

# PC3130 (AY2012/2013 sem 2)

## Suggested solutions

Throughout this solution sheet, the notation will follow Einstein summation convention unless otherwise specified.

### Question 1

**1a.** (AY2012/13 sem 2 notes, Chapter 1.1.2, page 14) Orbital angular momentum is defined as  $\vec{L} = \vec{x} \times \vec{p}$ , i.e. it has components  $L_i = \varepsilon_{ijk}x_jp_k$ . It has the commutation relation  $[L_i, L_j] = i\hbar\varepsilon_{ijk}L_k$ .

$$\begin{aligned} \mathbf{1ai.} \quad [L_i, L^2] &= [L_i, L_jL_j] = [L_i, L_j]L_j + L_j[L_i, L_j] \\ &= (i\hbar\varepsilon_{ijk}L_k)L_j + L_j(i\hbar\varepsilon_{ijk}L_k) \\ &= i\hbar(\varepsilon_{ijk}L_kL_j + \varepsilon_{ij'k'}L_{j'}L_{k'}) \quad (\text{relabelling indices, } j \rightarrow j', k \rightarrow k') \\ &= i\hbar(\varepsilon_{ijk}L_kL_j - \varepsilon_{ik'j'}L_{j'}L_{k'}) \\ &= i\hbar(\varepsilon_{ijk}L_kL_j - \varepsilon_{ijk}L_kL_j) \quad (\text{relabelling indices, } k' \rightarrow j, j' \rightarrow k) \\ &= 0 \end{aligned}$$

$$\begin{aligned} \mathbf{1aii.} \quad [L_i, x_j] &= [\varepsilon_{ilm}x_l p_m, x_j] = \varepsilon_{ilm}(x_l[p_m, x_j] + [x_l, x_j]p_m) \\ &= \varepsilon_{ilm}(x_l(-i\hbar\delta_{mj}) + 0) \quad \text{since } x_l \text{ and } x_j \text{ commute} \\ &= -i\hbar\varepsilon_{ilj}x_l \\ &= i\hbar\varepsilon_{ijl}x_l \\ &= i\hbar\varepsilon_{ijk}x_k \quad (\text{relabelling index, } l \rightarrow k) \end{aligned}$$

$$\begin{aligned} \mathbf{1aiii.} \quad [L_i, p_j] &= [\varepsilon_{ilm}x_l p_m, p_j] = \varepsilon_{ilm}(x_l[p_m, p_j] + [x_l, p_j]p_m) \\ &= \varepsilon_{ilm}(0 + (i\hbar\delta_{lj})p_m) \quad \text{since } p_m \text{ and } p_j \text{ commute} \\ &= i\hbar\varepsilon_{ijm}p_m \\ &= i\hbar\varepsilon_{ijk}p_k \quad (\text{relabelling index, } m \rightarrow k) \end{aligned}$$

$$\begin{aligned} [L_3, x^2] &= [L_3, x_jx_j] = [L_3, x_j]x_j + x_j[L_3, x_j] \\ &= (i\hbar\varepsilon_{3jk}x_k)x_j + x_j(i\hbar\varepsilon_{3jk}x_k) \\ &= i\hbar(\varepsilon_{3jk}x_kx_j + \varepsilon_{3j'k'}x_{j'}x_{k'}) \quad (\text{relabelling indices, } j \rightarrow j', k \rightarrow k') \\ &= i\hbar(\varepsilon_{3jk}x_kx_j - \varepsilon_{3k'j'}x_{j'}x_{k'}) \\ &= i\hbar(\varepsilon_{3jk}x_kx_j - \varepsilon_{3jk}x_kx_j) \quad (\text{relabelling indices, } k' \rightarrow j, j' \rightarrow k) \\ &= 0 \end{aligned}$$

$$\begin{aligned}
[L_3, p^2] &= [L_3, p_j p_j] = [L_3, p_j] p_j + p_j [L_3, p_j] \\
&= (i\hbar \varepsilon_{3jk} p_k) p_j + p_j (i\hbar \varepsilon_{3jk} p_k) \\
&= i\hbar (\varepsilon_{3jk} p_k p_j + \varepsilon_{3j'k'} p_{j'} p_{k'}) \quad (\text{relabelling indices, } j \rightarrow j', k \rightarrow k') \\
&= i\hbar (\varepsilon_{3jk} p_k p_j - \varepsilon_{3k'j'} p_{j'} p_{k'}) \\
&= i\hbar (\varepsilon_{3jk} p_k p_j - \varepsilon_{3jk} p_k p_j) \quad (\text{relabelling indices, } k' \rightarrow j, j' \rightarrow k) \\
&= 0
\end{aligned}$$

Since  $L_3$  commutes with  $x^2$  and  $p^2$  as shown above, it also commutes with any analytic function of  $x^2$  or  $p^2$ . Hence we have  $\left[ L_3, \frac{p^2}{2m} \right] = 0$  and  $[L_3, V(r)] = \left[ L_3, V(\sqrt{x^2}) \right] = 0$ , and therefore  $[L_3, H] = \left[ L_3, \frac{p^2}{2m} + V(r) \right] = [L_3, V(r)] + \left[ L_3, \frac{p^2}{2m} \right] = 0$ .

**1b.** Since  $[L_i, L^2] = 0$  (as shown in part 1ai), we also have  $[L_i^2, L^2] = 0$ . Also, by definition  $L^2 = L_1^2 + L_2^2 + L_3^2$ . Therefore,

$$\begin{aligned}
[L_1^2, L_2^2] &= [L_1^2, L^2 - L_1^2 - L_3^2] = [L_1^2, L^2] - [L_1^2, L_1^2] - [L_1^2, L_3^2] \\
&= 0 - 0 - [L_1^2, L_3^2] \\
&= [L_3^2, L_1^2]
\end{aligned}$$

By symmetry (permuting indices) we also get  $[L_3^2, L_1^2] = [L_2^2, L_3^2]$ , thus overall we have  $[L_1^2, L_2^2] = [L_2^2, L_3^2] = [L_3^2, L_1^2]$ .

Within the  $l = 1$  subspace, the  $|1, m\rangle$  states with  $m = -1, 0, 1$  form a complete basis. We shall therefore show that the above commutators vanish for all angular momentum states with  $l = 1$  by showing  $\langle 1, m' | [L_1^2, L_3^2] | 1, m \rangle = 0$  for all  $m, m' = -1, 0, 1$  (this necessarily implies that the commutators vanish in the  $l = 1$  subspace because any state in this subspace can be expressed as some linear combination of the  $|1, m\rangle$  states with  $m = -1, 0, 1$ ).

