Part II: Michaelmas 2020

Advanced Quantum Mechanics Question Sheet IV

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Question 1. Time evolution of spin

A spin 1/2 particle has gyromagnetic ratio γ , so that its magnetic moment is given by $\hat{\Gamma} = \gamma \hat{S}$ where \hat{S} is the spin operator.

Using Schrödinger's equation, show that the equation of motion for the spin state $|\psi(t)\rangle$ of such a particle in a magnetic field \boldsymbol{B} is

$$-\frac{1}{2}\gamma \left(\boldsymbol{B}\cdot\hat{\boldsymbol{\sigma}}\right)|\psi(t)\rangle = i\frac{\partial}{\partial t}|\psi(t)\rangle,$$

where $\hat{\boldsymbol{\sigma}}$ is a vector with the Pauli matrices $\hat{\sigma}_i$ as components.

 \boldsymbol{B} is a constant field in the z-direction with magnitude B_0 , and we choose

$$|\psi(0)\rangle = \cos(\theta/2)|\uparrow\rangle + \sin(\theta/2)|\downarrow\rangle$$
.

By representing the spin states as column vectors, show that at time t,

$$|\psi(t)\rangle = \cos(\theta/2) \exp(i\omega_0 t/2)|\uparrow\rangle + \sin(\theta/2) \exp(-i\omega_0 t/2)|\downarrow\rangle$$

where $\omega_0 = \gamma B_0$, and find the expectation values of the components of the magnetic moment $\hat{\boldsymbol{\mu}}$ at time t.

Using the general result

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

for the time evolution of the expectation value of an operator \hat{A} , show that for an arbitrarily varying magnetic field $\boldsymbol{B}(t)$ the magnetic moment operator satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\boldsymbol{\mu}}\rangle = \gamma\langle\hat{\boldsymbol{\mu}}\times\boldsymbol{B}(t)\rangle\,,$$

and demonstrate explicitly that the expectation values found above for the constant field satisfy this relation. Interpret your results physically.

Answer b: Time evolution of spin

The Hamiltonian for the interaction between a magnetic moment $\hat{\mu}$ and a magnetic field B is

$$\hat{H} = -\hat{\boldsymbol{\mu}} \cdot \boldsymbol{B} = -\gamma \hat{\boldsymbol{S}} \cdot \boldsymbol{B} = -\gamma \frac{\hbar}{2} \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{B}$$

Substituting into the time-dependent Schrödinger equation we have

$$-\frac{1}{2}\gamma \left(\boldsymbol{B}\cdot\hat{\boldsymbol{\sigma}}\right)|\psi(t)\rangle = i\frac{\partial}{\partial t}|\psi(t)\rangle,$$

For $\mathbf{B} = (0, 0, B_0)$, we have

$$-\frac{1}{2}\gamma B_0 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = i \frac{\partial}{\partial t} \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$$

with solutions

$$a(t) = A \exp(i\omega_0 t/2)$$
, $b(t) = B \exp(-i\omega_0 t/2)$.

Normalise by setting $A = \cos(\theta/2)$, $B = \sin(\theta/2)$, giving

$$|\psi(t)\rangle = \cos(\theta/2) \exp(i\omega_0 t/2) |\uparrow\rangle + \sin(\theta/2) \exp(-i\omega_0 t/2) |\downarrow\rangle$$
.

The expectation value of μ_x is

$$\langle \mu_x \rangle = \gamma \frac{\hbar}{2} \begin{pmatrix} a^* & b^* \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \gamma \frac{\hbar}{2} (a^*b + b^*a)$$
$$= \gamma \frac{\hbar}{2} \cos(\theta/2) \sin(\theta/2) \left[\exp(-i\omega_0 t) + \exp(i\omega_0 t) \right] = \gamma \frac{\hbar}{2} \sin\theta \cos(\omega_0 t) .$$

Similarly,

$$\langle \mu_y \rangle = -\gamma \frac{\hbar}{2} \sin \theta \sin(\omega_0 t); \qquad \langle \mu_z \rangle = \gamma \frac{\hbar}{2} \cos \theta.$$

