A e^{[A,B]}.$$

(iii) In the last part of the question, we now work with operators A, B that don't necessarily commute with their commutator. First we are asked to show that:

$$\frac{d}{d\lambda}\left(e^{\lambda A}Be^{-\lambda A}\right) = e^{\lambda A}[A,B]e^{-\lambda A}.$$

We simply take the derivative directly on the left hand side:

$$\frac{d}{d\lambda}\left(e^{\lambda A}Be^{-\lambda A}\right) = e^{\lambda A}ABe^{-\lambda A} - e^{\lambda A}BAe^{-\lambda A} = e^{\lambda A}[A,B]e^{-\lambda A},$$

as required. It is also useful to note that if we repeatedly take derivatives, we bring down more commutators, so that:

$$\frac{d^n}{d\lambda^n}\left(e^{\lambda A}Be^{-\lambda A}\right) = e^{\lambda A}\mathrm{ad}_A^n(B)e^{-\lambda A},$$

where we define the map ad_A by $\mathrm{ad}_A(B) = [A,B]$, so the nested commutators look like $\mathrm{ad}_A^2(B) = [A,[A,B]]$, $\mathrm{ad}_A^3(B) = [A,[A,[A,B]]]$ etc. We define $\mathrm{ad}_A^0(B) = B$.

Now to derive the final identity, let us consider the Taylor expansion of $e^{\lambda A}Be^{-\lambda A}$ about $\lambda = 0$. We have:

$$\begin{aligned}
e^A Be^{-A} &= \sum_{n=0}^{\infty}\frac{1}{n!}\frac{d^n}{d\lambda^n}\left(e^{\lambda A}Be^{-\lambda A}\right)\Big|_{\lambda=0} && \text{(Taylor's theorem)}\\
&= \sum_{n=0}^{\infty}\frac{1}{n!}\left(e^{\lambda A}\mathrm{ad}_A^n(B)e^{-\lambda A}\right)\Big|_{\lambda=0} && \text{(above work)}\\
&= \sum_{n=0}^{\infty}\frac{1}{n!}\mathrm{ad}_A^n(B) && \text{(setting } \lambda = 0\text{)}.
\end{aligned}$$

This identity is called *Hadamard's lemma*. Writing out the first few terms, we have:

$$B + [A,B] + \frac{1}{2}[A,[A,B]] + \cdots,$$

which is the required expression given in the question.

❊ **Comments**:

The product of exponentials is NOT the exponential of the sum. The most important takeaway from this question is $e^Ae^B \neq e^{A+B}$! Instead, for general operators A and B, we find:

$$e^Ae^B = \exp\left(\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n}\sum_{\substack{r_1+s_1>0\\ \vdots \\ r_n+s_n>0}}\frac{[A^{r_1}B^{s_1}\ldots A^{r_n}B^{s_n}]}{\left(\sum_{j=1}^{n}(r_j+s_j)\right)\cdot\left(\prod_{j=1}^{n}r_j!s_j!\right)}\right),$$

where the sum is over all non-negative values of r_i, s_i, and the notation $[A^{r_1}B^{s_1}\ldots A^{r_n}B^{s_n}]$ means

$$[A^{r_1}B^{s_1}\ldots A^{r_n}B^{s_n}] = \underbrace{[A,[A,\cdots[A}_{r_1},\underbrace{[B,[B,\cdots[B}_{s_1},\cdots\underbrace{[A,[A,\cdots[A}_{r_n},\underbrace{[B,[B,\cdots,B]}_{s_n}\cdots]\cdots].$$

Notice that this is zero if $s_n > 1$. This formula is called the *Baker-Campbell-Hausdorff identity*, and you will meet it properly in Part III Symmetries, Fields and Particles.

In this question, you are asked to prove a special case of the Baker-Campbell Hausdorff identity, when A and B both commute with their commutator $[A, B]$. This is very often the case in quantum mechanics; for example, if X is the position operator and P is the momentum operator, we have $[X, P] = i\hbar$ - hence both operators commute with their commutator.

Commutators are like derivatives. There is another interesting theoretical aspect to this question. We notice the following striking similarities:

Commutator identity	**Derivative identity**
$[A, B^n] = nB^{n-1}[A, B]$	$\frac{d}{dx}\left(f(x)^n\right) = nf(x)^{n-1}\frac{d}{dx}\left(f(x)\right)$
$[A, e^B] = e^B[A, B]$	$\frac{d}{dx}\left(e^{f(x)}\right) = e^{f(x)}\frac{d}{dx}\left(f(x)\right)$
$[A, BC] = [A, B]C + B[A, C]$	$\frac{d}{dx}\left(f(x)g(x)\right) = \frac{d}{dx}\left(f(x)\right)g(x) + f(x)\frac{d}{dx}\left(g(x)\right)$

We notice there's a symmetry between these identities if we replace:

$$[A, \cdot] \leftrightarrow d(\cdot)/dx, \qquad B \leftrightarrow f(x), \qquad C \leftrightarrow g(x).$$

It turns out that these identities generalise completely:

Theorem: If A and B commute with their commutator, $[A, f(B)] = f'(B)[A, B]$ for f analytic.

Proof: Since f is analytic, it is equal to its Taylor series locally. Near $B = 0$, we write: $f(B) = \sum_{n=0}^{\infty} \frac{f_n}{n!} B^n$, where f_n are just numbers. Then we have:

$$[A, f(B)] = \sum_{n=0}^{\infty} \frac{f_n}{n!}[A, B^n] = \left(\sum_{n=1}^{\infty} \frac{f_n}{(n-1)!} B^{n-1}\right)[A, B] = f'(B)[A, B]. \ \square$$

Hadamard's lemma. In the last part of the question, we proved an identity called *Hadamard's lemma*. One application of this lemma is to reverse some of the arguments in the symmetries section of the course. For example, recall that in lectures we showed:

$$\mathbf{P}/\hbar \text{ is the generator of translations} \quad \Rightarrow \quad [\mathbf{X}, \mathbf{P}] = i\hbar I, \text{ the canonical commutation relation,}$$

where I is the 3×3 identity matrix. We can show the reverse implication using Hadamard's lemma:

Theorem: The commutation relation $[\mathbf{X}, \mathbf{P}] = i\hbar I$ implies that $\mathbf{P}/\hbar$ is the infinitesimal generator of translations.

Proof: Assuming $[\mathbf{X}, \mathbf{P}] = i\hbar I$, we have that:

$$[\mathbf{P}/\hbar, \mathbf{X}] = -iI.$$

Consequently, $[\mathbf{P}/\hbar, [\mathbf{P}/\hbar, \mathbf{X}]] = 0$, and similarly all higher commutators vanish. Thus, using Hadamard's lemma, we have:

$$e^{i\mathbf{a}\cdot\mathbf{P}/\hbar}\mathbf{X}e^{-i\mathbf{a}\cdot\mathbf{P}/\hbar} = \frac{1}{0!}\mathbf{X} + \frac{1}{1!}i\mathbf{a}\cdot[\mathbf{P}, \mathbf{X}] = \mathbf{X} + \mathbf{a}. \quad \square$$

3. Let $X(t) = e^{iHt/\hbar}Xe^{-iHt/\hbar}$ and $P(t) = e^{iHt/\hbar}Pe^{-iHt/\hbar}$ where X and P are the usual position and momentum operators, and H is the Hamiltonian of the $d = 1$ harmonic oscillator. Show that:

$$X(t) = X\cos(\omega t) + \frac{1}{m\omega}P\sin(\omega t), \qquad P(t) = P\cos(\omega t) - m\omega X\sin(\omega t),$$

and interpret this result. Evaluate $[X(t), P(t)]$.

Solution: We evaluate the expressions for $X(t)$, $P(t)$ directly using Hadamard's lemma. To apply the lemma, we need to know the nested commutators:

$$\mathrm{ad}_H^n(X) = [\underbrace{H,[H,...,[H,[H}_{n\text{ times}},X]]...]], \qquad \mathrm{ad}_H^n(P) = [\underbrace{H,[H,...,[H,[H}_{n\text{ times}},P]]...]].$$

In this question, it's useful to note that these nested commutators obey $\mathrm{ad}_A^n(\lambda B) = \lambda\mathrm{ad}_A^n(B)$ for all constants $\lambda \in \mathbb{C}$, and $\mathrm{ad}_{\mu A}^n(B) = \mu^n\mathrm{ad}_A^n(B)$ for all constants $\mu \in \mathbb{C}$, by linearity of the commutator.

Let's being by evaluating the simple commutators $[H, X]$ and $[H, P]$. We have (recall H is the Hamiltonian of the harmonic oscillator):

$$[H,X] = \left[\frac{P^2}{2m} + \frac{1}{2}m\omega^2X^2, X\right] = \frac{1}{2m}[P^2,X] = \frac{P}{m}[P,X] = -\frac{i\hbar P}{m},$$

where the second from last equality follows from part (i) of Question 2 (since X and P are operators which commute with their commutator, $[X, P] = i\hbar$). Similarly, we have:

$$[H,P] = \left[\frac{P^2}{2m} + \frac{1}{2}m\omega^2X^2, P\right] = \frac{1}{2}m\omega^2[X^2,P] = m\omega^2X[X,P] = i\hbar m\omega^2X.$$

We can establish the following recursion relations between nested commutators:

$$\mathrm{ad}_H^n(X) = \mathrm{ad}_H^{n-1}([H,X]) = \mathrm{ad}_H^{n-1}\left(-\frac{i\hbar P}{m}\right) = \mathrm{ad}_H^{n-2}\left(-\frac{i\hbar}{m}[H,P]\right) = \mathrm{ad}_H^{n-2}(\hbar^2\omega^2X) = \hbar^2\omega^2\mathrm{ad}_H^{n-2}(X),$$

$$\mathrm{ad}_H^n(P) = \mathrm{ad}_H^{n-1}([H,P]) = \mathrm{ad}_H^{n-1}\left(i\hbar m\omega^2X\right) = \mathrm{ad}_H^{n-2}\left(i\hbar m\omega^2[H,X]\right) = \mathrm{ad}_H^{n-2}\left(\hbar^2\omega^2P\right) = \hbar^2\omega^2\mathrm{ad}_H^{n-2}(P).$$

Iterating these relations, we have:

$$\mathrm{ad}_H^n(X) = \begin{cases} \hbar^n\omega^nX & \text{if } n \text{ is even,} \\ -\dfrac{i\hbar^n\omega^n}{m\omega}P & \text{if } n \text{ is odd,} \end{cases} \qquad \mathrm{ad}_H^n(P) = \begin{cases} \hbar^n\omega^nP & \text{if } n \text{ is even,} \\ im\omega\hbar^n\omega^nX & \text{if } n \text{ is odd.} \end{cases}$$

Using Hadamard's lemma then, we have:

$$e^{iHt/\hbar}Xe^{-iHt/\hbar} = \sum_{n=0}^{\infty}\frac{1}{n!}\mathrm{ad}_{iHt/\hbar}^n(X) = \sum_{n=0}^{\infty}\frac{(it)^n}{n!\hbar^n}\mathrm{ad}_H^n(X) = \sum_{n=0}^{\infty}\frac{(-1)^n(t\omega)^{2n}}{(2n)!}X + \frac{1}{m\omega}\sum_{n=0}^{\infty}\frac{(-1)^n(t\omega)^{2n+1}}{(2n+1)!}P$$

$$= X\cos(\omega t) + \frac{1}{m\omega}P\sin(\omega t), \qquad \text{as required.}$$

Similarly, we have:

$$e^{iHt/\hbar}Pe^{-iHt/\hbar} = \sum_{n=0}^{\infty}\frac{1}{n!}\mathrm{ad}_{iHt/\hbar}^n(P) = \sum_{n=0}^{\infty}\frac{(it)^n}{n!\hbar^n}\mathrm{ad}_H^n(P) = \sum_{n=0}^{\infty}\frac{(-1)^n(t\omega)^{2n}}{(2n)!}P - m\omega\sum_{n=0}^{\infty}\frac{(-1)^n(t\omega)^{2n+1}}{(2n+1)!}X$$

$$= P\cos(\omega t) - m\omega X\sin(\omega t), \qquad \text{as required.}$$

Next we must interpret this result. We notice that these equations are precisely those of a *classical* harmonic oscillator with position $x(t)$ and momentum $p(t)$. To see this, recall that the equations of motion in classical physics are:

$$\frac{dx}{dt} = \frac{p}{m} \text{ (definition of momentum)} \qquad \text{and} \qquad \frac{dp}{dt} = -m\omega^2 x \text{ (Newton's second law)}.$$

We can solve these equations simultaneously, e.g. differentiating the first we get:

$$\frac{d^2x}{dt^2} = \frac{1}{m}\frac{dp}{dt} = -\omega^2 x \qquad \Rightarrow \qquad x(t) = A\cos(\omega t) + B\sin(\omega t).$$

Substituting this into the definition of momentum, we find:

$$p(t) = -A\omega m \sin(\omega t) + B\omega m \cos(\omega t).$$

Now imposing the conditions $x(0) = x_0$ and $p(0) = p_0$, we see that:

$$x(t) = x_0\cos(\omega t) + \frac{1}{m\omega}p_0\sin(\omega t), \qquad p(t) = p_0\cos(\omega t) - m\omega x_0 \sin(\omega t),$$

which are exactly the same as the quantum operators $X(t), P(t)$ equations of motion we derived above.

Aside: This is a completely generic phenomenon. Suppose that A is a standard time-independent quantum operator. We define a related time-dependent operator $A(t) = e^{iHt/\hbar}Ae^{-iHt/\hbar}$, which we call the *Heisenberg picture operator* corresponding to the *Schrödinger picture operator* A. This operator obeys an equation of motion given by:

$$\frac{dA(t)}{dt} = \frac{i}{\hbar}e^{iHt/\hbar}[H, A]e^{-iHt/\hbar} = \frac{i}{\hbar}[H, A(t)],$$

which is called the *Heisenberg equation of motion*. If you are taking the Part II Classical Dynamics course, you will eventually see that the observables $a(t)$ of classical systems obey a similar equation of motion:

$$\frac{da(t)}{dt} = \{H, a(t)\},$$

where $\{\cdot,\cdot\}$ is called the *Poisson bracket* and plays a similar role in classical mechanics as the commutator does in quantum mechanics.

When we *quantise* a classical system using *Dirac's canonical quantisation* (as is the case with the construction of the quantum harmonic oscillator), the key steps are: (i) we replace the classical observables $a(t)$ with quantum operators $A(t)$; (ii) we impose *canonical commutation relations* by promoting Poisson brackets $\{\cdot,\cdot\}$ to commutators of the form $\frac{i}{\hbar}[\cdot,\cdot]$. By the comparison of the above equations, it follows that whenever we quantise a classical system, the Heisenberg picture operators of the quantum system will obey the classical equations of motion.

Finally, we must evaluate the commutator $[X(t), P(t)]$. We have:

$$[X(t), P(t)] = [e^{itH/\hbar}Xe^{-itH/\hbar}, e^{itH/\hbar}Pe^{-itH/\hbar}] = e^{itH/\hbar}[X, P]e^{-itH/\hbar} = i\hbar e^{itH/\hbar}e^{-iHt/\hbar} = i\hbar.$$

4. A Fermi oscillator has Hilbert space $\mathcal{H} = \mathbb{C}^2$ and Hamiltonian $H = B^\dagger B$, where $B^2 = 0$, and

$$B^\dagger B + BB^\dagger = 1 \qquad (\text{the } \textit{anti}\text{commutator}).$$

Find the eigenvalues of H. If $|0\rangle$ is a state obeying $H|0\rangle = 0$ and $\langle 0|0\rangle = 1$, find $B|0\rangle$ and $B^\dagger|0\rangle$. Obtain a matrix representation of the operators B, $B^\dagger$ and H.

Solution: To find the spectrum of H, we use a similar analysis to that of the harmonic oscillator. First, we note the following commutation relation between H and B:

$$[H, B] = B^\dagger BB - BB^\dagger B = B^\dagger B^2 + B^\dagger B^2 - B = -B.$$

Here, we've used the fact that $BB^\dagger = 1 - B^\dagger B$ to obtain the final result. Similarly, we find the commutation relation:

$$[H, B^\dagger] = B^\dagger BB^\dagger - BB^\dagger B^\dagger = B^\dagger,$$

here using $(B^\dagger)^2 = 0$, the Hermitian conjugate of the condition $B^2 = 0$.

Now let $|E\rangle$ be an energy eigenstate with energy E, i.e. $H|E\rangle = E|E\rangle$. Then consider the effect of B and $B^\dagger$ on the energy of this state:

$$H(B|E\rangle) = BH|E\rangle + [H, B]|E\rangle = (E-1)B|E\rangle\,.$$

Thus B lowers the energy by one. Similarly, we find that

$$H(B^\dagger|E\rangle) = (E+1)B^\dagger|E\rangle\,,$$

so that $B^\dagger$ raises the energy by one. The norms of the states are given by:

$$||B|E\rangle||^2 = \langle E|B^\dagger B|E\rangle = \langle E|H|E\rangle = E, \qquad ||B^\dagger|E\rangle||^2 = \langle E|BB^\dagger|E\rangle = \langle E|1 - B^\dagger B|E\rangle = 1 - E.$$

which implies that $0 \leq E \leq 1$, since norms are non-negative.

Let $|E\rangle$ be an energy eigenstate of the oscillator. If its energy is not an integer, then we can lower with the operator B to get an energy eigenstate with negative energy. This is a contradiction, and hence $|E\rangle$ must have integer energy.

Finally, notice that the ground state $|0\rangle$ must have energy 0 (by applying B sufficiently many times), and the state $B^\dagger|0\rangle$ has energy 1. Thus the spectrum of H is $0, 1$.

Next, we must find $B|0\rangle$ and $B^\dagger|0\rangle$. We've already seen from the interpretation of B, $B^\dagger$ as raising and lowering operators that $B|0\rangle = 0$ and $B^\dagger|0\rangle \propto |1\rangle$. From the normalisation condition calculated above, we see that

$$B^\dagger|0\rangle = |1\rangle$$

precisely, where $|1\rangle$ is the first excited state.

Finally, to obtain matrix representations of the operators, let's write $|0\rangle$ as the vector $(1, 0)$ and $|1\rangle$ as the vector $(0, 1)$. Since $B|0\rangle = 0$, $B|1\rangle = |0\rangle$, $B^\dagger|0\rangle = |1\rangle$, $B^\dagger|1\rangle = 0$, $H|0\rangle = 0$ and $H|1\rangle = |1\rangle$, we find the matrix representations are:

$$B = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad B^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \qquad H = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Notice that as a sanity check, $H = B^\dagger B$ in this matrix form.

⁜ **Comments:** This question has an interpretation in terms of the *Pauli exclusion principle*, which you will meet later in the lecture course:

> **Pauli's Exclusion Principle:** Two identical fermionic particles cannot be in the same state simultaneously.

This helps us interpret the results above. First let's identify the state $|0\rangle$ as the state where the system has no particles present, and the state $|1\rangle$ as the state where the system has one fermionic particle in a particular state.

Then it makes sense to interpret:

- B is the *annihilation operator*. It removes one fermionic particle from the system.
- $B^\dagger$ is the *creation operator*. It adds one fermionic particle to the system.

This is consistent with our results. We have $B|0\rangle = 0$, since we can't remove any particles when there aren't any in the first place! We also have $B|1\rangle = |0\rangle$, as we'd expect.

Similarly, we have $B^\dagger|0\rangle = |1\rangle$, as we've added a fermionic particle to the system. Further, note that $B^\dagger|1\rangle = (B^\dagger)^2|0\rangle = 0$. This is the part that relates to the Pauli Exclusion Principle - we have tried to add two identical fermionic particles to the system in the same state. Therefore, the wavefunction vanishes as this is an impossible task.

This question leads us to think about some basic ideas in *quantum field theory*. The central idea is that we can 'create' particles out of the vacuum and 'annihilate' particles to leave only the vacuum again.

In quantum field theory, these 'particles' are in fact excitations of a quantum field. The corresponding Hamiltonian in a field theory is:

$$H = \int \frac{d^3\mathbf{q}}{(2\pi)^3} E_{\mathbf{q}} \cdot B^\dagger_{\mathbf{q}} B_{\mathbf{q}},$$

where $E_{\mathbf{q}} = \sqrt{m^2 + |\mathbf{q}|^2}$ is the relativistic energy of a particle of mass m and 3-momentum $\mathbf{q}$, and $B^\dagger_{\mathbf{q}}$, $B_{\mathbf{q}}$ are the raising and lowering operators, now dependent on the momentum $\mathbf{q}$.

For fermionic fields, we impose the anticommutation conditions

$$\{B_{\mathbf{q}}, B^\dagger_{\mathbf{q}'}\} = (2\pi)^3\delta(\mathbf{q}-\mathbf{q}'), \qquad \{B_{\mathbf{q}}, B_{\mathbf{q}'}\} = 0, \qquad \{B^\dagger_{\mathbf{q}}, B^\dagger_{\mathbf{q}'}\} = 0.$$

The reason we use anticommutation relations rather than commutation relations is related to the *spin-statistics theorem*, which you'll see later in the course, and will see proved in Part III Quantum Field Theory.

To create a particle from the field's vacuum state $|0\rangle$, we apply a normalised[1] version of the creation operator:

$$|p\rangle := \sqrt{2E_{\mathbf{p}}} B^\dagger_{\mathbf{p}} |0\rangle .$$

We interpret the state $|p\rangle$ as a state containing one fermionic particle of definite 4-momentum p. Indeed, we can check that this has the correct energy:

$$H|p\rangle = \int \frac{d^3\mathbf{q}}{(2\pi)^3}\sqrt{2E_{\mathbf{p}}}E_{\mathbf{q}} \cdot B^\dagger_{\mathbf{q}} B_{\mathbf{q}} B^\dagger_{\mathbf{p}}|0\rangle = \int \frac{d^3\mathbf{q}}{(2\pi)^3}\sqrt{2E_{\mathbf{p}}}E_{\mathbf{q}} \cdot B^\dagger_{\mathbf{q}}(2\pi)^3\delta^3(\mathbf{q}-\mathbf{p})|0\rangle = E_{\mathbf{p}}|p\rangle .$$

Further, we can add another particle of different momentum with no issue, defining the multiparticle state:

$$|p,p'\rangle = \sqrt{2E_{\mathbf{p}}}\sqrt{2E_{\mathbf{p}'}} B^\dagger_{\mathbf{p}} B^\dagger_{\mathbf{p}'}|0\rangle ,$$

but as soon as $p = p'$, the operator product $B^\dagger_{\mathbf{p}} B^\dagger_{\mathbf{p}}$ is both anticommuting and symmetric, so immediately cancels. It follows that the state $|p,p\rangle = 0$, consistent with the Pauli exclusion principle.

[1] The normalisation is to ensure Lorentz invariance, a point that is discussed in Part III Quantum Field Theory.

5. Consider a $d = 1$ quantum harmonic oscillator with classical frequency ω. For any $\alpha \in \mathbb{C}$, define the *coherent state* $|\alpha\rangle$ by

$$|\alpha\rangle = e^{\alpha A^\dagger - \bar{\alpha} A} |0\rangle ,$$

where $A^\dagger$ and A are the usual raising and lowering operators and $|0\rangle$ is the ground state of the oscillator.

(i) Show that $|\alpha\rangle$ is an eigenstate of A and find its eigenvalue. Compute the inner product between two different coherent states $|\alpha\rangle$ and $|\beta\rangle$. [*Hint: You may find it useful to use the results of the previous question.*] Does the set $\{|\alpha\rangle\}_{\alpha\in\mathbb{C}}$ of all coherent states form a basis of the Hilbert space?

(ii) A quantum oscillator is prepared to be in state $|\alpha\rangle$ at time $t = 0$. Show that subsequently it evolves to become the new coherent state $e^{-i\omega t/2} |e^{-i\omega t}\alpha\rangle$.

(iii) By expressing A and $A^\dagger$ in terms of X and P, sketch the position wavefunction of $|\alpha\rangle$ in the case that $\alpha \in \mathbb{R}$.

(iv) $(*)$ Now let $\alpha \in \mathbb{C}$ and compute $\langle\alpha|P|\alpha\rangle$. Hence give a physical interpretation of the coherent state for general complex α. Without further calculation, describe the shape and motion of both the position space and momentum space wavefunctions of a general coherent state as time passes.

Solution: (i) Let's begin by using Question 2 to rewrite $|\alpha\rangle$ in a more convenient form. Notice that the operators $\alpha A^\dagger$ and $-\bar{\alpha}A$ have the commutator:

$$[\alpha A^\dagger, -\bar{\alpha} A] = -|\alpha|^2 [A^\dagger, A] = |\alpha|^2,$$

using the fact that the harmonic oscillator raising and lowering operators obey the commutation relation $[A, A^\dagger] = 1$. Therefore, $\alpha A^\dagger$ and $-\bar{\alpha}A$ both commute with their commutator, so we can apply the results of Question 2.

We see that:

$$e^{\alpha A^\dagger - \bar{\alpha} A} = e^{-\frac{1}{2}|\alpha|^2} e^{\alpha A^\dagger + (-\bar{\alpha} A) + \frac{1}{2}|\alpha|^2} = e^{-\frac{1}{2}|\alpha|^2} e^{\alpha A^\dagger} e^{-\bar{\alpha} A},$$

using the identity $e^{A+B+\frac{1}{2}[A,B]} = e^A e^B$ from Question 2. Therefore, the state $|\alpha\rangle$ may be expressed as:

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} e^{\alpha A^\dagger} e^{-\bar{\alpha} A} |0\rangle .$$

Expanding the exponential, and using the fact that $A|0\rangle = 0$, we can simplify this representation to:

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} e^{\alpha A^\dagger} |0\rangle .$$

Let's begin the question now. First we want to show that $|\alpha\rangle$ is an eigenvector of A, and find its eigenvalue. We use the representation of $|\alpha\rangle$ we derived above:

$$A|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} A e^{\alpha A^\dagger} |0\rangle .$$

The operators here again remind us of the formulas from Question 2. This time, we note that $[A, \alpha A^\dagger] = \alpha$ so A and $\alpha A^\dagger$ both commute with their commutator. We then wish to apply the result $[A, e^B] = e^B [A, B]$. In this case, we find:

$$\begin{aligned}
A|\alpha\rangle &= e^{-\frac{1}{2}|\alpha|^2} e^{\alpha A^\dagger} A|0\rangle + e^{-\frac{1}{2}|\alpha|^2} [A, e^{\alpha A^\dagger}]|0\rangle && \text{(swapping } A \text{ and } e^{\alpha A^\dagger} \text{ order)} \\
&= e^{-\frac{1}{2}|\alpha|^2} [A, e^{\alpha A^\dagger}]|0\rangle && \text{(since } A|0\rangle = 0) \\
&= e^{-\frac{1}{2}|\alpha|^2} e^{\alpha A^\dagger} \alpha |0\rangle && \text{(by result } [A, e^B] = e^B [A, B]) \\
&= \alpha |\alpha\rangle .
\end{aligned}$$

Therefore, $|\alpha\rangle$ is indeed an eigenvector, with eigenvalue α.

Next, we are asked to find the inner product $\langle\alpha|\beta\rangle$ between two coherent states. Let's begin by computing the bra $\langle\alpha|$:

$$\langle\alpha| = |\alpha\rangle^\dagger = \left(e^{-\frac{1}{2}|\alpha|^2} e^{\alpha A^\dagger} |0\rangle\right)^\dagger = \left(e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{(\alpha A^\dagger)^n}{n!} |0\rangle\right)^\dagger = \langle 0| e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{(\bar{\alpha} A)^n}{n!} = \langle 0| e^{-\frac{1}{2}|\alpha|^2} e^{\bar{\alpha} A}.$$

Therefore, we see that

$$\langle\alpha|\beta\rangle = \langle 0| e^{-\frac{1}{2}|\alpha|^2} e^{\bar{\alpha} A} e^{-\frac{1}{2}|\beta|^2} e^{\beta A^\dagger} |0\rangle = e^{-\frac{1}{2}|\alpha|^2 - \frac{1}{2}|\beta|^2} \langle 0| e^{\bar{\alpha} A} e^{\beta A^\dagger} |0\rangle .$$

It would be a good idea to swap the orders of the exponentials, since we know that $e^{\bar{\alpha} A} |0\rangle = 1$, and correspondingly $\langle 0| e^{\beta A^\dagger} = 1$ since $A |0\rangle = 0$ and $\langle 0| A^\dagger = (A |0\rangle)^\dagger = 0$. In order to swap the exponentials, we'd like to use the result from Question 2:

$$e^A e^B = e^B e^A e^{[A,B]}.$$

In this case, we work with the operators $\bar{\alpha} A$ and $\beta A^\dagger$. We note that $[\bar{\alpha} A, \beta A^\dagger] = \bar{\alpha}\beta$, so $\bar{\alpha} A$ and $\beta A^\dagger$ certainly commute with their commutator. So the result of Question 2 applies, and we have:

$$e^{-\frac{1}{2}|\alpha|^2 - \frac{1}{2}|\beta|^2} \langle 0| e^{\alpha \bar{A}} e^{\beta A^\dagger} |0\rangle = e^{-\frac{1}{2}|\alpha|^2 - \frac{1}{2}|\beta|^2} \langle 0| e^{\beta A^\dagger} e^{\alpha \bar{A}} e^{\bar{\alpha}\beta} |0\rangle = e^{-\frac{1}{2}|\alpha|^2 - \frac{1}{2}|\beta|^2 + \bar{\alpha}\beta}.$$

Hence we have established that:

$$\langle\alpha|\beta\rangle = e^{-\frac{1}{2}|\alpha|^2 - \frac{1}{2}|\beta|^2 + \bar{\alpha}\beta}.$$

In particular, it follows that $\{|\alpha\rangle\}$ is *not* a basis of Hilbert space, since a basis of Hilbert space is defined to be a *maximal orthonormal set* contained with the Hilbert space (and not all $|\alpha\rangle$ are orthogonal).

Aside: We can go into a bit more detail about the properties of the states $\{|\alpha\rangle\}$. For example, we can show that these states do indeed *span* Hilbert space. To show this, consider evaluating the 'resolution of identity integral':

$$\int d^2\alpha \; |\alpha\rangle \langle\alpha| . \tag{$*$}$$

Note the measure $d^2\alpha$ integrates over the whole complex plane $\mathbb{C}$, since $\alpha \in \mathbb{C}$. Since we have an explicit form for $|\alpha\rangle$, we can check whether $(*)$ holds directly. We have:

$$\int d^2\alpha \; |\alpha\rangle \langle\alpha| = \int d^2\alpha \, e^{-|\alpha|^2} e^{\alpha A^\dagger} |0\rangle \langle 0| e^{\bar{\alpha} A} = \int d^2\alpha \, e^{-|\alpha|^2} \sum_{m,n=0}^{\infty} \frac{\alpha^m \bar{\alpha}^n}{m! n!} (A^\dagger)^m |0\rangle \langle 0| A^n.$$

Now recall from lectures that the energy eigenstates of the harmonic oscillator can be written as:

$$|m\rangle = \frac{(A^\dagger)^m}{\sqrt{m!}} |0\rangle .$$

Thus rewriting the bras and kets in our resolution of identity integral in terms of energy eigenstates, we have:

$$\int d^2\alpha \; |\alpha\rangle \langle\alpha| = \int d^2\alpha \, e^{-|\alpha|^2} \sum_{m,n=0}^{\infty} \frac{\alpha^m \bar{\alpha}^n}{\sqrt{m! n!}} |m\rangle \langle n| .$$

Why rewrite things in terms of the *energy eigenstates*? It's because the Hamiltonian is a *self-adjoint* or *Hermitian operator*; in particular, this means that its eigenstates form an orthonormal basis for Hilbert space. Hence the energy eigenstates span, so:

$$\sum_{n=0}^{\infty} |n\rangle \langle n| = 1,$$

which we will refer to later.

For now, let's tackle the looming integral. We need to evaluate:

$$\int d^2\alpha\, e^{-|\alpha|^2}\alpha^m\bar{\alpha}^n.$$

Let's work in polar coordinates. Write $\alpha = re^{i\theta}$. Then $d^2\alpha = rdrd\theta$, the standard polar measure. The integral splits into a product of integrals:

$$\int d^2\alpha\, e^{-|\alpha|^2}\alpha^m\bar{\alpha}^n = \left(\int_0^\infty dr\, r^{m+n+1}e^{-r^2}\right)\left(\int_0^{2\pi} d\theta\, e^{i(m-n)\theta}\right).$$

The angular integral can be computed easily:

$$\int_0^{2\pi} d\theta\, e^{i(m-n)\theta} = \begin{cases} 0 & \text{if } m \neq n \\ 2\pi & \text{otherwise.} \end{cases} = 2\pi\delta_{m,n}.$$

Hence we find:

$$\int d^2\alpha\, e^{-|\alpha|^2}\alpha^m\bar{\alpha}^n = 2\pi\delta_{m,n}\left(\int_0^\infty dr\, r^{2m+1}e^{-r^2}\right) = \pi\delta_{m,n}\left(\int_0^\infty d(r^2)\,(r^2)^m e^{-(r^2)}\right) = \pi\delta_{m,n}\Gamma(m+1).$$

In the final step, we have recognised the integral as the expression for the *gamma function*, which you will meet in Part II Further Complex Methods next term. For integers m, we have $\Gamma(m+1) = m!$. Therefore, we have shown that

$$\int d^2\alpha\ |\alpha\rangle\langle\alpha| = \pi\sum_{m=0}^{\infty}\frac{m!}{\sqrt{m!m!}}|m\rangle\langle m| = \pi,$$

using the resolution of the identity for eigenstates of the Hamiltonian, as we saw earlier. Therefore, we have the completeness relation:

$$\frac{1}{\pi}\int d^2\alpha\ |\alpha\rangle\langle\alpha| = 1.$$

It follows from this statement that the state $\{|\alpha\rangle\}$ certainly span Hilbert space, since for any $|\psi\rangle \in \mathcal{H}$, we have:

$$|\psi\rangle = 1\,|\psi\rangle = \frac{1}{\pi}\int d^2\alpha\,\langle\alpha|\psi\rangle\,|\alpha\rangle\,.$$

However, given any coherent state $|\beta\rangle$, we see that

$$|\beta\rangle = \frac{1}{\pi}\int d^2\alpha\ \langle\alpha|\beta\rangle\,|\alpha\rangle = \frac{1}{\pi}\int d^2\alpha\, e^{-\frac{1}{2}|\alpha|^2-\frac{1}{2}|\beta|^2-\bar{\alpha}\beta}\,|\alpha\rangle\,.$$

In particular, $e^{-\frac{1}{2}|\alpha|^2-\frac{1}{2}|\beta|^2-\bar{\alpha}\beta} \neq 0$ for $\alpha \neq \beta$. So $|\beta\rangle$ may be expressed as the linear combination of coherent states $|\alpha\rangle$ with *non-zero coefficients* for $|\alpha\rangle \neq |\beta\rangle$. It follows that the coefficients in an expansion of a generic state in terms of coherent states aren't unique (i.e. we don't have *linear independence*).

(ii) To examine how states evolve in time, we use Schrödinger's equation:

$$i\hbar\frac{d}{dt}|\psi\rangle = H\,|\psi\rangle\,.$$

This has the formal solution:

$$|\psi(t)\rangle = e^{-iHt/\hbar}\,|\psi(0)\rangle\,.$$

We want $|\psi(t)\rangle$, given that $|\psi(0)\rangle = |\alpha\rangle$, i.e. we initially begin with a coherent state. It follows that we must evaluate $e^{-iHt/\hbar}\,|\alpha\rangle$.

Carrying out the calculation, we have

$$
\begin{aligned}
e^{-iHt/\hbar}\left|\alpha\right\rangle &= e^{-\frac{1}{2}|\alpha|^2}e^{-iHt/\hbar}e^{\alpha A^\dagger}\left|0\right\rangle && \text{(definition of } |\alpha\rangle\text{)} \\
&= e^{-\frac{1}{2}|\alpha|^2}e^{-iHt/\hbar}\sum_{n=0}^{\infty}\frac{\alpha^n(A^\dagger)^n}{n!}\left|0\right\rangle && \text{(expanding exponential)} \\
&= e^{-\frac{1}{2}|\alpha|^2}e^{-iHt/\hbar}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\left|n\right\rangle && \left(\text{since } |n\rangle = (A^\dagger)^n\left|0\right\rangle/\sqrt{n!}\right) \\
&= e^{-\frac{1}{2}|\alpha|^2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}e^{-it\omega(n+\frac{1}{2})}\left|n\right\rangle && \left(\text{since } H\left|n\right\rangle = \hbar\omega\left(n+\frac{1}{2}\right)\left|n\right\rangle\right) \\
&= e^{-\frac{1}{2}|\alpha|^2}e^{-i\omega t/2}\sum_{n=0}^{\infty}\frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}}\left|n\right\rangle \\
&= e^{-i\omega t/2}e^{-\frac{1}{2}|\alpha e^{-i\omega t}|^2}\sum_{n=0}^{\infty}\frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}}\left|n\right\rangle \\
&= e^{-i\omega t/2}\left|\alpha e^{-i\omega t}\right\rangle,
\end{aligned}
$$

where in the last line, we've compared with the expansion of $|\alpha\rangle$ from earlier in the calculation - in particular, we've compared with line 3. This is the required result - it shows that if we start with a coherent state at time $t = 0$, we still have a coherent state at time $t > 0$.

(iii) We now wish to compute the position wavefunction of a coherent state, i.e. $\langle x|\alpha\rangle$. We are first asked to write down the expressions for A and $A^\dagger$ in terms of X and P; from lectures, we know that the appropriate expressions are:

$$
A = \frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega X + iP\right), \qquad A^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega X - iP\right).
$$

Inserting the expression for $A^\dagger$ into our expression $|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}e^{\alpha A^\dagger}\left|0\right\rangle$, we see that the position wavefunction is:

$$
\langle x|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}\left\langle x\right|\exp\left(\alpha\sqrt{\frac{m\omega}{2\hbar}}X - \frac{i\alpha P}{\sqrt{2m\hbar\omega}}\right)\left|0\right\rangle.
$$

To evaluate this matrix element, let's first break down the exponential sandwiched between the bra and the ket using the result of Question 2. Notice that

$$
\left[\alpha\sqrt{\frac{m\omega}{2\hbar}}X, -\frac{i\alpha P}{\sqrt{2m\hbar\omega}}\right] = -\frac{i\alpha^2}{2\hbar}[X,P] = \frac{\alpha^2}{2}.
$$

Therefore, both the relevant operators commute with their commutator, and so it follows:

$$
\exp\left(\alpha\sqrt{\frac{m\omega}{2\hbar}}X - \frac{i\alpha P}{\sqrt{2m\hbar\omega}}\right) = \exp\left(\alpha\sqrt{\frac{m\omega}{2\hbar}}X\right)\exp\left(-\frac{i\alpha P}{\sqrt{2m\hbar\omega}}\right)\exp\left(-\frac{\alpha^2}{4}\right).
$$

Therefore, the position wavefunction of the coherent state $|\alpha\rangle$ can be written as:

$$
\langle x|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2-\frac{\alpha^2}{4}}\left\langle x\right|\exp\left(\alpha\sqrt{\frac{m\omega}{2\hbar}}X\right)\exp\left(-\frac{i\alpha P}{\sqrt{2m\hbar\omega}}\right)\left|0\right\rangle.
$$

Acting to the left with the X-exponential, we're left with:

$$\langle x|\alpha\rangle = \exp\left(-\frac{1}{2}|\alpha|^2 - \frac{\alpha^2}{4}\right)\exp\left(\alpha\sqrt{\frac{m\omega}{2\hbar}}x\right)\langle x|\exp\left(-\frac{i\alpha P}{\sqrt{2m\hbar\omega}}\right)|0\rangle\,.$$

We now apply the result of Question 1(ii) which tells us that (since P generates translations):

$$\langle x|\exp\left(-\frac{i\alpha P}{\sqrt{2m\hbar\omega}}\right)|0\rangle = \psi_0\left(x - \frac{\alpha\hbar}{\sqrt{2m\hbar\omega}}\right).$$

where $\psi_0(x) = \langle x|0\rangle$ is the position wavefunction of the ground state of the oscillator. From lectures (or from looking it up in an appropriate book), we know that

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right).$$

So putting all the pieces together, we see that we have the final answer:

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

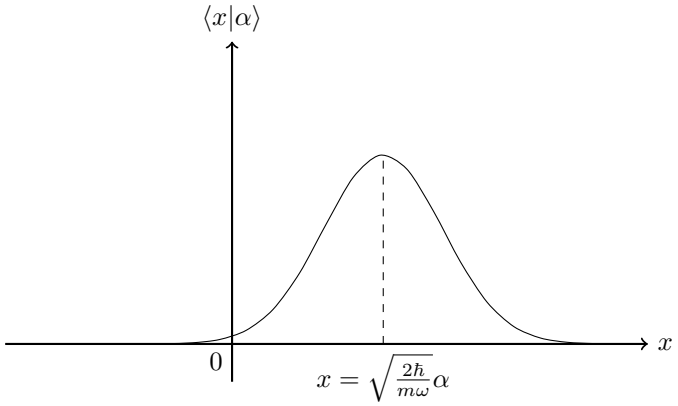
We can simplify further by combining the final two exponentials and completing the square. After some straightforward tidying up, we're left with:

$$\langle x|\alpha\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{1}{2}|\alpha|^2 + \frac{\alpha^2}{2}\right)\exp\left(-\frac{m\omega}{2\hbar}\left(x - \sqrt{\frac{2\hbar}{m\omega}}\alpha\right)^2\right).$$

This is just a Gaussian! We have to be a little careful, since it has a complex average proportional to α. However, in the case that α is real, this further simplifies to:

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

We know how to sketch a real Gaussian; in our case the result simply looks like:



There is an alternative, much easier, derivation of the position wavefunction.[2] We simply recall that $|\alpha\rangle$ is an eigenstate of A with eigenvalue α:

$$A\,|\alpha\rangle = \alpha\,|\alpha\rangle\,.$$

Taking the inner product with $|x\rangle$, we see that the wavefunctions obey:

$$\langle x|A|\alpha\rangle = \alpha\,\langle x|\alpha\rangle\,.$$

Therefore, writing down the position representation of A, we find the wavefunction obeys:

$$\frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega x + \hbar\frac{\partial}{\partial x}\right)\psi(x) = \alpha\psi(x).$$

This is a first order ODE for $\psi(x)$. Rearranging, we can put it into the form:

$$\frac{\partial\psi}{\partial x} = \frac{1}{\hbar}(\sqrt{2m\hbar\omega}\alpha - m\omega x)\psi.$$

Solving, we have:

$$\int\frac{d\psi}{\psi} = \frac{1}{\hbar}\int(\sqrt{2m\hbar\omega}\alpha - m\omega x)dx \qquad \Rightarrow \qquad \log|\psi| = \frac{1}{\hbar}\sqrt{2m\hbar\omega}\alpha x - \frac{m\omega x^2}{2\hbar} + C.$$

Therefore, the wavefunction is given by:

$$\psi(x) = A\exp\left(\sqrt{\frac{2m\omega}{\hbar}}\alpha x - \frac{m\omega x^2}{2\hbar}\right),$$

where the constant A is to ensure the normalisation of $\psi(x)$.

Since α is complex, it's useful to split it into real and imaginary parts to ensure we get our interpretation of the Gaussian right. Doing so, we have:

$$\psi(x) = A\exp\left(\sqrt{\frac{2m\omega}{\hbar}}i\,\mathrm{Im}(\alpha)x\right)\exp\left(\sqrt{\frac{2m\omega}{\hbar}}\,\mathrm{Re}(\alpha)x - \frac{m\omega x^2}{2\hbar}\right),$$

The imaginary part only contributes a phase, so we just ignore it. Completing the square in the exponent, we have

$$\psi(x) = A\exp\left(-\frac{m\omega}{2\hbar}\left(x - \sqrt{\frac{2\hbar}{m\omega}}\,\mathrm{Re}(\alpha)\right)^2\right),$$

where we've absorbed the constant term into A. We can calculate A, which is a normalisation constant required to make the integral of $|\psi(x)|^2$ equal to 1, using the standard Gaussian integral - we get the same result as above, i.e.

$$\psi(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}\left(x - \sqrt{\frac{2\hbar}{m\omega}}\,\mathrm{Re}(\alpha)\right)^2\right),$$

[2] Though the form of the question, asking us to write down X and P in terms of A and $A^\dagger$, suggests that we should use the first approach unfortunately.

(iv) Finally, we are asked to give a physical interpretation of the coherent state. To begin with, let's note some properties of the position wavefunction. We have:

- The position expectation $\langle\alpha|X|\alpha\rangle$ must be:

$$\langle\alpha|X|\alpha\rangle = \sqrt{\frac{2\hbar}{m\omega}}\,\mathrm{Re}(\alpha),$$

since this is the central value of the Gaussian.

- The position uncertainty (i.e. variance), $(\Delta X)^2 = \langle\alpha|(X - (\langle\alpha|X|\alpha\rangle))^2|\alpha\rangle$, must be equal to

$$(\Delta X)^2 = \frac{\hbar}{2m\omega},$$

by comparing the position probability distribution $|\psi(x)|^2$ with the general form of a Gaussian distribution

$$f(x) = A\exp\left(-\frac{(x-a)^2}{2\sigma^2}\right),$$

where the variance is given by σ^2.

We can apply the same analysis to the momentum wavefunction. Since the momentum wavefunction of the state $|\alpha\rangle$ is the Fourier transform of the position wavefunction of the system, it is *also a Gaussian* (we know from Part IB that the Fourier transform of a Gaussian is a Gaussian too)! Indeed, we have that:

$$f(x) = A\exp\left(-\frac{(x-a)^2}{2\sigma^2}\right) \qquad \text{has Fourier transform} \qquad \hat{f}(\omega) = A\sqrt{\frac{\sigma^2}{\hbar}}\exp\left(-\frac{\sigma^2\omega^2}{2\hbar^2}\right)\cdot\exp\left(-\frac{ia\omega}{\hbar}\right),$$

where the Fourier transform is defined by:

$$\hat{f}(\omega) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} f(x)e^{-i\omega x/\hbar}\,dx.$$

Note the factors of $\hbar$ relevant in the quantum mechanical case.

In particular, we note that the mean and variance will both change. We could either calculate how the mean changes, or just evaluate $\langle\alpha|P|\alpha\rangle$ directly, which is also very quick. To evaluate $\langle\alpha|P|\alpha\rangle$ directly, it's easiest to express P in terms of A and $A^\dagger$ first:

$$P = \sqrt{2m\hbar\omega}i\left(\frac{A^\dagger - A}{2}\right).$$

Therefore, we have:

$$\langle\alpha|P|\alpha\rangle = \frac{1}{2}\sqrt{2m\hbar\omega}\,ie^{-|\alpha|^2}\left(\langle 0|e^{\bar{\alpha}A}A^\dagger e^{\alpha A^\dagger}|0\rangle - \langle 0|e^{\bar{\alpha}A}Ae^{\alpha A^\dagger}|0\rangle\right)$$

$$= \frac{1}{2}\sqrt{2m\hbar\omega}\,ie^{-|\alpha|^2}\left(\langle 0|[e^{\bar{\alpha}A}, A^\dagger]e^{\alpha A^\dagger}|0\rangle - \langle 0|e^{\bar{\alpha}A}[A, e^{\alpha A^\dagger}]|0\rangle\right).$$

Recalling that $[A, A^\dagger] = 1$, we know that both A and $A^\dagger$ commute with their commutator, and hence we can evaluate the necessary commutators using Question 2. We have:

$$\langle\alpha|P|\alpha\rangle = \frac{1}{2}\sqrt{2m\hbar\omega}\,ie^{-|\alpha|^2}\left(\bar{\alpha}\,\langle 0|e^{\bar{\alpha}A}e^{\alpha A^\dagger}|0\rangle - \alpha\,\langle 0|e^{\bar{\alpha}A}e^{\alpha A^\dagger}|0\rangle\right)$$

$$= \frac{1}{2}\sqrt{2m\hbar\omega}\,i(\bar{\alpha} - \alpha) = \sqrt{2m\hbar\omega}\,\mathrm{Im}(\alpha).$$

Now we turn to the variance, for which it is simpler just to look at the Fourier transform. Note that the variance of the Gaussian $\psi(x)$ changes as:

$$\sigma^2 = \frac{\hbar}{m\omega} \mapsto \frac{\hbar^2}{\sigma^2} = \hbar m\omega.$$

Therefore, we find that the momentum wavefunction looks like

$$\hat{\psi}(p) \sim \exp\left(-\frac{1}{2\hbar m\omega}(x - \langle\alpha|P|\alpha\rangle)^2\right),$$

and so the probability distribution $|\hat{\psi}(p)|^2$ has the variance: $(\Delta P)^2 = \hbar m\omega/2$. To summarise, we see that:

- The momentum expectation $\langle\alpha|P|\alpha\rangle$ is given by

$$\langle\alpha|P|\alpha\rangle = \sqrt{2m\hbar\omega}\,\mathrm{Im}(\alpha).$$

- The momentum uncertainty is given by

$$(\Delta P)^2 = \frac{\hbar m\omega}{2}$$

We now have enough information to describe the physical interpretation of the states. There are various points we can make:

- Minimal uncertainty states. We notice that coherent states have position and momentum uncertainty which make the uncertainty principle an *equality*:

$$(\Delta X)^2(\Delta P)^2 = \frac{\hbar^2}{4} \qquad \Rightarrow \qquad (\Delta X)(\Delta P) = \frac{\hbar}{2}.$$

  This means that these states can have both their position and momentum defined in narrow ranges. In particular, coherent states are *approximately* eigenstates of both position and momentum:

$$X\,|\alpha\rangle \approx x\,|\alpha\rangle\,, \qquad P\,|\alpha\rangle \approx p\,|\alpha\rangle\,,$$

  with the error given by the uncertainties (ΔX) and (ΔP). In particular, this implies that these quantum states are *very close to their classical counterparts*. This is how coherent states were originally discovered.

- Approximately classical states. We mentioned in the previous point that coherent states must be very close to the equivalent classical system. An easy calculation in classical mechanics shows that the position and momentum of a time-dependent 1D *classical* harmonic oscillator are:

$$x(t) = A\cos(\omega t - \phi), \qquad p(t) = -Am\omega\sin(\omega t - \phi).$$

  Recall the expectation values for the position and momentum of the stationary coherent states were:

$$\langle\alpha|X|\alpha\rangle = \sqrt{\frac{2\hbar}{m\omega}}\,\mathrm{Re}(\alpha), \qquad \langle\alpha|P|\alpha\rangle = \sqrt{2m\hbar\omega}\,\mathrm{Im}(\alpha).$$

  From part (ii), we know that to add dynamics we set $\alpha \mapsto \alpha e^{-i\omega t}$. Therefore, we have

$$\langle\alpha|X|\alpha\rangle = \sqrt{\frac{2\hbar}{m\omega}}\,\mathrm{Re}(\alpha e^{-i\omega t}), \qquad \langle\alpha|P|\alpha\rangle = \sqrt{2m\hbar\omega}\,\mathrm{Im}(\alpha e^{-i\omega t}).$$

  Writing $\alpha = |\alpha|e^{i\phi}$, we see that the expectation values of the coherent states obey:

$$\langle\alpha|X|\alpha\rangle = \sqrt{\frac{2\hbar}{m\omega}}|\alpha|\cos(\omega t - \phi), \qquad \langle\alpha|P|\alpha\rangle = \sqrt{2m\hbar\omega}|\alpha|\sin(\phi - \omega t).$$

  These *exactly mirror* the classical solution, with $A = |\alpha|\sqrt{2\hbar/m\omega}$. So we once again see that coherent states are in a sense the states 'closest' to the classical system. There's a nice animation on the Wikipedia article on coherent states that demonstrates how the position wavefunction moves in time - the central value of the Gaussian moves just as the classical particle would move.[3]

[3] See https://en.wikipedia.org/wiki/Coherent_states#The_wavefunction_of_a_coherent_state.

6. (∗) In certain units where $\hbar = 2m = 1$, the relative motion of the atoms in a diatomic molecule can be modelled by the Hamiltonian

$$H_\nu = P^2 + \left(\nu + \frac{1}{2} - e^{-X}\right)^2,$$

where ν is a real parameter.

(i) Sketch the potential. Suggest a reason why it better describes the molecule's vibrations than the harmonic oscillator does.

(ii) Find a non-Hermitian operator A_ν that depends on ν such that

$$H_\nu = A_\nu^\dagger A_\nu + \nu + \frac{1}{4}.$$

What is the ground state of H_ν? Calculate the position space wavefunction of the ground state. For what range of ν is this state normalisable?

(iii) Let $|0, \nu\rangle$ be the ground state appropriate for parameter ν. Show that

$$A_\nu A_\nu^\dagger = A_{\nu-1}^\dagger A_{\nu-1} + 2\nu - 1,$$

and hence that $A_\nu^\dagger |0, \nu - 1\rangle$ is also an (unnormalised) eigenstate of H_ν.

(iv) Iterating this procedure, deduce an expression for the unnormalised nth eigenstate in terms of a sequence of raising operators acting on a ground state, for appropriate choices of the parameter. Hence find the bound state spectrum of H_ν. Show that the number of bound states is $\lfloor \nu + 1 \rfloor$. Do these states form a basis of the Hilbert space?

Solution: (i) We are first asked to sketch the function:

$$V(x) = \left(\nu + \frac{1}{2} - e^{-x}\right)^2.$$

We note that:

$$V'(x) = 2e^{-x}\left(\frac{1}{2} + \nu - e^{-x}\right),$$

so there is a stationary point at:

$$x = \log\left(\frac{2}{2\nu + 1}\right).$$

Since the argument of the logarithm has to be positive, a stationary point only exists when $2\nu + 1 > 0$, i.e. when $\nu > -1/2$. At the stationary point, V takes the value:

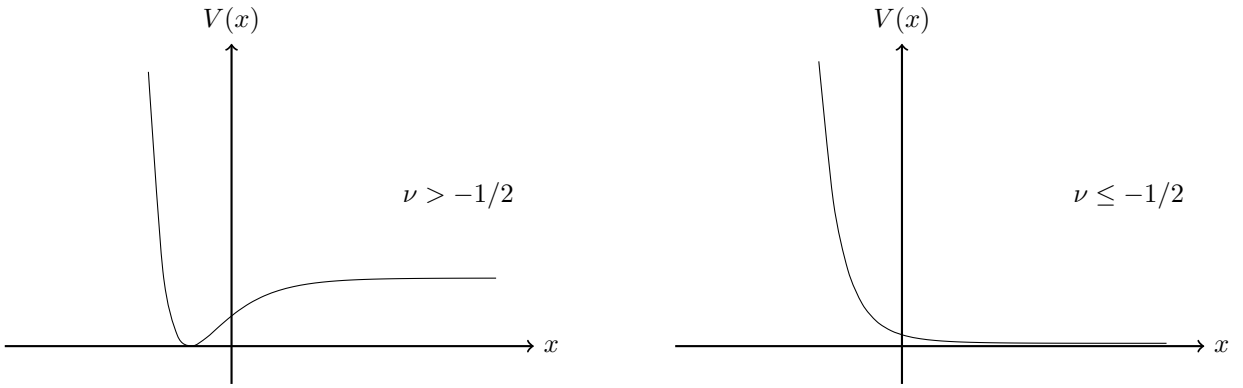
$$V\left(\log\left(\frac{2}{2\nu + 1}\right)\right) = 0.$$

Since $V(x) \geq 0$ for all x, the stationary point must be a minimum.

We also notice the asymptotic behaviour of the function:

- As $x \to \infty$, we have $V \to (\nu + 1/2)^2$.
- As $x \to -\infty$, we have $V \to \infty$.

Putting all this information together, there are two cases for what the graph looks like: (i) $\nu > -1/2$; (ii) $\nu \leq -1/2$. Sketching these two cases separately, we see:



We now need to interpret why $V(x)$ is a better potential for describing molecule's vibrations than the harmonic oscillator potential. First we note that X in this question represents the *relative position* of two atoms in a diatomic molecule. Therefore, for large X, the atoms are spaced far apart, and for small X, the atoms are close together.

When $\nu > -1/2$, we see from the form of the potential that as $X \to -\infty$, the potential becomes infinitely repulsive - the atoms are forced away from each other. As $X \to \infty$, the atoms become completely unaware of each other's existence. Finally, there is a well where for some range of energies, *bound states* can exist. This region describes the diatomic molecule as a whole - if the energy becomes larger, the atoms can break the bond and become free from one another.

When $\nu \leq -1/2$, there is no well, and hence the atoms can never join together to form a molecule. Whatever energy they have, they simply move away from one another.

Hence this is a better model because:

- It captures the possibility two atoms cannot form a molecule together ($\nu \leq -1/2$). This is not a feature of the harmonic oscillator.
- It allows for the chemical phenomenon of *bond breaking* given enough energy. This is also not a feature of the harmonic oscillator.

This potential is actually called a *Morse potential*, which you can find by searching Wikipedia.[4] The Wikipedia article also contains a nice diagram highlighting some of the features of the potential we discussed above.

The Morse potential is normally written in the form:

$$V(X) = D_e(1 - e^{-a(X-x_e)})^2 - D_e.$$

where D_e, a and x_e are constants. Since we can only measure energy differences, we can neglect the constant D_e from the Hamiltonian. Bringing the multiplicative D_e into the squared term, we have:

$$V(X) = \left(\sqrt{D_e} - e^{-a\log(\sqrt{D_e})(X-X_e)}\right)^2,$$

which suggests our form of the Morse potential has just selected

$$D_e = \left(\nu + \frac{1}{2}\right)^2, \qquad a\log(\sqrt{D_e}) = 1, \qquad X_e = 0.$$

[4] See https://en.wikipedia.org/wiki/Morse_potential.

(ii) We expect the operator A_ν to depend on e^{-X}, P from the form of the potential. From the desired form of the Hamiltonian, i.e. a product $A_\nu^\dagger A_\nu$, it makes sense to guess:

$$A_\nu = a + be^{-X} + ciP,$$

where a, b and c are real coefficients. Then:

$$A_\nu^\dagger A_\nu + \nu + \frac{1}{4} = (a + be^{-X} - ciP)(a + be^{-X} + ciP) + \nu + \frac{1}{4} = (a + be^{-X})^2 + P^2 + bci[e^{-X}, P] + \nu + \frac{1}{4}.$$

We can evaluate the commutator $[e^{-X}, P]$ using the result of Question 2:

$$[e^{-X}, P] = [-X, P]e^{-X} = -ie^{-X},$$

in units where $\hbar = 1$. It follows that:

$$A_\nu^\dagger A_\nu = (a + be^{-X})^2 + c^2P^2 + bce^{-X} + \nu + \frac{1}{4} = a^2 + (2ab + bc)e^{-X} + b^2e^{-2X} + c^2P^2 + \nu + \frac{1}{4}.$$

Comparing to the Hamiltonian:

$$H_\nu = P^2 + \left(\nu + \frac{1}{2} - e^{-X}\right)^2 = P^2 + \nu^2 + \nu + \frac{1}{4} - (2\nu + 1)e^{-X} + e^{-2X},$$

we see that a suitable choice of a, b and c to get the result we want is:

$$c = 1, \qquad a = \nu, \qquad b = -1.$$

Therefore we have:

$$H_\nu = A_\nu^\dagger A_\nu + \nu + \frac{1}{4},$$

where

$$A_\nu = \nu - e^{-X} + iP, \qquad A_\nu^\dagger = \nu - e^{-X} - iP.$$

The ground state $|0, \nu\rangle$ is an energy eigenstate of the Hamiltonian H_ν with minimal associated eigenvalue. Therefore, the ground state of the system will minimise $\langle 0, \nu|H_\nu|0, \nu\rangle$. Writing out H_ν using the form we derived above, we see that we must choose $|0, \nu\rangle$ to minimise:

$$\langle 0, \nu|H_\nu|0, \nu\rangle = \langle 0, \nu|A_\nu^\dagger A_\nu|0, \nu\rangle + \nu + \frac{1}{4} = ||A_\nu\,|0, \nu\rangle\,||^2 + \nu + \frac{1}{4}.$$

Therefore, the absolute best we could do to minimise the energy is to choose $|0, \nu\rangle$ such that $A_\nu\,|0, \nu\rangle = 0$. Then we would find that $|0, \nu\rangle$ had energy $\nu + 1/4$, which is the smallest the right hand side of the above equation can be.

But we have an explicit form for A_ν, so we can just check whether such a $|0, \nu\rangle$ exists. To produce such a $|0, \nu\rangle$, we can just write down its wavefunction, which must obey:

$$0 = \langle x|A_\nu|0, \nu\rangle = \left(\nu - e^{-x} + \frac{\partial}{\partial x}\right)\psi(x).$$

This is a simple, first-order ODE which we can solve exactly:

$$\frac{\partial\psi}{\partial x} = (-\nu + e^{-x})\psi \qquad \Rightarrow \qquad \int \frac{d\psi}{\psi} = \int(-\nu + e^{-x})dx \qquad \Rightarrow \qquad \psi(x) = Ae^{-\nu x - \exp(-x)},$$

where A is a constant of integration.

In order for this to be a bound state, it needs to be normalisable. In particular, we need

$$1 = |A|^2 \int_{-\infty}^{\infty} e^{-2\nu x - 2\exp(-x)} dx.$$

Making the substitution $u = 2e^{-x}$, we are left with:

$$1 = |A|^2 \int_0^{\infty} \frac{du}{u} e^{2\nu \log(u/2) - 2u} = \frac{|A|^2}{2^{2\nu}} \int_0^{\infty} du\, u^{2\nu-1} e^{-2u}.$$

We now just need to check when this integral converges.[5] Certainly this integral converges as $u \to \infty$, since e^{-2u} dominates the polynomial growth (or decay) of $u^{2\nu-1}$.

However, as $u \to 0$, the integrand looks like:

$$u^{2\nu-1} e^{-2u} \approx u^{2\nu-1},$$

and hence we get the approximate contribution to the integral (for $\epsilon \ll 1$):

$$\int_0^{\epsilon} u^{2\nu-1} = \left[\frac{u^{2\nu}}{2\nu}\right]_0^{\epsilon}.$$

Note in particular that if $2\nu < 0$, we get a divergence, but if $2\nu > 0$ everything is fine. If $2\nu = 0$, we also get a divergence, but a logarithmic one. Therefore, our state is normalisable if and only if $\nu > 0$.

This is almost in agreement with our prediction from part (i) about when we would get a bound state, i.e. $\nu > -1/2$. The physical reason that we only get bound states for $\nu > 0$ is that the potential well must be deep enough to be consistent with the uncertainty principle; if the well is shallow, there's only a few places we can be bound in, and hence the position uncertainty is small. It follows that the momentum may be very large - but then we could just escape out of the well! Therefore we only get bound states if the well is sufficiently deep, i.e. $\nu > 0$. We also anticipate that as ν grows, we will get more available bound states (which is consistent with what the question tells us in part (iv)).

To summarise our results, the ground state of the system for a specific ν is:

$$|0, \nu\rangle = A \int dx\, e^{-\nu x - \exp(-x)} |x\rangle .$$

and has energy $\nu + 1/4$. It is normalisable if and only if $\nu > 0$.

(iii) In this part, we are first asked to show that:

$$A_\nu A_\nu^\dagger = A_{\nu-1}^\dagger A_{\nu-1} + 2\nu - 1.$$

This is just an exercise in algebra. We have:

$$A_\nu A_\nu^\dagger - A_{\nu-1}^\dagger A_{\nu-1} = (\nu - e^{-X} + iP)(\nu - e^{-X} - iP) - (\nu - 1 - e^{-X} - iP)(\nu - 1 + e^{-X} + iP)$$

$$= \nu^2 - 2\nu e^{-X} + e^{-2X} + ie^{-X}P - iPe^{-X} + P^2 - (\nu-1)^2 + 2(\nu-1)e^{-X} - e^{-2X} + ie^{-X}P - iPe^{-X} - P^2$$

$$= \nu^2 - (\nu-1)^2 + 2i[e^{-X}, P] - 2e^{-X}.$$

[5] Some of you may recognise this integral as the *gamma function* $\Gamma(2\nu)$, in which case the convergence properties are well documented online. You'll see more about the gamma function and its properties in Part II Further Complex Methods next term, if you choose to take it.

Recalling that $[e^{-X}, P] = -ie^{-X}$ in units where $\hbar = 1$. Therefore, we're left with:

$$A_\nu A_\nu^\dagger - A_{\nu-1}^\dagger A_{\nu-1} = \nu^2 - (\nu-1)^2 = 2\nu - 1,$$

from which it follows that

$$A_\nu A_\nu^\dagger = A_{\nu-1}^\dagger A_{\nu-1} + 2\nu - 1,$$

as required.

Note that if we multiply this on the left by $A_\nu^\dagger$, we can write this identity in the following useful form:

$$A_\nu^\dagger A_\nu A_\nu^\dagger = A_\nu^\dagger A_{\nu-1}^\dagger A_{\nu-1} + (2\nu-1)A_\nu^\dagger$$

$$\Rightarrow \qquad \left(H_\nu - \nu - \frac{1}{4}\right) A_\nu^\dagger = A_\nu^\dagger \left(H_{\nu-1} - (\nu-1) - \frac{1}{4}\right) + (2\nu-1)A_\nu^\dagger$$

$$\Rightarrow \qquad H_\nu A_\nu^\dagger = A_\nu^\dagger (H_{\nu-1} + 2\nu).$$

Therefore, the identity we have proved really states 'we can move the Hamiltonian past the raising operator, as long as we decrease the value of ν to $\nu - 1$, and add 2ν'.

This form of the identity can help us to show that $A_\nu^\dagger |0, \nu-1\rangle$ is also an unnormalised eigenstate of H_ν. First, we recall from our earlier work that

$$H_\nu |0, \nu\rangle = \left(\nu + \frac{1}{4}\right) |0, \nu\rangle .$$

Therefore, we have:

$$H_\nu A_\nu^\dagger |0, \nu-1\rangle = A_\nu^\dagger (H_{\nu-1} + 2\nu) |0, \nu-1\rangle \qquad \text{(above identity)}$$

$$= A_\nu^\dagger \left(\nu - 1 + \frac{1}{4} + 2\nu\right) |0, \nu-1\rangle \qquad \text{(definition of } |0, \nu-1\rangle)$$

$$= \left(3\nu - \frac{3}{4}\right) A_\nu^\dagger |0, \nu-1\rangle .$$

So indeed $A_\nu^\dagger |0, \nu-1\rangle$ is indeed an eigenstate, with eigenvalue

$$3\nu - \frac{3}{4}.$$

There is the possibility that $A_\nu^\dagger |0, \nu-1\rangle$ may not be normalisable - this indeed occurs for some values of ν. We'll address this in part (iv).

(iv) We now try to find the full set of eigenstates of H_ν using the trick from (iii). First, let's notice that the reason the trick in (iii) worked is because it allowed us to commute H_ν past $A^\dagger_\nu$ to operate on the ground state $|0, \nu-1\rangle$, in the process converting H_ν to $H_{\nu-1}$.

It's reasonably clear that to generalise, we need to include an $A^\dagger_{\nu-1}$ for $H_{\nu-1}$ to swap with. So the next state we should consider is:

$$A^\dagger_\nu A^\dagger_{\nu-1} |0, \nu-2\rangle .$$

We see that this is also an eigenstates of H_ν, by the same method as (iii):

$$H_\nu A^\dagger_\nu A^\dagger_{\nu-1} |0, \nu-2\rangle = A^\dagger_\nu (H_{\nu-1} + 2\nu) A^\dagger_{\nu-1} |0, \nu-2\rangle$$

$$= A^\dagger_\nu A^\dagger_{\nu-1} (H_{\nu-2} + 2(\nu-1) + 2\nu) |0, \nu-2\rangle = \left(5\nu - \frac{15}{4}\right) A^\dagger_\nu A^\dagger_{\nu-1} |0, \nu-2\rangle .$$

We're now ready to state and prove a general result:

Theorem: For each $k = 1, ..., \lfloor \nu \rfloor$, we have that $A^\dagger_\nu A^\dagger_{\nu-1} ... A^\dagger_{\nu-k+1} |0, \nu-k\rangle$ is an (unnormalised) energy eigenstate of H_ν with energy eigenvalue:

$$E_k = (2k+1)\nu - k^2 + \frac{1}{4}.$$

Proof: We prove the result directly. We have:

$$H_\nu A^\dagger_\nu A^\dagger_{\nu-1} ... A^\dagger_{\nu-k+1} |0, \nu-k\rangle = A^\dagger_\nu (H_{\nu-1} + 2\nu) A^\dagger_{\nu-1} ... A^\dagger_{\nu-k+1} |0, \nu-k\rangle$$

$$= A^\dagger_\nu A^\dagger_{\nu-1} (H_{\nu-2} + 2\nu + 2(\nu-1)) A^\dagger_{\nu-2} ... A^\dagger_{\nu-k+1} |0, \nu-k\rangle$$

$$\vdots$$

$$= A^\dagger_\nu A^\dagger_{\nu-1} ... A^\dagger_{\nu-k+1} (H_{\nu-k} + 2\nu + ... + 2(\nu-k+1)) |0, \nu-k\rangle .$$

Acting with $H_{\nu-k}$, we see that this is indeed an eigenstate as we expected. The eigenvalue is:

$$E_k = \nu - k + \frac{1}{4} + 2(\nu + \nu - 1 + ... + \nu - k + 1) = (2k+1)\nu - k + \frac{1}{4} - 1 - 2 ... - (k-1)$$

$$= (2k+1)\nu - k + \frac{1}{4} - k(k-1) = (2k+1)\nu - k^2 + \frac{1}{4},$$

as required.

We now need to explain the limits on the range of k. This comes from the fact we need these states to be normalisable. We claim that if we start with a normalisable state $|0, \nu-k\rangle$, then the state $A^\dagger_\nu ... A^\dagger_{\nu-k+1} |0, \nu-k\rangle$ is normalisable too. Conversely, we claim that if we start with a non-normalisable state $|0, \nu-k\rangle$, then $A^\dagger_\nu ... A^\dagger_{\nu-k+1} |0, \nu-k\rangle$ is also non-normalisable.

Assuming that these claims are true, we have bound states only for $\nu - k > 0 \Rightarrow \nu > k$ (since $|0, \nu-k\rangle$ is normalisable if and only if $\nu - k > 0$, as we saw in part (ii)), i.e. k can be at most $\lfloor \nu \rfloor$. Including the ground state, which is not included in the Theorem, this indicates that there are $\lfloor \nu + 1 \rfloor$ bound states, as required by the question.

It's easiest to prove our claims by working in the position representation. Let $\psi(x)$ be the normalisable position wavefunction for the state normalisable state $|\psi\rangle$. Then

$$||A_{\nu-k}\,|\psi\rangle\,||^2 = \int_{-\infty}^{\infty} \psi^* \left(\nu - k - e^{-x} - \frac{\partial}{\partial x}\right)\left(\nu - k - e^{-x} + \frac{\partial}{\partial x}\right)\psi\, dx$$

$$= \int_{-\infty}^{\infty} \left((\nu-k)^2|\psi|^2 - 2e^{-x}(\nu-k)|\psi|^2 + e^{-2x}|\psi|^2 + \frac{\partial}{\partial x}\left(e^{-x}\psi\right) - e^{-x}\frac{\partial\psi}{\partial x} - \frac{\partial^2\psi}{\partial x^2}\right) dx.$$

Since $\psi, \psi', \psi'' \to 0$ as $|x| \to \infty$, this integral converges (provided $\psi, \psi', \psi'' \to 0$ faster than an exponential, which they do in the case of the ground state we observed). Conversely, if $|\psi\rangle$ is not normalisable, the first term in this expansion diverges. □

There's one extra point that we need to address, that wasn't mentioned in our formal proof above - we must ask ourselves: are there any bound states of the Hamiltonian H_ν that are *not* included in the sequence of states described in the Theorem (and are not the ground state)? For a standard harmonic oscillator, this point is dealt with by applying the lowering operator repeatedly to show that if we don't start with one of our special energy eigenstates, we generate states with energy less than the ground state.

We'll aim for something similar here. Let $|E, \nu+1\rangle$ be *any* eigenstate of $H_{\nu+1}$ with any energy E. It's possible this is not generated by the sequence of raising operators in the above Theorem. Now consider:

$$H_\nu A_{\nu+1}\,|E,\nu+1\rangle = \left(A_\nu^\dagger A_\nu + \nu + \frac{1}{4}\right) A_{\nu+1}\,|E,\nu+1\rangle\,.$$

Now applying our result from part (iii) in reverse, we have:

$$A_\nu^\dagger A_\nu = A_{\nu+1}A_{\nu+1}^\dagger - 2\nu - 1.$$

It follows that we can write:

$$H_\nu A_{\nu+1}\,|E,\nu+1\rangle = \left(A_{\nu+1}A_{\nu+1}^\dagger - \nu - \frac{3}{4}\right) A_{\nu+1}\,|E,\nu+1\rangle$$

$$= A_{\nu+1}(A_{\nu+1}^\dagger A_{\nu+1})\,|E,\nu+1\rangle - \left(\frac{3}{4} + \nu\right) A_{\nu+1}\,|E,\nu+1\rangle\,.$$

Recalling the form of $H_{\nu+1}$, we have

$$H_\nu A_{\nu+1}\,|E,\nu+1\rangle = A_{\nu+1}\left(H_{\nu+1} - \nu - \frac{5}{4}\right)|E,\nu+1\rangle - \left(\frac{3}{4} + \nu\right) A_{\nu+1}\,|E,\nu+1\rangle$$

$$= (E - 2(\nu+1))\,A_{\nu+1}\,|E,\nu+1\rangle\,.$$

It follows that $A_{\nu+1}\,|E,\nu+1\rangle$ is an energy eigenstate of H_ν with *lower energy*. Therefore, if $|E,\nu\rangle$ is an energy eigenstate of H_ν, it follows that $A_{\nu-k+1}...A_{\nu-1}A_\nu\,|E,\nu\rangle$ is an energy eigenstate of $H_{\nu-k}$, with energy

$$E - 2\nu - 2(\nu-1) - ... - 2(\nu-k+1) = E - 2\nu k + 2(1+2+...+(k-1)) = E - 2\nu k + \frac{2}{2}k(k-1)$$

$$= E - (2\nu+1)k + k^2.$$

For sufficiently large k, we will enter the region where $\nu - k < 0$, i.e. $\nu < k$, in which there is no normalisable ground state - indeed, there are no bound states by just looking at the shape of the potential. This will occur *unless* we hit the ground state of $H_{\nu-k}$, i.e. $|0, \nu - k\rangle$, with our sequence of lowering operators. Then applying the next operator in the sequence, $A_{\nu-k}$, will give zero, since if $A_{\nu-k+1}...A_{\nu-1}A_\nu |E, \nu\rangle \propto |0, \nu - k\rangle$, we see that

$$A_{\nu-k}A_{\nu-k+1}...A_{\nu-1}A_\nu |E, \nu\rangle \propto A_{\nu-k} |0, \nu - k\rangle = 0.$$

Our sequence of lowering operators then terminates.