We first recall that in terms of the raising/lowering operators, we have  $L_1 = \frac{L_+ + L_-}{2}$  and  $L_2 = \frac{L_+ - L_-}{2i}$ . Therefore we have

$$\begin{aligned}
L_1^2 &= \left( \frac{L_+ + L_-}{2} \right)^2 = \frac{1}{4} (L_+^2 + L_-^2 + L_+ L_- + L_- L_+) \\
L_2^2 &= \left( \frac{L_+ - L_-}{2i} \right)^2 = -\frac{1}{4} (L_+^2 + L_-^2 - L_+ L_- - L_- L_+)
\end{aligned}$$

To reduce clutter in the following steps, we also note that within the  $l = 1$  subspace, the “normalisation constants”  $\hbar\sqrt{l(l+1) - m(m \pm 1)}$  for the raising/lowering operators  $L_{\pm}$  take the value  $\hbar\sqrt{2}$  in all non-zero cases (as seen by substituting  $l = 1, m = -1, 0, 1$  into the expression), i.e. we have  $L_{\pm} |1, m\rangle = \hbar\sqrt{2} |1, m \pm 1\rangle$  in all non-zero cases.

For all  $m, m'$  within the  $l = 1$  subspace,

$$\begin{aligned}\langle 1, m' | [L_1^2, L_3^2] | 1, m \rangle &= \langle 1, m' | L_1^2 L_3^2 - L_3^2 L_1^2 | 1, m \rangle = \langle 1, m' | L_1^2 L_3^2 | 1, m \rangle - \langle 1, m' | L_3^2 L_1^2 | 1, m \rangle \\ &= \langle 1, m' | L_1^2 m^2 | 1, m \rangle - \langle 1, m' | m'^2 L_1^2 | 1, m \rangle \\ &= (m^2 - m'^2) \langle 1, m' | L_1^2 | 1, m \rangle\end{aligned}$$

We now consider two cases,  $m = \pm m'$  and  $m \neq \pm m'$ .

Case 1 ( $m = \pm m'$ ): We have  $(m^2 - m'^2) = 0$  and therefore  $\langle 1, m' | [L_1^2, L_3^2] | 1, m \rangle = 0$ .

Case 2 ( $m \neq \pm m'$ ): We first note that this necessarily implies exactly one of  $m, m'$  is 0 (and the other is  $\pm 1$ ), since the only values they can take are  $-1, 0, 1$ . If  $m = 0$ , then  $L_\pm^2 | 1, m \rangle = 0$  (since applying the raising/lowering operator twice to the  $m = 0$  state in the  $l = 1$  subspace gives zero) and thus  $\langle 1, m' | L_\pm^2 | 1, m \rangle = 0$ . If  $m' = 0$ , then since  $L_\pm^2 | 1, \mp 1 \rangle = 2\hbar^2 | 1, \pm 1 \rangle$  and  $L_\pm^2 | 1, \pm 1 \rangle = 0$ , we must have  $\langle 1, m' | L_\pm^2 | 1, m \rangle = 0$  (because the  $| 1, \pm 1 \rangle$  states are orthogonal to the  $| 1, 0 \rangle$  state).

(Alternative for  $m' = 0$ :  $L_+$  and  $L_-$  are the Hermitian conjugates of each other (since  $L_1$  and  $L_2$  are Hermitian), and thus  $\langle 1, 0 | L_\pm^2 = \left( (L_\pm^2)^\dagger | 1, 0 \rangle \right)^\dagger = (L_\mp^2 | 1, 0 \rangle)^\dagger = 0$ . Therefore  $\langle 1, m' | L_\pm^2 | 1, m \rangle = 0$  for  $m' = 0$ .)

Thus for this case,

$$\begin{aligned}\langle 1, m' | L_1^2 | 1, m \rangle &= \frac{1}{4} \langle 1, m' | (L_+^2 + L_-^2 + L_+ L_- + L_- L_+) | 1, m \rangle \\ &= \frac{1}{4} (0 + 0 + \langle 1, m' | L_+ L_- | 1, m \rangle + \langle 1, m' | L_- L_+ | 1, m \rangle) \\ &= \frac{1}{4} ((2\hbar^2 \text{ or } 0) \langle 1, m' | 1, m \rangle + (0 \text{ or } 2\hbar^2) \langle 1, m' | 1, m \rangle) \\ &= 0 \quad \text{since } m \neq \pm m' \text{ implies } m \neq m' \text{ and thus } \langle 1, m' | 1, m \rangle = 0\end{aligned}$$

and therefore  $\langle 1, m' | [L_1^2, L_3^2] | 1, m \rangle = 0$ .

Since the cases considered cover all possibilities, we have  $\langle 1, m' | [L_1^2, L_3^2] | 1, m \rangle = 0$  for all  $m, m'$  within the  $l = 1$  subspace. Therefore  $[L_1^2, L_3^2]$  vanishes within this subspace, and so do the other two commutators (since they are equal).

The  $| 1, -1 \rangle, | 1, 0 \rangle$  and  $| 1, 1 \rangle$  states form a complete basis for the  $l = 1$  subspace, and we shall hence express the common eigenstates of  $L_1^2, L_2^2$  and  $L_3^2$  (common eigenstates exist because these operators commute, as shown above) in terms of these states. As there are three states in the basis, the subspace has dimension 3.

We first note that  $| 1, -1 \rangle, | 1, 0 \rangle$  and  $| 1, 1 \rangle$  are eigenstates of  $L_3^2$  with eigenvalues  $\hbar^2, 0$  and  $\hbar^2$  respectively, i.e.  $| 1, -1 \rangle$  and  $| 1, 1 \rangle$  have the same eigenvalue, while  $| 1, 0 \rangle$  has a different one. Since they form a basis, one of the common eigenstates must be simply  $| 1, 0 \rangle$  itself, because any linear combination of  $| 1, 0 \rangle$  with  $| 1, -1 \rangle$  and/or  $| 1, 1 \rangle$  would *not* be an eigenstate of  $L_3^2$  (unless the coefficients for  $| 1, -1 \rangle$  and  $| 1, 1 \rangle$ , or  $| 1, 0 \rangle$ , are zero); this is easily seen by applying  $L_3^2$  to such a linear combination (noting the different eigenvalues).

By a similar line of reasoning, the remaining two common eigenstates must be linear combinations of  $|1, -1\rangle$  and  $|1, 1\rangle$  only, because adding a non-zero  $|1, 0\rangle$  component to such a linear combination would render it not an eigenstate of  $L_3^2$ . We also note that since  $|1, -1\rangle$  and  $|1, 1\rangle$  have the same eigenvalue (with respect to  $L_3^2$ ), any linear combination of them is automatically an eigenstate of  $L_3^2$ . It thus only remains to find out what linear combinations of the form  $a|1, 1\rangle + b|1, -1\rangle$  are eigenstates of both  $L_1^2$  and  $L_2^2$ . ( $a$  and  $b$  may be complex, but one of them can be chosen to be real and positive without loss of generality, because the global phase has no physical significance.)