These equations represent precession of the magnetic moment vector about the z axis with angular frequency ω_0 , with the magnetic moment vector at an angle θ to the z axis. For a general field $\mathbf{B}(t)$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\boldsymbol{\mu}}\rangle = \frac{i}{\hbar}\langle[-\gamma\hat{\boldsymbol{S}}\cdot\boldsymbol{B},\hat{\boldsymbol{\mu}}]\rangle = \frac{i\gamma^2}{\hbar}\langle\hat{\boldsymbol{S}}(\hat{\boldsymbol{S}}\cdot\boldsymbol{B}) - (\hat{\boldsymbol{S}}\cdot\boldsymbol{B})\hat{\boldsymbol{S}}\rangle.$$

In particular, for the x component,

$$\hat{S}_{x}(\hat{\boldsymbol{S}} \cdot \boldsymbol{B}) - (\hat{\boldsymbol{S}} \cdot \boldsymbol{B})\hat{S}_{x} = (\hat{S}_{x}\hat{S}_{y} - \hat{S}_{y}\hat{S}_{x})B_{y} + (\hat{S}_{x}\hat{S}_{z} - \hat{S}_{z}\hat{S}_{x})B_{z}$$

$$= (i\hbar\hat{S}_{z})B_{y} + (-i\hbar\hat{S}_{y})B_{z} = -i\hbar(\hat{\boldsymbol{S}} \wedge \boldsymbol{B})_{x},$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mu_{x}\rangle = \frac{i\gamma^{2}}{\hbar} \times -i\hbar\langle(\hat{\boldsymbol{S}} \wedge \boldsymbol{B})_{x}\rangle = \gamma^{2}\langle(\hat{\boldsymbol{S}} \wedge \boldsymbol{B})_{x}\rangle.$$

The same result must apply also to the y and z components, giving

$$\left| \frac{\mathrm{d}}{\mathrm{d}t} \langle \hat{\boldsymbol{\mu}} \rangle = \gamma \langle \hat{\boldsymbol{\mu}} \wedge \boldsymbol{B}(t) \rangle \right|.$$

The cross product of magnetic moment and magnetic field produces a torque which causes the magnetic moment to precess around the magnetic field.

Question c: Photon momentum

The total linear momentum operator $\hat{\boldsymbol{P}}$ for an electromagnetic field is

$$\hat{m{P}} = \sum_{m{k},\lambda} \hbar m{k} \, \hat{a}^{\dagger}_{m{k},\lambda} \hat{a}_{m{k},\lambda} \; .$$

Describe each of the terms in this expression. On what vector space does it act?

By generating a single photon state from the vacuum, show that a photon of wave vector \mathbf{k} (in any polarisation state λ) has linear momentum $\hbar \mathbf{k}$.

Similarly, the intrinsic (spin) angular momentum operator $\hat{\boldsymbol{J}}_{\mathrm{s}}$ is given by

$$\hat{m{J}}_{\mathrm{s}} = \hbar \sum_{m{k}} rac{m{k}}{|m{k}|} \left[\hat{a}^{\dagger}_{m{k},L} \hat{a}_{m{k},L} - \hat{a}^{\dagger}_{m{k},R} \hat{a}_{m{k},R}
ight] \; .$$

Again by generating a single photon state from the vacuum, show that for left-handed (right-handed) photons, the spin is oriented parallel to the photon direction of motion, with spin projection $+\hbar$ $(-\hbar)$.

Answer c: Photon momentum

The linear momentum operator for the EM field is

$$\hat{\boldsymbol{P}} = \sum_{\boldsymbol{k},\lambda} \hbar \boldsymbol{k} \, \hat{a}^{\dagger}_{\boldsymbol{k},\lambda} \hat{a}_{\boldsymbol{k},\lambda} \; .$$

Applying the total momentum operator \hat{P} to a single photon state $|\mathbf{k}, \lambda\rangle = \hat{a}_{\mathbf{k}, \lambda}^{\dagger} |0\rangle$ gives

$$\hat{\boldsymbol{P}}|\boldsymbol{k},\lambda\rangle = \hat{\boldsymbol{P}}\,\hat{a}_{\boldsymbol{k},\lambda}^{\dagger}|0\rangle = \left(\sum_{\boldsymbol{k}',\lambda'}\hbar\boldsymbol{k}'\,\hat{a}_{\boldsymbol{k}',\lambda'}^{\dagger}\hat{a}_{\boldsymbol{k}',\lambda'}\right)\hat{a}_{\boldsymbol{k},\lambda}^{\dagger}|0\rangle \ .$$