It follows that we need the energy of $A_{\nu-k+1}...A_{\nu-1}A_\nu |E, \nu\rangle$ to be the energy of the ground state of $H_{\nu-k}$, i.e. we require E and k to satisfy the relation:

$$E - (2\nu + 1)k + k^2 = \nu - k + \frac{1}{4} \qquad \Rightarrow \qquad E = E_k = (2k + 1)\nu - k^2 + \frac{1}{4}.$$

It follows that any energy eigenstate of H_ν that we start with, $|E, \nu\rangle$, must have the energy of one of the states we found earlier.

Finally, it's conceivable that some of our energy levels are degenerate, and there are yet more bound states. However, this is ruled out by the following Theorem:

Theorem: There are no degenerate bound states in one-dimensional quantum mechanics.

Proof: We can use a Part IB style quantum mechanics proof to show this result. Suppose that ψ_1 and ψ_2 are the position wavefunctions of two states of the same energy. Then we have:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_1}{\partial x^2} + V(x)\psi_1 = E\psi_1, \qquad -\frac{\hbar^2}{2m}\frac{\partial^2\psi_2}{\partial x^2} + V(x)\psi_2 = E\psi_2.$$

Multiplying the first equation by ψ_2, and the second by ψ_1, then subtracting from one another, we find:

$$\psi_2\frac{\partial^2\psi_1}{\partial x^2} - \psi_1\frac{\partial^2\psi_2}{\partial x^2} = 0.$$

Note we can write this as:

$$\frac{\partial}{\partial x}(\psi_2\psi_1' - \psi_1\psi_2') = 0 \qquad \Rightarrow \qquad \psi_2\psi_1' - \psi_1\psi_2' = \text{constant}.$$

Since these are bound states, as $|x| \to \infty$ we have $\psi_1, \psi_2 \to 0$. Therefore constant $= 0$. It follows that:

$$\frac{\psi_2'}{\psi_2} = \frac{\psi_1'}{\psi_1} \qquad \Rightarrow \qquad \psi_2 = c\psi_1$$

for some constant c. Therefore the states were the same all along, and hence there is no degeneracy. □

The final part of this question asks us whether the states we found above form a basis for Hilbert space. To frame this question another way, we must ask: do the wavefunctions of the states $|0, \nu\rangle$, $A_\nu^\dagger |0, \nu - 1\rangle$, etc, form a basis for the space of functions $L^2(\mathbb{R})$, i.e. the set of square-integrable functions?

The answer is *no*, since the space $L^2(\mathbb{R})$ is infinite-dimensional, but there are only finitely many states in our proposed basis.

7. Let $\mathbf{P}/\hbar$ and $\mathbf{J}/\hbar$ be the generators of translations and rotations respectively. By considering the effect of a rotation and translation on an arbitrary vector $\mathbf{v} \in \mathbb{R}^3$, show that

$$[J_i, P_j] = i\hbar\epsilon_{ijk}P_k.$$

Solution: Recall that to implement a classical symmetry S in quantum mechanics, we need to construct a unitary operator $U(S)$ that acts on Hilbert space. We can view our U operator as a map:

$$U : \{\text{classical symmetries}\} \to \{\text{unitary operators on Hilbert space}\}.$$

That is: to each classical symmetry, we assign a unitary operator acting on Hilbert space. An important property that we want from U is that it is a *homomorphism*:

$$U(S_1 \circ S_2) = U(S_1)U(S_2).$$

This just means: 'we can either form the composition of symmetries in the classical space of symmetries, $S_1 \circ S_2$, or in the quantum space of symmetries - the two approaches are equivalent'. This will be very important in this question. To work out the commutator $[J_i, P_j]$, we consider the difference between applying a rotation then a translation versus applying a translation then a rotation to a vector $\mathbf{v}$ *in the classical picture*, then use the homomorphism property to map to the *quantum picture*.

Let $R(\boldsymbol{\alpha})$ denote a *classical* rotation by angle $|\boldsymbol{\alpha}|$ anticlockwise around the axis $\hat{\boldsymbol{\alpha}}$. Similarly, let $T(\mathbf{a})$ denote a *classical* translation by a vector $\mathbf{a}$. Consider rotating a vector $\mathbf{v} \in \mathbb{R}^3$, and then translating it, in the classical space. The result of this operation is:

$$T(\mathbf{a})R(\boldsymbol{\alpha})\mathbf{v} = R(\boldsymbol{\alpha})\mathbf{v} + \mathbf{a}.$$

We could also have obtained this final result by translating the vector, then rotating it. However, we must modify the amount we translate by to make things work; in particular, we include a factor of the inverse rotation: $R^{-1}(\boldsymbol{\alpha}) = R(-\boldsymbol{\alpha})$:

$$R(\boldsymbol{\alpha})T(R(-\boldsymbol{\alpha})\mathbf{a})\mathbf{v} = R(\boldsymbol{\alpha})(\mathbf{v} + R(-\boldsymbol{\alpha})\mathbf{a}) = R(\boldsymbol{\alpha})\mathbf{v} + \mathbf{a}.$$

Comparing these two equations, and noting they hold for all $\mathbf{v}$, we have shown that the classical symmetries obey:

$$T(\mathbf{a})R(\boldsymbol{\alpha}) = R(\boldsymbol{\alpha})T(R(-\boldsymbol{\alpha})\mathbf{a}).$$

For $\boldsymbol{\alpha}$ infinitesimal, we can expand $R(-\boldsymbol{\alpha})\mathbf{a}$ in a more useful form:

Theorem: For $\boldsymbol{\alpha}$ infinitesimal, we have

$$R(\boldsymbol{\alpha})\mathbf{a} = \mathbf{a} + \boldsymbol{\alpha} \times \mathbf{a} + O(|\boldsymbol{\alpha}|^2).$$

Proof: Without loss of generality, align the z-axis with $\boldsymbol{\alpha}$, so we are rotating by an angle α anticlockwise about the z-axis. In these coordinates, $\boldsymbol{\alpha} = (0, 0, \alpha)$. Under the rotation, the vector $\mathbf{a} = (X, Y, Z)$ maps to the vector $R(\boldsymbol{\alpha})\mathbf{a}$, given by:

$$R(\boldsymbol{\alpha})\mathbf{a} = \begin{pmatrix} \cos(\alpha) & \sin(\alpha) & 0 \\ -\sin(\alpha) & \cos(\alpha) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} \cos(\alpha)X + \sin(\alpha)Y \\ -\sin(\alpha)X + \cos(\alpha)Y \\ Z \end{pmatrix}$$

Expanding in α, we have:

$$R(\boldsymbol{\alpha})\mathbf{a} = \begin{pmatrix} X + \alpha Y \\ -\alpha X + Y \\ Z \end{pmatrix} + O(\alpha^2) = \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} + \begin{pmatrix} \alpha Y \\ -\alpha X \\ Z \end{pmatrix} + O(\alpha^2).$$

Now notice that $\boldsymbol{\alpha} \times \mathbf{a} = (\alpha\, Y, -\alpha\, X, 0)$, so we have in fact shown that:

$$R(\boldsymbol{\alpha})\mathbf{a} = \mathbf{a} + \boldsymbol{\alpha} \times \mathbf{a} + O(|\boldsymbol{\alpha}|^2).$$

Since this final statement is coordinate-independent, it holds in complete generality. □

Therefore, our classical statement reads:

$$T(\mathbf{a})R(\boldsymbol{\alpha}) = R(\boldsymbol{\alpha})T(\mathbf{a} - \boldsymbol{\alpha} \times \mathbf{a}).$$

Applying our U homomorphism to transform these into quantum symmetries, we obtain:

$$U_T(\mathbf{a})U_R(\boldsymbol{\alpha}) = U_R(\boldsymbol{\alpha})U_T(\mathbf{a} - \boldsymbol{\alpha} \times \mathbf{a}).$$

Here, we have written $U(R(\boldsymbol{\alpha})) = U_R(\boldsymbol{\alpha})$ and $U_T(\mathbf{a}) = U(T(\mathbf{a}))$ to match up with the usual notation from lectures. We need the subscripts however to distinguish between the quantum translation and quantum rotations.

Now recall that $\mathbf{P}/\hbar$ is the infinitesimal generator of translations and $\mathbf{J}/\hbar$ is the infinitesimal generator of rotations. Therefore we can write this equation as:

$$\left(I - i\frac{\mathbf{a}\cdot\mathbf{P}}{\hbar}\right)\left(I - i\frac{\boldsymbol{\alpha}\cdot\mathbf{J}}{\hbar}\right) = \left(I - i\frac{\boldsymbol{\alpha}\cdot\mathbf{J}}{\hbar}\right)\left(I - i\frac{(\mathbf{a} - \boldsymbol{\alpha}\times\mathbf{a})\cdot\mathbf{P}}{\hbar}\right).$$

Expanding the exponentials and comparing the terms of order $O(\mathbf{a}, \boldsymbol{\alpha})$, we have:

$$\left(-i\frac{\mathbf{a}\cdot\mathbf{P}}{\hbar}\right)\left(-i\frac{\boldsymbol{\alpha}\cdot\mathbf{J}}{\hbar}\right) = i\frac{(\boldsymbol{\alpha}\times\mathbf{a})\cdot\mathbf{P}}{\hbar} + \left(-i\frac{\boldsymbol{\alpha}\cdot\mathbf{J}}{\hbar}\right)\left(-i\frac{\mathbf{a}\cdot\mathbf{P}}{\hbar}\right)$$

which simplifies to:

$$[\boldsymbol{\alpha}\cdot\mathbf{J}, \mathbf{a}\cdot\mathbf{P}] = i\hbar(\boldsymbol{\alpha}\times\mathbf{a})\cdot\mathbf{P}.$$

Writing this out in index notation, and noting that this holds for all infinitesimal $\mathbf{a}, \boldsymbol{\alpha}$, we find the required result:

$$[J_i, P_j] = i\hbar\epsilon_{ijk}P_k.$$

⁜ **Comments:** This question shows that **P** transforms like a *vector operator*, something that is explored more in David Skinner's notes and in Sakurai's book, *Modern Quantum Mechanics*.

This question is also discussed in David Skinner's notes in the section on *Transformations and Symmetries*, however the approach there is *not* entirely rigorous. Skinner's notes use the fact that

$$U([R(\boldsymbol{\alpha}), T(\mathbf{a})]) = U(R(\boldsymbol{\alpha})T(\mathbf{a}) - T(\mathbf{a})R(\boldsymbol{\alpha})) = [U_R(\boldsymbol{\alpha}), U_T(\mathbf{a})],$$

something which doesn't necessarily follow from the homomorphism property, since homomorphisms say *nothing* about linear combinations of terms, only about *products* of operators.

8. $(*)$ Consider a (spinless) free particle in $\mathbb{R}^3$. Galilean boosts with fixed velocity $\mathbf{v}$ act on the particle's Hilbert space through a time-independent unitary operator $U(\mathbf{v})$ defined by:

$$U^{-1}(\mathbf{v})\mathbf{X}(t)U(\mathbf{v}) = \mathbf{X}(t) + \mathbf{v}t,$$

where $\mathbf{X}(t)$ is the position operator in the Heisenberg picture.

(i) Show that $U(\mathbf{v}_1)U(\mathbf{v}_2) = U(\mathbf{v}_1 + \mathbf{v}_2)$ and that $U^{-1}(\mathbf{v})\mathbf{P}U(\mathbf{v}) = \mathbf{P} + m\mathbf{v}$. Hence express $U(\mathbf{v})$ in terms of $\mathbf{X}$, $\mathbf{P}$ and $\mathbf{v}$.

(ii) Let $T(\mathbf{a}) = e^{-i\mathbf{a}\cdot\mathbf{P}/\hbar}$ be the translation operator. Evaluate the composition of the operators

$$T^{-1}(\mathbf{a})U^{-1}(\mathbf{v})T(\mathbf{a})U(\mathbf{v}).$$

Is this compatible with what you'd expect classically for the corresponding sequence of boosts and translations?

Solution: (i) The defining equation of the boost operator is given in the question as:

$$U^{-1}(\mathbf{v})\mathbf{X}(t)U(\mathbf{v}) = \mathbf{X}(t) + \mathbf{v}t.$$

Thus the result of applying two successive boosts, with parameters $\mathbf{v}_1$ and $\mathbf{v}_2$ respectively, is:

$$U^{-1}(\mathbf{v}_2)U^{-1}(\mathbf{v}_1)\mathbf{X}(t)U(\mathbf{v}_1)U(\mathbf{v}_2) = U^{-1}(\mathbf{v}_2)(\mathbf{X}(t) + \mathbf{v}_1 t)U(\mathbf{v}_2) = \mathbf{X}(t) + \mathbf{v}_2 t + \mathbf{v}_1 t.$$

The result of applying a single boost with parameter $\mathbf{v}_1 + \mathbf{v}_2$ is:

$$U^{-1}(\mathbf{v}_1 + \mathbf{v}_2)\mathbf{X}(t)U(\mathbf{v}_1 + \mathbf{v}_2) = \mathbf{X}(t) + (\mathbf{v}_1 + \mathbf{v}_2)t.$$

Thus we have shown:

$$U^{-1}(\mathbf{v}_1 + \mathbf{v}_2)\mathbf{X}(t)U(\mathbf{v}_1 + \mathbf{v}_2) = U^{-1}(\mathbf{v}_2)U^{-1}(\mathbf{v}_1)\mathbf{X}(t)U(\mathbf{v}_1)U(\mathbf{v}_2).$$

Rearranging this relationship, we find:

$$\mathbf{X}(t)U(\mathbf{v}_1 + \mathbf{v}_2)U^{-1}(\mathbf{v}_2)U^{-1}(\mathbf{v}_1) = U(\mathbf{v}_1 + \mathbf{v}_2)U^{-1}(\mathbf{v}_2)U^{-1}(\mathbf{v}_1)\mathbf{X}(t)$$

$$\Rightarrow \qquad [\mathbf{X}(t), U(\mathbf{v}_1 + \mathbf{v}_2)U^{-1}(\mathbf{v}_2)U^{-1}(\mathbf{v}_1)] = \mathbf{0}.$$

Now let's consider the action of the operator $U(\mathbf{v}_1 + \mathbf{v}_2)U^{-1}(\mathbf{v}_2)U^{-1}(\mathbf{v}_1)$ on the position basis $|\mathbf{x}\rangle$. We claim that $|\mathbf{x}\rangle$ is mapped to $|\mathbf{x}\rangle$ for all $\mathbf{x} \in \mathbb{R}^3$; this is easily verified, since (at time $t = 0$):

$$\mathbf{X}U(\mathbf{v}_1 + \mathbf{v}_2)U^{-1}(\mathbf{v}_2)U^{-1}(\mathbf{v}_1)\,|\mathbf{x}\rangle = U(\mathbf{v}_1 + \mathbf{v}_2)U^{-1}(\mathbf{v}_2)U^{-1}(\mathbf{v}_1)\mathbf{X}\,|\mathbf{x}\rangle = \mathbf{x}U(\mathbf{v}_1 + \mathbf{v}_2)U^{-1}(\mathbf{v}_2)U^{-1}(\mathbf{v}_1)\,|\mathbf{x}\rangle\,.$$

hence $U(\mathbf{v}_1 + \mathbf{v}_2)U^{-1}(\mathbf{v}_2)U^{-1}(\mathbf{v}_1)\,|\mathbf{x}\rangle \propto |\mathbf{x}\rangle$ for each $\mathbf{x} \in \mathbb{R}^3$. But all the U's are unitary operators (given in the question), so are norm-preserving, hence we have:

$$U(\mathbf{v}_1 + \mathbf{v}_2)U^{-1}(\mathbf{v}_2)U^{-1}(\mathbf{v}_1)\,|\mathbf{x}\rangle = |\mathbf{x}\rangle$$

for all $|\mathbf{x}\rangle$. Therefore $U(\mathbf{v}_1 + \mathbf{v}_2)U^{-1}(\mathbf{v}_2)U^{-1}(\mathbf{v}_1) = I$ on a basis, and hence it follows that:

$$U(\mathbf{v}_1 + \mathbf{v}_2) = U(\mathbf{v}_1)U(\mathbf{v}_2),$$

as required.

To see how the Galilean boost operator acts on momentum, we need to relate $\mathbf{X}(t)$ to $\mathbf{P}(t)$. For a non-relativistic Hamiltonian H (this is the only context in which considering Galilean boosts makes sense!) given by

$$H = \frac{\mathbf{P}^2}{2m},$$

(recall the particle is free) we know that Heisenberg's equation of motion gives:

$$\dot{\mathbf{X}}(t) = -\frac{i}{\hbar}[H, \mathbf{X}(t)] = -\frac{i}{2m\hbar}[\mathbf{P}^2(t), \mathbf{X}(t)] = \frac{1}{m}\mathbf{P}(t),$$

and hence it follows that $\mathbf{P}(t) = m\dot{\mathbf{X}}(t)$. Thus taking the time-derivative of the defining equation of the boost $U(\mathbf{v})$, we get the required result:

$$U^{-1}(\mathbf{v})\dot{\mathbf{X}}(t)U(\mathbf{v}) = \dot{\mathbf{X}}(t) + \mathbf{v} \qquad \Rightarrow \qquad U^{-1}(\mathbf{v})\mathbf{P}(t)U(\mathbf{v}) = \mathbf{P}(t) + m\mathbf{v}.$$

Finally, we must express $U(\mathbf{v})$ in terms of $\mathbf{X}$, $\mathbf{P}$ and $\mathbf{v}$. So far, we have the two equations:

$$U^{-1}(\mathbf{v})\mathbf{X}(t)U(\mathbf{v}) = \mathbf{X}(t) + \mathbf{v}t$$

$$U^{-1}(\mathbf{v})\mathbf{P}(t)U(\mathbf{v}) = \mathbf{P}(t) + m\mathbf{v}.$$

Setting $t = 0$ in the first equation shows that $[\mathbf{X}, U(\mathbf{v})] = 0$. This commutation relation shows that $U(\mathbf{v})$ *does not depend on* $\mathbf{P}$, as we will prove in the following Theorem:

Theorem: Let A be an operator depending only on position $\mathbf{X}$ and momentum $\mathbf{P}$, i.e. $A = A(\mathbf{X}, \mathbf{P})$. Suppose that $[A, \mathbf{X}] = 0$. Then A is a independent of $\mathbf{P}$.

Proof: By assumption, we have for all $|\psi\rangle$, $[A, \mathbf{X}]\,|\psi\rangle = 0$. Let the momentum wavefunction of $|\psi\rangle$ be $\tilde{\psi}(\mathbf{p})$. Then the momentum wavefunction of $[A, \mathbf{X}]\,|\psi\rangle$ is

$$A(-i\hbar\nabla_{\mathbf{p}}\tilde{\psi}) + i\hbar\nabla_{\mathbf{p}}(A\tilde{\psi}) = 0,$$

which is equal to zero since $[A, \mathbf{P}]\,|\psi\rangle = 0$. This holds since $\mathbf{X} = -i\hbar\nabla_{\mathbf{p}}$ in the momentum basis, which is a fact we can verify through a brief calculation in the style of Examples Sheet 1. Note we've committed an abuse of notation and written A to mean the operator acting on both the Hilbert space, and the momentum wavefunction.

Using the Leibniz rule, we may rewrite this condition as: $(\nabla_{\mathbf{p}}A)\tilde{\psi} = 0$. This equation must hold for all momentum wavefunctions $\tilde{\psi}(\mathbf{p})$, and hence it follows that A is independent of $\mathbf{P}$. The result follows. □

It follows that $U(\mathbf{v})$ is a function of $\mathbf{X}$ (and the constant $\mathbf{v}$) only. Thus, we consider commuting $\mathbf{P}(t)$ and $U(\mathbf{v})$ in the momentum transformation equation when $t = 0$. We find that:

$$\mathbf{P} + m\mathbf{v} = U^{-1}(\mathbf{v})\mathbf{P}U(\mathbf{v}) = \mathbf{P} + U^{-1}(\mathbf{v})[\mathbf{P}, U(\mathbf{v})] = \mathbf{P} + U^{-1}(\mathbf{v})\frac{\partial U(\mathbf{v})}{\partial \mathbf{X}}[\mathbf{P}, \mathbf{X}] = \mathbf{P} - i\hbar U^{-1}(\mathbf{v})\frac{\partial U(\mathbf{v})}{\partial \mathbf{X}}$$

Here, we used the result from the Comments of Examples Sheet 1, Question 2, that $[\mathbf{P}, f(\mathbf{X})] = f'(\mathbf{X})[\mathbf{P}, \mathbf{X}]$. Reading off from the above equation, we see that we must solve the equation:

$$\frac{\partial U(\mathbf{v})}{\partial \mathbf{X}} = \frac{i}{\hbar}m\mathbf{v}U(\mathbf{v}).$$

This has the solution:

$$U(\mathbf{v}) = e^{im\mathbf{v}\cdot\mathbf{X}/\hbar},$$

which expresses $U(\mathbf{v})$ in terms of $\mathbf{X}$ and $\mathbf{v}$ as required.

(ii) We are now asked to evaluate the composition of operators:

$$T^{-1}(\mathbf{a})U^{-1}(\mathbf{a})T(\mathbf{a})U(\mathbf{v}) = e^{i\mathbf{a}\cdot\mathbf{P}/\hbar}e^{-im\mathbf{v}\cdot\mathbf{X}/\hbar}e^{-i\mathbf{a}\cdot\mathbf{P}/\hbar}e^{im\mathbf{v}\cdot\mathbf{X}/\hbar}.$$

To do so, we would like to reverse the order of the two central operators. We can use a result from Question 2:

$$e^A e^B = e^B e^A e^{[A,B]}$$

for operators A and B which both commute with their commutator $[A, B]$. In this case, we have:

$$e^{-im\mathbf{v}\cdot\mathbf{X}/\hbar}e^{-i\mathbf{a}\cdot\mathbf{P}/\hbar} = e^{-i\mathbf{a}\cdot\mathbf{P}/\hbar}e^{-im\mathbf{v}\cdot\mathbf{X}/\hbar}\exp\left(\left[-\frac{im\mathbf{v}\cdot\mathbf{X}}{\hbar}, -\frac{i\mathbf{a}\cdot\mathbf{P}}{\hbar}\right]\right) = \exp\left(-\frac{m}{\hbar^2}a_j v_i[X_i, P_j]\right) = \exp\left(-\frac{im}{\hbar}\mathbf{a}\cdot\mathbf{v}\right).$$

Hence the result is:

$$T^{-1}(\mathbf{a})U^{-1}(\mathbf{v})T(\mathbf{a})U(\mathbf{v}) = e^{-im\mathbf{a}\cdot\mathbf{v}/\hbar}.$$

An alternative, slightly quicker, method relies on the result:

$$U^{-1}(\mathbf{v})f(\mathbf{P})U(\mathbf{v}) = f(U^{-1}\mathbf{P}U(\mathbf{v})) = f(\mathbf{P} + m\mathbf{v}).$$

This can be seen to be true by writing out f in a power series, and then inserting $U(\mathbf{v})$'s and $U^{-1}(\mathbf{v})$'s everywhere. In our case, we have:

$$T^{-1}(\mathbf{a})U^{-1}(\mathbf{v})T(\mathbf{a})U(\mathbf{v}) = e^{i\mathbf{a}\cdot\mathbf{P}/\hbar}U^{-1}(\mathbf{v})e^{-i\mathbf{a}\cdot\mathbf{P}/\hbar}U(\mathbf{v}) = e^{i\mathbf{a}\cdot\mathbf{P}/\hbar}e^{-i\mathbf{a}\cdot(\mathbf{P}+m\mathbf{v})/\hbar} = e^{-im\mathbf{a}\cdot\mathbf{v}/\hbar},$$

combining the exponents in the final step because they commute.

In the classical picture, we'd have (with a slight abuse of notation, using the same symbols to denote operators on Hilbert space and on classical phase space):

$$\begin{aligned} T^{-1}(\mathbf{a})U^{-1}(\mathbf{v})T(\mathbf{a})U(\mathbf{v})\mathbf{x} &= T^{-1}(\mathbf{a})U^{-1}(\mathbf{v})T(\mathbf{a})(\mathbf{x} + \mathbf{v}t) \\ &= T^{-1}(\mathbf{a})U^{-1}(\mathbf{v})(\mathbf{x} + \mathbf{v}t + \mathbf{a}) \\ &= T^{-1}(\mathbf{a})(\mathbf{x} + \mathbf{a}) \\ &= \mathbf{x}. \end{aligned}$$

This holds for all classical positions $\mathbf{x} \in \mathbb{R}^3$, and so we see that classically, $T^{-1}(\mathbf{a})U^{-1}(\mathbf{a})T(\mathbf{a})U(\mathbf{v})$ is the identity operator.

Therefore, it looks like the quantum result is not compatible with the classical result. But the quantum result *is* the same as the identity *up to an unobservable phase* (recall overall phases are unimportant in quantum mechanics, because we always take the modulus squared before obtaining observable results). Therefore, the results are completely compatible.

Part II: Principles of Quantum Mechanics
Examples Sheet 2 Solutions

Please send all comments and corrections to jmm232@cam.ac.uk.

1. Let $\hat{\mathbf{n}}$ be the unit vector in the direction with polar coordinates (θ, ϕ) and let $\boldsymbol{\sigma}$ be the Pauli matrices. Find the eigenvectors of $\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}$. Hence show that the state of a spin-$\frac{1}{2}$ particle in which a measurement of the component of spin along $\hat{\mathbf{n}}$ is certain to yield $\hbar/2$ is

$$|\uparrow_{\hat{\mathbf{n}}}\rangle = \sin\left(\frac{\theta}{2}\right) e^{i\phi/2} |\downarrow\rangle + \cos\left(\frac{\theta}{2}\right) e^{-i\phi/2} |\uparrow\rangle\,, \qquad (*)$$

where $|\uparrow\rangle, |\downarrow\rangle$ are the usual eigenstates of S_z. Obtain the corresponding expression for $|\downarrow_{\hat{\mathbf{n}}}\rangle$. Explain why each of the coefficients in $(*)$ has modulus $1/\sqrt{2}$ when $\theta = \pi/2$, and why $\langle\uparrow \mid \uparrow_{\hat{\mathbf{n}}}\rangle = 0$ at $\theta = \pi$.

Solution: The unit vector is $\hat{\mathbf{n}} = (\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta))$, so

$$\hat{\mathbf{n}} \cdot \boldsymbol{\sigma} = \sin(\theta)\cos(\phi)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \sin(\theta)\sin(\phi)\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \cos(\theta)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} \cos(\theta) & \sin(\theta)e^{-i\phi} \\ \sin(\theta)e^{i\phi} & -\cos(\theta) \end{pmatrix}.$$

The eigenvalues of this matrix, λ, obey:

$$0 = \det\begin{pmatrix} \cos(\theta) - \lambda & \sin(\theta)e^{-i\phi} \\ \sin(\theta)e^{i\phi} & -\cos(\theta) - \lambda \end{pmatrix} = -\cos^2(\theta) + \lambda^2 - \sin^2(\theta) = (\lambda - 1)(\lambda + 1),$$

hence the eigenvalues are ± 1.

The eigenvector $(x, y)^T$ corresponding to the eigenvalue $+1$ obeys:

$$\begin{aligned} (\cos(\theta) - 1)x + \sin(\theta)e^{-i\phi}y &= 0 \\ \sin(\theta)e^{i\phi}x - (\cos(\theta) + 1)y &= 0. \end{aligned}$$

Recalling the trigonometric formulae:

$$\cos(\theta) - 1 = -2\sin^2\left(\frac{\theta}{2}\right), \qquad \cos(\theta) + 1 = 2\cos^2\left(\frac{\theta}{2}\right), \qquad \sin(\theta) = 2\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right),$$

we can rewrite these equations as:

$$\begin{aligned} \sin\left(\frac{\theta}{2}\right) e^{i\phi/2}x - \cos\left(\frac{\theta}{2}\right) e^{-i\phi/2}y &= 0 \\ \sin\left(\frac{\theta}{2}\right) e^{i\phi/2}x - \cos\left(\frac{\theta}{2}\right) e^{-i\phi/2}y &= 0. \end{aligned}$$

Hence an eigenvector corresponding to the eigenvalue $+1$ is:

$$\begin{pmatrix} \cos\left(\frac{1}{2}\theta\right) e^{-i\phi/2} \\ \sin\left(\frac{1}{2}\theta\right) e^{i\phi/2} \end{pmatrix}$$

By similar calculation, an eigenvector corresponding to the eigenvalue -1 is:

$$\begin{pmatrix} \sin\left(\frac{1}{2}\theta\right) e^{i\phi/2} \\ -\cos\left(\frac{1}{2}\theta\right) e^{-i\phi/2} \end{pmatrix}$$

Let's now relate these results to the spin operator $\mathbf{S}$. Recall that the spin operator for a spin-$\frac{1}{2}$ particle can be written as $\mathbf{S} = \frac{1}{2}\hbar\boldsymbol{\sigma}$, where $\boldsymbol{\sigma}$ is the vector of Pauli matrices. Hence the spin of the particle in the $\hat{\mathbf{n}}$ direction is $\hat{\mathbf{n}} \cdot \mathbf{S} = \frac{1}{2}\hbar\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}$, which is directly related to the matrix we've just been studying!

For a state $|\uparrow_{\hat{\mathbf{n}}}\rangle$ to have definite spin $\frac{1}{2}\hbar$ in the direction $\hat{\mathbf{n}}$, we need the state to be an eigenvector of $\hat{\mathbf{n}} \cdot \mathbf{S}$. That is, we need:

$$\hat{\mathbf{n}} \cdot \mathbf{S} \, |\uparrow_{\hat{\mathbf{n}}}\rangle = \frac{1}{2}\hbar\hat{\mathbf{n}} \cdot \boldsymbol{\sigma} \, |\uparrow_{\hat{\mathbf{n}}}\rangle = \frac{1}{2}\hbar \, |\uparrow_{\hat{\mathbf{n}}}\rangle \, ,$$

i.e. $|\uparrow_{\hat{\mathbf{n}}}\rangle$ is an eigenvector of $\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}$ with eigenvalue $+1$. But we've already found this eigenvector, and hence

$$|\uparrow_{\hat{\mathbf{n}}}\rangle = \sin\left(\frac{\theta}{2}\right) e^{i\phi/2} \, |\downarrow\rangle + \cos\left(\frac{\theta}{2}\right) e^{-i\phi/2} \, |\uparrow\rangle \, ,$$

as required (note this state is normalised; if we'd chosen another eigenvector in the above, we may have had to normalise at this point). Similarly, we have:

$$|\downarrow_{\hat{\mathbf{n}}}\rangle = \sin\left(\frac{\theta}{2}\right) e^{i\phi/2} \, |\uparrow\rangle - \cos\left(\frac{\theta}{2}\right) e^{-i\phi/2} \, |\downarrow\rangle \, .$$

At $\theta = \pi$, our unit vector is pointing in the direction of the negative z-axis, i.e. it corresponds to the particle having spin-down. Therefore, if we measure the spin in the z-direction, we will *definitely* see spin-down with probability 1. In particular, we have:

$$|\uparrow_{\hat{\mathbf{n}}}\rangle = |\downarrow\rangle$$

with this direction of $\hat{\mathbf{n}}$. It follows that $\langle\uparrow \mid \uparrow_{\hat{\mathbf{n}}}\rangle = 0$, i.e. the amplitude for seeing the system in the spin-up state is zero.

When $\theta = \pi/2$, the unit vector $\hat{\mathbf{n}}$ lies in the xy plane. Therefore, if we measure the system's spin in the z-direction, we will have equal probability of obtaining spin-up (i.e. the unit vector $\hat{\mathbf{n}}$ pointing along the positive z-axis) and obtaining spin-down (i.e. the unit vector $\hat{\mathbf{n}}$ pointing along the negative z-axis). It follows that we must have:

$$|\uparrow_{\hat{\mathbf{n}}}\rangle = \frac{1}{\sqrt{2}} \, |\downarrow\rangle + \frac{1}{\sqrt{2}} \, |\uparrow\rangle \, ,$$

which is what we found in the earlier part of the question.

2. For a spin-$\frac{1}{2}$ particle, the spin operator is $\mathbf{S} = \hbar\boldsymbol{\sigma}/2$, where $\boldsymbol{\sigma}$ is the vector $(\sigma_1, \sigma_2, \sigma_3)$, each entry of which is a Pauli matrix.

(i) Without multiplying matrices, explain why the Pauli matrices obey

$$\sigma_i\sigma_j = \delta_{ij}I + i\epsilon_{ijk}\sigma_k,$$

for $i, j, k \in \{1, 2, 3\}$, where I is the identity matrix. Hence show that $\mathbf{a}\cdot\boldsymbol{\sigma}\mathbf{b}\cdot\boldsymbol{\sigma} = \mathbf{a}\cdot\mathbf{b}I + i(\mathbf{a}\times\mathbf{b})\cdot\boldsymbol{\sigma}$ for any two vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^3$.

(ii) Hence show that $e^{-i\boldsymbol{\alpha}\cdot\mathbf{S}/\hbar} = \cos\left(\frac{\alpha}{2}\right) I - i\sin\left(\frac{\alpha}{2}\right)\hat{\boldsymbol{\alpha}}\cdot\boldsymbol{\sigma}$ for a spin-$\frac{1}{2}$ particle.

(iii) A particle of spin-$\frac{1}{2}$ interacts with a uniform, homogeneous magnetic field $\mathbf{B}$ via the Hamiltonian $H = -\gamma\mathbf{B}\cdot\mathbf{S}$, where γ is a constant. If the particle's spin is initially prepared to be in some state $|\chi\rangle$, show that the probability its spin is found to be in an orthogonal state $|\chi'\rangle$ a time t later is $|\langle\chi'|\hat{\mathbf{B}}\cdot\boldsymbol{\sigma}|\chi\rangle|^2\sin^2(\omega t)$, where ω is a frequency you should specify.

(iv) Obtain the Heisenberg equation of motion for $\mathbf{S}(t)$ with this Hamiltonian.

(v) Hence show that the spin operator in the Heisenberg picture is:

$$\mathbf{S}(t) = \cos(2\omega t)\mathbf{S} + (1-\cos(2\omega t))\hat{\mathbf{B}}(\hat{\mathbf{B}}\cdot\mathbf{S}) - \sin(2\omega t)\hat{\mathbf{B}}\times\mathbf{S}.$$

Solution: (i) Let's split the product into a commutator and an anti-commutator as follows:

$$\sigma_i\sigma_j = \frac{1}{2}(\sigma_i\sigma_j + \sigma_j\sigma_i) + \frac{1}{2}(\sigma_i\sigma_j - \sigma_j\sigma_i) = \frac{1}{2}\{\sigma_i, \sigma_j\} + \frac{1}{2}[\sigma_i, \sigma_j].$$

We will evaluate $\{\sigma_i, \sigma_j\}$ and $[\sigma_i, \sigma_j]$ in order to verify the identity. The form of the question suggests that we are allowed to assume that the Pauli matrices are related to the spin operator $\mathbf{S}$ (for spin-$\frac{1}{2}$ particles) via $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$. Indeed, it's reasonable to take this as the definition of the Pauli matrices. This relation immediately gives us the commutator we want:

$$[\sigma_i, \sigma_j] = \frac{4}{\hbar^2}[S_i, S_j] = \frac{4}{\hbar^2}i\hbar\epsilon_{ijk}S_k = 2i\epsilon_{ijk}\sigma_k.$$

It remains to show that the anticommutator $\{\sigma_i, \sigma_j\} = 2\delta_{ij}$. In order to do this, it's best to start by finding the diagonal elements of this anticommutator, i.e. $\{\sigma_i, \sigma_i\} = 2\sigma_i^2$ (with no summation here!).

To find σ_i^2, note that we can relate the square of this Pauli matrix to the square of the corresponding spin component: $\sigma_i^2 = \frac{4}{\hbar^2}S_i^2$. Now note that we can always rotate our coordinates so that $S_i = S_z$; then, since the eigenvalues of S_z are $\pm\hbar/2$, it follows that the eigenvalues of S_z^2 are both $\hbar^2/4$. In particular, it must be the case that

$$S_i^2 = S_z^2 = \frac{\hbar^2}{4}I,$$

and thus we must have $S_i^2 = \frac{1}{4}\hbar^2 I$ for all i. It follows that $\sigma_i^2 = 1$ for all i.

To get $\{\sigma_i, \sigma_j\}$ for $i \neq j$, there are a couple of tricks we could use:

- Method 1: Write the anticommutator as the square of a raising operator.
  Since $S_i^2 = \frac{1}{4}\hbar^2 I$ for all i, we have for $i \neq j$:

$$\{S_i, S_j\} = S_iS_j + S_jS_i = -i(S_i + iS_j)^2 - iS_i^2 + iS_j^2 = -i(S_i + iS_j)^2.$$

For $i \neq j$, we can rotate our coordinates so that $S_i + iS_j = S_x + iS_y$; hence, we see that

$$\{S_i, S_j\} = -iS_+^2,$$

where S_+ is the usual spin angular momentum raising operator. Now note that $S_+^2 = 0$. This follows because we can't ever put two more units of spin into our system - if we are at spin $1/2$ we would raise to spin $5/2$, and if we are at spin $-1/2$ we would raise to spin $3/2$, both of which are impossible for spin-$1/2$ particles. It follows that

$$\{S_i, S_j\} = 0 = \{\sigma_i, \sigma_j\}$$

for $i \neq j$. Combining with the result $\sigma_i^2 = 1$, we see $\{\sigma_i, \sigma_j\} = 2\delta_{ij}$.

- Method 2: Consider $\hat{n}_i\hat{n}_j\{\sigma_i, \sigma_j\}$.
For any unit vector $\hat{\mathbf{n}}$, we can rotate our coordinates such that $\hat{\mathbf{n}} = \hat{\mathbf{e}}_z$. Then:

$$(\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})^2 = \sigma_3^2 = 1,$$

using our earlier result. Hence we have $(\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})^2 = 1$ for any unit vector $\hat{\mathbf{n}}$. Applying this to the anti-commutator, we have:

$$\hat{n}_i\hat{n}_j\{\sigma_i, \sigma_j\} = (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})^2 + (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})^2 = 2(\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})^2 = 2I = 2\hat{n}_i\hat{n}_j\delta_{ij},$$

which gives $\{\sigma_i, \sigma_j\} = 2\delta_{ij}I$ as required.

The final part of this question follows immediately when we write things out in suffix notation:

$$(\mathbf{a} \cdot \boldsymbol{\sigma})(\mathbf{b} \cdot \boldsymbol{\sigma}) = a_i b_j \sigma_i \sigma_j = a_i b_j (\delta_{ij} I + i\epsilon_{ijk}\sigma_k) = (\mathbf{a} \cdot \mathbf{b})I + i(\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma}.$$

(ii) First, note that the exponential can be written as:

$$\exp\left(-\frac{i\boldsymbol{\alpha} \cdot \mathbf{S}}{\hbar}\right) = \exp\left(-\frac{i\boldsymbol{\alpha} \cdot \boldsymbol{\sigma}}{2}\right),$$

in terms of the Pauli matrices $\boldsymbol{\sigma}$, using the definition of $\mathbf{S}$. We would like to expand this exponential, the result of which will be to obtain lots of powers of $\boldsymbol{\alpha} \cdot \boldsymbol{\sigma}$. Thus it will be useful to consider the value of: $(\boldsymbol{\alpha} \cdot \boldsymbol{\sigma})^p$. We can simplify this whenever there are two Pauli matrices next to one another using the identity we proved in part (i). In particular, we have:

$$(\boldsymbol{\alpha} \cdot \boldsymbol{\sigma})^2 = \alpha_i \alpha_j \sigma_i \sigma_j = \alpha_i \alpha_j (\delta_{ij} I + i\epsilon_{ijk}\sigma_k) = |\boldsymbol{\alpha}|^2 I.$$

and hence we deduce that $(\boldsymbol{\alpha} \cdot \boldsymbol{\sigma})^p = |\boldsymbol{\alpha}|^p I$ for p even, and $(\boldsymbol{\alpha} \cdot \boldsymbol{\sigma})^p = |\boldsymbol{\alpha}|^{p-1}\boldsymbol{\alpha} \cdot \boldsymbol{\sigma}$ for p odd.

We are now ready to expand the matrix exponential. We have:

$$\begin{aligned}
\exp\left(-\frac{i\boldsymbol{\alpha} \cdot \sigma}{2}\right) &= \sum_{n=0}^{\infty} \frac{(-i)^n (\boldsymbol{\alpha} \cdot \boldsymbol{\sigma})^n}{2^n n!} \\
&= \sum_{n=0}^{\infty} \frac{(-i)^{2n} (\boldsymbol{\alpha} \cdot \boldsymbol{\sigma})^{2n}}{2^{2n}(2n)!} + \sum_{n=0}^{\infty} \frac{(-i)^{2n+1} (\boldsymbol{\alpha} \cdot \boldsymbol{\sigma})^{2n+1}}{2^{2n+1}(2n+1)!} && \text{(splitting into even and odd terms)} \\
&= \sum_{n=0}^{\infty} \frac{(-1)^n |\boldsymbol{\alpha}|^{2n}}{2^{2n}(2n)!} - \frac{i}{|\boldsymbol{\alpha}|} \sum_{n=0}^{\infty} \frac{(-1)^{2n} |\boldsymbol{\alpha}|^{2n+1}}{2^{2n+1}(2n+1)!} && \text{(using } (\boldsymbol{\alpha} \cdot \boldsymbol{\sigma})^p \text{ result)} \\
&= \cos\left(\frac{|\boldsymbol{\alpha}|}{2}\right) I - i \sin\left(\frac{|\boldsymbol{\alpha}|}{2}\right) \hat{\boldsymbol{\alpha}} \cdot \boldsymbol{\sigma} && \text{(definitions of sine, cosine)},
\end{aligned}$$

which is the required result.

(iii) As usual, we use the time-dependent Schrödinger equation. We have the formal solution of the Schrödinger equation:

$$i\hbar\frac{d\left|\psi\right\rangle}{dt} = H\left|\psi\right\rangle \qquad \Rightarrow \qquad \left|\psi(t)\right\rangle = e^{-iHt/\hbar}\left|\psi(0)\right\rangle = e^{-iHt/\hbar}\left|\chi\right\rangle,$$

where we have used the fact that we are initially in the spin state $\left|\psi(0)\right\rangle = \left|\chi\right\rangle$. We now insert the given Hamiltonian and evaluate the right hand side:

$$\exp\left(-\frac{iHt}{\hbar}\right)\left|\chi\right\rangle = \exp\left(\frac{\gamma it}{\hbar}\mathbf{B}\cdot\mathbf{S}\right)\left|\chi\right\rangle = \left(\cos\left(\frac{\gamma tB}{2}\right)I + i\sin\left(\frac{\gamma tB}{2}\right)\hat{\mathbf{B}}\cdot\boldsymbol{\sigma}\right)\left|\chi\right\rangle,$$

using the result from part (ii), with $\boldsymbol{\alpha} = -\gamma t\mathbf{B}$. Contracting with some orthogonal state $\left|\chi'\right\rangle$, we have:

$$\left\langle\chi'\right|\left(\cos\left(\frac{\gamma tB}{2}\right)I + i\sin\left(\frac{\gamma tB}{2}\right)\hat{\mathbf{B}}\cdot\boldsymbol{\sigma}\right)\left|\chi\right\rangle = \left\langle\chi'|\hat{\mathbf{B}}\cdot\boldsymbol{\sigma}|\chi\right\rangle i\sin\left(\frac{\gamma tB}{2}\right).$$

The desired probability is the modulus squared of this amplitude. We have:

$$\left|\left\langle\chi'|\hat{\mathbf{B}}\cdot\boldsymbol{\sigma}|\chi\right\rangle\right|^2\sin^2\left(\frac{\gamma tB}{2}\right),$$

which is exactly of the required form. In particular the frequency is $\omega = \gamma B/2$.

(iv) The Heisenberg equation of motion is:

$$\frac{d\mathbf{S}(t)}{dt} = \frac{i}{\hbar}[H, \mathbf{S}(t)],$$

hence we must evaluate $[H, \mathbf{S}(t)]$. Since

$$[H, \mathbf{S}(t)] = [e^{iHt/\hbar}He^{-iHt/\hbar}, e^{iHt/\hbar}\mathbf{S}e^{-iHt/\hbar}] = e^{iHt/\hbar}[H, \mathbf{S}]e^{-iHt/\hbar},$$

it's sufficient to evaluate the Schrödinger picture commutator first, and then transform the result to the Heisenberg picture. We have:

$$[H, S_i] = -\gamma B_j[S_j, S_i] = -\gamma B_j i\hbar\epsilon_{jik}S_k = \gamma i\hbar(\mathbf{B}\times\mathbf{S})_i.$$

Hence we have:

$$[H, \mathbf{S}(t)] = \gamma i(\mathbf{B}\times\mathbf{S}(t)) \qquad \Rightarrow \qquad \frac{d\mathbf{S}(t)}{dt} = -\gamma\mathbf{B}\times\mathbf{S}(t).$$

(v) We now solve the vector equation we derived in part (iv). Note first that $\mathbf{S}(0) = \mathbf{S}$, where $\mathbf{S}$ is the Schrödinger picture spin operator, which implies that $\dot{\mathbf{S}}(0) = -\gamma\mathbf{B}\times\mathbf{S}$, so we have some initial conditions. Turning to the equation itself, we can differentiate to get:

$$\frac{d^2\mathbf{S}(t)}{dt^2} = -\gamma\mathbf{B}\times\left(\frac{d\mathbf{S}(t)}{dt}\right) = \gamma^2\mathbf{B}\times(\mathbf{B}\times\mathbf{S}(t)) = \gamma^2\left(\mathbf{B}(\mathbf{B}\cdot\mathbf{S}(t)) - B^2\mathbf{S}(t)\right),$$

where in the last equality, we used Lagrange's formula for the vector triple product, $\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) = \mathbf{b}(\mathbf{a}\cdot\mathbf{c}) - \mathbf{c}(\mathbf{a}\cdot\mathbf{b})$.

To solve this equation, consider splitting $\mathbf{S}(t)$ into a part that is parallel to $\mathbf{B}$ and a part that is perpendicular to $\mathbf{B}$. We write:

$$\mathbf{S}(t) = \mathbf{S}_{\parallel}(t) + \mathbf{S}_{\perp}(t), \qquad \text{where} \qquad \mathbf{S}_{\parallel}(t) = (\hat{\mathbf{B}}\cdot\mathbf{S}(t))\hat{\mathbf{B}}, \quad \mathbf{S}_{\perp}(t) = \mathbf{S}(t) - (\hat{\mathbf{B}}\cdot\mathbf{S}(t))\hat{\mathbf{B}}.$$

The parallel part satisfies the differential equation (recall $\mathbf{B}$ is constant):

$$\frac{d^2\mathbf{S}_{\parallel}}{dt^2} = \frac{d^2}{dt^2}\left[(\hat{\mathbf{B}}\cdot\mathbf{S}(t))\hat{\mathbf{B}}\right] = \gamma^2\left(\mathbf{B}\cdot\hat{\mathbf{B}}(\mathbf{B}\cdot\mathbf{S}(t)) - B^2(\mathbf{S}(t)\cdot\hat{\mathbf{B}})\right)\hat{\mathbf{B}} = \mathbf{0},$$

hence we can write $\mathbf{S}_{\parallel}(t) = \mathbf{A}_0 + \mathbf{A}_1 t$, for constant vectors $\mathbf{A}_0, \mathbf{A}_1$. Note that $\mathbf{S}_{\parallel}(0) = (\hat{\mathbf{B}}\cdot\mathbf{S})\hat{\mathbf{B}}$ and $\dot{\mathbf{S}}_{\parallel}(0) = (\hat{\mathbf{B}}\cdot\dot{\mathbf{S}}(0))\hat{\mathbf{B}} = -\gamma(\hat{\mathbf{B}}\cdot(\mathbf{B}\times\mathbf{S}))\hat{\mathbf{B}} = \mathbf{0}$, so we see that the constants are given by $\mathbf{A}_0 = (\hat{\mathbf{B}}\cdot\mathbf{S})\hat{\mathbf{B}}$ and $\mathbf{A}_1 = \mathbf{0}$.

The perpendicular part satisfies the differential equation:

$$\frac{d^2\mathbf{S}_\perp}{dt^2} = \frac{d^2}{dt^2}\left[\mathbf{S}(t) - (\hat{\mathbf{B}}\cdot\mathbf{S}(t))\hat{\mathbf{B}}\right] = \gamma^2\left(\mathbf{B}(\mathbf{B}\cdot\mathbf{S}(t)) - B^2\mathbf{S}(t)\right) - \gamma^2\mathbf{S}(t)\left(B(\mathbf{B}\cdot\mathbf{S}(t)) - B^2(\hat{\mathbf{B}}\cdot\mathbf{S})\right)$$

$$= -\gamma^2B^2\left(\mathbf{S}(t) - (\hat{\mathbf{B}}\cdot\mathbf{S}(t))\hat{\mathbf{B}}\right) = -\gamma^2B^2\mathbf{S}_\perp(t),$$

which has the solution:

$$\mathbf{S}_\perp(t) = \mathbf{A}_2\cos(\gamma Bt) + \mathbf{A}_3\sin(\gamma Bt),$$

for some constant vectors $\mathbf{A}_2$, $\mathbf{A}_3$. These are again fixed by the initial conditions; this time we have:

$$\mathbf{S}_\perp(0) = \mathbf{S} - (\hat{\mathbf{B}}\cdot\mathbf{S})\hat{\mathbf{B}}, \qquad \dot{\mathbf{S}}_\perp(0) = -\gamma B(\hat{\mathbf{B}}\times\mathbf{S}),$$

and hence:

$$\mathbf{S}_\perp(t) = \left(\mathbf{S} - (\hat{\mathbf{B}}\cdot\mathbf{S})\hat{\mathbf{B}}\right)\cos(\gamma Bt) - (\hat{\mathbf{B}}\times\mathbf{S})\sin(\gamma Bt).$$

Putting everything together, we have:

$$\mathbf{S}(t) = (\hat{\mathbf{B}}\cdot\mathbf{S})\hat{\mathbf{B}} + \left(\mathbf{S} - (\hat{\mathbf{B}}\cdot\mathbf{S})\hat{\mathbf{B}}\right)\cos(\gamma Bt) - (\hat{\mathbf{B}}\times\mathbf{S})\sin(\gamma Bt)$$

$$= \cos(2\omega t)\mathbf{S} + (1-\cos(2\omega t))\hat{\mathbf{B}}(\hat{\mathbf{B}}\cdot\mathbf{S}) - \sin(2\omega t)\hat{\mathbf{B}}\times\mathbf{S},$$

as required (recall $\omega = \gamma B/2$ from part (iii)).

3. A spin-$1/2$ particle interacts with a time-varying magnetic field such that:

$$H = -\gamma \mathbf{B}(t) \cdot \mathbf{S} \qquad \text{where} \qquad \mathbf{B}(t) = B_0 \hat{\mathbf{z}} + b\left(\hat{\mathbf{x}}\cos(\omega_1 t) + \hat{\mathbf{y}}\sin(\omega_1 t)\right).$$

Let $|\psi(t)\rangle$ be the state of the particle at time t and let $U(\omega_1 t\hat{\mathbf{z}})$ be the rotation operator around the $\hat{\mathbf{z}}$-axis through the time-dependent angle $\omega_1 t$.

(i) Define $|\chi(t)\rangle$ by $|\psi(t)\rangle = U(\omega_1 t\hat{\mathbf{z}})\,|\chi(t)\rangle$. Show that $|\chi(t)\rangle$ obeys the time-dependent Schrödinger equation with Hamiltonian $H_{\text{eff}} = -\gamma \mathbf{B}_{\text{eff}} \cdot \mathbf{S}$, where $\mathbf{B}_{\text{eff}}$ is a time-independent magnetic field you should specify.

(ii) Hence show that $\langle \mathbf{S} \rangle_{\psi(t)} = R(\omega_1 t\hat{\mathbf{z}})R(-\gamma t \mathbf{B}_{\text{eff}})\,\langle \mathbf{S} \rangle_{\psi(0)}$, where $R(\boldsymbol{\alpha})$ is a rotation matrix in $\mathbb{R}^3$.

(iii) Draw a sketch to illustrate how $\langle \mathbf{S} \rangle_{\psi(t)}$ varies in time.

Solution: (i) Let's write $|\psi\rangle := |\psi(t)\rangle$, $|\chi\rangle := |\chi(t)\rangle$ and $U := U(\omega_1 t\hat{\mathbf{z}})$ to save on notation. Then $|\psi\rangle = U\,|\chi\rangle$. Since $|\psi\rangle$ is the state of the system, it obeys the Schrödinger equation:

$$i\hbar \frac{d\,|\psi\rangle}{dt} = H\,|\psi\rangle\,.$$

Writing this in terms of $|\chi\rangle$, we have:

$$i\hbar \frac{dU}{dt}\,|\chi\rangle + i\hbar U \frac{d\,|\chi\rangle}{dt} = HU\,|\chi\rangle\,.$$

Rearranging, we have:

$$i\hbar \frac{d\,|\chi\rangle}{dt} = U^{-1}HU\,|\chi\rangle - i\hbar U^{-1}\frac{dU}{dt}\,|\chi\rangle = \left(U^{-1}HU - i\hbar U^{-1}\frac{dU}{dt}\right)|\chi\rangle =: H_{\text{eff}}\,|\chi\rangle\,.$$

So we see that we must evaluate:

$$H_{\text{eff}} = U^{-1}HU - i\hbar U^{-1}\frac{dU}{dt}. \qquad (*)$$

Let's start with the term $U^{-1}HU$. There are essentially two ways to proceed:

· 1. Algebraic method. Note that we can write U and H in matrix form, since they act on a spin-$1/2$ Hilbert space. In particular, H can be written as:

$$H = -\gamma \mathbf{B}\cdot\mathbf{S} = -\frac{\hbar\gamma}{2}\mathbf{B}\cdot\boldsymbol{\sigma} = -\frac{\hbar\gamma}{2}\begin{pmatrix} B_0 & b(\cos(\omega_1 t) - i\sin(\omega_1 t)) \\ b(\cos(\omega_1 t) + i\sin(\omega_1 t)) & -B_0 \end{pmatrix} = -\frac{\hbar\gamma}{2}\begin{pmatrix} B_0 & be^{-i\omega_1 t} \\ be^{i\omega_1 t} & -B_0 \end{pmatrix},$$

using the definitions of the Pauli matrices. Similarly, we can write:

$$U = U(\omega_1 t\hat{\mathbf{z}}) = \exp\left(-\frac{i\omega_1 t S_3}{\hbar}\right) = \exp\left(-\frac{i\omega_1 t\sigma_3}{2}\right) = \begin{pmatrix} e^{-i\omega_1 t/2} & 0 \\ 0 & e^{i\omega_1 t/2} \end{pmatrix},$$

since the third Pauli matrix is given by $\sigma_3 = \text{diag}\{1, -1\}$. The task of evaluating $U^{-1}HU$ now simply comes down to matrix multiplication; we have:

$$\begin{aligned} U^{-1}HU &= -\frac{\hbar\gamma}{2}\begin{pmatrix} e^{i\omega_1 t/2} & 0 \\ 0 & e^{-i\omega_1 t/2} \end{pmatrix}\begin{pmatrix} B_0 & be^{-i\omega_1 t} \\ be^{i\omega_1 t} & -B_0 \end{pmatrix}\begin{pmatrix} e^{-i\omega_1 t/2} & 0 \\ 0 & e^{i\omega_1 t/2} \end{pmatrix} \\ &= -\frac{\hbar\gamma}{2}\begin{pmatrix} B_0 & b \\ b & -B_0 \end{pmatrix}. \end{aligned}$$

Notice that the right hand side is precisely the same as the matrix form of the original Hamiltonian H, except with $\omega_1 \mapsto 0$. Thus we have:

$$U^{-1}HU = -\gamma\left(B_0\hat{\mathbf{z}} + b\hat{\mathbf{x}}\right)\cdot\mathbf{S}.$$

- 2. GEOMETRIC METHOD. Instead of doing all the algebra above, we could use some results from the course. Recall that in quantum mechanics, a *vector operator* $\mathbf{V}$ transforms under the rotation operator $U(\boldsymbol{\alpha})$ as:

$$U(\boldsymbol{\alpha})^{-1}\mathbf{V}U(\boldsymbol{\alpha}) = R(\boldsymbol{\alpha})\mathbf{V}, \tag{†1}$$

where $R(\boldsymbol{\alpha})$ is the 3×3 special orthogonal matrix corresponding to a rotation by $|\boldsymbol{\alpha}|$ anticlockwise about the axis $\hat{\boldsymbol{\alpha}}$. If we neglect space and focus on spin, the rotation operator can be written in the form $U(\boldsymbol{\alpha}) = \exp\left(-i\boldsymbol{\alpha}\cdot\mathbf{S}/\hbar\right)$.

Expanding (†1) infinitesimally, we find (using the standard arguments from lectures and Examples Sheet 1) that:

$$[S_i, V_j] = i\hbar\epsilon_{ijk}V_k. \tag{†2}$$

We also know from Examples Sheet 1 that this commutation relation (†2) implies the finite transformation law (†1) using Hadamard's lemma (see the Comments on Examples Sheet 1, Question 2). In particular, (†1) and (†2) are equivalent conditions for an operator $\mathbf{V}$ to be a vector operator.

Recalling the spin algebra $[S_i, S_j] = i\hbar\epsilon_{ijk}S_k$, we see that the spin operator $\mathbf{S}$ itself is a vector operator, and hence transforms under rotations as:

$$U(\boldsymbol{\alpha})^{-1}\mathbf{S}U(\boldsymbol{\alpha}) = R(\boldsymbol{\alpha})\mathbf{S}.$$

This can immediately be applied to our question; we have:

$$U^{-1}HU = -\gamma\mathbf{B}\cdot\left(U^{-1}(\omega_1 t\hat{\mathbf{z}})\mathbf{S}U(\omega_1 t\hat{\mathbf{z}})\right) = -\gamma\mathbf{B}\cdot\left(R(\omega_1 t\hat{\mathbf{z}})\mathbf{S}\right).$$

Now, recall that rotation matrices are orthogonal (i.e. $R^T = R^{-1}$), hence we can move the rotation from acting on the spin operator $\mathbf{S}$ to instead acting on the magnetic field $\mathbf{B}$:

$$\mathbf{B}\cdot\left(R(\omega_1 t\hat{\mathbf{z}})\mathbf{S}\right) = B_i R(\omega_1 t\hat{\mathbf{z}})_{ij}S_j = R(-\omega_1 t\hat{\mathbf{z}})_{ji}B_i S_j = \left(R(-\omega_1 t\hat{\mathbf{z}})\mathbf{B}\right)\cdot\mathbf{S}.$$

Hence we have:

$$U^{-1}HU = -\gamma\left(R(-\omega_1 t\hat{\mathbf{z}})\mathbf{B}\right)\cdot\mathbf{S} = -\gamma\left(B_0\hat{\mathbf{z}} + b\hat{\mathbf{x}}\right)\cdot\mathbf{S},$$

which is precisely the result we obtained above by algebraic means.

It now remains to evaluate the term involving the derivative, $U^{-1}(dU/dt)$. This is simpler, and we can do it directly:

$$-i\hbar U^{-1}\frac{dU}{dt} = -\omega_1\exp\left(\frac{i\omega_1 tS_3}{\hbar}\right)\exp\left(-\frac{i\omega_1 tS_3}{\hbar}\right)S_3 = -\omega_1 S_3.$$

It follows that $(*)$ can be rewritten as:

$$H_{\text{eff}} = -\gamma\left(B_0\hat{\mathbf{z}} + b\hat{\mathbf{x}}\right)\cdot\mathbf{S} - \omega_1 S_3 = -\gamma\left(\left(B_0 + \frac{\omega_1}{\gamma}\right)\hat{\mathbf{z}} + b\hat{\mathbf{x}}\right)\cdot\mathbf{S}.$$

Hence we have indeed shown that $H_{\text{eff}} = -\gamma\mathbf{B}_{\text{eff}}\cdot\mathbf{S}$, with

$$\mathbf{B}_{\text{eff}} = \left(B_0 + \frac{\omega_1}{\gamma}\right)\hat{\mathbf{z}} + b\hat{\mathbf{x}}.$$

We now see the significance of defining $|\chi(t)\rangle := U(-\omega_1 t\hat{\mathbf{z}})\,|\psi(t)\rangle$. The original magnetic field $\mathbf{B}(t)$ consisted of a background field $B_0\hat{\mathbf{z}}$ pointing in the z-direction, together with a rotating, dynamical magnetic field $b\hat{\mathbf{x}}\cos(\omega_1 t) + b\hat{\mathbf{y}}\sin(\omega_1 t)$. The idea of defining the state $|\chi(t)\rangle$ is to boost the state $|\psi(t)\rangle$ into the rotating frame, so that the rotating part of the field becomes non-dynamical, and hence easier to work with.

We see that indeed the new field is non-dynamical, but we have also acquired an additional contribution to the background field pointing in the $\hat{\mathbf{z}}$ direction. The origin of this contribution is the fact that we have changed reference frames from an initial inertial frame to a rotating, non-inertial frame, and hence we acquire some additional energy term (which crops up in the quantum-mechanical Hamiltonian) to account for the fictitious forces that arise in the non-inertial frame.

(ii) Next, we are asked to derive a particular formula for $\langle \mathbf{S} \rangle_{\psi(t)}$, the expected value of the spin when the system is in the state $|\psi(t)\rangle$, i.e. the expected value of the spin at time t. We would like to derive a formula such that $\langle \mathbf{S} \rangle_{\psi(t)}$ can be written in terms of $\langle \mathbf{S} \rangle_{\psi(0)}$, hence we will need to think about time-evolution of the system.

The standard time-dependent Schrödinger equation for the state $|\psi(t)\rangle$, given by:

$$i\hbar \frac{d\,|\psi(t)\rangle}{dt} = H(t)\,|\psi(t)\rangle$$

does *not* have the formal solution $|\psi(t)\rangle = e^{-iH(t)t/\hbar}\,|\psi(0)\rangle$ in this case, because the *Hamiltonian is time-dependent*. In particular, differentiating this formula solution, we will get additional terms arising that correspond to time-derivatives of the Hamiltonian, and we see the equation is *not* satisfied by this solution.[6]

Instead, in this question we have derived a Schrödinger equation for $|\chi(t)\rangle$ in the rotating frame, where the effective Hamiltonian is *not* time-dependent. We can thus use the formal solution of the Schrödinger equation here:

$$i\hbar \frac{d\,|\chi(t)\rangle}{dt} = H_{\text{eff}}\,|\chi(t)\rangle \qquad \Rightarrow \qquad |\chi(t)\rangle = e^{-iH_{\text{eff}}t/\hbar}\,|\chi(0)\rangle = e^{i\gamma t \mathbf{B}_{\text{eff}}\cdot\mathbf{S}/\hbar}\,|\chi(0)\rangle = U(-\gamma t \mathbf{B}_{\text{eff}})\,|\chi(0)\rangle\,.$$

We can use this result to evaluate $\langle \mathbf{S} \rangle_{\psi(t)}$, by passing to the states $|\chi(t)\rangle$ first, performing the reverse time-evolution back to $t = 0$, then restoring the states $|\psi(0)\rangle$. We have:

$$\begin{aligned}
\langle \mathbf{S} \rangle_{\psi(t)} &= \langle \psi(t)|\mathbf{S}|\psi(t)\rangle \\
&= \langle \chi(t)|U^\dagger(\omega_1 t\hat{\mathbf{z}})\mathbf{S}U(\omega_1 t\hat{\mathbf{z}})|\chi(t)\rangle \\
&= \langle \chi(t)|R(\omega_1 t\hat{\mathbf{z}})\mathbf{S}|\chi(t)\rangle && (\mathbf{S} \text{ is a vector operator; see above 'geometric method'}) \\
&= R(\omega_1 t\hat{\mathbf{z}})\,\langle \chi(t)|\mathbf{S}|\chi(t)\rangle && (R \text{ acts on components of } \mathbf{S}\text{, not on Hilbert space}) \\
&= R(\omega_1 t\hat{\mathbf{z}})\,\langle \chi(0)|U^\dagger(-\gamma t\mathbf{B}_{\text{eff}})\mathbf{S}U(-\gamma t\mathbf{B}_{\text{eff}})|\chi(0)\rangle && (\text{time evolution of } |\chi(t)\rangle \text{ from above}) \\
&= R(\omega_1 t\hat{\mathbf{z}})\,\langle \chi(0)|R(-\gamma t\mathbf{B}_{\text{eff}})\mathbf{S}|\chi(0)\rangle && (\mathbf{S} \text{ is a vector operator; see above 'geometric method'}) \\
&= R(\omega_1 t\hat{\mathbf{z}})R(-\gamma t\mathbf{B}_{\text{eff}})\,\langle \chi(0)|\mathbf{S}|\chi(0)\rangle && (R \text{ acts on components of } \mathbf{S}\text{, not on Hilbert space}) \\
&= R(\omega_1 t\hat{\mathbf{z}})R(-\gamma t\mathbf{B}_{\text{eff}})\,\langle \psi(0)|\mathbf{S}|\psi(0)\rangle && (|\psi(0)\rangle = U(\mathbf{0})\,|\chi(0)\rangle = |\chi(0)\rangle) \\
&= R(\omega_1 t\hat{\mathbf{z}})R(-\gamma t\mathbf{B}_{\text{eff}})\,\langle \mathbf{S} \rangle_{\psi(0)}\,.
\end{aligned}$$

Hence we have established $\langle \mathbf{S} \rangle_{\psi(t)} = R(\omega_1 t\hat{\mathbf{z}})R(-\gamma t\mathbf{B}_{\text{eff}})\,\langle \mathbf{S} \rangle_{\psi(0)}$, as required.

(iii) The motion of $\langle \mathbf{S} \rangle_{\psi(t)}$ is that of a *spinning top*, of the type you study in Part II Classical Dynamics. There is a constant rotation around the $\hat{\mathbf{z}}$ axis, coupled with another rotation around that $\hat{\mathbf{B}}_{\text{eff}}$ axis which can combine in three possible ways, depending on how fast the relative rotations are:[7]

[6] We will see how to deal with time-dependent Hamiltonians later in the course when we study the *interaction picture*, where we find that the formal solution of the above equation is given by the *time-ordered exponential* of the Hamiltonian acting on the state $|\psi(0)\rangle$.

[7] See Figure 44, page 70 of David Tong's Part II Classical Dynamics notes for better pictures.

4. Write down the 3×3 matrix that represents S_x for a spin-1 system in the basis in which $S_z = \mathrm{diag}\{\hbar, 0, -\hbar\}$.

An unpolarised beam of spin-1 particles enters a Stern-Gerlach filter that passes only particles with $S_z = \hbar$. On exiting this filter, the beam enters a second filter that passes only particles with $S_x = \hbar$ and then finally it encounters a filter that passes only particles with $S_z = -\hbar$. What fraction of the initial particles make it right through?

Solution: We saw in lectures that the relevant matrix was:

$$S_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

It will be useful to know the eigenvectors and eigenvalues of the matrix S_x. Via a quick calculation, we find the normalised eigenvectors, and corresponding eigenvalues, are:

$$\begin{pmatrix} 1/2 \\ -\sqrt{2}/2 \\ 1/2 \end{pmatrix}, \text{ with eigenvalue } -\hbar, \qquad \begin{pmatrix} 1/2 \\ \sqrt{2}/2 \\ 1/2 \end{pmatrix}, \text{ with eigenvalue } \hbar, \text{ and} \qquad \begin{pmatrix} -1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \end{pmatrix}, \text{ with eigenvalue } 0.$$

It's also useful to know the eigenvectors and eigenvalues of the matrix S_z. Trivially, its normalised eigenvectors and corresponding eigenvalues are:

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \text{ with eigenvalue } \hbar, \qquad \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \text{ with eigenvalue } 0, \text{ and} \qquad \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \text{ with eigenvalue } -\hbar.$$

Let's tackle the Stern-Gerlach filter part of the question now. The term 'unpolarised' means that the initial beam contains an equal mix of all possible spin states of the particles. Thus we assume that $1/3$ of the initial particles are in the spin state $|1,1\rangle$, $1/3$ of the initial particles are in the spin state $|1,0\rangle$ and $1/3$ of the initial particles are in the spin state $|1,-1\rangle$, where $|s,\sigma\rangle$ denotes a spin state with total spin 1 and spin σ in the z-direction, as usual.

The first filter passes only particles with $S_z = \hbar$, that is, only particles in the state $|1,1\rangle$ are allowed through. Therefore $1/3$ of the particles make it through the first filter, and the state of all particles making it through the first filter must be:

$$|\psi\rangle = |1,1\rangle.$$

We now want to pass this state through an S_x-filter. Therefore, we rewrite the state in terms of S_x eigenvectors. This is an easy exercise in linear algebra, leading to: $|\psi\rangle = |1,1\rangle =$

$$\underbrace{\frac{1}{2}\left(\frac{1}{2}|1,1\rangle - \frac{\sqrt{2}}{2}|1,0\rangle + \frac{1}{2}|1,-1\rangle\right)}_{S_x \text{ eigenvector with eigenvalue } -\hbar} + \underbrace{\frac{1}{2}\left(\frac{1}{2}|1,1\rangle + \frac{\sqrt{2}}{2}|1,0\rangle + \frac{1}{2}|1,-1\rangle\right)}_{S_x \text{ eigenvector with eigenvalue } \hbar} - \frac{\sqrt{2}}{2}\underbrace{\left(-\frac{1}{\sqrt{2}}|1,1\rangle + \frac{1}{\sqrt{2}}|1,-1\rangle\right)}_{S_x \text{ eigenvector with eigenvalue } 0}.$$

Now the second filter passes only particles with $S_x = \hbar$, so only particles in the eigenstate with S_x-eigenvalue $\hbar$ make it through. Looking at the amplitudes, only $(1/2)^2 = 1/4$ of the remaining particles make it through this filter. The state after passing through the filter reduces to:

$$|\psi\rangle = \frac{1}{2}|1,1\rangle + \frac{\sqrt{2}}{2}|1,0\rangle + \frac{1}{2}|1,-1\rangle.$$

The final filter passes only states with $S_z = -\hbar$, i.e. particles in the state $|1,-1\rangle$. Again, by considering the amplitudes of $|\psi\rangle$, only $(1/2)^2 = 1/4$ of the remaining particles make it through this final filter. Hence a fraction of $\frac{1}{3} \cdot \frac{1}{4} \cdot \frac{1}{4} = 1/48$ of the particles make it through the whole thing.

5. Let $R = |\mathbf{X}|$ and $P_r = (\hat{\mathbf{X}} \cdot \mathbf{P} + \mathbf{P} \cdot \hat{\mathbf{X}})/2$ be operators corresponding to the radial coordinate and momenta. Evaluate $[R, P_r]$.

The radial Hamiltonian of a hydrogen atom in a state of definite total angular momentum labelled by l is

$$H_l = \frac{P_r^2}{2\mu} + V_{\text{eff}}(R) = \frac{\hbar^2}{2\mu}\left(\frac{P_r^2}{\hbar^2} + \frac{l(l+1)}{R^2} - \frac{2}{a_0 R}\right),$$

where μ is the reduced mass and $a_0 = 4\pi\epsilon_0\hbar^2/\mu e^2$ is the Bohr radius.

(i) Sketch the effective potential for various $l \in \mathbb{N}_0$. By considering their minima, show that for any fixed $E < 0$, there is a maximum value of l beyond which bound states of energy E cannot exist.

(ii) Let A_l be the dimensionless operator

$$A_l = \frac{a_0}{\sqrt{2}}\left(\frac{1}{(l+1)a_0} - \frac{l+1}{R} + \frac{i}{\hbar}P_r\right).$$

Express H_l in terms of A_l and its Hermitian adjoint, and show that

$$[A_l^\dagger, A_l] = \frac{a_0^2\mu}{\hbar^2}(H_{l+1} - H_l).$$

Hence show that $A_l H_l = H_{l+1} A_l$.

(iii) Let $|E, l\rangle$ obey $H_l |E, l\rangle = E |E, l\rangle$. Show that $A_l |E, l\rangle$ is an eigenstate of H_{l+1} with the same eigenvalue E. What is the interpretation of the radial wavefunction $\langle r|A_l|E, l\rangle$?

(iv) Explain why there must exist an $l_{\text{max}} \in \mathbb{N}_0$ such that $A_{l_{\text{max}}} |E, l_{\text{max}}\rangle = 0$. Deduce that $|E, l_{\text{max}}\rangle$ has energy:

$$E = -\frac{\hbar^2}{2\mu a_0^2}\frac{1}{(l_{\text{max}}+1)^2},$$

and hence that the energy levels of hydrogen are

$$E = -\frac{\hbar^2}{2\mu a_0^2 n^2}$$

with orbital angular momentum $l \in \{0, 1, ..., n-1\}$.

Solution: We are first asked to find the commutator $[R, P_r]$. We have;

$$[R, P_r] = \left[|\mathbf{X}|, \frac{\hat{\mathbf{X}} \cdot \mathbf{P} + \mathbf{P} \cdot \hat{\mathbf{X}}}{2}\right] = \frac{1}{2}[|\mathbf{X}|, \hat{\mathbf{X}} \cdot \mathbf{P}] + \frac{1}{2}[|\mathbf{X}|, \mathbf{P} \cdot \hat{\mathbf{X}}].$$

We now apply the result from the comments of Examples Sheet 1, Question 2. Recall that $[A, f(B)] = f'(B)[A, B]$ for operators A, B that commute with their commutator $[A, B]$. In our particular case then, we will use the result:

$$[P_j, f(\mathbf{X})] = [P_j, X_i]\frac{\partial}{\partial X_i} f(\mathbf{X}) = -i\hbar\frac{\partial}{\partial X_j} f(\mathbf{X}).$$

Using index notation, we have:

$$[R, P_r] = \frac{1}{2}\left[\sqrt{X_i X_i}, \frac{X_j}{\sqrt{X_k X_k}} P_j\right] + \frac{1}{2}\left[\sqrt{X_i X_i}, P_j \frac{X_j}{\sqrt{X_k X_k}}\right]$$

$$= \frac{1}{2}\frac{X_j}{\sqrt{X_k X_k}}\left[\sqrt{X_i X_i}, P_j\right] + \frac{1}{2}\left[\sqrt{X_i X_i}, P_j\right]\frac{X_j}{\sqrt{X_k X_k}} \qquad \text{(Leibniz identity, functions of } \mathbf{X} \text{ commute)}$$

Thus we see we need only evaluate the commutator $[\sqrt{X_iX_i}, P_j]$. Using the result we stated above, we have:

$$[\sqrt{X_iX_i}, P_j] = -[P_j, \sqrt{X_iX_i}] = i\hbar\frac{\partial}{\partial X_j}(\sqrt{X_iX_i}) = \frac{i\hbar X_j}{\sqrt{X_iX_i}}.$$

Substituting this into the above, we find the result $[R, P_r] = i\hbar$, as required.