To be an eigenstate of  $L_1^2$ , we require

$$\begin{aligned} L_1^2(a|1, 1\rangle + b|1, -1\rangle) &= \lambda(a|1, 1\rangle + b|1, -1\rangle) \\ \frac{1}{4}(L_+^2 + L_-^2 + L_+L_- + L_-L_+)(a|1, 1\rangle + b|1, -1\rangle) &= \lambda a|1, 1\rangle + \lambda b|1, -1\rangle \\ \frac{1}{4}(0 + 2\hbar^2 b|1, 1\rangle + 2\hbar^2 a|1, -1\rangle + 0 + 2\hbar^2 a|1, 1\rangle + 0 + 0 + 2\hbar^2 b|1, -1\rangle) &= \lambda a|1, 1\rangle + \lambda b|1, -1\rangle \\ \frac{\hbar^2}{2}((a+b)|1, 1\rangle + (a+b)|1, -1\rangle) &= \lambda a|1, 1\rangle + \lambda b|1, -1\rangle \end{aligned}$$

This gives us the system of equations  $\frac{\hbar^2}{2}(a+b) = \lambda a$ ,  $\frac{\hbar^2}{2}(a+b) = \lambda b$ . Subtracting the second equation from the first, we get  $\lambda(a-b) = 0$ , with the solutions

$a = b$ : Then  $\frac{\hbar^2}{2}(a+a) = \lambda a$ , and so  $\lambda = \hbar^2$ . Choosing  $a$  to be real and positive without loss of generality, and normalising the state, we have  $a = \frac{1}{\sqrt{2}}$ ,  $b = \frac{1}{\sqrt{2}}$ .

$\lambda = 0$ : Then  $\frac{\hbar^2}{2}(a+b) = 0$ , and so  $a = -b$ . Choosing  $a$  to be real and positive without loss of generality, and normalising the state, we have  $a = \frac{1}{\sqrt{2}}$ ,  $b = -\frac{1}{\sqrt{2}}$ .

Therefore, the linear combinations of  $|1, -1\rangle$  and  $|1, 1\rangle$  that are also eigenstates of  $L_1^2$  are  $\frac{1}{\sqrt{2}}|1, -1\rangle \pm \frac{1}{\sqrt{2}}|1, 1\rangle$  (or scalar multiples thereof). They have different eigenvalues with respect to  $L_1^2$ , are orthogonal to each other and  $|1, 0\rangle$  (and thus together with  $|1, 0\rangle$  must be a basis for this subspace, as it has dimension 3), and we have shown earlier that  $|1, 0\rangle$  must be one of the common eigenstates of  $L_1^2$ ,  $L_2^2$  and  $L_3^2$ ; hence, they must be precisely the common eigenstates we are looking for (the two common eigenstates other than  $|1, 0\rangle$  cannot be a linear combination of both these two states, because such a combination would not be an eigenstate of  $L_1^2$  due to the different eigenvalues). (Alternatively, one can explicitly verify this by applying  $L_2^2$  to these states and showing they are indeed eigenstates of  $L_2^2$ .)

In summary, the common eigenstates of  $L_1^2$ ,  $L_2^2$  and  $L_3^2$  are  $|1, 0\rangle$ ,  $\frac{1}{\sqrt{2}}|1, -1\rangle + \frac{1}{\sqrt{2}}|1, 1\rangle$  and  $\frac{1}{\sqrt{2}}|1, -1\rangle - \frac{1}{\sqrt{2}}|1, 1\rangle$  (or scalar multiples thereof).

(Remark: It can be verified that with respect to each of the operators  $L_1^2$ ,  $L_2^2$  and  $L_3^2$ , two of the common eigenstates have eigenvalue  $\hbar^2$  and one has eigenvalue 0, as expected by symmetry. However, the state with eigenvalue 0 is different for each operator.)

## Question 2

**2ai.** The magnetic field in this case is constant and uniform, thus as stated in the question, a possible magnetic vector potential is simply

$$\vec{A} = \frac{1}{2}\vec{B} \times \vec{x} = \frac{1}{2}(0, 0, B_0) \times (x_1, x_2, x_3) = \frac{B_0}{2}(-x_2, x_1, 0)$$

(Alternatively, by definition any vector field  $\vec{A}$  that satisfies  $\nabla \times \vec{A} = \vec{B}$  is a valid vector potential, thus we can simply verify explicitly that  $\nabla \times \vec{A} = \nabla \times \frac{B_0}{2}(-x_2, x_1, 0) = (0, 0, B_0)$ .)

We note also that this choice of magnetic vector potential follows the Coulomb gauge (i.e.  $\nabla \cdot \vec{A} = 0$ ), since  $\nabla \cdot \frac{B_0}{2}(-x_2, x_1, 0) = \frac{B_0}{2}(\partial_1(-x_2) + \partial_2(x_1) + \partial_3(0)) = 0$ .

**2aii.** This derivation is essentially identical to that presented in lecture (AY2012/13 sem 2 notes, Chapter 2) apart from the presence of an electric field in the  $z$ -direction, so some steps have been skimmed over for brevity. Refer to notes for full details. Note, however, that the energy levels as given in this question do not appear to be entirely correct unless additional constraints are specified on the particle's  $x_3$ -motion, as described later.

The Hamiltonian is  $\frac{(\vec{p}-q\vec{A})^2}{2m} + V(\vec{x})$ . We note that since  $\vec{p} = -i\hbar\nabla$ , we have by product rule  $\vec{p} \cdot (\vec{A}\psi) = (\vec{p} \cdot \vec{A})\psi + \vec{A} \cdot (\vec{p}\psi)$ . The  $(\vec{p} - q\vec{A})^2$  term thus expands to give

$$\begin{aligned} (\vec{p} - q\vec{A})^2 &= \vec{p}^2 + q^2\vec{A}^2 - q\vec{p} \cdot \vec{A} - q\vec{A} \cdot \vec{p} \\ &= \vec{p}^2 + q^2\vec{A}^2 - q(\vec{p} \cdot \vec{A}) - 2q\vec{A} \cdot \vec{p} \\ &= \vec{p}^2 + q^2\vec{A}^2 - 0 - 2q\vec{A} \cdot \vec{p} \quad \text{since } (\vec{p} \cdot \vec{A}) = -i\hbar\nabla \cdot \vec{A} = 0 \text{ (Coulomb gauge)} \\ &= \vec{p}^2 + q^2\vec{A}^2 - 2q\left(\frac{1}{2}\vec{B} \times \vec{x}\right) \cdot \vec{p} \\ &= \vec{p}^2 + q^2\vec{A}^2 - q\vec{B} \cdot (\vec{x} \times \vec{p}) \\ &= \vec{p}^2 + q^2\vec{A}^2 - q\vec{B} \cdot \vec{L} \\ &= \vec{p}^2 + q^2\frac{B_0^2}{4}((-x_2)^2 + x_1^2 + 0^2) - q(0, 0, B_0) \cdot (L_1, L_2, L_3) \\ &= \vec{p}^2 + \frac{q^2B_0^2}{4}(x_1^2 + x_2^2) - qB_0L_3 \end{aligned}$$

Since in this case  $V(\vec{x}) = 0$ , the Hamiltonian can thus be expressed as

$$\begin{aligned} H &= \frac{1}{2m} \left( \vec{p}^2 + \frac{q^2B_0^2}{4}(x_1^2 + x_2^2) - qB_0L_3 \right) + 0 \\ &= H_{2D} + H_{free} - \frac{qB_0}{2m}L_3 \\ &= \left[ H_{2D} - \frac{qB_0}{2m}\hbar(N_+ - N_-) \right] + H_{free} \end{aligned}$$

where  $H_{2D} = \frac{1}{2m} (p_1^2 + p_2^2) + \frac{q^2 B_0^2}{8m} (x_1^2 + x_2^2)$  is the Hamiltonian of a 2-dimensional harmonic oscillator (in the  $x_1$ - $x_2$  plane) with angular frequency  $\omega = \sqrt{\frac{q^2 B_0^2}{4m^2}} = \frac{qB_0}{2m}$ , and  $H_{free} = \frac{p_3^2}{2m}$  is the Hamiltonian of a 1-dimensional free particle (along the  $x_3$  axis).

