1. **2010 Exam Q1(d):** An electron in a hydrogen atom is in an excited state with $l = 2$. What are the possible values of its total angular momentum quantum number j? List the possible values of m_j and the degeneracy of each.

2. **2010 Exam Q3** In a 2-electron system, the total spin has x-component

$$\hat{S}_x = \hat{S}_{1x} \otimes \hat{I} + \hat{I} \otimes \hat{S}_{2x}$$

(a) Evaluate the results of applying $\hat{S}_x$ to each of the "direct product" basis vectors, i.e.

$$|1\rangle = |\uparrow\rangle|\uparrow\rangle; \quad |2\rangle = |\uparrow\rangle|\downarrow\rangle; \quad |3\rangle = |\downarrow\rangle|\uparrow\rangle; \quad |4\rangle = |\downarrow\rangle|\downarrow\rangle.$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ are the spin-up and spin-down eigenstates of $\hat{S}_z$.

(The x-Pauli matrix $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$).

Hence show that the matrix representing $\hat{S}_x$ in the direct product basis is

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

[8 marks]

(b) An alternative basis:

$$|\mathrm{I}\rangle = (|1\rangle + |2\rangle + |3\rangle + |4\rangle)/2; \quad |\mathrm{II}\rangle = (|1\rangle - |4\rangle)/\sqrt{2};$$

$$|\mathrm{III}\rangle = (|1\rangle - |2\rangle - |3\rangle + |4\rangle)/2; \quad |\mathrm{IV}\rangle = (|2\rangle - |3\rangle)/\sqrt{2}.$$

consists of eignevectors of S_x. Evaluate the matrix representation of $\hat{S}_x$ in this basis by using the matrix of eigenvectors to perform a unitary transform from the direct product basis. Verify that the transformed matrix is diagonal and hence find the eigenvalues associated with each eigenvector. [10 marks]

(c) Is this the only possible eigenbasis for $\hat{S}_x$? Briefly explain why. [3 marks]

(d) What is different between the state $|\mathrm{IV}\rangle$ and the other three eigenkets? What are the possible value(s) that a measurement of S_y might yield for this state? [4 marks]

3. **2010 Exam Q4(d)** The normalized ground state wave function of the simple harmonic oscillator is

$$\langle x|0\rangle = K \exp\left(-\frac{m\omega x^2}{2\hbar}\right).$$

where K is a normalizing factor. Using the operator $\hat{a}^\dagger$, or otherwise, find the wave function for the first excited state (you need not find the normalisation factor).

[6 marks]

Hint: $\hat{a}$ (not $\hat{a}^\dagger$) is given by

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

1. Possible values of total angular momentum $\mathbf{J} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$: $J^2 = j(j+1)\hbar^2$, $L^2 = l(l+1)\hbar^2$, $S^2 = s(s+1)\hbar^2$. j, l, and s are all quantised and positive: l must have integer values; j and s can also have half-integer values. Maximum value of j is $j_{\max} = l + s$, minimum value $j_{\min} = |l - s|$. In between, values decrease in steps of one. Electrons have $s = \frac{1}{2}$, so for $l = 2$,

$$j_{\max} = 5/2, \quad j_{\min} = 3/2$$

and there are no intermediate values.

Possible values of m_j run from j to $-j$ in unit steps, hence

j	$5/2$	$3/2$	degeneracy
	$5/2$		1
	$3/2$	$3/2$	2
m_j	$1/2$	$1/2$	2
	$-1/2$	$-1/2$	2
	$-3/2$	$-3/2$	2
	$-5/2$		1