(i) The effective potential is:

$$V_{\text{eff}}(R) = \frac{\hbar^2}{2\mu}\left(\frac{l(l+1)}{R^2} - \frac{2}{a_0 R}\right).$$

We focus on $R > 0$, since R is a radial coordinate. We note the following behaviour:

- As $R \to \infty$, we have $V_{\text{eff}}(R) \to 0$; this happens independently of the angular momentum quantum number l.
- As $R \to 0$, the effective potential behaves like a $1/R^2$ potential:

  $$V_{\text{eff}}(R) \sim \frac{\hbar^2 l(l+1)}{2\mu a_0 R}.$$

  Therefore, as $R \to 0$, the effective potential tends to $+\infty$ like $1/R^2$. The graph is steeper here for larger values of the angular momentum quantum number l.

  This applies for all values of l except for $l = 0$. When $l = 0$, the potential just looks like a $-1/R$ potential, and decays to $-\infty$ at the origin.
- The potential crosses $V = 0$ when:

  $$\frac{l(l+1)}{R^2} - \frac{2}{a_0 R} = 0 \qquad \Rightarrow \qquad R = \frac{1}{2}a_0 l(l+1).$$

  Hence as the angular momentum quantum number l increases, the R value where the potential crosses the $V = 0$ axis increases.
- Finally, the potential has stationary points when:

  $$0 = V'_{\text{eff}}(R) = \frac{\hbar^2}{2\mu}\left(-\frac{2l(l+1)}{R^3} + \frac{2}{a_0 R^2}\right) \qquad \Rightarrow \qquad R = a_0 l(l+1).$$

  This occurs at twice the R value where the potential crosses the $V = 0$ axis, and hence V has a negative value at this stationary point. Eventually, $V \to 0$ as $R \to \infty$, so this must be a *minimum*.

  The value of V at the minimum is given by:

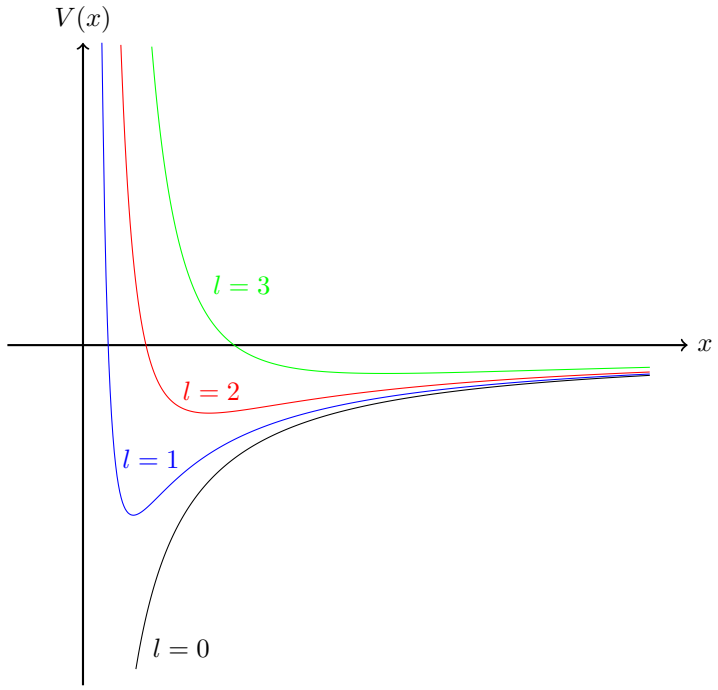
  $$V_{\text{eff}}(a_0 l(l+1)) = -\frac{\hbar^2}{2\mu a_0^2 l(l+1)}.$$

  Hence as l increases, the value of V at this minimum approaches zero. Thus the minimum well becomes shallower and shallower. This will make it more and more difficult to find bound states at higher values of l.

  This analysis applies to all values of l, except $l = 0$, where there is no minimum. The graph just looks like a $1/R$ graph.

With this analysis, we are able to draw the required diagrams, which are given on the next page.

We note that for any energy $E < 0$, there exist values of l where we can have bound states (even if it's just $l = 0$). However, as l increases, the minimum increases to a point where it occurs at some value greater than E. Therefore, bound states of energy $E < 0$ can no longer exist after this point. Hence there is a maximum value of l beyond which bound states of energy E cannot exist, as required.



(ii) In this part of the question, we are asked to express H_l in terms of the lowering and raising operators A_l and $A_l^\dagger$. As usual we expect something of the form:

$$H_l \sim (\cdots)A_l^\dagger A_l + (\cdots),$$

so let's begin by considering the product of operators $A_l^\dagger A_l$. We have:

$$A_l^\dagger A_l = \frac{a_0^2}{2}\left(\frac{1}{(l+1)a_0} - \frac{l+1}{R} - \frac{iP_r}{\hbar}\right)\left(\frac{1}{(l+1)a_0} - \frac{l+1}{R} + \frac{iP_r}{\hbar}\right)$$

$$= \frac{a_0^2}{2}\left(\frac{1}{a_0^2(l+1)^2} - \frac{1}{a_0 R} + \frac{iP_r}{(l+1)a_0\hbar} - \frac{1}{a_0 R} + \frac{(l+1)^2}{R^2} - \frac{i(l+1)}{\hbar}\cdot\frac{1}{R}\cdot P_r \right.$$
$$\left. - \frac{iP_r}{(l+1)a_0\hbar} + \frac{i(l+1)}{\hbar}\cdot P_r \cdot \frac{1}{R} + \frac{P_r^2}{\hbar^2}\right)$$

$$= \frac{a_0^2}{2}\left(\frac{1}{a_0^2(l+1)^2} - \frac{2}{a_0 R} + \frac{(l+1)^2}{R^2} - \frac{i(l+1)}{\hbar}\cdot\left[\frac{1}{R}, P_r\right] + \frac{P_r^2}{\hbar^2}\right)$$

To evaluate $[1/R, P_r]$, we can again use the result from Examples Sheet 1: if A, B commute with their commutator, then $[A, f(B)] = f'(B)[A, B]$. We know that $[R, P_r] = i\hbar$ from our earlier work, so R and P_r certainly commute with their commutator. Thus we have:

$$\left[\frac{1}{R}, P_r\right] = -\left[P_r, \frac{1}{R}\right] = i\hbar\frac{\partial}{\partial R}\left(\frac{1}{R}\right) = -\frac{i\hbar}{R^2}.$$

It follows that:

$$A_l^\dagger A_l = \frac{a_0^2}{2}\left(\frac{1}{a_0^2(l+1)^2} - \frac{2}{a_0 R} + \frac{(l+1)^2}{R^2} - \frac{(l+1)}{R^2} + \frac{P_r^2}{\hbar^2}\right) = \frac{a_0^2}{2}\left(\frac{1}{a_0^2(l+1)^2} - \frac{2}{a_0 R} + \frac{l(l+1)}{R^2} + \frac{P_r^2}{\hbar^2}\right).$$

Rewriting this in terms of the Hamiltonian, we have:

$$A_l^\dagger A_l = \frac{1}{2(l+1)^2} + \frac{a_0^2\mu}{\hbar^2}H_l.$$

Rearranging, we have:

$$H_l = \frac{\hbar^2}{a_0^2\mu}A_l^\dagger A_l - \frac{\hbar^2}{2a_0^2\mu(l+1)^2}.$$

We are also asked to find the commutator $[A_l^\dagger, A_l] = A_l^\dagger A_l - A_l A_l^\dagger$. We have already evaluated $A_l^\dagger A_l$, so we just need to find $A_l A_l^\dagger$. By exactly the same calculation as above, we find the result:

$$A_l A_l^\dagger = \frac{1}{2(l+1)^2} + \frac{a_0^2\mu}{\hbar^2}H_{l+1}.$$

Hence we have the required result:

$$[A_l^\dagger, A_l] = A_l^\dagger A_l - A_l A_l^\dagger = \frac{a_0^2\mu}{\hbar^2}(H_{l+1} - H_l).$$

Finally, we need to show $A_l H_l = H_{l+1}A_l$. To do so, let's consider $[A_l, H_l]$, since we effectively want to move an annihilation operator to the right of the Hamiltonian H_l. We have:

$$[A_l, H_l] = \left[A_l, \frac{\hbar^2}{a_0^2\mu}A_l^\dagger A_l - \frac{\hbar^2}{2a_0^2\mu(l+1)^2}\right] = \frac{\hbar^2}{a_0^2\mu}[A_l, A_l^\dagger A_l] = \frac{\hbar^2}{a_0^2\mu}[A_l, A_l^\dagger]A_l = (H_{l+1} - H_l)A_l,$$

using the result for the commutator $[A_l^\dagger, A_l]$ from above. Writing out this result in full, we see:

$$A_l H_l - H_l A_l = H_{l+1}A_l - H_l A_l \qquad \Rightarrow \qquad A_l H_l = H_{l+1}A_l,$$

which is the required result.

(iii) We are given that $|E, l\rangle$ is an energy eigenstate of H_l, i.e. $H_l|E, l\rangle = E|E, l\rangle$. We want to show that $A_l|E, l\rangle$ is an eigenstate of H_{l+1} with the same energy eigenvalue E; we can simply use the result from (ii). We have:

$$H_{l+1}A_l|E, l\rangle = A_l H_l|E, l\rangle = EA_l|E, l\rangle,$$

as required.

The radial wavefunction $\langle r|A_l|E, l\rangle$ is simply the wavefunction of an energy eigenstate of hydrogen with orbital angular momentum labelled by $l + 1$.

(iv) For the last part of the question, we are asked the find the energy spectrum of the hydrogen atom. First, we know from part (i) that given a fixed energy E, if we increase the angular momentum quantum number enough to say some value l_{max}, there does not exist a bound state with energy E *and* angular momentum quantum number $l_{\text{max}} + 1$.

Since $A_l \left|E, l\right\rangle$ is an energy eigenstate of the system with energy E and angular momentum quantum number $l + 1$, it follows that we can construct energy eigenstates:

$$A_l \left|E, l\right\rangle \propto \left|E, l+1\right\rangle, \qquad A_{l+1}A_l \left|E, l\right\rangle \propto \left|E, l+2\right\rangle, \qquad ... \qquad A_{l+k-1}...A_l \left|E, l\right\rangle \propto \left|E, l+k\right\rangle.$$

We cannot do this indefinitely since for a fixed energy there is a maximum possible angular momentum quantum number, so it follows there is some l_{max} such that $A_{l_{\text{max}}} \left|E, l_{\text{max}}\right\rangle = 0$. Taking the norm of this equation, we have:

$$0 = ||A_{l_{\text{max}}} \left|E, l_{\text{max}}\right\rangle||^2 = \langle E, l_{\text{max}}|A^\dagger_{l_{\text{max}}} A_{l_{\text{max}}}|E, l_{\text{max}}\rangle$$

$$= \langle E, l_{\text{max}}|\frac{1}{2(l_{\text{max}}+1)^2} + \frac{a_0^2\mu}{\hbar^2}H_{l_{\text{max}}}|E, l_{\text{max}}\rangle = \frac{1}{2(l_{\text{max}}+1)^2} + \frac{a_0^2\mu}{\hbar^2}E,$$

from which it follows that

$$E = -\frac{\hbar^2}{2a_0^2\mu(l_{\text{max}}+1)^2},$$

as required.

This analysis applies to *all* energy eigenstates $\left|E, l\right\rangle$, and hence it follows that all energies are of this form. So generically our energies look like:

$$E = -\frac{\hbar^2}{2a_0^2\mu n^2},$$

where $n = l_{\text{max}} + 1$. We can get this from states of orbital angular momentum:

$$l \in \{0, ..., n-1\},$$

as we saw above (note that each of these l values corresponds to a state space $\{\left|k, m\right\rangle\}$ which contains $2l + 1$ states, $m \in \{-l, -l+1..., l\}$, so this shows that the degeneracy of the hydrogen energy levels is $(2 \cdot 0 + 1) + (2 \cdot 1 + 1) + \cdots + (2 \cdot (n-1) + 1) = n^2$). If we wanted to be completely rigorous about this final answer, we would need to *construct* the states giving rise to these energies to show they actually existed - this construction is very similar to the work we did for Question 6, Sheet 1, and is definitely for enthusiasts only.

⁕ **Comments:** This question is discussed in David Skinner's notes for this course in the chapter on *Dynamical Symmetries*, in particular the section on the gross structure of hydrogen.

Notice also that the methods we used to solve this question are similar to those used in Examples Sheet 1, Question 6. There, the parameter ν plays a similar role to the angular momentum quantum number l in this question. Here, however, we are moving *horizontally* through different values of l at fixed values of E rather than *diagonally* through different values of ν and E at the same time. The standard harmonic oscillator moves *vertically* only, with raising/lowering operators *only* affecting E and no other parameters.

6. (∗) Consider a $d = 2$ isotropic harmonic oscillator of frequency ω.

   (i) Construct combinations of the raising and lowering operators of the 2D oscillator that obey the same $\mathfrak{so}(3)$ algebra as angular momentum in 3D.

   (ii) Show how all the states of the 2D oscillator fit into representations of $\mathfrak{so}(3)$.

Solution: (i) Recall that the raising and lowering operators, $A_x, A_x^\dagger, A_y, A_y^\dagger$, of the 2D oscillator obey the algebra:

$$[A_i, A_j^\dagger] = \delta_{ij}, \qquad [A_i, A_j] = [A_i^\dagger, A_j^\dagger] = 0,$$

as you saw in lectures. In this question, we are asked to construct combinations J_+, J_-, J_3 of the raising and lowering operators such that these operators obey the angular momentum algebra, $[J_+, J_-] = 2\hbar J_3$ and $[J_3, J_\pm] = \pm\hbar J_\pm$ (this algebra is called the $\mathfrak{so}(3)$ algebra, as mentioned in the question).

To make the construction, we re-analyse the raising and lowering operators, giving them a new interpretation. Let us say that the interpretation of $A_x^\dagger$ is to create a unit of angular momentum $+\hbar/2$, whilst A_x destroys a unit of angular momentum $+\hbar/2$. Similarly, let us say that the interpretation of $A_y^\dagger$ is to create an 'anti-unit' of angular momentum $-\hbar/2$, whilst A_y destroys an 'anti-unit' of angular momentum $-\hbar/2$. The angular momentum of a given state is then a difference of the number of units of angular momentum and the number of anti-units of angular momentum:

$$J_3 = \frac{\hbar}{2}\left(A_x^\dagger A_x - A_y^\dagger A_y\right).$$

To increase angular momentum by $\hbar$, we destroy an anti-unit of angular momentum $-\hbar/2$ and create a unit of angular momentum $\hbar/2$. Similarly, to decrease angular momentum by $\hbar$, we destroy a unit of angular momentum $\hbar/2$ and create an anti-unit of angular momentum $-\hbar/2$. Hence we define raising and lowering operators for angular momentum via:

$$J_+ = \hbar A_x^\dagger A_y, \qquad J_- = \hbar A_y^\dagger A_x.$$

It turns out that these operators indeed obey the angular momentum algebra $\mathfrak{so}(3)$! We can verify this directly; for the first commutation relation $[J_+, J_-]$, we have:

$$\begin{aligned}
[J_+, J_-] &= \hbar^2\left(A_x^\dagger A_y A_y^\dagger A_x - A_y^\dagger A_x A_x^\dagger A_y\right) \\
&= \hbar^2\left(A_x^\dagger A_x [A_y, A_y^\dagger] + A_x^\dagger A_x A_y^\dagger A_y - A_y^\dagger A_y [A_x, A_x^\dagger] - A_y^\dagger A_y A_x^\dagger A_x\right) \\
&= \hbar^2\left(A_x^\dagger A_x - A_y^\dagger A_y\right) = 2\hbar J_3,
\end{aligned}$$

as anticipated. For the remaining commutation relations, we have:

$$\begin{aligned}
[J_3, J_+] &= \frac{1}{2}\hbar^2\left(A_x^\dagger A_x A_x^\dagger A_y - A_y^\dagger A_y A_x^\dagger A_y - A_x^\dagger A_y A_x^\dagger A_x + A_x^\dagger A_y A_y^\dagger A_y\right) \\
&= \frac{1}{2}\hbar^2\left(A_x^\dagger A_y [A_x, A_x^\dagger] + (A_x^\dagger)^2 A_x A_y - A_y^\dagger A_x^\dagger (A_y)^2 - (A_x^\dagger)^2 A_x A_y + A_x^\dagger A_y [A_y, A_y^\dagger] + A_y^\dagger A_x^\dagger (A_y)^2\right) \\
&= \hbar^2 A_x^\dagger A_y = \hbar J_+.
\end{aligned}$$

Similarly, we have $[J_3, J_-] = -\hbar J_-$ (e.g. by exchanging $x \leftrightarrow y$, under which $J_3 \mapsto -J_3$). Hence this construction has reproduced the $\mathfrak{so}(3)$ algebra as required.

(ii) The Hilbert space of the 2D harmonic oscillator is spanned by states of the form:

$$|n_x, n_y\rangle = \frac{(A_x)^{n_x}}{\sqrt{n_x!}} \frac{(A_y)^{n_y}}{\sqrt{n_y!}} |0,0\rangle ,$$

where $|0,0\rangle$ is the vacuum state. We must split these states into 'representations' of the algebra $J_\pm, J_3$. Here, the question is talking about *irreducible representations*, which are *minimal subspaces which 'transforms amongst themselves' under the algebra*. That is, we would like to split the Hilbert space $\mathcal{H}$ into subspaces $\mathcal{H}_\alpha$ such that:

$$J_\pm \mathcal{H}_\alpha \subseteq \mathcal{H}_\alpha, \qquad J_3 \mathcal{H}_\alpha \subseteq \mathcal{H}_\alpha,$$

(this is the 'transforming amongst themselves' condition) such that there do not exist subspaces $U_\alpha \leq \mathcal{H}_\alpha$ such that $J_\pm U_\alpha \subseteq U_\alpha$, $J_3 U_\alpha \subseteq U_\alpha$ (this is the 'minimality' condition).

To construct this decomposition, let's start by considering what happens when we act with $J_\pm$, J_3, as defined above, on each of the basis states for the 2D harmonic oscillator:

$$J_+ |n_x, n_y\rangle = \hbar A_x^\dagger A_y |n_x, n_y\rangle = \hbar\sqrt{(n_x+1)n_y}\, |n_x+1, n_y-1\rangle ,$$

$$J_- |n_x, n_y\rangle = \hbar A_y^\dagger A_x |n_x, n_y\rangle = \hbar\sqrt{n_x(n_y+1)}\, |n_x-1, n_y+1\rangle ,$$

$$J_3 |n_x, n_y\rangle = \frac{1}{2}\hbar \left(A_x^\dagger A_x - A_y^\dagger A_y\right) |n_x, n_y\rangle = \frac{1}{2}\hbar \left(n_x - n_y\right) |n_x, n_y\rangle ,$$

where we have used the standard action of the harmonic oscillator raising and lowering operators (namely $A|n\rangle = \sqrt{n}\,|n-1\rangle$ and $A^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle$, generalised to the 2D oscillator appropriately). In particular, this shows explicitly that J_+ raises the J_3 eigenvalue of a state by $\hbar$, and J_- lowers the J_3 eigenvalue of a state by 1.

It's also useful to construct the operator $\mathbf{J}^2 = J_3^2 + \frac{1}{2}(J_+J_- + J_-J_+)$. You can prove quickly that $[J_3, \mathbf{J}^2] = [J_\pm, \mathbf{J}^2] = 0$ (as anticipated given the analogy with the angular momentum algebra). Hence this operator commutes with the entire algebra; we call an operator which is quadratic in the generators of the algebra and commutes with all elements of the algebra a *Casimir element*. This operator acts on the basis of states via:

$$\begin{aligned}\mathbf{J}^2 |n_x, n_y\rangle &= \frac{1}{4}\hbar^2 (n_x - n_y)^2 |n_x, n_y\rangle + \frac{1}{2}\hbar^2 \left(n_x^2 (n_y+1)^2 + (n_x+1)^2 n_y^2\right) |n_x, n_y\rangle \\ &= \hbar^2 \left(\frac{n_x+n_y}{2}\right)\left(\frac{n_x+n_y}{2}+1\right) |n_x, n_y\rangle ,\end{aligned}$$

where we have written the eigenvalue in the form $\hbar^2 j(j+1)$ in analogy with the action of $\mathbf{J}^2$ as an angular momentum operator. This suggests that we should define subspaces:

$$\mathcal{H}_j = \text{span}\left\{ |n_x, n_y\rangle : \frac{n_x+n_y}{2} = j \right\}.$$

These subspaces cover the 2D harmonic oscillator Hilbert space $\mathcal{H}$ by varying the values of j. Furthermore, each $\mathcal{H}_j$ is an irreducible representation, since acting with J_+, J_-, J_3 does not affect the $\mathbf{J}^2$ eigenvalue (since these operators all commute with $\mathbf{J}^2$), so J_+, J_-, J_3 acting on $\mathcal{H}_j$ keeps us inside the space $\mathcal{H}_j$. Moreover, there's no smaller subspace inside $\mathcal{H}_j$ which transforms amongst itself, since we can get between all states in $\mathcal{H}_j$ using the raising and lowering operators $J_\pm$.

⁕ **Comments:** The significance of this question is explored much more deeply in the Part III Symmetries, Fields and Particles course (and knowing material from that is definitely beyond the scope of this course!). The question is also discussed in J. J. Sakurai's *Modern Quantum Mechanics* in Section 3.8, if you would like to read more details.

Part II: Principles of Quantum Mechanics
Examples Sheet 3 Solutions

Please send all comments and corrections to jmm232@cam.ac.uk.

Background: the Clebsch-Gordan formula for addition of angular momentum

It's very often the case in quantum mechanics that we want to combine two systems with angular momentum. For example, all particles have some fixed *spin* s, and their spatial wavefunction can be decomposed into a sum of *orbital angular momentum* eigenstates. Thus the Hilbert space of a particle of spin-s can be written in the form:

$$\mathcal{H}_{\text{particle}} = \mathcal{H}_s \otimes (\mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \cdots) = \mathcal{H}_s \otimes \left(\bigoplus_{l=0}^{\infty} \mathcal{H}_l \right),$$

where $\mathcal{H}_k = \mathcal{H}_s$, $\mathcal{H}_l$ is an angular momentum Hilbert space, with total angular momentum eigenvalue j; i.e. it is of the form:

$$\mathcal{H}_k = \{|k,k\rangle, |k,k-1\rangle, |k,k-2\rangle, ..., |k,-(k-2)\rangle, |k,-(k-1)\rangle, |k,-k\rangle\}.$$

Notice that the total angular momentum (of any type, spin, orbital, or spin plus orbital), $\mathbf{K}^2 = K_1^2 + K_2^2 + K_3^2$, is constant on the space $\mathcal{H}_k$, returning the eigenvalue $\hbar^2 k(k+1)$ when it acts on any state $|k,\kappa\rangle$. Note also that the Hilbert space $\mathcal{H}_{\text{particle}}$ is composed of a factor $\mathcal{H}_s$, which comes from the spin angular momentum of the particle (note the value of s is fixed), and a factor $\mathcal{H}_0 \oplus \mathcal{H}_1 \oplus ...$, corresponding to the fact that the particle's spatial wavefunction can be expressed as some (possible infinite) linear combination of *orbital angular momentum eigenstates* (which in the position basis are associated Legendre polynomials).

It is very common in the physics literature to abbreviate angular momentum Hilbert spaces via: $\underline{k} = \mathcal{H}_k$, so our Hilbert space can be written instead as:

$$\mathcal{H}_{\text{particle}} = \underline{s} \otimes \left(\bigoplus_{l=0}^{\infty} \underline{l} \right).$$

So far, this formula treats the two types of angular momentum as distinct factors of the space. However, it is often the case that we are instead interested in the *total angular momentum*, $\mathbf{J} = \mathbf{L} + \mathbf{S}$ of the particle; it would be nice if we could decompose the space $\mathcal{H}_{\text{particle}}$ into eigenspaces of $\mathbf{J}^2$ to answer questions about total angular momentum more easily. To achieve this, note that the tensor product distributes over the direct sum of vector spaces, so we can rewrite this formula as:

$$\mathcal{H}_{\text{particle}} = \bigoplus_{l=0}^{\infty} \underline{s} \otimes \underline{l}.$$

Hence the key question we need to answer is: how do we decompose $\underline{k_1} \otimes \underline{k_2}$, for two different angular momentum systems $\underline{k_1}, \underline{k_2}$, into eigenspaces of $\mathbf{K}^2 = (\mathbf{K}_1 + \mathbf{K}_2)^2$? As you discussed in lectures, we use an algorithm for the 'addition of angular momentum'; in general, we find the famous *Clebsch-Gordan formula*:

Theorem: (The Clebsch-Gordan formula) We have:

$$\underline{k_1} \otimes \underline{k_2} = (\underline{k_1 + k_2}) \oplus (\underline{k_1 + k_2 - 1}) \oplus \cdots \oplus (\underline{|k_1 - k_2| + 1}) \oplus (\underline{|k_1 - k_2|}) = \bigoplus_{k=|k_1-k_2|}^{k_1+k_2} \underline{k}.$$

The spaces on the right are labelled by their $\mathbf{K}^2 = (\mathbf{K}_1 + \mathbf{K}_2)^2$ angular momentum quantum number. This relates to the 'addition of angular momentum' algorithm, since we first find the top state $|k_1 + k_2, k_1 + k_2\rangle = |k_1, k_1\rangle |k_2, k_2\rangle$, then lower repeatedly to obtain all other states in $\underline{k_1 + k_2}$; we then find the state $|k_1 + k_2 - 1, k_1 + k_2 - 1\rangle$ using orthogonality, and lower repeatedly to obtain all other states in $\underline{k_1 + k_2 - 1}$, etc.

Solutions to Examples Sheet 3

1. Consider the addition of angular momentum 3 to angular momentum 1. Express the states

$$|4,4\rangle, |4,3\rangle, |3,3\rangle, |3,2\rangle, |2,2\rangle, |2,1\rangle$$

of the combined system in terms of the states of the subsystems.

Solution: The highest angular momentum state here is $|4,4\rangle$, so we begin by simply writing down the standard answer:

$$|4,4\rangle = |3,3\rangle\,|1,1\rangle\,.$$

To obtain $|4,3\rangle$, we apply the lowering operator $J_- = J_{1-} + J_{2-}$. We have:

$$J_-\,|4,4\rangle = J_{1-}\,|3,3\rangle\,|1,1\rangle + |3,3\rangle\,J_{2-}\,|1,1\rangle$$

$$\Rightarrow \qquad \hbar\sqrt{4(4+1)-4(4-1)}\,|4,3\rangle = \hbar\sqrt{3(3+1)-3(3-1)}\,|3,2\rangle\,|1,1\rangle + |3,3\rangle\,\hbar\sqrt{1(1+1)-1(1-1)}\,|1,0\rangle$$

$$\Rightarrow \qquad |4,3\rangle = \sqrt{\frac{3}{4}}\,|3,2\rangle\,|1,1\rangle + \sqrt{\frac{1}{4}}\,|3,3\rangle\,|1,0\rangle\,.$$

Since we will eventually need to construct $|2,2\rangle$ by considering orthogonality with $|3,2\rangle$ and $|4,2\rangle$, we will also need to construct $|4,2\rangle$. Applying the lowering operator again, we have:

$$J_-\,|4,3\rangle = \sqrt{\frac{3}{4}}J_{1-}\,|3,2\rangle\,|1,1\rangle + \sqrt{\frac{3}{4}}\,|3,2\rangle\,J_{2-}\,|1,1\rangle + \sqrt{\frac{1}{4}}J_{1-}\,|3,3\rangle\,|1,0\rangle + \sqrt{\frac{1}{4}}\,|3,3\rangle\,J_{2-}\,|1,0\rangle$$

$$\begin{aligned}\Rightarrow\ \sqrt{4(4+1)-3(3-1)}\,|4,2\rangle = {}& \sqrt{\frac{3}{4}}\sqrt{3(3+1)-2(2-1)}\,|3,1\rangle\,|1,1\rangle + \sqrt{\frac{3}{4}}\,|3,2\rangle\,\sqrt{1(1+1)-1(1-1)}\,|1,0\rangle \\ & + \sqrt{\frac{1}{4}}\sqrt{3(3+1)-3(3-1)}\,|3,2\rangle\,|1,0\rangle + \sqrt{\frac{1}{4}}\,|3,3\rangle\,\sqrt{1(1+1)-0(0-1)}\,|1,-1\rangle\end{aligned}$$

$$\Rightarrow \qquad \sqrt{14}\,|4,2\rangle = \sqrt{\frac{15}{2}}\,|3,1\rangle\,|1,1\rangle + 2\sqrt{\frac{3}{2}}\,|3,2\rangle\,|1,0\rangle + \sqrt{\frac{1}{2}}\,|3,3\rangle\,|1,-1\rangle$$

$$\Rightarrow \qquad |4,2\rangle = \sqrt{\frac{15}{28}}\,|3,1\rangle\,|1,1\rangle + \sqrt{\frac{3}{7}}\,|3,2\rangle\,|1,0\rangle + \sqrt{\frac{1}{28}}\,|3,3\rangle\,|1,-1\rangle$$

Thankfully, we are not asked to calculate $|4,1\rangle$!

The next state we wish to obtain is $|3,3\rangle$. Recall that to start working on a new $\mathbf{J}^2$ eigenvalue, we start from the highest state possible again, and write it as a general linear combination of all states such that $m = m_1 + m_2$.

$$|3,3\rangle = a\,|3,3\rangle\,|1,0\rangle + b\,|3,2\rangle\,|1,1\rangle\,,$$

for some coefficients a and b. Now use the fact that $\langle 4,3|3,3\rangle = 0$ and $\langle 3,3|3,3\rangle = 1$. This gives us two simultaneous equations, which allows us to deduce the values of a and b. We have:

$$|a|^2 + |b|^2 = 1, \qquad a + \sqrt{3}b = 0.$$

From these equations, it follows that $a = -\sqrt{3}b$, and b can be chosen to be $-1/2$. Therefore $a = \sqrt{3}/2$. It follows that:

$$|3,3\rangle = \sqrt{\frac{3}{4}}\,|3,3\rangle\,|1,0\rangle - \sqrt{\frac{1}{4}}\,|3,2\rangle\,|1,1\rangle\,.$$

To obtain $|3,2\rangle$, just apply the lowering operator as per usual. We have:

$$J_-\,|3,3\rangle = \sqrt{\frac{3}{4}}J_{1-}\,|3,3\rangle\,|1,0\rangle + \sqrt{\frac{3}{4}}\,|3,3\rangle\,J_{2-}\,|1,0\rangle - \sqrt{\frac{1}{4}}J_{1-}\,|3,2\rangle\,|1,1\rangle - \sqrt{\frac{1}{4}}\,|3,2\rangle\,J_{2-}\,|1,1\rangle$$

$$\Rightarrow \qquad \sqrt{6}\,|3,2\rangle = \sqrt{\frac{3}{4}}\sqrt{6}\,|3,2\rangle\,|1,0\rangle + \sqrt{\frac{3}{4}}\sqrt{2}\,|3,3\rangle\,|1,-1\rangle - \sqrt{\frac{1}{4}}\sqrt{10}\,|3,1\rangle\,|1,1\rangle - \sqrt{\frac{1}{4}}\sqrt{2}\,|3,2\rangle\,|1,0\rangle$$

$$\Rightarrow \qquad |3,2\rangle = \sqrt{\frac{3}{4}}\,|3,2\rangle\,|1,0\rangle + \sqrt{\frac{1}{4}}\,|3,3\rangle\,|1,-1\rangle - \sqrt{\frac{5}{12}}\,|3,1\rangle\,|1,1\rangle - \sqrt{\frac{1}{12}}\,|3,2\rangle\,|1,0\rangle$$

$$\Rightarrow \qquad |3,2\rangle = \sqrt{\frac{1}{3}}\,|3,2\rangle\,|1,0\rangle + \sqrt{\frac{1}{4}}\,|3,3\rangle\,|1,-1\rangle - \sqrt{\frac{5}{12}}\,|3,1\rangle\,|1,1\rangle\,.$$

Note in the last step, we combined $\sqrt{3/4}$ and $-\sqrt{1/12}$ via:

$$\sqrt{\frac{3}{4}} - \sqrt{\frac{1}{12}} = \frac{\sqrt{3}}{2} - \frac{1}{2\sqrt{3}} = \frac{3\sqrt{3}}{6} - \frac{\sqrt{3}}{6} = \frac{\sqrt{3}}{3} = \frac{1}{\sqrt{3}}.$$

Next, we are asked to find $|2,2\rangle$. Again, we recall that to start working on a new $\mathbf{J}^2$ eigenvalue, we start from the highest state possible again, and write it as a general linear combination of all states such that $m = m_1 + m_2$. This time, we have:

$$|2,2\rangle = a\,|3,3\rangle\,|1,-1\rangle + b\,|3,2\rangle\,|1,0\rangle + c\,|3,1\rangle\,|1,1\rangle\,.$$

There are three conditions that fix the values of a, b and c, namely: $\langle 2,2|2,2\rangle = 1$, $\langle 3,2|2,2\rangle = 0$ and $\langle 4,2|2,2\rangle = 0$. Applying each of these conditions, we find the three simultaneous equations:

$$|a|^2 + |b|^2 + |c|^2 = 1, \qquad \sqrt{\frac{1}{4}}a + \sqrt{\frac{1}{3}}b - \sqrt{\frac{5}{12}}c = 0, \qquad \sqrt{\frac{1}{28}}a + \sqrt{\frac{3}{7}}b + \sqrt{\frac{15}{28}}c = 0.$$

Simplifying the second two equations, we have:

$$|a|^2 + |b|^2 + |c|^2 = 1, \qquad \frac{1}{2}a + \frac{\sqrt{3}}{3}b - \frac{1}{2}\sqrt{\frac{5}{3}}c = 0, \qquad \frac{1}{2}a + \sqrt{3}b + \frac{\sqrt{15}}{2}c = 0.$$

Solving the last two equations simultaneously, we have:

$$b = -\frac{a}{\sqrt{3}}, \qquad c = \frac{a}{\sqrt{15}}.$$

Using the last condition, we see that we can choose $a = \sqrt{15/21} = \sqrt{5/7}$. Thus we have:

$$|2,2\rangle = \sqrt{\frac{5}{7}}\,|3,3\rangle\,|1,-1\rangle - \sqrt{\frac{5}{21}}\,|3,2\rangle\,|1,0\rangle + \sqrt{\frac{1}{21}}\,|3,1\rangle\,|1,1\rangle\,.$$

Finally, we need to find the state $|2,1\rangle$. This is just obtained by applying the lowering operator to $|2,2\rangle$. We have:

$$\begin{aligned} J_- |2,2\rangle = &\sqrt{\frac{5}{7}} J_{1-} |3,3\rangle |1,-1\rangle + \sqrt{\frac{5}{7}} |3,3\rangle J_{2-} |1,-1\rangle - \sqrt{\frac{5}{21}} J_{1-} |3,2\rangle |1,0\rangle \\ &- \sqrt{\frac{5}{21}} |3,2\rangle J_{2-} |1,0\rangle + \sqrt{\frac{1}{21}} J_{1-} |3,1\rangle |1,1\rangle + \sqrt{\frac{1}{21}} |3,1\rangle J_{2-} |1,1\rangle \end{aligned}$$

$$\Rightarrow \sqrt{4} |2,1\rangle = \sqrt{\frac{30}{7}} |3,2\rangle |1,-1\rangle - \sqrt{\frac{50}{21}} |3,1\rangle |1,0\rangle - \sqrt{\frac{10}{21}} |3,2\rangle |1,-1\rangle + \sqrt{\frac{12}{21}} |3,0\rangle |1,1\rangle + \sqrt{\frac{2}{21}} |3,1\rangle |1,0\rangle$$

$$\Rightarrow |2,1\rangle = \sqrt{\frac{15}{14}} |3,2\rangle |1,-1\rangle - \sqrt{\frac{25}{42}} |3,1\rangle |1,0\rangle - \sqrt{\frac{5}{42}} |3,2\rangle |1,-1\rangle + \sqrt{\frac{1}{7}} |3,0\rangle |1,1\rangle + \sqrt{\frac{1}{42}} |3,1\rangle |1,0\rangle .$$

We can simplify some of the coefficients as follows:

$$\sqrt{\frac{15}{14}} - \sqrt{\frac{5}{42}} = \frac{\sqrt{5}}{\sqrt{7}} \left(\sqrt{\frac{3}{2}} - \sqrt{\frac{1}{6}} \right) = \sqrt{\frac{5}{7}} \left(\sqrt{\frac{3}{2}} - \frac{\sqrt{3}}{3\sqrt{2}} \right) = \frac{2}{3} \sqrt{\frac{15}{14}} = \sqrt{\frac{10}{21}},$$

$$\sqrt{\frac{1}{42}} - \sqrt{\frac{25}{42}} = -\frac{4}{\sqrt{42}} = -\sqrt{\frac{16}{42}} = -\sqrt{\frac{8}{21}}.$$

Thus we obtain:

$$|2,1\rangle = \sqrt{\frac{10}{21}} |3,2\rangle |1,-1\rangle - \sqrt{\frac{8}{21}} |3,1\rangle |1,0\rangle + \sqrt{\frac{1}{7}} |3,0\rangle |1,1\rangle .$$

2. State $|s, \sigma\rangle$ are formed by combining the states $|1, \sigma_1\rangle$, $|1, \sigma_2\rangle$ of two subsystems, each having spin $s = 1$.

(a) Show that the states of the combined system with $s = 2, 0$ are symmetric under the interchange $\sigma_1 \leftrightarrow \sigma_2$, whereas those with $s = 1$ are antisymmetric.

(b) Two identical spin 1 particles, whose centre of mass is at rest, have combined spin **S**, relative orbital angular momentum **L** and total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$. Let (j, l, s) denote the quantum numbers corresponding to the operators $(\mathbf{J}^2, \mathbf{L}^2, \mathbf{S}^2)$ of the combined system. Show that $l + s$ must be even. If $j = 1$, what are the possible values of l and s?

Solution: (a) For this part of the question, let's compute the states of the combined system using the algorithm for the addition of angular momentum, so that we can have some more practice (in general however, we can just compute the symmetry properties of the top states, then note that $S_- = S_{1-} + S_{2-}$ preserves any symmetry properties under lowering). Here, we are adding angular momentum 1 to angular momentum 1, so the first state of the combined system that we should consider is:

$$|2, 2\rangle = |1, 1\rangle\,|1, 1\rangle\,.$$

To obtain $|2, 1\rangle$, we apply the lowering operator $J_- = J_{1-} + J_{2-}$. We obtain:

$$\hbar\sqrt{2(2+1) - 2(2-1)}\,|2, 1\rangle = \hbar\sqrt{1(1+1) - 1(1-1)}\,|1, 0\rangle\,|1, 1\rangle + \hbar\sqrt{1(1+1) - 1(1-1)}\,|1, 1\rangle\,|1, 0\rangle$$

$$\Rightarrow \qquad |2, 1\rangle = \sqrt{\frac{1}{2}}\,|1, 0\rangle\,|1, 1\rangle + \sqrt{\frac{1}{2}}\,|1, 1\rangle\,|1, 0\rangle\,.$$

Applying the lowering operator again, we have:

$$\begin{aligned}\hbar\sqrt{2(2+1) - 1(1-1)}\,|2, 0\rangle = \hbar\sqrt{\frac{1}{2}}\sqrt{1(1+1)}\,|1, -1\rangle\,|1, 1\rangle \\ + 2\hbar\sqrt{\frac{1}{2}}\sqrt{1(1+1) - 1(1-1)}\,|1, 0\rangle\,|1, 0\rangle + \sqrt{\frac{1}{2}}\sqrt{1(1+1)}\,|1, 1\rangle\,|1, -1\rangle\end{aligned}$$

$$\Rightarrow \qquad |2, 0\rangle = \sqrt{\frac{1}{6}}\,|1, -1\rangle\,|1, 1\rangle + \sqrt{\frac{4}{6}}\,|1, 0\rangle\,|1, 0\rangle + \sqrt{\frac{1}{6}}\,|1, 1\rangle\,|1, -1\rangle\,.$$

Again, applying the lowering operator:

$$\begin{aligned}\hbar\sqrt{2(2+1)}\,|2, -1\rangle = \sqrt{\frac{1}{6}}\hbar\sqrt{1(1+1) - 1(1-1)}\,|1, -1\rangle\,|1, 0\rangle + \sqrt{\frac{4}{6}}\hbar\sqrt{1(1+1)}\,|1, -1\rangle\,|1, 0\rangle \\ + \sqrt{\frac{4}{6}}\hbar\sqrt{1(1+1)}\,|1, 0\rangle\,|1, -1\rangle + \sqrt{\frac{1}{6}}\hbar\sqrt{1(1+1) - 1(1-1)}\,|1, 0\rangle\,|1, -1\rangle\end{aligned}$$

$$\Rightarrow \qquad |2, -1\rangle = \sqrt{\frac{1}{2}}\,|1, -1\rangle\,|1, 0\rangle + \sqrt{\frac{1}{2}}\,|1, 0\rangle\,|1, -1\rangle\,.$$

A final application of the lowering operator gives:

$$|2, -2\rangle = |1, -1\rangle\,|1, -1\rangle\,.$$

Scanning all these states, we see they are symmetric under swapping $\sigma_1 \leftrightarrow \sigma_2$ in each of the tensor product basis states. So indeed the composite system states with total spin quantum number 2 are symmetric under this exchange.

Next, we want to construct the composite states with total spin quantum number 1. The first state is $|1,1\rangle$, which we express as a general linear combination of the tensor product states that have the correct sum of J_3 eigenvalues:

$$|1,1\rangle = a\,|1,1\rangle\,|1,0\rangle + b\,|1,0\rangle\,|1,1\rangle\,.$$

The orthogonality relation $\langle 2,1|1,1\rangle$ and the normalisation condition $\langle 1,1|1,1\rangle$ together imply the two simultaneous equations:

$$|a|^2 + |b|^2 = 1, \qquad a + b = 0.$$

From this, it follows that we can choose:

$$|1,1\rangle = \sqrt{\frac{1}{2}}\,|1,1\rangle\,|1,0\rangle - \sqrt{\frac{1}{2}}\,|1,0\rangle\,|1,1\rangle\,.$$

Applying the lowering operator, we have:

$$\hbar\sqrt{1(1+1)-1(1-1)}\,|1,0\rangle = \sqrt{\frac{1}{2}}\hbar\sqrt{1(1+1)}\,|1,1\rangle\,|1,-1\rangle - \sqrt{\frac{1}{2}}\sqrt{1(1+1)}\,|1,-1\rangle\,|1,1\rangle$$

$$\Rightarrow \qquad |1,0\rangle = \sqrt{\frac{1}{2}}\,|1,1\rangle\,|1,-1\rangle - \sqrt{\frac{1}{2}}\,|1,-1\rangle\,|1,1\rangle\,.$$

Applying the lowering operator once more, we have:

$$\hbar\sqrt{1(1+1)}\,|1,-1\rangle = \sqrt{\frac{1}{2}}\hbar\sqrt{1(1+1)-1(1-1)}\,|1,0\rangle\,|1,-1\rangle - \sqrt{\frac{1}{2}}\sqrt{1(1+1)-1(1-1)}\,|1,-1\rangle\,|1,0\rangle$$

$$\Rightarrow \qquad |1,-1\rangle = \sqrt{\frac{1}{2}}\,|1,0\rangle\,|1,-1\rangle - \sqrt{\frac{1}{2}}\,|1,-1\rangle\,|1,0\rangle\,.$$

Again scanning these states, we see they are all antisymmetric under swapping $\sigma_1 \leftrightarrow \sigma_2$ in each of the tensor product basis states. Thus we see the composite system states with total spin quantum number 1 are antisymmetric under this exchange, as required.

The only remaining composite state is $|0,0\rangle$, which we write as the general linear combination of tensor product states with $m_1 + m_2 = 0$. We have:

$$|0,0\rangle = a\,|1,1\rangle\,|1,-1\rangle + b\,|1,-1\rangle\,|1,1\rangle + c\,|1,0\rangle\,|1,0\rangle\,.$$

Using the two orthogonality conditions $\langle 2,0|0,0\rangle = 0$ and $\langle 1,0|0,0\rangle = 0$, together with the normalisation condition $\langle 0,0|0,0\rangle = 1$, we have the three simultaneous equations:

$$a + 2c + b = 0, \qquad a - b = 0, \qquad |a|^2 + |b|^2 + |c|^2 = 1$$

We notice that a valid solution is $a = b = -c = \sqrt{1/3}$. Therefore, we have:

$$|0,0\rangle = \sqrt{\frac{1}{3}}\,|1,1\rangle\,|1,-1\rangle + \sqrt{\frac{1}{3}}\,|1,-1\rangle\,|1,1\rangle - \sqrt{\frac{1}{3}}\,|1,0\rangle\,|1,0\rangle\,.$$

Again, we see that this is clearly symmetric under exchange of $\sigma_1 \leftrightarrow \sigma_2$ in all the tensor product basis states. So we're done.

(b) First note that since the particles are spin-1, they must be *bosons*, by the spin-statistics theorem. In particular, their joint wavefunction is symmetric under exchange of the particles.

We know from part (a) that the total spin angular momentum quantum number for the two particles can be either $s = 0, 1$ or 2. In the case that $s = 0, 2$, the spin state is symmetric under exchange of the particles, while if $s = 1$, the spin state is antisymmetric under exchange of the particles.

We also know from lectures that if we exchange two particles with total orbital angular momentum quantum number l, we pick up a factor of $(-1)^l$ in the wavefunction.

Therefore, if $s = 0, 2$, and we exchange the particles, we pick up a total factor of $1 \cdot (-1)^l$ in the wavefunction. This must be 1 for the particles to be bosons, and hence we require l even. If $s = 1$, we pick up a total factor of $-1 \cdot (-1)^l$ in the wavefunction under particle exchange. Hence we require l odd to ensure bosonic statistics of the system.

In all cases then, we have that $l + s$ is even, as required.

For the final part, consider combining the total orbital angular momentum of the system with the total spin angular momentum of the system. We know from the Clebsch-Gordan formula that the possible total angular momentum quantum numbers of the resulting composite system are:

$$j \in \{l + s, \qquad l + s - 1, \qquad ..., \qquad |l - s|\}.$$

Hence for the three possible values of s, we see:

- If $s = 0$, the only possible j value is l. Hence we need $l = 1$ for $j = 1$. But then $l + s = 0 + 1 = 1$ is odd, which is forbidden.
- If $s = 1$, then the possible j values are $j \in \{l + 1, ..., |l - 1|\}$. If $l = 0$, $l + s$ is not even. If $l = 1$, then $j \in \{2, 1, 0\}$, so this is consistent. If $l = 2$, then $j = l + s$ is not even. Finally, if $l = 3$ or above, then $\{l + 1, ..., |l - 1|\}$ does not include $j = 1$. Hence the only consistent pairing here is $s = 1, l = 1$.
- Finally, if $s = 2$, the possible j values are $\{l + 2, l + 1, l, |l - 1|, |l - 2|\}$. If $l = 0$, then this list only contains $\{2\}$, and hence $j = 2$, so this is impossible. If $l = 2$, then this list contains $\{4, 3, 2, 1, 0\}$, so $j = 1$ is on the list, and this is consistent. If $l = 4$ or above, then the list no longer contains 1. Thus the only consistent pairing here is $s = 2, l = 2$.

So the possible combinations are: $s = 1$ and $l = 1$, or $s = 2$ and $l = 2$.

⁜ **Comments:** In this question, we explore an interesting result related to antisymmetry/symmetry of angular momentum eigenstates in a composite system. The features we see here are completely general: it turns out that when we add angular momentum j to angular momentum j, the resulting system of states contains alternating antisymmetric and symmetric 'columns' of states. A full proof of this fact is given on Richard Chapling's website.[8]

[8] https://rc476.user.srcf.net/pqm/Sheet3.pdf. The relevant question is currently listed as Examples Sheet 3, Question 7.

3. Three spin-1 particles are governed by the Hamiltonian $H = (2\lambda/\hbar^2)(\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_1)$, where $\mathbf{S}_i$ is the spin operator of the ith particle and λ is a positive constant. Find the eigenvalues and corresponding degeneracies of the Hamiltonian in the cases that:

(i) each particle is distinguishable;

(ii) all three particles are identical and all have the same spatial wavefunction.

Solution: Before starting this question, it's useful to notice that we can rewrite the Hamiltonian in terms of the magnitude of the total spin squared $\mathbf{S}^2 = (\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3)^2$, and the magnitudes of the individual spins squared, $\mathbf{S}_1^2, \mathbf{S}_2^2, \mathbf{S}_3^2$, since:

$$2\mathbf{S}_1 \cdot \mathbf{S}_2 + 2\mathbf{S}_2 \cdot \mathbf{S}_3 + 2\mathbf{S}_3 \cdot \mathbf{S}_1 = (\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3)^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2 - \mathbf{S}_3^2 = \mathbf{S}^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2 - \mathbf{S}_3^2.$$

Hence, the Hamiltonian can be written as:

$$H = \frac{\lambda}{\hbar^2}\left(\mathbf{S}^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2 - \mathbf{S}_3^2\right).$$

Furthermore, since each of the subsystems $1, 2, 3$ has spin-1, we know that $\mathbf{S}_i^2$ is constant on subsystem i, returning the value $\hbar^2 1(1+1) = 2\hbar^2$ on all states in the subsystem. Thus we $\mathbf{S}_i^2 = 2\hbar^2$, and it follows:

$$H = \frac{\lambda}{\hbar^2}\mathbf{S}^2 - 6\lambda.$$

We can now begin the question proper.

(i) For the first part, the Hilbert space of the particles is given by $\underline{1} \otimes \underline{1} \otimes \underline{1}$, since there are no symmetry restrictions on the particles (because they are *distinguishable*). By the Clebsch-Gordan formula, we can expand this in terms of eigenspaces of $\mathbf{S}^2$ via:

$$\begin{aligned}
\underline{1} \otimes \underline{1} \otimes \underline{1} &= \underline{1} \otimes (\underline{0} \oplus \underline{1} \oplus \underline{2}) \\
&= (\underline{1} \otimes \underline{0}) \oplus (\underline{1} \otimes \underline{1}) \oplus (\underline{1} \otimes \underline{2}) \\
&= \underline{1} \oplus (\underline{0} \oplus \underline{1} \oplus \underline{2}) \oplus (\underline{1} \oplus \underline{2} \oplus \underline{3}) \\
&= \underline{0} \oplus \underline{1} \oplus \underline{1} \oplus \underline{1} \oplus \underline{2} \oplus \underline{2} \oplus \underline{3}. \qquad (*)
\end{aligned}$$

In particular, since $\underline{k} = \{|k,k\rangle, ..., |k,-k\rangle\}$ has dimension $2k+1$, we see that there is $2\cdot 0+1 = 1$ state with $\mathbf{S}^2$-eigenvalue $\hbar^2 0\cdot(0+1) = 0$, there are $3\cdot(2\cdot 1+1) = 9$ states with $\mathbf{S}^2$-eigenvalue $\hbar^2 1\cdot(1+1) = 2\hbar^2$, there are $2\cdot(2\cdot 2+1) = 10$ states with $\mathbf{S}^2$-eigenvalue $\hbar 2\cdot(2+1) = 6\hbar^2$, and there are $2\cdot 3+1 = 7$ states with $\mathbf{S}^2$-eigenvalue $\hbar^2 3\cdot(3+1) = 12\hbar^2$. Note this makes a total of $1+9+10+7 = 27$ states, which is in agreement with the dimension of the tensor product space $\underline{1}\otimes\underline{1}\otimes\underline{1}$.

In particular, turning to the Hamiltonian, we see that we have:

- One state with energy $\frac{\lambda}{\hbar^2}\cdot 0 - 6\lambda = -6\lambda$;
- 9 states with energy $\frac{\lambda}{\hbar^2}\cdot 2\hbar^2 - 6\lambda = -4\lambda$;
- 10 states with energy $\frac{\lambda}{\hbar^2}\cdot 6\hbar^2 - 6\lambda = 0$;
- 7 states with energy $\frac{\lambda}{\hbar^2}\cdot 12\hbar^2 - 6\lambda = 6\lambda$.

(ii) The second part is a little bit trickier, because the Hilbert space for the particles *isn't* $\underline{1} \otimes \underline{1} \otimes \underline{1}$. This is because the particles are identical, so we must instead restrict to the completely symmetric subspace of $\underline{1} \otimes \underline{1} \otimes \underline{1}$, which we will write as:

$$\mathrm{Sym}(\underline{1} \otimes \underline{1} \otimes \underline{1}).$$

There's no nice Clebsch-Gordan formula that can be used to decompose this space; instead we have to do some work. First, let's try to construct a basis for $\mathrm{Sym}(\underline{1} \otimes \underline{1} \otimes \underline{1})$ to know what kind of states we're dealing with.

Note first that the dimension of $\mathrm{Sym}(\underline{1} \otimes \underline{1} \otimes \underline{1})$ is quite straightforward to compute; since the general state in $\underline{1} \otimes \underline{1} \otimes \underline{1}$ is of the form $|\sigma_1\sigma_2\sigma_3\rangle := |1, \sigma_1\rangle\,|1, \sigma_2\rangle\,|1, \sigma_3\rangle$ where $\sigma_i = -1, 0, 1$, it suffices to count the number of different choices of $\sigma_1\sigma_2\sigma_3$, *up to permutations*, which are distinct from one another. Since there aren't that many combinations, we can just write out some lists of $\sigma_1\sigma_2\sigma_3$ that are the same up to permutations:

- If all three of the σ_i are the same, the state is automatically symmetric. Hence $|111\rangle$, $|000\rangle$ and $|-1,-1,-1\rangle$ are all distinct basis states in $\mathrm{Sym}(\underline{1} \otimes \underline{1} \otimes \underline{1})$; we have counted three states this way.
- Consider now states with two 1's. If we additionally have a zero, the relevant states $|110\rangle$, $|101\rangle$ and $|011\rangle$, which all must combine together as a single state in the symmetric subspace:

  $$\frac{1}{\sqrt{3}}(|110\rangle + |101\rangle + |011\rangle).$$

  Similarly if we additionally had a -1, we'd get a single state proportional to $|1,1,-1\rangle + |1,-1,1\rangle + |-1,1,1\rangle$. Hence there are two states in the symmetric subspace with two of the σ_i given by 1. The same argument applies to having two of the σ_i given by 0, or two of the σ_1 given by -1, hence we have counted six states this way.
- Finally, suppose that all the σ_i are distinct. There is a unique state in the symmetric subspace that looks like this, given by:

  $$\frac{1}{\sqrt{6}}\left(|1,0,-1\rangle + |1,-1,0\rangle + |0,1,-1\rangle + |0,-1,1\rangle + |-1,0,1\rangle + |-1,1,0\rangle\right).$$

Hence the dimension of $\mathrm{Sym}(\underline{1} \otimes \underline{1} \otimes \underline{1})$ is precisely 10. We can now use this information to save us some work:

- Let's note that $|111\rangle \in \mathrm{Sym}(\underline{1}\otimes\underline{1}\otimes\underline{1})$ is the top angular momentum eigenstate, and hence has $\mathbf{S}^2$ quantum number 3. Thus it lives in an angular momentum space $\underline{3}$ (if it inhabited $\underline{j}$ for $j > 3$, then we would have state of higher $\mathbf{S}^2$ quantum number, which would contradict the obvious physical fact that $|111\rangle$ is the top angular momentum eigenstate of the system). In particular, all elements of this $\underline{3}$ space, which are generated by acting with the lowering operator $S_- = S_{1-} + S_{2-} + S_{3-}$ on $|111\rangle$, are symmetric since the lowering operator itself is symmetric. So we have accounted for a total of $2 \cdot 3 + 1 = 7$ basis states of $\mathrm{Sym}(\underline{1} \otimes \underline{1} \otimes \underline{1})$, all of which have $\mathbf{S}^2$ quantum number 3, and hence $\mathbf{S}^2$-eigenvalue $\hbar^2 3 \cdot (3+1) = 12\hbar^2$. Using the above work in the distinguishable case, it follows these 7 states have energy 6λ.
- There are 3 basis states remaining. Choosing to arrange these states in eigenspaces of $\mathbf{S}^2$, we see that we can write the space spanned by these 3 remaining states as $\underline{j_1} \oplus \underline{j_2} \oplus ... \oplus \underline{j_n}$ for some $j_1, ..., j_n$. However, on the grounds of dimension, the only possible splittings are:

  $$\underline{0} \oplus \underline{0} \oplus \underline{0}, \qquad \underline{0} \oplus \underline{\frac{1}{2}} \qquad \text{or} \qquad \underline{1}.$$

  But if we have an $\mathbf{S}^2$ eigenspace in the symmetric subspace $\mathrm{Sym}(\underline{1} \otimes \underline{1} \otimes \underline{1})$, then it also must exist in the overall space $\underline{1} \otimes \underline{1} \otimes \underline{1}$. But looking at $(*)$ only one of these options is a subspace, namely $\underline{1}$. Thus we must have three states of $\mathbf{S}^2$ quantum number 1, i.e. $\mathbf{S}^2$-eigenvalue $\hbar^2 1 \cdot (1+1) = 2\hbar^2$, i.e. energy -4λ.

In summary, in the case that the particles are identical, there are energy levels -4λ with degeneracy 3, and 6λ with degeneracy 7.

4. Consider the isotropic harmonic oscillator in three dimensions, with potential $V(\mathbf{X}) = V_0 + \frac{1}{2}m\omega^2\mathbf{X}^2$.

   (i) Write down the allowed energy eigenvalues. What is the degeneracy of the nth level?

   (ii) $(*)$ In a simple model of the atomic nucleus, each nucleon (proton or neutron, each with spin-$\frac{1}{2}$) moves in the harmonic potential $V(r)$ above, interpreted as being created by the other nucleons. Explain why the nuclear isotopes $^4\mathrm{H}$, $^{16}\mathrm{O}$ and $^{40}\mathrm{Ca}$ are especially stable.

   [Helium, oxygen and calcium have atomic numbers $Z = 2, 8$ and 20, respectively. All protons are identical.]

Solution: (i) The possible energy eigenvalues are just:

$$E_{n_1 n_2 n_3} = V_0 + \hbar\omega\left(n_1 + n_2 + n_3 + \frac{3}{2}\right), \qquad n_1, n_2, n_3 \geq 0,$$

i.e. the sum of the energies of three independent harmonic oscillators, all of frequency ω. Since the sum of n_1, n_2 and n_3 is an integer, the distinct energy levels are (in increasing order):

$$V_0 + \hbar\omega \cdot \frac{3}{2}, \qquad V_0 + \hbar\omega \cdot \left(1 + \frac{3}{2}\right), \qquad V_0 + \hbar\omega \cdot \left(2 + \frac{3}{2}\right), \qquad \text{etc.}$$

Hence the nth energy level has energy:

$$E = V_0 + \hbar\omega\left(n + \frac{3}{2}\right).$$

To determine the degeneracy, we simply need to find the number of states of the system that give rise to this particular energy. This is equivalent to determining the number of possible combinations of integers n_1, n_2 and $n_3 \geq 0$ such that

$$n = n_1 + n_2 + n_3,$$

for n given. This can be accomplished with a counting technique called *stars and bars*:

Theorem: The number of ways to partition the integer n into a sum $n = n_1 + n_2 + n_3$ of three non-negative integers $n_1, n_2, n_3 \geq 0$ is $\frac{1}{2}(n+2)(n+1)$.

Proof: Suppose that we represent the integer n by a list of n *stars*:

$$\underbrace{\star\star\star\ldots\star}_{n \text{ times}}.$$

To partition n up into three sets, we insert two *bars*, for example for $n = 4$ we could have:

$$\star\star\,|\,\star\,|\star, \qquad \text{or} \qquad \star\star\star\star||$$

which we read as $4 = 2 + 1 + 1$, and $4 = 4 + 0 + 0$, respectively. In general, we will have n stars and 2 bars, and any permutation of these items will give a different valid partition. The number of valid permutations is then:

$$\frac{(n+2)!}{n! \cdot 2!} = \frac{1}{2}(n+2)(n+1).$$

since we have n identical stars and 2 identical bars, which we cannot distinguish. □

Thus the degeneracy of the nth level is just:

$$\frac{1}{2}(n+2)(n+1).$$

(ii) $(*)$ Recall that each nucleon has spin-$1/2$, and so in particular all nucleons are fermions. They therefore obey the Pauli exclusion principle - no two identical fermions may be in the same state simultaneously.

As we saw in part (i), the nth energy level has a degeneracy

$$\frac{1}{2}(n+2)(n+1)$$

coming from its spatial (harmonic oscillator) part. However, since we are now dealing with particles that have two possible spin states, there is also a twofold degeneracy from the spin. Hence there are:

$$(n+2)(n+1)$$

degenerate states all at the nth energy level. Since identical fermions cannot occupy the same state, there are effectively $(n+2)(n+1)$ available states for each proton to be in if it is at the nth energy level; the same goes for each neutron.

Now let's think about how this relates to stability. Considering each isotope in turn:

- The helium nucleus has 2 protons and 2 neutrons. The lowest energy level has degeneracy $(0+2)(0+1) = 2$, and hence we can assign this energy level two neutrons and two protons. This makes the helium nucleus particularly stable because it does not have energy levels that are not filled with particles; this makes the helium nucleus less likely to lose or gain nucleons than a nucleus that had an unfilled outer energy level.
- The oxygen nucleus has 8 protons and 8 neutrons. As we've seen, there are 2 available states at the lowest energy level. There are also $(1+2)(1+1) = 6$ available states at the first excited energy level. Therefore we can put 2 protons and 2 neutrons into the lowest energy level, and 6 protons and 6 neutrons into the first excited energy level. Again, this makes the oxygen nucleus particularly stable because we have a filled outer energy level.
- Finally, the calcium nucleus has 20 protons and 20 neutrons. In the second excited energy level, there are $(2+2)(2+1) = 12$ available states. Since $12+6+2 = 20$, we can fill the first three energy levels with protons and neutrons. Again, we have stability because we have a filled outer energy level.

5. In this question you should assume total angular momentum and parity are conserved in the decay process.

Show that a particle of spin 1 cannot decay into two identical particles of spin 0. The ρ-meson has spin-1 and can decay into two spinless π-mesons (pions) with different electric charges. If the intrinsic parity of any pion is negative, what is the intrinsic parity of the ρ-meson?

Solution: These decay questions can be a bit tricky to get your head round, but I think there are two important tools that will help you out:

- Always assume that the decaying particle starts in its rest frame. We can then assume that the initial orbital angular momentum is $l_{\text{LHS}} = 0$, and hence the initial total angular momentum is equal to the spin, i.e. $j_{\text{LHS}} = s_{\text{LHS}}$.
- Draw a table summarising all the particles' properties! This can be very helpful when organising your thoughts.

Let's begin by considering a decay $X \to Y + Y$, where X has spin-1 and Y has spin-0. Constructing a table of the particles' properties, we have:

Particle property	X	**First** Y	**Second** Y
Intrinsic parity	η_X	η_Y	η_Y
Total ang. mom. (j)	1	?	
Orbital ang. mom. (l)	0	?	
Spin (s)	1	0	0

The cells that cross both Y columns are supposed to represent properties of the $Y + Y$ composite system.

Now, we have a lot of unknown values in both Y columns. Let's try to fix some of these unknowns by thinking about conservation and addition of angular momentum:

- Let's begin by using *conservation of total angular momentum*. This means that the total angular momentum of X must be equal to the total angular momentum of the composite system $Y + Y$.

  The decaying particle X has total angular momentum quantum number $j = 1$. Therefore, since total angular momentum is conserved, the composite $Y + Y$ system must also have angular momentum quantum number $j = 1$.

- We can add the spin momenta of the two Y particles using addition of angular momenta. Since both Y particles have spin zero, the only spin state in the composite system is $|0, 0\rangle = |0, 0\rangle \otimes |0, 0\rangle$. It follows that the composite system has total spin zero.

Modifying our table to include these results, we have:

Particle property	X	**First** Y	**Second** Y
Intrinsic parity	η_X	η_Y	η_Y
Total ang. mom. (j)	1	1	
Orbital ang. mom. (l)	0	?	
Spin (s)	1	0	

We should now think about the allowed orbital angular momentum quantum numbers of the composite $Y + Y$ system. We know that we can add the orbital angular momentum of the $Y + Y$ system to the spin angular momentum of the $Y + Y$ system to get the total angular momentum of the $Y + Y$ system. We know from lectures that when we add the orbital angular momentum l to the spin angular momentum 0 we must get a result in the range:

$$\{l + 0, l + 0 - 1, ..., |l - 0|\} = \{l\}.$$

In this case, the range is trivially just l. Thus we have $l = j = 1$. Entering this into the table, we have:

Particle property	X	**First** Y	**Second** Y
Intrinsic parity	η_X	η_Y	η_Y
Total ang. mom. (j)	1	1	
Orbital ang. mom. (l)	0	1	
Spin (s)	1	0	

We must now explain why the decay $X \to Y + Y$ cannot happen. First notice that since both Y particles have spin zero, they must be *bosons* by the spin-statistics theorem. Hence under exchange of one of the Y particles with the other Y particle, we must pick up a $+1$ in the wavefunction, since they are identical.

However, we know from lectures that under exchange of the Y particles, we pick up a factor of $(-1)^l$ from the spatial wavefunction of the Y particles, where l is their orbital angular momentum. It follows that in this case, we obtain a sign: $(-1)^1 = -1$. This is a contradiction, hence this decay cannot occur.

In the second part of this question we are asked to consider the decay $\rho \to \pi^+ + \pi^-$, where ρ has spin-1 and the $\pi^\pm$ particles have spin-0. Everything in our above argument goes through just as before, except for the identical particles argument at the end, giving the table:

Particle property	ρ	π^+	π^-
Intrinsic parity	η_ρ	-1	-1
Total ang. mom. (j)	1	1	
Orbital ang. mom. (l)	0	1	
Spin (s)	1	0	

Note that we have entered the pions' intrinsic parity, which is given as -1. To determine the intrinsic parity of the ρ-meson, we use the fact that parity is conserved during the interaction.

We know from lectures that acting with the parity operator on the left hand side returns a sign $\eta_\rho(-1)^0 = \eta_\rho$. On the right hand side, we get a sign $\eta_{\pi^+}\eta_{\pi^-}(-1)^1 = -1$. Therefore, by conservation of parity, $\eta_\rho = -1$.

6. In this question you should assume total angular momentum and parity are conserved in the decay process.

A particle X is observed to undergo the decays $X \to \rho^+ + \pi^+$ and $X \to K + K$, where the kaon K has spin-0. What is the lowest value of the spin of X that is consistent with this, and what is the corresponding intrinsic parity of X?

Solution: Let's begin by constructing the relevant tables for the decays. Consider first the decay $X \to K + K$. We make the following observations:

- If we view the decaying X in its rest frame, we can set the initial orbital angular momentum eigenvalue to 0. Further, setting the spin of X to s, we have that the total angular momentum before the decay is $j = s$, since we are adding angular momentum 0 to angular momentum s, and this can only produce states of angular momentum s.
- By conservation of total angular momentum, the total angular momentum quantum number of the composite $K+K$ system must be $j = s$.
- Since each kaon K has spin-0, it follows that the composite system $K + K$ must have spin 0 (since we are adding spin 0 to spin 0).

Thus we have the table of particle properties:

Particle property	X	K	K
Intrinsic parity	η_X	η_K	η_K
Total ang. mom. (j)	s	s	
Orbital ang. mom. (l)	0	$?$	
Spin (s)	s	0	

Let the orbital angular momentum quantum number on the right hand side be l'. Then, by considering addition of the orbital angular momentum on the right hand side to the spin angular momentum, we see that we must have:

$$s \in \{l + 0, ..., |l - 0|\} = \{l\} \qquad \Rightarrow \qquad l = s.$$

Hence inserting this value, we have the complete table:

Particle property	X	K	K
Intrinsic parity	η_X	η_K	η_K
Total ang. mom. (j)	s	s	
Orbital ang. mom. (l)	0	s	
Spin (s)	s	0	

Considering parity conservation, we have $\eta_X(-1)^0 = \eta_K^2(-1)^s$, which implies that $\eta_X = (-1)^s$.

Also note that since the kaons are spin-0 particles, they are *bosons* by the spin-statistics theorem. It follows that under exchange of the two identical kaons on the right hand side, we pick up a sign $1 = (-1)^s$ in the wavefunction. So s is an even integer, and hence the intrinsic parity of X is $\eta_X = 1$.

Let's move to the other decay process. As a first observation, let us note that ρ^+ is exactly the same as a neutral ρ-meson, except it carries a positive charge. Therefore, from Question 4 we know that ρ^+ has spin 1 and intrinsic parity $\eta_{\rho^+} = -1$.

We now construct a table for the decay $X \to \rho^+ + \pi^+$. We have:

Particle property	X	ρ^+	π^+
Intrinsic parity	1	-1	-1
Total ang. mom. (j)	s	s	
Orbital ang. mom. (l)	0	?	
Spin (s)	s	1	0

Considering addition of the two spin angular momenta on the right hand side, we note that the composite $\rho^+ + \pi^+$ can have any spin in the range $\{1+0, ..., |1-0|\} = \{1\}$. Hence we can complete the table as:

Particle property	X	ρ^+	π^+
Intrinsic parity	1	-1	-1
Total ang. mom. (j)	s	s	
Orbital ang. mom. (l)	0	?	
Spin (s)	s	1	

Let the orbital angular momentum quantum number on the right hand side be l. Then we know from addition of angular momentum that we must have:

$$s \in \{l+1, l, ...|l-1|\}.$$

Considering parity of both sides, we also arrive at the condition $1 = (-1)^l$, from which it follows that l is even.

Let's put together everything we know. First, we know that s is an even integer. So we should test $s = 0, 2, ...$ in turn and see which is the first value consistent with all the conditions we have derived.

- $s = 0$ is consistent with the decay $X \to K + K$. However, for $s = 0$ to be consistent with the decay $X \to \rho^+ + \pi^+$, we would need

  $$0 \in \{l+1, l, ..., |l-1|\}$$

  for some value of l, which is itself an even integer. Note $l = 0$ does not work, since then we have $0 \in \{1\}$, a contradiction. Note $l = 2$ also fails, since we then have $0 \in \{3, 2, 1\}$. It quickly becomes apparent that higher values of l are less and less useful. Thus $s = 0$ does not work.

- $s = 2$ is consistent with the decay $X \to K + K$. For $s = 2$ to be consistent with the decay $X \to \rho^+ + \pi^+$, we need

  $$2 \in \{l+1, l, ..., |l-1|\}$$

  for some even integer l. But we have just seen that $l = 2$ works. Thus $s = 2$ is the lowest allowed value of s.

7. A $d = 1$ harmonic oscillator of mass m and frequency ω is perturbed by $\Delta = \lambda X^4$. By expressing the position operator X in terms of the raising and lowering operators A and $A^\dagger$, show that the first order change in energy in the nth excited state is:

$$\delta E_n = 3\lambda(2n^2 + 2n + 1)\left(\frac{\hbar}{2m\omega}\right)^2.$$

What is the radius of convergence in λ of perturbation theory here?

Solution: Recall that the raising and lowering operators are given by:

$$A = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega X + iP), \qquad A^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega X - iP),$$

hence the position operator is given in terms of the raising and lowering operators as:

$$X = \sqrt{\frac{\hbar}{2m\omega}}\left(A + A^\dagger\right).$$

Since we are working with a $d = 1$ harmonic oscillator, all energy levels are non-degenerate, so we're safe to use non-degenerate perturbation theory. Recall from lectures that the first order correction to the nth energy level is:

$$\delta E_n = \langle n|\Delta|n\rangle = \lambda\langle n|X^4|n\rangle.$$

Inserting the expression for X in terms of the raising and lowering operators, we have:

$$\delta E_n = \lambda\langle n|(A + A^\dagger)^4|n\rangle\left(\frac{\hbar}{2m\omega}\right)^2.$$

It remains to evaluate the matrix element. This takes some care, as we can't just expand using the binomial theorem, since A and $A^\dagger$ do not commute. We have:

$$(A + A^\dagger)^4 = (A + A^\dagger)^2(A + A^\dagger)^2 = (A^2 + AA^\dagger + A^\dagger A + {A^\dagger}^2)(A^2 + AA^\dagger + A^\dagger A + {A^\dagger}^2)$$

$$\begin{aligned} &= A^4 + A^3A^\dagger + A^2A^\dagger A + A^2{A^\dagger}^2 + AA^\dagger A^2 + AA^\dagger AA^\dagger + AA^\dagger{}^2A + AA^\dagger{}^3 \\ &+A^\dagger A^3 + A^\dagger A^2A^\dagger + A^\dagger AA^\dagger A + A^\dagger AA^\dagger{}^2 + A^\dagger{}^2A^2 + A^\dagger{}^2AA^\dagger + A^\dagger{}^3A + A^\dagger{}^4. \end{aligned}$$

This looks like a pretty horrible mess! However, with some careful thought, we can decide which of these terms we care about, and which we can just throw away. For example:

- A^4 can just be thrown away. This is because $A^4|n\rangle \propto |n-4\rangle$, and $\langle n|n-4\rangle = 0$. Thus we just get zero when we take the matrix element.
- $A^3A^\dagger$ can just be thrown away. Again, we see $A^3A^\dagger|n\rangle \propto |n-2\rangle$, and $\langle n|n-2\rangle = 0$.
- …etc. These considerations imply we need *exactly two lowering operators and two raising operators* in terms that produce a non-zero element when sandwiched between $\langle n|$ and $|n\rangle$.