Since the Hamiltonian can be separated into a sum of a Hamiltonian for motion in the  $x_1$ - $x_2$  plane (this includes the  $\frac{qB_0}{2m} L_3$  term) and a Hamiltonian for motion along the  $x_3$  axis, the motions are uncoupled. We thus use the  $|n_+, n_-, k_3\rangle$  basis, where  $k_3$  is the wavenumber associated with the free-particle motion along the  $x_3$  axis. Using this basis, the eigenvalues of  $H_{2D}$  are  $(n_+ + n_- + 1) \hbar\omega$ , while the eigenvalues of  $-\frac{qB_0}{2m} \hbar (N_+ - N_-)$  are  $-\frac{qB_0}{2m} \hbar (n_+ - n_-)$ .

However, the eigenvalues of  $H_{free}$  can take any non-negative real value (namely,  $\frac{\hbar^2 k_3^2}{2m}$ ). To eliminate this energy, we need to either confine the particle to a plane parallel to the  $x_1$ - $x_2$  plane, or change to a reference frame such that the  $x_3$ -component of the particle energy vanishes. With this constraint, the eigenvalues of the Hamiltonian (and hence the allowed energies) are then

$$\begin{aligned} E &= (n_+ + n_- + 1) \hbar\omega - \frac{qB_0}{2m} \hbar (n_+ - n_-) = (n_+ + n_- + 1) \hbar \frac{qB_0}{2m} - (n_+ - n_-) \hbar \frac{qB_0}{2m} \\ &= (2n_- + 1) \hbar \frac{qB_0}{2m} \\ &= \left(n_- + \frac{1}{2}\right) \hbar \frac{qB_0}{m} \end{aligned}$$

In summary, the allowed energies are thus  $E = \left(n + \frac{1}{2}\right) \hbar\omega_1$  where  $\omega_1 = \frac{qB_0}{m}$  and  $n$  is a non-negative integer, as desired.

**2b.** Consider the electric dipole moment under the coordinate transformation  $\vec{x} \rightarrow -\vec{x}$ . Since this is only a change of coordinates, it does not affect the physical quantity  $\langle nlm | \vec{d} | nlm \rangle$ . (An alternative approach is to note that space inversion is a unitary operation, and thus we have  $\langle nlm |' \vec{d} | nlm \rangle' = \langle nlm | U^\dagger U \vec{d} U^\dagger U | nlm \rangle = \langle nlm | \vec{d} | nlm \rangle$ .) Therefore, we have

$$\begin{aligned} \langle nlm | \vec{d} | nlm \rangle &= \langle nlm |' \vec{d} | nlm \rangle' = \langle nlm |' q\vec{x}' | nlm \rangle' \\ &= q \langle nlm | (-1)^l (-\vec{x}) (-1)^l | nlm \rangle \\ &= q(-1)^{2l+1} \langle nlm | \vec{x} | nlm \rangle \\ &= -q \langle nlm | \vec{x} | nlm \rangle \\ &= -\langle nlm | \vec{d} | nlm \rangle \end{aligned}$$

Since  $\langle nlm | \vec{d} | nlm \rangle = -\langle nlm | \vec{d} | nlm \rangle$ , we must thus have  $\langle nlm | \vec{d} | nlm \rangle = 0$ .

The third component of the electric dipole moment of the  $|\psi\rangle = \frac{1}{\sqrt{2}}(|2, 0, 0\rangle + |2, 1, 0\rangle)$  state is given by

$$\begin{aligned}
\langle\psi|d_3|\psi\rangle &= \frac{1}{2}(\langle 2, 0, 0| + \langle 2, 1, 0|)d_3(|2, 0, 0\rangle + |2, 1, 0\rangle) \\
&= \frac{1}{2}(\langle 2, 0, 0|d_3|2, 0, 0\rangle + \langle 2, 0, 0|d_3|2, 1, 0\rangle + \langle 2, 1, 0|d_3|2, 0, 0\rangle + \langle 2, 1, 0|d_3|2, 1, 0\rangle) \\
&= \frac{1}{2}(\langle 2, 0, 0|d_3|2, 1, 0\rangle + \langle 2, 1, 0|d_3|2, 0, 0\rangle) \text{ since } \langle nlm|\vec{d}|nlm\rangle = 0 \text{ as shown earlier} \\
&= \frac{1}{2}(\langle 2, 0, 0|d_3|2, 1, 0\rangle + \langle 2, 0, 0|d_3|2, 1, 0\rangle^*) \text{ since } x_3 \text{ is Hermitian (an observable)} \\
&\text{(Alternatively, the two terms could be evaluated individually if desired)} \\
&= \text{Re}(\langle 2, 0, 0|d_3|2, 1, 0\rangle)
\end{aligned}$$

We thus just need to evaluate  $\langle 2, 0, 0|d_3|2, 1, 0\rangle$ , i.e.  $\langle 2, 0, 0|qx_3|2, 1, 0\rangle$ :

$$\begin{aligned}
\langle 2, 0, 0|qx_3|2, 1, 0\rangle &= \langle 2, 0, 0|qr \cos \theta|2, 1, 0\rangle \\
&= q \int (R_{2,0}(r)Y_0^0(\theta, \phi))^* r \cos \theta (R_{2,1}(r)Y_1^0(\theta, \phi)) d^3r \\
&= q \int_{4\pi} \int_0^\infty (R_{2,0}(r)Y_0^0(\theta, \phi))^* r \cos \theta (R_{2,1}(r)Y_1^0(\theta, \phi)) r^2 dr d\Omega \\
&= q \left( \int_{4\pi} Y_0^0(\theta, \phi)^* \cos \theta Y_1^0(\theta, \phi) d\Omega \right) \left( \int_0^\infty R_{2,0}(r)^* R_{2,1}(r) r^3 dr \right) \\
&= q \langle 0, 0|\cos \theta|1, 0\rangle \left( \int_0^\infty R_{2,0}(r)R_{2,1}(r)r^3 dr \right) \text{ since } R_{2,0}(r) \text{ is real} \\
&= q \sqrt{\frac{(1+0)(1-0)}{(2+1)(2-1)}} \left( -\frac{9}{\sqrt{3}}a_0 \right) \text{ by the given formulae} \\
&= q \sqrt{\frac{1}{3}} \left( -\frac{9}{\sqrt{3}}a_0 \right) \\
&= -3qa_0
\end{aligned}$$

Therefore  $\langle\psi|d_3|\psi\rangle = \text{Re}(\langle 2, 0, 0|d_3|2, 1, 0\rangle) = -3qa_0$ , as desired.

**Important note:** If you wish to evaluate  $\int_0^\infty R_{2,0}(r)R_{2,1}(r)r^3 dr$  explicitly rather than use the provided result, note that the normalisation factor given in the question for the  $R_{2,1}(r)$  function is incorrect — it should be  $\frac{1}{\sqrt{24}}$ , not  $\frac{1}{\sqrt{2}}$ .