2. (a) Recalling that $\hat{S}_i = \frac{\hbar}{2}\sigma_i$, the given Pauli matrix shows that the effect of the single-particle S_x operator is to swap spin-up for spin-down, and vice-versa, and multiply the state vector by $\hbar/2$. Using the rule:

$$A \otimes B|a\rangle|b\rangle = (A|a\rangle) \otimes (B|b\rangle)\,,$$

we have

$$\begin{aligned}
S_x|1\rangle &= \hbar/2(|\downarrow\rangle|\uparrow\rangle + |\uparrow\rangle|\downarrow\rangle) = \hbar/2(|3\rangle + |2\rangle) \\
S_x|2\rangle &= \hbar/2(|\downarrow\rangle|\downarrow\rangle + |\uparrow\rangle|\uparrow\rangle) = \hbar/2(|4\rangle + |1\rangle) \\
S_x|3\rangle &= \hbar/2(|\uparrow\rangle|\uparrow\rangle + |\downarrow\rangle|\downarrow\rangle) = \hbar/2(|1\rangle + |4\rangle) \\
S_x|4\rangle &= \hbar/2(|\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\uparrow\rangle) = \hbar/2(|2\rangle + |3\rangle)
\end{aligned}$$

The given matrix is the one that leads to these results in matrix notation, where

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \text{etc.}$$

(b) We can change the basis of an operator, here to the "Roman" (R) from the "arabic" (a) basis, by writing:

$$[S_x]^{(R)} = [S^{aR}]^\dagger [S_x]^{(a)} [S^{aR}]$$

where $[S^{aR}]$ is the "Roman-to-arabic" conversion matrix, i.e. the matrix of eigenvectors, which consists of columns which are the "Roman" eigenvectors in the "arabic" basis (and rows vice-versa):

$$\begin{aligned}
[S_x]^{(R)} &= \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & 0 & \frac{-1}{2} \\ \frac{1}{2} & \frac{-1}{2} & \frac{-1}{2} & \frac{1}{2} \\ 0 & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 \end{pmatrix} \frac{\hbar}{2} \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{-1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & 0 & \frac{-1}{2} & \frac{-1}{\sqrt{2}} \\ \frac{1}{2} & \frac{-1}{\sqrt{2}} & \frac{1}{2} & 0 \end{pmatrix} \\
&= \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & 0 & \frac{-1}{2} \\ \frac{1}{2} & \frac{-1}{2} & \frac{-1}{2} & \frac{1}{2} \\ 0 & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 \end{pmatrix} \frac{\hbar}{2} \begin{pmatrix} 1 & 0 & -1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & -1 & 0 \end{pmatrix} \\
&= \frac{\hbar}{2} \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \hbar \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}
\end{aligned}$$

As required, this is diagonal, and so we can just read the eigenvalues off the diagonal, viz: $|I\rangle$: $\hbar$; $|II\rangle$: 0; $|III\rangle$: $-\hbar$; $|IV\rangle$: 0.

(c) This is not the only possible eigenbasis for $\hat{S}_x$, because the eigenvalue zero is degenerate. Hence any pair of orthogonal vectors in the $S_x = 0$ eigenspace could be used as part of an $\hat{S}_x$ eigenbasis.

(d) State $|IV\rangle$ is the spin-singlet state corresponding to total-spin $S = 0$; the other eigenkets are triplet states corresponding to $S = 1$, i.e. $S^2 = 2\hbar^2$. The spin-singlet state has the property that it has a zero spin eigenvalue for measurement along any direction, in particular a measurement of S_y will definitely yield $S_y = 0$.

3. From the given expression for $\hat{a}$ you can take the adjoint, recalling that $\hat{x}$ and $\hat{p}$ are Hermitian:

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

You should know that $\hat{a}^\dagger|n\rangle \propto |n+1\rangle$, and in particular the first excited state can be got from the ground state via $|1\rangle \propto \hat{a}^\dagger|0\rangle$ (you may also remember the proportionality constant, $\sqrt{n+1}$, but it's not needed here). In the position representation this becomes

$$\langle x|1\rangle \propto \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{i}{m\omega} \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \langle x|0\rangle.$$

So

$$\langle x|1\rangle \propto \sqrt{\frac{m\omega}{2\hbar}}\left(x-\frac{\hbar}{m\omega}\left[\frac{-m\omega 2x}{2\hbar}\right]\right)\exp\left[\frac{-m\omega x^2}{2\hbar}\right]=\sqrt{\frac{m\omega}{2\hbar}}2\,x\exp\left[\frac{-m\omega x^2}{2\hbar}\right].$$

(The constant factors at the front of this expression can be omitted, as they will be absorbed into the normalization constant).