Thus the matrix element reduces to:

$$\langle n|A^2{A^\dagger}^2 + AA^\dagger AA^\dagger + AA^\dagger{}^2A + A^\dagger A^2A^\dagger + A^\dagger AA^\dagger A + A^\dagger{}^2A^2|n\rangle.$$

It remains to work out the contributions from each of the terms. We use the important identities:

$$A^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle\,, \qquad A\,|n\rangle = \sqrt{n}\,|n-1\rangle\,,$$

which you should have seen in lectures. Considering each term in turn then, we have:

- $\langle n|A^2{A^\dagger}^2|n\rangle = \sqrt{(n+1)(n+2)}\,\langle n|A^2|n+2\rangle = \sqrt{(n+2)^2(n+1)^2}\,\langle n|n\rangle = (n+2)(n+1).$
- $\langle n|AA^\dagger AA^\dagger|n\rangle = \sqrt{(n+1)^4} = (n+1)^2.$
- $\langle n|A{A^\dagger}^2A|n\rangle = \sqrt{n^2(n+1)^2} = n(n+1).$
- $\langle n|A^\dagger A^2A^\dagger|n\rangle = \sqrt{(n+1)^2n^2} = n(n+1).$
- $\langle n|A^\dagger AA^\dagger A|n\rangle = \sqrt{n^4} = n^2.$
- $\langle n|{A^\dagger}^2A^2|n\rangle = \sqrt{n^2(n-1)^2} = n(n-1).$

Therefore the matrix element is:

$$\langle n|(A^\dagger + A)^4|n\rangle = (n+2)(n+1) + (n+1)^2 + n(n+1) + n(n+1) + n^2 + n(n-1)$$

$$= 6n^2 + 6n + 3.$$

Hence assembling everything, we get the first order change in energy:

$$\delta E_n = 3\lambda(2n^2 + 2n + 1)\left(\frac{\hbar}{2m\omega}\right)^2,$$

as required.

We are now asked to comment on the radius of convergence of perturbation theory. Notice the following facts:

- We know that perturbation theory converges for $\lambda = 0$, since then our corrections are all trivially zero.
- For $\lambda < 0$, there are *no bound states* of the system, since our potential becomes:

$$V(X) = \frac{1}{2}m\omega^2X^2 + \lambda X^4$$

  which is clearly not bounded below as $X \to \pm\infty$. Quantum tunnelling thus allows any particle to escape to infinity.

From the second point, it follows that perturbation theory *must* fail to converge for $\lambda < 0$, else it would predict an additional bound state in the $\lambda < 0$ case of some finite energy.

But now recall from some analysis course that power series converge in a *disk* in the complex plane, centred on the place where we are expanding around. Our disk is centred on $\lambda = 0$, but cannot include any of the region $\lambda < 0$. Therefore the radius of convergence of the perturbation series is 0.

8. A particle of mass m is confined by the infinite square well potential

$$V(x) = \begin{cases} 0 & \text{when } |x| < a, \\ \infty & \text{when } |x| > a. \end{cases}$$

(i) Show that, to first order in λ, the energy levels of this particle are unchanged when the potential is perturbed by $\delta V(x) = \lambda x/a$.

(ii) Show that the ground-state wavefunction *is* changed, becoming

$$\psi_\lambda(x) = \frac{1}{\sqrt{a}}\cos(\pi x/2a) + \frac{16\lambda}{\pi^2 E_1\sqrt{a}} \sum_{n=2,4,\ldots} (-1)^{n/2} \frac{n}{(n^2-1)^3} \sin(n\pi x/2a) + O(\lambda^2),$$

where E_1 is the ground state energy. Explain why this wavefunction does not have well-defined parity.

(iii) Write down a formula giving the second order correction to the energy of the ground state energy. Will this second order correction be positive or negative? Detailed calculation is not required.

(iv) $(*)$ Suppose now that the initial well is only finitely deep. Will perturbation theory converge? Comment on the relevance of this to the Stark effect in hydrogen.

Solution: We should begin by finding the energy levels and energy eigenstates of the unperturbed system. It's easiest to do this in the position representation, then we must solve the simple problem of finding the wavefunction and energies of a 'particle in a box', just as we did in Part IB Quantum Mechanics. Recall that the wavefunction $\psi_n(x)$ for the nth eigenstate satisfies the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_n}{\partial x^2} + V(x)\psi_n = E_n\psi_n,$$

where

$$V(x) = \begin{cases} 0 & \text{when } |x| < a, \\ \infty & \text{when } |x| > a. \end{cases}$$

Thus we immediately deduce that $\psi_n(x) = 0$ for $|x| > a$ (i.e. outside the box), and inside the box we have:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_n}{\partial x^2} = E_n\psi_n \qquad \Rightarrow \qquad \psi_n = A_n \sin\left(\sqrt{\frac{2mE_n}{\hbar^2}}(x-a)\right).$$

Continuity of the wavefunction at $x = \pm a$ demands that we have $\psi(\pm a) = 0$. Imposing these conditions fixes the energies to be:

$$E_n = \frac{n^2\pi^2\hbar^2}{8ma^2}, \qquad \text{for } n > 0,$$

just as we found in Part IB Quantum Mechanics. The undisturbed eigenstates are thus:

$$\psi_n(x) = A_n \sin\left(\frac{n\pi}{2a}(x-a)\right).$$

The normalisation constant can be obtained by considering:

$$1 = \int_{-a}^{a} \psi_n(x)^*\psi_n(x) = \int_{-a}^{a} |A_n|^2 \sin^2\left(\frac{n\pi(x-a)}{2a}\right) dx = |A_n|^2 a \qquad \Rightarrow \qquad A_n = \sqrt{\frac{1}{a}}.$$

Thus we have:

$$\psi_n(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{n\pi(x-a)}{2a}\right).$$

As a final note, observe that we are working in one dimension. So (as we saw on Sheet 1) the energy levels must be non-degenerate, and hence non-degenerate perturbation theory will apply throughout this question.

(i) Let's start doing some perturbation theory. We know from lectures that the first order change in energy of the nth level due to the presence of the perturbation is given by the formula:

$$\frac{\langle n|\delta V|n\rangle}{\langle n|n\rangle} = \frac{\langle n|\mathbf{X}\lambda/a|n\rangle}{\langle n|n\rangle},$$

where $|n\rangle$ is the nth energy eigenstate of the system. Working in the position representation, we see that:

$$\frac{\lambda}{a}\cdot\langle n|\mathbf{X}|n\rangle = \frac{\lambda}{a}\cdot\int_{-a}^{a} x\sin^2\left(\frac{n\pi(x-a)}{2a}\right)dx.$$

This integral has an odd integrand and we are integrating over a symmetric domain, hence it is zero. So we immediately deduce that the change in energy due to the perturbation at first order is 0, as required.

(ii) The ground state in this case is given by $n = 1$ (the $n = 0$ eigenstate vanishes). Using the result from lectures for the change to a wavefunction due to a perturbation, the perturbed ground state wavefunction in this case is (to first order):

$$\begin{aligned}\psi_\lambda(x) &= \psi_1(x) + \lambda\sum_{m\neq 1}\frac{\langle m|\delta V|1\rangle}{E_1 - E_m}\psi_m(x)\\ &= \frac{1}{\sqrt{a}}\sin\left(\frac{\pi(x-a)}{2a}\right) + \frac{\lambda}{a^2}\sum_{m\neq 1}\frac{\psi_m(x)}{E_1-E_m}\int_{-a}^{a} x\sin\left(\frac{m\pi(x-a)}{2a}\right)\sin\left(\frac{\pi(x-a)}{2a}\right)dx\end{aligned}$$

Recalling the energy levels, we have: $E_1 - E_m = \dfrac{\pi^2\hbar^2}{8ma^2}(1-m^2) = E_1(1-m^2)$. Hence the perturbed ground state wavefunction may be written as:

$$\psi_\lambda(x) = \frac{1}{\sqrt{a}}\sin\left(\frac{\pi(x-a)}{2a}\right) - \frac{\lambda}{a^2E_1}\sum_{m\neq 1}\frac{\psi_m(x)}{(m-1)(m+1)}\int_{-a}^{a} x\sin\left(\frac{m\pi(x-a)}{2a}\right)\sin\left(\frac{\pi(x-a)}{2a}\right)dx.$$

To perform the integral, recall the trigonometric 'product to sum formula':

$$\sin(A)\sin(B) = \frac{1}{2}(\cos(A-B) - \cos(A+B)).$$

We then have:

$$\int_{-a}^{a} x\sin\left(\frac{m\pi(x-a)}{2a}\right)\sin\left(\frac{\pi(x-a)}{2a}\right)dx = \frac{1}{2}\int_{-a}^{a} x\left(\cos\left(\frac{(m-1)\pi x}{2a}\right) - \cos\left(\frac{(m+1)\pi x}{2a}\right)\right)dx.$$

Integrating both terms by parts, we have:

$$\frac{1}{2}\left[\left[\frac{x\sin\left(\frac{(m-1)\pi(x-a)}{2a}\right)}{\frac{(m-1)\pi}{2a}}\right]_{-a}^{a} - \int_{-a}^{a}\frac{\sin\left(\frac{(m-1)\pi(x-a)}{2a}\right)}{\frac{(m-1)\pi}{2a}}dx - \left[\frac{x\sin\left(\frac{(m+1)\pi(x-a)}{2a}\right)}{\frac{(m+1)\pi}{2a}}\right]_{-a}^{a} + \int_{-a}^{a}\frac{\sin\left(\frac{(m+1)\pi(x-a)}{2a}\right)}{\frac{(m+1)\pi}{2a}}dx\right]$$

$$= \frac{1}{2}\left[-\int_{-a}^{a}\frac{\sin\left(\frac{(m-1)\pi(x-a)}{2a}\right)}{\frac{(m-1)\pi}{2a}}dx + \int_{-a}^{a}\frac{\sin\left(\frac{(m+1)\pi(x-a)}{2a}\right)}{\frac{(m+1)\pi}{2a}}dx\right]$$

$$= \frac{1}{2}\left[-\left[\frac{\cos\left(\frac{(m-1)\pi(x-a)}{2a}\right)}{\left(\frac{(m-1)\pi}{2a}\right)^2}\right]_{-a}^{a} + \left[\frac{\cos\left(\frac{(m+1)\pi(x-a)}{2a}\right)}{\left(\frac{(m+1)\pi}{2a}\right)^2}\right]_{-a}^{a}\right].$$

Hence the integral evaluates to:

$$\frac{1}{2}\left(\left(\frac{2a}{(m-1)\pi}\right)^2(1-(-1)^{m-1})-\left(\frac{2a}{(m+1)\pi}\right)^2(1-(-1)^{m+1})\right).$$

Note there are singularities at $m=1$ and $m=-1$, but these are not included in our summation, so we can ignore them. We notice also that for m odd, we get zero. Otherwise, we just get:

$$\left(\frac{2a}{(m-1)\pi}\right)^2-\left(\frac{2a}{(m+1)\pi}\right)^2=\frac{4a^2}{\pi^2}\left(\frac{1}{(m-1)^2}-\frac{1}{(m+1)^2}\right)=\frac{4a^2}{\pi^2}\cdot\frac{4m}{(m-1)^2(m+1)^2}.$$

Substituting this into the formula for the perturbed wavefunction, we have:

$$\psi_\lambda(x)=\frac{1}{\sqrt{a}}\sin\left(\frac{\pi(x-a)}{2a}\right)-\frac{16\lambda}{\pi^2\sqrt{a}E_1}\sum_{m=2,4,\ldots}\frac{m}{(m^2-1)^3}\sin\left(\frac{m\pi(x-a)}{2a}\right).$$

Notice that

$$\sin\left(\frac{\pi(x-a)}{2a}\right)=\sin\left(\frac{\pi x}{2a}-\frac{\pi}{2}\right)=\cos\left(\frac{\pi x}{2a}\right),$$

and

$$\sin\left(\frac{m\pi(x-a)}{2a}\right)=\sin\left(\frac{m\pi x}{2a}-\frac{m\pi}{2}\right)=(-1)^{m/2+1}\sin\left(\frac{m\pi x}{2a}\right)\qquad\text{when } m\in 2\mathbb{Z}.$$

Then the formula

$$\psi_\lambda(x)=\frac{1}{\sqrt{a}}\cos\left(\frac{\pi x}{2a}\right)+\frac{16\lambda}{\pi^2\sqrt{a}E_1}\sum_{m=2,4,\ldots}\frac{(-1)^{m/2}m}{(m^2-1)^3}\sin\left(\frac{m\pi x}{2a}\right)$$

follows, as required.

We are now asked to explain why this function does *not* have well-defined parity. This is simply a case of the perturbed potential no longer being invariant under parity; since the perturbed potential is

$$V(x)=\frac{\lambda x}{a}$$

in the region $-a<x<a$, it is not invariant under parity $\mathcal{P}:x\to -x$.

It follows that parity is *not* a symmetry of the Hamiltonian anymore, and so the parity operator Π does *not* commute with the Hamiltonian, i.e. $[\Pi,H]\neq 0$. Thus the eigenstates of H are *not* simultaneously eigenstates of Π, and are hence do *not* have well-defined parity.

(iii) We know from lectures that the second-order correction to the ground state wavefunction is:

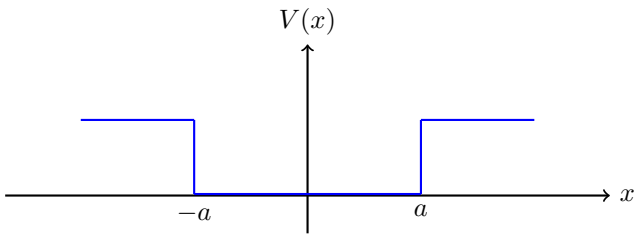
$$\lambda^2\sum_{m\neq 1}\frac{|\langle m|\delta V|1\rangle|^2}{E_1-E_m}.$$

The numerator of the sum is non-negative, but the denominator of the sum obeys

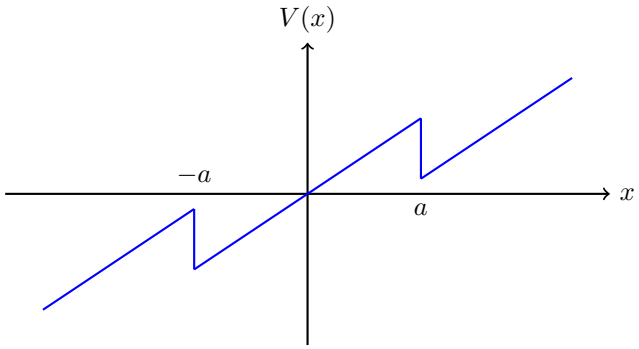
$$E_1-E_m=E_1(1-m^2)<0$$

for all $m>1$, and hence is always negative. It follows that the second-order correction is negative.

(iv) For a well of finite-depth, the unperturbed potential looks like:



Hence, in the presence the perturbation $\delta V(x) = \lambda x/a$, the modified potential looks like:



The new potential in the presence of the perturbation is therefore *unbounded below* for all $\lambda \neq 0$. Hence there are *no bound states* of the perturbed system for $\lambda \neq 0$. In particular, perturbation theory must fail to converge for all $\lambda \neq 0$, else it would predict the existence of a new bound state. It follows that the perturbation expansion has zero radius of convergence.

Finally, we are asked to comment on the relevance of this result to the Stark effect in hydrogen. To relate the two, we view the finite potential well drawn above as a crude approximation to the potential of the hydrogen atom. We view this potential as being the potential in the direction of one of the coordinate axes, say. For a deep enough well, the electron can exist in a bound state in the atom, just as in the full theory of the hydrogen atom.

We should view the perturbation as the result of applying an *electric field* to the atom in the direction of the x-coordinate axis. The result is that the atom becomes *polarised*, represented by graph of the perturbed potential above. Just as in the real Stark effect, described in David Skinner's notes in the chapter on perturbation theory, we notice that:

- To first order, there is no change in the energies - this is the 'quadratic' nature of the Stark effect. This is a result of the unperturbed states being of definite parity.
- In the perturbed system, the wavefunction is modified so that it is no longer a state of definite parity. This reflects the fact that the atom is now polarised, so the electron is more likely to be on one side of the atom than on the other.

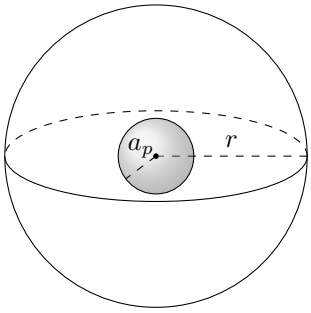
❊ **Comments:** You can read more about the quadratic Stark effect in David Skinner's notes for this course, in the chapter on perturbation theory.

9. An atomic nucleus has finite size and inside the electrostatic potential $\Phi(r)$ deviates from Ze/r. Take the proton's radius to be $a_p \approx 10^{-15}\,\mathrm{m}$ and its charge density to be uniform. Treating the difference between $\Phi(r)$ and Ze/r as a perturbation of the gross structure Hamiltonian of the hydrogen, calculate the first order change in the energy of the ground state of hydrogen. [*Hint: Use the fact that $a_p \ll a_0$ (the Bohr radius) to approximate the integral you encounter.*]

Why is the change in energy of any state with $l \geq 1$ extremely small?

Solution: For a point-like atomic nucleus, an orbiting electron experiences a Coulomb potential. However, if the atomic nucleus has finite extent, we know from Part IB Electromagnetism that the potential will differ from the Coulomb potential on the inside of the nucleus - this question is about investigating the effect of treating the change in the potential inside the nucleus as a perturbation. The inclusion of a finite nuclear radius should have an effect on the electron's wavefunction - indeed, we expect it to be very unlikely for the electron to found *inside* the nucleus, a possibility that is now admitted!

First, we should calculate the electrostatic potential due to a sphere of charge, which is how we are now modelling the atomic nucleus. This requires some basic electrostatics from Part IB Electromagnetism. Consider inserting a *Gaussian surface*, in this case a sphere of radius r, around or within a sphere of charge Ze and radius a_p:



The symmetry of the problem implies that the electric field due to the charged sphere is a function only of the radius r, hence $\mathbf{E} \equiv \mathbf{E}(r)$. We also note that the electric field is completely radial, i.e. $\mathbf{E} \equiv E_r(r)\hat{\mathbf{r}}$. Now we apply *Gauss' law* in integral form:

$$\int_S \mathbf{E} \cdot \mathbf{dA} = \frac{Q}{\epsilon_0},$$

where Q is the charge contained within the surface S. In words, this says that the electric field flux through a closed surface is equal to the charge contained inside the volume enclosed by the surface (with some conventional factor $1/\epsilon_0$).

In this case, the integral on the left hand side is easily evaluated, because $\mathbf{E} = \mathbf{E}(r)$. Thus we get:

$$\int_S \mathbf{E} \cdot \mathbf{dA} = 4\pi r^2 \hat{\mathbf{r}} \cdot \mathbf{E}(r) = 4\pi r^2 E_r(r).$$

Depending on the radius of the Gaussian surface, this can be equal to different things. Gauss' law gives:

$$4\pi\epsilon_0 r^2 E_r(r) = \begin{cases} Ze & \text{if } r > a_p \\ Ze\left(\dfrac{r}{a_p}\right)^3 & \text{if } r \leq a_p. \end{cases}$$

Recall that the electric potential ϕ (which is again a function only of the radius r in this case) is defined by

$$\mathbf{E} = E_r \hat{\mathbf{r}} = -\nabla\phi = -\frac{d\phi}{dr}\hat{\mathbf{r}}.$$

In our case then, the electric potential obeys:

$$\frac{d\phi}{dr} = \begin{cases} -\dfrac{Ze}{4\pi\epsilon_0 r^2} & \text{if } r > a_p \\ -\dfrac{Ze}{4\pi\epsilon_0 r^2}\left(\dfrac{r}{a_p}\right)^3 & \text{if } r \leq a_p. \end{cases}$$

Performing the integrals, and imposing the conditions $\phi(r) \to 0$ as $r \to \infty$ and continuity at $r = a_p$, we have:

$$\phi(r) = \begin{cases} \dfrac{Ze}{4\pi\epsilon_0 r} & \text{if } r > a_p \\ \dfrac{3Ze}{8\pi\epsilon_0 a_p} - \dfrac{Zer^2}{8\pi\epsilon_0 a_p^3} & \text{if } r \leq a_p \end{cases} = \begin{cases} \dfrac{Ze}{4\pi\epsilon_0 r} & \text{if } r > a_p \\ \dfrac{Ze}{8\pi\epsilon_0 a_p}\left(3 - \left(\dfrac{r}{a_p}\right)^2\right) & \text{if } r \leq a_p. \end{cases}$$

The form of the question now suggests that we should be working in units where $4\pi\epsilon_0 = 1$ (we are told the potential outside of the sphere of charge is Ze/r), hence our final answer is:

$$\phi(r) = \begin{cases} \dfrac{Ze}{r} & \text{if } r > a_p \\ \dfrac{Ze}{2a_p}\left(3 - \left(\dfrac{r}{a_p}\right)^2\right) & \text{if } r \leq a_p. \end{cases}$$

To obtain the Hamiltonian, we need the energy of the system. Recall that Newton's second law can be written as $\mathbf{F} = -\nabla V$, where V is the potential energy of the system. Also recall that the Lorentz force law states $\mathbf{F} = -e\mathbf{E} = e\nabla\phi$ (note the charge on an electron here is $-e$) for electrons in the presence of an electric field. Comparing these expressions, it follows that the potential energy of this system is:

$$V(r) = -e\phi(r) = \begin{cases} -\dfrac{Ze^2}{r} & \text{if } r > a_p \\ -\dfrac{Ze^2}{2a_p}\left(3 - \left(\dfrac{r}{a_p}\right)^2\right) & \text{if } r \leq a_p. \end{cases}$$

and hence the Hamiltonian is given by:

$$H = \frac{\mathbf{P}^2}{2m} + V(r) = \frac{\mathbf{P}^2}{2m} + \begin{cases} -\dfrac{Ze^2}{r} & \text{if } r > a_p \\ -\dfrac{Ze^2}{2a_p}\left(3 - \left(\dfrac{r}{a_p}\right)^2\right) & \text{if } r \leq a_p. \end{cases}$$

We can write this in the form $H = H_0 + \Delta$, where H_0 is the Hamiltonian for an atom with nuclear charge Ze, and with the nucleus treated as a point, and Δ given by:

$$\Delta = \begin{cases} 0 & \text{if } r > a_p \\ \dfrac{Ze^2}{r} - \dfrac{Ze^2}{2a_p}\left(3 - \left(\dfrac{r}{a_p}\right)^2\right) & \text{if } r \leq a_p. \end{cases}$$

We now view Δ as a perturbation. We would like to calculate the change in the ground state state energy to first order. Since the ground state of hydrogen is non-degenerate, we can use non-degenerate perturbation theory. In particular, we can just quote from lectures that the required change in energy is:

$$\langle 1,0,0|\Delta|1,0,0\rangle\,,$$

where $|n,l,m\rangle = |1,0,0\rangle$ is the ground state of the electron in an unperturbed atom with nuclear charge Ze. Recall (or look up) that the ground state has the wavefunction:

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi}a_0^{3/2}}\exp\left(-\frac{r}{a_0}\right),$$

where a_0 is the Bohr radius. Therefore,

$$\langle 1,0,0|\Delta|1,0,0\rangle = \frac{4\pi}{\pi a_0^3}\int_0^{a_p} e^{-2r/a_0}\left(\frac{Ze^2}{r} - \frac{Ze^2}{2a_p}\left(3-\left(\frac{r}{a_p}\right)^2\right)\right)r^2\,dr$$

$$\approx \frac{4}{a_0^3}\int_0^{a_p}\left(\frac{Ze^2}{r} - \frac{Ze^2}{2a_p}\left(3-\left(\frac{r}{a_p}\right)^2\right)\right)r^2\,dr.$$

In the final line, we have approximated $e^{-2r/a_0} \approx 1$ for $r < a_p \ll a_0$. Hence we can evaluate the integral to get the change in energy:

$$\langle 1,0,0|\Delta|1,0,0\rangle \approx \frac{4}{a_0^3}\left(\frac{Ze^2a_p^2}{2} - \frac{Ze^2}{2a_p}\left(a_p^3 - \frac{a_p^3}{5}\right)\right) = \frac{4Ze^2a_p^2}{5a_0^3}.$$

Finally, we are asked why the change in energy is very small for $l \geq 1$. This has a simple physical explanation: for $l \geq 1$, the electron has angular momentum. It is therefore excited, and hence is very unlikely to be near the proton anyway - so the electron mostly 'sees' the proton as pointlike for $l \geq 1$.

10. An isotropic harmonic oscillator $d = 2$ has mass m and frequency ω.

(i) Write down a basis of its energy eigenstates.

(ii) What is the energy and degeneracy of the nth excited state?

(iii) The oscillator is perturbed by small potential $\delta V = \lambda xy$. Show that this perturbation lifts the degeneracy of the first excited state, producing states with energies $2\hbar\omega \pm \lambda\hbar/2m\omega$. What are the corresponding eigenstates?

(iv) Which states remain degenerate in the presence of this perturbation?

(v) $(*)$ What is the radius of convergence (in λ) of this perturbation series?

Solution: (i) The basis of energy eigenstates is:

$$\left\{ |nm\rangle = |n\rangle \otimes |m\rangle = \frac{(A_x^\dagger)^n}{\sqrt{n!}} |0\rangle \otimes \frac{(A_y^\dagger)^m}{\sqrt{m!}} |0\rangle : n, m \in \mathbb{Z}_0^+ \right\},$$

where $A_x^\dagger$ and $A_y^\dagger$ are the raising operators for the oscillator in the x and y directions respectively.

(ii) The energy of the nth excited state is $E_n = \hbar\omega(n+1)$. By the same 'stars and bars' argument as in Question 3, the degeneracy of this energy level is

$$\frac{(n+1)!}{n!} = n + 1.$$

(iii) We know from lectures that we must diagonalise the perturbation in the degenerate subspace, then find the eigenvalues of the resulting matrix.

In this case, the degenerate subspace is simply span$\{|10\rangle, |01\rangle\}$, i.e. the span of the state that is minimally excited in the x-direction and the state that is minimally excited in the y-direction. It follows that the matrix of the perturbation in this subspace is:

$$\begin{pmatrix} \langle 10|\delta V|10\rangle & \langle 10|\delta V|01\rangle \\ \langle 01|\delta V|10\rangle & \langle 01|\delta V|01\rangle \end{pmatrix} = \lambda \begin{pmatrix} \langle 10|XY|10\rangle & \langle 10|XY|01\rangle \\ \langle 01|XY|10\rangle & \langle 01|XY|01\rangle \end{pmatrix}$$

The best way to proceed now is to write X and Y in terms of the raising and lowering operators in order to evaluate the matrix elements. Recall from the lectures on the harmonic oscillator:

$$X = \sqrt{\frac{\hbar}{2m\omega}} \left(A_x + A_x^\dagger\right), \qquad Y = \sqrt{\frac{\hbar}{2m\omega}} \left(A_y + A_y^\dagger\right).$$

The first matrix element is thus:

$$\begin{aligned} \langle 10|XY|10\rangle &= \frac{\hbar}{2m\omega} \langle 10|(A_x + A_x^\dagger)(A_y + A_y^\dagger)|10\rangle \\ &= \frac{\hbar}{2m\omega} \langle 10|A_xA_y + A_xA_y^\dagger + A_x^\dagger A_y + A_x^\dagger A_y^\dagger|10\rangle \\ &= 0 \qquad \text{(acting to left with } A_y^\dagger\text{, and to right with } A_y\text{)}. \end{aligned}$$

By symmetry, we have $\langle 01|XY|01\rangle = 0$ also.

The off-diagonal matrix elements can be evaluated similarly:

$$\begin{aligned}
\langle 10|XY|01\rangle &= \frac{\hbar}{2m\omega}\langle 10|(A_x + A_x^\dagger)(A_y + A_y^\dagger)|01\rangle \\
&= \frac{\hbar}{2m\omega}\langle 10|A_xA_y + A_xA_y^\dagger + A_x^\dagger A_y + A_x^\dagger A_y^\dagger|01\rangle \\
&= \frac{\hbar}{2m\omega}\langle 10|10\rangle && (A_x^\dagger|0\rangle = |1\rangle, A_y|1\rangle = |0\rangle) \\
&= \frac{\hbar}{2m\omega} && (|10\rangle \text{ normalised})
\end{aligned}$$

By symmetry, we have $\langle 01|XY|10\rangle = \hbar/2m\omega$ also. Therefore the matrix of the perturbation in the relevant degenerate subspace is:

$$\frac{\hbar\lambda}{2m\omega}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}.$$

The eigenvalues of the matrix

$$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

obey the characteristic equation $\mu^2 - 1 = 0$, hence they are $\mu = \pm 1$. The associated eigenvectors are:

$$\begin{pmatrix}1\\ 1\end{pmatrix} \qquad \text{and} \qquad \begin{pmatrix}1\\ -1\end{pmatrix}.$$

Hence the eigenvalues of the perturbation in the relevant degenerate subspace are: $\pm\hbar\lambda/2m\omega$, with respective eigenstates

$$\frac{|10\rangle + |01\rangle}{\sqrt{2}} \qquad \text{and} \qquad \frac{|10\rangle - |01\rangle}{\sqrt{2}}.$$

The energy level $E_1 = 2\hbar\omega$ splits to the two energy levels:

$$2\hbar\omega \pm \frac{\hbar\lambda}{2m\omega}$$

under the perturbation. It follows that the initial twofold degeneracy is indeed lifted.

(iv) There are a couple of ways of doing this part, depending on whether you have done part (v) or not. We have:

- Method 1: Direct method. The most direct method is just to evaluate the matrix of the perturbation in a general degenerate subspace, then diagonalise it to check whether it has any repeated eigenvalues. In general, we want to evaluate matrix elements of the form:

  $$\langle n'm'|XY|nm\rangle\,.$$

  As before, we can evaluate these by writing X and Y in terms of raising and lowering operators. We have:

  $$\begin{aligned}
  \langle n'm'|XY|nm\rangle &= \frac{\hbar}{2m\omega}\langle n'|(A_x + A_x^\dagger)|n\rangle\,\langle m'|(A_y + A_y^\dagger)|m\rangle \\
  &= \frac{\hbar}{2m\omega}\left(\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}\right)\left(\sqrt{m}\delta_{m',m-1} + \sqrt{m+1}\delta_{m',m+1}\right).
  \end{aligned}$$

  In particular, we can arrange the matrix of the perturbation to be *symmetric* and *tridiagonal*, with zeroes along the diagonal. Furthermore, all the entries in the subleading and superleading diagonals of the matrix are clearly non-zero. We can thus invoke a mysterious result from linear algebra: *the eigenvalues of a symmetric tridiagonal matrix with non-zero entries in all of the subleading and superleading diagonal slots are all distinct.* It follows that all degeneracy is lifted.

- Method 2: Using exact solution, i.e. part (v). We know that the exact solution expanded to first order is:

$$E = \hbar\omega \left[(n_1 + n_2 + 1) + \frac{\lambda}{2m\omega^2} (n_1 - n_2) + O(\lambda^2) \right].$$

Therefore the degeneracy of the energy level $E = \hbar\omega (n_1 + n_2 + 1)$ is always lifted, since the pairs (n_1, n_2) that give a constant E always have distinct differences, e.g. $(n_1, n_2) = (3, 0), (2, 1), (1, 2), (0, 3)$ all have distinct differences $3, 1, -1, -3$. So the energy levels are all completely split and no degeneracy remains.

(v) $(*)$ To determine the radius of convergence of the perturbation series, we use a trick. We notice that in fact this 'perturbed' harmonic oscillator isn't really a perturbed oscillator at all - it's just an anisotropic harmonic oscillator, oscillating along different axes to the standard x, y axes. In particular, we can write the Hamiltonian as:

$$H = \frac{\mathbf{P}^2}{2m} + \frac{1}{2}m\omega^2 X^2 + \frac{1}{2}m\omega^2 Y^2 + \lambda XY$$

$$= \frac{\mathbf{P}^2}{2m} + \frac{1}{2}m\omega^2 \left(1 + \frac{\lambda}{m\omega^2}\right) \left(\frac{X+Y}{\sqrt{2}}\right)^2 + \frac{1}{2}m\omega^2 \left(1 - \frac{\lambda}{m\omega^2}\right) \left(\frac{X-Y}{\sqrt{2}}\right)^2.$$

It immediately follows that the energy levels of the 'perturbed' oscillator are given by:

$$E = \hbar\omega\sqrt{1 + \frac{\lambda}{m\omega^2}} \left(n_1 + \frac{1}{2}\right) + \hbar\omega\sqrt{1 - \frac{\lambda}{m\omega^2}} \left(n_2 + \frac{1}{2}\right),$$

where n_1, n_2 are non-negative integers. Expanding for $\lambda \ll 1$, the energy levels are:

$$E = \hbar\omega \left[(n_1 + n_2 + 1) + \frac{\lambda}{2m\omega^2} (n_1 - n_2) + O(\lambda^2) \right]$$

Choosing $n_1 = 1, n_2 = 0$ and $n_1 = 0, n_2 = 1$, we arrive at the 'split' energy levels we found in part (iii). In particular, we see that our perturbative expansion of the energy levels in λ will converge provided the expansion of the square roots

$$\sqrt{1 \pm \frac{\lambda}{m\omega^2}}$$

in λ converges. But by the binomial theorem, the disk on which the Taylor series of these square roots converges is:

$$\left|\frac{\lambda}{m\omega^2}\right| < 1 \qquad \Rightarrow \qquad |\lambda| < m\omega^2.$$

Hence the radius of convergence of the perturbation series in this question is $m\omega^2$.

Part II: Principles of Quantum Mechanics
Examples Sheet 4 Solutions

Please send all comments and corrections to jmm232@cam.ac.uk.

1. Suppose a system has a basis of just two orthonormal states $|1\rangle$ and $|2\rangle$, with respect to which the total Hamiltonian has the matrix representation

$$\begin{pmatrix} E_1 & V_0 e^{i\omega t} \\ V_0 e^{-i\omega t} & E_2 \end{pmatrix},$$

where V_0 is independent of time. At $t = 0$, the system is in state $|1\rangle$. Show that the probability of a transition from state $|1\rangle$ to state $|2\rangle$ in time interval t is

$$P(t) = \frac{4V_0^2}{(E_1 - E_2 + \hbar\omega)^2} \sin^2\left(\frac{(E_1 - E_2 + \hbar\omega)t}{2\hbar}\right) + O(V_0^3),$$

to lowest non-trivial order in V_0. Solve this two-state problem exactly to find the true value of $P(t)$ and hence state conditions necessary for the perturbative approach to be valid here.

Solution: In this question, we are expected to treat the V_0 parts of the Hamiltonian as a time-dependent perturbation, and hence we must use the results of time-dependent perturbation theory. Let's take this opportunity to recall the key points of the theory:

Time-dependent perturbation theory: The key feature of time-dependent perturbation theory is the introduction of a new quantum-mechanical picture: the *interaction picture*. Given a Hamiltonian $H = H_0 + \Delta(t)$, where $\Delta(t)$ is the time-dependent perturbation to the Hamiltonian H_0, we define the *interaction picture* states and operators by:

$$|\psi_I(t)\rangle = e^{iH_0 t/\hbar} |\psi_S(t)\rangle, \qquad \mathcal{O}_I(t) = e^{iH_0 t/\hbar} \mathcal{O}_S e^{-iH_0 t/\hbar},$$

where $|\psi_S(t)\rangle$ is a state in the Schrödinger picture and $\mathcal{O}_S$ is an operator in the Schrödinger picture.

The interesting thing about the interaction picture is that it separates out the time evolution due to the part of the Hamiltonian H_0 and the time evolution due to the part of the Hamiltonian $\Delta(t)$. We can see this by deriving some equations of motion:

$$i\hbar \frac{d|\psi_I(t)\rangle}{dt} = i\hbar \frac{d}{dt}\left(e^{iH_0 t/\hbar} |\psi_S(t)\rangle\right) = -e^{iH_0 t/\hbar} H_0 |\psi_S(t)\rangle + e^{iH_0 t/\hbar} H |\psi_S(t)\rangle$$

$$= -e^{iH_0 t/\hbar} H_0 e^{-iH_0 t/\hbar} |\psi_I(t)\rangle + e^{iH_0 t/\hbar} H e^{-iH_0 t/\hbar} |\psi_I(t)\rangle = \Delta_I(t) |\psi_I(t)\rangle$$

Note we use the Schrödinger equation in the second equality to evaluate $i\hbar d|\psi_S(t)\rangle/dt$. Similarly we have:

$$i\hbar \frac{d\mathcal{O}_I(t)}{dt} = i\hbar \frac{d}{dt}\left(e^{iH_0 t/\hbar} \mathcal{O}_S(t) e^{-iH_0 t/\hbar}\right) = [\mathcal{O}_I(t), H_0] + i\hbar e^{iH_0 t/\hbar} \frac{\partial \mathcal{O}_S(t)}{\partial t} e^{-iH_0 t/\hbar}.$$

We see that time-evolution of interaction picture states is governed by a Schrödinger equation involving the perturbed part of the Hamiltonian in the interaction picture, $\Delta_I(t)$, whilst time-evolution of interaction picture operators is governed by a modified version of the Heisenberg equation involving the unperturbed part of the Hamiltonian, H_0.

In general, to work out the state of the system at time t, our plan is to solve the interaction picture Schrödinger equation for the interaction picture state $|\psi_I(t)\rangle$, then transform back to the Schrödinger picture to find $|\psi_S(t)\rangle$.

Unfortunately, since $\Delta_I(t)$ is time-dependent, we cannot solve the equation

$$i\hbar\frac{d\,|\psi_I(t)\rangle}{dt} = \Delta_I(t)\,|\psi_I(t)\rangle \tag{$*$}$$

for $|\psi_I(t)\rangle$ using the standard exponential solution that we would use for the Schrödinger equation. However, there *is* a formal solution, which we can find as follows.

First, we recast the equation $(*)$ as an integral equation:

$$|\psi_I(t)\rangle = |\psi_I(t_0)\rangle - \frac{i}{\hbar}\int_{t_0}^{t} dt_1\,\Delta_I(t_1)\,|\psi_I(t_1)\rangle\,.$$

Now recursively substitute the expression for $|\psi_I(t)\rangle$ into itself:

$$|\psi_I(t)\rangle = |\psi_I(t_0)\rangle - \frac{i}{\hbar}\int_{t_0}^{t} dt\,\Delta_I(t_1)\,|\psi_I(t_0)\rangle + \left(-\frac{i}{\hbar}\right)^2\int_{t_0}^{t} dt_1\,\Delta_I(t_1)\int_{t_0}^{t_1} dt_2\,\Delta_I(t_2)\,|\psi_I(t_0)\rangle + \cdots$$

$$= \left(I - \frac{i}{\hbar}\int_{t_0}^{t} dt\,\Delta_I(t_1) + \left(-\frac{i}{\hbar}\right)^2\int_{t_0}^{t}\int_{t_0}^{t_1} dt_1\,dt_2\,\Delta_I(t_1)\Delta_I(t_2) + \cdots\right)|\psi_I(t_0)\rangle\,.$$

We have thus found a series solution to the equation. We notice that the series resembles the expansion of an exponential (albeit without any factorials), and hence we define the *time-ordered exponential*:

$$\mathrm{Texp}\left(-\frac{i}{\hbar}\Delta\right) = I - \frac{i}{\hbar}\int_{t_0}^{t} dt\,\Delta_I(t_1) + \left(-\frac{i}{\hbar}\right)^2\int_{t_0}^{t}\int_{t_0}^{t_1} dt_1\,dt_2\,\Delta_I(t_1)\Delta_I(t_2) + \cdots$$

so that we can write the solution to the equation $(*)$ as:

$$|\psi_I(t)\rangle = \mathrm{Texp}\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt'\,\Delta_I(t')\right)|\psi_I(t_0)\rangle\,,$$

in analogy with the formal solution to the regular Schrödinger equation, without a time-dependent Hamiltonian. This formula is called *Dyson's formula*.

It is now possible to transform back to the Schrödinger picture if required:

$$e^{iH_0t/\hbar}\,|\psi_S(t)\rangle = \mathrm{Texp}\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt'\,e^{iH_0t'/\hbar}\Delta(t')e^{-iH_0t'/\hbar}\right)e^{iH_0t_0/\hbar}\,|\psi_S(t_0)\rangle$$

$$\Rightarrow \qquad |\psi_S(t)\rangle = e^{-iH_0t/\hbar}\mathrm{Texp}\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt'\,e^{iH_0t'/\hbar}\Delta(t')e^{-iH_0t'/\hbar}\right)e^{iH_0t_0/\hbar}\,|\psi_S(t_0)\rangle\,,$$

from which we can compute interesting quantities and answer interesting questions.

Let's apply these results to the question we are interested in. We start in the initial state $|1\rangle$ at time $t = 0$, and the H_0 and $\Delta(t)$ are given by:

$$H_0 = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}, \qquad \Delta(t) = \begin{pmatrix} 0 & V_0 e^{i\omega t} \\ V_0 e^{-i\omega t} & 0 \end{pmatrix}.$$

Therefore, Dyson's formula tells us that after a time t we will be in the state $|\psi_S(t)\rangle =$

$$\begin{pmatrix} e^{-iE_1 t/\hbar} & 0 \\ 0 & e^{-iE_2 t/\hbar} \end{pmatrix} \mathrm{Texp}\left(-\frac{i}{\hbar}\int_0^t dt' \begin{pmatrix} e^{iE_1 t'/\hbar} & 0 \\ 0 & e^{iE_2 t'/\hbar} \end{pmatrix} \begin{pmatrix} 0 & V_0 e^{i\omega t'} \\ V_0 e^{-i\omega t'} & 0 \end{pmatrix} \begin{pmatrix} e^{-iE_1 t'/\hbar} & 0 \\ 0 & e^{-iE_2 t'/\hbar} \end{pmatrix} \right) \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$= \begin{pmatrix} e^{-iE_1 t/\hbar} & 0 \\ 0 & e^{-iE_2 t/\hbar} \end{pmatrix} \mathrm{Texp}\left(-\frac{i}{\hbar} V_0 \int_0^t dt' \begin{pmatrix} 0 & e^{i(E_1 - E_2 + \hbar\omega)t'/\hbar} \\ e^{i(E_2 - E_1 - \hbar\omega)t'/\hbar} & 0 \end{pmatrix} \right) \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Notice that we have written $|1\rangle$ in column vector notation, consistent with the matrix notation that we have used for the operators. Expanding the time-ordered exponential and keeping only the first two terms, we have:

$$|\psi_S(t)\rangle = \begin{pmatrix} e^{-iE_1 t/\hbar} & 0 \\ 0 & e^{-iE_2 t/\hbar} \end{pmatrix} \left(I - \frac{i}{\hbar} V_0 \int_0^t dt' \begin{pmatrix} 0 & e^{i(E_1 - E_2 + \hbar\omega)t'/\hbar} \\ e^{i(E_2 - E_1 - \hbar\omega)t'/\hbar} & 0 \end{pmatrix} + \cdots \right) \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$= \begin{pmatrix} e^{-iE_1 t/\hbar} & 0 \\ 0 & e^{-iE_2 t/\hbar} \end{pmatrix} \left(I - \frac{i}{\hbar} V_0 \begin{pmatrix} 0 & \frac{\hbar}{i} \cdot \frac{e^{i(E_1 - E_2 + \hbar\omega)t/\hbar} - 1}{E_1 - E_2 + \hbar\omega} \\ \frac{\hbar}{i} \cdot \frac{e^{i(E_2 - E_1 - \hbar\omega)t/\hbar} - 1}{E_2 - E_1 - \hbar\omega} & 0 \end{pmatrix} + \cdots \right) \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$= \begin{pmatrix} e^{-iE_1 t/\hbar} \\ 0 \end{pmatrix} - \frac{V_0 e^{-iE_2 t/\hbar}}{E_2 - E_1 - \hbar\omega} \begin{pmatrix} 0 \\ e^{i(E_2 - E_1 - \hbar\omega)t/\hbar} - 1 \end{pmatrix} + O(V_0^2).$$

It follows that

$$\langle 2|\psi_S(t)\rangle = -\frac{V_0 e^{-iE_1 t/\hbar}(e^{i(E_2 - E_1 - \hbar\omega)t/\hbar} - 1)}{E_2 - E_1 - \hbar\omega} + O(V_0^2),$$

and so the required probability is:

$$|\langle 2|\psi_S(t)\rangle|^2 = \frac{V_0^2}{(E_1 - E_2 + \hbar\omega)^2} \left(e^{i(E_2 - E_1 - \hbar\omega)t/\hbar} - 1 \right) \left(e^{-i(E_2 - E_1 - \hbar\omega)t/\hbar} - 1 \right) + O(V_0^3)$$

$$= \frac{V_0^2}{(E_1 - E_2 + \hbar\omega)^2} \left(2 - 2\cos\left(\frac{(E_1 - E_2 + \hbar\omega)t}{\hbar} \right) \right) + O(V_0^3)$$

$$= \frac{4V_0^2}{(E_1 - E_2 + \hbar\omega)^2} \sin^2\left(\frac{(E_1 - E_2 + \hbar\omega)t}{2\hbar} \right) + O(V_0^3),$$

as was to be shown.

We are now asked to solve the system exactly, and hence compare the exact probability with the perturbative result. Let's write the state of the system at a general time t as:

$$|\psi_S(t)\rangle = a_1(t)\,|1\rangle + a_2(t)\,|2\rangle = \begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix},$$

where $a_1(t)$, $a_2(t)$ are the time-dependent coefficients of $|1\rangle$, $|2\rangle$. We are interested in the probability of measuring the system to be in the state $|2\rangle$ at time t; this probability is given in terms of the $a_i(t)$ as $P(t) = |a_2(t)|^2$.

Since $|\psi_S(t)\rangle$ obeys the Schrödinger equation, we have:

$$i\hbar \frac{d}{dt}\begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix} = H\begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix} = \begin{pmatrix} E_1 & V_0 e^{i\omega t} \\ V_0 e^{-i\omega t} & E_2 \end{pmatrix}\begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix}.$$

Reading off the two rows of this matrix equation, we see that we have a coupled system of first-order ODEs:

$$i\hbar \dot{a}_1(t) = E_1 a_1(t) + V_0 e^{i\omega t} a_2(t) \tag{1}$$

$$i\hbar \dot{a}_2(t) = V_0 e^{-i\omega t} a_1(t) + E_2 a_2(t). \tag{2}$$

Since $|\psi_S(0)\rangle = |1\rangle$, we also have the initial conditions $a_1(0) = 1, a_2(0) = 0$. It remains to use this system of ODEs to determine $a_2(t)$.

Let's eliminate $a_1(t)$ from these equations. First, differentiate equation (2) to get:

$$i\hbar \ddot{a}_2(t) = E_2 \dot{a}_2(t) - i\omega V_0 e^{-i\omega t} a_1(t) + V_0 e^{-i\omega t}\dot{a}_1(t).$$

Now eliminate $\dot{a}_1(t)$ from this equation using equation (1):

$$\begin{aligned} i\hbar \ddot{a}_2(t) &= E_2 \dot{a}_2(t) - i\omega V_0 e^{-i\omega t} a_1(t) + \frac{V_0 e^{-i\omega t}}{i\hbar}\left(V_0 e^{i\omega t} a_2(t) + E_1 a_1(t)\right) \\ &= E_2 \dot{a}_2(t) - \frac{iV_0^2}{\hbar} a_2(t) - \left(i\omega V_0 e^{-i\omega t} + \frac{iE_1 V_0 e^{-i\omega t}}{\hbar}\right) a_1(t). \end{aligned}$$

Finally, eliminate $a_1(t)$ from this equation using equation (2):

$$\begin{aligned} i\hbar \ddot{a}_2(t) &= E_2 \dot{a}_2(t) - \frac{iV_0^2}{\hbar} a_2(t) + \left(\frac{E_1}{\hbar} + \omega\right)\left(\hbar \dot{a}_2(t) + iE_2 a_2(t)\right) \\ &= (E_1 + E_2 + \hbar\omega)\dot{a}_2(t) + \left(\frac{iE_1E_2}{\hbar} + i\omega E_2 - \frac{iV_0^2}{\hbar}\right) a_2(t). \end{aligned}$$

This is a second-order ODE for $a_2(t)$ with constant coefficients. The auxiliary equation of this ODE is:

$$i\hbar\lambda^2 - (E_1 + E_2 + \hbar\omega)\lambda + \left(\frac{iV_0^2}{\hbar} - i\omega E_2 - \frac{iE_1E_2}{\hbar}\right) = 0,$$

which has the solutions:

$$\begin{aligned} \lambda_\pm &= \frac{E_1 + E_2 + \hbar\omega \pm \sqrt{(E_1 + E_2 + \hbar\omega)^2 + 4\left(V_0^2 - \hbar\omega E_2 - E_1E_2\right)}}{2i\hbar} \\ &= \frac{E_1 + E_2 + \hbar\omega \pm \sqrt{(E_1 - E_2 + \hbar\omega)^2 + 4V_0^2}}{2i\hbar} \end{aligned}$$

We can now quote the solution of the ODE, which is:

$$a_2(t) = Ae^{\lambda_- t} + Be^{\lambda_+ t},$$

where A and B are time-independent complex constants. To fix the constants, recall the initial conditions. We have $a_2(0) = 0$, which gives $A + B = 0$, i.e. $B = -A$.

Since $a_1(0) = 1$, we can use equation (2) to determine that $\dot{a}_2(0) = -iV_0/\hbar$. It follows that

$$A\lambda_- + B\lambda_+ = -\frac{iV_0}{\hbar} \qquad \Rightarrow \qquad A = -\frac{iV_0}{\hbar(\lambda_- - \lambda_+)} = \frac{V_0}{\sqrt{(E_1 - E_2 + \hbar\omega)^2 + 4V_0^2}}.$$

Therefore:

$$a_2(t) = \frac{V_0}{\sqrt{(E_1 - E_2 + \hbar\omega)^2 + 4V_0^2}} \left(e^{\lambda_- t} - e^{\lambda_+ t}\right).$$

The quantity we are interested in is $P(t) = |a_2(t)|^2$, which is given by:

$$P(t) = |a_2(t)|^2 = \frac{V_0^2}{(E_1 - E_2 + \hbar\omega)^2 + 4V_0^2} \left(e^{\lambda_- t} - e^{\lambda_+ t}\right)\left(e^{-\lambda_- t} - e^{-\lambda_+ t}\right)$$

since both λ_- and λ_+ are pure imaginary, and so $\lambda_\pm^* = -\lambda_\pm$. Multiplying everything out, we find:

$$P(t) = \frac{V_0^2}{(E_1 - E_2 + \hbar\omega)^2 + 4V_0^2} \left(2 - e^{(\lambda_- - \lambda_+)t} - e^{-(\lambda_- - \lambda_+)t}\right)$$

$$= \frac{2V_0^2}{(E_1 - E_2 + \hbar\omega)^2 + 4V_0^2} \left(1 - \cos\left(\frac{\lambda_- - \lambda_+}{i}\right)\right)$$

$$= \frac{4V_0^2}{(E_1 - E_2 + \hbar\omega)^2 + 4V_0^2} \sin^2\left(\frac{t\sqrt{(E_1 - E_2 + \hbar\omega)^2 + 4V_0^2}}{2\hbar}\right).$$

We can compare this to the perturbative result by expanding in V_0. We can expand $((E_1 - E_2 + \hbar\omega)^2 + 4V_0^2)^{-1}$ using the binomial theorem; similarly we can expand $\sqrt{(E_1 - E_2 + \hbar\omega)^2 + 4V_0^2}$ using the binomial theorem. We can then expand $\sin^2(...)$ using a Taylor series, which is everywhere convergent. Notice that this approach exactly reproduces the work from above.

Therefore, we see that the only thing that could stop a series expansion in V_0 from converging are the binomial expansions, which have radius of convergence:

$$\frac{4V_0^2}{(E_1 - E_2 + \hbar\omega)^2} < 1.$$

2. A particle of mass m and charge e is contained within a cubical box of side a. Initially the particle is in the stationary state of energy $3\pi^2\hbar^2/2ma^2$. At time $t = 0$, a uniform electric field of strength E is switched on parallel to one of the edges of the cube. Obtain an expression to second order in e for the probability of measuring the particle to have energy $3\pi^2\hbar^2/ma^2$ at time t.

Solution: Let's describe the box as

$$B = \{0 \leq x \leq a, 0 \leq y \leq a, 0 \leq z \leq a\}.$$

The potential of the system is then:

$$V(\mathbf{x}) = \begin{cases} 0 & \text{for } \mathbf{x} \in B, \\ \infty & \text{for } \mathbf{x} \notin B. \end{cases}$$

Suppose the applied electric field is in the z direction, so that $\mathbf{E}(t) = (0, 0, EH(t))$, where $H(t)$ is the Heaviside step function (recall the electric field is turned on at time $t = 0$, and is of strength E). An electric potential for this electric field is such that $\mathbf{E}(t) = -\nabla\phi(\mathbf{x}, t)$, and hence we can choose

$$\phi(\mathbf{x}, t) = -EzH(t).$$

Therefore, the energy of the particle due to the electric field is $-eEzH(t)$.

It follows that the Hamiltonian of the system is:

$$H = \frac{\mathbf{P}^2}{2m} + V(\mathbf{X}) - eEZH(t).$$

We treat $eEZH(t)$ as a time-dependent perturbation, hence we write the Hamiltonian as

$$H = H_0 + \Delta(t), \qquad \text{with } H_0 = \frac{\mathbf{P}^2}{2m} + V(\mathbf{X}), \qquad \Delta(t) = -eEZH(t).$$

We are given that the system starts at time $t = 0$ in the energy eigenstate of H_0 of energy $3\pi^2\hbar^2/2ma^2$, so it makes sense to start by finding the energy eigenstates of H_0, a simple 'particle in a box', and their respective eigenvalues.

The position wavefunction of a particle in a box must be zero outside of the box, since there is infinite potential outside and we cannot have a particle of infinite energy. Inside the box, an energy eigenstate must obey the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{x})\psi = E\psi, \qquad \text{with boundary conditions} \qquad \psi(\pm a/2, \mathbf{y}, \mathbf{z}) = \psi(\mathbf{x}, \pm a/2, \mathbf{z}) = \psi(\mathbf{x}, \mathbf{y}, \pm a/2) = 0.$$

We can use separation of variables to write the wavefunction in the form $\psi(\mathbf{x}) = \psi_x(x)\psi_y(y)\psi_z(z)$. Then each ψ_i satisfies an equation of the form:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_i}{\partial x_i^2} + V(\mathbf{x})\psi_i = E_i\psi_i,$$

where $E_x + E_y + E_z = E$ is a constant. Inside the box, this simplifies to:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_i}{\partial x_i^2} = E_i\psi_i \qquad \Rightarrow \qquad \psi_i(x_i) = A_i \sin\left(\sqrt{\frac{2mE_i}{\hbar^2}}x_i\right) + B_i \cos\left(\sqrt{\frac{2mE_i}{\hbar^2}}x_i\right),$$

where A_i and B_i are constants. Now use the boundary conditions $\psi_i(0) = 0, \psi_i(a) = 0$. Then it follows that $B_i = 0$, and E_i is quantised as follows:

$$\psi_{in}(x_i) = A_{in} \sin\left(\frac{n\pi x_i}{a}\right), \qquad E_{in} = \hbar^2 n^2 \pi^2 / 2ma^2.$$

It follows that a basis of energy eigenstates for the system is:

$$\psi_{n_x n_y n_z}(\mathbf{x}) = A_{xyz} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{a}\right) \sin\left(\frac{n_z \pi z}{a}\right),$$

where $\psi_{n_z n_y n_z}$ has energy

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2ma^2} \left(n_x^2 + n_y^2 + n_z^2\right),$$

and A_{xyz} is a normalisation constant. This normalisation constant obeys:

$$|A_{xyz}|^2 \int_0^a dx \int_0^a dy \int_0^a dz \, \sin^2\left(\frac{n_x \pi x}{a}\right) \sin^2\left(\frac{n_y \pi y}{a}\right) \sin^2\left(\frac{n_z \pi z}{a}\right) = 1.$$

Since

$$\int_0^a dx_i \, \sin^2\left(\frac{n_i \pi x_i}{a}\right) = \frac{a}{2},$$

It follows that the normalisation constant can be chosen to be

$$A_{xyz} = \sqrt{\frac{8}{a^3}}.$$

Thus the basis of energy eigenstates is:

$$\psi_{n_x n_y n_z}(\mathbf{x}) = \sqrt{\frac{8}{a^3}} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{a}\right) \sin\left(\frac{n_z \pi z}{a}\right).$$

We write the state with position space wavefunction $\psi_{n_x n_y n_z}$ as $|n_x n_y n_z\rangle$.

Now we know the energy eigenstates of the free Hamiltonian, let's think about what the question wants us to calculate. Initially, the particle is in a state of energy $3\pi^2\hbar^2/2ma^2$. There is only one such state: $|111\rangle$, hence we must initially be in this state.

We want to calculate the probability that we are in a state of energy $3\pi^2\hbar^2/ma^2$ at time $t > 0$. At time $t = 0$, it's clear that the only states that have energy $3\pi^2\hbar^2/ma^2$ are $|112\rangle$, $|121\rangle$ and $|211\rangle$. However we must be very careful - at time $t > 0$, these states are no longer eigenstates because of the presence of the perturbation. Hence they are *not* states of energy $3\pi^2\hbar^2/ma^2$!

So what can we do? It initially looks like we have to solve the full perturbed system exactly to work out the energy eigenstates. However, it turns out this is not really necessary - we can instead show that the states $|112\rangle$, $|121\rangle$ and $|211\rangle$ are good approximations to the states which have energy $3\pi^2\hbar^2/ma^2$ at time $t > 0$.

Lemma: The states of the perturbed system with energy $3\pi^2\hbar^2/ma^2$ at time $t > 0$ are of the form $|112\rangle + |\phi_{112}\rangle$, $|121\rangle + |\phi_{121}\rangle$ and $|211\rangle + |\phi_{211}\rangle$, where the states $|\phi_{112}\rangle$, $|\phi_{121}\rangle$ and $|\phi_{211}\rangle$ have wavefunctions of order $O(e)$.

Proof: Let $|E\rangle$ be an energy eigenstate of the unperturbed Hamiltonian H_0 with energy $3\pi^2\hbar^2/ma^2$, i.e. one of $|112\rangle$, $|121\rangle$ and $|211\rangle$. Let $|E\rangle + |\phi(t)\rangle$ be an energy eigenstates of the full Hamiltonian $H_0 + \Delta(t)$ with energy $3\pi^2\hbar^2/ma^2$. Then we must have:

$$(H_0 + \Delta(t))(|E\rangle + |\phi(t)\rangle) = \frac{3\pi^2\hbar^2}{ma^2}(|E\rangle + |\phi(t)\rangle).$$

Acting with H_0 on $|E\rangle$, we find:

$$\frac{3\pi^2\hbar^2}{ma^2}|E\rangle + H_0|\phi(t)\rangle + \Delta(t)|E\rangle + \Delta(t)|\phi(t)\rangle = \frac{3\pi^2\hbar^2}{ma^2}|E\rangle + \frac{3\pi^2\hbar^2}{ma^2}|\phi(t)\rangle .$$

Cancelling the $|E\rangle$ term on both sides, we're left with:

$$H_0|\phi(t)\rangle + \Delta(t)|E\rangle + \Delta(t)|\phi(t)\rangle = \frac{3\pi^2\hbar^2}{ma^2}|\phi(t)\rangle . \qquad (*)$$

Recall that $H_0 = O(e^0)$, since it contains no e dependence. We also have $\Delta(t) = O(e)$. We now ask: what is the order of $|\phi(t)\rangle$ in e?

Suppose that $|\phi(t)\rangle = O(e^0)$, i.e. $|\phi(t)\rangle$ contains a constant, e-independent term in its perturbative expansion in e. Then comparing terms of order e^0 in $(*)$, we have:

$$H_0|\phi(t)\rangle = \frac{3\pi^2\hbar^2}{ma^2}|\phi(t)\rangle .$$

That is, $|\phi(t)\rangle$ is an energy eigenstate of the non-perturbed Hamiltonian of energy $3\pi^2\hbar^2/ma^2$. But then we would have:

$$(H_0 + \Delta(t))(|E\rangle + |\phi(t)\rangle) = \frac{3\pi^2\hbar^2}{ma^2}(|E\rangle + |\phi(t)\rangle) \qquad \Rightarrow \qquad \Delta(t)(|E\rangle + |\phi(t)\rangle)) = 0,$$

and looking at the position representation of $\Delta(t)$, we see that this equation can only hold if $|E\rangle + |\phi(t)\rangle = 0$; this is a contradiction, since the state was supposed to have energy $3\pi^2\hbar^2/ma^2$.

Thus we must have $|\phi(t)\rangle = O(e^1)$ at least. □

Let's apply this to the question. Dyson's formula gives the state of the system at time $t > 0$ as:

$$|\psi_S(t)\rangle = e^{-iH_0t/\hbar}\mathrm{Texp}\left(-\frac{i}{\hbar}\int_0^t dt'\, e^{iH_0t'/\hbar}\Delta(t')e^{-iH_0t'/\hbar}\right)|111\rangle .$$

Expanding the time-ordered exponential to first order in e, we have:

$$|\psi_S(t)\rangle = e^{-iH_0t/\hbar}\left(I - \frac{i}{\hbar}\int_0^t dt'\, e^{iH_0t'/\hbar}\Delta(t')e^{-iH_0t'/\hbar} + O(e^2)\right)|111\rangle .$$

We want to find the probability that the system is in on of the states $|112\rangle + |\phi_{112}\rangle$, $|121\rangle + |\phi_{121}\rangle$ or $|211\rangle + |\phi_{211}\rangle$ at time t. We can find this by taking the inner product with $|\psi_S(t)\rangle$; let $|E\rangle$ denote one of $|112\rangle$, $|121\rangle$ and $|211\rangle$ and let $|\phi\rangle$ denote the respective state $|\phi_{\dots}\rangle$. Then:

$$(\langle E| + \langle\phi|)|\psi_S(t)\rangle = (\langle E| + \langle\phi|)\, e^{-iH_0t/\hbar}\left(I - \frac{i}{\hbar}\int_{t_0}^t dt'\, e^{iH_0t'/\hbar}\Delta(t')e^{-iH_0t'/\hbar} + O(e^2)\right)|111\rangle$$

$$= \underbrace{\langle E|e^{-iH_0t/\hbar}|111\rangle}_{O(e^0)} + \underbrace{\langle\phi|e^{-iH_0t/\hbar}|111\rangle - \frac{i}{\hbar}\int_{t_0}^t dt'\ \langle E|e^{iH_0t'/\hbar}\Delta(t')e^{-iH_0t'/\hbar}|111\rangle}_{O(e^1)} + O(e^2).$$

Acting with the exponentials of the H_0's appropriately, and noting that $\langle E|111\rangle = 0$ since the unperturbed energy eigenstates are orthogonal, we can simplify this to:

$$(\langle E| + \langle \phi|)\,|\psi_S(t)\rangle = e^{-iE_{111}t/\hbar}\,\langle \phi|111\rangle - \frac{i}{\hbar}\int_0^t dt'\, e^{i(E-E_{111})t'/\hbar}\,\langle E|\Delta(t')|111\rangle + O(e^2).$$

So we get the normal first order formula for time-dependent perturbation theory, plus a correction $e^{-iE_{111}t/\hbar}\,\langle\phi|111\rangle$ from the fact that our free states are no longer energy eigenstates of the system. We must compute $\langle\phi|111\rangle$ to establish this correction term. We have:

Lemma: The correction $\langle\phi|111\rangle$ is given by:

$$\langle\phi|111\rangle = \frac{2ma^2}{3\pi^2\hbar^2}\,\langle E|\Delta(t)|111\rangle\,.$$

Proof: Recall that $|E\rangle + |\phi\rangle$ obeys:

$$(H_0 + \Delta(t))(\langle E\rangle + \langle\phi\rangle) = \frac{3\pi^2\hbar^2}{ma^2}(\langle E\rangle + \langle\phi\rangle)$$

which, by comparing terms of order $O(e^1)$, can be reduced to:

$$H_0\,\langle\phi\rangle + \Delta(t)\,\langle E\rangle = \frac{3\pi^2\hbar^2}{ma^2}\,\langle\phi\rangle\,.$$

Take the inner product with $|111\rangle$. Then we have:

$$\langle 111|H_0|\phi\rangle + \langle 111|\Delta(t)|E\rangle = \frac{3\pi^2\hbar^2}{ma^2}\,\langle 111|\phi\rangle\,.$$

Acting on $\langle 111|$ to the left with H_0 gives:

$$\frac{3\pi^2\hbar^2}{2ma^2}\,\langle 111|\phi\rangle + \langle 111|\Delta(t)|E\rangle = \frac{3\pi^2\hbar^2}{ma^2}\,\langle 111|\phi\rangle\,,$$

which we can rearrange to:

$$\langle 111|\phi\rangle = \frac{2ma^2}{3\pi^2\hbar^2}\,\langle 111|\Delta(t)|E\rangle\,.$$

Taking the complex conjugate gives the result. □

Hence we have the final result:

$$(\langle E| + \langle \phi|)\,|\psi_S(t)\rangle = \frac{2ma^2e^{-iE_{111}t/\hbar}}{3\pi^2\hbar^2}\,\langle E|\Delta(t)|111\rangle - \frac{i}{\hbar}\int_0^t dt'\, e^{i(E-E_{111})t'/\hbar}\,\langle E|\Delta(t')|111\rangle + O(e^2).$$

To simplify further, we need to compute the matrix element $\langle E|\Delta(t)|111\rangle$. Recalling that $\Delta(t) = -eEZH(t)$ (where E is the strength of the applied electric field - careful not to confuse it with $|E\rangle$!) we have

$$\langle E|\Delta(t)|111\rangle = -eEH(t)\,\langle E|Z|111\rangle\,.$$

Now we just compute $\langle E|Z|111\rangle$ for each possible $|E\rangle$:

- For $|E\rangle = |112\rangle$, we have:

$$\langle 112|Z|111\rangle = \frac{8}{a^3}\int_0^a dx\int_0^a dy\int_0^a dz\,z\,\sin^2\left(\frac{\pi x}{a}\right)\sin^2\left(\frac{\pi y}{a}\right)z\sin\left(\frac{2\pi z}{a}\right)\sin\left(\frac{\pi z}{a}\right)$$

$$= \frac{2}{a}\int_0^a dz\,z\sin\left(\frac{2\pi z}{a}\right)\sin\left(\frac{\pi z}{a}\right).$$

  Now using the identity $\sin(A)\sin(B) = \frac{1}{2}\left(\cos(A-B) - \cos(A+B)\right)$, we can simplify this integral to:

$$\langle 112|Z|111\rangle = \frac{1}{a}\int_0^a dz\,z\left(\cos\left(\frac{\pi z}{a}\right) - \cos\left(\frac{3\pi z}{a}\right)\right),$$

  which can be evaluated using integration by parts to give:

$$\langle 112|Z|111\rangle = -\frac{16a}{9\pi^2}.$$

- For $|E\rangle = |121\rangle$ and $|E\rangle = |211\rangle$, we immediately get zero for the matrix element, since the integral is over orthogonal sines.

Hence we see that the required amplitude is just:

$$\left(\langle 112| + \langle\phi_{112}|\right)|\psi_S(t)\rangle = \frac{32ma^3eEe^{-iE_{111}t/\hbar}}{27\pi^4\hbar^2} - \frac{16aeEi}{9\pi^2\hbar}\int_0^t dt'\,e^{i(E-E_{111})t'/\hbar} + O(e^2)$$

$$= \frac{16aeE}{9\pi^2}\left(\frac{2ma^2}{3\pi^2\hbar^2}e^{-iE_{111}t/\hbar} - \frac{e^{i(E-E_{111})t/\hbar}-1}{E-E_{111}}\right) + O(e^2)$$

Recall that $E_{111} = 3\pi^2\hbar^2/2ma^2$, and $E = 3\pi^2\hbar^2/ma^2$, and hence we have:

$$E - E_{111} = \frac{3\pi^2\hbar^2}{2ma^2} = E_{111} \qquad \Rightarrow \qquad \frac{1}{E-E_{111}} = \frac{2ma^2}{3\pi^2\hbar^2}.$$

Hence we see that the required amplitude is just:

$$\begin{aligned}\left(\langle 112| + \langle\phi_{112}|\right)|\psi_S(t)\rangle &= \frac{32ma^3eE}{27\pi^4\hbar^2}\left(1 + e^{-iE_{111}t/\hbar} - e^{iE_{111}t/\hbar}\right) + O(e^2)\\ &= \frac{32ma^3eE}{27\pi^4\hbar^2}\left(1 - 2i\sin\left(\frac{E_{111}t}{\hbar}\right)\right) + O(e^2)\end{aligned}$$

The required probability, given by the modulus squared of the amplitude, is therefore:

$$P(t) = \frac{1024m^2a^6e^2E^2}{729\pi^8\hbar^4}\left(1 + 4\sin^2\left(\frac{3\pi^2\hbar t}{2ma^2}\right)\right) + O(e^3).$$

3. A harmonic oscillator of angular frequency ω is acted on by the time-dependent perturbation

$$\frac{q\mathcal{E}X}{\sqrt{\pi}\tau}\exp\left(-\frac{t^2}{\tau^2}\right)$$

for all t, where X is the position operator and $q, \mathcal{E}$ and τ are constants. Show that in first-order perturbation theory, the only allowed transition from the ground state is to the first excited state. If the perturbation acts from very early times to very late times, find the probability that this transition takes place, correct to order $\mathcal{E}^2$.

By expanding $U_I(t)$ to *second* non-trivial order, calculate the corresponding probability for a transition from the ground state to the second excited state.

Solution: We want to compute the probability of a transition from the ground state $|0\rangle$ at time $t = t_1$ say, to any other state at time $t = t_2$. By Dyson's formula, we know that if we start in the ground state at $|0\rangle$ at time $t = t_1$, at time $t = t_2$ we will be in the state:

$$|\psi_S(t_2)\rangle = e^{-iH_0t_2/\hbar}\mathrm{Texp}\left(-\frac{i}{\hbar}\int_{t_1}^{t_2}dt'\,e^{iH_0t'/\hbar}\frac{q\mathcal{E}X}{\sqrt{\pi}\tau}\exp\left(-\frac{t'^2}{\tau^2}\right)e^{-iH_0t'/\hbar}\right)e^{iH_0t_1/\hbar}\,|0\rangle\,,$$

where H_0 is the Hamiltonian of the unperturbed oscillator. Expanding the time-ordered exponential, we have:

$$|\psi_S(t_2)\rangle = e^{-iH_0(t_2-t_1)/\hbar}\,|0\rangle - \frac{i}{\hbar}\frac{q\mathcal{E}e^{-iH_0t_2/\hbar}}{\sqrt{\pi}\tau}\int_{t_1}^{t_2}dt'\,\exp\left(-\frac{t'^2}{\tau^2}\right)e^{iH_0t'/\hbar}Xe^{-iH_0t'/\hbar}e^{iH_0t_1/\hbar}\,|0\rangle + O(\mathcal{E}^2)$$

We want the probability that we will be in the excited state $|n\rangle$ at time $t = t_2$. Hence we take the inner product of the above equation with the state $|n\rangle$ to get:

$$\langle n|\psi_S(t_2)\rangle = \langle n|\,e^{-iH_0(t_2-t_1)/\hbar}\,|0\rangle - \frac{i}{\hbar}\frac{q\mathcal{E}}{\sqrt{\pi}\tau}\int_{t_1}^{t_2}dt'\,\exp\left(-\frac{t'^2}{\tau^2}\right)\langle n|\,e^{-iH_0t_2/\hbar}e^{iH_0t'/\hbar}Xe^{-iH_0t'/\hbar}e^{iH_0t_1/\hbar}\,|0\rangle + O(\mathcal{E}^2)$$

We first evaluate the matrix elements. The matrix element involved in the zeroth order contribution can be evaluated by acting with the exponential on $|0\rangle$:

$$\langle n|e^{-iH_0(t_2-t_1)/\hbar}|0\rangle = e^{-i(t_2-t_1)\omega/2}\,\langle n|0\rangle = e^{-i(t_2-t_1)\omega/2}\delta_{n0}.$$

The matrix element involved in the integral can be evaluated by first acting to the left and right, as appropriate, with the exponentials leaving:

$$\langle n|\,e^{-iH_0t_2/\hbar}e^{iH_0t'/\hbar}Xe^{-iH_0t'/\hbar}e^{iH_0t_1/\hbar}\,|0\rangle = e^{-i(n+1/2)t_2\omega}e^{int'\omega}e^{it_1\omega/2}\,\langle n|X|0\rangle\,.$$

To evaluate $\langle n|X|0\rangle$, we expand X into raising and lowering operators. We have:

$$\langle n|X|0\rangle = \sqrt{\frac{\hbar}{2m\omega}}\,\langle n|(A+A^\dagger)|0\rangle = \sqrt{\frac{\hbar}{2m\omega}}\,\langle n|1\rangle = \sqrt{\frac{\hbar}{2m\omega}}\delta_{n1}.$$

Hence we see that:

$$\langle n|\psi_S(t_2)\rangle = e^{-i(t_2-t_1)\omega/2}\delta_{n0} - \frac{i}{\hbar}e^{-i(n+1/2)t_2\omega}e^{it_1\omega/2}\frac{q\mathcal{E}}{\sqrt{\pi}\tau}\sqrt{\frac{\hbar}{2m\omega}}\int_{t_1}^{t_2}dt'\,e^{int'\omega}\exp\left(-\frac{t'^2}{\tau^2}\right)\delta_{n1} + O(\mathcal{E}^2).$$

Thus, at first order, we find that only $\langle 0|\psi_S\rangle$ and $\langle 1|\psi_S\rangle$ are non-vanishing. Since a transition from the ground state to the ground state is not much of a transition, we indeed see that the only allowed transition is to the first excited state.

We should interpret the phrases 'very early' and 'very late' times as instructing us to set $t_1 = -\infty$ and $t_2 = \infty$. However, this will result in divergence exponentials if we take this limit straight away. So let's evaluate everything with arbitrary t_1, t_2 and then take the correct limit towards the end of the calculation.

The amplitude for the transition to the first excited state is:

$$\langle 1|\psi_S(t_2)\rangle = -\frac{i}{\hbar}e^{-3it_2\omega/2}e^{it_1\omega/2}\frac{q\mathcal{E}}{\sqrt{\pi}\tau}\sqrt{\frac{\hbar}{2m\omega}}\int_{t_1}^{t_2} dt'\, e^{it'\omega}\exp\left(-\frac{t'^2}{\tau^2}\right) + O(\mathcal{E}^2).$$

The relevant integral we need to evaluate is:

$$\int_{t_1}^{t_2} dt'\, e^{it'\omega}\exp\left(-\frac{t'^2}{\tau^2}\right) = e^{-\frac{1}{4}\omega^2\tau^2}\int_{t_1}^{t_2} dt'\, \exp\left(-\frac{(t-\frac{1}{2}i\omega\tau^2)^2}{\tau^2}\right).$$

In the limit $t_1 \to -\infty$ and $t_2 \to \infty$, this integral becomes a complex Gaussian integral. This can't really be evaluated using real techniques (though some may say you can just substitute $u = t - \frac{1}{2}i\omega\tau$, this is in fact incorrect), but *can* be computed using contour integration. However, we reserve this calculation for courses such as Part II Asymptotic Methods and Part II Further Complex Methods.