### Question 3

**3a.** This derivation is essentially identical to that presented in lecture (AY2012/13 sem 2 notes, Chapter 4), so some steps have been skimmed over for brevity. Refer to notes for full details.

Consider an arbitrary vector  $\vec{A}$  rotated about the axis  $\hat{n}$  by an infinitesimal angle  $\varepsilon$ . Let the change be denoted  $\delta\vec{A}$ , and the angle between  $\vec{A}$  and  $\hat{n}$  be denoted  $\theta$ .

The direction of  $\delta\vec{A}$  is perpendicular to both  $\vec{A}$  and  $\hat{n}$ , and thus can be specified by the unit vector  $\frac{\hat{n} \times \vec{A}}{|\hat{n} \times \vec{A}|} = \frac{\hat{n} \times \vec{A}}{|\vec{A}| \sin \theta}$ .

The magnitude of  $\delta\vec{A}$  can be seen by geometry to be  $(|\vec{A}| \sin \theta) \varepsilon$ .

Therefore we have  $\delta\vec{A} = \frac{\hat{n} \times \vec{A}}{|\vec{A}| \sin \theta} (|\vec{A}| \sin \theta) \varepsilon = \varepsilon \hat{n} \times \vec{A}$ , in other words  $\vec{A}' = \vec{A} + \varepsilon \hat{n} \times \vec{A} = (1 + \varepsilon \hat{n} \times) \vec{A}$ . The rotation operator  $\mathfrak{R}_{\hat{n}}(\varepsilon)$  in physical space is thus  $\mathfrak{R}_{\hat{n}}(\varepsilon) = 1 + \varepsilon \hat{n} \times$ .

To find the rotation operator in Hilbert space, we use  $\psi'(\vec{x}') = \psi(\vec{x})$  and apply a Taylor expansion since  $\varepsilon$  is infinitesimal:

$$\psi'(\vec{x}') = \psi(\vec{x}) = \psi(\mathfrak{R}_{\hat{n}}(\varepsilon)^{-1} \vec{x}') = \psi(\vec{x}' - \varepsilon \hat{n} \times \vec{x}') = \psi(\vec{x}') - \varepsilon (\hat{n} \times \vec{x}') \cdot \nabla \psi(\vec{x}') + O(\varepsilon^2)$$

Relabelling  $\vec{x}'$  as  $\vec{x}$ , and recalling  $\vec{p} = \frac{\hbar}{i} \nabla$  and  $\vec{L} = \vec{x} \times \vec{p}$ , we obtain

$$\begin{aligned} \psi'(\vec{x}) &= \psi(\vec{x}) - \varepsilon (\hat{n} \times \vec{x}) \cdot \nabla \psi(\vec{x}) + O(\varepsilon^2) = \psi(\vec{x}) - \frac{i}{\hbar} \varepsilon ((\hat{n} \times \vec{x}) \cdot \vec{p}) \psi(\vec{x}) + O(\varepsilon^2) \\ &= \psi(\vec{x}) - \frac{i}{\hbar} \varepsilon (\hat{n} \cdot \vec{L}) \psi(\vec{x}) + O(\varepsilon^2) \end{aligned}$$

Since  $\psi'(\vec{x}) = \langle \vec{x} | R | \psi \rangle$ , the coordinate representation  $R_c$  of  $R$  is hence  $R_c = 1 - \frac{i}{\hbar} \varepsilon (\hat{n} \cdot \vec{L})$ .

We now consider a multicomponent wavefunction  $\psi_i(\vec{x})$ . We then have  $\psi'_i(\vec{x}') = \pi_{ij} \psi_j(\vec{x})$ . Repeating the previous procedure gives

$$\psi'_i(\vec{x}) = \pi_{ij} \left[ \psi_j(\vec{x}) - \frac{i}{\hbar} \varepsilon (\hat{n} \cdot \vec{L}) \psi_j(\vec{x}) + O(\varepsilon^2) \right]$$

We assume that for infinitesimal rotations,  $\pi_{ij} = \delta_{ij} - \frac{i}{\hbar} \varepsilon (\hat{n} \cdot \vec{S})_{ij}$ . This hence gives

$$\begin{aligned} \psi'_i(\vec{x}) &= \left[ \delta_{ij} - \frac{i}{\hbar} \varepsilon (\hat{n} \cdot \vec{S})_{ij} \right] \left[ \psi_j(\vec{x}) - \frac{i}{\hbar} \varepsilon (\hat{n} \cdot \vec{L}) \psi_j(\vec{x}) + O(\varepsilon^2) \right] \\ &= \psi_i(\vec{x}) - \frac{i}{\hbar} \varepsilon (\hat{n} \cdot \vec{L}) \psi_i(\vec{x}) - \frac{i}{\hbar} \varepsilon (\hat{n} \cdot \vec{S})_{ij} \psi_j(\vec{x}) + O(\varepsilon^2) \\ &= \left( 1 - \frac{i}{\hbar} \varepsilon (\hat{n} \cdot \vec{L}) - \frac{i}{\hbar} \varepsilon (\hat{n} \cdot \vec{S})_{ij} \right) \psi_j(\vec{x}) + O(\varepsilon^2) \end{aligned}$$

Defining  $\vec{J} = \vec{L} + \vec{S}$  and keeping terms to order  $\varepsilon$ , we have  $\psi'_i(\vec{x}) = \left(1 - \frac{i}{\hbar}\varepsilon (\hat{n} \cdot \vec{J})\right)_{ij} \psi_j(\vec{x})$ , and therefore  $R_{\hat{n}}(\varepsilon) = 1 - \frac{i}{\hbar}\varepsilon (\hat{n} \cdot \vec{J})$ .

To find the finite rotation operator, we use the fact that  $R_{\hat{n}}(\theta + \delta\theta) = R_{\hat{n}}(\delta\theta)R_{\hat{n}}(\theta)$ . Letting  $\delta\theta$  be infinitesimal and applying the previous result, we hence have

$$R_{\hat{n}}(\theta + \delta\theta) = \left(1 - \frac{i}{\hbar}\delta\theta (\hat{n} \cdot \vec{J})\right) R_{\hat{n}}(\theta) = R_{\hat{n}}(\theta) - \frac{i}{\hbar}\delta\theta (\hat{n} \cdot \vec{J}) R_{\hat{n}}(\theta)$$

$$\begin{aligned} \text{Rearranging terms gives us } \frac{R_{\hat{n}}(\theta + \delta\theta) - R_{\hat{n}}(\theta)}{\delta\theta} &= -\frac{i}{\hbar} (\hat{n} \cdot \vec{J}) R_{\hat{n}}(\theta) \\ \implies \frac{d}{d\theta} R_{\hat{n}}(\theta) &= -\frac{i}{\hbar} (\hat{n} \cdot \vec{J}) R_{\hat{n}}(\theta) \\ \implies R_{\hat{n}}(\theta) &= \exp\left(-\frac{i}{\hbar}\theta (\hat{n} \cdot \vec{J})\right) \end{aligned}$$

**3b.** Since the expectation value of an observable should remain unchanged under rotation, we have  $\langle \psi | Q | \psi \rangle = \langle \psi' | Q' | \psi' \rangle$ , i.e.  $\langle \psi | Q | \psi \rangle = \langle \psi | R^\dagger Q' R | \psi \rangle$ . Since this holds for any arbitrary state  $|\psi\rangle$ , this implies  $Q = R^\dagger Q' R$ . As rotation is unitary, we have  $R^{-1} = R^\dagger$ , and thus  $Q = R^\dagger Q' R \implies Q' = R Q R^\dagger$ .