The commutation relation $[\hat{a}_{\boldsymbol{k},\lambda},\hat{a}^{\dagger}_{\boldsymbol{k}',\lambda'}] = \delta_{\boldsymbol{k}',\boldsymbol{k}} \delta_{\lambda'\lambda}$ allows the rightmost pair of operators to be reordered as

$$\hat{a}_{\mathbf{k}',\lambda'}\hat{a}_{\mathbf{k},\lambda}^{\dagger} = \delta_{\mathbf{k}'\mathbf{k}}\delta_{\lambda'\lambda} + \hat{a}_{\mathbf{k},\lambda}^{\dagger}\hat{a}_{\mathbf{k}',\lambda'}.$$

Since $\hat{a}_{\mathbf{k}',\lambda'}|0\rangle = 0$, we then obtain

$$\hat{a}_{\mathbf{k}',\lambda'}\hat{a}_{\mathbf{k},\lambda}^{\dagger}|0\rangle = \delta_{\mathbf{k}'\mathbf{k}}\delta_{\lambda'\lambda}|0\rangle$$
.

Hence

$$\hat{\boldsymbol{P}}|\boldsymbol{k},\lambda\rangle = \sum_{\boldsymbol{k}',\lambda'} \hbar \boldsymbol{k}' \, \hat{a}^{\dagger}_{\boldsymbol{k}',\lambda'} \delta_{\boldsymbol{k}'\boldsymbol{k}} \delta_{\lambda'\lambda} |0\rangle = \hbar \boldsymbol{k} \, \hat{a}^{\dagger}_{\boldsymbol{k},\lambda} |0\rangle \; .$$

Thus photons have linear momentum $\hbar \mathbf{k}$:

$$\hat{m{P}}|m{k},\lambda
angle = \hbarm{k}|m{k},\lambda
angle$$
 .

The intrinsic angular momentum operator is

$$\hat{\boldsymbol{J}}_{\mathrm{S}} = \hbar \sum_{\boldsymbol{k}} \frac{\boldsymbol{k}}{|\boldsymbol{k}|} \left[\hat{a}_{\boldsymbol{k},L}^{\dagger} \hat{a}_{\boldsymbol{k},L} - \hat{a}_{\boldsymbol{k},R}^{\dagger} \hat{a}_{\boldsymbol{k},R} \right] .$$

Operating with \hat{J}_{S} on a right-handed single photon state $|k,R\rangle = \hat{a}_{k,R}^{\dagger}|0\rangle$ gives

$$\hat{\boldsymbol{J}}_{\mathrm{S}}|\boldsymbol{k},R\rangle = \hat{\boldsymbol{J}}_{\mathrm{S}}\hat{a}_{\boldsymbol{k},R}^{\dagger}|0\rangle = \hbar \sum_{\boldsymbol{k}'} \frac{\boldsymbol{k}'}{|\boldsymbol{k}'|} \left[\hat{a}_{\boldsymbol{k}',L}^{\dagger}\hat{a}_{\boldsymbol{k}',L} - \hat{a}_{\boldsymbol{k}',R}^{\dagger}\hat{a}_{\boldsymbol{k}',R}\right]\hat{a}_{\boldsymbol{k},R}^{\dagger}|0\rangle \ .$$

The operators $\hat{a}_{k',L}$ and $\hat{a}_{k,R}^{\dagger}$ commute, and $\hat{a}_{k',L}|0\rangle = 0$. Hence the first term on the right-hand side vanishes, leaving just the second term:

$$\hat{\boldsymbol{J}}_{\mathrm{S}}|\boldsymbol{k},R\rangle = -\hbar\sum_{\boldsymbol{k}'} rac{\boldsymbol{k}'}{|\boldsymbol{k}'|} \hat{a}^{\dagger}_{\boldsymbol{k}',R} \hat{a}_{\boldsymbol{k}',R} \hat{a}^{\dagger}_{\boldsymbol{k},R} |0\rangle \ .$$

Inverting the order of the rightmost two operators,

$$\hat{a}_{\mathbf{k}',R}\hat{a}_{\mathbf{k},R}^{\dagger} = \delta_{\mathbf{k}'\mathbf{k}}\delta_{\lambda'\lambda} + \hat{a}_{\mathbf{k},R}^{\dagger}\hat{a}_{\mathbf{k}',R} ,$$

and using $\hat{a}_{\mathbf{k}',R}|0\rangle = 0$ then gives

$$\boxed{ \hat{\boldsymbol{J}}_{\mathrm{S}} |\boldsymbol{k},R\rangle = -\hbar \frac{\boldsymbol{k}}{|\boldsymbol{k}|} \hat{a}_{\boldsymbol{k},R}^{\dagger} |0\rangle } \ .$$

Hence right-handed photons possess an intrinsic angular momentum oriented opposite to the photon direction of motion, with spin projection $-\hbar$ along the photon direction.