After completing the calculation, we find that the integral we need is:

$$e^{-\frac{1}{4}\omega^2\tau^2}\int_{-\infty}^{\infty} dt'\, \exp\left(-\frac{(t'-\frac{1}{2}i\omega\tau^2)^2}{\tau^2}\right) = \tau\sqrt{\pi}e^{-\frac{1}{4}\omega^2\tau^2}.$$

The probability of this transition is therefore:

$$|\langle 1|\psi_S(t_2)\rangle|^2 = \frac{q^2\mathcal{E}^2}{2\hbar m\omega\pi\tau^2}\left(\tau\sqrt{\pi}e^{-\frac{1}{4}\omega^2\tau^2}\right)^2 + O(\mathcal{E}^3)$$

$$= \frac{q^2\mathcal{E}^2}{2\hbar m\omega}e^{-\frac{1}{2}\omega^2\tau^2} + O(\mathcal{E}^3).$$

We are now asked to do something a lot more difficult: evaluate the leading order probability for transition from the ground state to the second excited state. We know that the zeroth order and first order terms in the Dyson expansion do not contribute; therefore we must evaluate the second order term - this, as it turns out, is very difficult.

Recalling the definition of the time-ordered exponential in the general theory of time-dependent perturbation theory, we can immediately write down the second order term in the Dyson expansion for $|\psi_S(t_2)\rangle$:

$$\langle 2|\psi_S(t_2)\rangle = -\langle 2|\, e^{-iH_0t_2/\hbar}\frac{q^2\mathcal{E}^2}{\pi\hbar^2\tau^2}\int_{t_1}^{t_2} dt'\int_{t_1}^{t'} dt''\, \exp\left(-\frac{t'^2}{\tau^2}-\frac{t''^2}{\tau^2}\right)e^{iH_0t'/\hbar}Xe^{-iH_0t'/\hbar}e^{iH_0t''/\hbar}Xe^{-iH_0t''/\hbar}e^{iH_0t_1/\hbar}\,|0\rangle$$
$$+ O(\mathcal{E}^3)$$

Acting to the left on the states with the exponentials, we can simplify some things. We can throw away any overall phases (i.e. ones we are not integrating over), because they will just get squared away when we take the modulus to find the probability. The result is that we have (up to a phase) the simplified expression:

$$\langle 2|\psi_S(t_2)\rangle = \frac{q^2\mathcal{E}^2}{\pi\hbar^2\tau^2}\int_{t_1}^{t_2} dt'\int_{t_1}^{t'} dt''\, e^{5i\omega t'/2}\exp\left(-\frac{t'^2}{\tau^2}-\frac{t''^2}{\tau^2}\right)\langle 2|\, Xe^{-iH_0t'/\hbar}e^{iH_0t''/\hbar}X\,|0\rangle\, e^{-i\omega t''/2} + O(\mathcal{E}^3)$$

To further simplify things, we need to evaluate the matrix element:

$$\langle 2|\, X e^{-iH_0 t'/\hbar} e^{iH_0 t''/\hbar} X\, |0\rangle\,.$$

To do so, it's convenient to eliminate the time-evolution operators in the middle by inserting a complete set of states:

$$\langle 2|X e^{-iH_0 t'/\hbar} e^{iH_0 t''/\hbar} X|0\rangle = \sum_{n=0}^{\infty} \langle 2|\, X e^{-iH_0 t'/\hbar}\, |n\rangle\, \langle n|\, e^{iH_0 t''/\hbar} X\, |0\rangle\,.$$

Operating on the states $|n\rangle$ and $\langle n|$ using the exponentials, we're left with:

$$\sum_{n=0}^{\infty} e^{-i(n+1/2)\omega t'} e^{i(n+1/2)\omega t''}\, \langle 2|\, X\, |n\rangle\, \langle n|\, X\, |0\rangle\,.$$

These look like tractable matrix elements! We have:

$$\langle n|X|0| = \sqrt{\frac{\hbar}{2m\omega}}\, \langle n|A + A^\dagger|0\rangle = \sqrt{\frac{\hbar}{2m\omega}}\delta_{n1}, \qquad \langle 2|X|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\, \langle 2|A + A^\dagger|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{2}\delta_{n1} + \sqrt{3}\delta_{n3}).$$

Inserting these into the sum, we see that only one term survives:

$$\langle 2|\, X e^{-iH_0 t'/\hbar} e^{iH_0 t''/\hbar} X\, |0\rangle = \frac{\sqrt{2}\hbar}{2m\omega} e^{-3i\omega t'/2} e^{3i\omega t''/2}$$

Hence we must evaluate:

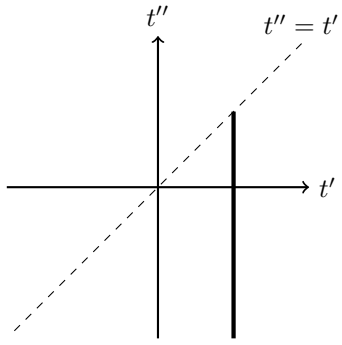
$$\langle 2|\psi_S(t_2)\rangle = \frac{q^2\mathcal{E}^2}{\sqrt{2}m\omega\pi\hbar\tau^2} \int_{t_1}^{t_2} dt' \int_{t_1}^{t'} dt''\, e^{i\omega t'} e^{i\omega t''} \exp\left(-\frac{t'^2}{\tau^2} - \frac{t''^2}{\tau^2}\right) + O(\mathcal{E}^3)$$

in the limit as $t_1 \to -\infty$ and $t_2 \to \infty$. The main part of this calculation will be the evaluation of the double integral:

$$I = \int_{-\infty}^{\infty} dt' \int_{-\infty}^{t'} dt''\, e^{i\omega t'} e^{i\omega t''} \exp\left(-\frac{t'^2}{\tau^2} - \frac{t''^2}{\tau^2}\right).$$

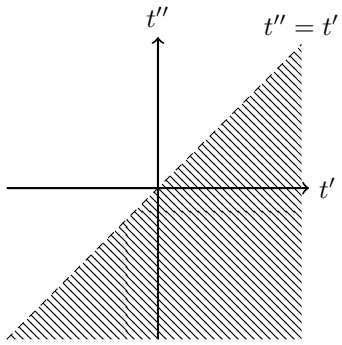
We notice that the inner integral is a Gaussian integral, and hence has no closed form solution. Therefore, we should expect to have to massage the integral a bit first in order to get it into a nice form.

When we have double integrals like this, it's always helpful to think about what region of the plane we're integrating over. The inner integral says: for a fixed value of t', integrate over all values of t'' from $-\infty$ up to t'. That is, we integrate over the region $-\infty < t'' < t'$. Graphically, this looks like:



The thick strip shows the range of t'' for a fixed value of t', from $-\infty$ up to t'.

The outer integral then ranges over all possible values of t', and hence the region of integration in the plane is:

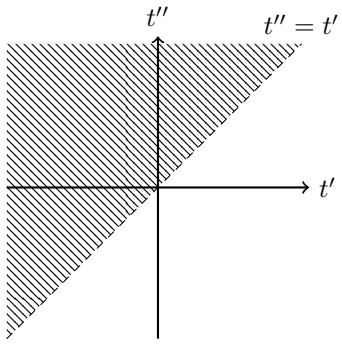


Thus, we can succinctly write the region of the plane over which we are integrating as $t'' \leq t'$.

Now comes the clever trick. The prime labels in the integral are arbitrary, so we can swap $t' \leftrightarrow t''$, which gives:

$$I = \int_{-\infty}^{\infty} dt'' \int_{-\infty}^{t''} dt' \, e^{i\omega t''} e^{i\omega t'} \exp\left(-\frac{t''^2}{\tau^2} - \frac{t'^2}{\tau^2}\right).$$

Note that the integrand itself is unchanged - that is, we are integrating the same function. However, the region of integration is now $t' \leq t''$, which looks like:



Hence we see that

$$\begin{aligned} I + I &= \int_{-\infty}^{\infty} dt' \int_{-\infty}^{t'} dt'' \, e^{i\omega t'} e^{i\omega t''} \exp\left(-\frac{t'^2}{\tau^2} - \frac{t''^2}{\tau^2}\right) + \int_{-\infty}^{\infty} dt'' \int_{-\infty}^{t''} dt' \, e^{i\omega t''} e^{i\omega t'} \exp\left(-\frac{t''^2}{\tau^2} - \frac{t'^2}{\tau^2}\right) \\ &= \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} dt'' e^{i\omega t'} e^{i\omega t''} \exp\left(-\frac{t'^2}{\tau^2} - \frac{t''^2}{\tau^2}\right). \end{aligned}$$

That is, we see that twice the integral is the same as integrating the function over the whole $t't''$ plane. We can separate the integral over the whole plane into a product (using a result from Part IA Vector Calculus):

$$2I = \left(\int_{-\infty}^{\infty} dt' \, e^{i\omega t'} \exp\left(-\frac{t'^2}{\tau^2}\right)\right)\left(\int_{-\infty}^{\infty} dt'' \, e^{i\omega t''} \exp\left(-\frac{t''^2}{\tau^2}\right)\right) = \left(\int_{-\infty}^{\infty} dt' e^{i\omega t'} \exp\left(-\frac{t'^2}{\tau^2}\right)\right)^2$$

We discussed the value of the integral on the right hand side earlier in the question. Hence we have found that:

$$I = \frac{1}{2}\left(\tau\sqrt{\pi}e^{-\frac{1}{4}\omega\tau^2}\right)^2 = \frac{1}{2}\tau^2\pi e^{-\frac{1}{2}\omega^2\tau^2}.$$

Hence the amplitude is:

$$\langle 2|\psi_S(\infty)\rangle = \frac{q^2\mathcal{E}^2}{\sqrt{2}m\omega\pi\hbar\tau^2}\cdot\frac{1}{2}\tau^2\pi e^{-\frac{1}{2}\omega^2\tau^2} + O(\mathcal{E}^3)$$

and so the required probability of the transition is:

$$|\,\langle 2|\psi_S(\infty)\rangle\,|^2 = \frac{q^4\mathcal{E}^4}{8m^2\omega^2\hbar^2}e^{-\omega^2\tau^2} + O(\mathcal{E}^5).$$

⁜ **Comments:** In this question, we calculated a second-order contribution to a transition probability. We found that the integral was very difficult to compute, and needed some tricks.

In quantum field theory, integrals of this form are absolutely ubiquitous. However, there is a general fact that helps in their evaluation. For time-dependent operators $\mathcal{O}_1$, $\mathcal{O}_2$, $\mathcal{O}_3$, ... $\mathcal{O}_n$, we want to evaluate the integral:

$$\int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{t_1} dt_2 \int_{-\infty}^{t_2} dt_3 ... \int_{-\infty}^{t_{n-1}} dt_n\, \mathcal{O}_1(t_1)...\mathcal{O}_n(t_n).$$

Using a similar method to the one used in this questions, we can show that:

$$\int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{t_1} dt_2 \int_{-\infty}^{t_2} dt_3 ... \int_{-\infty}^{t_{n-1}} dt_n\, \mathcal{O}_1(t_1)...\mathcal{O}_n(t_n) = \frac{1}{n!}\int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} dt_3 ... \int_{-\infty}^{\infty} dt_n\, T\{\mathcal{O}_1(t_1)...\mathcal{O}_n(t_n)\}$$

where $T\{\mathcal{O}_1(t_1)...\mathcal{O}_n(t_n)\}$ is the *time-ordering* of the string of operators, which is defined by

$$T\{\mathcal{O}_1(t_1)...\mathcal{O}_n(t_n)\} = \mathcal{O}_1(t_{i_1})...\mathcal{O}_n(t_{i_n})$$

in the region of integration space where $t_{i_1} \geq t_{i_2} \geq ... \geq t_{i_n}$ and $i_1, i_2, ..., i_n$ is some permutation of $1, 2, ..., n$. This explains why we call it the 'time-ordering' of the operators - we just rearrange them so that the operator with earliest time argument acts first, then the operator with the second earliest time argument acts second, etc. We have different time orderings in different regions of integration space.

At first sight, this doesn't look much better! However, there is another theorem, proved in Part III Quantum Field Theory, that further simplifies things. *Wick's Theorem* allows us to write a time-ordered string of operators as:

$$T\{\mathcal{O}_1...\mathcal{O}_n\} = \text{sum over all possible normal-ordered contractions of the string } \mathcal{O}_1...\mathcal{O}_n.$$

Here, a *contraction* deletes a pair of operators $\mathcal{O}_i$ and $\mathcal{O}_j$ and replaces them by a numeric factor called a *propagator*, and *normal-ordering* moves all annihilation (lowering) operators to the right of the string, and all creation (raising) operators to the left of the string. Normal-ordered operators are particularly useful, since when we compute a matrix element, all annihilation operators act immediately on the state and kill it if appropriate, and we don't have to worry about any commutation. This streamlines calculations that are otherwise quite difficult.

This expansion of the time-ordering of a string of operators is the basis of the Feynman diagram expansion used in quantum field theory (at least in the *canonical formalism*).

4. A particle travelling in one dimension with momentum $p = \hbar k > 0$ encounters the steep-sided potential well $V(x) = -V_0 < 0$ for $|x| < a$. Use Fermi's golden rule to show that the probability the particle will be reflected by the well is

$$P_{\text{reflect}} \approx \frac{V_0^2}{4E^2} \sin^2(2ka),$$

where $E = p^2/2m$. Show that in the limit $E \gg V_0$ this result is consistent with the exact result for the reflection probability. [*Hint: Adopt periodic boundary conditions to normalise the wavefunctions of the initial and final states.*]

Solution: The hint instructs us to adopt periodic boundary conditions to normalise the wavefunctions. Therefore, let's restrict the real line to $[-L/2, L/2]$, and then take $L \to \infty$ at the end. We'll adopt periodic boundary conditions on this interval.

We know from Part IB Quantum Mechanics that an incoming scattering state of momentum $p = \hbar k$ has the wavefunction:

$$\psi_k(x) = \frac{e^{ikx}}{\sqrt{L}},$$

where the factor of $1/\sqrt{L}$ is there to ensure normalisation on the interval $[-L/2, L/2]$:

$$\frac{1}{L} \int_{-L/2}^{L/2} e^{-ikx} e^{ikx}\, dx = 1.$$

For the wavefunction to be obey periodic boundary conditions at the ends of the interval, we require

$$e^{ikL/2} = e^{-ikL/2} \qquad \Rightarrow \qquad e^{ikL} = 1 \qquad \Rightarrow \qquad k = \frac{2n\pi}{L},\ n \in \mathbb{Z}.$$

Thus momentum is quantised in units of $2\pi/L$. Let's call the incoming state with this momentum $|n\rangle$.

When the state is reflected, it could in principle have a new momentum, say $p' = \hbar k'$. This new momentum must be in the opposite direction to the incoming momentum, so if $p > 0$, we must have $p' < 0$. Otherwise, the wavefunction of the reflected state has exactly the same form:

$$\psi_{k'}(x) = \frac{e^{ik'x}}{\sqrt{L}}.$$

Again, periodicity implies quantisation of momentum, so we have $k' = 2n'\pi/L$ for some $n' \in \mathbb{Z}$. Let's call the reflected state $|k'\rangle$.

If we were watching our experiment to see if a wave of momentum k' was reflected, we would want to calculated the transition probability of the process $|k\rangle \to |k'\rangle$ in the presence of the potential well $V(x)$. In order to so perturbatively, let's treat $V(x)$ as a small perturbation to the zero potential. In particular, the unperturbed Hamiltonian is then simply $H_0 = P^2/2m$. If we start in the initial state $|k\rangle$, Fermi's Golden rule says that the rate of transition to the state $|k'\rangle$ (i.e. the probability per unit time) is just:

$$\Gamma(|k\rangle \to |k'\rangle) = \frac{2\pi}{\hbar} |\langle k'|V|k\rangle|^2 \delta(E_{k'} - E_k).$$

The relevant matrix element here is:

$$\langle k'|V|k\rangle = -\frac{V_0}{L} \int_{-a}^{a} e^{-ik'x} e^{ikx}\, dx = -\frac{2V_0}{L} \frac{\sin((k-k')a)}{k-k'}.$$

Hence we can already simplify the rate to:

$$\Gamma(|k\rangle \to |k'\rangle) = \frac{8\pi V_0^2}{\hbar(k-k')^2 L^2} \sin^2((k-k')a) \delta(E_{k'} - E_k).$$

To get the *total* probability of reflection, let's think about things physically. As an experimenter, we would be able to determine the momentum of the incoming particle because we make the particle ourselves in the lab. However, when the particle is reflected, it could gain any old momentum (in reality, only one value of the momentum corresponds to reflection). Thus to get the total probability of reflection, we need to integrate over all possible outgoing momenta (for L large enough, we can treat k as continuous).

To do this in practice, we define a *differential rate* for our process by:

$$d\Gamma(|k\rangle \to \{|l\rangle : l \in (k', k' + dk')\}) = \frac{8\pi V_0^2}{\hbar(k-k')^2 L^2} \sin^2((k-k')a)\delta(E_{k'} - E_k)n(k')dk'.$$

Here, the differential rate is the probability per unit time of transition from a specific state $|k\rangle$ to any final state $|l\rangle$. The function $n(k')$ is called the *density of states* and $n(k')dk'$ is the number of states with momentum in the interval $(k', k' + dk')$.

Our next objective is to determine the density of states $n(k')$. Since momentum is quantised in units of $2\pi/L$, each state occupies an effective area $2\pi/L$ in k' space. Therefore, the density of states is given by:

$$n(k')dk' = \frac{dk'}{2\pi/L} = \frac{L}{2\pi}dk'.$$

Substituting in the formula for $n(k')$, and integrating both sides with respect to k', we get (recalling that the rate is the probability per unit time):

$$\frac{dP}{dt} = \frac{4V_0^2}{\hbar L} \int_{k'_{\text{min}}}^{k'_{\text{max}}} \frac{\sin^2((k-k')a)}{(k-k')^2} \delta(E_{k'} - E_k)\, dk'.$$

where P is the probability of reflection. To perform the integral, we recall that

$$\delta(E_{k'} - E_k) = \delta\left(\frac{\hbar^2 k'^2}{2m} - \frac{\hbar^2 k^2}{2m}\right) = \frac{m\delta(k'-k)}{\hbar^2 k} + \frac{m\delta(k'+k)}{\hbar^2 k},$$

where we have used the result from Part IB Methods that

$$\delta(f(x)) = \sum_{\text{roots } x_0 \text{ of } f(x)} \frac{\delta(x - x_0)}{|f'(x_0)|}.$$

We recognise that the delta function $\delta(k'-k)$ corresponds to transmission, since p and p' will then have the same sign (in particular, we notice that $k' = k$ must be excluded from the range of integration $[k'_{\text{min}}, k'_{\text{max}}]$). Thus dropping the $\delta(k'-k)$ term, we find:

$$\frac{dP}{dt} = \frac{mV_0^2}{\hbar^3 k^3 L} \sin^2(2ka).$$

To finish, we need to integrate over t. But everything on the right is a time-independent constant; therefore we can just integrate immediately. The range of integration is from the time when the wave was sent in to the time when it returns to its initial location. Assuming on average that the wave reflects from the location $x = 0$, the wave must travel a distance L at a velocity $v = p/m$. Thus the time taken is $t = L/(p/m)$. Substituting this in, we have:

$$P = \frac{mV_0^2}{\hbar^3 k^3 L} \sin^2(2ka) \cdot \frac{L}{p/m} = \frac{m^2 V_0^2}{\hbar^3 k^3 p} \sin^2(2ka) = \frac{m^2 V_0^2}{p^4} \sin^2(2ka) = \frac{V_0^2 \sin^2(2ka)}{4E^2},$$

using $p = \hbar k$ and $E = p^2/2m$. This is the required probability.

We are now asked to repeat the question to find the exact result. This is essentially a problem from Part IB Quantum Mechanics, where you learned how to solve scattering problems.

A scattering state for this potential has a wavefunction ψ obeying:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \psi\begin{cases}-V_0 & \text{for } |x| < a \\ 0 & \text{otherwise}\end{cases} = E\psi.$$

Letting $E = \hbar^2k^2/2m$ and $E + V_0 = \hbar^2\kappa^2/2m$, we see immediately that

$$\psi = \begin{cases} e^{ikx} + Re^{e-ikx} & \text{for } x < -a \\ Ae^{i\kappa x} + Be^{-i\kappa x} & \text{for } |x| < a \\ Te^{ikx} & \text{for } x > a. \end{cases}$$

Here, we have set the constant in front of e^{ikx} to 1 in the region $x < -a$ without loss of generality. It is then clear that the reflection amplitude is R and the transmission amplitude is T.

To fix the values of R, A, B and T, we use continuity of ψ and ψ' at the boundaries $x = -a$ and $x = a$. This implies the system of simultaneous equations:

$$\begin{aligned} e^{-ika} + Re^{ika} &= Ae^{-i\kappa a} + Be^{\kappa a} \\ ike^{-ika} - ikRe^{ika} &= i\kappa Ae^{-i\kappa a} - i\kappa Be^{i\kappa a} \\ Ae^{i\kappa a} + Be^{-i\kappa a} &= Te^{ika} \\ i\kappa Ae^{i\kappa a} - i\kappa Be^{-i\kappa a} &= ikTe^{ika}. \end{aligned}$$

Solving the third and fourth equations simultaneously, we can find expression for A and B in terms of R and T:

$$A = \left(\frac{k+\kappa}{2\kappa}\right)Te^{i(k-\kappa)a}, \qquad B = \left(\frac{\kappa-k}{2\kappa}\right)Te^{i(k+\kappa)a}.$$

Substituting back into the first and second equation, we can solve simultaneously for R and T. We find the reflection amplitude to be:

$$R = \frac{ie^{-2ika}(k^2-\kappa^2)\sin(2\kappa a)}{(\kappa^2+k^2)i\sin(2\kappa a) - 2\kappa k\cos(2\kappa a)},$$

and hence the reflection probability is:

$$|R|^2 = \frac{(k^2-\kappa^2)^2\sin^2(2\kappa a)}{(\kappa^2+k^2)^2\sin^2(2\kappa a) + 4\kappa^2k^2\cos^2(2\kappa a)}.$$

Note that

$$k^2 - \kappa^2 = -\frac{2mV_0}{\hbar^2},$$

and in the limit $E \gg V_0, \kappa \approx k$. So replace $k^2 + \kappa^2 \approx 2k^2, 4\kappa^2k^2 \approx 4k^4$. Then we have

$$|R|^2 \approx \frac{m^2V_0^2}{k^4\hbar^4}\sin^2(2ka) = \frac{V_0^2\sin^2(2ka)}{4E^2},$$

which indeed agrees with the Fermi's Golden Rule approach.

5. Consider the driven quantum harmonic oscillator with Hamiltonian

$$H = \hbar\omega\left(A^\dagger A + \frac{1}{2}\right) + \hbar\left(f^*(t)A + f(t)A^\dagger\right).$$

Taking H_0 to be the standard oscillator Hamiltonian, show that the perturbation in the interaction picture is

$$V_I(t) = \hbar\left(\tilde{f}^*(t)A + \tilde{f}(t)A^\dagger\right),$$

where $\tilde{f}(t) = e^{i\omega t}f(t)$.

Define an operator $U(g)$ by $U(g) := e^{gA^\dagger - g^*A}$, where $g = g(t)$. Show that

$$U(g) = e^{-|g|^2/2}e^{gA^\dagger}e^{-g^*A}.$$

By taking the time-derivative of this expression, deduce that the time evolution operator in the interaction picture can be written as

$$U_I(t) = U(g)\exp\left(-\int_0^t \mathrm{Im}\left(\dot{g}^*g\right)\,dt'\right),$$

for the choice

$$g(t) = -i\int_0^t \tilde{f}(t')\,dt'.$$

At $t = 0$ the oscillator is initially in its ground state $|0\rangle$. In the case that $f(t) = e^{-i\omega t}f_0$, where f_0 is a constant, show that at time t the oscillator is in the coherent state

$$|\psi_S(t)\rangle = e^{-|f_0|^2t^2/2}e^{-i\omega t/2}e^{-itf(t)A^\dagger}|0\rangle$$

in the Schrödinger picture. Comment on the relevance of this model to the operation of a laser.

Solution: The perturbation in the interaction picture is given by:

$$V_I(t) = e^{iH_0t/\hbar}Ve^{-iH_0t/\hbar} = \hbar e^{iH_0t/\hbar}\left(f^*(t)A + f(t)A^\dagger\right)e^{-iH_0t/\hbar}.$$

Since $\hbar$, $f^*(t)$ and $f(t)$ are constants, we just need to be able to evaluate the operator products:

$$e^{iH_0t/\hbar}Ae^{-iH_0t/\hbar}, \qquad e^{iH_0t/\hbar}A^\dagger e^{-iH_0t/\hbar}.$$

The first product can be evaluated using a trick. Define $F(t) = e^{iH_0t/\hbar}Ae^{-iH_0t/\hbar}$. Then

$$\frac{dF}{dt} = \frac{i}{\hbar}\left(e^{iH_0t/\hbar}H_0Ae^{-iH_0t/\hbar} - e^{iH_0t/\hbar}AH_0e^{-iH_0t/\hbar}\right) = \frac{i}{\hbar}e^{iH_0t/\hbar}[H_0, A]e^{-iH_0t/\hbar}.$$

Now:

$$[H_0, A] = \hbar\omega[A^\dagger A, A] = \hbar\omega[A^\dagger, A]A = -\hbar\omega A.$$

Thus we have:

$$\frac{dF}{dt} = \frac{i}{\hbar}\left(-\hbar\omega e^{iH_0t/\hbar}Ae^{-iH_0t/\hbar}\right) = -i\omega F.$$

This is a simple differential equation for F. At time $t = 0$, we know that $F = A$, and hence the solution is just

$$F(t) = Ae^{-i\omega t}.$$

Finally, notice that the other operator product we are interested in is just $F^\dagger(t) = e^{iH_0t/\hbar}A^\dagger e^{-iH_0t/\hbar} = A^\dagger e^{i\omega t}$. Thus the perturbation in the interaction picture is:

$$V_I(t) = \hbar\left(f^*(t)e^{-i\omega t}A + f(t)e^{i\omega t}A^\dagger\right) = \hbar\left(\tilde{f}^*(t)A + \tilde{f}(t)A^\dagger\right),$$

as required.

In the next part of the question, we define an operator $U(g) = e^{gA^\dagger - g^*A}$ which depends on a time-dependent function $g(t)$. We are asked to prove an equivalent form for this operator. First note that $[gA^\dagger, -g^*A] = |g|^2$, so $gA^\dagger$ and $-g^*A$ both commute with their commutator. Thus we can apply the result of Examples Sheet 1, Question 2 to write:

$$U(g) = e^{gA^\dagger - g^*A} = e^{-\frac{1}{2}|g|^2} e^{gA^\dagger - g^*A + \frac{1}{2}[gA^\dagger, -g^*A]} = e^{-\frac{1}{2}|g|^2} e^{gA^\dagger} e^{-g^*A}.$$

as required.

Using the chain rule, the time-derivative of $U(g)$ is given by:

$$\frac{dU}{dt} = -\frac{1}{2}\left(\dot{g}g^* + g\dot{g}^*\right) e^{-\frac{1}{2}|g|^2} e^{gA^\dagger} e^{-g^*A} + \dot{g}A^\dagger e^{-\frac{1}{2}|g|^2} e^{gA^\dagger} e^{-g^*A} - \dot{g}^* e^{-\frac{1}{2}|g|^2} e^{gA^\dagger} A e^{-g^*A}.$$

We can commute the A past $e^{gA^\dagger}$ using the result of Examples Sheet 1, Question 2. We have

$$e^{gA^\dagger} A = A e^{gA^\dagger} + [e^{gA^\dagger}, A] = A e^{gA^\dagger} - g e^{gA^\dagger},$$

since $[A, A^\dagger] = 1$. Therefore,

$$\frac{dU}{dt} = \left(-\frac{1}{2}\dot{g}g^* + \frac{1}{2}\dot{g}^* g + \dot{g}A^\dagger - \dot{g}^* A\right) U = \left(-\frac{i}{2}\,\mathrm{Im}(\dot{g}^* g) + \dot{g}A^\dagger - \dot{g}^* A\right) U.$$

For the suggested choice

$$g(t) = -i \int_0^t \tilde{f}(t')\, dt',$$

we have

$$\dot{g}A^\dagger - \dot{g}^* A = -i\tilde{f}(t)A^\dagger - i\tilde{f}^*(t)A = -\frac{i}{\hbar} V_I,$$

by the earlier work, where we found the perturbation in the interaction picture. It follows that the differential equation for U can be written as:

$$\frac{dU}{dt} = \left(-\frac{i}{2}\,\mathrm{Im}(\dot{g}^* g) - \frac{i}{\hbar} V_I\right) U.$$

Now recall from lectures that the time-evolution operator of the system in the interaction picture, $U_I(t)$, obeys the defining differential equation:

$$i\hbar \frac{dU_I}{dt} = V_I U_I, \qquad U_I(0) = I.$$

This is similar to the equation for $U(g)$, but that equation also contains an additional term on the right hand side. We therefore guess a solution $U_I(t) = U(g)H(t)$, for some unknown operator $H(t)$.

Now, since $U(g(0)) = U(0) = I$, the initial condition translates to $H(0) = I$. The differential equation itself becomes:

$$i\hbar \frac{dU}{dt} H(t) + i\hbar U(g) \frac{dH}{dt} = V_I U(g) H(t).$$

Inserting the expression we derived above for dU/dt, and cancelling appropriately, we find:

$$\frac{\hbar}{2}\,\mathrm{Im}(\dot{g}^* g) H(t) + i\hbar \frac{dH}{dt} = 0 \qquad \Rightarrow \qquad \frac{dH}{dt} = \frac{i}{2}\,\mathrm{Im}(\dot{g}^* g) H(t), \qquad H(0) = I.$$

This equation has the solution:

$$H(t) = \exp\left(\frac{i}{2}\int_0^t \mathrm{Im}(\dot{g}^* g)\, dt'\right),$$

and hence the time-evolution operator for the interaction picture is indeed

$$U_I(t) = U(g)\exp\left(\frac{i}{2}\int_0^t \mathrm{Im}(\dot{g}^* g)\, dt'\right).$$

Finally, we are asked to restrict to the case $f(t) = e^{-i\omega t} f_0$, and consider evolution of the system starting from the state $|0\rangle$ at time $t = 0$. In this case, we have

$$g(t) = -i\int_0^t \tilde{f}(t')\, dt' = -i\int_0^t f_0\, dt' = -if_0 t.$$

Therefore:

$$U_I(t) = U(-if_0 t)\exp\Bigg(\underbrace{\frac{i}{2}\int_0^t \mathrm{Im}((-if_0)^*(-if_0 t'))\, dt'}_{0}\Bigg) = U(-if_0 t).$$

Recalling the definition of $U(g)$, we have

$$U_I(t) = e^{-f_0^2 t^2/2} e^{-if_0 t A^\dagger} e^{-if_0 t A}.$$

At time $t = 0$, the system starts in the state $|0\rangle$. The interaction picture version of this state is just $|0_I\rangle = e^{iH_0 \cdot 0/\hbar}|0\rangle = |0\rangle$. After a time t, the system will have evolved to the interaction picture state:

$$|\psi_I(t)\rangle = U_I(t)|0_I\rangle = e^{-f_0^2 t^2/2} e^{-if_0 t A^\dagger} e^{-if_0 t A}|0\rangle.$$

Notice that $e^{-if_0 t A}|0\rangle = |0\rangle$, which we can see by expanding the exponential. Hence we have:

$$|\psi_I(t)\rangle = e^{-f_0^2 t^2/2} e^{-if_0 t A^\dagger}|0\rangle.$$

Restoring the interaction picture state to the Schrödinger picture, we have:

$$|\psi_S(t)\rangle = e^{-iH_0 t/\hbar} e^{-f_0^2 t^2/2} e^{-if_0 t A^\dagger}|0\rangle.$$

To get the result in the question, we must commute $e^{-iH_0 t/\hbar}$ past $e^{-if_0 t A^\dagger}$. This is quite difficult unless we remember that we are acting on the state $|0\rangle$ with these operators. We have:

$$\begin{aligned}
e^{-iH_0 t/\hbar} e^{-if_0 t A^\dagger}|0\rangle &= e^{-iH_0 t/\hbar}\sum_{n=0}^{\infty}\frac{(-if_0 t A^\dagger)^n}{n!}|0\rangle && \text{(definition of exponential)}\\
&= e^{-iH_0 t/\hbar}\sum_{n=0}^{\infty}\frac{(-if_0 t)^n}{\sqrt{n!}}|n\rangle && (|n\rangle = (A^\dagger)^n|0\rangle/\sqrt{n!})\\
&= \sum_{n=0}^{\infty}\frac{(-if_0 t)^n}{\sqrt{n!}} e^{-i\omega t(n+1/2)}|n\rangle && \text{(acting on } |n\rangle \text{ with } e^{-iH_0 t/\hbar})\\
&= e^{-i\omega t/2}\sum_{n=0}^{\infty}\frac{(-if_0 t e^{-i\omega t} A^\dagger)^n}{n!}|0\rangle\\
&= e^{-i\omega t/2} e^{-itf(t)A^\dagger}|0\rangle.
\end{aligned}$$

Hence we find $|\psi_S(t)\rangle = e^{-f_0^2 t^2/2} e^{-i\omega t/2} e^{-itf(t)A^\dagger}|0\rangle$, as required.

Alternative solution using coherent states: There is a much quicker way of doing this part of the question if we remember some results from Examples Sheet 1. There, we defined a *coherent state* of the harmonic oscillator by:

$$|\alpha\rangle = e^{\alpha A^\dagger - \bar{\alpha} A} |0\rangle = U(\alpha) |0\rangle ,$$

where $U(\alpha)$ is the U operator in this question with $g = \alpha$. In this question, we want to find the interaction picture state of the system at time t, given it starts in the interaction picture state $|0_I\rangle = |0\rangle$. This state is given by:

$$|\psi_I(t)\rangle = U(-if_0 t) |0\rangle ,$$

as we saw above. But now we identify that the right hand side is a coherent state of the harmonic oscillator, namely $|-if_0 t\rangle$. Moving back to the Schrödinger picture, we can write:

$$|\psi_S(t)\rangle = e^{-iH_0 t/\hbar} |-if_0 t\rangle .$$

This should be interpreted as a time-evolution operator for the harmonic oscillator, H_0, acting on a coherent state $-if_0 t$. Recall from Examples Sheet 1 that to evolve a coherent state in time we simply multiply the whole state by $e^{-i\omega t/2}$ and multiply the argument of the coherent state by $e^{-i\omega t}$. Hence we have:

$$|\psi_S(t)\rangle = e^{-i\omega t/2} |-ie^{-i\omega t} f_0 t\rangle = e^{-i\omega t/2} |-itf(t)\rangle$$

Finally, recall from the solution to Examples Sheet 1, Question 5, we can write the coherent state $|\alpha\rangle$ as:

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} e^{\alpha A^\dagger} |0\rangle ,$$

and hence we have:

$$|\psi_S(t)\rangle = e^{-i\omega t/2} |-itf(t)\rangle = e^{-i\omega t/2} e^{-\frac{1}{2}t^2 f_0^2} e^{-itf(t)A^\dagger} |0\rangle ,$$

which is the required form.

The very last part of this question asks us to comment on the relevance of this model to the operation of a laser. The relevant physical facts are:

- In quantum optics, the state of a laser is such that (i) it has an indefinite number of photons; (ii) it has a precisely defined phase. It turns out that both these conditions are satisfied by the *coherent states* of Examples Sheet 1; we shall describe why as follows.

  Let us suppose that the number of photons in a laser beam is a quantum observable N. If there is one photon, the system has energy E_1, if there are two photons, the system has energy E_2, etc. One good way of describing the possible states of the system is through the *harmonic oscillator* energy levels. That is, the one photon state corresponds to the state $|1\rangle$ of the harmonic oscillator, the two photon state corresponds to the state $|2\rangle$ of the harmonic oscillator, etc.

  Notice that the raising and lowering operators correspond to *creation* and *annihilation* of photons in this model. That is, $A^\dagger |n\rangle$ has one more photon than the state $|n\rangle$, and $A |n\rangle$ has one less photon.

  The state $\{|n\rangle\}$ of the harmonic oscillator are not very good at satisfying the laser state conditions (i) and (ii) though. Each state $|n\rangle$ has a definite number of photons, so cannot satisfy (i). *However*, a coherent state such as $|\alpha\rangle$ from Examples Sheet 1 is a superposition over all possible $\{|n\rangle\}$ and hence describes a state of a laser without a definite number of photons. Furthermore, we can interpret the fixed phase of the complex number α as the phase of the laser, and the modulus $|\alpha|$ of the complex number as the amplitude of the electromagnetic radiation composing the laser. Thus *coherent states are the physical states for lasers*.

- In this question, we effectively start with a coherent state $|0\rangle$ at time $t = 0$ which evolves to a coherent state $e^{-i\omega t/2} |-itf(t)\rangle$ at time t. Notice in particular that the amplitude of the laser is growing in time as $|-itf(t)| = t$. This corresponds to increasing intensity of the laser over time, as we build up the power of the laser. Hence this model describes an experimental setup where we create and power up a laser.

6. Let $\rho = \sum_{i,j} \rho_{ij} |i\rangle \langle j|$ be the density operator of some quantum system. Show that the system is in a pure state if and only if every row of the matrix ρ_{ij} is a multiple of the first row, and every column is a multiple of the first column.

Solution: Suppose the system is in some pure state

$$|\psi\rangle = \sum_i c_i |i\rangle .$$

Then the density operator takes the form:

$$\rho = |\psi\rangle \langle\psi| = \left(\sum_i c_i |i\rangle\right)\left(\sum_j c_j^* \langle j|\right) = \sum_{i,j} c_i c_j^* |i\rangle \langle j| .$$

Hence the density matrix has entries $\rho_{ij} = c_i c_j^*$. Writing out the matrix explicitly, we see it is of the form:

$$\begin{pmatrix} c_1c_1^* & c_1c_2* & c_1c_3^* & \cdots & c_1c_N^* \\ c_2c_1^* & c_2c_2^* & c_2c_3^* & \cdots & c_2c_N^* \\ c_3c_1^* & c_3c_2^* & c_3c_3^* & \cdots & c_3c_N^* \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_Nc_1^* & c_Nc_2^* & c_Nc_3^* & \cdots & c_Nc_N^* \end{pmatrix} .$$

We may assume without loss of generality that $c_1 > 0$ (else we can rearrange the basis vectors $|i\rangle$ until it is). It follows that the second row is c_2/c_1 times the first, the third row is c_3/c_1 times the first, etc, and the second column is c_2^*/c_1^* times the first, the third column is c_3^*/c_1^* times the first, etc. This show that every row is a multiple of the first row and every column is a multiple of the first column.

We must now prove the converse, which is slightly more tricky. We will use the following fact about density matrices:

Lemma: The diagonal entries of a density matrix are non-negative real numbers.

Proof: In some basis, the density operator can be written as:

$$\rho = \sum_\alpha p_\alpha |\alpha\rangle \langle\alpha| ,$$

where p_α are real, non-negative numbers (since they are probabilities). Transforming to an arbitrary basis $\{|i\rangle\}$, we expand:

$$|\alpha\rangle = \sum_i a_{\alpha i} |i\rangle .$$

The density operator then becomes:

$$\rho = \sum_{\alpha,i,j} p_\alpha a_{\alpha i} a_{\alpha j}^* |i\rangle \langle j| .$$

It follows that the density matrix is $\rho_{ij} = p_\alpha a_{\alpha i} a_{\alpha j}^*$. The diagonal entries are $\rho_{ii} = p_\alpha |a_{\alpha i}|^2 \geq 0$. □

We can now begin our proof. Suppose that our system has a density matrix ρ_{ij} whose rows are all a multiple of the first row, and whose columns are all a multiple of the first column. We know from the above Lemma that ρ_{ij} has non-negative diagonal entries. Furthermore, we know from lectures that $\mathrm{tr}(\rho) = 1$, and hence not all of the diagonal entries can be zero. Thus we can arrange for ρ_{11} to be real and positive by rearranging the basis vectors.

Let $\rho_{11} = |a_1|^2$ for some complex number $a_1 \neq 0$ (it can have any phase). Since $a_1 \neq 0$, we can write the entire first row's entries in the form

$$|a_1|^2, \qquad a_1 a_2^*, \qquad a_1 a_3^*, \qquad \cdots \qquad a_1 a_N^*$$

where $a_2^* = \rho_{12}/a_1, a_3^* = \rho_{13}/a_1$, etc.

Since all the rows of ρ_{ij} are multiples of the first row, we must be able to write the density matrix in the form:

$$\begin{pmatrix} |a_1|^2 & a_1 a_2^* & a_1 a_3^* & \cdots & a_1 a_N^* \\ b_2|a_1|^2 & b_2 a_1 a_2^* & b_2 a_1 a_3^* & \cdots & b_2 a_1 a_N^* \\ b_3|a_1|^2 & b_3 a_1 a_2^* & b_3 a_1 a_3^* & \cdots & b_3 a_1 a_N^* \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b_N|a_1|^2 & b_N a_1 a_2^* & b_N a_1 a_3^* & \cdots & b_N a_1 a_N^* \end{pmatrix},$$

for some numbers $b_2, b_3 ... b_N$. But recall from lectures that the density matrix is Hermitian, and so

$$\begin{aligned} b_2|a_1|^2 = a_1^* a_2 \qquad &\Rightarrow \qquad b_2 = a_2/a_1, \\ b_3|a_1|^2 = a_1^* a_3 \qquad &\Rightarrow \qquad b_3 = a_3/a_1, \\ &\vdots \\ b_N|a_1|^2 = a_1^* a_N \qquad &\Rightarrow \qquad b_N = a_N/a_1. \end{aligned}$$

It follows that the density matrix is

$$\rho_{ij} = \begin{pmatrix} a_1 a_1^* & a_1 a_2 * & a_1 a_3^* & \cdots & a_1 a_N^* \\ a_2 a_1^* & a_2 a_2^* & a_2 a_3^* & \cdots & a_2 a_N^* \\ a_3 a_1^* & a_3 a_2^* & a_3 a_3^* & \cdots & a_3 a_N^* \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_N a_1^* & a_N a_2^* & a_N a_3^* & \cdots & a_N a_N^* \end{pmatrix}$$

This is exactly the form of the density matrix we found in the forward direction proof. It follows that the density operator is:

$$\rho = \left(\sum_i a_i |i\rangle \right) \left(\sum_j a_j \langle j| \right),$$

which is the density operator for a pure state. This completes our proof.

7. Show that the entropy $S(\rho) = -\mathrm{tr}_{\mathcal{H}}(\rho \log(\rho))$ obeys $S(U\rho U^\dagger) = S(\rho)$ for any unitary operator U, and hence that the entropy is both time-independent and independent of the choice of basis on $\mathcal{H}$.

A composite system is formed from two uncorrelated subsystems A and B. Both subsystems are in impure states, with the numbers $\{p_{A_i}\}$ and $\{p_{B_r}\}$ being the probabilities of the members of the complete sets of states $\{|A;i\rangle\}$ and $\{|B;r\rangle\}$ respectively. Show that the entropy of the composite system is the sum of the entropies of the two subsystems. What is the relevance of this result for thermodynamics?

Solution: For the first part, recall that we saw in lectures:

$$S(\rho) = -\mathrm{tr}_{\mathcal{H}}(\rho \log(\rho)) = -\sum_r \rho_r \log(\rho_r),$$

where ρ_r are the eigenvalues of the density operator ρ.

To establish $S(U\rho U^\dagger) = S(\rho)$, we simply note that $U\rho U^\dagger$ has the same eigenvalues as ρ. This is true since $U\rho U^\dagger$ is identical to ρ after the change of basis $|i\rangle \mapsto U^\dagger |i\rangle$.

The fact that S is independent of basis choice follows almost immediately. Under a unitary change of basis, ρ transforms to $U\rho U^\dagger$ for some unitary matrix U, so our former result $S(U\rho U^\dagger) = S(\rho)$ precisely states that entropy is independent of basis.

Finally, we can also use this result to show that entropy is time-independent. In the Heisenberg picture, all time-dependence is contained in the operators; in particular, in the Heisenberg picture we can write the density operator as $\rho_H(t) = U(t)\rho_S U(t)^{-1}$ where ρ_S is the time-independent Schrödinger picture density operator.

We are now asked to show that entropy is an additive quantity, i.e. the entropy of a composite system is the sum of the entropies of the subsystems of which it is composed, provided the two subsystems are uncorrelated.

Since our two systems are uncorrelated, the probability that our composite system is in the state $|A;i\rangle \otimes |B;j\rangle$ is simply $p_{ir} = p_{Ai}p_{Br}$ (independent probabilities multiply). It follows that the density operator for the whole composite system is just $\rho = \mathrm{diag}(p_{11}, p_{12}, p_{13}, ...)$ with basis vectors appropriately arranged. It follows that the entropy of the whole system is simply:

$$S = -\sum_{i,r} p_{ir} \log(p_{ir}) = -\sum_{i,r} p_{Ai}p_{Br}(\log(p_{Ai}) + \log(p_{Br}))$$

$$= -\underbrace{\left(\sum_r p_{Br}\right)}_{1} \sum_i p_{Ai} \log(p_{Ai}) - \underbrace{\left(\sum_i p_{Ai}\right)}_{1} \sum_r p_{Br} \log(p_{Br}) = S_A + S_B,$$

and hence we're done.

This result shows that entropy is an *extensive* thermodynamic quantity. That is, if we double the size of a system, we have twice as much entropy. This is in contrast to an *intensive* thermodynamic quantity, which does not dependent on the size of the system. Some examples of extensive quantities are entropy and mass, and some examples of intensive quantities are temperature and density.

You'll discuss extensive and intensive quantities in much more detail in the Part II Statistical Physics course, if you decide to take it.

8. Let $\mathcal{H}_1$, $\mathcal{H}_2$ and $\mathcal{H}_3$ each describe two-state systems, and let $\{|\uparrow\rangle, |\downarrow\rangle\}$ form a basis of ach $\mathcal{H}_i$, where $\sigma_z |\uparrow\rangle = |\uparrow\rangle$, $\sigma_z |\downarrow\rangle = -|\downarrow\rangle$ with σ_z a Pauli matrix.

(i) Compute $\sigma_x |\uparrow\rangle$, $\sigma_x |\downarrow\rangle$, $\sigma_y |\uparrow\rangle$ and $\sigma_y |\downarrow\rangle$, where σ_x and σ_y are the other two Pauli matrices.

(ii) Consider the state

$$|\mathsf{GHZ}\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle |\uparrow\rangle |\uparrow\rangle - |\downarrow\rangle |\downarrow\rangle |\downarrow\rangle \right) \in \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3,$$

known as the *Greenberger, Horne and Zeilinger* state. Show that this state obeys

$$\sigma_y \otimes \sigma_y \otimes \sigma_x |\mathsf{GHZ}\rangle = \sigma_y \otimes \sigma_x \otimes \sigma_y |\mathsf{GHZ}\rangle = \sigma_x \otimes \sigma_y \otimes \sigma_y |\mathsf{GHZ}\rangle = |\mathsf{GHZ}\rangle , \tag{$*$}$$

whilst

$$\sigma_x \otimes \sigma_x \otimes \sigma_x |\mathsf{GHZ}\rangle = -|\mathsf{GHZ}\rangle . \tag{$\dagger$}$$

(iii) Suppose we try to reproduce these results in a hidden variable theory, by assigning functions

$$s_i : \mathbb{R}^3 \times \mathbb{R}^n \to \{-1, +1\}$$

to each of the three subsystems, where the classical value of the spin is entirely determined by the axis $\mathbf{a} \in \mathbb{R}^3$ along which the spin is measured and the value $\mathbf{v} \in \mathbb{R}^n$ of the hidden variables. What constraints must these classical spins obey if they are to be compatible with ($*$) and ($\dagger$)? Is this possible?

Solution: (i) For this part, let's work in matrix and vector notation. Then we know from lectures that:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Using this notation, it's immediately clear that

$$\sigma_x |\uparrow\rangle = |\downarrow\rangle , \qquad \sigma_x |\downarrow\rangle = |\uparrow\rangle , \qquad \sigma_y |\uparrow\rangle = i |\downarrow\rangle , \qquad \sigma_y |\downarrow\rangle = -i |\uparrow\rangle .$$

(ii) We simply use the result from (i). We have, for example:

$$\sigma_y \otimes \sigma_y \otimes \sigma_x |\mathsf{GHZ}\rangle = \frac{1}{\sqrt{2}} \sigma_y \otimes \sigma_y \otimes \sigma_x \left(|\uparrow\rangle |\uparrow\rangle |\uparrow\rangle - |\downarrow\rangle |\downarrow\rangle |\downarrow\rangle \right) = \frac{1}{\sqrt{2}} \left(i^2 |\downarrow\rangle |\downarrow\rangle |\downarrow\rangle - (-i)^2 |\uparrow\rangle |\uparrow\rangle |\uparrow\rangle \right) = |\mathsf{GHZ}\rangle .$$

Completely analogously, we get the other required results.

(iii) Let $\mathbf{e}_i$ be the unit vector in the i direction. From part (ii) of the question, we know that the functions s_i must obey the conditions:

$$s_1(\mathbf{e}_y, \mathbf{v}) s_2(\mathbf{e}_y, \mathbf{v}) s_3(\mathbf{e}_x, \mathbf{v}) = +1, \qquad s_1(\mathbf{e}_y, \mathbf{v}) s_2(\mathbf{e}_x, \mathbf{v}) s_3(\mathbf{e}_y, \mathbf{v}) = +1, \qquad s_1(\mathbf{e}_x, \mathbf{v}) s_2(\mathbf{e}_y, \mathbf{v}) s_3(\mathbf{e}_y, \mathbf{v}) = +1,$$

$$s_1(\mathbf{e}_x, \mathbf{v}) s_2(\mathbf{e}_x, \mathbf{v}) s_3(\mathbf{e}_x, \mathbf{v}) = -1$$

for any values of the hidden variables $\mathbf{v}$. However, the first three constraints also imply: $s_1(\mathbf{e}_x, \mathbf{v}) s_2(\mathbf{e}_x, \mathbf{v}) s_3(\mathbf{e}_x, \mathbf{v})$

$$\begin{aligned}
&= s_1(\mathbf{e}_x, \mathbf{v}) s_1(\mathbf{e}_y, \mathbf{v})^2 s_2(\mathbf{e}_x, \mathbf{v}) s_2(\mathbf{e}_y, \mathbf{v})^2 s_3(\mathbf{e}_x, \mathbf{v}) s_3(\mathbf{e}_y, \mathbf{v})^2 && \text{(since } s_i^2 = 1) \\
&= (s_1(\mathbf{e}_x, \mathbf{v}) s_2(\mathbf{e}_y, \mathbf{v}) s_3(\mathbf{e}_y, \mathbf{v})) (s_1(\mathbf{e}_y, \mathbf{v}) s_2(\mathbf{e}_x, \mathbf{v}) s_3(\mathbf{e}_y, \mathbf{v})) (s_1(\mathbf{e}_y, \mathbf{v}) s_2(\mathbf{e}_y, \mathbf{v}) s_3(\mathbf{e}_x, \mathbf{v})) \\
&= (+1)(+1)(+1) \\
&= +1,
\end{aligned}$$

which contradicts the fourth constraint. Hence hidden variable theories are inconsistent with quantum mechanics. This is a simplified proof of *Bell's Theorem*, which you saw in lectures.

Part II: Principles of Quantum Mechanics
Past Paper Solutions

Please send all comments and corrections to jmm232@cam.ac.uk.

2014, Paper 1, Section II, 33A

Let $\hat{x}, \hat{p}$ and $H(\hat{x}, \hat{p}) = \hat{p}^2/2m + V(\hat{x})$ be the position operator, momentum operator and Hamiltonian for a particle moving in one dimension. Let $|\psi\rangle$ be the state vector for the particle. The position and momentum eigenstates have inner products

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

Show that

$$\langle x|\hat{p}|\psi\rangle = -i\hbar\frac{\partial}{\partial x}\psi(x) \qquad \text{and} \qquad \langle p|\hat{x}|\psi\rangle = i\hbar\frac{\partial}{\partial p}\tilde{\psi}(p)$$

where $\psi(x)$ and $\tilde{\psi}(p)$ are the wavefunctions in the position representation and momentum representation, respectively. Show how $\psi(x)$ and $\tilde{\psi}(p)$ may be expressed in terms of each other.

For general $V(\hat{x})$, express $\langle p|V(\hat{x})|\psi\rangle$ in terms of $\tilde{\psi}(p)$, and hence write down the time-independent Schrödinger equation in the momentum representation satisfied by $\tilde{\psi}(p)$.

Consider now the case $V(x) = -(\hbar^2\lambda/m)\delta(x), \lambda > 0$. Show that there is a bound state with energy $E = -\epsilon, \epsilon > 0$, with wavefunction $\tilde{\psi}(p)$ satisfying

$$\tilde{\psi}(p) = \frac{\hbar\lambda}{\pi}\frac{1}{2m\epsilon + p^2}\int_{-\infty}^{\infty}\tilde{\psi}(p')\,dp'.$$

Hence show that there is a unique value for ϵ and determine this value.

Solution: To show the initial results, we use the *completeness relations*, or *resolution of identity*, for the $|x\rangle$ and $|p\rangle$ bases:

$$\int dx\ |x\rangle\langle x| = I, \qquad \int dp\ |p\rangle\langle p| = I,$$

where I is the identity operator. Inserting these relations into $\langle x|\hat{p}|\psi\rangle$ and $\langle p|\hat{x}|\psi\rangle$ respectively, we have

$$\begin{aligned}
\langle x|\hat{p}|\psi\rangle &= \int dp\ \langle x|\hat{p}|p\rangle\langle p|\psi\rangle && \text{(inserting identity)}\\
&= \int dp\, p\,\langle x|p\rangle\langle p|\psi\rangle && \text{(since } \hat{p}\,|p\rangle = p\,|p\rangle\text{)}\\
&= \int dp\, p\left(\frac{1}{\sqrt{2\pi\hbar}}\exp\left(ipx/\hbar\right)\right)\langle p|\psi\rangle && \text{(given form of } \langle x|p\rangle \text{ in question)}\\
&= -i\hbar\frac{\partial}{\partial x}\left(\int dp\,\frac{1}{\sqrt{2\pi\hbar}}\exp\left(ipx/\hbar\right)\langle p|\psi\rangle\right) && (-i\hbar\partial_x(\exp(ipx/\hbar)) = p\exp(ipx/\hbar))\\
&= -i\hbar\frac{\partial}{\partial x}\left(\int dp\ \langle x|p\rangle\langle p|\psi\rangle\right) && \text{(given form of } \langle x|p\rangle \text{ in question)}\\
&= -i\hbar\frac{\partial}{\partial x}\psi(x) && \text{(resolution of identity, and } \psi(x) = \langle x|\psi\rangle\text{)}.
\end{aligned}$$

The argument for $\langle p|\hat{x}|\psi\rangle$ is exactly the same; all we need to do this time is remember that the inner product on Hilbert space exhibits *conjugate symmetry* $\langle p|x\rangle = \overline{\langle x|p\rangle}$, which is the origin of the minus sign in the result. Explicitly, we have

$$\begin{aligned}
\langle p|\hat{x}|\psi\rangle &= \int dx\ \langle p|\hat{x}|x\rangle \langle x|\psi\rangle && \text{(inserting identity)} \\
&= \int dx\, x \langle p|x\rangle \langle x|\psi\rangle && \text{(since } \hat{x}\,|x\rangle = x\,|x\rangle\text{)} \\
&= \int dx\, x \left(\frac{1}{\sqrt{2\pi\hbar}} \exp\left(-ipx/\hbar\right)\right) \langle x|\psi\rangle && \text{(given } \langle x|p\rangle = \overline{\langle p|x\rangle}\text{)} \\
&= i\hbar\frac{\partial}{\partial p}\left(\int dx\, \frac{1}{\sqrt{2\pi\hbar}} \exp\left(-ipx/\hbar\right) \langle x|\psi\rangle\right) && (i\hbar\partial_p(\exp(-ipx/\hbar)) = x\exp(-ipx/\hbar)) \\
&= i\hbar\frac{\partial}{\partial p}\left(\int dx\ \langle p|x\rangle \langle x|\psi\rangle\right) && \text{(given } \langle x|p\rangle = \overline{\langle p|x\rangle}\text{)} \\
&= i\hbar\frac{\partial}{\partial p}\tilde{\psi}(p) && \text{(resolution of identity, and } \tilde{\psi}(p) = \langle p|\psi\rangle\text{)}.
\end{aligned}$$

Recall that the position and momentum wavefunctions are related by a *Fourier transform* (in some special normalisation), which we can prove by inserting a resolution of identity as appropriate:

$$\begin{aligned}
\psi(x) &= \langle x|\psi\rangle && \text{(definition)} \\
&= \int dp\ \langle x|p\rangle \langle p|\psi\rangle && \text{(inserting identity)} \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int dp\, e^{ipx/\hbar}\tilde{\psi}(p) && \text{(given } \langle x|p\rangle\text{)}.
\end{aligned}$$

Similarly,

$$\begin{aligned}
\tilde{\psi}(p) &= \langle p|\psi\rangle && \text{(definition)} \\
&= \int dx\ \langle p|x\rangle \langle p|\psi\rangle && \text{(inserting identity)} \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int dx\, e^{-ipx/\hbar}\psi(x) && \text{(given } \langle x|p\rangle = \overline{\langle p|x\rangle}\text{)}.
\end{aligned}$$

Next, we are asked to express $\langle p|V(\hat{x})|\psi\rangle$ in terms of $\tilde{\psi}(p)$. We know that to construct $\tilde{\psi}(p)$ we must get a $\langle p|\psi\rangle$ somehow; this would suggest inserting a momentum resolution of identity. But that would leave $\langle p|V(\hat{x})|p'\rangle$ say, which is not easy to simplify - we must *also* insert a position resolution of identity to give $V(\hat{x})$ something to act on. Thus we have:

$$\begin{aligned}
\langle p|V(\hat{x})|\psi\rangle &= \iint dx dp'\ \langle p|V(\hat{x})|x\rangle \langle x|p'\rangle \langle p'|\psi\rangle && \text{(inserting two identities)} \\
&= \frac{1}{2\pi\hbar} \iint dx\, dp'\, V(x) e^{ix(p'-p)/\hbar}\tilde{\psi}(p') && (V(\hat{x})\,|x\rangle = V(x)\,|x\rangle, \tilde{\psi}(p') = \langle p'|\psi\rangle \text{ and given } \langle x|p\rangle = \overline{\langle p|x\rangle}) \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int dp'\, \tilde{V}(p-p')\tilde{\psi}(p') && \text{(where } \tilde{V} \text{ is the Fourier transform of } V\text{)} \\
&= \frac{1}{\sqrt{2\pi\hbar}}(\tilde{V} * \tilde{\psi})(p) && (* \text{ denotes convolution}).
\end{aligned}$$

Here, we have introduced the Fourier transform of the potential, given in this normalisation by:

$$\tilde{V}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int dx\, V(x) e^{-ipx/\hbar}.$$

We have also used the definition of the *convolution* of two functions:

$$(f * g)(u) = \int du'\, f(u - u') g(u').$$

Using the result we found for $\langle p|V(\hat{x})|\psi\rangle$, we are asked to find the time-independent Schrödinger equation in the momentum representation. Recall that the representation-independent form of the time-independent Schrödinger equation reads:

$$\hat{H}\,|\psi\rangle = E\,|\psi\rangle\,,$$

where the Hamiltonian is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}),$$

as specified in the question. Contracting the representation-independent form with $\langle p|$ on the left, we will find the representation of this equation in the momentum basis:

$$\langle p| \left(\frac{\hat{p}^2}{2m} + V(\hat{x}) \right) |\psi\rangle = \langle p|E|\psi\rangle \qquad \Rightarrow \qquad \frac{p^2}{2m}\tilde{\psi}(p) + \frac{1}{\sqrt{2\pi\hbar}}(\tilde{V} * \tilde{\psi})(p) = E\tilde{\psi}(p),$$

using $\langle p|\,\hat{p}^2 = p^2\,\langle p|$, and the result we derived above for the momentum representation of the potential.

We are now asked to specialise to a delta function potential $V(x) = -(\hbar^2\lambda/m)\delta(x)$, for $\lambda > 0$. To write down the time-independent Schrödinger equation explicitly in this case, we need to first evaluate the Fourier transform of this potential:

$$\tilde{V}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int dx\, V(x) e^{-ipx/\hbar} = -\frac{\hbar^2\lambda}{m\sqrt{2\pi\hbar}} \int dx\, \delta(x) e^{-ipx/\hbar} = -\frac{\hbar^2\lambda}{m\sqrt{2\pi\hbar}},$$

using the delta function to absorb the integral. Note that $\tilde{V}(p)$ is a constant, independent of p, so in particular the convolution with $\tilde{\psi}$ in the momentum representation of the time-independent Schrödinger equation reduces to:

$$(\tilde{V} * \tilde{\psi})(p) = \int_{-\infty}^{\infty} dp'\, \tilde{V}(p - p')\tilde{\psi}(p') = -\frac{\hbar^2\lambda}{m\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp'\, \tilde{\psi}(p').$$

Thus, the time-independent Schrödinger equation for a bound state with energy $E = -\epsilon$, becomes:

$$\frac{p^2}{2m}\tilde{\psi}(p) - \frac{\hbar\lambda}{2\pi m} \int_{-\infty}^{\infty} dp'\, \tilde{\psi}(p') = -\epsilon\tilde{\psi}(p) \qquad \Rightarrow \qquad \tilde{\psi}(p) = \frac{\hbar\lambda}{\pi(2m\epsilon + p^2)} \int_{-\infty}^{\infty} dp'\, \tilde{\psi}(p'), \tag{†}$$

as required.

It remains to find the value of ϵ. It's not completely obvious how to do this - so far, all we've done is derive a horrible integral equation for $\tilde{\psi}(p)$! However, there is a trick to finish. Notice that if we integrate both sides with respect to p over the domain $p \in (-\infty, \infty)$, we obtain

$$\int_{-\infty}^{\infty} dp\, \tilde{\psi}(p) = \left(\int_{-\infty}^{\infty} dp\, \frac{\hbar\lambda}{\pi(2m\epsilon + p^2)} \right) \int_{-\infty}^{\infty} dp'\, \tilde{\psi}(p'),$$

since the integral of $\tilde{\psi}(p')$ over $p' \in (-\infty, \infty)$ is just a constant, independent of p. The remaining integral on the right hand side can be performed exactly; we recognise it as an arctangent integral:

$$\int_{-\infty}^{\infty} dp\, \frac{\hbar\lambda}{\pi(2m\epsilon + p^2)} = \frac{\hbar\lambda}{\pi} \left[\frac{1}{\sqrt{2m\epsilon}} \arctan\left(\frac{p}{\sqrt{2m\epsilon}} \right) \right]_{-\infty}^{\infty} = \frac{\hbar\lambda}{\pi} \cdot \frac{1}{\sqrt{2m\epsilon}} \cdot \left(\frac{\pi}{2} - -\frac{\pi}{2} \right) = \frac{\hbar\lambda}{\sqrt{2m\epsilon}}.$$

Hence, substituting the result into the above, we have:

$$\int_{-\infty}^{\infty} dp\, \tilde{\psi}(p) = \frac{\hbar\lambda}{\sqrt{2m\epsilon}} \int_{-\infty}^{\infty} dp'\, \tilde{\psi}(p')$$

Thus we see that

$$\int_{-\infty}^{\infty} dp\, \tilde{\psi}(p) = 0,$$

and hence $\tilde{\psi}(p) = 0$ by (†), *unless* ϵ takes the specific value:

$$\frac{\hbar\lambda}{\sqrt{2m\epsilon}} = 1 \qquad \Rightarrow \qquad \epsilon = \frac{\hbar^2\lambda^2}{2m}.$$

2014, Paper 2, Section II, 33A

(i) Let a and $a^\dagger$ be the annihilation and creation operators, respectively, for a simple harmonic oscillator whose Hamiltonian is

$$H_0 = \omega\left(a^\dagger a + \frac{1}{2}\right).$$

with $[a, a^\dagger] = 1$. Explain how the set of eigenstates $\{|n\rangle : n = 0, 1, 2, \dots\}$ of H_0 is obtained and deduce the corresponding eigenvalues. Show that

$$a|0\rangle = 0,$$

$$a|n\rangle = \sqrt{n}\,|n-1\rangle, \quad n \geq 1,$$

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle, \quad n \geq 0.$$

(ii) Consider a system whose unperturbed Hamiltonian is

$$H_0 = \left(a^\dagger a + \frac{1}{2}\right) + 2\left(b^\dagger b + \frac{1}{2}\right),$$

where $[a, a^\dagger] = 1$, $[b, b^\dagger] = 1$ and all other commutators are zero. Find the degeneracies of the eigenvalues of H_0 with energies $E_0 = \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}$ and $\frac{11}{2}$.

The system is perturbed so that it is now described by the Hamiltonian

$$H = H_0 + \lambda H',$$

where $H' = (a^\dagger)^2 b + a^2 b^\dagger$. Using degenerate perturbation theory, calculate to $O(\lambda)$ the energies of the eigenstates associated with the level $E_0 = \frac{9}{2}$.

Write down the eigenstates, to $O(\lambda)$, associated with these perturbed energies. By explicit evaluation show that they are in fact exact eigenstates of H with these energies as eigenvalues.

Solution: (i) We can deduce the energy eigenstates of H_0 as follows. Let's begin by noticing that the spectrum of H_0 is bounded below, since for any normalised eigenstate $|E\rangle$ of H_0 of energy E, we have:

$$E = \langle E|H_0|E\rangle = \omega\langle E|a^\dagger a|E\rangle + \frac{1}{2}\omega = \omega||a|E\rangle||^2 + \frac{1}{2}\omega \geq \frac{1}{2}\omega.$$

Now suppose that $|E\rangle$ is an energy eigenstate of H_0 with energy E. We note that $a|E\rangle$ is also an energy eigenstate of H_0:

$$\begin{aligned}
H_0(a|E\rangle) &= \omega\left(a^\dagger a + \frac{1}{2}\right)a|E\rangle && \text{(definition of } H_0\text{)}\\
&= \omega\left(aa^\dagger + [a^\dagger, a] + \frac{1}{2}\right)a|E\rangle && \text{(commuting } a, a^\dagger\text{)}\\
&= a\omega\left(a^\dagger a + [a^\dagger, a] + \frac{1}{2}\right)|E\rangle && \text{(taking out } a \text{ to left)}\\
&= aH_0|E\rangle - \omega a|E\rangle && \text{(definition of } H_0\text{, and } [a^\dagger, a] = -1\text{)}\\
&= (E-\omega)(a|E\rangle) && \text{(since } H_0|E\rangle = E|E\rangle\text{)}
\end{aligned}$$

Thus $|E\rangle$, $a|E\rangle$, $a^2|E\rangle$, ... , $a^n|E\rangle$ is a sequence of energy eigenstates of H_0 with increasingly lower energies E, $E-\omega$, $E-2\omega$, ... , $E-n\omega$. Unless this sequence suddenly terminates, then we will find that H_0 has a spectrum that is unbounded below.

It follows that there must exist a non-negative integer n such that $a^{n+1}|E\rangle = 0$. In particular (assuming that H_0 has *some* energy eigenstate $|E\rangle$), this proves the existence of a state $|0\rangle$ ($= a^n|E\rangle$) such that $a|0\rangle = 0$. We see that this state has energy:

$$H_0|0\rangle = \omega\left(a^\dagger a + \frac{1}{2}\right)|0\rangle = \frac{1}{2}\omega|0\rangle\,.$$

Looking at the energies of our sequence from above ($E, E-\omega, E-2\omega, \ldots, E-n\omega$) we also see that this implies

$$E - n\omega = \frac{1}{2}\omega \qquad \Rightarrow \qquad E = \omega\left(n + \frac{1}{2}\right),$$

for some non-negative integer n.

So far we have shown that there exists a state $|0\rangle$ of minimal energy $\frac{1}{2}\omega$, and any eigenstate $|n\rangle$ of H_0 must have energy of the form $E_n = \omega\left(n + \frac{1}{2}\right)$ for some non-negative integer n. We now *inductively construct* a state of energy E_n for each n.

Suppose that $|n\rangle$ is a state of energy E_n, as described above. Then $a^\dagger|n\rangle$ is an eigenstate of H_0 with energy E_{n+1}:

$$\begin{aligned}
H_0(a^\dagger|n\rangle) &= \omega\left(a^\dagger a + \frac{1}{2}\right)a^\dagger|n\rangle && \text{(definition of } H_0\text{)}\\
&= \omega\left(a^\dagger a^\dagger a + a^\dagger[a,a^\dagger] + \frac{1}{2}a^\dagger\right)|n\rangle && \text{(commuting } a^\dagger, a\text{)}\\
&= a^\dagger\omega\left(a^\dagger a + [a,a^\dagger] + \frac{1}{2}\right)|n\rangle && \text{(taking out } a^\dagger \text{ to left)}\\
&= a^\dagger H_0|n\rangle + \omega a|n\rangle && \text{(definition of } H_0\text{, and } [a,a^\dagger] = +1\text{)}\\
&= (E_n + \omega)(a^\dagger|n\rangle) && \text{(since } H_0|n\rangle = E_n|n\rangle\text{)}\\
&= E_{n+1}a^\dagger|n\rangle
\end{aligned}$$

where the last equality follows since $E_n + \omega = \omega(n + \frac{1}{2}) + \omega = \omega(n + 1 + \frac{1}{2}) = E_{n+1}$.

Hence we have found $a^\dagger|n\rangle \propto |n+1\rangle$. We can find the appropriate normalisation of the state as follows:

$$||a^\dagger|n\rangle||^2 = \langle n|aa^\dagger|n\rangle = \langle n|a^\dagger a|n\rangle + \langle n|[a,a^\dagger]|n\rangle = \omega^{-1}\langle n|(H_0 - \omega/2)|n\rangle + 1 = n+1.$$

Thus we can consistently choose $a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$. In particular, dividing through by the normalisation and iterating, we have constructed the eigenstates of H_0:

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle\,, \qquad \text{with energies} \qquad E_n = \omega\left(n + \frac{1}{2}\right).$$

The energy eigenstates are non-degenerate, since we are working in one dimension. Hence these are precisely all the energy eigenstates and energy eigenvalues.

We are also asked to quickly derive the result $a|n\rangle = \sqrt{n}\,|n-1\rangle$. We already saw that $a|n\rangle$ is an energy eigenstate of energy $E_n - \omega = E_{n-1}$, hence we already have $a|n\rangle \propto |n-1\rangle$. We can find the proportionality constant similar to before:

$$||a|n\rangle||^2 = \langle n|a^\dagger a|n\rangle = \omega^{-1}\langle n|(H_0 - \omega/2)|n\rangle = n.$$

Hence we have $a|n\rangle = \sqrt{n}\,|n-1\rangle$, as required.

(ii) Since all the a's and all the b's commute, the given Hamiltonian can be equivalently viewed as a tensor product:

$$H_0 = \left(a^\dagger a + \frac{1}{2}\right) \otimes I + I \otimes 2\left(b^\dagger b + \frac{1}{2}\right)$$

acting on the Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$, the product of a harmonic oscillator of frequency $\omega = 1$ and another harmonic oscillator of frequency $\omega = 2$, with basis given by:

$$|n, m\rangle := |n\rangle \otimes |m\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle \otimes \frac{(b^\dagger)^m}{\sqrt{m!}} |0\rangle ,$$

where $n, m \geq 0$. The state $|n, m\rangle$ has energy

$$E_{n,m} = n + \frac{1}{2} + 2\left(m + \frac{1}{2}\right) = n + 2m + \frac{3}{2}.$$

We are asked to find the degeneracy of lots of energy levels. We have:

- $E_0 = \frac{3}{2}$ is only possible if $n = m = 0$. Thus we have degeneracy 1.
- $E_0 = \frac{5}{2}$ requires $n + 2m = 1$. This is only possible if $n = 1, m = 0$. Thus we have degeneracy 1.
- $E_0 = \frac{7}{2}$ requires $n + 2m = 2$. This is possibly only if $n = 2, m = 0$ *or* $n = 0, m = 1$. Thus we have degeneracy 2.
- $E_0 = \frac{9}{2}$ requires $n+2m = 3$. Again, we see there are two possibilities here: $(n, m) = (3, 0), (1, 1)$. Hence we have degeneracy 2.
- $E_0 = \frac{11}{2}$ requires $n+2m = 4$. There are three options here: $(n, m) = (4, 0), (2, 1), (0, 2)$; hence we have threefold degeneracy.

We are now given a perturbation of the Hamiltonian:

$$\lambda H' = \lambda \left((a^\dagger)^2 b + a^2 b^\dagger\right) .$$

We are asked to calculate the first-order corrections to the energy level $E_0 = \frac{9}{2}$ in the presence of this perturbation. Recall that the way to do this is to *diagonalise the perturbation in the degenerate subspace*.

The basis states of the degenerate subspace are in this case those corresponding to $(n, m) = (3, 0)$ and $(1, 1)$, i.e. $|3, 0\rangle$, $|1, 1\rangle$. The matrix of $\lambda H'$ in this subspace can be calculated as follows:

- The first matrix element is:

  $$\langle 1, 1|\lambda H'|1, 1\rangle = \lambda \langle 1, 1|(a^\dagger)^2 b + a^2 b^\dagger|1, 1\rangle .$$

  Acting with $(a^\dagger)^2$ to the left annihilates $\langle 1, 1|$. Acting to the right with a^2 (recall all the a's and b's commute) annihilates $|1, 1\rangle$. So we find:

  $$\langle 1, 1|\lambda H'|1, 1\rangle = 0.$$

- The second matrix element is:

  $$\langle 1, 1|\lambda H'|3, 0\rangle = \lambda \langle 1, 1|(a^\dagger)^2 b + a^2 b^\dagger|3, 0\rangle .$$

  We see that the first term includes a b, which annihilates $|3, 0\rangle$ to the right. The action of the second term of $|3, 0\rangle$ is given by the relations we derived in part (i):

  $$a^2 b^\dagger |3, 0\rangle = \sqrt{3 \cdot 2}\, |1, 1\rangle = \sqrt{6}\, |1, 1\rangle .$$

  Hence we see $\langle 1, 1|\lambda H'|3, 0\rangle = \lambda\sqrt{6}$.

- The third matrix element is:

$$\langle 3,0|\lambda H'|1,1\rangle = \overline{\langle 1,1|\lambda H'|3,0\rangle} = \lambda\sqrt{6},$$

by conjugate symmetry.