By geometric considerations, we would expect  $J_2$  to transform to  $J_2 \cos \theta - J_1 \sin \theta$  under a rotation of angle  $\theta$  about the  $x_3$ -axis. We shall now proceed to verify this algebraically, using power series expansions. Noting that  $R_{\hat{k}}(-\theta) = e^{\frac{i}{\hbar}\theta J_3} = R_{\hat{k}}(\theta)^\dagger$ , we shall ease the intermediate calculations slightly by instead showing that  $R_{\hat{k}}(\theta)^\dagger J_2 R_{\hat{k}}(\theta) = J_2 \cos \theta + J_1 \sin \theta$ , then substituting  $\theta \rightarrow -\theta$  to obtain the desired result  $R_{\hat{k}}(\theta) J_2 R_{\hat{k}}(\theta)^\dagger = J_2 \cos \theta - J_1 \sin \theta$ .

We first note that  $\frac{d}{d\theta} R_{\hat{k}}(\theta) = \frac{d}{d\theta} e^{-\frac{i}{\hbar}\theta J_3} = -\frac{i}{\hbar} J_3 R_{\hat{k}}(\theta)$ , and similarly  $\frac{d}{d\theta} R_{\hat{k}}(\theta)^\dagger = \frac{i}{\hbar} J_3 R_{\hat{k}}(\theta)^\dagger$ .

Also, since  $R_{\hat{k}}(\theta)$  has a power series expansion in terms of  $J_3$  and no other operators, it commutes with  $J_3$  (similarly for  $R_{\hat{k}}(\theta)^\dagger$ ).

Denote  $R_{\hat{k}}(\theta)^\dagger J_2 R_{\hat{k}}(\theta)$  as  $f(\theta)$ . We shall show by induction that

$$f^{(n)}(\theta) = \begin{cases} (-1)^{\frac{n}{2}} R_{\hat{k}}(\theta)^\dagger J_2 R_{\hat{k}}(\theta) & \text{if } n \text{ is even} \\ (-1)^{\frac{n-1}{2}} R_{\hat{k}}(\theta)^\dagger J_1 R_{\hat{k}}(\theta) & \text{if } n \text{ is odd} \end{cases}$$

Denoting the above statement as  $P(n)$ , we shall show the base case  $P(0)$  to be true, then show that for any non-negative even number  $m$ , we have  $P(m) \implies P(m+1) \implies P(m+2)$ , thereby proving  $P(n)$  to be true for all  $n \in \mathbb{Z}_{\geq 0}$  by induction.

Base case  $P(0)$ :  $f(\theta) = (-1)^0 R_{\hat{k}}(\theta)^\dagger J_2 R_{\hat{k}}(\theta) = R_{\hat{k}}(\theta)^\dagger J_2 R_{\hat{k}}(\theta)$  is indeed true.

Inductive step: Assume  $P(m)$  is true for some non-negative even  $m$ . Then we have  $f^{(m)}(\theta) = (-1)^{\frac{m}{2}} R_{\hat{k}}(\theta)^\dagger J_2 R_{\hat{k}}(\theta)$ , and thus

$$\begin{aligned}
f^{(m+1)}(\theta) &= \frac{d}{d\theta} \left( (-1)^{\frac{m}{2}} R_{\hat{k}}(\theta)^\dagger J_2 R_{\hat{k}}(\theta) \right) \\
&= (-1)^{\frac{m}{2}} \left( \left( \frac{d}{d\theta} R_{\hat{k}}(\theta)^\dagger \right) J_2 R_{\hat{k}}(\theta) + R_{\hat{k}}(\theta)^\dagger J_2 \left( \frac{d}{d\theta} R_{\hat{k}}(\theta) \right) \right) \\
&= (-1)^{\frac{m}{2}} \left( \left( \frac{i}{\hbar} J_3 R_{\hat{k}}(\theta)^\dagger \right) J_2 R_{\hat{k}}(\theta) + R_{\hat{k}}(\theta)^\dagger J_2 \left( -\frac{i}{\hbar} J_3 R_{\hat{k}}(\theta) \right) \right) \\
&= (-1)^{\frac{m}{2}} \left( \frac{i}{\hbar} \right) (R_{\hat{k}}(\theta)^\dagger J_3 J_2 R_{\hat{k}}(\theta) - R_{\hat{k}}(\theta)^\dagger J_2 J_3 R_{\hat{k}}(\theta)) \text{ since } R_{\hat{k}}(\theta)^\dagger \text{ commutes with } J_3 \\
&= (-1)^{\frac{m}{2}} \left( \frac{i}{\hbar} \right) R_{\hat{k}}(\theta)^\dagger (J_3 J_2 - J_2 J_3) R_{\hat{k}}(\theta) \\
&= (-1)^{\frac{m}{2}} \left( \frac{i}{\hbar} \right) R_{\hat{k}}(\theta)^\dagger (-i\hbar J_1) R_{\hat{k}}(\theta) \text{ since } [J_3, J_2] = -i\hbar J_1 \\
&= (-1)^{\frac{m}{2}} R_{\hat{k}}(\theta)^\dagger J_1 R_{\hat{k}}(\theta)
\end{aligned}$$

therefore  $P(m+1)$  is true (noting that  $m+1$  is odd). We also hence have, similarly,

$$\begin{aligned}
f^{(m+2)}(\theta) &= \frac{d}{d\theta} \left( (-1)^{\frac{m}{2}} R_{\hat{k}}(\theta)^\dagger J_1 R_{\hat{k}}(\theta) \right) \\
&= (-1)^{\frac{m}{2}} \left( \left( \frac{i}{\hbar} J_3 R_{\hat{k}}(\theta)^\dagger \right) J_1 R_{\hat{k}}(\theta) + R_{\hat{k}}(\theta)^\dagger J_1 \left( -\frac{i}{\hbar} J_3 R_{\hat{k}}(\theta) \right) \right) \\
&= (-1)^{\frac{m}{2}} \left( \frac{i}{\hbar} \right) R_{\hat{k}}(\theta)^\dagger (J_3 J_1 - J_1 J_3) R_{\hat{k}}(\theta) \text{ since } R_{\hat{k}}(\theta)^\dagger \text{ commutes with } J_3 \\
&= (-1)^{\frac{m+2}{2}} R_{\hat{k}}(\theta)^\dagger J_2 R_{\hat{k}}(\theta) \text{ since } [J_3, J_1] = i\hbar J_2
\end{aligned}$$

therefore  $P(m+2)$  is true (noting that  $m+2$  is even). Hence we have shown that for any non-negative even  $m$ , we have  $P(m) \implies P(m+1) \implies P(m+2)$ .