Question d: Coherent states

Show that

$$\frac{\partial}{\partial \beta} \left(e^{-\beta \hat{a}^{\dagger}} \hat{a} e^{\beta \hat{a}^{\dagger}} \right) = 1$$

By subsequently integrating the result, show that

$$e^{-\beta \hat{a}^{\dagger}} \hat{a} e^{\beta \hat{a}^{\dagger}} = \beta + \hat{a}$$
.

Using this expression, show that $|\beta\rangle = Ne^{\beta\hat{a}^{\dagger}}|0\rangle$ is a coherent state, i.e. $\hat{a}|\beta\rangle = \beta|\beta\rangle$, where N is a normalisation factor. Show that N is given by $N = e^{-|\beta|^2/2}$.

Calculate the expectation values, $x_0 = \langle \hat{x} \rangle$ and $p_0 = \langle \hat{p} \rangle$, with respect to $|\beta\rangle$ and, by considering $\langle \hat{x}^2 \rangle$ and $\langle \hat{p}^2 \rangle$, show that

$$(\Delta p)^2 (\Delta x)^2 = \frac{\hbar^2}{4} \,,$$

where $(\Delta p)^2 = \langle (\hat{p} - \langle \hat{p} \rangle)^2 \rangle$ (and similarly $(\Delta x)^2$).

Hint: Remember how the creation and annihilation operators are related to the phase space operators \hat{x} and \hat{p} . Also, note that taking the Hermitian conjugate of the eigenvalue equation $\hat{a}|\beta\rangle = \beta|\beta\rangle$ leads to the relation $\langle\beta|\hat{a}^{\dagger} = \langle\beta|\beta^*$.

Show that the eigenvalue equation $\hat{a}|\beta\rangle = \beta|\beta\rangle$ translates to the equation

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

for the coordinate representation, $\psi(x)$, of the coherent state. Show that this equation has the solution

$$\psi(x) = N \exp\left[-\frac{(x-x_0)^2}{4(\Delta x)^2} + i\frac{p_0 x}{\hbar}\right],$$

where x_0 and p_0 are defined in part (b) above.

By expressing $|\beta\rangle$ in the number basis, show that

$$|\beta(t)\rangle = e^{-i\omega t/2}|\beta e^{-i\omega t}\rangle$$
.

As a result, deduce expressions for $x_0(t)$ and $p_0(t)$ and show they represent solutions to the classical equations of motion. How does the width of the coherent state wavepacket evolve with time?

Answer d: Coherent states

(a) Differentiating the left hand side of the given expression with respect to β , one obtains

$$e^{-\beta \hat{a}^{\dagger}}\underbrace{\left[\hat{a},\hat{a}^{\dagger}\right]}_{=1}e^{\beta \hat{a}^{\dagger}}=1$$
.

Integrating, we therefore have that $e^{-\beta \hat{a}^{\dagger}} \hat{a} e^{\beta \hat{a}^{\dagger}} = \beta$ + "integration constant". By setting $\beta = 0$ we can deduce that the "constant" must be the operator \hat{a} , yielding the required result. Using this result, we have that

$$e^{-\beta \hat{a}^\dagger} \hat{a} |\beta\rangle = e^{-\beta \hat{a}^\dagger} \hat{a} N e^{\beta \hat{a}^\dagger} |0\rangle = N(\beta + \hat{a}) |0\rangle = N\beta |0\rangle \,.$$

Multiplying through by $e^{+\beta \hat{a}^{\dagger}}$ then shows that $\hat{a}|\beta\rangle = \beta|\beta\rangle$, and thus that $|\beta\rangle$ is a coherent state.