- The final matrix element is:

$$\langle 3,0|\lambda H'|3,0\rangle = \lambda \langle 3,0|(a^\dagger)^2 b + a^2 b^\dagger|3,0\rangle .$$

The first term annihilates $|3,0\rangle$ via b acting to the right. The second term annihilates $\langle 3,0|$ via $b^\dagger$ acting to the left. Hence we find:

$$\langle 3,0|\lambda H'|3,0\rangle = 0.$$

It follows that the matrix of $\lambda H'$ in the degenerate subspace, with the basis $\{|1,1\rangle, |3,0\rangle\}$, is given by:

$$\lambda H'\Big|_{\text{degnerate subspace}} = \lambda \begin{pmatrix} 0 & \sqrt{6} \\ \sqrt{6} & 0 \end{pmatrix} = \lambda\sqrt{6} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

By inspection, we see that the eigenvalues and the eigenvectors of this matrix are simply:

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} \text{ with eigenvalue } \lambda\sqrt{6}, \qquad \begin{pmatrix} 1 \\ -1 \end{pmatrix} \text{ with eigenvalue } -\lambda\sqrt{6}.$$

Hence the perturbed states and their energies are given by:

$$|1,1\rangle \pm |3,0\rangle \quad \text{ with energy } \quad \frac{9}{2} \pm \lambda\sqrt{6},$$

to first order in λ.

Finally, we are asked to verify that these states are exact eigenstates of the perturbed Hamiltonian. We already know that these states are exact eigenstates of $\lambda H'$ by the work above (they are literally eigenvectors of the matrix of $\lambda H'$!); that is:

$$\lambda H' \left(|1,1\rangle \pm |3,0\rangle\right) = \pm\lambda\sqrt{6} \left(|1,1\rangle \pm |3,0\rangle\right).$$

Hence, by linearity, we need only check the action of H_0 on these eigenstates:

$$H_0 \left(|1,1\rangle \pm |3,0\rangle\right) = E_{1,1}|1,1\rangle \pm E_{3,0}|3,0\rangle = \frac{9}{2}\left(|1,1\rangle \pm |3,0\rangle\right)$$

Hence we indeed have:

$$\left(H_0 + \lambda H'\right)\left(|1,1\rangle \pm |3,0\rangle\right) = \left(\frac{9}{2} \pm \lambda\sqrt{6}\right)\left(|1,1\rangle \pm |3,0\rangle\right),$$

as required.

2014, Paper 3, Section II, 33A

Let $\mathbf{J} = (J_1, J_2, J_3)$ and $|jm\rangle$ denote the standard angular-momentum operators and states so that, in units where $\hbar = 1$,

$$\mathbf{J}^2 |jm\rangle = j(j+1) |jm\rangle , \quad J_3 |jm\rangle = m |jm\rangle .$$

Show that $U(\theta) = \exp(-i\theta J_2)$ is unitary. Define

$$J_i(\theta) = U(\theta) J_i U^{-1}(\theta), \qquad \text{for } i = 1, 2, 3$$

and

$$|jm\rangle_\theta = U(\theta) |jm\rangle .$$

Find expressions for $J_1(\theta)$, $J_2(\theta)$ and $J_3(\theta)$ as linear combinations of J_1, J_2 and J_3. Briefly explain why $U(\theta)$ represents rotation of $\mathbf{J}$ through angle θ about the 2-axis.

Show that

$$J_3(\theta) |jm\rangle_\theta = m |jm\rangle_\theta . \tag{$*$}$$

Express $|10\rangle_\theta$ as a linear combination of the states $|1m\rangle$, $m = -1, 0, 1$. By expressing J_1 in terms of $J_\pm$, use $(*)$ to determine the coefficients in this expansion.

A particle of spin 1 is in the state $|10\rangle$ at time $t = 0$. It is subject to the Hamiltonian

$$H = -\mu \mathbf{B} \cdot \mathbf{J},$$

where $\mathbf{B} = (0, B, 0)$. At time t the value of J_3 is measured and found to be $J_3 = 0$. At time $2t$ the value of J_3 is measured again and found to be $J_3 = 1$. Show that the joint probability for these two values to be measured is:

$$\frac{1}{8} \sin^2 (2\mu B t) .$$

[*The following result may be quoted:* $J_\pm |jm\rangle = \sqrt{(j \mp m)(j \pm m + 1)} \, |j \, m \pm 1\rangle$.]

Solution: First, we are asked to show that the given operator $U(\theta)$ is unitary. We have:

$$U(\theta)U(\theta)^\dagger = \exp(-i\theta J_2)) \exp(-i\theta J_2)^\dagger = \exp(-i\theta J_2) \exp\left(i\theta J_2^\dagger\right) .$$

We can take the dagger inside the exponential by considering the expansion of the exponential as a series, for example. Since $\mathbf{J}$ is an observable, is is Hermitian, and in particular its components are Hermitian. Thus $J_2^\dagger = J_2$. Finally, we can combine the exponentials because their arguments commute, so we have:

$$U(\theta)U(\theta)^\dagger = \exp(-i\theta J_2) \exp(i\theta J_2) = \exp(-i\theta J_2 + i\theta J_2) = \exp(0) = I.$$

Thus $U(\theta)$ is unitary, as required.

We are now given that $J_i(\theta) = U(\theta) J_i U(\theta)^{-1}$. We would like to write the right hand side in terms of J_1, J_2 and J_3. Since we have a parameter θ on both sides of the equation, we remember a trick that can sometimes work in quantum mechanics to simplify things: differentiate with respect to that parameter![1] We have:

$$\frac{dJ_i(\theta)}{d\theta} = \frac{dU(\theta)}{d\theta} J_i U(\theta)^{-1} + U(\theta) J_i \frac{dU(\theta)^{-1}}{d\theta}.$$

[1] See for example, Examples Sheet 1, Question 2 or Examples Sheet 4, Question 5.

The derivatives are given by:

$$\frac{dU(\theta)}{d\theta} = \frac{d}{d\theta}\left(\exp\left(-i\theta J_2\right)\right) = \exp\left(-i\theta J_2\right)\left(-iJ_2\right) = U(\theta)(-iJ_2),$$

and

$$\frac{dU(\theta)^{-1}}{d\theta} = \frac{d}{d\theta}\left(\exp\left(i\theta J_2\right)\right) = iJ_2\exp\left(i\theta J_2\right) = iJ_2U(\theta)^{-1}.$$

If we wanted to derive these results really carefully, we'd use the series expansion of the exponential. Note that it doesn't matter which side we pull out the $\pm iJ_2$ to, since $\pm iJ_2$ commutes with $\exp\left(\pm i\theta J_2\right)$. Substituting these derivatives into the above, we have the differential equation:

$$\frac{dJ_i(\theta)}{d\theta} = U(\theta)(-iJ_2)J_iU(\theta)^{-1} + U(\theta)J_i(iJ_2)U(\theta)^{-1} = -iU(\theta)[J_2, J_i]U(\theta)^{-1}.$$

Using the standard angular-momentum commutation relations

$$[J_2, J_i] = i\epsilon_{2ik}J_k,$$

this simplifies to:

$$\frac{dJ_i(\theta)}{d\theta} = \epsilon_{2ik}U(\theta)J_kU(\theta)^{-1} = \epsilon_{2ik}J_k(\theta).$$

Writing out in components, we have:

$$\frac{dJ_1(\theta)}{d\theta} = -J_3(\theta), \qquad \frac{dJ_2(\theta)}{d\theta} = 0, \qquad \frac{dJ_3(\theta)}{d\theta} = J_1(\theta).$$

The second equation has the trivial solution $J_2(\theta) = J_2(0) = J_2$. The remaining coupled equations can be solved by differentiating both equations:

$$\frac{d^2J_1(\theta)}{d\theta^2} = -\frac{dJ_3(\theta)}{d\theta} = -J_1(\theta), \qquad \frac{d^2J_3(\theta)}{d\theta^2} = \frac{dJ_1(\theta)}{d\theta} = -J_3(\theta).$$

Using the boundary conditions $J_1(0) = J_1$, $J_3(0) = J_3$ and

$$\left.\frac{dJ_1}{d\theta}\right|_{\theta=0} = -J_3, \qquad \left.\frac{dJ_3}{d\theta}\right|_{\theta=0} = J_1,$$

from the first order equations, the second-order equations have the solutions:

$$J_1(\theta) = \cos(\theta)J_1 - \sin(\theta)J_3, \qquad J_3(\theta) = \sin(\theta)J_1 + \cos(\theta)J_3.$$

Altogether then, we see that

$$\mathbf{J}(\theta) = \begin{pmatrix} J_1(\theta) \\ J_2(\theta) \\ J_3(\theta) \end{pmatrix} = U(\theta)\mathbf{J}U(\theta)^{-1} = \begin{pmatrix} \cos(\theta) & 0 & -\sin(\theta) \\ 0 & 1 & 0 \\ \sin(\theta) & 0 & \cos(\theta) \end{pmatrix} \begin{pmatrix} J_1 \\ J_2 \\ J_3 \end{pmatrix}.$$

Hence $U(\theta)$ acts on the operator $\mathbf{J}$ as a rotation by angle θ about the 2-axis, as required.

We are now asked to consider the action of $U(\theta)$ on states. First, we look at the state $|jm\rangle_\theta = U(\theta)\,|jm\rangle$. This is an eigenstate of $J_3(\theta)$:

$$J_3(\theta)\,|jm\rangle_\theta = U(\theta)J_3U(\theta)^{-1}U(\theta)\,|jm\rangle = U(\theta)J_3\,|jm\rangle = mU(\theta)\,|jm\rangle = m\,|jm\rangle_\theta\,,$$

as required.

We are now asked to express $|10\rangle_\theta$ in terms of the states $|1m\rangle$ for $m = -1, 0, 1$. But why should we be able to achieve this in the first place? It is because $|10\rangle_\theta$ is an eigenvector of $\mathbf{J}^2$ with eigenvalue $1(1+1)$, and hence must be in the eigenspace $\mathrm{span}\{|1m\rangle : m = -1, 0, 1\}$. We can see this by noting:

$$\mathbf{J}^2 |10\rangle_\theta = \mathbf{J}^2 U(\theta) |10\rangle = U(\theta)\mathbf{J}^2 |10\rangle = 1(1+1)U(\theta) |10\rangle = 1(1+1) |10\rangle_\theta ,$$

where we have used the fact that J_2 commutes with $\mathbf{J}^2$, which implies $U(\theta)$ commutes with $\mathbf{J}^2$.

Therefore, let's write:

$$|10\rangle_\theta = a |1,-1\rangle + b |10\rangle + c |11\rangle$$

for some complex coefficients a, b and c. Now, let's recap what we know about both sides: (i) both sides are eigenstates of $J_3(\theta)$ with eigenvalues 0; (ii) both sides are eigenstates of $\mathbf{J}^2$ with eigenvalue $1(1+1)$; (iii) both sides are normalised states. Condition (ii) is trivially satisfied, but (i) and (iii) will give us more information.

Acting on both sides with $J_3(\theta)$ then, we have:

$$0 = J_3(\theta) |10\rangle_\theta = (\sin(\theta)J_1 + \cos(\theta)J_3) (a |1,-1\rangle + b |10\rangle + c |11\rangle) ,$$

where we have expressed $J_3(\theta)$ in terms of J_1 and J_3 using our earlier work. Now recalling that the angular momentum raising and lowering operators are defined by $J_\pm := J_1 \pm iJ_2$, we see that we can write J_1 in terms of the angular momentum raising and lowering operators as:

$$J_1 = \frac{J_+ + J_-}{2}.$$

In our case, we will use the facts $J_+ |1m\rangle = \sqrt{(1-m)(2+m)}\,|1m\rangle$ and $J_- |1m\rangle = \sqrt{(1+m)(2-m)}\,|1m\rangle$ given in the question, together with $J_3 |1m\rangle = m |1m\rangle$. Thus, the right hand side reduces to:

$$0 = \left(\sin(\theta)\left(\frac{J_+ + J_-}{2}\right) + \cos(\theta)J_3\right) (a |1,-1\rangle + b |10\rangle + c |11\rangle)$$

$$= \frac{\sqrt{2}\sin(\theta)}{2} (a |10\rangle + b |11\rangle + b |1,-1\rangle + c |10\rangle) + \cos(\theta) (-a |1,-1\rangle + c |11\rangle) .$$

Comparing coefficients, we see that we require:

$$\frac{\sqrt{2}\sin(\theta)}{2} b = -c\cos(\theta), \qquad a = -c, \qquad \text{and} \qquad \frac{\sqrt{2}\sin(\theta)}{2} c = a\cos(\theta).$$

Eliminating a, b in favour of c leaves: $|10\rangle_\theta = -c |1,-1\rangle - \sqrt{2}\cot(\theta)c |10\rangle + c |11\rangle$. Requiring the correct normalisation then gives the equation:

$$2|c|^2 \left(1 + \cot^2(\theta)\right) = 1 \qquad \Rightarrow \qquad c = \frac{\sin(\theta)}{\sqrt{2}},$$

up to an arbitrary phase. Thus we have:

$$|10\rangle_\theta = -\frac{\sin(\theta)}{\sqrt{2}} |1,-1\rangle - \cos(\theta) |10\rangle + \frac{\sin(\theta)}{\sqrt{2}} |11\rangle$$

up to an arbitrary phase.

For the final part of the question, we are told that a spin one particle is subject to the Hamiltonian:

$$H = -\mu \mathbf{B} \cdot \mathbf{J} = -\mu B J_2.$$

In particular, this implies that the time-evolution operator associated to this Hamiltonian is given by:

$$U_T(t) = \exp(-iHt) = \exp(i\mu B t J_2) = U(-\mu B t),$$

where $U(\theta) = U(-\mu B t)$ is a rotation operator as studied in this question.

Initially, we are told the system is in the state $|10\rangle$. Evolving using the time-evolution operator for a time t, we have:

$$U_T(t)|10\rangle = U(-\mu B t)|10\rangle = |10\rangle_{-\mu B t} = \frac{\sin(\mu B t)}{\sqrt{2}}|1,-1\rangle - \cos(\mu B t)|10\rangle - \frac{\sin(\mu B t)}{\sqrt{2}}|11\rangle,$$

using the expression we found earlier in the question for $|10\rangle_\theta$. We see that the probability of measuring $J_3 = 0$ at time t is given by:

$$\cos^2(\mu B t).$$

Supposing that we indeed measure this eigenvalue, then we immediately collapse to the eigenstate $|10\rangle$ after the measurement. Evolving for a further time t, we get to the exact same state again. The probability of measuring $J_3 = 1$ at time t if we start from the state $|10\rangle$ is given simply by:

$$\frac{1}{2}\sin^2(\mu B t).$$

Hence the required joint probability of measuring $J_3 = 0$ at time t *and* $J_3 = 1$ at time $2t$ is given by:

$$\frac{1}{2}\sin^2(\mu B t)\cos^2(\mu B t) = \frac{1}{8}\sin^2(2\mu B t),$$

as required.

2014, Paper 4, Section II, 32A

Define the *interaction picture* for a quantum mechanical system with Schrödinger picture Hamiltonian $H_0+V(t)$ and explain why the interaction and Schrödinger pictures give the same physical predictions for transition rates between eigenstates of H_0. Derive the equation of motion for the interaction picture states $|\overline{\psi(t)}\rangle$.

A system consists of just two states $|1\rangle$ and $|2\rangle$, with respect to which

$$H_0 = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}, \qquad V(t) = \hbar\lambda \begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix}.$$

Writing the interaction picture state as $|\overline{\psi(t)}\rangle = a_1(t)\,|1\rangle + a_2(t)\,|2\rangle$, show that the interaction picture equation of motion can be written as:

$$i\dot{a}_1(t) = \lambda e^{i\mu t} a_2(t), \qquad i\dot{a}_2(t) = \lambda e^{-i\mu t} a_1(t), \tag{$*$}$$

where $\mu = \omega - \omega_{21}$ and $\omega_{21} = (E_2 - E_1)/\hbar$. Hence show that $a_2(t)$ satisfies

$$\ddot{a}_2 + i\mu\dot{a}_2 + \lambda^2 a_2 = 0.$$

Given that $a_2(0) = 0$, show that the solution takes the form

$$a_2(t) = \alpha e^{-i\mu t/2}\sin(\Omega t),$$

where Ω is a frequency to be determined and α is a complex constant of integration.

Substitute this solution for $a_2(t)$ into $(*)$ to determine $a_1(t)$ and, by imposing the normalisation condition $|||\overline{\psi(t)}\rangle||^2 = 1$ at $t = 0$, show that $|\alpha|^2 = \lambda^2/\Omega^2$.

At time $t = 0$, the system is in state $|1\rangle$. Write down the probability of finding the system in the state $|2\rangle$ at time t.

Solution: The *interaction picture* for a quantum mechanical system is defined in terms of *interaction states* and *interaction operators*, which are given in terms of their Schrödinger picture counterparts (written $|\psi_S\rangle$ and A_S respectively) by:

$$|\psi_I(t)\rangle = e^{iH_0 t/\hbar}\,|\psi_S(t)\rangle\,, \qquad A_I(t) = e^{iH_0 t/\hbar} A_S e^{-iH_0 t/\hbar},$$

where $U_0(t) = e^{-iH_0 t/\hbar}$ is the time-evolution operator of the free Hamiltonian H_0, and $e^{iH_0 t/\hbar}$ is its inverse.

Physical predictions of the theory are given entirely in terms of matrix elements of the theory, and since for any two states $|\psi\rangle$, $|\phi\rangle$ and any operator A in either the Schrödinger picture or the interaction picture, we have:

$$\langle\phi_S|A_S|\psi_S\rangle = \langle\phi_S|e^{-iH_0 t/\hbar}e^{iH_0 t/\hbar}A_S e^{-iH_0 t/\hbar}e^{iH_0 t/\hbar}|\psi_S\rangle = \langle\phi_I|A_I(t)|\psi_I\rangle\,,$$

we see that the predictions of the two pictures are entirely equivalent.

Finally, we are asked to derive the equation of motion for interaction pictures states. Acting on an interaction picture state $|\psi_I\rangle$ with a time derivative, we have

$$i\hbar\frac{\partial}{\partial t}\,|\psi_I(t)\rangle = i\hbar\frac{\partial}{\partial t}\left(e^{iH_0 t/\hbar}\,|\psi_S(t)\rangle\right) = -H_0 e^{iH_0 t/\hbar}\,|\psi_S(t)\rangle + e^{iH_0 t/\hbar}(H_0 + V(t))\,|\psi_S(t)\rangle\,,$$

using Schrödinger's equation for the Schrödinger picture state $|\psi_S(t)\rangle$. Since H_0 commutes with $e^{iH_0 t/\hbar}$, we can simplify the right hand side leaving:

$$i\hbar\frac{\partial}{\partial t}\,|\psi_I(t)\rangle = e^{iH_0 t/\hbar}V(t)\,|\psi_S(t)\rangle = e^{iH_0 t/\hbar}V(t)e^{-iH_0 t/\hbar}e^{iH_0 t/\hbar}\,|\psi_S(t)\rangle = V_I(t)\,|\psi_I(t)\rangle$$

$$\Rightarrow \qquad i\hbar\frac{\partial}{\partial t}\,|\psi_I(t)\rangle = V_I(t)\,|\psi_I(t)\rangle\,,$$

which is the interaction picture equation of motion as required.

For the rest of the question, we work with a specific two-state system with given $H_0, V(t)$; throughout we will write states as column vectors and operators as 2×2 matrices. Let's begin by noting that for the given H_0, the inverse of the free time-evolution operator is given by:

$$e^{iH_0 t/\hbar} = \begin{pmatrix} e^{iE_1 t/\hbar} & 0 \\ 0 & e^{iE_2 t/\hbar} \end{pmatrix}.$$

It follows that the interaction term $V(t)$ in the interaction picture is given by:

$$\begin{aligned} e^{iH_0 t/\hbar} V(t) e^{-iH_0 t/\hbar} &= \hbar\lambda \begin{pmatrix} e^{iE_1 t/\hbar} & 0 \\ 0 & e^{iE_2 t/\hbar} \end{pmatrix} \begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix} \begin{pmatrix} e^{-iE_1 t/\hbar} & 0 \\ 0 & e^{-iE_2 t/\hbar} \end{pmatrix} \\ &= \hbar\lambda \begin{pmatrix} 0 & \exp\left(it\left(\frac{E_1 - E_2}{\hbar} + \omega\right)\right) \\ \exp\left(it\left(\frac{E_2 - E_1}{\hbar} - \omega\right)\right) & 0 \end{pmatrix} \\ &= \hbar\lambda \begin{pmatrix} 0 & e^{i\mu t} \\ e^{-i\mu t} & 0 \end{pmatrix}, \end{aligned}$$

where $\mu = \omega - (E_2 - E_1)/\hbar$ is defined in the question. Since the state $|\psi_I(t)\rangle = (a_1(t), a_2(t))$ is given in column vector form, it follows the the interaction picture equation of motion can be written in the form:

$$i\hbar \frac{\partial}{\partial t} |\psi_I(T)\rangle = V_I(t) |\psi_I(t)\rangle \qquad \Rightarrow \qquad i \begin{pmatrix} \dot{a}_1 \\ \dot{a}_2 \end{pmatrix} = \begin{pmatrix} 0 & \lambda e^{i\mu t} \\ \lambda e^{-i\mu t} & 0 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}.$$

Hence we have the coupled system of equations:

$$i\dot{a}_1 = \lambda e^{i\mu t} a_2, \qquad i\dot{a}_2 = \lambda e^{-i\mu t} a_1,$$

as required.

We must now solve these equations in the way specified by the question. First, we can decouple the equations as suggested. Differentiating the second, we have:

$$i\ddot{a}_2 = -i\lambda\mu e^{-i\mu t} a_1 + \lambda e^{-i\mu t} \dot{a}_1 = \mu \dot{a}_2 - i\lambda^2 a_2,$$

substituting for $\lambda e^{-i\mu t} a_1$ and $\dot{a}_1$ using the original equations. Simplifying, we get the equation:

$$\ddot{a}_2 + i\mu \dot{a}_2 + \lambda^2 a_2 = 0,$$

as required.

This is a second order linear differential equation with constant coefficients. Its auxiliary equation is given by:

$$\epsilon^2 + i\mu\epsilon + \lambda^2 = 0 \qquad \Rightarrow \qquad \epsilon_\pm = -\frac{i\mu}{2} \pm \frac{i}{2}\sqrt{\mu^2 + 4\lambda^2}.$$

It follows that the solutions are given by:

$$a_2(t) = \alpha e^{-i\mu t/2} \sin\left(\frac{\sqrt{\mu^2 + 4\lambda^2}}{2} t\right) + \beta e^{-i\mu t/2} \cos\left(\frac{\sqrt{\mu^2 + 4\lambda^2}}{2} t\right).$$

Given the initial condition $a_2(0) = 0$, we have $\beta = 0$. So the particular solution in our case is:

$$a_2(t) = \alpha e^{-i\mu t/2} \sin\left(\frac{\sqrt{\mu^2 + 4\lambda^2}}{2} t\right),$$

as required. We see that the frequency Ω in the question is given by:

$$\Omega = \frac{\sqrt{\mu^2 + 4\lambda^2}}{2}.$$

It remains to determine $a_1(t)$. Simply looking at the original coupled system of equations, we see that:

$$a_1(t) = \frac{i\dot{a}_2(t)}{\lambda} e^{i\mu t},$$

so we need only differentiate $a_2(t)$ to obtain $a_1(t)$. Carrying this out, we find the result:

$$a_1(t) = \frac{i\alpha}{\lambda} e^{i\mu t/2} \left(\Omega \cos(\Omega t) - \frac{i\mu}{2} \sin(\Omega t) \right).$$

The normalisation condition at time $t = 0$ then determines:

$$|a_1(0)|^2 + |a_2(0)|^2 = 1 \qquad \Rightarrow \qquad |\alpha|^2 \frac{\Omega^2}{\lambda^2} + 0 = 1 \qquad \Rightarrow \qquad |\alpha|^2 = \frac{\lambda^2}{\Omega^2},$$

as required.

Finally, we are told that the system is in state $|1\rangle$ at time $t = 0$, i.e. we have $a_2(0) = 0$. We know from all our above work that the probability of finding the system is state $|2\rangle$ at time $t = 0$ is given by:

$$|a_2(t)|^2 = |\alpha|^2 \sin^2(\Omega t) = \frac{\lambda^2}{\Omega^2} \sin^2(\Omega t).$$

2015, Paper 1, Section II, 31A

If A and B are operators which each commute with their commutator $[A, B]$, show that

$$F(\lambda) = e^{\lambda A} e^{\lambda B} e^{-\lambda(A+B)} \qquad \text{satisfies} \qquad F'(\lambda) = \lambda [A, B] F(\lambda).$$

By solving this differential equation for $F(\lambda)$, deduce that

$$e^A e^B = e^{\frac{1}{2}[A,B]} e^{A+B}.$$

The annihilation and creation operators for a harmonic oscillator of mass m and frequency ω are defined by

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i}{m\omega} \hat{p} \right), \qquad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i}{m\omega} \hat{p} \right).$$

Write down an expression for the general normalised eigenstate $|n\rangle$ ($n = 0, 1, 2, \ldots$) of the oscillator Hamiltonian H in terms of the ground state $|0\rangle$. What is the energy eigenvalue E_n of the state $|n\rangle$?

Suppose the oscillator is now subject to a small perturbation so that it is described by the modified Hamiltonian $H + \epsilon V(\hat{x})$ with $V(\hat{x}) = \cos(\mu \hat{x})$. Show that

$$V(\hat{x}) = \frac{1}{2} e^{-\gamma^2/2} \left(e^{i\gamma a^\dagger} e^{i\gamma a} + e^{-i\gamma a^\dagger} e^{-i\gamma a} \right),$$

where γ is a constant, to be determined. Hence show that to $O(\epsilon^2)$ the shift in the ground state energy as a result of the perturbation is

$$\epsilon e^{-\mu^2 \hbar / 4m\omega} - \epsilon^2 e^{-\mu^2 \hbar / 2m\omega} \frac{1}{\hbar\omega} \sum_{p=1}^{\infty} \frac{1}{(2p)! 2p} \left(\frac{\mu^2 \hbar}{2m\omega} \right)^{2p}.$$

[*Standard results of perturbation theory may be quoted without proof.*]

Solution: The first part of this question is the same as Examples Sheet 1, Question 2; it's discussed in much more detail there. Taking the derivative, we have:

$$F'(\lambda) = e^{\lambda A} A e^{\lambda B} e^{-\lambda(A+B)} + e^{\lambda A} e^{\lambda B} B e^{-\lambda(A+B)} - e^{\lambda A} e^{\lambda B} (A+B) e^{\lambda(A+B)} = e^{\lambda A} [A, e^{\lambda B}] e^{-\lambda(A+B)}.$$

We see that we need to evaluate the commutator $[A, e^{\lambda B}]$. We evaluate this in two steps:

- First, we evaluate $[A, B^n]$. Recall that if A, B both commute with their commutator, then commutators are like derivatives as we saw on Examples Sheet 1. So $[A, B^n] = nB^{n-1}[A, B]$ should be our guess.

  We can prove this guess by induction. The base case $n = 1$ is trivial. Suppose the result is true for $n = k$ and consider $n = k + 1$. Then we have:

  $$[A, B^{k+1}] = [A, B^k] B + B^k [A, B] = k B^{k-1} [A, B] B + B^k [A, B] = (k+1) B^k [A, B],$$

  using the induction hypothesis and the fact that A and B both commute with their commutator. The result follows by inducion.

- Using this result, we can evaluate $[A, e^{\lambda B}]$. Expanding the exponential in its Taylor series, we have:

  $$[A, e^{\lambda B}] = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} [A, B^n] = \lambda \sum_{n=1}^{\infty} \frac{\lambda^{n-1}}{n!} n B^{n-1} [A, B] = \lambda e^{\lambda B} [A, B].$$

Substituting this into our earlier expression for $F'(\lambda)$ (and recalling we can commute $[A, B]$ past A, B everywhere), we get the final result:

$$F'(\lambda) = \lambda [A, B] e^{\lambda A} e^{\lambda B} e^{-\lambda(A+B)} = \lambda [A, B] F(\lambda).$$

We must now solve this differential equation. The equation is separable, and we have

$$\int \frac{dF}{F} = [A,B]\int \lambda\, d\lambda \qquad \Rightarrow \qquad F(\lambda) = C\exp\left(\frac{\lambda^2}{2}[A,B]\right),$$

where C is some λ-independent operator of integration. Setting $\lambda = 0$ and noting $F(0) = I$ in its original definition, we have $C = I$. It follows that

$$F(\lambda) = \exp\left(\frac{\lambda^2}{2}[A,B]\right) = e^{\lambda A}e^{\lambda B}e^{-\lambda(A+B)}.$$

Set $\lambda = 1$ in the two expressions for $F(\lambda)$ and compare to find:

$$e^A e^B = e^{\frac{1}{2}[A,B]}e^{A+B},$$

as required.

The next part of the question asks us about the harmonic oscillator. Recall that the one-dimensional harmonic oscillator has eigenstates

$$|n\rangle = \frac{(a^\dagger)^n\,|0\rangle}{\sqrt{n!}}, \qquad \text{with energy eigenvalues} \qquad E_n = \hbar\omega\left(n+\frac{1}{2}\right),$$

where $|0\rangle$ is the ground state of the oscillator, and $n = 0, 1, 2, \ldots$.

We are now given a perturbation to this oscillator of the form $V(\hat{x}) = \cos(\mu\hat{x})$. We are asked to express this in a different form. Recalling the exponential expression for cosine, we have:

$$V(\hat{x}) = \frac{1}{2}\left(e^{i\mu\hat{x}} + e^{-i\mu\hat{x}}\right).$$

It suffices to expand $e^{i\mu\hat{x}}$, and then flip $\mu \mapsto -\mu$ for the other exponential. From the given expressions for a and $a^\dagger$, we see that we can express $\hat{x}$ as:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(a^\dagger + a\right).$$

Recalling that a and $a^\dagger$ commute with their commutator, and $[a, a^\dagger] = 1$, we see that we can expand the desired exponential via the formula $e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}$:

$$\exp\left(i\mu\hat{x}\right) = \exp\left(i\mu\sqrt{\frac{\hbar}{2m\omega}}\left(a^\dagger + a\right)\right) = \exp\left(i\mu\sqrt{\frac{\hbar}{2m\omega}}a^\dagger\right)\exp\left(i\mu\sqrt{\frac{\hbar}{2m\omega}}a\right)\exp\left(\frac{\mu^2}{2}\cdot\frac{\hbar}{2m\omega}[a^\dagger, a]\right).$$

Set $\gamma = \mu\sqrt{\hbar/2m\omega}$. Then we have

$$e^{i\mu\hat{x}} = e^{-\frac{1}{2}\gamma^2}e^{i\gamma a^\dagger}e^{-i\gamma a^\dagger},$$

and flipping $\mu \mapsto -\mu$ sends $\gamma \mapsto -\gamma$, so we see that

$$V(\hat{(x)}) = \cos(\mu\hat{x}) = \frac{1}{2}e^{-\frac{1}{2}\gamma^2}\left(e^{i\gamma a^\dagger}e^{i\gamma a} + e^{-i\gamma a^\dagger}e^{-i\gamma a}\right),$$

as required.

We now use some standard results from perturbation theory. From lectures, we know that the shift in the ground state energy of the system in the presence of the perturbation is given by:

$$\epsilon \langle 0|V|0\rangle + \epsilon^2 \sum_{m\neq 0} \frac{|\langle m|V|0\rangle|^2}{E_0 - E_m},$$

and so we see that we must evaluate the generic matrix element $\langle m|V|0\rangle$. Let's first consider the simpler matrix element $\langle m|e^{i\gamma a^\dagger}e^{i\gamma a}|0\rangle$, since we will then be able to deduce $\langle m|V|0\rangle$. We have:

$$\begin{aligned}
\langle m|e^{i\gamma a^\dagger}e^{i\gamma a}|0\rangle &= \langle m|e^{i\gamma a^\dagger}\left(I + i\gamma a + \cdots\right)|0\rangle \\
&= \langle m|e^{i\gamma a^\dagger}|0\rangle && (a|0\rangle = 0) \\
&= \sum_{n=0}^{\infty} \frac{(i\gamma)^n}{\sqrt{n!}} \langle m|\frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle && (\text{expanding exponential}) \\
&= \sum_{n=0}^{\infty} \frac{(i\gamma)^n}{\sqrt{n!}} \langle m|n\rangle && (|n\rangle = (a^\dagger)^n|0\rangle/\sqrt{n!}) \\
&= \frac{(i\gamma)^m}{\sqrt{m!}} && (\langle m|n\rangle = \delta_{mn})
\end{aligned}$$

and hence we have (by flipping $\gamma \mapsto -\gamma$:

$$\langle m|V|0\rangle = \frac{1}{2}e^{-\frac{1}{2}\gamma^2}\left(\frac{(i\gamma)^m}{\sqrt{m!}} + \frac{(-i\gamma)^m}{\sqrt{m!}}\right) = \frac{1}{2}e^{-\frac{1}{2}\gamma^2}\frac{(i\gamma)^m}{\sqrt{m!}}(1 + (-1)^m).$$

We see that there are two cases, depending on the parity of m:

$$\langle 2p+1|V|0\rangle = 0, \qquad \langle 2p|V|0\rangle = e^{-\frac{1}{2}\gamma^2}\frac{(-\gamma)^p}{\sqrt{(2p)!}}.$$

Putting everything together, we get the shift in energy:

$$\begin{aligned}
&\epsilon e^{-\frac{1}{2}\gamma^2} + \epsilon^2 \sum_{p=1}^{\infty} \frac{e^{-\gamma^2}(-\gamma)^{2p}}{(2p)!\cdot(E_0 - E_{2p})} = \epsilon e^{-\frac{1}{2}\gamma^2} - \frac{\epsilon^2}{\hbar\omega}e^{-\gamma^2}\sum_{p=1}^{\infty}\frac{(-\gamma)^{2p}}{(2p)!\cdot(2p)} \\
&= \epsilon \exp\left(-\frac{\mu^2\hbar}{4m\omega}\right) - \frac{\epsilon^2}{\hbar\omega}\exp\left(-\frac{\mu^2\hbar}{2m\omega}\right)\sum_{p=1}^{\infty}\frac{1}{(2p)!\cdot(2p)}\left(\frac{\mu^2\hbar}{2m\omega}\right)^{2p},
\end{aligned}$$

as required.

2015, Paper 2, Section II, 31A

Express the spin operator $\mathbf{S}$ for a particle of spin $\frac{1}{2}$ in terms of the Pauli matrices $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ where

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Show that $(\mathbf{n} \cdot \boldsymbol{\sigma})^2 = I$ for any unit vector $\mathbf{n}$ and deduce that

$$e^{-i\theta \mathbf{n}\cdot\mathbf{S}/\hbar} = I\cos(\theta/2) - i(\mathbf{n}\cdot\boldsymbol{\sigma})\sin(\theta/2).$$

The space of states V for a particle of spin-$\frac{1}{2}$ has basis states $|\uparrow\rangle, |\downarrow\rangle$, which are eigenstates of S_3 with eigenvalues $\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$ respectively. If the Hamiltonian for the particle is $H = \frac{1}{2}\alpha\hbar\sigma_1$, find

$$e^{-itH/\hbar}\,|\uparrow\rangle \qquad \text{and} \qquad e^{-itH/\hbar}\,|\downarrow\rangle\,,$$

as linear combinations of the basis states.

The space of states for a system of two spin-$\frac{1}{2}$ particles is $V \otimes V$. Write down explicit expressions for the joint eigenstates of $\mathbf{J}^2$ and J_3, where $\mathbf{J}$ is the sum of the spin operators for the particles.

Suppose that the two-particle system has Hamiltonian $H = \frac{1}{2}\lambda\hbar\,(\sigma_1 \otimes I + I \otimes \sigma_1)$ and that at time $t = 0$ the system is in the state with J_3 eigenvalue $\hbar$. Calculate the probability that at time $t > 0$, the system will be measured to be in the state with $\mathbf{J}^2$ eigenvalue zero.

Solution: The spin operator is given by $\mathbf{S} = \frac{1}{2}\hbar\boldsymbol{\sigma}$ where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the vector of Pauli matrices.

Let $\hat{\mathbf{n}} = (x, y, z)$ be a unit vector. Then

$$\hat{\mathbf{n}}\cdot\boldsymbol{\sigma} = \begin{pmatrix} z & x - iy \\ x + iy & z \end{pmatrix} \qquad \Rightarrow \qquad (\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})^2 = \begin{pmatrix} x^2 + y^2 + z^2 & 0 \\ 0 & x^2 + y^2 + z^2 \end{pmatrix} = I,$$

as required. We can therefore deduce:

$$\begin{aligned} e^{-i\theta\hat{\mathbf{n}}\cdot\mathbf{S}/\hbar} &= \sum_{n=0}^{\infty} \left(\frac{-i\theta}{\hbar}\right)^n \frac{(\hat{\mathbf{n}}\cdot\mathbf{S})^n}{n!} \\ &= \sum_{n=0}^{\infty} \left(-\frac{i\theta}{2}\right)^n \frac{(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})^n}{n!} \\ &= \sum_{n=0}^{\infty} \left(-\frac{i\theta}{2}\right)^{2n} \frac{(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})^{2n}}{(2n)!} + \sum_{n=0}^{\infty} \left(-\frac{i\theta}{2}\right)^{2n+1} \frac{(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})^{2n+1}}{(2n+1)!} \\ &= I\sum_{n=0}^{\infty} \left(\frac{\theta}{2}\right)^{2n} \frac{(-1)^n}{(2n)!} - i(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}) \sum_{n=0}^{\infty} \left(\frac{\theta}{2}\right)^{2n+1} \frac{(-1)^n}{(2n+1)!} \\ &= I\cos\left(\frac{\theta}{2}\right) - i(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})\sin\left(\frac{\theta}{2}\right), \end{aligned}$$

which is the required identity.

We are now asked to consider a spin-$\frac{1}{2}$ particle in the presence of the Hamiltonian $H = \frac{1}{2}\alpha\hbar\sigma_1 = \alpha S_1$. The time-evolution operator in this instance is given by:

$$e^{-iHt/\hbar} = e^{-it\alpha S_1/\hbar},$$

so we choose $\theta = \alpha t$ in the previous work, giving

$$e^{-iHt/\hbar} = I\cos\left(\frac{\alpha t}{2}\right) - i\sigma_1 \sin\left(\frac{\alpha t}{2}\right).$$

Now note that $\sigma_1 |\uparrow\rangle = |\downarrow\rangle, \sigma_1 |\downarrow\rangle = |\uparrow\rangle$, using the matrix form of σ_1. Hence we can work out:

$$e^{-iHt/\hbar}|\uparrow\rangle = \cos\left(\frac{\alpha t}{2}\right)|\uparrow\rangle - i\sin\left(\frac{\alpha t}{2}\right)|\downarrow\rangle, \qquad \text{and,} \qquad e^{-iHt/\hbar}|\downarrow\rangle = \cos\left(\frac{\alpha t}{2}\right)|\downarrow\rangle - i\sin\left(\frac{\alpha t}{2}\right)|\uparrow\rangle.$$

We now consider a joint system of two spin-$\frac{1}{2}$ particles. We know from lectures, and our practice on the examples sheets, the the formulae for the joint eigenstates of $\mathbf{J}^2$, J_3 are simply:

$$|1,1\rangle = |\uparrow\rangle|\uparrow\rangle, \qquad |1,0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\uparrow\rangle\right), \qquad |1,-1\rangle = |\downarrow\rangle|\downarrow\rangle$$

and

$$|0,0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\right).$$

We are now given that the Hamiltonian of the joint system is

$$H = \frac{1}{2}\lambda\hbar\left(\sigma_1 \otimes I - I \otimes \sigma_1\right),$$

from which it follows that the time evolution operator of the joint system is:

$$e^{-iHt/\hbar} = e^{-it\sigma_1\otimes I/\hbar}e^{+itI\otimes\sigma_1/\hbar},$$

since operators from the different subsystems will commute. We are told that at time $t = 0$ we are in the eigenstate $|1,1\rangle = |\uparrow\rangle|\uparrow\rangle$ (the eigenstate of the total J_3 with eigenvalue $\hbar$), and hence after a time t we will be in the state:

$$|\psi\rangle = e^{-iHt/\hbar}|1,1\rangle = e^{-it\sigma_1/\hbar}|\uparrow\rangle e^{+it\sigma_1/\hbar}|\downarrow\rangle = \left(\cos\left(\frac{\lambda t}{2}\right)|\uparrow\rangle - i\sin\left(\frac{\lambda t}{2}\right)|\downarrow\rangle\right)\left(\cos\left(\frac{\lambda t}{2}\right)|\uparrow\rangle + i\sin\left(\frac{\lambda t}{2}\right)|\downarrow\rangle\right),$$

using the result we derived earlier in the question about the action of this form of Hamiltonian on individual spin-$\frac{1}{2}$ systems. This can be expanded to give:

$$|\psi\rangle = \cos^2\left(\frac{\lambda t}{2}\right)|\uparrow\rangle|\uparrow\rangle + i\cos\left(\frac{\lambda t}{2}\right)\sin\left(\frac{\lambda t}{2}\right)|\uparrow\rangle|\downarrow\rangle - i\sin\left(\frac{\lambda t}{2}\right)\cos\left(\frac{\lambda t}{2}\right)|\downarrow\rangle|\uparrow\rangle + \sin^2\left(\frac{\lambda t}{2}\right)|\downarrow\rangle|\downarrow\rangle.$$

We want the probability of measuring the $\mathbf{J}^2$ eigenvalue 0 at time $t = 0$. This corresponds to the probability $|\langle 0,0|\psi\rangle|^2$; the relevant amplitude is given by:

$$\langle 0,0|\psi\rangle = \frac{1}{\sqrt{2}}\left(i\cos\left(\frac{\lambda t}{2}\right)\sin\left(\frac{\lambda t}{2}\right)\right) + \frac{1}{\sqrt{2}}\left(i\sin\left(\frac{\lambda t}{2}\right)\cos\left(\frac{\lambda t}{2}\right)\right) = \frac{i}{\sqrt{2}}\sin\left(\lambda t\right),$$

and hence the required probability is

$$\frac{1}{2}\sin^2\left(\lambda t\right).$$

2015, Paper 3, Section II, 31A

Let $|j,m\rangle$ denote the normalised joint eigenstates of $\mathbf{J}^2$ and J_3 where $\mathbf{J}$ is the angular momentum operator for a quantum system. State clearly the possible values of the quantum numbers j and m and write down the corresponding eigenvalues in units with $\hbar = 1$.

Consider two quantum systems with angular momentum states $|\frac{1}{2},r\rangle$ and $|j,m\rangle$. The eigenstates corresponding to their combined angular momentum can be written as

$$|J,M\rangle = \sum_{r,m} C^{JM}_{rm}\,|\tfrac{1}{2},r\rangle\,|j,m\rangle\,,$$

where C^{JM}_{rm} are Clebsch-Gordan coefficients for addition of angular momenta $\frac{1}{2}$ and j. What are the possible values of J and what is a necessary condition relating r, m and M in order that $C^{JM}_{rm} \neq 0$?

Calculate the values of C^{JM}_{rm} for $j = 2$ and for all $M \geq \frac{3}{2}$. Use the sign convention that $C^{JJ}_{rm} > 0$ when m takes its maximum value.

A particle X with spin $\frac{3}{2}$ and intrinsic parity η_X is at rest. It decays into two particles A and B with spin $\frac{1}{2}$ and spin 0, respectively. Both A and B have intrinsic parity -1. The relative orbital angular momentum quantum number for the two particle system is l. What are the possible values of l for the cases $\eta_X = +1$ and $\eta_X = -1$?

Suppose particle X is prepared in the state $|\frac{3}{2},\frac{3}{2}\rangle$ before it decays. Calculate the probability P for particle A to be found in the state $|\frac{1}{2},\frac{1}{2}\rangle$ given that $\eta_X = +1$.

What is the probability P if instead $\eta_X = -1$?

[*Units with $\hbar = 1$ should be used throughout. You may also use without proof*

$$J_-\,|j,m\rangle = \sqrt{(j+m)(j-m+1)}\,|j,m-1\rangle\,.]$$

Solution: As we know from lectures, the possible values for j and m are:

$$j \in \{0,\tfrac{1}{2},1,\tfrac{3}{2},2,\dots\} = \tfrac{1}{2}\mathbb{Z}^+_0, \qquad m \in \{-j,-(j-1),\dots,j-1,j\}\,.$$

The eigenvalues corresponding to $|j,m\rangle$ are such that $\mathbf{J}^2\,|j,m\rangle = j(j+1)\,|j,m\rangle$ and $J_3\,|j,m\rangle = m\,|j,m\rangle$ in units where $\hbar = 1$.

Recall that when we add two angular momentum systems with fixed j values j_1 and j_2, the possible total J values of the resulting composite system lie in the range:

$$J \in \{j_1+j_2, j_1+j_2-1,\dots,|j_1-j_2|\},$$

corresponding to a quantised set of steps from having the subsystems' angular momenta maximally aligned to the subsystems' angular momenta minimally aligned. In our case, the subsystems have j values $j_1 = j$ and $j_2 = \frac{1}{2}$, and hence

$$J \in \{j+\tfrac{1}{2}, j-\tfrac{1}{2}\} \quad \text{if } j \geq \tfrac{1}{2}, \qquad J = \tfrac{1}{2} \quad \text{if } j = 0.$$

Since the total J_3 operator on the composite system is given by $J_3 = J_{3,1}\otimes I + I\otimes J_{3,2}$, we have:

$$\sum_{r,m} C^{JM}_{rm}\,M\,|\tfrac{1}{2},r\rangle\,|j,m\rangle = M\,|J,M\rangle = J_3\,|J,M\rangle = \sum_{r,m} C^{JM}_{rm}\,(r+m)\,|\tfrac{1}{2},r\rangle\,|j,m\rangle\,,$$

i.e. the required necessary condition is $r+m=M$.

We are now asked to perform an addition of angular momentum calculation explicitly, where we must add angular momentum 2 to angular momentum $\frac{1}{2}$. The highest state is, as usual, given by:

$$|\tfrac{5}{2},\tfrac{5}{2}\rangle = |2,2\rangle\,|\tfrac{1}{2},\tfrac{1}{2}\rangle\,.$$

Applying the lowering operator $J_- = J_{-,1}\otimes I + I\otimes J_{-,2}$ to both sides, and using the formula given in the question, we find:

$$J_-\,|\tfrac{5}{2},\tfrac{5}{2}\rangle = J_{-,1}\,|2,2\rangle\,|\tfrac{1}{2},\tfrac{1}{2}\rangle + |2,2\rangle\,J_{-,2}\,|\tfrac{1}{2},\tfrac{1}{2}\rangle$$

$$\Rightarrow \qquad |\tfrac{5}{2},\tfrac{3}{2}\rangle = \sqrt{\frac{4}{5}}\,|2,1\rangle\,|\tfrac{1}{2},\tfrac{1}{2}\rangle + \sqrt{\frac{1}{5}}\,|2,2\rangle\,|\tfrac{1}{2},-\tfrac{1}{2}\rangle\,.$$

Lowering again would give us an M value less than $3/2$, and we are not asked for such states. We see that the next state we need to construct then is $|\frac{3}{2},\frac{3}{2}\rangle$, which can be found by using orthogonality to $|\frac{5}{2},\frac{3}{2}\rangle$ as usual. By inspection then, the appropriate orthogonal state is:

$$|\tfrac{3}{2},\tfrac{3}{2}\rangle = \sqrt{\frac{1}{5}}\,|2,1\rangle\,|\tfrac{1}{2},\tfrac{1}{2}\rangle - \sqrt{\frac{4}{5}}\,|2,2\rangle\,|\tfrac{1}{2},-\tfrac{1}{2}\rangle\,.$$

We are now asked to apply our work to a decay process question. We are given the decay $X \to A + B$, where X is a spin-$\frac{3}{2}$ particle and A and B are spin-$\frac{1}{2}$ and spin-0 particles respectively. We are also given that A and B both have intrinsic parity -1.

Since angular momentum $1/2$ added to angular momentum 0 is just the same as angular momentum $1/2$ again, we can add the spins of A and B to get total spin $1/2$. If we assume we start in the rest frame of X, we can take its initial orbital angular momentum to be 0, so combining its spin angular momentum and orbital angular momentum we get total angular momentum $3/2$ before the decay; by conservation of total angular momentum this is also the total angular momentum after the decay. Hence we can construct the following table:

Particle property	X	A	B
Intrinsic parity	η_X	-1	-1
Total ang. mom. (j)	$3/2$	$3/2$	
Orbital ang. mom. (l)	0	l	
Spin (s)	$3/2$	$1/2$	

We have written the total orbital angular momentum after the decay as l. By considering addition of the orbital angular momentum and the spin angular momentum of the $A + B$ system to give the total angular momentum of the $A + B$ system, we see that we must have:

$$\tfrac{3}{2} \in \{l + \tfrac{1}{2}, \ldots, |l - \tfrac{1}{2}|\}\,.$$

It follows that $l = 1$ or $l = 2$. We can deduce the value of l given the value of η_X using parity conservation:

- If $\eta_X = 1$, then parity conservation tells us that $1\cdot(-1)^0 = (-1)\cdot(-1)\cdot(-1)^l$, and hence $l = 2$.
- If $\eta_X = -1$, then parity conservation tells us that $(-1)\cdot(-1)^0 = (-1)\cdot(-1)\cdot(-1)^l$, and hence $l = 1$.

Finally, we are asked to calculate some probabilities.

- First, given $\eta_X = 1$ and we start in the total angular momentum state $|\frac{3}{2}, \frac{3}{2}\rangle$, we must compute the probability that A will be in the spin state $|\frac{1}{2}, \frac{1}{2}\rangle$ after the decay. By conservation of total angular momentum, the total angular momentum state on the right hand side is given by:

$$|\tfrac{3}{2}, \tfrac{3}{2}\rangle = \sqrt{\frac{1}{5}}\,|2,1\rangle_{\text{orbital}}\,|\tfrac{1}{2}, \tfrac{1}{2}\rangle_{A+B\,\text{spin}} - \sqrt{\frac{4}{5}}\,|2,2\rangle_{\text{orbital}}\,|\tfrac{1}{2}, -\tfrac{1}{2}\rangle_{A+B\,\text{spin}}\,,$$

  where we have split the state into the orbital angular momentum contribution and the spin angular momentum contribution, using the fact that $l = 2$ when $\eta = 1$ and the total $A + B$ spin is $1/2$, so we can apply the results from the beginning of the question.

  We see that the probability that the total $A + B$ spin will be in the state $|\frac{1}{2}, \frac{1}{2}\rangle$ is given by $P = 1/5$, and since B has zero spin, this is equivalent to A having the spin state $|\frac{1}{2}, \frac{1}{2}\rangle$. Thus the required probability is $P = 1/5$.

- We are now asked to repeat the calculation given $\eta_X = -1$. This time we need to split $|\frac{3}{2}, \frac{3}{2}\rangle$ across two subsystems of orbital angular momentum $l = 1$ and spin angular momentum $s = \frac{1}{2}$. But now $|\frac{3}{2}, \frac{3}{2}\rangle$ is the highest angular momentum state in addition of angular momentum 1 to angular momentum $\frac{1}{2}$, so we trivially have:

$$|\tfrac{3}{2}, \tfrac{3}{2}\rangle = |1,1\rangle_{\text{orbital}}\,|\tfrac{1}{2}, \tfrac{1}{2}\rangle_{A+B\,\text{spin}}\,.$$

  Hence we see the probability that A will be in the spin state $|\frac{1}{2}, \frac{1}{2}\rangle$ is $P = 1$.

2015, Paper 4, Section II, 30A

The Hamiltonian for a quantum system in the Schrödinger picture is $H_0 + \lambda V(t)$, where H_0 is independent of time and the parameter λ is small. Define the interaction picture corresponding to this Hamiltonian and derive a time evolution equation for interaction picture states.

Suppose that $|\chi\rangle$ and $|\phi\rangle$ are eigenstates of H_0 with distinct eigenvalues E and E', respectively. Show that if the system is in state $|\chi\rangle$ at time zero then the probability of measuring it to be in state $|\phi\rangle$ at time t is

$$\frac{\lambda^2}{\hbar^2}\left|\int_0^t dt'\,\langle\phi|V(t')|\chi\rangle\, e^{i(E'-E)t'/\hbar}\right|^2 + O(\lambda^3).$$

Let H_0 be the Hamiltonian for an isotropic three-dimensional harmonic oscillator of mass m and frequency ω, with $\chi(r)$ being the ground state wavefunction (where $r = |\mathbf{x}|$) and $\phi_i(\mathbf{x}) = (2m\omega/\hbar)^{1/2} x_i \chi(r)$ being wavefunctions for the states at the first excited energy level ($i = 1, 2, 3$). The oscillator is in its ground state at $t = 0$ when a perturbation

$$\lambda V(t) = \lambda \hat{x}_3 e^{-\mu t}$$

is applied, with $\mu > 0$, and H_0 is then measured after a very large time has elapsed. Show that to first order in perturbation theory the oscillator will be found in one particular state at the first excited energy level with probability

$$\frac{\lambda^2}{2\hbar m\omega(\mu^2+\omega^2)},$$

but that the probability that it will be found in either of the other excited states is zero (to this order).

[*You may use the fact that* $4\pi\int_0^\infty r^4|\chi(r)|^2\,dr = \dfrac{3\hbar}{2m\omega}$.]

Solution: The *interaction picture* for a quantum mechanical system is defined in terms of *interaction states* and *interaction operators*, which are given in terms of their Schrödinger picture counterparts (written $|\psi_S\rangle$ and A_S respectively) by:

$$|\psi_I(t)\rangle = e^{iH_0 t/\hbar}\,|\psi_S(t)\rangle\,, \qquad A_I(t) = e^{iH_0 t/\hbar} A_S e^{-iH_0 t/\hbar},$$

where $U_0(t) = e^{-iH_0 t/\hbar}$ is the time-evolution operator of the free Hamiltonian H_0, and $e^{iH_0 t/\hbar}$ is its inverse.

We are also asked to derive the equation of motion for interaction pictures states. Acting on an interaction picture state $|\psi_I\rangle$ with a time derivative, we have

$$i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = i\hbar\frac{\partial}{\partial t}\left(e^{iH_0 t/\hbar}\,|\psi_S(t)\rangle\right) = -H_0 e^{iH_0 t/\hbar}\,|\psi_S(t)\rangle + e^{iH_0 t/\hbar}(H_0 + \lambda V(t))\,|\psi_S(t)\rangle\,,$$

using Schrödinger's equation for the Schrödinger picture state $|\psi_S(t)\rangle$. Since H_0 commutes with $e^{iH_0 t/\hbar}$, we can simplify the right hand side leaving:

$$i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = e^{iH_0 t/\hbar}\lambda V(t)\,|\psi_S(t)\rangle = e^{iH_0 t/\hbar}\lambda V(t) e^{-iH_0 t/\hbar} e^{iH_0 t/\hbar}\,|\psi_S(t)\rangle = \lambda V_I(t)\,|\psi_I(t)\rangle$$

$$\Rightarrow \qquad i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = \lambda V_I(t)\,|\psi_I(t)\rangle\,,$$

which is the interaction picture equation of motion as required.

Next we are asked to establish the probability of measuring the system to be in the free-Hamiltonian eigenstate $|\phi\rangle$ at time t, if it is in the free-Hamiltonian eigenstate $|\chi\rangle$ at time $t = 0$. First we recall that interaction picture predictions are equivalent to Schrödinger picture predictions, hence it is equivalent to find the probability working in the interaction picture.

Next, we need to deal with the interaction picture equation of motion itself. Notice that by direct integration, we can recast the interaction picture equation of motion as an integral equation:

$$i\hbar\,|\psi_I(t)\rangle = i\hbar\,|\psi_I(0)\rangle + \int_0^t \lambda V_I(t')\,|\psi_I(t')\rangle\;dt'.$$

The integrand on the right hand side involves a $|\psi_I(t')\rangle$; if we express this in terms of the right hand side we can get an iterative series in λ as a result. Truncating at the first order, we obtain the approximation:

$$i\hbar\,|\psi_I(t)\rangle \approx i\hbar\,|\psi_I(0)\rangle + \lambda\int_0^t V_I(t')\,|\psi_I(0)\rangle\;dt'.$$

Recall $|\psi_I(0)\rangle = |\chi\rangle$ is given. We want to find $\langle\phi|\psi_I(t)\rangle$, which is then given by:

$$i\hbar\,\langle\phi|\psi_I(t)\rangle \approx i\hbar\,\langle\phi|\chi\rangle + \lambda\int_0^t \langle\phi|V_I(t')|\chi\rangle\;dt'.$$

Expanding $V_I(t') = e^{iH_0t'/\hbar}V(t')e^{-iH_0t'/\hbar}$ and acting on the free-Hamiltonian eigenstates with the relevant operators leaves us with:

$$i\hbar\,\langle\phi|\psi_I(t)\rangle \approx i\hbar\,\langle\phi|\chi\rangle + \lambda\int_0^t e^{i(E'-E)t'/\hbar}\,\langle\phi|V(t')|\chi\rangle\;dt'.$$

Assuming that $|\chi\rangle, |\phi\rangle$ have distinct eigenvalues E and E', they are orthogonal, and hence we're left with the probability:

$$|\,\langle\phi|\psi_I(t)\rangle\,|^2 = \frac{\lambda^2}{\hbar^2}\left|\int_0^t e^{i(E'-E)t'/\hbar}\,\langle\phi|V(t')|\chi\rangle\;dt'\right|^2,$$

as required.

For the next part, we are asked to apply the bookwork to three examples. Let's kill three birds with one stone, and just stack all the given wavefunctions in a vector, and in an abuse of notation write $|\boldsymbol{\phi}\rangle = (|\phi_1\rangle\,, |\phi_2\rangle\,, |\phi_3\rangle)^T$. Then:

$$\langle\boldsymbol{\phi}|V(t')|\chi\rangle = \iiint_{\mathbb{R}^3} dV\,\left(\frac{2m\omega}{\hbar}\right)^{1/2}\mathbf{x}\chi(r)^*x_3e^{-\mu t'}\chi(r) = \left(\frac{2m\omega}{\hbar}\right)^{1/2}\iiint_{\mathbb{R}^3} dV\begin{pmatrix}x_1x_3\\x_2x_3\\x_3^2\end{pmatrix}|\chi(r)|^2e^{-\mu t'},$$

using the formulae for the given wavefunctions, and the position representation of the given $V(t')$. Switching to spherical polars, we're left with:

$$\langle\boldsymbol{\phi}|V(t')|\chi\rangle = \left(\frac{2m\omega}{\hbar}\right)^{1/2}e^{-\mu t'}\int_0^\infty\int_0^{2\pi}\int_0^{\pi}\begin{pmatrix}r^4\sin^2(\theta)\cos(\phi)\cos(\theta)\\r^4\sin^2(\theta)\sin(\phi)\cos(\theta)\\r^4\cos^2(\theta)\sin(\theta)\end{pmatrix}|\chi(r)|^2\,d\theta d\phi dr.$$

Notice that the ϕ_1, ϕ_2 terms drop out, since the integrals over $\cos(\phi), \sin(\phi)$ vanish. Thus the transition probability to ϕ_1, ϕ_2 is zero.

Evaluating the integrals for the remaining state ϕ_3, in particular using the hint in the question for the radial integral, we have:

$$\langle \phi_3 | V(t') | \chi \rangle = \left(\frac{2m\omega}{\hbar} \right)^{1/2} e^{-\mu t'} \int_0^{\infty} \int_0^{2\pi} \int_0^{\pi} r^4 \cos^2(\theta) \sin(\theta) |\chi(r)|^2 \, d\theta d\phi dr$$

$$= 2\pi e^{-\mu t'} \cdot \frac{3\hbar}{8\pi m\omega} \cdot \left(\frac{2m\omega}{\hbar} \right)^{1/2} \int_0^{\pi} \cos^2(\theta) \sin(\theta) \, d\theta = \frac{3\hbar e^{-\mu t'}}{4m\omega} \cdot \left(\frac{2m\omega}{\hbar} \right)^{1/2} \cdot \left[-\frac{\cos^3(\theta)}{3} \right]_0^{\pi}$$

$$= e^{-\mu t'} \left(\frac{\hbar}{2m\omega} \right)^{1/2}.$$

Notice that since ϕ_3 is an excited state of the 3D harmonic oscillator, it has energy $\hbar\omega(1 + \frac{3}{2})$, and hence its difference in energy with the ground state is simply $\hbar\omega(1 + \frac{3}{2}) - \frac{3}{2}\hbar\omega = \hbar\omega$. Hence the probability of being in the state ϕ_3 after a very long time ($t \to \infty$) is given by:

$$\frac{\lambda^2}{\hbar^2} \left(\frac{\hbar}{2m\omega} \right) \left| \int_0^t e^{(i\omega - \mu)t'} \, dt' \right|^2 = \frac{\lambda^2}{2m\hbar\omega} \left| -\frac{1}{i\omega - \mu} \right|^2 = \frac{\lambda^2}{2\hbar m\omega(\mu^2 + \omega^2)},$$

as required.

2016, Paper 1, Section II, 31A

A particle in one dimension has position and momentum operators $\hat{x}$ and $\hat{p}$ whose eigenstates obey

$$\langle x|x'\rangle = \delta(x-x'), \qquad \langle p|p'\rangle = \delta(p-p'), \qquad \langle x|p\rangle = (2\pi\hbar)^{-1/2}e^{ixp/\hbar}.$$

For a state $|\psi\rangle$, define the position-space and momentum-space wavefunctions $\psi(x)$ and $\tilde{\psi}(p)$ and show how each of these can be expressed in terms of the other.

Write down the translation operator $U(\alpha)$ and check that your expression is consistent with the property that $U(\alpha)\,|x\rangle = |x+\alpha\rangle$. For a state $|\psi\rangle$, relate the position-space and momentum-space wavefunctions for $U(\alpha)\,|\psi\rangle$ to $\psi(x)$ and $\tilde{\psi}(p)$ respectively.

Now consider a harmonic oscillator with mass m, frequency ω, and annihilation and creation operators

$$a = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right), \qquad a^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right).$$

Let $\psi_n(x)$ and $\tilde{\psi}_n(p)$ be the wavefunctions corresponding to the normalised energy eigenstates $|n\rangle$, where $n = 01, 2, \ldots$.

(i) Express $\psi_0(x-\alpha)$ explicitly in terms of the wavefunctions $\psi_n(x)$.

(ii) Given that $\tilde{\psi}_n(p) = f_n(u)\tilde{\psi}_0(p)$, where the f_n are polynomials and $u = (2/\hbar m\omega)^{1/2}p$, show that

$$e^{-i\gamma u} = e^{-\gamma^2/2}\sum_{n=0}^{\infty}\frac{\gamma^n}{\sqrt{n!}}f_n(u) \qquad \text{for any real } \gamma.$$

[*You may quote standard results for a harmonic oscillator. You may also use, without proof,* $e^{A+B} = e^Ae^Be^{-\frac{1}{2}[A,B]}$ *for operators* A *and* B *which each commute with* $[A,B]$.]

Solution: The *position-space wavefunction* of the state $|\psi\rangle$ is defined by $\psi(x) = \langle x|\psi\rangle$ and the *momentum-space wavefunction* of the state $|\psi\rangle$ is defined by $\tilde{\psi}(p) = \langle p|\psi\rangle$. These definitions ensure the $\psi(x)$, $\tilde{\psi}(p)$ are the components of the state $|\psi\rangle$ with respect to the position basis $\{|x\rangle\}$ and the momentum basis $\{|p\rangle\}$ respectively:

$$|\psi\rangle = \int dx\,\psi(x)\,|x\rangle = \int dp\,\tilde{\psi}(p)\,|p\rangle\,.$$

To express the position-space wavefunction in terms of the momentum-space wavefunction, we use *resolution of identity* of the momentum basis:

$$\int dp\ |p\rangle\,\langle p| = I,$$

which shows us that:

$$\psi(x) = \langle x|\psi\rangle = \int dp\ \langle x|p\rangle\,\langle p|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int dp\,e^{ixp/\hbar}\tilde{\psi}(p).$$

Hence we see that the position-space wavefunction is the Fourier transform (with some special normalisation) of the momentum-space wavefunction. Similarly, using resolution of identity of the position basis:

$$\int dx\ |x\rangle\,\langle x| = I,$$

we can express the momentum-space wavefunction in terms of the position-space wavefunction:

$$\tilde{\psi}(p) = \langle p|\psi\rangle = \int dx\ \langle p|x\rangle\,\langle x|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int dx\,e^{-ixp/\hbar}\psi(x).$$

Again, they are related by a Fourier transform (with some special normalisation).

Depending on what iteration of the course we want to take as our starting point, there are two ways in which we might define the translation operator:

- We could define the translation operator $U(\alpha)$ to be the unitary operator obeying the operator equation:

$$U(\alpha)^{-1}\hat{x}U(\alpha) = \hat{x} + \alpha,$$

where $\hat{x}$ is the position operator. By multiplying through with $U(\alpha)$, we can rewrite this equation as a commutator:

$$[\hat{x}, U(\alpha)] = \alpha U(\alpha).$$

We can then show that $U(\alpha)\,|x\rangle$ is an eigenstate of the position operator $\hat{x}$ with eigenvalue $x + \alpha$ by noting:

$$\hat{x}U(\alpha)\,|x\rangle = ([\hat{x}, U(\alpha)] + U(\alpha)\hat{x})\,|x\rangle = (x+\alpha)U(\alpha)\,|x\rangle\,.$$

Hence $U(\alpha)\,|x\rangle = \lambda\,|x+\alpha\rangle$. To find the constant of proportionality, consider for example:

$$\langle x'|U(\alpha)^{-1}\hat{x}U(\alpha)|x\rangle = \langle x'|\hat{x}+\alpha|x\rangle \qquad \Rightarrow \qquad |\lambda|^2\,\langle x'+\alpha|\hat{x}|x+\alpha\rangle = (x+\alpha)\delta(x'-x)$$

$$\Rightarrow \qquad |\lambda|^2(x+\alpha)\delta(x'-x) = (x+\alpha)\delta(x'-x).$$

Hence we see that $|\lambda| = 1$, and so without loss of generality we can choose $\lambda = 1$.[2]

- Another definition we might use for the translation operator is $U(\alpha) = e^{-i\alpha\hat{p}/\hbar}$, where $\hat{p}$ is the momentum operator. We then note that:

$$U(\alpha)\,|x\rangle = \int dp\, e^{-i\alpha\hat{p}/\hbar}\,|p\rangle\,\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int dp\, e^{-i(x+\alpha)p/\hbar}\,|p\rangle = \int dp\;\langle p|x+\alpha\rangle\,|p\rangle = |x+\alpha\rangle\,.$$

Either way, we arrive at the result $U(\alpha)\,|x\rangle = |x+\alpha\rangle$. Now let's determine how $U(\alpha)$ affects the position and momentum-space wavefunctions of a generic state $|\psi\rangle$. To determine the effect of $U(\alpha)$ on the position-space wavefunction, we consider:

$$\langle x|U(\alpha)|\psi\rangle = \left(U(\alpha)^\dagger\,|x\rangle\right)^\dagger\,|\psi\rangle = (U(-\alpha)\,|x\rangle)^\dagger\,|\psi\rangle = \langle x-\alpha|\psi\rangle = \psi(x-\alpha).$$

For the momentum-space wavefunction, we either recall that $U(\alpha) = e^{-i\alpha\hat{p}/\hbar}$ by definition of the translation operator, or by momentum as the generator of translations, which gives us:

$$\langle p|U(\alpha)|\psi\rangle = \langle p|e^{-i\alpha\hat{p}/\hbar}|\psi\rangle = e^{-i\alpha p/\hbar}\,\langle p|\psi\rangle = e^{-i\alpha p/\hbar}\tilde{\psi}(p).$$

(i) We now move on to the harmonic oscillator part of the question. First we are asked to express the translated ground-state position-wavefunction $\psi_0(x-\alpha)$ in terms of all the other position-wavefunctions of the oscillator's states. We have:

$$\psi_0(x-\alpha) = \langle x-\alpha|0\rangle = \langle x|U(\alpha)|0\rangle = \langle x|\exp\left(-\frac{i\alpha\hat{p}}{\hbar}\right)|0\rangle\,.$$

Expressing the momentum $\hat{p}$ in terms of the raising and lowering operators, we will then be able to act on the ground state $|0\rangle$ efficiently. By computing $a - a^\dagger$, we have

$$\hat{p} = i\left(\frac{\hbar m\omega}{2}\right)^{1/2}\left(a^\dagger - a\right).$$

[2] In principle, λ could depend on x and α and then things become a lot more complicated - but this is really not something you need to worry about in this course.

We would now like to compute the exponential of $-i\alpha\hat{p}/\hbar$. To do this, we will need to use the identity given in the question for the exponential of the sum of two operators both of which commute with their commutator:

$$\exp\left(-\frac{i\alpha}{\hbar}\cdot i\left(\frac{\hbar m\omega}{2}\right)^{1/2}\left(a^\dagger - a\right)\right) = \exp\left(\alpha\left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(a^\dagger - a\right)\right)$$

$$= \exp\left(\alpha\left(\frac{m\omega}{2\hbar}\right)^{1/2}a^\dagger\right)\exp\left(-\alpha\left(\frac{m\omega}{2\hbar}\right)^{1/2}a\right)\exp\left(-\frac{1}{2}\alpha^2\left(\frac{m\omega}{2\hbar}\right)\right).$$

Hence:

$$\psi_0(x-\alpha) = \exp\left(-\frac{\alpha^2 m\omega}{4\hbar}\right)\langle x|\exp\left(\alpha\left(\frac{m\omega}{2\hbar}\right)^{1/2}a^\dagger\right)|0\rangle \qquad \text{(since } e^a \sim I + a + a^2 + \cdots\text{)}$$

$$= \exp\left(-\frac{\alpha^2 m\omega}{4\hbar}\right)\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\left(\frac{m\omega}{2\hbar}\right)^{n/2}\langle x|\frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle$$

$$= \exp\left(-\frac{\alpha^2 m\omega}{4\hbar}\right)\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\left(\frac{m\omega}{2\hbar}\right)^{n/2}\psi_n(x).$$

(ii) For the last part of the question, we are told something about $\tilde{\psi}_n(p)$ for each n, which is the momentum-space wavefunction corresponding to the position space wavefunction $\psi_n(x)$. Recall from the very beginning of the question, to go between the two we take a Fourier transform. Therefore, let's take the Fourier transform of the equation we derived in part (ii).

On the left hand side, we have:

$$\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}dx\, e^{-ixp/\hbar}\psi_0(x-\alpha) = \frac{e^{-ip\alpha/\hbar}}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}du\, e^{-iup/\hbar}\psi_0(u) = e^{-ip\alpha/\hbar}\tilde{\psi}_0(p),$$

using the substitution $u = x - \alpha$ in the second step. We could also have seen this from the fact that we found the momentum wavefunction of $U(\alpha)\,|\psi_0\rangle$ was $e^{-ip\alpha/\hbar}\tilde{\psi}_0(p)$, and the momentum wavefunction is the Fourier transform of the position wavefunction $\psi_0(x-\alpha)$.

On the right hand side, we have:

$$\exp\left(-\frac{\alpha^2 m\omega}{4\hbar}\right)\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\left(\frac{m\omega}{2\hbar}\right)^{n/2}f_n(u)\tilde{\psi}_0(p),$$

where the f_n are some unknown functions. Putting everything together and setting $\gamma = \alpha(m\omega/2\hbar)^{1/2}$, and using $u = (2/\hbar m\omega)^{1/2}p$ as given, we arrive at the result:

$$e^{-i\gamma u} = e^{-\gamma^2/2}\sum_{n=0}^{\infty}\frac{\gamma^n}{\sqrt{n!}}f_n(u).$$

Since α was arbitrary, this holds for arbitrary γ too, as required.

2016, Paper 2, Section II, 32A

(a) Let $|jm\rangle$ be standard, normalised angular momentum eigenstates with labels specifying eigenvalues for $\mathbf{J}^2$ and J_3. Taking units in which $\hbar = 1$,

$$J_\pm |jm\rangle = \{(j \mp m)(j \pm m + 1)\}^{1/2} |j\, m \pm 1\rangle \,.$$

Check the coefficients above by computing norms of states, quoting any angular momentum commutation relations that you require.

(b) Two particles, each of spin $s > 0$, have combined spin states $|JM\rangle$. Find expressions for all such states with $M = 2s - 1$ in terms of product states.

(c) Suppose that the particles in part (b) move about their centre of mass with a spatial wavefunction that is a spherically symmetric function of relative position. If the particles are identical, what spin states $|J\, 2s-1\rangle$ are allowed? Justify your answer.

(d) Now consider two particles of spin 1 that are not identical and are both at rest. If the 3-component of the spin of each particle is zero, what is the probability that their total, combined spin is zero?

Solution: (a) We have:

$$\begin{aligned}
||J_+ |jm\rangle\,||^2 &= \langle jm|J_- J_+|jm\rangle && (\text{since } J_+^\dagger = J_-)\\
&= \langle jm|(J_x - iJ_y)(J_x + iJ_y)|jm\rangle \\
&= \langle jm|\mathbf{J}^2 - J_z^2 + i[J_x, J_y]|jm\rangle \\
&= \langle jm|\mathbf{J}^2 - J_z^2 - J_z|jm\rangle && (\text{since } [J_x, J_y] = iJ_z)\\
&= j(j+1) - m^2 - m \\
&= (j-m)(j+m+1),
\end{aligned}$$

using $\mathbf{J}^2 |jm\rangle = j(j+1)|jm\rangle$ and $J_z |jm\rangle = m|jm\rangle$. This verifies the normalisation as required (up to an arbitrary phase).

The argument is almost identical for $J_-|jm\rangle$; we have:

$$\begin{aligned}
||J_- |jm\rangle\,||^2 &= \langle jm|J_+ J_-|jm\rangle && (\text{since } J_-^\dagger = J_+)\\
&= \langle jm|(J_x + iJ_y)(J_x - iJ_y)|jm\rangle \\
&= \langle jm|\mathbf{J}^2 - J_z^2 - i[J_x, J_y]|jm\rangle \\
&= \langle jm|\mathbf{J}^2 - J_z^2 + J_z|jm\rangle && (\text{since } [J_x, J_y] = iJ_z)\\
&= j(j+1) - m^2 + m \\
&= (j+m)(j-m+1),
\end{aligned}$$

and we're done.