Thus by induction,  $P(n)$  is true for all  $n \in \mathbb{Z}_{\geq 0}$ . We note that this in turn gives us

$$\begin{aligned}
f^{(n)}(0) &= \begin{cases} (-1)^{\frac{n}{2}} R_{\hat{k}}(0)^\dagger J_2 R_{\hat{k}}(0) & \text{if } n \text{ is even} \\ (-1)^{\frac{n-1}{2}} R_{\hat{k}}(0)^\dagger J_1 R_{\hat{k}}(0) & \text{if } n \text{ is odd} \end{cases} \\
&= \begin{cases} (-1)^{\frac{n}{2}} J_2 & \text{if } n \text{ is even} \\ (-1)^{\frac{n-1}{2}} J_1 & \text{if } n \text{ is odd} \end{cases} \quad \text{since } R_{\hat{k}}(0)^\dagger = R_{\hat{k}}(0) = 1
\end{aligned}$$

Finally, we consider the power series expansion of  $f(\theta)$  (since the exponential function is analytic) to obtain

$$\begin{aligned}
f(\theta) &= \sum_{n=0}^{\infty} \left( \frac{\theta^n}{n!} f^{(n)}(0) \right) = \sum_{\text{even } n}^{\infty} \left( \frac{\theta^n}{n!} (-1)^{\frac{n}{2}} J_2 \right) + \sum_{\text{odd } n}^{\infty} \left( \frac{\theta^n}{n!} (-1)^{\frac{n-1}{2}} J_1 \right) \\
&= J_2 \sum_{\text{even } n}^{\infty} \left( \frac{\theta^n}{n!} (-1)^{\frac{n}{2}} \right) + J_1 \sum_{\text{odd } n}^{\infty} \left( \frac{\theta^n}{n!} (-1)^{\frac{n-1}{2}} \right) \\
&= J_2 \cos \theta + J_1 \sin \theta
\end{aligned}$$

Therefore we have shown that  $R_{\hat{k}}(\theta)^\dagger J_2 R_{\hat{k}}(\theta) = J_2 \cos \theta + J_1 \sin \theta$ . Substituting  $\theta \rightarrow -\theta$  gives us  $R_{\hat{k}}(\theta) J_2 R_{\hat{k}}(\theta)^\dagger = J_2 \cos \theta - J_1 \sin \theta$ , as expected.

(Remark: If known, the identity  $e^A B e^{-A} = B + [A, B] + \frac{1}{2!} [A, [A, B]] + \frac{1}{3!} [A, [A, [A, B]]] \dots$  (see the Baker-Campbell-Hausdorff formula, which is related) can be used instead to derive this desired result. The identity itself may be demonstrated by various methods such as differentiating with respect to a parameter, or expanding  $e^A$  and  $e^{-A}$  as power series and multiplying terms appropriately, or by an argument similar to the above procedure.)

Using the power series expansion of the exponential function, and recalling that  $R_{\hat{k}}(\theta)$  is unitary (i.e.  $R_{\hat{k}}(\theta)^\dagger R_{\hat{k}}(\theta) = R_{\hat{k}}(\theta) R_{\hat{k}}(\theta)^\dagger = 1$ ), we have

$$\begin{aligned}
R_{\hat{k}}(\pi) e^{-\frac{i}{\hbar} \alpha J_2} R_{\hat{k}}(\pi)^\dagger &= R_{\hat{k}}(\pi) \left( \sum_{n=0}^{\infty} \frac{1}{n!} \left( -\frac{i}{\hbar} \alpha J_2 \right)^n \right) R_{\hat{k}}(\pi)^\dagger \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} \left( -R_{\hat{k}}(\pi) \frac{i}{\hbar} \alpha J_2 R_{\hat{k}}(\pi)^\dagger \right)^n \quad \text{since } R_{\hat{k}}(\pi)^\dagger R_{\hat{k}}(\pi) = 1 \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} \left( -\frac{i}{\hbar} \alpha (J_2 \cos \pi - J_1 \sin \pi) \right)^n \quad \text{by the previous result} \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{i}{\hbar} \alpha J_2 \right)^n \\
&= e^{\frac{i}{\hbar} \alpha J_2}, \text{ as desired.}
\end{aligned}$$

(This method generalises to other functions with power series expansions as well.)

## Question 4

**4a.** This derivation is essentially identical to that presented in lecture (AY2012/13 sem 2 notes, Chapter 4), so some steps have been skimmed over for brevity. Refer to notes for full details. To avoid confusion with the particle subscripts, this answer uses subscripts  $x, y, z$  instead of 1, 2, 3 to denote the Cartesian components of the angular momenta.

We show that the components of  $\vec{J}$  satisfy the angular momentum commutation relations  $[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k$ , hence the eigenvalues of  $J^2$  and  $J_z$  can be written as  $j(j+1)\hbar^2$  and  $m\hbar$  respectively, where  $j$  is a non-negative integer or half-integer and  $m$  increases in integer steps from  $-j$  to  $j$  (inclusive).

$J_1^2, J_2^2, J_{1z}$  and  $J_{2z}$  commute and thus can have common eigenstates  $|\alpha, j_1, j_2, m_1, m_2\rangle$ . We show that  $J_z|\alpha, j_1, j_2, m_1, m_2\rangle = (m_1 + m_2)\hbar|\alpha, j_1, j_2, m_1, m_2\rangle$  (where  $J_z = J_{1z} + J_{2z}$ ) and thus  $|\alpha, j_1, j_2, m_1, m_2\rangle$  are also eigenstates of  $J_z$ , with eigenvalue  $(m_1 + m_2)\hbar$ . Therefore, we have  $m = m_1 + m_2$ .

We now use a counting method to find the allowed values of  $j$  in terms of  $j_1$  and  $j_2$ . Let  $c_m$  be the number of states  $|j, m\rangle$  for a fixed  $m$ , and  $d_j$  be the number of states  $|j, m\rangle$  for a fixed  $m$  and  $j$ . We note that  $d_j = 1$  if and only if that particular combination of  $j, m$  is allowed, and  $d_j = 0$  otherwise. Since  $|m| \leq j$  and taking  $m \geq 0$ , we have

$$c_m = d_m + d_{m+1} + d_{m+2} + \dots$$

$$c_{m+1} = d_{m+1} + d_{m+2} + \dots$$

and thus  $d_m = c_m - c_{m+1}$ . Tabulating values of  $c_m$ , we have

$m_1$	$m_2$	$m = m_1 + m_2$	$c_m$
$j_1$	$j_2$	$j_1 + j_2$	1
$j_1$ $j_1 - 1$	$j_2 - 1$ $j_2$	$j_1 + j_2 - 1$	2
$j_1$ $\vdots$ $j_1 - n$	$j_2 - n$ $\vdots$ $j_2$	$j_1 + j_2 - n$	$n + 1$

From the table, we have  $c_{j_1+j_2} = 1$ ,  $c_{j_1+j_2-1} = 2$  and so on, increasing by one each time, up until a certain point (to be discussed below). Therefore we have  $d_{j_1+j_2} = 1 - 0 = 1$ ,  $d_{j_1+j_2-1} = 2 - 1 = 1$ , and so on, up until that point, i.e. those values of  $j$  are allowed.