To normalise to uinty, set

$$1 = \langle \beta | \beta \rangle = N \langle 0 | e^{\beta^* \hat{a}} | \beta \rangle = N \langle 0 | \sum_{n=0}^{\infty} \frac{(\beta^* \hat{a})^n}{n!} | \beta \rangle = N \sum_{n=0}^{\infty} \frac{(\beta^* \beta)^n}{n!} \langle 0 | \beta \rangle = N^2 e^{|\beta|^2}$$

where, in the last step, we have used $\langle 0|\beta\rangle=N\langle 0|e^{\beta\hat{a}^{\dagger}}|0\rangle=N.$ Thus $N=e^{-|\beta|^2/2},$ as required.

(b) For the harmonic oscillator, the creation and annihilation operators are related to the phase space operators by $\hat{x} = \sqrt{(\hbar/2m\omega)}(\hat{a} + \hat{a}^{\dagger})$, and $\hat{p} = -i\sqrt{(\hbar m\omega/2)}(\hat{a} - \hat{a}^{\dagger})$. Therefore, we have

$$\langle \hat{x} \rangle = \sqrt{\frac{\hbar}{2m\omega}} (\beta + \beta^*), \qquad \langle \hat{p} \rangle = -i\sqrt{\frac{\hbar m\omega}{2}} (\beta - \beta^*).$$

Then, using the identity $(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$, we have

$$\langle \hat{x}^2 \rangle = \frac{\hbar}{2m\omega} \langle \beta | (\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger \hat{a} + (\hat{a}^\dagger)^2) | \beta \rangle = \frac{\hbar}{2m\omega} (1 + (\beta + \beta^*)^2),$$

$$\langle \hat{p}^2 \rangle = -\frac{\hbar m\omega}{2} \langle \beta | (\hat{a}^2 - \hat{a}\hat{a}^\dagger - \hat{a}^\dagger \hat{a} + (\hat{a}^\dagger)^2) | \beta \rangle = \frac{\hbar m\omega}{2} (1 - (\beta - \beta^*)^2).$$

As a result, we find that $(\Delta x)^2 = \hbar/(2m\omega)$ and $(\Delta p)^2 = \hbar m\omega/2$, leading to the required expression.

- (c) The equation follows simply from the definion of the operator \hat{a} and the solution may be checked by substitution.
- (d) Using the time evolution of the stationary states, $|n(t)\rangle = e^{-iE_nt/\hbar}|n(0)\rangle$, where $E_n = \hbar\omega(n+1/2)$, it follows that

$$|\beta(t)\rangle = e^{-i\omega t/2}e^{-|\beta|^2/2}\sum_{n=0}^{\infty}\frac{\beta^n}{\sqrt{n!}}e^{-in\omega t}|n\rangle = e^{-i\omega t/2}|e^{-i\omega t}\beta\rangle.$$

Therefore, during the time evolution, the coherent state form is preserved, and the centre of mass and momentum follow that of the classical oscillator,

$$x_0(t) = A\cos(\varphi + \omega t), \qquad p_0(t) = -m\omega A\sin(\varphi + \omega t).$$

The width of the wavepacket remains constant.

Question 4. Addition of angular momenta

Consider the addition of two angular momenta, $\ell_1=2$ and $\ell_2=1$. By drawing a diagram similar to that of Figure 9 of Handout VI, tabulate the possible values of the

corresponding quantum numbers m_1 , m_2 and $M = m_1 + m_2$ (relating to \hat{L}_z), and show that the values of M correspond to the expected values L = 3, 2, 1 of the total angular momentum quantum number L.

Repeat for the case $\ell_1 = 3$, $\ell_2 = 1$.

(†) For the case $\ell_1 = 2$ and $\ell_2 = 1$, the state $|L, M\rangle = |3, 3\rangle$ can be written down straightforwardly as $|\ell_1, m_1\rangle \otimes |\ell_2, m_2\rangle = |2, 2\rangle \otimes |1, 1\rangle$. Use ladder operators to construct the state $|L, M\rangle = |3, 2\rangle$ as a linear combination of the product states $|\ell_1, m_1\rangle \otimes |\ell_2, m_2\rangle$, and then orthogonality to construct the state $|L, M\rangle = |2, 2\rangle$.