(b) To construct the spin states of the composite system, we use the standard angular momentum algorithm to add angular momentum s to angular momentum s. The highest angular momentum state is:

$$|2s, 2s\rangle = |s, s\rangle\,|s, s\rangle\,.$$

Applying the lowering operator $J_- = J_{-,1} \otimes I + I \otimes J_{-,2}$ to both sides, we have (using the formulae from part (a)):

$$\sqrt{4s}\,|2s, 2s-1\rangle = \sqrt{2s}\,|s, s-1\rangle\,|s, s\rangle + \sqrt{2s}\,|s, s\rangle\,|s, s-1\rangle$$

$$\Rightarrow \qquad |2s, 2s-1\rangle = \frac{1}{\sqrt{2}}\,|s, s-1\rangle\,|s, s\rangle + \frac{1}{\sqrt{2}}\,|s, s\rangle\,|s, s-1\rangle\,.$$

The only other state the question wants us to construct is $|2s-1, 2s-1\rangle$, which we construct using orthogonality to $|2s, 2s-1\rangle$. By inspection, we see that we need:

$$|2s-1, 2s-1\rangle = \frac{1}{\sqrt{2}}\,|s, s-1\rangle\,|s, s\rangle - \frac{1}{\sqrt{2}}\,|s, s\rangle\,|s, s-1\rangle\,,$$

up to an arbitrary phase.

(c) In the next part of the question, we are asked which of the states we constructed in (b), of the form $|J, 2s-1\rangle$, are allowed if we are given further that the particles are *identical*.

Note that we are given that the particles move around their centre of mass frame, so the only sign contribution from orbital angular momentum is $(-1)^0 = 1$.

Therefore, under particle exchange, we need only be concerned with the sign that arises from exchange of the particles' spin states. The state $|2s, 2s-1\rangle$ is *symmetric* under the exchange of the particles, so in the case that we are in the state $|2s, 2s-1\rangle$, we pick up an overall sign $+1$ under the particles' exchange. This is only valid if the particles are bosons; equivalently, by the spin-statistics theorem, the particles have integral spin.

The state $|2s-1, 2s-1\rangle$ is *antisymmetric* under the exchange of the particles, so we pick up an overall sign -1 under particle exchange. This is only valid if the particles are fermions; equivalently, by the spin-statistics theorem, the particles have *half*-integral spin.

(d) We are essentially told that we are in the state $|1, 0\rangle\,|1, 0\rangle$ of the composite system. We must express this in terms of the total angular momentum eigenstates of the composite system, and in particular determine the projection onto $|0, 0\rangle$, which is the state where the composite system has total spin 0.

Starting from the top, we have the states of the composite system:

$$|2, 2\rangle = |1, 1\rangle\,|1, 1\rangle$$

$$|2, 1\rangle = \frac{1}{\sqrt{2}}\left(|1, 0\rangle\,|1, 1\rangle + |1, 1\rangle\,|1, 0\rangle\right)$$

$$|2, 0\rangle = \frac{1}{\sqrt{6}}\left(|1, -1\rangle\,|1, 1\rangle + 2\,|1, 0\rangle\,|1, 0\rangle + |1, 1\rangle\,|1, -1\rangle\right),$$

by repeatedly lowering using $J_- = J_{-,1} \otimes I + I \otimes J_{-,2}$.

We can obtain $|1,1\rangle$ by orthogonality to $|2,1\rangle$; this was already discussed in part (b). We can then generate the following states:

$$|1,1\rangle = \frac{1}{\sqrt{2}}\left(|1,1\rangle\,|1,0\rangle - |1,0\rangle\,|1,1\rangle\right)$$

$$|1,0\rangle = \frac{1}{\sqrt{2}}\left(|1,1\rangle\,|1,-1\rangle - |1,-1\rangle\,|1,1\rangle\right).$$

Finally, to construct $|0,0\rangle$ we use orthogonality to $|2,0\rangle$ and $|1,0\rangle$. Generally, $|0,0\rangle$ will be some linear combination:

$$|0,0\rangle = \alpha\,|1,0\rangle\,|1,0\rangle + \beta\,|1,1\rangle\,|1,-1\rangle + \gamma\,|1,-1\rangle\,|1,1\rangle\,.$$

but the required orthogonality conditions imply that:

$$\beta - \gamma = 0, \qquad \beta + 2\alpha + \gamma = 0.$$

Solving these equations in terms of β, we see that $\gamma = \beta$ and $\alpha = -\beta$. Hence the state can be written as:

$$|0,0\rangle = \frac{1}{\sqrt{3}}\left(-\,|1,0\rangle\,|1,0\rangle + |1,1\rangle\,|1,-1\rangle + |1,-1\rangle\,|1,1\rangle\right).$$

after appropriate normalisation and a choice of arbitrary phase. It follows that the projection $\langle 0,0|\,(|1,0\rangle\,|1,0\rangle)$ is given by $1/\sqrt{3}$, and hence the required probability is just:

$$\frac{1}{3}.$$

2016, Paper 3, Section II, 31A

A three-dimensional oscillator has Hamiltonian

$$H = \frac{1}{2m}\left(\hat{p}_1^2 + \hat{p}_2^2 + \hat{p}_3^2\right) + \frac{1}{2}m\omega^2\left(\alpha^2\hat{x}_1^2 + \beta^2\hat{x}_2^2 + \gamma^2\hat{x}_3^2\right),$$

where the constants $m, \omega, \alpha, \beta, \gamma$ are real and positive. Assuming a unique ground state, construct the general normalised eigenstate of H and give a formula for its energy eigenvalue. [*You may quote without proof results for a one-dimensional harmonic oscillator of mass m and frequency ω that follow from writing $\hat{x} = (\hbar/2m\omega)^{1/2}(a + a^\dagger)$ and $\hat{p} = (\hbar m\omega/2)^{1/2} i(a^\dagger - a)$.*]

List all states in the four lowest energy levels of H in the cases:

(i) $\alpha < \beta < \gamma < 2\alpha$;

(ii) $\alpha = \beta$ and $\gamma = \alpha + \epsilon$, where $0 < \epsilon \ll \alpha$.

Now consider H with $\alpha = \beta = \gamma = 1$ subject to a perturbation

$$\lambda m\omega^2\left(\hat{x}_1\hat{x}_2 + \hat{x}_2\hat{x}_3 + \hat{x}_3\hat{x}_1\right),$$

where λ is small. Compute the changes in energies for the ground state and the states at the first excited level of the original Hamiltonian, working to the leading order at which non-zero corrections occur. [*You may quote without proof results from perturbation theory.*]

Explain briefly why some energy levels of the perturbed Hamiltonian will be exactly degenerate. [*Hint: Compare with (ii) above.*]

Solution: We are allowed to 'quote without proof results for a one-dimensional harmonic oscillator'. So let us recall that writing $\hat{x}, \hat{p}$ in terms of raising and lowering operators for a one-dimensional harmonic oscillator with ground state $|0\rangle$, we can write the nth eigenstate as

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle,$$

which has energy $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$.

The given Hamiltonian can be viewed as the tensor product:

$$H = H_1 \otimes H_2 \otimes H_3,$$

where H_1, H_2, H_3 are the Hamiltonians for harmonic oscillators in the x, y and z directions respectively, with frequencies $\alpha\omega$, $\beta\omega$ and $\gamma\omega$ respectively. It follows that we can solve each of these individual oscillators using the one-dimensional method; coupled with the fact that there is a unique overall ground state $|0\rangle = |0\rangle \otimes |0\rangle \otimes |0\rangle$, we immediately have that the general eigenstate of H is given by:

$$|n_1 n_2 n_3\rangle = \frac{(a_1^\dagger)^{n_1}}{\sqrt{n_1!}}\frac{(a_2^\dagger)^{n_2}}{\sqrt{n_2!}}\frac{(a_3^\dagger)^{n_3}}{\sqrt{n_3!}}|000\rangle,$$

where a_1, a_2, a_3 are the lowering operators for the Hamiltonians H_1, H_2, H_3 respectively. The energy of the state $|E_{n_1 n_2 n_3}\rangle$ is given by:

$$E_{n_1 n_2 n_3} = \hbar\alpha\omega\left(n_1 + \frac{1}{2}\right) + \hbar\omega\beta\left(n_2 + \frac{1}{2}\right) + \hbar\omega\gamma\left(n_3 + \frac{1}{2}\right) = \frac{1}{2}\hbar\omega\left(\alpha + \beta + \gamma\right) + \hbar\omega\left(\alpha n_1 + \beta n_2 + \gamma n_3\right).$$

(i) We are now asked to state the four lowest energy levels in the case $\alpha < \beta < \gamma < 2\alpha$. Looking at the expression we wrote down above for the energy levels $E_{n_1 n_2 n_3}$, we see that the lowest energy levels are:

$$E_{000} < E_{100} < E_{010} < E_{001}.$$

It is clear from the general form of $E_{n_1 n_2 n_3}$ that these energy levels are all non-degenerate in this case.

(ii) If $\alpha = \beta, \gamma = \alpha + \epsilon, 0 < \epsilon \ll \alpha$, then the general expression for the energy levels becomes:

$$E_{n_1 n_2 n_3} = \frac{3}{2}\hbar\omega\alpha + \frac{1}{2}\hbar\omega\epsilon + \hbar\omega\alpha\left(n_1 + n_2 + \left(1 + \frac{\epsilon}{\alpha}\right) n_3\right)$$

It's clear from writing $E_{n_1 n_2 n_3}$ in this form that the lowest energies levels are now $E_{000} < E_{100} = E_{010} < E_{001} < E_{200} = E_{110} = E_{020}$.

The first energy level E_{000} and the third energy level E_{001} are clearly both non-degenerate, whilst the second energy level $E_{100} = E_{010}$ has twofold degeneracy and the fourth energy level $E_{200} = E_{110} = E_{020}$ has threefold degeneracy.

For the next part of the question, we assume that $\alpha = \beta = \gamma = 1$, and add a perturbation:

$$\Delta = \lambda m\omega^2 \left(\hat{x}_1\hat{x}_2 + \hat{x}_2\hat{x}_3 + \hat{x}_3\hat{x}_1\right)$$

to the system. For practical purposes, it is useful to expand this perturbation in terms of raising and lowering operators. Recall that

$$\hat{x}_i = \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(a_i + a_i^\dagger\right)$$

for each spatial coordinate, and hence we can write the perturbation as:

$$\Delta = \frac{1}{2}\lambda\hbar\omega\left((a_1 + a_1^\dagger)(a_2 + a_2^\dagger) + (a_2 + a_2^\dagger)(a_3 + a_3^\dagger) + (a_3 + a_3^\dagger)(a_1 + a_1^\dagger)\right)$$

$$= \frac{1}{2}\lambda\hbar\omega\left(a_1a_2 + a_1a_2^\dagger + a_1^\dagger a_2^\dagger + a_1^\dagger a_2 + a_2a_3 + a_2a_3^\dagger + a_2^\dagger a_3 + a_2^\dagger a_3^\dagger + a_3a_1 + a_3a_1^\dagger + a_3^\dagger a_1 + a_3^\dagger a_1^\dagger\right).$$

We are now asked to determine the change in energy to the ground state and the first excited states (which will be $|100\rangle$, $|010\rangle$ and $|001\rangle$ in the case that $\alpha = \beta = \gamma = 1$) of our original system, to lowest non-zero order in perturbation theory.

The ground state is non-degenerate, and hence we can apply the result of non-degenerate perturbation theory. The first-order change in energy to the ground state is simply:

$$\langle 000|\Delta|000\rangle = 0,$$

by considering acting to the left or the right respectively with each of the raising and lowering operators. The second-order change in the energy is:

$$\sum_{\substack{n_1 n_2 n_3 \\ \neq 000}} \frac{|\langle n_1 n_2 n_3|\Delta|000\rangle|^2}{E_{000} - E_{n_1 n_2 n_3}},$$

and so we see that we must compute a general matrix element $\langle n_1 n_2 n_3|\Delta|000\rangle$. Using the expression for Δ in terms of the raising and lowering operators this is not too bad, since all the lowering operators will just annihilate $|000\rangle$ so we can ignore these terms:

$$\langle n_1 n_2 n_3|\Delta|000\rangle = \frac{1}{2}\lambda\hbar\omega\langle n_1 n_2 n_3|a_1^\dagger a_2^\dagger + a_2^\dagger a_3^\dagger + a_3^\dagger a_1^\dagger|000\rangle$$

$$= \frac{1}{2}\hbar\lambda\omega\left(\delta_{n_1 1}\delta_{n_2 1}\delta_{n_3 0} + \delta_{n_1 0}\delta_{n_2 1}\delta_{n_3 1} + \delta_{n_1 1}\delta_{n_2 0}\delta_{n_3 1}\right).$$

Hence we get the second order change in energy:

$$\left(\frac{1}{2}\hbar\lambda\omega\right)^2 \cdot \left(\frac{1}{E_{000}-E_{110}}+\frac{1}{E_{000}-E_{101}}+\frac{1}{E_{000}-E_{011}}\right) = -\frac{3\hbar\omega\lambda^2}{8}.$$

Now consider the change in energy to the first excited state $|100\rangle$, $|010\rangle$, $|001\rangle$. Since these states are degenerate, we must use degenerate perturbation theory here. We need to *diagonalise the perturbation in the degenerate subspace*. This can be achieved by first finding the matrix of Δ in the degenerate subspace. We notice:

- The action of the perturbation on the state $|100\rangle$ is given by:

$$\begin{aligned}\Delta|100\rangle &= \frac{1}{2}\hbar\lambda\omega\left(a_1a_2^\dagger + a_1^\dagger a_2^\dagger + a_3^\dagger a_1 + a_3^\dagger a_1^\dagger\right)|100\rangle \\ &= \frac{1}{2}\hbar\lambda\omega\left(|010\rangle + \sqrt{2}\,|210\rangle + |111\rangle + |001\rangle + \sqrt{2}\,|201\rangle\right),\end{aligned}$$

  and hence we have the matrix elements $\langle 100|\Delta|100\rangle = 0$, $\langle 010|\Delta|100\rangle = \frac{1}{2}\hbar\lambda\omega$ and $\langle 001|\Delta|100\rangle = \frac{1}{2}\hbar\lambda\omega$.

- By symmetry (the perturbation is symmetry under the cyclic symmetry $1\mapsto 2, 2\mapsto 3, 3\mapsto 1$), we can deduce that the other matrix elements are given similarly by:

$$\langle 010|\Delta|010\rangle = 0, \qquad \langle 100|\Delta|010\rangle = \frac{1}{2}\hbar\lambda\omega, \qquad \langle 001|\Delta|010\rangle = \frac{1}{2}\hbar\lambda\omega$$

$$\langle 001|\Delta|001\rangle = 0, \qquad \langle 100|\Delta|001\rangle = \frac{1}{2}\hbar\lambda\omega, \qquad \langle 010|\Delta|001\rangle = \frac{1}{2}\hbar\lambda\omega.$$

It follows that with respect to the basis $\{|100\rangle, |010\rangle, |001\rangle\}$, the matrix of Δ in the degenerate subspace is given by

$$\Delta\big|_{\text{degenerate subspace}} = \frac{1}{2}\hbar\lambda\omega\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix}.$$

We can determine the eigenvalues of this matrix to be:

$$-\frac{1}{2}\hbar\lambda\omega, \qquad -\frac{1}{2}\hbar\lambda\omega, \qquad \hbar\lambda\omega.$$

Hence we see that the energy level is split into two new energy levels, one of which has degeneracy two and the other has zero degeneracy (at least at first order in perturbation theory).

Finally, we are asked to show that the degeneracy two energy level that we found in the previous part of the question is exactly degenerate at all orders in perturbation theory. This can be achieved by diagonalising the perturbation. Note that the perturbed potential part of the Hamiltonian in this instance can be written in the form:

$$V(\hat{\mathbf{x}}) = \frac{1}{2}m\omega^2\left(\hat{x}_1^2+\hat{x}_2^2+\hat{x}_3^2+2\lambda\hat{x}_1\hat{x}_2+2\lambda\hat{x}_2\hat{x}_3+2\lambda\hat{x}_1\hat{x}_3\right).$$

This is a quadratic form, and can be written in matrix form as:

$$V(\hat{\mathbf{x}}) = \frac{1}{2}m\omega^2\begin{pmatrix}1&\lambda&\lambda\\\lambda&1&\lambda\\\lambda&\lambda&1\end{pmatrix}.$$

Note there are no ordering ambiguities, because all the components of position commute. The eigenvalues of the matrix are $1-\lambda$, $1-\lambda$ and $2\lambda+1$, hence there exists coordinates $\hat{X}$, $\hat{Y}$ and $\hat{Z}$ in which this quadratic form can be diagonalised to:

$$\frac{1}{2}m\omega^2\left((1-\lambda)\hat{X}^2+(1-\lambda)\hat{Y}^2+((1-\lambda)+3\lambda)\hat{Z}^2\right).$$

Hence the perturbation makes our oscillator into an anisotropic oscillator of type (ii), which we saw had exactly degenerate energy levels.

2016, Paper 4, Section II, 31A

(a) Consider a quantum system with Hamiltonian $H = H_0 + V$, where H_0 is independent of time. Define the interaction picture corresponding to this Hamiltonian and derive an expression for the time derivative of an operator in the interaction picture, assuming it is independent of time in the Schrödinger picture.

(b) The Pauli matrices $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ satisfy

$$\sigma_i \sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k.$$

Explain briefly how these properties allow $\boldsymbol{\sigma}$ to be used to describe a quantum system with spin-$\frac{1}{2}$.

(c) A particle with spin-$\frac{1}{2}$ has position and momentum operators $\hat{\mathbf{x}} = (\hat{x}_1, \hat{x}_2, \hat{x}_3)$ and $\hat{\mathbf{p}} = (\hat{p}_1, \hat{p}_2, \hat{p}_3)$. The unitary operator corresponding to a rotation through an angle θ about an axis $\mathbf{n}$ is $U = \exp(-i\theta \mathbf{n} \cdot \mathbf{J}/\hbar)$ where $\mathbf{J}$ is the total angular momentum. Check this statement by considering the effect of an infinitesimal rotation on $\hat{\mathbf{x}}$, $\hat{\mathbf{p}}$ and $\boldsymbol{\sigma}$.

(d) Suppose that the particle in part (c) has Hamiltonian $H = H_0 + V$ with

$$H_0 = \frac{1}{2m}\hat{\mathbf{p}}^2 + \alpha \mathbf{L} \cdot \boldsymbol{\sigma} \qquad \text{and} \qquad V = B\sigma_3,$$

where $\mathbf{L}$ is the orbital angular momentum and α, B are constants. Show that all components of $\mathbf{J}$ are independent of time in the interaction picture. Is this true in the Heisenberg picture?

[*You may quote commutation relations of* $\mathbf{L}$ *with* $\hat{\mathbf{x}}$ *and* $\hat{\mathbf{p}}$.]

Solution: (a) The *interaction picture* for a quantum mechanical system is defined in terms of *interaction states* and *interaction operators*, which are given in terms of their Schrödinger picture counterparts (written $|\psi_S\rangle$ and A_S respectively) by:

$$|\psi_I(t)\rangle = e^{iH_0 t/\hbar} |\psi_S(t)\rangle, \qquad A_I(t) = e^{iH_0 t/\hbar} A_S e^{-iH_0 t/\hbar},$$

where $U_0(t) = e^{-iH_0 t/\hbar}$ is the time-evolution operator of the free Hamiltonian H_0, and $e^{iH_0 t/\hbar}$ is its inverse.

We are now asked to derive the equation of motion for interaction pictures operators. Acting on an interaction picture operator $A_I(t)$ with a time derivative, we have

$$i\hbar \frac{dA_I}{dt} = i\hbar \frac{d}{dt}\left(e^{iH_0 t/\hbar} A_S e^{-iH_0 t/\hbar}\right) = i\hbar \left(e^{iH_0 t/\hbar}\left(\frac{iH_0}{\hbar} A_S - A_S \frac{iH_0}{\hbar}\right) e^{-iH_0 t/\hbar}\right)$$

$$= e^{iH_0 t/\hbar}[A_S, H_0] e^{-iH_0 t/\hbar} = [A_I(t), H_0],$$

using the identity $e^A[B, C]e^{-A} = [e^A B e^{-A}, e^A C e^{-A}]$ in the very last step.

(b) We claim that expressing $\mathbf{S} = \frac{1}{2}\hbar\boldsymbol{\sigma}$ leads to the correct spin algebra for a spin-$\frac{1}{2}$ particle. The correct commutation relations follow for S_i, S_j because of the ϵ_{ijk} part of the Pauli matrix identity:

$$[S_i, S_j] = \frac{1}{4}\hbar^2[\sigma_i, \sigma_j] = \frac{1}{4}\hbar^2 (\sigma_i\sigma_j - \sigma_j\sigma_i) = \frac{1}{4}\hbar^2 (i\epsilon_{ijk}\sigma_k - i\epsilon_{jik}\sigma_k) = i\hbar\epsilon_{ijk}S_k.$$

The δ_{ij} part of the Pauli matrix identity guarantees that along any direction, we have $(\hat{\mathbf{n}} \cdot \mathbf{S})^2 = \frac{1}{4}\hbar^2$; that is, the magnitude of the particle's spin is definitely $\hbar/2$ measured in any particular direction; this is required for a spin-$1/2$ particle. We have:

$$(\hat{\mathbf{n}} \cdot \mathbf{S})^2 = \frac{\hbar^2}{4}\left(\hat{n}_1^2\sigma_1^2 + \hat{n}_2^2\sigma_2^2 + \hat{n}_3^2\sigma_3^2\right) = \frac{\hbar^2}{4}.$$

(c) Let's consider the effect of this rotation operator on a general vector operator $\mathbf{V}$. We have:

$$\exp\left(\frac{i\theta\mathbf{n}\cdot\mathbf{J}}{\hbar}\right)\mathbf{V}\exp\left(\frac{-i\theta\mathbf{n}\cdot\mathbf{J}}{\hbar}\right)=\left(I+\frac{i\theta\mathbf{n}\cdot\mathbf{J}}{\hbar}\right)\mathbf{V}\left(I-\frac{i\theta\mathbf{n}\cdot\mathbf{J}}{\hbar}\right)+O(\theta^2)$$

$$=\mathbf{V}+\frac{i\theta}{\hbar}[\mathbf{n}\cdot\mathbf{J},\mathbf{V}]+O(\theta^2).$$

Now recall that for any vector operator, be it position $\hat{\mathbf{x}}$, momentum $\hat{\mathbf{p}}$, or spin $\mathbf{S}=\frac{1}{2}\hbar\boldsymbol{\sigma}$[3], we have the canonical commutation relation with $\mathbf{J}$ given by:

$$[J_i,V_j]=i\hbar\epsilon_{ijk}V_k.$$

Hence in this instance, we get the result:

$$\exp\left(\frac{i\theta\mathbf{n}\cdot\mathbf{J}}{\hbar}\right)V_j\exp\left(\frac{-i\theta\mathbf{n}\cdot\mathbf{J}}{\hbar}\right)=V_j-\theta n_i\epsilon_{ijk}V_k+O(\theta^2)=V_j+[\theta\mathbf{n}\times\mathbf{V}]_j+O(\theta^2),$$

which can be rewritten as:

$$\exp\left(\frac{i\theta\mathbf{n}\cdot\mathbf{J}}{\hbar}\right)\mathbf{V}\exp\left(\frac{-i\theta\mathbf{n}\cdot\mathbf{J}}{\hbar}\right)=\mathbf{V}+\theta\mathbf{n}\times\mathbf{V}+O(\theta^2),$$

which is indeed the way an infinitesimal rotation should act on a vector (we can see this, for example, by choosing coordinate where $\mathbf{n}=(0,0,1)$, and then expanding the corresponding rotation matrix $R(\theta)$ in small θ).

(d) We are now asked to show that J_i is independent of time in the interaction picture. Let's write $J_i^I(t)$ for the interaction picture angular momentum, and J_i for the Schrödinger picture angular momentum. By part (a), the interaction picture operator evolves as:

$$i\hbar\frac{dJ_i^I(t)}{dt}=[J_i^I(t),H_0]=e^{iH_0t/\hbar}[J_i,H_0]e^{-iH_0t/\hbar}.$$

We can evaluate the commutator $[J_i,H_0]$ using the given expression for H_0. In index notation, we have:

$$[J_i,H_0]=\frac{1}{2m}[J_i,p_kp_k]+\frac{\alpha}{m\hbar}[J_i,L_kS_k]=\frac{1}{2m}\left([J_i,p_k]p_k+p_k[J_i,p_k]\right)+\frac{\alpha}{m\hbar}\left([J_i,L_k]S_k+L_k[J_i,S_k]\right).$$

Using the commutation relation for J_i with a vector operator, we have

$$[J_i,H_0]=\frac{1}{2m}\left(\epsilon_{ikj}p_jp_k+\epsilon_{ikj}p_kp_j\right)+\frac{\alpha}{m\hbar}\left(\epsilon_{ikj}L_jS_k+\epsilon_{ikj}L_kS_j\right)=0,$$

since both terms are the product of something antisymmetric on k,j and something symmetric on k,j. We deduce that

$$\frac{dJ_i^I(t)}{dt}=0,$$

as required.

In the Heisenberg picture, we instead must use the Heisenberg equation of motion:

$$i\hbar\frac{dJ_i^H(t)}{dt}=[J_i^H(t),H]=e^{iHt/\hbar}[J_i,H]e^{-iHt/\hbar},$$

where $H=H_0+B\sigma_3$ is the full Hamiltonian here. We have already seen that $[J_i,H_0]=0$. So we are left to evaluate the commutator:

$$[J_i,B\sigma_3]=\frac{2B}{\hbar}[J_i,S_3]=\frac{2B}{\hbar}i\hbar\epsilon_{i3k}S_k=i\hbar B\epsilon_{i3k}\sigma_k.$$

Hence we're left with:

$$\frac{dJ_i^H(t)}{dt}=B\epsilon_{i3k}e^{iHt/\hbar}\sigma_ke^{-iHt/\hbar}\neq 0,$$

unless $i=3$. So the vector $\mathbf{J}^H(t)$ in the Heisenberg picture is *not* independent of time.

[3] Well, technically spin is a pseudovector, but here it doesn't matter because pseudovectors transform in the same way as vectors under rotations.

2017, Paper 1, Section II, 32C

The position and momentum operators of the harmonic oscillator can be written as

$$\hat{x} = \left(\frac{\hbar}{2m\omega}\right)^{1/2} \left(a + a^\dagger\right), \qquad \hat{p} = \left(\frac{\hbar m\omega}{2}\right)^{1/2} i\left(a^\dagger - a\right),$$

where m is the mass, ω is the frequency, and the Hamiltonian is

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

Assuming that $[\hat{x}, \hat{p}] = i\hbar$, derive the commutation relations for a and $a^\dagger$. Construct the Hamiltonian in terms of a and $a^\dagger$. Assuming that there is a unique ground state, explain how all other energy eigenstates can be constructed from it. Determine the energy of each of these eigenstates.

Consider the modified Hamiltonian

$$H' = H + \lambda\hbar\omega\left(a^2 + {a^\dagger}^2\right),$$

where λ is a dimensionless parameter. Use perturbation theory to calculate the modified energy levels to second order in λ, quoting any standard formulae that you require. Show that the modified Hamiltonian can be written in the form

$$H' = \frac{1}{2m}(1 - 2\lambda)\hat{p}^2 + \frac{1}{2}m\omega^2(1 + 2\lambda)\hat{x}^2.$$

Assuming $|\lambda| < 1/2$, calculate the modified energies exactly. Show that the results are compatible with those obtained from perturbation theory.

Solution: First we are asked to derive the commutation relations for a and $a^\dagger$. We trivially have the commutation relations $[a, a] = 0$ and $[a^\dagger, a^\dagger] = 0$. Substituting the given forms for $\hat{x}, \hat{p}$ into the commutation relation $[\hat{x}, \hat{p}] = i\hbar$, we can derive $[a, a^\dagger]$ as follows:

$$\begin{aligned}
i\hbar &= [\hat{x}, \hat{p}] && \text{(given commutation relation)} \\
&= \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(\frac{\hbar m\omega}{2}\right)^{1/2} i\left[a + a^\dagger, a^\dagger - a\right] && \text{(given forms of } \hat{x}, \hat{p}) \\
&= \frac{i\hbar}{2}\left([a, a^\dagger] - [a^\dagger, a]\right) && \text{(linearity of commutator, and } [a, a] = [a^\dagger, a^\dagger] = 0) \\
&= i\hbar[a, a^\dagger] && \text{(antisymmetry of commutator).}
\end{aligned}$$

We conclude that $[a, a^\dagger] = 1$. By the antisymmetry of the commutator, we also have $[a^\dagger, a] = -1$.

Next we are asked to write the Hamiltonian in terms of a and $a^\dagger$. Inserting the expressions for $\hat{x}, \hat{p}$ in terms of $a, a^\dagger$ into

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

we have

$$\begin{aligned}
H &= -\frac{1}{2m}\left(\frac{\hbar m\omega}{2}\right)\left(a^\dagger - a\right)^2 + \frac{1}{2}m\omega^2\left(\frac{\hbar}{2m\omega}\right)\left(a + a^\dagger\right)^2 \\
&= -\frac{\hbar\omega}{4}\left((a^\dagger)^2 - a^\dagger a - aa^\dagger + a^2\right) + \frac{\hbar\omega}{4}\left(a^2 + aa^\dagger + a^\dagger a + (a^\dagger)^2\right) \\
&= \frac{\hbar\omega}{2}\left(a^\dagger a + aa^\dagger\right).
\end{aligned}$$

Commuting $a^\dagger$ past a, we have the final form of the Hamiltonian:

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

We can construct the energy eigenstates of H as follows. Let's begin by noticing that the spectrum of H is bounded below, since for any normalised eigenstate $|E\rangle$ of H of energy E, we have:

$$E = \langle E|H|E\rangle = \hbar\omega\,\langle E|a^\dagger a|E\rangle + \frac{1}{2}\hbar\omega = \hbar\omega||a\,|E\rangle\,||^2 + \frac{1}{2}\hbar\omega \geq \frac{1}{2}\hbar\omega.$$

We are given that we can assume the existence of a unique ground state $|0\rangle$, which is such that the energy of H is minimised. Thus we assume that $|0\rangle$ obeys $a\,|0\rangle = 0$. In particular, it then follows that $H\,|0\rangle = \frac{1}{2}\hbar\omega\,|0\rangle$.

Now suppose that $|E\rangle$ is any energy eigenstate of H with energy E. We note that $a\,|E\rangle$ is also an energy eigenstate of H:

$$\begin{aligned}
H(a\,|E\rangle) &= \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)a\,|E\rangle && \text{(above form of } H\text{)}\\
&= \hbar\omega\left(aa^\dagger + [a^\dagger, a] + \frac{1}{2}\right)a\,|E\rangle && \text{(commuting } a, a^\dagger\text{)}\\
&= a\hbar\omega\left(a^\dagger a + [a^\dagger, a] + \frac{1}{2}\right)|E\rangle && \text{(taking out } a \text{ to left)}\\
&= aH\,|E\rangle - \hbar\omega a\,|E\rangle && \text{(above form of } H\text{, and } [a^\dagger, a] = -1\text{)}\\
&= (E - \hbar\omega)(a\,|E\rangle) && \text{(since } H\,|E\rangle = E\,|E\rangle\text{)}
\end{aligned}$$

Thus $|E\rangle$, $a\,|E\rangle$, $a^2\,|E\rangle$, ... , $a^n\,|E\rangle$ is a sequence of energy eigenstates of H with increasingly lower energies E, $E - \hbar\omega$, $E - 2\hbar\omega$, ... , $E - n\hbar\omega$. Unless this sequence suddenly terminates, then we will find that H has a spectrum that is unbounded below. It follows that there must exist a non-negative integer n such that $a^{n+1}\,|E\rangle = 0$. In particular, we must hit the ground state at some point, by uniqueness - it follows that $a^n\,|E\rangle = |0\rangle$ for some integer n. In particular, looking at the energies of our sequence from above (E, $E - \hbar\omega$, $E - 2\hbar\omega$, ... , $E - n\hbar\omega$) we see that this implies

$$E - n\hbar\omega = \frac{1}{2}\hbar\omega \qquad \Rightarrow \qquad E = \hbar\omega\left(n + \frac{1}{2}\right),$$

for some non-negative integer n.

So far we have shown that any eigenstate $|n\rangle$ of H must have energy of the form $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$ for some non-negative integer n. We now *inductively construct* a state of energy E_n for each n. Suppose that $|n\rangle$ is a state of energy E_n, as described above. Then $a^\dagger\,|n\rangle$ is an eigenstate of H with energy E_{n+1}:

$$\begin{aligned}
H(a^\dagger\,|n\rangle) &= \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)a^\dagger\,|n\rangle && \text{(above form of } H\text{)}\\
&= \hbar\omega\left(a^\dagger a^\dagger a + a^\dagger[a, a^\dagger] + \frac{1}{2}a^\dagger\right)|n\rangle && \text{(commuting } a^\dagger, a\text{)}\\
&= a^\dagger\hbar\omega\left(a^\dagger a + [a, a^\dagger] + \frac{1}{2}\right)|n\rangle && \text{(taking out } a^\dagger \text{ to left)}
\end{aligned}$$

$$= a^\dagger H \left|n\right\rangle + \hbar\omega a \left|n\right\rangle \qquad \text{(above form of } H\text{, and } [a, a^\dagger] = +1)$$

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

$$= E_{n+1} a^\dagger \left|n\right\rangle$$

where the last equality follows since $E_n + \hbar\omega = \hbar\omega(n + \frac{1}{2}) + \hbar\omega = \hbar\omega(n + 1 + \frac{1}{2}) = E_{n+1}$.

Hence we have found $a^\dagger \left|n\right\rangle \propto \left|n+1\right\rangle$. We can find the appropriate normalisation of the state as follows:

$$||a^\dagger \left|n\right\rangle||^2 = \langle n|aa^\dagger|n\rangle = \langle n|a^\dagger a|n\rangle + \langle n|[a, a^\dagger]|n\rangle = \hbar^{-1}\omega^{-1} \left\langle n\right| (H - \hbar\omega/2) \left|n\right\rangle + 1 = n + 1.$$

Thus we can consistently choose $a^\dagger \left|n\right\rangle = \sqrt{n+1} \left|n+1\right\rangle$. In particular, dividing through by the normalisation and iterating, we have constructed the eigenstates of H:

$$\left|n\right\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} \left|0\right\rangle, \qquad \text{with energies} \qquad E_n = \hbar\omega\left(n + \frac{1}{2}\right).$$

The energy eigenstates are non-degenerate, since we are working in one dimension. Hence these are precisely all the energy eigenstates and energy eigenvalues.

We now consider a perturbed harmonic oscillator. Recall that for a perturbed Hamiltonian $H' = H + \Delta H$, the modification to the nth energy level is given by:

$$\delta E_n = \langle n|\Delta H|n\rangle + \sum_{m\neq n} \frac{|\left\langle m\right|\Delta H\left|n\right\rangle|^2}{E_n - E_m},$$

where H' is the perturbation to the Hamiltonian and $\left|m\right\rangle$ is the mth excited state, in this case given by

$$\frac{(a^\dagger)^m}{\sqrt{m!}} \left|0\right\rangle$$

as we saw above. In our case, the relevant matrix element we need to evaluate is:

$$\begin{aligned}
\langle m|\Delta H|n\rangle &= \frac{\lambda\hbar\omega}{\sqrt{m!\cdot n!}} \langle 0|a^m(a^2 + {a^\dagger}^2)(a^\dagger)^n|0\rangle \\
&= \frac{\lambda\hbar\omega}{\sqrt{m!\cdot n!}} \left(\langle 0|a^{m+2}(a^\dagger)^n|0\rangle + \langle 0|a^m(a^\dagger)^{n+2}|0\rangle\right) \\
&= \lambda\hbar\omega\left(\sqrt{(m+2)(m+1)} \left\langle m+2\right|\left.n\right\rangle + \sqrt{(n+2)(n+1)} \left\langle m\right|\left.n+2\right\rangle\right) \\
&= \lambda\hbar\omega\left(\sqrt{(m+2)(m+1)}\delta_{m+2,n} + \sqrt{(n+2)(n+1)}\delta_{m,n+2}\right).
\end{aligned}$$

It follows that the modification to the nth energy levels is given by:

$$\delta E_n = \lambda^2\hbar^2\omega^2\left(\frac{n(n-1)}{E_n - E_{n-2}} + \frac{(n+2)(n+1)}{E_n - E_{n+2}}\right) = \lambda^2\hbar\omega\left(\frac{n(n-1)}{2} - \frac{(n+2)(n+1)}{2}\right) = -\lambda^2\hbar\omega(2n+1).$$

Hence the modified energy levels are given by $\tilde{E}_n = \hbar\omega\left(n + \frac{1}{2} - \lambda^2(2n+1)\right)$.

Finally, we are asked to derive the exact energy levels for this perturbation and hence demonstrate that our perturbative expansion is consistent. To do this, let's expand the perturbation in terms of $\hat{x}$ and $\hat{p}$. First note that we can write the raising and lowering operators as:

$$a = \frac{1}{\sqrt{2\hbar m\omega}} \left(m\omega\hat{x} + i\hat{p}\right), \qquad a^\dagger = \frac{1}{\sqrt{2\hbar m\omega}} \left(m\omega\hat{x} - i\hat{p}\right).$$

Hence we can write the perturbation as:

$$\Delta H = \lambda\hbar\omega \left(a^2 + {a^\dagger}^2\right) = \frac{\lambda\hbar\omega}{2\hbar m\omega} \left(2m^2\omega^2\hat{x}^2 - 2\hat{p}^2 + im\omega\hat{x}\hat{p} + im\omega\hat{p}\hat{x} - im\omega\hat{x}\hat{p} - im\omega\hat{p}\hat{x}\right) = \frac{\lambda}{m} \left(m^2\omega^2\hat{x}^2 - \hat{p}^2\right).$$

Thus indeed the perturbed Hamiltonian can be rewritten in the form:

$$H' = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 + \lambda m\omega^2\hat{x}^2 - \frac{\lambda}{m}\hat{p}^2 = \frac{(1-2\lambda)}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2(1+2\lambda)\hat{x}^2.$$

Define an effective mass $m' = m/(1-2\lambda)$. Then we can rewrite H' in harmonic oscillator form as:

$$H = \frac{1}{2m'}\hat{p}^2 + \frac{1}{2}m'\omega^2(1-4\lambda^2)\hat{x}^2.$$

Hence this is a harmonic oscillator with frequency $\omega\sqrt{1-4\lambda^2}$. It follows that its energy levels are:

$$E_n = \hbar\omega\sqrt{1-4\lambda^2}\left(n + \frac{1}{2}\right) = \hbar\omega\left(n + \frac{1}{2}\right) - 2\lambda^2\hbar\omega\left(n + \frac{1}{2}\right) + O(\lambda^4) = \hbar\omega\left(n + \frac{1}{2} - \lambda^2\left(2n+1\right)\right) + O(\lambda^4),$$

which is consistent with the result we got from perturbation theory.

2017, Paper 2, Section II, 32C

Let $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ be a set of Hermitian operators obeying

$$[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k \qquad \text{and} \qquad (\mathbf{n}\cdot\boldsymbol{\sigma})^2 = 1, \tag{$*$}$$

where $\mathbf{n}$ is any unit vector. Show that $(*)$ implies that

$$(\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma}) = \mathbf{a}\cdot\mathbf{b} + i(\mathbf{a}\times\mathbf{b})\cdot\boldsymbol{\sigma}$$

for any vectors $\mathbf{a}$ and $\mathbf{b}$. Explain, with reference to the properties $(*)$, how $\boldsymbol{\sigma}$ can be related to the intrinsic angular momentum $\mathbf{S}$ for a particle of spin-$\frac{1}{2}$.

Show that the operators $P_\pm = \frac{1}{2}(1 \pm \mathbf{n}\cdot\boldsymbol{\sigma})$ are Hermitian and obey

$$P_\pm^2 = P_\pm, \qquad P_+P_- = P_-P_+ = 0.$$

Show how $P_\pm$ can be used to write any state $|\chi\rangle$ as a linear combination of eigenstates of $\mathbf{n}\cdot\boldsymbol{\sigma}$. Use this to deduce that if the system is in a normalised state $|\chi\rangle$ when $\mathbf{n}\cdot\boldsymbol{\sigma}$ is measured, then the results ± 1 will be obtained with probabilities

$$||P_\pm|\chi\rangle||^2 = \frac{1}{2}\left(1 \pm \langle\chi|\mathbf{n}\cdot\boldsymbol{\sigma}|\chi\rangle\right).$$

If $|\chi\rangle$ is a state corresponding to the system having spin up along a direction defined by a unit vector $\mathbf{m}$, show that a measurement will find the system to have spin up along $\mathbf{n}$ with probability $\frac{1}{2}(1 + \mathbf{n}\cdot\mathbf{m})$.

Solution: From $(*)$, we first notice:

$$(\mathbf{a}\cdot\boldsymbol{\sigma})^2 = (|\mathbf{a}|\hat{\mathbf{a}}\cdot\boldsymbol{\sigma})^2 = |\mathbf{a}|^2,$$

for any vector $\mathbf{a}$. Hence we have:

$$|\mathbf{a}+\mathbf{b}|^2 = ((\mathbf{a}+\mathbf{b})\cdot\boldsymbol{\sigma})^2 = (\mathbf{a}\cdot\boldsymbol{\sigma})^2 + (\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma}) + (\mathbf{b}\cdot\boldsymbol{\sigma})(\mathbf{a}\cdot\boldsymbol{\sigma}) + (\mathbf{b}\cdot\boldsymbol{\sigma})^2 = |\mathbf{a}|^2 + |\mathbf{b}|^2 + (\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma}) + (\mathbf{b}\cdot\boldsymbol{\sigma})(\mathbf{a}\cdot\boldsymbol{\sigma}).$$

Commuting $(\mathbf{a}\cdot\boldsymbol{\sigma})$ past $(\mathbf{b}\cdot\boldsymbol{\sigma})$, we have:

$$(\mathbf{b}\cdot\boldsymbol{\sigma})(\mathbf{a}\cdot\boldsymbol{\sigma}) = b_i a_j \sigma_i\sigma_j = b_i a_j \sigma_j\sigma_i + b_i a_j[\sigma_i, \sigma_j] = (\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma}) + 2ib_i a_j \epsilon_{ijk}\sigma_k = (\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma}) + 2i(\mathbf{b}\times\mathbf{a})\cdot\boldsymbol{\sigma}.$$

Putting everything together, we have:

$$2(\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma}) = |\mathbf{a}+\mathbf{b}|^2 - |\mathbf{a}|^2 - |\mathbf{b}|^2 + 2i(\mathbf{a}\times\mathbf{b})\cdot\boldsymbol{\sigma}.$$

Expanding the norms, and dividing by two, we're left with the result:

$$(\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma}) = \mathbf{a}\cdot\mathbf{b} + i(\mathbf{a}\times\mathbf{b})\cdot\boldsymbol{\sigma},$$

as required.

By setting $S_i = \frac{1}{2}\hbar\sigma_i$, we see that S_i has all the properties of the spin operator for a spin-$\frac{1}{2}$ particle. Namely, it obeys the correct commutation algebra:

$$[S_i, S_j] = \frac{\hbar^2}{4}[\sigma_i, \sigma_j] = \frac{\hbar^2}{2} i\epsilon_{ijk}\sigma_k = i\hbar\epsilon_{ijk}S_k.$$

We also have $(\hat{\mathbf{n}}\cdot\mathbf{S})^2 = \frac{1}{4}\hbar^2$; that is, the magnitude of the particle's spin is definitely $\hbar/2$ measured along any particular direction; this is required for a spin-$1/2$ particle. We have:

$$(\hat{\mathbf{n}}\cdot\mathbf{S})^2 = \frac{\hbar^2}{4}(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})^2 = \frac{\hbar^2}{4}.$$

We are given in the question that the operator $\boldsymbol{\sigma}$ are Hermitian. The given $P_\pm$ operators obey:

$$P_\pm^\dagger = \frac{1}{2}\left(1 \pm \mathbf{n}\cdot\boldsymbol{\sigma}\right)^\dagger = \frac{1}{2}\left(1 \pm \mathbf{n}\cdot\boldsymbol{\sigma}^\dagger\right) = \frac{1}{2}(1 \pm \mathbf{n}\cdot\boldsymbol{\sigma}) = P_\pm,$$

hence they are Hermitian as required.

We can prove the given identities directly. First, we have:

$$P_\pm^2 = \frac{1}{2}(1 \pm \mathbf{n}\cdot\boldsymbol{\sigma})\cdot\frac{1}{2}(1 \pm \mathbf{n}\cdot\boldsymbol{\sigma}) = \frac{1}{4}\left(1 \pm 2\mathbf{n}\cdot\boldsymbol{\sigma} + (\mathbf{n}\cdot\boldsymbol{\sigma})^2\right) = \frac{1}{2}(1 \pm \mathbf{n}\cdot\boldsymbol{\sigma}) = P_\pm,$$

as required. We also have:

$$P_+P_- = \frac{1}{4}(1 + \mathbf{n}\cdot\boldsymbol{\sigma})(1 - \mathbf{n}\cdot\boldsymbol{\sigma}) = \frac{1}{4}(1 - (\mathbf{n}\cdot\boldsymbol{\sigma})^2) = 0,$$

and similarly

$$P_-P_+ = \frac{1}{4}(1 - \mathbf{n}\cdot\boldsymbol{\sigma})(1 + \mathbf{n}\cdot\boldsymbol{\sigma}) = \frac{1}{4}(1 - (\mathbf{n}\cdot\boldsymbol{\sigma})^2) = 0.$$

The notation and properties of $P_\pm$ leads us to think that we should interpret them as *projection operators*. With this interpretation, we hope to be able to write any state as:

$$|\chi\rangle = P_+|\chi\rangle + P_-|\chi\rangle.$$

This actually follows trivially, since $P_+ + P_- = \frac{1}{2}(1 + \mathbf{n}\cdot\boldsymbol{\sigma}) + \frac{1}{2}(1 - \mathbf{n}\cdot\boldsymbol{\sigma}) = 1$. It remains to show that $P_+|\chi\rangle$ and $P_-|\chi\rangle$ are eigenstates of $\mathbf{n}\cdot\boldsymbol{\sigma}$. We have:

$$(\mathbf{n}\cdot\boldsymbol{\sigma})P_\pm|\chi\rangle = \frac{1}{2}\left((\mathbf{n}\cdot\boldsymbol{\sigma}) \pm (\mathbf{n}\cdot\boldsymbol{\sigma})^2\right)|\chi\rangle = \pm\frac{1}{2}\left(1 \pm \mathbf{n}\cdot\boldsymbol{\sigma}\right)|\chi\rangle = \pm P_\pm|\chi\rangle.$$

Hence $P_\pm|\chi\rangle$ are indeed eigenstates of $\mathbf{n}\cdot\boldsymbol{\sigma}$ with eigenvalues ±1 respectively.

We can now make the deduction in the question. Suppose that $|\chi\rangle$ is a normalised eigenstate. As we saw above, we can write $|\chi\rangle = P_+|\chi\rangle + P_-|\chi\rangle$. By the Born rule, on measuring the observable $\mathbf{n}\cdot\boldsymbol{\sigma}$, the probability of obtaining ±1 is then the norm of the projection of $|\chi\rangle$ onto the corresponding eigenstates of $\mathbf{n}\cdot\boldsymbol{\sigma}$ with eigenvalues ±1, which we found earlier were simply $P_\pm|\chi\rangle$. Hence we have:

$$\mathrm{Prob}(+1) = \left(\langle\chi|P_+^\dagger\right)|\chi\rangle = \left(\langle\chi|P_+\right)\left(P_+|\chi\rangle + P_-|\chi\rangle\right) = \langle\chi|P_+^2|\chi\rangle = ||P_+|\chi\rangle||^2 = \langle\chi|P_+|\chi\rangle = \frac{1}{2}\left(1 + \langle\chi|\mathbf{n}\cdot\boldsymbol{\sigma}|\chi\rangle\right),$$

using the properties $P_+^\dagger = P_+$, $P_+^2 = P_+$ and $P_+P_- = 0$ we derived earlier. Similarly, we find:

$$\mathrm{Prob}(-1) = ||P_-|\chi\rangle||^2 = \frac{1}{2}\left(1 - \langle\chi|\mathbf{n}\cdot\boldsymbol{\sigma}|\chi\rangle\right).$$

Finally, we are told that $|\chi\rangle$ is an eigenstate of $\mathbf{m}\cdot\boldsymbol{\sigma}$ with eigenvalue $+1$ (this is the meaning of the phrase '$|\chi\rangle$ is in the spin-up state along the direction defined by the unit vector $\mathbf{m}$'). Hence we have $\mathbf{m}\cdot\boldsymbol{\sigma}|\chi\rangle = |\chi\rangle$. In particular, the probability of finding the state to have spin-up in the $\mathbf{n}$ direction is given by the above work to be:

$$\begin{aligned}\frac{1}{2}\left(1 + \langle\chi|\mathbf{n}\cdot\boldsymbol{\sigma}|\chi\rangle\right) &= \frac{1}{2}\left(1 + \langle\chi|(\mathbf{n}\cdot\boldsymbol{\sigma})(\mathbf{m}\cdot\boldsymbol{\sigma})|\chi\rangle\right)\\ &= \frac{1}{2}\left(1 + \mathbf{n}\cdot\mathbf{m} + i\,\langle\chi|(\mathbf{n}\times\mathbf{m})\cdot\boldsymbol{\sigma}|\chi\rangle\right),\end{aligned}$$

using the identity we proved at the very start of the question for $(\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma})$. Finally, note that $\langle\chi|(\mathbf{n}\times\mathbf{m})\cdot\boldsymbol{\sigma}|\chi\rangle = 0$, since $\mathbf{n}\times\mathbf{m}$ is orthogonal to $\mathbf{m}$, and $|\chi\rangle$ is an eigenstate which is definitely spin-up in the $\mathbf{m}$ direction. On measurement of $(\mathbf{n}\times\mathbf{m})\cdot\boldsymbol{\sigma}$ then, the chance of getting spin-up and the change of getting spin-down when in the state $|\chi\rangle$ are equal, and hence the expectation of the measurement is zero. Hence we have the required probability.

2017, Paper 3, Section II, 32C

The angular momentum operators $\mathbf{J} = (J_1, J_2, J_3)$ obey the commutation relations

$$[J_3, J_\pm] = \pm J_\pm, \qquad [J_+, J_-] = 2J_3,$$

where $J_\pm = J_1 \pm iJ_2$.

A quantum mechanical system involves the operators $a, a^\dagger, b$ and $b^\dagger$ such that

$$[a, a^\dagger] = [b, b^\dagger] = 1, \qquad [a, b] = [a^\dagger, b] = [a, b^\dagger] = [a^\dagger, b^\dagger] = 0.$$

Define $K_+ = a^\dagger b$, $K_- = ab^\dagger$ and $K_3 = \frac{1}{2}(a^\dagger a - b^\dagger b)$. Show that $K_\pm$ and K_3 obey the same commutation relations as $J_\pm$ and J_3.

Suppose that the system is in the state $|0\rangle$ such that $a|0\rangle = b|0\rangle = 0$. Show that $(a^\dagger)^2|0\rangle$ is an eigenstate of K_3. Let $K^2 = \frac{1}{2}(K_+K_- + K_-K_+) + K_3^2$. Show that $(a^\dagger)^2|0\rangle$ is an eigenstate of K^2 and find the eigenvalue. How many other states do you expect to find with the same value of K^2? Find them.

Solution: This whole question is made significantly easier if we just work out the commutation relations between $K_\pm$, K_3 and $a, a^\dagger, b, b^\dagger$ from the off. Notice first that since all the a's commute with all the b's, we have:

$$[K_3, a] = \frac{1}{2}[a^\dagger a, a] = -\frac{1}{2}a, \qquad [K_3, a^\dagger] = \frac{1}{2}[a^\dagger a, a^\dagger] = \frac{1}{2}a^\dagger,$$

$$[K_3, b] = -\frac{1}{2}[b^\dagger b, b] = \frac{1}{2}b, \qquad [K_3, b^\dagger] = -\frac{1}{2}[b^\dagger b, b^\dagger] = -\frac{1}{2}b^\dagger.$$

For the $K_\pm$ commutation relations with $a, a^\dagger, b, b^\dagger$, we have:

$$[K_+, a] = [a^\dagger b, a] = -b, \qquad [K_+, b] = [a^\dagger b, b] = 0, \qquad [K_+, a^\dagger] = [a^\dagger b, a^\dagger] = 0, \qquad [K_+, b^\dagger] = [a^\dagger b, b^\dagger] = a^\dagger,$$

$$[K_-, a] = [ab^\dagger, a] = 0, \qquad [K_-, b] = [ab^\dagger, b] = -a, \qquad [K_-, a^\dagger] = [ab^\dagger, a^\dagger] = b^\dagger, \qquad [K_-, b^\dagger] = [ab^\dagger, b^\dagger] = 0.$$

Hence we have:

$$[K_+, K_-] = [a^\dagger b, K_-] = a^\dagger[b, K_-] + [a^\dagger, K_-]b = a^\dagger a - b^\dagger b = 2K_3,$$

as required. Similarly, we have:

$$[K_3, K_+] = [K_3, a^\dagger b] = [K_3, a^\dagger]b + a^\dagger[K_3, b] = \frac{1}{2}a^\dagger b + \frac{1}{2}a^\dagger b = K_+,$$

and

$$[K_3, K_-] = [K_3, ab^\dagger] = [K_3, a]b^\dagger + a[K_3, b^\dagger] = -\frac{1}{2}ab^\dagger - \frac{1}{2}ab^\dagger = -K_-.$$

So indeed we have the required results:

$$[K_+, K_-] = 2K_3, \qquad [K_3, K_\pm] = \pm K_\pm,$$

This tells us that we should view K_3, $K_\pm$ as angular momentum operators, since they obey the angular momentum commutation algebra (recall that the commutation algebra is all we need to assume to derive the special form of the eigenvalues of J_3, J^2, so the same applies to K_3, K^2 here).

Next we are asked to construct some eigenstates for K_3, K^2. First, we are asked to show that $(a^\dagger)^2 |0\rangle$ is an eigenstate of K_3. First, we note that

$$K_3 |0\rangle = 0,$$

since all annihilation operators are on the right of the expression for K_3. Hence we have:

$$K_3(a^\dagger)^2 |0\rangle = \left([K_3, (a^\dagger)^2] + (a^\dagger)^2 K_3\right) |0\rangle = \left([K_3, a^\dagger]a^\dagger + a^\dagger[K_3, a^\dagger]\right) |0\rangle = (a^\dagger)^2 |0\rangle ,$$

using $[K_3, a^\dagger] = \frac{1}{2}a^\dagger$ from above. Thus we deduce that indeed $(a^\dagger)^2 |0\rangle$ is an eigenstate of K_3 with eigenvalue $+1$.

Next, we are asked to determine the K^2 eigenvalue of $(a^\dagger)^2 |0\rangle$. We first note that $K_+ |0\rangle = K_- |0\rangle = 0$, since again we can just annihilate $|0\rangle$ using annihilation operators in $K_\pm$. Thus we have:

$$\begin{aligned} K^2(a^\dagger)^2 |0\rangle &= \left(\frac{1}{2}(K_+K_- + K_-K_+) + K_3^2\right)(a^\dagger)^2 |0\rangle \\ &= \left(K_+K_- + \frac{1}{2}[K_-, K_+] + K_3^2\right)(a^\dagger)^2 |0\rangle \\ &= \left(K_+K_- - K_3 + K_3^2\right)(a^\dagger)^2 |0\rangle \\ &= [K_+K_-, (a^\dagger)^2] |0\rangle , \end{aligned}$$

recalling that $K_3(a^\dagger)^2 |0\rangle = (a^\dagger)^2 |0\rangle$ from above. It remains to evaluate the commutator. We have:

$$[K_+K_-, (a^\dagger)^2] |0\rangle = [K_+, (a^\dagger)^2]K_- |0\rangle + K_+[K_-, (a^\dagger)^2] |0\rangle = K_+\left([K_-, a^\dagger]a^\dagger + a^\dagger[K_-, a^\dagger]\right) |0\rangle$$

$$= 2K_+a^\dagger b^\dagger |0\rangle = 2(a^\dagger)^2 bb^\dagger |0\rangle = 2(a^\dagger)^2[b, b^\dagger] |0\rangle = 2(a^\dagger)^2 |0\rangle .$$

Hence we have $K^2(a^\dagger)^2 |0\rangle = 1(1+1)(a^\dagger)^2 |0\rangle$, i.e. the eigenvalue is $2 = 1(1+1)$. This implies that we are working with a representation of the angular momentum eigenstate $|1, 1\rangle$. Therefore, we know from the general theory of angular momentum that there will be *two* more eigenstates with K^2 eigenvalue $2 = 1(1+1)$, corresponding to the angular momentum eigenstates $|1, 0\rangle$ and $|1, -1\rangle$. We should expect to obtain them using the raising and lowering operators, so we hope they are given by:

$$K_-(a^\dagger)^2 |0\rangle \qquad \text{and} \qquad K_-^2(a^\dagger)^2 |0\rangle .$$

We can find the K_3 eigenvalues of these states quite easily:

$$K_3K_-(a^\dagger)^2 |0\rangle = [K_3, K_-](a^\dagger)^2 |0\rangle + K_-(a^\dagger)^2 |0\rangle = -K_-(a^\dagger)^2 |0\rangle + K_-(a^\dagger)^2 |0\rangle = 0,$$

and

$$K_3K_-^2(a^\dagger)^2 |0\rangle = [K_3, K_-^2](a^\dagger)^2 |0\rangle + K_-^2(a^\dagger)^2 |0\rangle = -2K_-^2(a^\dagger)^2 |0\rangle + K_-^2(a^\dagger)^2 |0\rangle = -K_-^2(a^\dagger)^2 |0\rangle ,$$

so we get the expected eigenvalues of 0 and -1.

It remains to show that these are also eigenstates of K^2 with eigenvalue $1(1+1)$. To do so, it's useful to quickly work out $[K^2, K_-]$. We have:

$$\begin{aligned} [K^2, K_-] &= \frac{1}{2}[K_+K_-, K_-] + \frac{1}{2}[K_-K_+, K_-] + [K_3^2, K_-] \\ &= \frac{1}{2}[K_+, K_-]K_- + \frac{1}{2}K_-[K_+, K_-] + K_3[K_3, K_-] + [K_3, K_-]K_3 \\ &= K_3K_- + K_-K_3 - K_3K_- - K_-K_3 = 0. \end{aligned}$$

Therefore, we see that (just as expected from the angular momentum algebra), K^2 and K_- commute. It follows that $K_-(a^\dagger)^2 |0\rangle$ and $K_-^2(a^\dagger)^2 |0\rangle$ indeed have the K^2 eigenvalue $1(1+1)$ as required.

2017, Paper 4, Section II, 32C

The Hamiltonian for a quantum system in the Schrödinger picture is

$$H_0 + \lambda V(t),$$

where H_0 is independent of time and the parameter λ is small. Define the interaction picture corresponding to this Hamiltonian and derive a time evolution equation for interaction picture states.

Let $|n\rangle$ and $|m\rangle$ be eigenstates of H_0 with distinct eigenvalues E_n and E_m respectively. Show that if the system was in the state $|n\rangle$ in the remote past, then the probability of measuring it to be in a different state $|m\rangle$ at time t is

$$\frac{\lambda^2}{\hbar^2}\left|\int_{-\infty}^{t} dt' \ \langle m|V(t')|n\rangle \, e^{i(E_m-E_n)t'/\hbar}\right|^2 + O(\lambda^3).$$

Let the system be a simply harmonic oscillator with $H_0 = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$, where $[a, a^\dagger] = 1$. Let $|0\rangle$ be the ground state which obeys $a\,|0\rangle = 0$. Suppose

$$V(t) = e^{-p|t|}(a + a^\dagger),$$

with $p > 0$. In the remote past the system was in the ground state. Find the probability, to lowest non-trivial order in λ, for the system to be in the first excited state in the far future.

Solution: The *interaction picture* for a quantum mechanical system is defined in terms of *interaction states* and *interaction operators*, which are given in terms of their Schrödinger picture counterparts (written $|\psi_S\rangle$ and A_S respectively) by:

$$|\psi_I(t)\rangle = e^{iH_0 t/\hbar}\,|\psi_S(t)\rangle\,, \qquad A_I(t) = e^{iH_0 t/\hbar} A_S e^{-iH_0 t/\hbar},$$

where $U_0(t) = e^{-iH_0 t/\hbar}$ is the time-evolution operator of the free Hamiltonian H_0, and $e^{iH_0 t/\hbar}$ is its inverse.

We are also asked to derive the equation of motion for interaction pictures states. Acting on an interaction picture state $|\psi_I\rangle$ with a time derivative, we have

$$i\hbar\frac{\partial}{\partial t}\,|\psi_I(t)\rangle = i\hbar\frac{\partial}{\partial t}\left(e^{iH_0 t/\hbar}\,|\psi_S(t)\rangle\right) = -H_0 e^{iH_0 t/\hbar}\,|\psi_S(t)\rangle + e^{iH_0 t/\hbar}(H_0 + \lambda V(t))\,|\psi_S(t)\rangle\,,$$

using Schrödinger's equation for the Schrödinger picture state $|\psi_S(t)\rangle$. Since H_0 commutes with $e^{iH_0 t/\hbar}$, we can simplify the right hand side leaving:

$$i\hbar\frac{\partial}{\partial t}\,|\psi_I(t)\rangle = e^{iH_0 t/\hbar}\lambda V(t)\,|\psi_S(t)\rangle = e^{iH_0 t/\hbar}\lambda V(t) e^{-iH_0 t/\hbar} e^{iH_0 t/\hbar}\,|\psi_S(t)\rangle = \lambda V_I(t)\,|\psi_I(t)\rangle$$

$$\Rightarrow \qquad i\hbar\frac{\partial}{\partial t}\,|\psi_I(t)\rangle = \lambda V_I(t)\,|\psi_I(t)\rangle\,,$$

which is the interaction picture equation of motion as required.

Next we are asked to establish the probability of measuring the system to be in the free-Hamiltonian eigenstate $|m\rangle$ at time t, if it is in the free-Hamiltonian eigenstate $|n\rangle$ at time $t = -\infty$. First we recall that interaction picture predictions are equivalent to Schrödinger picture predictions, hence it is equivalent to find the probability working in the interaction picture.

Next, we need to deal with the interaction picture equation of motion itself. Notice that by direct integration, we can recast the interaction picture equation of motion as an integral equation:

$$i\hbar\,|\psi_I(t)\rangle = i\hbar\,|\psi_I(-\infty)\rangle + \int_{-\infty}^{t} \lambda V_I(t')\,|\psi_I(t')\rangle\;dt'.$$

The integrand on the right hand side involves a $|\psi_I(t')\rangle$; if we express this in terms of the right hand side we can get an iterative series in λ as a result. Truncating at the first order, we obtain the approximation:

$$i\hbar\,|\psi_I(t)\rangle \approx i\hbar\,|\psi_I(-\infty)\rangle + \lambda\int_{-\infty}^{t} V_I(t')\,|\psi_I(0)\rangle\;dt' + O(\lambda^2).$$

Recall $|\psi_I(-\infty)\rangle = |n_I\rangle \propto |n\rangle$ is given. We want to find $|\,\langle m_I|\psi_I(t)\rangle\,|^2 = |\,\langle m|\psi_I(t)\rangle\,|^2$, which can be found by computing:

$$i\hbar\,\langle m|\psi_I(t)\rangle \approx i\hbar\,\langle m|n\rangle + \lambda\int_{-\infty}^{t} \langle m|V_I(t')|n\rangle\;dt' + O(\lambda^2).$$

Expanding $V_I(t') = e^{iH_0t'/\hbar}V(t')e^{-iH_0t'/\hbar}$ and acting on the free-Hamiltonian eigenstates with the relevant operators leaves us with:

$$i\hbar\,\langle m|\psi_I(t)\rangle \approx i\hbar\,\langle m|n\rangle + \lambda\int_{-\infty}^{t} e^{i(E_m-E_n)t'/\hbar}\,\langle m|V(t')|n\rangle\;dt' + O(\lambda^2).$$

Assuming that $|n\rangle, |m\rangle$ have distinct eigenvalues E_n and E_m, they are orthogonal, and hence we're left with the probability:

$$|\,\langle m|\psi_I(t)\rangle\,|^2 = \frac{\lambda^2}{\hbar^2}\left|\int_{-\infty}^{t} e^{i(E_m-E_n)t'/\hbar}\,\langle m|V(t')|n\rangle\;dt'\right|^2 + O(\lambda^3),$$

as required. Note we get an $O(\lambda^3)$ correction from cross-terms when we square ($O(\lambda)\cdot O(\lambda^2) = O(\lambda^3)$).

We are now asked to apply the above work to an example. We are given $|n\rangle = |0\rangle$, $|m\rangle = |1\rangle = a^\dagger|0\rangle$ and $t = \infty$ (we are looking at the 'far future'). We are also given the interaction $V(t)$. First, we work out the matrix element $\langle 1|V(t)|0\rangle$. We have:

$$\langle 1|e^{-p|t|}(a+a^\dagger)|0\rangle = e^{-p|t|}\,\langle 0|aa^\dagger|0\rangle = e^{-p|t|}\,\langle 0|[a,a^\dagger]|0\rangle = e^{-p|t|}.$$

The difference in energy between the levels is simply $E_1 - E_0 = \frac{3}{2}\hbar\omega - \frac{1}{2}\hbar\omega = \hbar\omega$. Hence we must evaluate the integral:

$$\int_{-\infty}^{\infty} e^{(i\omega t' - p|t'|)}\,dt' = \left[\frac{e^{(i\omega+p)t'}}{i\omega+p}\right]_{-\infty}^{0} + \left[\frac{e^{(i\omega-p)t'}}{i\omega-p}\right]_{0}^{\infty} = \frac{1}{i\omega+p} - \frac{1}{i\omega-p} = \frac{2p}{\omega^2+p^2}.$$

It follows that the required probability is:

$$\frac{4p^2\lambda^2}{\hbar^2(\omega^2+p^2)^2}.$$

2018, Paper 1, Section II, 33D

A one-dimensional harmonic oscillator has Hamiltonian

$$H = \hbar\omega\left(A^\dagger A + \frac{1}{2}\right)$$

where $[A, A^\dagger] = 1$. Show that $A\,|n\rangle = \sqrt{n}\,|n-1\rangle$, where $H\,|n\rangle = \hbar\omega(n+\frac{1}{2})\,|n\rangle$ and $\langle n|n\rangle = 1$.

The oscillator is perturbed by adding a new term λX^4 to the Hamiltonian. Given that

$$A = \frac{m\omega X - iP}{\sqrt{2m\hbar\omega}},$$

show that the ground state of the perturbed system is

$$|0_\lambda\rangle = |0\rangle - \frac{\hbar\lambda}{4m^2\omega^3}\left(3\sqrt{2}\,|2\rangle + \sqrt{\frac{3}{2}}\,|4\rangle\right),$$

to first order in λ. [*You may use the fact that, in non-degenerate perturbation theory, a perturbation Δ causes the first-order shift*

$$|m^{(1)}\rangle = \sum_{n\neq m}\frac{\langle n|\Delta|m\rangle}{E_m - E_n}\,|n\rangle$$

in the mth energy level.]

Solution: To show that $A\,|n\rangle = \sqrt{n-1}\,|n-1\rangle$, we first show that $A\,|n\rangle$ is an eigenstate of H; we then find the proportionality constant. We have:

$$\begin{aligned}
HA\,|n\rangle &= \hbar\omega\left(A^\dagger A + \frac{1}{2}\right)A\,|n\rangle && \text{(definition of } H\text{)}\\
&= \hbar\omega\left(AA^\dagger + [A^\dagger, A] + \frac{1}{2}\right)A\,|n\rangle && \text{(commuting } A, A^\dagger\text{)}\\
&= \hbar\omega A\left(A^\dagger A + \frac{1}{2}\right)|n\rangle + [A^\dagger, A]\hbar\omega A\,|n\rangle\\
&= AH\,|n\rangle - \hbar\omega A\,|n\rangle\\
&= \hbar\omega\left((n-1) + \frac{1}{2}\right)A\,|n\rangle && \text{(since } H\,|n\rangle = \hbar\omega\left(n+\frac{1}{2}\right)|n\rangle\text{)}.
\end{aligned}$$

It follows that $A\,|n\rangle \propto |n-1\rangle$. To find the normalisation, note that

$$||A\,|n\rangle\,||^2 = \langle n|A^\dagger A|n\rangle = \langle n|\left(\frac{H}{\hbar\omega} - \frac{1}{2}\right)|n\rangle = \frac{1}{\hbar\omega}\langle n|H|n\rangle - \frac{1}{2} = n + \frac{1}{2} - \frac{1}{2} = n.$$

It follows that we can set $A\,|n\rangle = \sqrt{n}\,|n-1\rangle$ (there is in principle an arbitrary phase, but we can set this to 1 without loss of generality).

It is also useful to note that $A^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle$; this follows by an almost identical proof.

We are now asked to calculate the ground state of the system in the presence of a perturbation $\Delta = \lambda X^4$ to first-order in λ. Using the hint, the first-order change to the ground state is given by:

$$|0^{(1)}\rangle = \lambda \sum_{n=1}^{\infty} \frac{\langle n|X^4|0\rangle}{E_0 - E_n} |n\rangle \,.$$

Hence we must now calculate the matrix elements $\langle n|X^4|0\rangle$. To do so, it's best to express X in terms of the raising and lowering operators:

$$A = \frac{m\omega X - iP}{\sqrt{2m\hbar\omega}}, \qquad A^\dagger = \frac{m\omega X + iP}{\sqrt{2m\hbar\omega}} \qquad \Rightarrow \qquad X = \sqrt{\frac{\hbar}{2m\omega}} \left(A^\dagger + A\right).$$

Thus we have:

$$X^4 = \frac{\hbar^2}{4m^2\omega^2} \left(A^\dagger + A\right)^4$$

We now wish to expand $\left(A^\dagger + A\right)^4$. This is quite difficult, because A and $A^\dagger$ do not commute, so we can't just write down the binomial expansion of this expression. However, things are made much easier by instead considering $X^4 |0\rangle$. Then we can ignore any term in the expansion of $\left(A^\dagger + A\right)^4$ that ends in an A, because the A will simply annihilate $|0\rangle$. Hence we have:

$$X^4 |0\rangle = \frac{\hbar^2}{4m^2\omega^2} \left(A^\dagger + A\right)^4 |0\rangle$$

$$= \frac{\hbar^2}{4m^2\omega^2} \left((A^\dagger)^4 + A(A^\dagger)^3 + A^\dagger A(A^\dagger)^2 + (A^\dagger)^2 AA^\dagger + A^2(A^\dagger)^2 + AA^\dagger AA^\dagger + A^\dagger A^2 A^\dagger + A^3 A^\dagger\right)|0\rangle \,.$$

Now notice that some terms in this expansion give zero. In particular, if we do not raise with $A^\dagger$ sufficiently many times, then lower with A too many times, we will get zero. The terms that vanish are those involving the last two operators $A^\dagger A^2 A^\dagger$, $A^3 A^\dagger$.

Furthermore, we lose any terms that act on $|0\rangle$ and only produce $|0\rangle$, because we will contract with $\langle n|$ for $n \geq 1$. The terms that disappear are $A^2(A^\dagger)^2$ and $AA^\dagger AA^\dagger$.

Hence we only need to evaluate the vastly simplified expression:

$$\begin{aligned}
\langle n| X^4 |0\rangle &= \frac{\hbar^2}{4m^2\omega^2} \langle n| \left((A^\dagger)^4 + A(A^\dagger)^3 + A^\dagger A(A^\dagger)^2 + (A^\dagger)^2 AA^\dagger\right)|0\rangle \\
&= \frac{\hbar^2}{4m^2\omega^2} \left(\sqrt{4\cdot 3\cdot 2\cdot 1}\,\langle n|4\rangle + \sqrt{3\cdot 3\cdot 2\cdot 1}\,\langle n|2\rangle + \sqrt{2\cdot 2\cdot 2\cdot 1}\,\langle n|2\rangle + \sqrt{2\cdot 1\cdot 1\cdot 1}\,\langle n|2\rangle\right) \\
&= \frac{\hbar^2}{4m^2\omega^2} \left(2\sqrt{6}\,\delta_{n4} + 6\sqrt{2}\,\delta_{n2}\right).
\end{aligned}$$

Noting that $E_0 - E_4 = \frac{1}{2}\hbar\omega - \hbar\omega\left(4 + \frac{1}{2}\right) = -4\hbar\omega$ and $E_0 - E_2 = -2\hbar\omega$, we have the required result:

$$|0^{(1)}\rangle = -\frac{\lambda\hbar}{4m^2\omega^3} \left(\frac{6\sqrt{2}}{2}|2\rangle + \frac{2\sqrt{6}}{4}|4\rangle\right) = -\frac{\lambda\hbar}{4m^2\omega^3} \left(3\sqrt{2}\,|2\rangle + \sqrt{\frac{3}{2}}\,|4\rangle\right).$$

⁂ **Comments from the Examiner:** *This question required some simple bookwork, followed by a calculation in perturbation that both lecturer and examiner thought some would find tricky. Both lecturer and examiner were completely wrong. The question was way too straightforward and the vast majority of students got full marks.*

2018, Paper 2, Section II, 34D

Explain what is meant by the *intrinsic parity* of a particle. In each of the decay processes below, parity is conserved.

A deuteron (d^+) has intrinsic parity $\eta_d = +1$ and spin $s = 1$. A negatively charge pion (π^-) has spin $s = 0$. The ground state of a hydrogenic 'atom' formed from a deuteron and a pion decays to two identical neutrons (n), each of spin $s = \frac{1}{2}$ and parity $\eta_n = +1$. Deduce the intrinsic parity of the pion.

The Δ^- particle has spin $s = \frac{3}{2}$ and decays as

$$\Delta^- \to \pi^- + n.$$

What are the allowed values of the orbital angular momentum? In the centre of mass frame, the vector $\mathbf{r}_\pi - \mathbf{r}_n$ joining the pion to the neutron makes an angle θ to the $\hat{\mathbf{z}}$-axis. The final state is an eigenstate of J_z and the spatial probability distribution is proportional to $\cos^2(\theta)$. Deduce the intrinsic parity of the Δ^-. [*Hint: You may use the fact that the first three Legendre polynomials are given by* $P_0(x) = 1, P_1(x) = x, P_2(x) = \frac{1}{2}(3x^2 - 1)$.]

Solution: The classical *parity* operator $\mathcal{P} : \mathbb{R}^3 \to \mathbb{R}^3$ acts via $\mathcal{P}(\mathbf{x}) = -\mathbf{x}$. Let its representation on Hilbert space as a unitary operator be given by $\Pi = U(\mathcal{P})$, and let $|P; \mathbf{x}\rangle$ denote the state of some particle P definitely at the position $\mathbf{x}$. Then the *intrinsic parity* of the particle P is the constant $\eta_P = \pm 1$ such that

$$\Pi\,|P; \mathbf{x}\rangle = \eta_P\,|P; -\mathbf{x}\rangle\,.$$

This is extended by linearity when P is not in a definite location (i.e. its spatial wavefunction is not a delta function).