$c_m$  stops increasing when the possible values of  $m_1$  in the first column and/or  $m_2$  in the second column cover all values they can take (i.e. all values in integer steps from  $-j_1$  to  $j_1$  or  $-j_2$  to  $j_2$  respectively), whichever occurs first. It can be seen that this occurs after  $2j_1$  and/or  $2j_2$  steps, whichever is smaller. The value of  $j$  at which this occurs is  $(j_1 + j_2) - \min(2j_1, 2j_2) = |j_1 - j_2|$ , thus we have  $d_j = 0$  from this point onwards. (Alternative: Draw a diagram as in the example in the lecture notes.)

Therefore, the allowed values of  $j$  are  $j_1 + j_2, j_1 + j_2 - 1, \dots, |j_1 - j_2|$ .

**4b.** We recall that  $\langle j_1, j_2, m_1, m_2 | j_1, j_2, j, m \rangle = 0$  whenever  $m \neq m_1 + m_2$ . For the  $|1, \frac{1}{2}, \frac{3}{2}, \frac{3}{2}\rangle$  state, we have  $j_1 = 1$ ,  $j_2 = \frac{1}{2}$  and  $m = \frac{3}{2}$ . Therefore, the only values of  $m_1$  and  $m_2$  which can satisfy  $m_1 + m_2 = m = \frac{3}{2}$  are  $m_1 = 1$  and  $m_2 = \frac{1}{2}$ , since  $-j_1 \leq m_1 \leq j_1$  and  $-j_2 \leq m_2 \leq j_2$ . Hence, the coupled state in terms of the uncoupled states must simply be  $|1, \frac{1}{2}, \frac{3}{2}, \frac{3}{2}\rangle = |1, 1\rangle |\frac{1}{2}, \frac{1}{2}\rangle$ , since all the other coefficients are zero. (If desired, one can explicitly verify using the formula provided that  $\langle 1, \frac{1}{2}, 1, \frac{1}{2} | 1, \frac{1}{2}, \frac{3}{2}, \frac{3}{2} \rangle = \langle 1, \frac{1}{2}, \frac{3}{2} - \frac{1}{2}, \frac{1}{2} | 1, \frac{1}{2}, 1 + \frac{1}{2}, \frac{3}{2} \rangle = \sqrt{\frac{1 + \frac{3}{2} + \frac{1}{2}}{2(1) + 1}} = 1$ , as expected.)

For the  $|1, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\rangle$  state, we again have  $j_1 = 1$ ,  $j_2 = \frac{1}{2}$ , but this time  $m = -\frac{1}{2}$  can be formed in two ways from sums of the possible values of  $m_1$  and  $m_2$ , namely  $m_1 = -1, m_2 = \frac{1}{2}$  and  $m_1 = 0, m_2 = -\frac{1}{2}$ . We evaluate the corresponding Clebsch-Gordan coefficients with the provided formulae:

$$\langle 1, \frac{1}{2}, -1, \frac{1}{2} | 1, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \rangle = \langle 1, \frac{1}{2}, -\frac{1}{2} - \frac{1}{2}, \frac{1}{2} | 1, \frac{1}{2}, 1 - \frac{1}{2}, \frac{3}{2} \rangle = -\sqrt{\frac{1 - (-\frac{1}{2}) + \frac{1}{2}}{2(1) + 1}} = -\sqrt{\frac{2}{3}}$$

$$\langle 1, \frac{1}{2}, 0, -\frac{1}{2} | 1, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \rangle = \langle 1, \frac{1}{2}, -\frac{1}{2} + \frac{1}{2}, \frac{1}{2} | 1, \frac{1}{2}, 1 - \frac{1}{2}, \frac{3}{2} \rangle = \sqrt{\frac{1 + (-\frac{1}{2}) + \frac{1}{2}}{2(1) + 1}} = \sqrt{\frac{1}{3}}$$

The mod-squared sum of these coefficients is 1, as expected. (Again,  $\langle j_1, j_2, m_1, m_2 | j_1, j_2, j, m \rangle = 0$  for the other values of  $m_1, m_2$  since  $m \neq m_1 + m_2$  for those values.) Therefore, the coupled state in terms of the uncoupled states is  $|1, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\rangle = \sqrt{\frac{1}{3}} |1, 0\rangle |\frac{1}{2}, -\frac{1}{2}\rangle - \sqrt{\frac{2}{3}} |1, -1\rangle |\frac{1}{2}, \frac{1}{2}\rangle$ .

As seen from the above result, the coefficient for the component with the spin- $\frac{1}{2}$  particle (i.e. the electron) in spin-down is  $\sqrt{\frac{1}{3}}$ . Therefore, the probability of measuring the electron spin to be down is  $\frac{1}{3}$ .

(Remark: One can verify against a table of Clebsch-Gordan coefficients that these are indeed the correct values for the coefficients.)

**4c.** For ease of notation, we shall denote the  $n^{\text{th}}$ -energy-level one-particle wavefunctions by  $\psi_n(x_i) = \sqrt{\frac{2}{b}} \sin\left(\frac{n\pi x_i}{b}\right)$ .

Since the particles have half-integer spin, they are fermions. Therefore, the state must be antisymmetric under particle interchange, and the particles must all be in different states. As the particles are assumed to all be in the same spin state, the spatial wavefunction must be antisymmetric and the one-particle wavefunctions must all be different.

Therefore, the wavefunction of the ground state  $\phi_0$  is

$$\phi_0(x_1, x_2, x_3) = \frac{1}{\sqrt{6}}(\psi_1(x_1)\psi_2(x_2)\psi_3(x_3) + \psi_2(x_1)\psi_3(x_2)\psi_1(x_3) + \psi_3(x_1)\psi_1(x_2)\psi_2(x_3) \\ - \psi_1(x_1)\psi_3(x_2)\psi_2(x_3) - \psi_3(x_1)\psi_2(x_2)\psi_1(x_3) - \psi_2(x_1)\psi_1(x_2)\psi_3(x_3))$$

$$\text{with energy } (1^2 + 2^2 + 3^2)\frac{\hbar^2\pi^2}{2mb^2} = 14\frac{\hbar^2\pi^2}{2mb^2}.$$

The wavefunction of the first excited state  $\phi_1$  is

$$\phi_1(x_1, x_2, x_3) = \frac{1}{\sqrt{6}}(\psi_1(x_1)\psi_2(x_2)\psi_4(x_3) + \psi_2(x_1)\psi_4(x_2)\psi_1(x_3) + \psi_4(x_1)\psi_1(x_2)\psi_2(x_3) \\ - \psi_1(x_1)\psi_4(x_2)\psi_2(x_3) - \psi_4(x_1)\psi_2(x_2)\psi_1(x_3) - \psi_2(x_1)\psi_1(x_2)\psi_4(x_3))$$

$$\text{with energy } (1^2 + 2^2 + 4^2)\frac{\hbar^2\pi^2}{2mb^2} = 21\frac{\hbar^2\pi^2}{2mb^2}.$$

Solutions provided by: Ernest Tan