Now for the decay processes. For the first, we have the table of given data:

Particle property	d^+	π^-	**First** n	**Second** n
Intrinsic parity	1	η_π	1	1
Total ang. mom. (j)	j		$?$	
Orbital ang. mom. (l)	0		l	
Spin (s)	1	0	$\frac{1}{2}$	$\frac{1}{2}$

Note that we've set the orbital angular momenta of the left hand side to 0 without loss of generality, by an appropriate choice of origin about which to measure the orbital angular momentum of the system.

Now, we can add the spin angular momenta of the deuteron d^+ and pion π^- to get spin 1. Similarly, we can add the total spin angular momenta of the d^+, π^- system to the total orbital angular momenta of the d^+, π^- system to find that $j = 1$. By conservation of angular momentum, we can also fill in the total angular momentum of the n, n pair as $j = 1$ too:

Particle property	d^+	π^-	**First** n	**Second** n
Intrinsic parity	1	η_π	1	1
Total ang. mom. (j)	1		1	
Orbital ang. mom. (l)	0		l	
Spin (s)	1		$\frac{1}{2}$	$\frac{1}{2}$

We now add the spin angular momenta of the n, n pair. This is a little more complicated as there are two options:

- The spins are aligned, in which case we get total spin 1. Writing $|\uparrow\rangle = |\frac{1}{2}, \frac{1}{2}\rangle$, $|\downarrow\rangle = |\frac{1}{2}, -\frac{1}{2}\rangle$, we see that the total spin eigenstates are given by:

$$|1,1\rangle = |\uparrow\rangle\,|\uparrow\rangle \qquad |1,0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle\,|\downarrow\rangle + |\downarrow\rangle\,|\uparrow\rangle\right) \qquad |1,-1\rangle = |\downarrow\rangle\,|\downarrow\rangle\,.$$

  In particular, on exchange of the neutrons, the spin state is *symmetric*.

- The spins are anti-aligned, in which case we get total spin 0. The total spin eigenstates are given by:

$$|0,0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle\,|\downarrow\rangle - |\downarrow\rangle\,|\uparrow\rangle\right).$$

  On exchange of the neutrons, the spin state is *antisymmetric*.

Using this to fill in the table further, we have:

Particle property	d^+	π^-	**First** n	**Second** n
Intrinsic parity	1	η_π	1	1
Total ang. mom. (j)	1		1	
Orbital ang. mom. (l)	0		l	
Spin (s)	1		1 (symm.) or 0 (antisymm.)	

We can now decide on the value of the orbital angular momenta of the n, n pair l. Let's run through the possible cases:

- If the pair has total spin 0, then we must have $l = 1$ to ensure that the spin plus the orbital angular momentum can produce the total angular momentum $j = 1$. But then on exchanging the n, n pair we pick up a factor of $(-1)^1 = -1$ from the spatial wavefunction and a factor of -1 from the spin wavefunction, so a total factor of $+1$. This contradicts the fact that the particles are *fermions* (which follows from the *spin-statistics theorem*, since they have spin $\frac{1}{2}$).

- If the pair has total spin 1, we can have either $l = 0$ or $l = 1$. In the case that $l = 0$, exchange of the n, n pair gives a factor of $(-1)^0 = +1$ from the spatial wavefunction, and a factor of $+1$ from the spin wavefunction, again giving a total factor of $+1$ - a contradiction.

  Hence we must have $l = 1$. We can check using the same method that this is consistent with the particles being fermions.

To finish, we find the parity of the pion π^-. By conservation of parity, we have

$$1 \cdot \eta_{\pi^-} \cdot (-1)^0 = 1 \cdot 1 \cdot (-1)^1 \qquad \Rightarrow \qquad \eta_{\pi^-} = -1.$$

Note that we must use the factors of intrinsic parity and the factors of $(-1)^l$ from the spatial wavefunctions on both sides.

In the last part of the question, we are presented with another decay process $\Delta^- \to \pi^- + n$. Filling in all the given data (and the data we derived above for the π^-) in a table, we have:

Particle property	Δ^0	π^-	n
Intrinsic parity	η_{Δ^-}	-1	1
Total ang. mom. (j)	$3/2$	$3/2$	
Orbital ang. mom. (l)	0	l	
Spin (s)	$3/2$	$1/2$	

Note that we have also filled in some extra bits and pieces, just as we normally do. In particular, we have chosen to work in the rest frame for the decaying Δ^-, and so $l = 0$ on the left hand side. This means that the total angular momentum on the left hand side is $3/2$, since we are given the spin of the Δ^- is $3/2$, and adding angular momentum $3/2$ to angular momentum 0 can only result in angular momentum $3/2$.

We have also added together the spins of the neutron and the pion, since angular momentum 0 added to angular momentum $1/2$ can only result in angular momentum $1/2$. Finally, we have imposed conservation of total angular momentum to declare that the total angular momentum of the neutron-pion system is $3/2$.

We can now find the possible values of the orbital angular momentum of the neutron-pion system. We note that angular momentum l must be added to angular momentum $1/2$ to give angular momentum $3/2$, and hence we have:

$$\tfrac{3}{2} \in \left\{ \tfrac{1}{2} + l, \tfrac{1}{2} + l - 1, \tfrac{1}{2} + l - 2, \ldots, \left| \tfrac{1}{2} - l \right| \right\}.$$

It follows that the allowed values of l are just $l = 1$ or $l = 2$.

In the last part of the question, we are told that the spatial probability distribution of the system is proportional to $\cos^2(\theta)$, hence its spatial wavefunction must be proportional to $\cos(\theta)$. Recall from lectures that the spatial wavefunction for a system with total orbital angular momentum quantum number l and L_z quantum number m is proportional to the associated Legendre polynomial $P_l^m(\cos(\theta))$; in general, the system will have spatial wavefunction which is some superposition of these functions for different l and different m.

However, for $m \neq 0$, all associated Legendre polynomials $P_l^m(\cos(\theta))$ have a dependence on $\sin(\theta)$, so we can ignore $m \neq 0$, leaving only the Legendre polynomials given in the hint - scanning the functions given there implies $l = 1$.[4]
From this, we can deduce the intrinsic parity of the Δ^- using parity conservation:

$$\eta_{\Delta^-}(-1)^0 = (-1) \cdot (+1) \cdot (-1)^1 \qquad \Rightarrow \qquad \eta_{\Delta^-} = +1.$$

✻ **Comments from the Examiner:** *This was a fairly tricky question on the parity of particles in various decay processes. It is close to questions on the examples sheet, but is a topic that students often have trouble with. This was the case here. A couple of students got full marks with beautifully succinct answers of around $1/2$ a page, and a few others did well. But most struggled to appreciate the subtle correlation between the spin and angular momentum due to the anti-symmetric nature of the wavefunction. Given the large number of poor attempts, I was fairly generous in marking.*

[4] Technically, this argument is still rather unsatisfactory. The Hilbert space of the right hand side is given by $\mathcal{H}_{1/2} \otimes (\mathcal{H}_1 \oplus \mathcal{H}_2)$, the tensor product of the spin Hilbert space and the orbital angular momentum Hilbert space (which is composed of two summands, corresponding to two possibilities for l). Expanding using the Clebsch-Gordan formula, we get the result: $(\mathcal{H}_{1/2} \oplus \mathcal{H}_{3/2}) \oplus (\mathcal{H}_{3/2} \oplus \mathcal{H}_{5/2})$. Since the system must have definite total angular momentum $j = 3/2$, it follows our state is in some superposition of states drawn from the first occurrence and second occurrences of $\mathcal{H}_{3/2}$. Using the fact J_z is fixed, the problem boils down to writing out $|\frac{3}{2}, m\rangle$ in terms of states of $\mathcal{H}_{1/2} \otimes \mathcal{H}_1$ and $\mathcal{H}_{1/2} \otimes \mathcal{H}_2$; analysing the orbital angular momentum projections of these states eventually leads to the correct result but is clearly beyond the scope of the question.

2018, Paper 3, Section II, 34D

A quantum system is prepared in the ground state $|0\rangle$ at time $t = 0$. It is subjected to a time-varying Hamiltonian $H = H_0 + \Delta(t)$. Show that, to first order in $\Delta(t)$, the system evolves as

$$|\psi(t)\rangle = \sum_k c_k(t) e^{-iE_k t/\hbar} |k\rangle ,$$

where $H_0 |k\rangle = E_k |k\rangle$ and

$$c_k(t) = \frac{1}{i\hbar} \int_0^t \langle k|\Delta(t')|0\rangle \, e^{i(E_k - E_0)t'/\hbar} \, dt'.$$

A large number of hydrogen atoms, each in the ground state, are subjected to an electric field

$$\mathbf{E}(t) = \begin{cases} \mathbf{0} & \text{for } t < 0, \\ \hat{\mathbf{z}} \mathcal{E}_0 \exp(-t/\tau) & \text{for } t > 0, \end{cases}$$

where $\mathcal{E}_0$ is a constant. Show that the fraction of atoms found in the state $|n, l, m\rangle = |2, 1, 0\rangle$ is, after a long time and to lowest non-trivial order in $\mathcal{E}_0$,

$$\frac{2^{15}}{3^{10}} \frac{a_0^2 e^2 \mathcal{E}_0^2}{\hbar^2(\omega^2 + 1/\tau^2)}$$

where $\hbar\omega$ is the energy difference between the $|2, 1, 0\rangle$ and $|1, 0, 0\rangle$ states, e is the electron charge and a_0 the Bohr radius. What fraction of atoms lie in the $|2, 0, 0\rangle$ state?

[*Hint: You may assume the hydrogenic wavefunctions*

$$\langle \mathbf{r}|1, 0, 0\rangle = \frac{2}{\sqrt{4\pi}} \frac{1}{a_0^{3/2}} \exp\left(-\frac{r}{a_0}\right) \qquad \textit{and} \qquad \langle \mathbf{r}|2, 1, 0\rangle = \frac{1}{\sqrt{4\pi}} \frac{1}{(2a_0)^{3/2}} \frac{r}{a_0} \cos(\theta) \exp\left(-\frac{r}{2a_0}\right)$$

and the integral

$$\int_0^\infty r^m e^{-\alpha r} \, dr = \frac{m!}{\alpha^{m+1}}$$

for m a positive integer.]

Solution: For the first part of the question, it is useful to introduce the *interaction picture* and derive an equation of motion in the interaction picture. Recall that the *interaction picture* for a quantum mechanical system is defined in terms of *interaction states* and *interaction operators*, which are given in terms of their Schrödinger picture counterparts (written $|\psi_S\rangle$ and A_S respectively) by:

$$|\psi_I(t)\rangle = e^{iH_0 t/\hbar} |\psi_S(t)\rangle , \qquad A_I(t) = e^{iH_0 t/\hbar} A_S e^{-iH_0 t/\hbar},$$

where $U_0(t) = e^{-iH_0 t/\hbar}$ is the time-evolution operator of the free Hamiltonian H_0, and $e^{iH_0 t/\hbar}$ is its inverse.

Acting on an interaction picture state $|\psi_I\rangle$ with a time derivative, we have

$$i\hbar \frac{\partial}{\partial t} |\psi_I(t)\rangle = i\hbar \frac{\partial}{\partial t} \left(e^{iH_0 t/\hbar} |\psi_S(t)\rangle \right) = -H_0 e^{iH_0 t/\hbar} |\psi_S(t)\rangle + e^{iH_0 t/\hbar} (H_0 + \Delta(t)) |\psi_S(t)\rangle ,$$

using Schrödinger's equation for the Schrödinger picture state $|\psi_S(t)\rangle$.

Since H_0 commutes with $e^{iH_0t/\hbar}$, we can simplify the right hand side leaving:

$$i\hbar\frac{\partial}{\partial t}\left|\psi_I(t)\right\rangle = e^{iH_0t/\hbar}\Delta(t)\left|\psi_S(t)\right\rangle = e^{iH_0t/\hbar}\Delta(t)e^{-iH_0t/\hbar}e^{iH_0t/\hbar}\left|\psi_S(t)\right\rangle = \Delta_I(t)\left|\psi_I(t)\right\rangle$$

$$\Rightarrow \qquad i\hbar\frac{\partial}{\partial t}\left|\psi_I(t)\right\rangle = \Delta_I(t)\left|\psi_I(t)\right\rangle,$$

which is the interaction picture equation of motion.

We now want to express the Schrödinger state at time t in terms of energy eigenstates of the free Hamiltonian, to first order in $\Delta(t)$. Let

$$\left|\psi_S(t)\right\rangle = \sum_k a_k(t)\left|k\right\rangle.$$

We can find the coefficients by computing $\langle k|\psi_S(t)\rangle$. Relating this to the interaction picture state, this is equivalent to computing

$$\langle k|\psi_S(t)\rangle = \langle k|e^{-iH_0t/\hbar}|\psi_I(t)\rangle = e^{-iE_kt/\hbar}\left\langle k|\psi_I(t)\right\rangle,$$

so it's sufficient to compute $\langle k|\psi_I(t)\rangle$.

We can do so by solving the interaction picture equation of motion. Notice that by direct integration, we can recast the interaction picture equation of motion as an integral equation:

$$i\hbar\left|\psi_I(t)\right\rangle = i\hbar\left|\psi_I(0)\right\rangle + \int_0^t \Delta_I(t')\left|\psi_I(t')\right\rangle\, dt'.$$

The integrand on the right hand side involves a $|\psi_I(t')\rangle$; if we express this in terms of the right hand side we can get an iterative series in Δ as a result. Truncating at the first order, we obtain the approximation:

$$i\hbar\left|\psi_I(t)\right\rangle \approx i\hbar\left|\psi_I(0)\right\rangle + \int_0^t \Delta_I(t')\left|\psi_I(0)\right\rangle\, dt' + O(\Delta^2).$$

Recall $|\psi_I(0)\rangle = |0\rangle$ is given (since at $t = 0$ the inverse of the time-evolution operator is just I). We want to find $\langle k|\psi_I(t)\rangle$, which is then given by:

$$i\hbar\left\langle k|\psi_I(t)\right\rangle \approx i\hbar\left\langle k|0\right\rangle + \int_0^t \left\langle k|\Delta_I(t')|0\right\rangle\, dt' + O(\Delta^2).$$

Expanding $\Delta_I(t') = e^{iH_0t'/\hbar}\Delta(t')e^{-iH_0t'/\hbar}$ and acting on the free-Hamiltonian eigenstates with the relevant operators leaves us with:

$$i\hbar\left\langle k|\psi_I(t)\right\rangle \approx i\hbar\left\langle k|0\right\rangle + \int_0^t e^{i(E_k-E_0)t'/\hbar}\left\langle k|\Delta(t')|0\right\rangle\, dt' + O(\Delta^2).$$

Relating this back to the coefficients of the Schrödinger picture state, we have

$$a_k(t) = e^{-iE_kt/\hbar}\left(\left\langle k|0\right\rangle + \frac{1}{i\hbar}\int_0^t e^{i(E_k-E_0)t'/\hbar}\left\langle k|\Delta(t')|0\right\rangle\, dt' + O(\Delta^2)\right)$$

This is almost the formula in the question, but there's something different when $k = 0$ - in fact, the formula in the question is just wrong! It neglects the most important transition of them all, which is simply the lack of a transition.

We are now asked to apply this work to a specific example. We are given $t = \infty$ (the transition takes place after a long time), $|0\rangle = |1,0,0\rangle$ (we are working with the ground state of hydrogen, namely $|1,0,0\rangle$) and we are interested in the coefficient of $|2,1,0\rangle$ in the expansion of the Schrödinger state, since we want the probability of finding the system in the state $|2,1,0\rangle$ after a long time (the probability will be the same as the expected fraction of atoms). Finally, we are given that the system is perturbed by an *electric field*, and hence we need to figure out how the perturbation affects the Hamiltonian. First, note that an electric potential for the given electric field is:

$$\phi = z\mathcal{E}_0 \exp\left(-t/\tau\right) H(t),$$

where $H(t)$ is the Heaviside step function. Hence the perturbed Hamiltonian is: $H = H_{\text{hydrogen}} - eZ\mathcal{E}_0 \exp\left(-t/\tau\right) H(t)$.

In particular, we can write the required probability as:

$$\frac{e^2\mathcal{E}_0^2}{\hbar^2}\left|\int_0^\infty \langle 2,1,0|Z|1,0,0\rangle\, e^{-t'/\tau} e^{i\omega t'}\, dt'\right|^2$$

We must now calculate the matrix element in the integral. This is given by the volume integral:

$$\langle 2,1,0|Z|1,0,0\rangle = \frac{1}{4\sqrt{2}\pi a_0^4}\int_{\mathbb{R}^3} dV\, rz\cos(\theta)\exp\left(-\frac{3r}{2a_0}\right)$$

Moving into spherical polar coordinates, we set $z = r\cos(\theta)$. Then we must evaluate the integral:

$$\frac{1}{4\sqrt{2}\pi a_0^4}\int_0^{2\pi} d\phi \int_0^\pi d\theta \int_0^\infty dr\, r^4 \sin(\theta)\cos^2(\theta)\exp\left(-\frac{3r}{2a_0}\right) = \frac{1}{2\sqrt{2}a_0^4}\left(\int_0^\pi d\theta\, \sin(\theta)\cos^2(\theta)\right)\left(\int_0^\infty dr\, r^4\exp\left(-\frac{3r}{2a_0}\right)\right).$$

The angular integral gives:

$$\int_0^\pi d\theta\, \sin(\theta)\cos^2(\theta) = \left[-\frac{\cos^3(\theta)}{3}\right]_0^\pi = \frac{2}{3}.$$

The radial integral gives:

$$\int_0^\infty dr\, r^4\exp\left(-\frac{3r}{2a_0}\right) = \frac{4!}{(3/2a_0)^5} = \frac{2^8 a_0^5}{3^4}.$$

Putting everything together, the matrix element gives:

$$\langle 2,1,0|\hat{\mathbf{Z}}|1,0,0\rangle = \frac{1}{2\sqrt{2}a_0^4}\cdot\frac{2}{3}\cdot\frac{2^8 a_0^5}{3^4} = \frac{2^{15/2}a_0}{3^5}.$$

The required probability is thus:

$$\frac{2^{15}}{3^{10}}\cdot\frac{a_0^2e^2\mathcal{E}_0^2}{\hbar^2}\left|\int_0^\infty e^{-t'/\tau}e^{i\omega t'}\, dt'\right|^2 = \frac{2^{15}}{3^{10}}\cdot\frac{a_0^2e^2\mathcal{E}_0^2}{\hbar^2}\cdot\frac{1}{\omega^2+1/\tau^2},$$

as required.

Finally, we are asked what fraction of atoms will be in the state $|2,0,0\rangle$, i.e. what is the probability of a transition to $|2,0,0\rangle$ after a very long time. Since the wavefunction for $|2,0,0\rangle$ is spherically symmetric, all θ-dependence will come from the $z = r\cos(\theta)$ and the measure $dV = r^2\sin(\theta)$. Hence our angular integral will be an integral over $\sin(\theta)\cos(\theta)$, from 0 to 2π, which gives zero. Hence there will be zero atoms in this state.

⁕ **Comments from the Examiner:** *This question, on the interaction picture, got a range of answers. Most students could do the book-work at the beginning. But you had to think to figure out what matrix element to compute, and then keep your head when doing it. I thought it was a good question which separated the students.*

2018, Paper 4, Section II, 33D

The spin operators obey the commutation relations $[S_i, S_j] = i\hbar\epsilon_{ijk}S_k$. Let $|s,\sigma\rangle$ be an eigenstate of the spin operators S_z and $\mathbf{S}^2$, with $S_z|s,\sigma\rangle = \sigma\hbar|s,\sigma\rangle$ and $\mathbf{S}^2|s,\sigma\rangle = s(s+1)\hbar^2|s,\sigma\rangle$. Show that

$$S_\pm|s,\sigma\rangle = \sqrt{s(s+1)-\sigma(\sigma\pm1)}\hbar|s,\sigma\pm1\rangle\,,$$

where $S_\pm = S_x \pm iS_y$. When $s=1$, use this to derive the explicit matrix representation

$$S_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}$$

in a basis in which S_z is diagonal.

A beam of atoms, each with spin 1, is polarised to have spin $+\hbar$ along the direction $\mathbf{n} = (\sin(\theta), 0, \cos(\theta))$. This beam enters a Stern-Gerlach filter that splits the atoms according to their spin along the $\hat{\mathbf{z}}$-axis. Show that $N_+/N_- = \cot^4(\theta/2)$, where N_+ (respectively N_-) is the number of atoms emerging from the filter with spins parallel (respectively anti-parallel) to $\hat{\mathbf{z}}$.

Solution: We must first show that $S_\pm|s,\sigma\rangle$ are eigenstates of both S_z and $\mathbf{S}^2$ with the claimed eigenvalues. First, we have:

$$\begin{aligned}
S_zS_\pm|s,\sigma\rangle &= S_z(S_x \pm iS_y)|s,\sigma\rangle && \text{(definition of } S_\pm\text{)}\\
&= (S_x \pm iS_y)S_z|s,\sigma\rangle + ([S_z,S_x] \pm i[S_z,S_y])|s,\sigma\rangle && \text{(commuting } S_z \text{ past)}\\
&= \hbar\sigma S_\pm|s,\sigma\rangle + i\hbar(S_y \mp iS_x)|s,\sigma\rangle && \text{(given commutation relations, } S_z|s,\sigma\rangle = \hbar\sigma|s,\sigma\rangle\text{)}\\
&= \hbar\sigma S_\pm|s,\sigma\rangle \pm \hbar(S_x \pm iS_y)|s,\sigma\rangle\\
&= \hbar(\sigma\pm1)S_\pm|s,\sigma\rangle\,.
\end{aligned}$$

Notice also that $\mathbf{S}^2$ commutes with S_i, since

$$[\mathbf{S}^2, S_i] = [S_jS_j, S_i] = S_j[S_j,S_i] + [S_j,S_i]S_j = i\hbar\epsilon_{jik}S_jS_k + i\hbar\epsilon_{jik}S_kS_j = i\hbar\epsilon_{jik}(S_jS_k + S_kS_j) = 0,$$

since we have a symmetric quantity multiplied by an antisymmetric quantity. Therefore we can deduce $[\mathbf{S}^2, S_\pm] = 0$, and it follows that

$$\mathbf{S}^2S_\pm|s,\sigma\rangle = S_\pm\mathbf{S}^2|s,\sigma\rangle = \hbar^2s(s+1)S_\pm|s,\sigma\rangle\,.$$

Therefore, we have shown $S_\pm|s,\sigma\rangle \propto |s,\sigma\pm1\rangle$.

It remains to find the proportionality constants. To do so, let's first notice that:

$$\mathbf{S}^2 = S_x^2 + S_y^2 + S_z^2 = (S_x \mp iS_y)(S_x \pm iS_y) \mp i[S_x,S_y] + S_z^2 = S_\mp S_\pm \pm \hbar S_z + S_z^2.$$

Hence it follows that:

$$S_\pm S_\mp = \mathbf{S}^2 - S_z^2 \mp \hbar S_z.$$

Thus on taking the norm of $S_\pm|s,\sigma\rangle$ we get (noting $S_\pm^\dagger = S_\mp$):

$$||S_\pm|s,\sigma\rangle||^2 = \langle s,\sigma|S_\mp S_\pm|s,\sigma\rangle = \langle s,\sigma|\mathbf{S}^2 - S_z^2 \mp \hbar S_z|s,\sigma\rangle = \hbar^2s(s+1) - \hbar^2\sigma^2 \mp \hbar^2\sigma = \hbar^2(s(s+1) - \sigma(\sigma\pm1)).$$

Hence taking the square root, we see (up to an arbitrary phase) we get the required result:

$$S_\pm|s,\sigma\rangle = \sqrt{s(s+1)-\sigma(\sigma\pm1)}\hbar|s,\sigma\pm1\rangle\,.$$

We are now asked to derive the matrix form for S_x for a spin 1 particle. In this case, we know from the general theory that a basis that diagonalises S_z is $\mathrm{span}\{|1,-1\rangle, |1,0\rangle, |1,1\rangle\}$. Hence we should aim to find the matrix elements of S_x in this basis.

To do so, it is first sensible to express S_x in terms of the raising and lowering operators. We have:

$$S_\pm = S_x \pm iS_y \qquad \Rightarrow \qquad S_x = (S_+ + S_-)/2.$$

Hence, acting on each of the basis states with S_x in turn, we have:

- Consider acting on $|1,-1\rangle$ with S_x. We get:

$$S_x|1,-1\rangle = \frac{1}{2}S_+|1,-1\rangle + \frac{1}{2}S_-|1,-1\rangle = \frac{1}{2}\sqrt{1(1+1)-(-1)((-1)+1)}\hbar\,|1,0\rangle = \frac{\hbar}{\sqrt{2}}|1,0\rangle.$$

  Hence $\langle 1,-1|S_x|1,-1\rangle = 0$, $\langle 1,0|S_x|1,-1\rangle = \hbar/\sqrt{2}$ and $\langle 1,1|S_x|1,-1\rangle = 0$.

- Now consider acting on $|1,0\rangle$ with S_x. We have:

$$S_x|1,0\rangle = \frac{1}{2}S_+|1,0\rangle + \frac{1}{2}S_-|1,0\rangle = \frac{\hbar}{\sqrt{2}}|1,1\rangle + \frac{\hbar}{\sqrt{2}}|1,-1\rangle.$$

  Hence $\langle 1,-1|S_x|1,0\rangle = \hbar/\sqrt{2}$, $\langle 1,0|S_x|1,0\rangle = 0$ and $\langle 1,1|S_x|1,1\rangle = 0$.

- Finally, consider acting on $|1,1\rangle$ with S_x. We have:

$$S_x|1,1\rangle = \frac{1}{2}S_+|1,1\rangle + \frac{1}{2}S_-|1,1\rangle = \frac{\hbar}{\sqrt{2}}|1,0\rangle.$$

  Hence $\langle 1,-1|S_x|1,1\rangle = 0$, $\langle 1,-1|S_x|1,0\rangle = \hbar/\sqrt{2}$ and $\langle 1,-1|S_x|1,-1\rangle = 0$.

It follows that the required matrix is indeed: $S_x = \dfrac{\hbar}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}$. Note also that in this basis, $S_z = \mathrm{diag}\{-\hbar, 0, \hbar\}$.

We are now given that a beam of atoms definitely has spin $+\hbar$ along the axis $\mathbf{n} = (\sin(\theta), 0, \cos(\theta))$. Hence its corresponding quantum state $|\psi\rangle$ must be such that $(\mathbf{n}\cdot\mathbf{S})|\psi\rangle = \hbar|\psi\rangle$. That is, $|\psi\rangle$ must be an eigenvector of the matrix

$$\sin(\theta)S_x + \cos(\theta)S_z = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}-\sqrt{2}\cos(\theta) & \sin(\theta) & 0\\ \sin(\theta) & 0 & \sin(\theta)\\ 0 & \sin(\theta) & \sqrt{2}\cos(\theta)\end{pmatrix}.$$

with eigenvalue $+\hbar$. Since we know there will be an eigenvector with eigenvalue $+\hbar$, we can simply derive simultaneous equations for the coefficients in $|\psi\rangle = (a,b,c)$. We see that these coefficients must obey:

$$-\sqrt{2}\cos(\theta)a + b\sin(\theta) = \sqrt{2}a, \qquad \sin(\theta)a + \sin(\theta)c = \sqrt{2}b, \qquad \sin(\theta)b + \sqrt{2}\cos(\theta)c = \sqrt{2}c.$$

In fact, we don't even need to solve these equations. The number of particles N_- emerging from the filter with spins anti-parallel to $\hat{\mathbf{z}}$ will simply be proportional to $|a|^2$, the probability of measuring the initial state $|\psi\rangle$ to have spin anti-parallel to $\hat{\mathbf{z}}$. Similarly, $|c|^2$ is proportional to N_+, with the same constant of proportionality, so the ratio we are looking for is just $N_-/N_+ = |c|^2/|a|^2 = |c/a|^2$.

Hence, we simply eliminate b from the first and third equations to deduce:

$$c(1-\cos(\theta)) = a(1+\cos(\theta)) \qquad \Rightarrow \qquad \left|\frac{c}{a}\right|^2 = \frac{(1+\cos(\theta))^2}{(1-\cos(\theta))^2} = \frac{\left(2\cos^2(\theta/2)\right)^2}{\left(2\sin^2(\theta/2)\right)^2} = \cot^4\left(\frac{\theta}{2}\right).$$

✳ **Comments from the Examiner:** *A straightforward question on the algebra of spin. Students could answer this very well.*

2019, Paper 1, Section II, 33B

A $d = 3$ isotropic harmonic oscillator of mass μ and frequency ω has lowering operators

$$\mathbf{A} = \frac{1}{\sqrt{2\mu\hbar\omega}} \left(\mu\omega\mathbf{X} + i\mathbf{P}\right)$$

where **X** and **P** are the position and momentum operators. Assuming the standard commutation relations for **X** and **P**, evaluate the commutators $[A_i^\dagger, A_j^\dagger], [A_i, A_j]$ and $[A_i, A_j^\dagger]$ for $i, j = 1, 2, 3$, among the components of the raising and lowering operators.

How is the ground state $|\mathbf{0}\rangle$ of the oscillator defined? How are normalised higher excited states obtained from $|\mathbf{0}\rangle$? [You should determine the appropriate normalisation constant for each energy eigenstate.]

By expressing the orbital angular momentum operator **L** in terms of the raising and lowering operators, show that each first excited state of the isotropic oscillator has total orbital angular momentum quantum number $l = 1$, and find a linear combination $|\psi\rangle$ of these first excited states obeying $L_z |\psi\rangle = +\hbar |\psi\rangle$ and $|| \, |\psi\rangle \, || = 1$.

Solution: The canonical commutation relations between the components of **X** and **P** are given by $[X_i, X_j] = 0, [P_i, P_j] = 0$, and $[X_i, P_j] = i\hbar\delta_{ij} = -[P_j, X_i]$. Hence we have:

$$[A_i^\dagger, A_j^\dagger] = \frac{1}{2\mu\hbar\omega} \left[\mu\omega X_i - iP_i, \mu\omega X_j - iP_j\right] = \frac{1}{2\mu\hbar\omega} \left(-i\mu\omega[X_i, P_j] - i\mu\omega[P_i, X_j]\right) = 0,$$

$$[A_i, A_j] = \frac{1}{2\mu\hbar\omega} \left[\mu\omega X_i + iP_i, \mu\omega X_j + iP_j\right] = \frac{1}{2\mu\hbar\omega} \left(i\mu\omega[X_i, P_j] + i\mu\omega[P_i, X_j]\right) = 0,$$

$$[A_i, A_j^\dagger] = \frac{1}{2\mu\hbar\omega} \left[\mu\omega X_i + iP_i, \mu\omega X_j - iP_j\right] = \frac{1}{2\mu\hbar\omega} \left(-i\mu\omega[X_i, P_j] + i\mu\omega[P_i, X_j]\right) = \frac{1}{\hbar} \left(-i(i\hbar\delta_{ij})\right) = \delta_{ij},$$

Recall that the Hamiltonian for a 3D isotropic oscillator is given by:

$$H = \hbar\omega \left(\mathbf{A}^\dagger \cdot \mathbf{A} + \frac{3}{2}\right) = \hbar\omega \left(A_j^\dagger A_j + \frac{3}{2}\right),$$

where the summation convention is implied. The ground state of the oscillator is defined by $\mathbf{A} |\mathbf{0}\rangle = \mathbf{0}$. To produce higher energy states, we use the raising operators $A_i^\dagger$; let's show how these act. First, it's useful to note the commutation relation between H and $A_i^\dagger$; we have:

$$[H, A_i^\dagger] = \hbar\omega \left[A_j^\dagger A_j, A_i^\dagger\right] = \hbar\omega A_j^\dagger [A_j, A_i^\dagger] = \hbar\omega A_i^\dagger.$$

Now suppose that $|E\rangle$ is an energy eigenstate of energy E, i.e. $H |E\rangle = E |E\rangle$. Then $A_i^\dagger |E\rangle$ is also an energy eigenstate, but of higher energy:

$$H A_i^\dagger |E\rangle = A_i^\dagger H |E\rangle + [H, A_i^\dagger] |E\rangle = (E + \hbar\omega) A_i^\dagger |E\rangle$$

Hence starting from the ground state, we can build up excited states by applying the creation operators $A_i^\dagger$. In particular, using the fact that orthogonal oscillator directions commute, we have the general (non-normalised) energy eigenstate:

$$(A_x^\dagger)^{n_x} (A_y^\dagger)^{n_y} (A_z^\dagger)^{n_z} |\mathbf{0}\rangle$$

has energy $\hbar\omega(n_x + n_y + n_z + 3/2)$.

We now need to find the normalisation of these states. It's useful to prove a quick result (which is a special case of Examples Sheet 1, Question 2(i)):

Lemma: We have the following commutation relation (where the summation convention is *not* used):

$$[A_i, (A_i^\dagger)^n] = n(A_i^\dagger)^{n-1}.$$

Proof: We can use induction. In the cases $n = 0, 1$, the result is immediate by the commutation relations. Now assume the result for $n = k$ and consider the case $n = k + 1$. We have:

$$[A_i, (A_i^\dagger)^{k+1}] = [A_i, (A_i^\dagger)^k]A_i^\dagger + A_i^\dagger[A_i, (A_i^\dagger)^k] = k(A_i^\dagger)^{k-1}A_i^\dagger + A_i^\dagger\left(k(A_i^\dagger)^{k-1}\right) = (k+1)(A_i^\dagger)^k.$$

Hence we're done, by induction. □

Let's now apply this result to normalise the state $(A_x^\dagger)^{n_x}(A_y^\dagger)^{n_y}(A_z^\dagger)^{n_z}\,|\mathbf{0}\rangle$. Since all orthogonal directions of the oscillator commute, we have:

$$||(A_x^\dagger)^{n_x}(A_y^\dagger)^{n_y}(A_z^\dagger)^{n_z}\,|\mathbf{0}\rangle\,||^2 = \langle\mathbf{0}|A_x^{n_x}(A_x^\dagger)^{n_x}A_y^{n_y}(A_y^\dagger)^{n_y}A_z^{n_z}(A_z^\dagger)^{n_z}|\mathbf{0}\rangle\,.$$

Now note that commuting any of the annihilation operators A_i past their respective power of creation operators, $(A_i^\dagger)^{n_i}$, will give zero when A_i acts on the vacuum, leaving just the commutator. Hence we have, using the Lemma from above:

$$\langle\mathbf{0}|A_x^{n_x-1}[A_x, (A_x^\dagger)^{n_x}]A_y^{n_y-1}[A_y, (A_y^\dagger)^{n_y}]A_z^{n_z-1}[A_z, (A_z^\dagger)^{n_z}]|\mathbf{0}\rangle$$

$$= n_x n_y n_z\,\langle\mathbf{0}|A_x^{n_x-1}(A_x^\dagger)^{n_x-1}A_y^{n_y-1}(A_y^\dagger)^{n_y-1}A_z^{n_z-1}(A_z^\dagger)^{n_z-1}|\mathbf{0}\rangle\,.$$

Hence we have established the recurrence relation:

$$||(A_x^\dagger)^{n_x}(A_y^\dagger)^{n_y}(A_z^\dagger)^{n_z}\,|\mathbf{0}\rangle\,||^2 = n_x n_y n_z||(A_x^\dagger)^{n_x-1}(A_y^\dagger)^{n_y-1}(A_z^\dagger)^{n_z-1}\,|\mathbf{0}\rangle\,||^2.$$

Repeated application of this recurrence relation gives:

$$|n_x, n_y, n_z\rangle = \frac{(A_x^\dagger)^{n_x}}{\sqrt{(n_x)!}}\frac{(A_y^\dagger)^{n_y}}{\sqrt{(n_y)!}}\frac{(A_z^\dagger)^{n_z}}{\sqrt{(n_z)!}}\,|\mathbf{0}\rangle$$

as the correctly normalised versions of our states.

The orbital angular momentum is given by: $L_i = \epsilon_{ijk}X_jP_k$. To write this in terms of raising and lowering operators, note that the relations:

$$\mathbf{A} = \frac{1}{\sqrt{2\mu\hbar\omega}}\left(\mu\omega\mathbf{X} + i\mathbf{P}\right), \qquad \mathbf{A}^\dagger = \frac{1}{\sqrt{2\mu\hbar\omega}}\left(\mu\omega\mathbf{X} - i\mathbf{P}\right)$$

imply that

$$\mathbf{X} = \sqrt{\frac{\hbar}{2\mu\omega}}\left(\mathbf{A} + \mathbf{A}^\dagger\right), \qquad \mathbf{P} = \sqrt{\frac{\mu\hbar\omega}{2}}i\left(\mathbf{A}^\dagger - \mathbf{A}\right).$$

Hence the angular momentum can be written as:

$$L_i = \epsilon_{ijk}X_jP_k = \frac{i\hbar}{2}\epsilon_{ijk}\left(A_j + A_j^\dagger\right)\left(A_k^\dagger - A_k\right) = \frac{i\hbar}{2}\epsilon_{ijk}\left(A_jA_k^\dagger - A_j^\dagger A_k\right) = i\hbar\epsilon_{ijk}A_jA_k^\dagger,$$

where in the last step, we relabelled the indices of the final term, and used the commutation relation $[A_k^\dagger, A_j] = -\delta_{jk}$.

Let's act with L_i on each of the first excited states $|1,0,0\rangle$, $|0,1,0\rangle$ and $|0,0,1\rangle$ (since we will later need to know how L_z acts on each of these states too). Each of these states can be written in the form $A_l^\dagger |\mathbf{0}\rangle$, hence we evaluate:

$$L_i A_l^\dagger |\mathbf{0}\rangle = i\hbar\epsilon_{ijk} A_j A_k^\dagger A_l^\dagger |\mathbf{0}\rangle = i\hbar\epsilon_{ijk} A_k^\dagger [A_j, A_l^\dagger] |\mathbf{0}\rangle = i\hbar\epsilon_{ilk} A_k^\dagger |\mathbf{0}\rangle .$$

It follows that $\mathbf{L}^2$ acting on each of these states gives:

$$\mathbf{L}^2 A_l^\dagger |\mathbf{0}\rangle = L_i L_i A_l^\dagger |\mathbf{0}\rangle = i\hbar\epsilon_{ilk} L_i A_k^\dagger |\mathbf{0}\rangle = -\hbar^2 \epsilon_{ilk}\epsilon_{ikj} A_j^\dagger |\mathbf{0}\rangle .$$

Simplifying the Levi-Civita symbols, we have:

$$\mathbf{L}^2 A_l^\dagger |\mathbf{0}\rangle = -\hbar^2 \left(\delta_{lk}\delta_{kj} - \delta_{lj}\delta_{kk}\right) A_j^\dagger |\mathbf{0}\rangle = 2\hbar^2 A_l^\dagger |\mathbf{0}\rangle .$$

It follows that each of $|1,0,0\rangle$, $|0,1,0\rangle$ and $|0,0,1\rangle$ is indeed an eigenvalue of $\mathbf{L}^2$ with eigenvalue $\hbar^2 1(1+1)$, which corresponds to the quantum number $l = 1$, as required.

Finally, we must construct a normalised linear combination of these states that is also an eigenstates of L_z with eigenvalue $+\hbar$. Earlier, we computed $L_i A_l^\dagger |\mathbf{0}\rangle$. Restricting just to $L_z A_l^\dagger |\mathbf{0}\rangle$, we see that

$$L_z A_x^\dagger |\mathbf{0}\rangle = i\hbar A_y^\dagger |\mathbf{0}\rangle , \qquad L_z A_y^\dagger |\mathbf{0}\rangle = -i\hbar A_x^\dagger |\mathbf{0}\rangle , \qquad L_z A_z^\dagger |\mathbf{0}\rangle = 0.$$

Hence taking the linear combination $|1,0,0\rangle + i\,|0,1,0\rangle = (A_x^\dagger + iA_y^\dagger) |\mathbf{0}\rangle$ does the job; we have:

$$L_z \left(|1,0,0\rangle + i\,|0,1,0\rangle\right) = i\hbar\,|0,1,0\rangle + i(-i)\hbar\,|1,0,0\rangle = \hbar\left(|1,0,0\rangle + i\,|0,1,0\rangle\right) .$$

It remains to normalise this state; since $|1,0,0\rangle$ and $|0,1,0\rangle$ are already normalised, we can simply use:

$$\frac{|1,0,0\rangle + i\,|0,1,0\rangle}{\sqrt{2}}.$$

⁜ **Comments from the Examiner:** *A very popular question. Many candidates were no doubt attracted by the easy bookwork in the first section however the latter parts on the 3D oscillator were more challenging. Surprisingly many candidates were unable to reproduce the correct normalisation of the eigenstates or even the defining condition of the ground state (the fact that it is a zero eigenvector of all the annihilation operators). Constructing the required linear combination for the final part of the question also proved challenging to many although one did not need to complete this perfectly to obtain an* α.

2019, Paper 2, Section II, 33B

(a) Let $|i\rangle$ and $|j\rangle$ be two eigenstate of a time-independent Hamiltonian H_0 separated in energy by $\hbar\omega_{ij}$. At time $t = 0$ the system is perturbed by a small, time-independent operator V. The perturbation is turned off at time $t = T$. Show that if the system is initially in the state $|i\rangle$, the probability of transition to a state $|j\rangle$ is approximately:

$$P_{ij} = 4|\langle i|V|j\rangle|^2 \frac{\sin^2(\omega_{ij}T/2)}{(\hbar\omega_{ij})^2}.$$

(b) An uncharged particle with spin one-half and magnetic moment μ travels at speed v through a region of uniform magnetic field $\mathbf{B} = (0, 0, B)$. Over a length L of its path, an additional perpendicular magnetic field b is applied. The spin-dependent part of the Hamiltonian is:

$$H(t) = \begin{cases} -\mu(B\sigma_z + b\sigma_x) & \text{while } 0 < t < L/v, \\ -\mu B\sigma_z & \text{otherwise,} \end{cases}$$

where σ_z and σ_x are Pauli matrices. The particle initially has its spin aligned along the direction of $\mathbf{B} = (0, 0, B)$. Find the probability that it makes a transition to the state with opposite spin:

(i) by assuming $b \ll B$ and using your result from part (a);

(ii) by finding the exact evolution of state.

[Hint: for any 3-vector $\mathbf{a}$, $e^{i\mathbf{a}\cdot\boldsymbol{\sigma}} = \cos(a)I + i\sin(a)\hat{\mathbf{a}}\cdot\boldsymbol{\sigma}$, *where* I *is the* 2×2 *identity matrix,* $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, $a = |\mathbf{a}|$ *and* $\hat{\mathbf{a}} = \mathbf{a}/|\mathbf{a}|$*.]*

Solution: (a) For the first part, it is useful to introduce the *interaction picture*. We define interaction picture states $|\psi(t)\rangle_I$ and operators $O_I(t)$ in terms of their Schrödinger counterparts via the equations:

$$|\psi(t)\rangle_I = e^{iH_0t/\hbar}|\psi(t)\rangle_S, \qquad O_I(t) = e^{iH_0t/\hbar}O_S(t)e^{-iH_0t/\hbar}.$$

This definition implies that the interaction picture states obey the equation of motion:

$$i\hbar\frac{d|\psi(t)\rangle_I}{dt} = -e^{iH_0t/\hbar}H_0|\psi(t)\rangle_S + e^{iH_0t/\hbar}(H_0+V)|\psi(t)\rangle_S = e^{iH_0t/\hbar}Ve^{-iH_0t/\hbar}e^{iH_0t/\hbar}|\psi(t)\rangle_S = V_I(t)|\psi(t)\rangle_I.$$

Recasting this as an integral equation, we have:

$$|\psi(t)\rangle_I = |\psi(0)\rangle_I - \frac{i}{\hbar}\int_0^t dt'\, V_I(t')|\psi(t')\rangle_I.$$

Repeatedly substituting this equation into itself, we can produce a perturbative expansion of $|\psi(t)\rangle_I$ in powers of the perturbation V. Hence to first order, we have the result:

$$|\psi(t)\rangle_I = |\psi(0)\rangle_I - \frac{i}{\hbar}\int_0^t dt'\, V_I(t')|\psi(0)\rangle_I.$$

Rewriting everything in terms of the Schrödinger picture again, we get:

$$|\psi(t)\rangle_S = e^{-iH_0t/\hbar}|\psi(0)\rangle_S - \frac{i}{\hbar}\int_0^t dt'\, e^{iH_0(t'-t)/\hbar}Ve^{-iH_0t'/\hbar}|\psi(0)\rangle_S.$$

Next, let's insert some of the data from the question. We want to know information about a transition from the H_0 eigenstate $|i\rangle$ at time $t = 0$ to the H_0 eigenstate $|j\rangle$ at time $t = T$. Let $H_0 |i\rangle = E_i |i\rangle$ and $H_0 |j\rangle = E_j |j\rangle$. Then the required transition amplitude is given by:

$$\langle j|\psi(T)\rangle_S = e^{-iE_jT/\hbar} \langle j|i\rangle - \frac{i}{\hbar} \int_0^T dt' e^{iE_j(t'-T)/\hbar} \langle j|V|i\rangle e^{-iE_it'/\hbar}.$$

Notice the right hand side contains the overall phase $e^{-iE_jT/\hbar}$ which is removed on taking the modulus squared, so let's just ignore it. Notice also that $\langle j|V|i\rangle$ is time-independent, so can be taken out of the integral. Finally, let's assume that $|i\rangle$, $|j\rangle$ are distinct eigenstates with distinct energy eigenvalues so that $\langle j|i\rangle = 0$ and $\hbar\omega_{ij} = E_i - E_j \neq 0$. Then we're left with:

$$\langle j|\psi(T)\rangle_S = -\frac{i}{\hbar} \langle j|V|i\rangle \int_0^T dt' e^{-i\omega_{ij}t'} = -\frac{i}{\hbar} \langle j|V|i\rangle \left[\frac{e^{-i\omega_{ij}T} - 1}{-i\omega_{ij}}\right] = -e^{-i\omega_{ij}T/2} \cdot \langle j|V|i\rangle \frac{2i\sin(\omega_{ij}T/2)}{\hbar\omega_{ij}}.$$

Hence the transition probability is:

$$|\langle j|\psi(T)\rangle_S|^2 = 4|\langle j|V|i\rangle|^2 \frac{\sin^2(\omega_{ij}T/2)}{(\hbar\omega_{ij})^2},$$

as required.

(b) (i) Let $|\uparrow\rangle$, $|\downarrow\rangle$ be a basis of spin-z eigenstates for the spin Hilbert space of the particle, with $\sigma_z |\uparrow\rangle = |\uparrow\rangle$ and $\sigma_z |\downarrow\rangle = -|\downarrow\rangle$. The free Hamiltonian in this problem $H_0 = -\mu B\sigma_z$, and hence $|\uparrow\rangle$ and $|\downarrow\rangle$ are eigenstates of H_0:

$$H_0 |\uparrow\rangle = -\mu B |\uparrow\rangle, \qquad H_0 |\downarrow\rangle = \mu B |\downarrow\rangle.$$

Initially, our particle is in the state $|\uparrow\rangle$, where its spin is aligned with the z-axis. We want to find the probability that the spin is reversed, i.e. the particle lies in the state $|\downarrow\rangle$, at time $T = L/v$. The difference in particle energies is $\hbar\omega_{\uparrow\downarrow} = 2\mu B$.

The perturbation is $V = -\mu b\sigma_x$, and hence the relevant matrix element in the application of the method from (a) is:

$$\langle\downarrow|V|\uparrow\rangle = -\mu b \langle\downarrow| \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} |\uparrow\rangle . = -\mu b \langle\downarrow|\downarrow\rangle = -\mu b.$$

It follows from the results of part (a) that the transition probability is simply:

$$P_{\uparrow\downarrow} = \frac{4\mu^2 b^2 \sin^2(\mu BL/\hbar v)}{4\mu^2 B^2} = \frac{b^2 \sin^2(\mu BL/\hbar v)}{B^2}.$$

(b) (ii) We are now asked to solve the same problem exactly. Starting at time $t = 0$ and ending at time $t = T = L/v$, we have that the Hamiltonian applied to the system is $H = -\mu(B\sigma_z + b\sigma_x)$. Recalling that H generates time-translations, we can apply the exponentiated form of this operator to the state $|\uparrow\rangle$ to see how it evolves in time. At time $t = T = L/v$, the state will have evolved to:

$$e^{-iHT/\hbar} |\uparrow\rangle = e^{i\mu T(B\sigma_z + b\sigma_x)/\hbar} |\uparrow\rangle = \left(\cos\left(\frac{\mu T\sqrt{b^2+B^2}}{\hbar}\right) + i\sin\left(\frac{\mu T\sqrt{b^2+B^2}}{\hbar}\right)\left(\frac{b}{\sqrt{b^2+B^2}}\sigma_x + \frac{B}{\sqrt{b^2+B^2}}\sigma_z\right)\right)|\uparrow\rangle,$$

using the hint with the vector $\mathbf{a} = (b\mu t/\hbar, 0, B\mu t/\hbar)$.

Taking the inner product with $\langle\downarrow|$, we get the amplitude for the transition. This is given by:

$$\langle\downarrow|e^{-iHT/\hbar}|\uparrow\rangle = \frac{ib}{\sqrt{b^2+B^2}}\sin\left(\frac{\mu T\sqrt{b^2+B^2}}{\hbar}\right),$$

using $\sigma_x|\uparrow\rangle = |\downarrow\rangle$, $\sigma_z|\uparrow\rangle = |\uparrow\rangle$. Taking the modulus squared, we arrive at the exact probability:

$$\frac{b^2}{b^2+B^2}\sin\left(\frac{\mu L\sqrt{b^2+B^2}}{\hbar v}\right).$$

To first order in b/B, this gives exactly the same result as we got in part (b)(ii).

⁜ **Comments from the Examiner:** *This question on time-dependent perturbation theory attracted significantly fewer attempts than the others on this course. Part b) required a careful application of the bookwork asked for part a). The final part requiring the exact diagonalisation of the Hamiltonian required some familiarity with the properties of the Pauli matrices and the correct use of the identity given in the hint. Several attempts took a wrong turning at this point leading to incorrect expressions for the eigenvalues.*

2019, Paper 3, Section II, 33B

Consider the Hamiltonian $H = H_0 + V$, where V is a small perturbation. If $H_0|n\rangle = E_n|n\rangle$, write down an expression for the eigenvalues of H, correct to second order in the perturbation, assuming the energy levels of H_0 are non-degenerate.

In a certain three-state system, H_0 and V take the form:

$$H_0 = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_3 \end{pmatrix} \qquad \text{and} \qquad V = V_0\begin{pmatrix} 0 & \epsilon & \epsilon^2 \\ \epsilon & 0 & 0 \\ \epsilon^2 & 0 & 0 \end{pmatrix},$$

with V_0 and ϵ real, positive constants and $\epsilon \ll 1$.

(a) Consider first the case $E_1 = E_2 \neq E_3$ and $|\epsilon V_0/(E_3 - E_2)| \ll 1$. Use the results of degenerate perturbation theory to obtain the energy eigenvalues correct to order ϵ.

(b) Now consider the different case $E_3 = E_2 \neq E_1$ and $|\epsilon V_0/(E_2 - E_1)| \ll 1$. Use the results of non-degenerate perturbation theory to obtain the energy eigenvalues correct to order ϵ^2. Why is it not necessary to use degenerate perturbation theory in this case?

(c) Obtain the exact energy eigenvalues in case (b), and compare these to your perturbative results by expanding to second order in ϵ.

➽ **Solution:** From lectures, we know that the energy eigenvalues of H are given by:

$$E_n' = E_n + \langle n|V|n\rangle + \sum_{m\neq n}\frac{|\langle n|V|m\rangle|^2}{E_n - E_m} + \cdots \qquad (*)$$

to second order in the perturbation, assuming the energy levels are non-degenerate.

(a) In the case $E_1 = E_2 \neq E_3$, we must apply the results of degenerate perturbation theory. The key result states that the shifts in the energy eigenvalues are given by the eigenvalues of the matrix of the perturbation, projected into the degenerate subspace.

In our case, the degenerate subspace is spanned by the vectors $|1\rangle$ and $|2\rangle$, hence the matrix of the perturbation projected into the degenerate subspace is:

$$V_0 \begin{pmatrix} 0 & \epsilon \\ \epsilon & 0 \end{pmatrix}.$$

Diagonalising, we see that the eigenvalues will satisfy:

$$\lambda^2 - V_0^2\epsilon^2 = 0 \qquad \Rightarrow \qquad \lambda = \pm V_0\epsilon.$$

Hence the energy level $E_1 = E_2$ splits into the energy levels $E_1' = E_1 + V_0\epsilon$ and $E_2' = E_2 - V_0\epsilon$ under the perturbation, to first order in ϵ.

What happens to the energy level E_3? Since the perturbation only couples the energy eigenstates $|1\rangle$, $|2\rangle$ at order ϵ (note the coupling between $|3\rangle$ and $|1\rangle$ is of order ϵ^2), the perturbation has no effect on the energy eigenstate $|3\rangle$. We have, to order ϵ, $E_3' = E_3$.

(b) We are now asked to consider the different case $E_3 = E_2 \neq E_1$. The unperturbed system here is degenerate, but we do not need to apply degenerate perturbation theory - why?

The answer is that the perturbation does not mix degenerate states in this case. That is, $|3\rangle$ and $|2\rangle$ are not mixed by the perturbation, i.e. $\langle 3|V|2\rangle = \langle 2|V|3\rangle = 0$. We can imagine that the zero matrix elements cancel the zero denominators $E_3 - E_2, E_2 - E_3$ in the expansion $(*)$; essentially we are saying $0/0 = 0$.

For a slightly more rigorous argument, we can consider instead a basic Hamiltonian with energy eigenvalues E_1, E_2, E_3 all distinct. The perturbation series $(*)$ is then valid. In the limit $E_1 \to E_2$, the series blows up because $\langle 2|V|1\rangle$ and $\langle 1|V|2\rangle$ are finite and non-zero; therefore the series breaks down and we have to use degenerate perturbation theory. In the limit $E_2 \to E_3$ however, the series does *not* blow up, because $\langle 3|V|1\rangle = \langle 1|V|3\rangle = 0$ for all values of E_2, E_3.

Now we have justified the use of non-degenerate perturbation theory, let's apply it. The shift in the first energy level is:

$$\begin{aligned} E_1' &= E_1 + \langle 1|V|1\rangle + \frac{|\langle 1|V|2\rangle|^2}{E_1 - E_2} + \frac{|\langle 1|V|3\rangle|^2}{E_1 - E_3} + \cdots \\ &= E_1 + \frac{V_0^2\epsilon^2}{E_1 - E_2} + \cdots. \end{aligned}$$

The shift in the remaining energy levels is:

$$\begin{aligned} E_2' &= E_2 + \langle 2|V|2\rangle + \frac{|\langle 2|V|1\rangle|^2}{E_2 - E_1} + \cdots \\ &= E_2 + \frac{V_0^2\epsilon^2}{E_2 - E_1} + \cdots, \end{aligned}$$

and

$$\begin{aligned} E_3' &= E_3 + \langle 3|V|3\rangle + \frac{|\langle 3|V|1\rangle|^2}{E_3 - E_1} + \cdots \\ &= E_3 + \cdots. \end{aligned}$$

In particular, we see that the energy level $E_2 = E_3$ splits into two energy levels under the perturbation.

(c) We now obtain the exact energy eigenvalues in case (b). We must diagonalise the matrix:

$$\begin{pmatrix} E_1 & V_0\epsilon & V_0\epsilon^2 \\ V_0\epsilon & E_2 & 0 \\ V_0\epsilon^2 & 0 & E_2 \end{pmatrix}.$$

The eigenvalues are given by the equation:

$$0 = \det \begin{pmatrix} E_1-\lambda & V_0\epsilon & V_0\epsilon^2 \\ V_0\epsilon & E_2-\lambda & 0 \\ V_0\epsilon^2 & 0 & E_2-\lambda \end{pmatrix} = (E_2-\lambda)\left[(E_1-\lambda)(E_2-\lambda) - V_0^2\epsilon^2\right] - V_0^2\epsilon^4(E_2-\lambda).$$

Factorising, we have:

$$0 = (E_2-\lambda)\left(\lambda^2 - (E_1+E_2)\lambda + E_1E_2 - V_0^2(\epsilon^2+\epsilon^4)\right).$$

Hence we get the energy eigenvalue $\lambda = E_2 = E_3$ (consistent with one of the ones we found in part (b) - now we know that the result is not just valid to order $O(\epsilon^2)$, but to all orders), together with the eigenvalues:

$$\lambda_\pm = \frac{E_1+E_2 \pm \sqrt{(E_1+E_2)^2 - 4(E_1E_2 - V_0^2(\epsilon^2+\epsilon^4))}}{2}$$

$$= \frac{E_1+E_2 \pm \sqrt{(E_1-E_2)^2 + 4V_0^2(\epsilon^2+\epsilon^4)}}{2}.$$

Hence, we have the spectrum:

$$E_2, \qquad \frac{E_1+E_2+\sqrt{(E_1-E_2)^2+4V_0^2(\epsilon^2+\epsilon^4)}}{2}, \qquad \frac{E_1+E_2-\sqrt{(E_1-E_2)^2+4V_0^2(\epsilon^2+\epsilon^4)}}{2}.$$

In the case $|\epsilon V_0/(E_2-E_1)| \ll 1$, we can expand the second two energy eigenvalues using the binomial expansion:

$$\sqrt{(E_1-E_2)^2+4V_0^2(\epsilon^2+\epsilon^4)} = (E_1-E_2)\sqrt{1+\frac{4V_0^2(\epsilon^2+\epsilon^4)}{(E_2-E_1)^2}} = (E_1-E_2)\left(1 - \frac{2V_0^2(\epsilon^2+\epsilon^4)}{(E_2-E_1)^2} + \cdots\right).$$

Retaining only the terms in ϵ^2, we're left with:

$$(E_1-E_2) - \frac{2V_0^2\epsilon^2}{E_1-E_2}.$$

Hence the second two energy eigenvalues can be expanded as:

$$E_2 + \frac{V_0^2\epsilon^2}{E_2-E_1}, \qquad \text{and} \qquad E_1 + \frac{V_0^2\epsilon^2}{E_1-E_2},$$

which exactly match the expressions we found in part (b).

⁜ **Comments from the Examiner:** *A popular question on perturbation theory which most found relatively easy. The question tested the understanding of both the degenerate and non-degenerate cases which was demonstrated in most attempts. The final part of the question simply required finding the eigenvalues of a 3×3 matrix and candidates who got that far were rewarded with some easy marks.*

2019, Paper 4, Section II, 32B

Define the *spin raising* and *spin lowering* operators S_+ and S_-. Show that

$$S_\pm |s,\sigma\rangle = \hbar\sqrt{s(s+1)-\sigma(\sigma\pm 1)}\,|s,\sigma\pm 1\rangle\,,$$

where $S_z|s,\sigma\rangle = \hbar\sigma|s,\sigma\rangle$ and $\mathbf{S}^2|s,\sigma\rangle = \hbar^2 s(s+1)|s,\sigma\rangle$.

Two spin-$\frac{1}{2}$ particles, with spin operators $\mathbf{S}^{(1)}$ and $\mathbf{S}^{(2)}$, have Hamiltonian

$$H = \alpha\mathbf{S}^{(1)}\cdot\mathbf{S}^{(2)} + \mathbf{B}\cdot(\mathbf{S}^{(1)}-\mathbf{S}^{(2)}),$$

where α and $\mathbf{B} = (0,0,B)$ are constants. Express H in terms of the two particles' spin raising and spin lowering operators $S_\pm^{(1)}$, $S_\pm^{(2)}$ and the corresponding z-components $S_z^{(1)}$, $S_z^{(2)}$. Hence find the eigenvalues of H. Show that there is a unique ground state in the limit $B\to 0$ and that the first excited state is triply degenerate in this limit. Explain this degeneracy by considering the action of the combined spin operator $\mathbf{S}^{(1)}+\mathbf{S}^{(2)}$ on the energy eigenstates.

Solution: Let $\mathbf{S} = (S_x, S_y, S_z)$ be the spin operator. The spin raising and spin lowering operators are defined by:

$$S_\pm = S_x \pm iS_y.$$

To determine the action of $S_\pm$ on the states $|s,\sigma\rangle$, consider the commutation relations between $S_\pm$ and S_z, $\mathbf{S}^2$. Using the fundamental spin commutation relations $[S_i,S_j] = i\hbar\epsilon_{ijk}S_k$ and $[\mathbf{S}^2,S_i]=0$, we have:

$$[S_z,S_\pm] = [S_z,S_x\pm iS_y] = i\hbar S_y \mp i(i\hbar)S_x = \pm\hbar S_\pm \qquad \text{and} \qquad [\mathbf{S}^2,S_\pm]=0.$$

With this information, we can determine that $S_\pm|s,\sigma\rangle \propto |s,\sigma\pm1\rangle$, since:

$$\mathbf{S}^2 S_\pm|s,\sigma\rangle = S_\pm\mathbf{S}^2|s,\sigma\rangle = \hbar^2 s(s+1)S_\pm|s,\sigma\rangle$$

and

$$S_zS_\pm|s,\sigma\rangle = S_\pm S_z|s,\sigma\rangle + [S_z,S_\pm]|s,\sigma\rangle = \hbar\sigma S_\pm|s,\sigma\rangle \pm \hbar S_\pm|s,\sigma\rangle = \hbar(\sigma\pm1)S_\pm|s,\sigma\rangle\,.$$

To determine the constant of proportionality, notice that we can write the total spin operator as:

$$\mathbf{S}^2 = S_x^2+S_y^2+S_z^2 = (S_x\mp iS_y)(S_x\pm iS_y)\mp i[S_x,S_y]+S_z^2 = S_\mp S_\pm \pm \hbar S_z + S_z^2.$$

Hence we can compute the norm:

$$||S_\pm|s,\sigma\rangle||^2 = \langle s,\sigma|S_\mp S_\pm|s,\sigma\rangle = \langle s,\sigma|\mathbf{S}^2 - S_z^2 \mp \hbar S_z|s,\sigma\rangle = \hbar^2 s(s+1)-\hbar^2\sigma^2\mp\hbar^2\sigma = \hbar^2\left(s(s+1)-\sigma(\sigma\pm1)\right).$$

It follows that:

$$S_\pm|s,\sigma\rangle = \hbar\sqrt{s(s+1)-\sigma(\sigma\pm1)}\,|s,\sigma\pm1\rangle\,,$$

as required.

To express the given Hamiltonian in terms of the spin raising and spin lowering operators, it's useful to rewrite S_x and S_y in terms of the raising and lowering operators. We note that we have:

$$S_x = \frac{1}{2}(S_+ + S_-)\,, \qquad S_y = \frac{1}{2i}(S_+ - S_-)\,.$$

Hence, in the expression for the Hamiltonian, we have:

$$\begin{aligned}\mathbf{S}^{(1)}\cdot\mathbf{S}^{(2)} &= S_x^{(1)}S_x^{(2)} + S_y^{(1)}S_y^{(2)} + S_z^{(1)}S_z^{(2)} \\ &= \frac{1}{4}\left(S_+^{(1)} + S_-^{(1)}\right)\left(S_+^{(2)} + S_-^{(2)}\right) - \frac{1}{4}\left(S_+^{(1)} - S_-^{(1)}\right)\left(S_+^{(2)} - S_-^{(2)}\right) + S_z^{(1)}S_z^{(2)} \\ &= \frac{1}{2}S_+^{(1)}S_-^{(2)} + \frac{1}{2}S_-^{(1)}S_+^{(2)} + S_z^{(1)}S_z^{(2)}.\end{aligned}$$

We also have:

$$\mathbf{B}\cdot(\mathbf{S}^{(1)} - \mathbf{S}^{(2)}) = B(S_z^{(1)} - S_z^{(2)}).$$

Hence the final expression for the Hamiltonian is:

$$H = \frac{\alpha}{2}\left(S_+^{(1)}S_-^{(2)} + S_-^{(1)}S_+^{(2)}\right) + \alpha S_z^{(1)}S_z^{(2)} + B(S_z^{(1)} - S_z^{(2)}).$$

We now wish to find the eigenvalues of H. The vector space that H acts on is spanned by the states $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$, where the first slot denotes the spin state of the first particle and the second slot denotes the spin states of the second particle. Acting on each of these basis elements in turn, we can determine the matrix of H in this basis, and hence diagonalise H conveniently.

Acting with H on each of the basis elements then, we have:

- On the first basis element $|\uparrow\uparrow\rangle$, both $S_+^{(1)}S_-^{(2)}$ and $S_-^{(1)}S_+^{(2)}$ annihilate the state, since they try to add too much angular momentum or take away too much angular momentum to the states. Hence, using $S_z|\uparrow\rangle = \frac{1}{2}\hbar|\uparrow\rangle$, we're left with:
$$H|\uparrow\uparrow\rangle = \frac{1}{4}\alpha\hbar^2|\uparrow\uparrow\rangle + \frac{1}{2}B\hbar|\uparrow\uparrow\rangle - \frac{1}{2}B\hbar|\uparrow\uparrow\rangle = \frac{1}{4}\alpha\hbar^2|\uparrow\uparrow\rangle.$$
- Similarly, on the final basis element $|\downarrow\downarrow\rangle$, we have (using $S_z|\downarrow\rangle = -\frac{1}{2}\hbar|\downarrow\rangle$):
$$H|\downarrow\downarrow\rangle = \frac{1}{4}\alpha\hbar^2|\downarrow\downarrow\rangle.$$
- On the basis element $|\uparrow\downarrow\rangle$, the raising and lowering operators do not necessarily give zero. We have that $S_+^{(1)}S_-^{(2)}$ annihilates the state, but $S_-^{(1)}S_+^{(2)}$ gives:
$$S_-^{(1)}S_+^{(2)}|\uparrow\downarrow\rangle = \hbar^2|\downarrow\uparrow\rangle.$$
Thus the whole Hamiltonian acts as:
$$H|\uparrow\downarrow\rangle = \frac{\alpha\hbar^2}{2}|\downarrow\uparrow\rangle - \frac{1}{4}\alpha\hbar^2|\uparrow\downarrow\rangle + \frac{1}{2}B\hbar(|\uparrow\downarrow\rangle + |\uparrow\downarrow\rangle) = \frac{\alpha\hbar^2}{2}|\downarrow\uparrow\rangle - \left(\frac{1}{4}\alpha\hbar^2 - B\hbar\right)|\uparrow\downarrow\rangle.$$
- Similarly, the Hamiltonian acts on the basis element $|\downarrow\uparrow\rangle$ as:
$$H|\downarrow\uparrow\rangle = \frac{\alpha\hbar^2}{2}|\uparrow\downarrow\rangle - \left(\frac{1}{4}\alpha\hbar^2 + B\hbar\right)|\downarrow\uparrow\rangle.$$

We can now write down the matrix form of the Hamiltonian and diagonalise it to find the energy levels. In the basis we used above, $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$, we have:

$$H = \begin{pmatrix} \frac{1}{4}\alpha\hbar^2 & 0 & 0 & 0 \\ 0 & -(\frac{1}{4}\alpha\hbar^2 - B\hbar) & \frac{1}{2}\alpha\hbar^2 & 0 \\ 0 & \frac{1}{2}\alpha\hbar^2 & -(\frac{1}{4}\alpha\hbar^2 + B\hbar) & 0 \\ 0 & 0 & 0 & \frac{1}{4}\alpha\hbar^2 \end{pmatrix}$$

Clearly we have the eigenvalue $\alpha\hbar^2$ corresponding to the eigenstates $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$. We can find additional energy eigenvalues and eigenvectors by diagonalising the 2×2 submatrix contained in H. The eigenvalues obey:

$$0 = \det \begin{pmatrix} -(\frac{1}{4}\alpha\hbar^2 - B\hbar) - \lambda & \frac{1}{2}\alpha\hbar^2 \\ \frac{1}{2}\alpha\hbar^2 & -(\frac{1}{4}\alpha\hbar^2 + B\hbar) - \lambda \end{pmatrix} = \left(\frac{1}{4}\alpha\hbar^2 - B\hbar + \lambda\right)\left(\frac{1}{4}\alpha\hbar^2 + B\hbar + \lambda\right) - \frac{1}{4}\alpha^2\hbar^4.$$

Simplifying, we see that we need to solve the quadratic:

$$0 = \lambda^2 + \frac{1}{2}\alpha\hbar^2\lambda - \frac{3}{16}\alpha^2\hbar^4 - B^2\hbar^2$$

Using the quadratic formula, we have:

$$\lambda = \frac{-\frac{1}{2}\alpha\hbar^2 \pm \sqrt{\frac{1}{4}\alpha^2\hbar^4 + \frac{3}{4}\alpha^2\hbar^4 + 4B^2\hbar^2}}{2} = -\frac{1}{4}\alpha\hbar^2 \pm \sqrt{\frac{1}{4}\alpha^2\hbar^4 + B^2\hbar^2}$$

Hence the energy eigenvalues are:

$$\frac{1}{4}\alpha\hbar^2, \qquad \frac{1}{4}\alpha\hbar^2, \qquad -\frac{1}{4}\alpha\hbar^2 + \sqrt{\frac{1}{4}\alpha^2\hbar^4 + B^2\hbar^2}, \qquad -\frac{1}{4}\alpha\hbar^2 - \sqrt{\frac{1}{4}\alpha^2\hbar^4 + B^2\hbar^2}.$$

In the limit $B \to 0$, the energy eigenvalues reduce to:

$$\frac{1}{4}\alpha\hbar^2, \qquad \frac{1}{4}\alpha\hbar^2, \qquad \frac{1}{4}\alpha\hbar^2, \qquad -\frac{3}{4}\alpha\hbar^2.$$

The associated eigenvectors can be determined easily in this limit too, showing the degeneracy. The first two energy eigenvalues arise from the states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ as we have seen. The remaining come from eigenvectors of the matrix:

$$\begin{pmatrix} -\frac{1}{4}\alpha\hbar^2 & \frac{1}{2}\alpha\hbar^2 \\ \frac{1}{2}\alpha\hbar^2 & -\frac{1}{4}\alpha\hbar^2 \end{pmatrix} = -\frac{\alpha\hbar^2}{4}\begin{pmatrix} 1 & -2 \\ -2 & 1 \end{pmatrix}.$$

Simply guessing $(1, 1)^T$ as an eigenvector gives the eigenvalue $\frac{1}{4}\alpha\hbar^2$; since this is a symmetric matrix, the other eigenvector can be chosen to be orthogonal, so choose $(1, -1)^T$ to be the other eigenvector. We see this has eigenvalue $-\frac{3}{4}\alpha\hbar^2$ as expected. Hence we see:

- The state $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$ has the energy eigenvalue $-\frac{3}{4}\alpha\hbar^2$. This is the unique eigenvector (up to normalisation) associated with this eigenvalue, hence is the unique ground state (i.e. lowest energy state) of the system.
- The states $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$ and $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ all have energy eigenvalue $\frac{1}{4}\alpha\hbar^2$. They span a space of dimension 3, hence this energy level is threefold degenerate as required.

Finally, we are asked to explain the threefold degeneracy by considering the action of the total spin $\mathbf{S} = \mathbf{S}^{(1)} + \mathbf{S}^{(2)}$ on the energy eigenstates. Considering just the z-component, we have:

$$S_z \left|\uparrow\uparrow\right\rangle = \left(S_z^{(1)} + S_z^{(2)}\right) \left|\uparrow\uparrow\right\rangle = \hbar \left|\uparrow\uparrow\right\rangle .$$

Similarly:

$$S_z \left|\downarrow\downarrow\right\rangle = -\hbar \left|\downarrow\downarrow\right\rangle ,$$

and

$$S_z \left(\left|\uparrow\downarrow\right\rangle + \left|\downarrow\uparrow\right\rangle\right) = 0.$$

It follows that the states $\{\left|\uparrow\uparrow\right\rangle , \left|\uparrow\downarrow\right\rangle + \left|\downarrow\uparrow\right\rangle , \left|\downarrow\downarrow\right\rangle\}$ are the S_z eigenvectors of a spin-1 system, corresponding to spins $S_z = \hbar$, $S_z = 0$ and $S_z = -\hbar$ respectively.

Let's see if we can relate this to the Hamiltonian. Consider taking the square of the combined spin operator $\mathbf{S}^2 = (\mathbf{S}^{(1)} + \mathbf{S}^{(2)})^2$. We get:

$$\mathbf{S}^2 = (\mathbf{S}^{(1)})^2 + (\mathbf{S}^{(2)})^2 + 2\mathbf{S}^{(1)} \cdot \mathbf{S}^{(2)} = \frac{3}{2}\hbar^2 + 2\mathbf{S}^{(1)} \cdot \mathbf{S}^{(2)},$$

since $\mathbf{S}^{(i)}$ are both spin operators for spin-$\frac{1}{2}$ particles, hence we have $(\mathbf{S}^{(i)})^2 = 3\hbar^2/4$. It follows that the Hamiltonian, in the limit $B \to 0$, can be written in the form:

$$H = \alpha \mathbf{S}^{(1)} \cdot \mathbf{S}^{(2)} = \frac{3}{2}\alpha \mathbf{S}^2 - \frac{1}{4}\alpha\hbar^2.$$

Hence the Hamiltonian is a linear function of the total spin of the system, $\mathbf{S}^2$. In particular, the eigenvectors of $\mathbf{S}^2$ will precisely be the eigenvectors of H. Note, however, that H does not care about the alignment of the total spin, governed by S_z.

When the total spin is $\mathbf{S}^2 = 0$, there is only one possible alignment, i.e. $S_z = 0$. When the total spin is $\mathbf{S}^2 = \hbar^2$, there are three possible alignments, $S_z = \hbar$, $S_z = 0$ and $S_z = -\hbar$, corresponding to a threefold degeneracy.

This also relates to the symmetry of the system. We see that if we rotate the total spin $\mathbf{S}$, we can map between $S_z = \hbar$, $S_z = 0$ and $S_z = -\hbar$, however the Hamiltonian is unchanged, since it depends only on the square of the spin $\mathbf{S}^2$. The rotational invariance implies that we get the observed degeneracy. The rotational invariance is broken by the additional B-dependent term, and hence we do not get the same degeneracy when $B \neq 0$. Indeed, the B-dependent term is $B(S_z^{(1)} - S_z^{(2)})$ which is only invariant under the subgroup of rotations which fixes the z-axis; this subgroup leads to a two-fold degeneracy as it acts on a space of dimension 2, rather than a three-fold degeneracy from the full rotational invariance.

⁜ **Comments from the Examiner:** *Another very popular question. Most candidates were able to reproduce the bookwork for the first half of the question and this was sufficient to achieve at least a β in most cases. The middle section of the question, in which an explicit diagonalisation of the given Hamiltonian was required was more demanding but was completed in almost half of the attempts almost always resulting in an α. The best answers correctly described the role of rotational symmetry in the $B \to 0$ limit as an explanation of the resulting degeneracies.*