[The angular momentum ladder operators
$$\hat{L}_{\pm}$$
 act as
$$\hat{L}_{\pm}|L,m_L\rangle = \hbar\sqrt{L(L+1)-m_L(m_L\pm1)}|L,m_L\pm1\rangle \ .$$
]

Verify that the states obtained in (b) are the same as would be written down using the tables of Clebsch-Gordan coefficients appended to this examples sheet (see the table labelled $2 \otimes 1$).

Using the $2 \otimes 1$ table, write down the state $|L, M\rangle = |1, -1\rangle$ as a linear combination of the $|\ell_1, m_1\rangle \otimes |\ell_2, m_2\rangle$ states.

Show that the scalar product $\hat{\boldsymbol{L}}_1 \cdot \hat{\boldsymbol{L}}_2$ of two angular momentum operators can be expressed as

$$\hat{\boldsymbol{L}}_1 \cdot \hat{\boldsymbol{L}}_2 = \frac{1}{2} (\hat{L}_1)_+ (\hat{L}_2)_- + \frac{1}{2} (\hat{L}_1)_- (\hat{L}_2)_+ + (\hat{L}_1)_z (\hat{L}_2)_z ,$$

where $(\hat{L}_{1,2})_{\pm} = (\hat{L}_{1,2})_x \pm i(\hat{L}_{1,2})_y$ are ladder operators. By operating directly with $(\hat{L}_1 + \hat{L}_2)^2$ and $(\hat{L}_1)_z + (\hat{L}_2)_z$, verify that the linear combination of product states written down in (\dagger) does indeed have total angular momentum quantum numbers L = 1 and M = -1.

Convince yourself that each table of Clebsch-Gordan coefficients corresponds to a unitary (in fact, orthogonal) matrix. For the cases $j_1 \otimes j_2 = (1/2) \otimes (1/2)$, $1 \otimes 1$, $(3/2) \otimes (3/2)$ and $2 \otimes 2$ (for which $j_1 = j_2$), what is the symmetry of the total angular momentum eigenstates $|j, m_j\rangle$ for each possible value of j under interchange of the labels 1 and 2?

Answer h: Addition of angular momenta

(a) For the case $\ell_1 = 2$, $\ell_2 = 1$, the possible ways of forming each value of $M = m_1 + m_2$ can be tabulated as

The largest value of M is M=3, so the largest value of L must be L=3. There must also be a state with M=2 corresponding to L=3, but the table contains two states with M=2. Therefore there must be a state with L=2 as well. We need two states with M=1, one for each of the L=3,2 multiplets, but the table lists three states with M=1, so there must be an L=1 state as well. With L=3,2,1, all of the M states are now accounted for.

For the case $\ell_1 = 3$, $\ell_2 = 1$, we can again form a table:

Following the same logic as before, we see that sets of states with L = 4, 3, 2 just account for all the entries in the table.

(b) To construct the states explicitly, we start with the $|L, M\rangle = |3, 3\rangle$ state, which can be formed in only one way, viz. $|3, 3\rangle = |2, 2\rangle \otimes |1, 1\rangle$. Operating with the lowering operator $\hat{L}_{-} = (\hat{L}_{1})_{-} + (\hat{L}_{2})_{-}$, and recalling that

$$\hat{L}_{-}|\ell,m\rangle = \sqrt{\ell(\ell+1) - m(m-1)}\hbar|\ell,m-1\rangle,$$

we then obtain

$$\sqrt{6}\hbar|3,2\rangle = \sqrt{2}\hbar|2,2\rangle \otimes |1,0\rangle + \sqrt{4}\hbar|2,1\rangle \otimes |1,1\rangle \ ,$$

where the first term on the right hand side comes from lowering the $\ell_2 = 1$ state with $(\hat{L}_2)_-$ and the second from lowering the $\ell_1 = 2$ state with $(\hat{L}_1)_-$. Hence

$$\boxed{|3,2\rangle = \sqrt{1/3}|2,2\rangle \otimes |1,0\rangle + \sqrt{2/3}|2,1\rangle \otimes |1,1\rangle}.$$
 (1)

The state $|2,2\rangle$ must be the orthogonal linear combination,

$$\boxed{|2,2\rangle = \sqrt{2/3}|2,2\rangle \otimes |1,0\rangle - \sqrt{1/3}|2,1\rangle \otimes |1,1\rangle}.$$
 (2)

Further states could be computed in the same way if required.

(c) The column headed J=3, M=+2 in the 2×1 table of Clebsch-Gordan coefficients contains two entries, 1/3 and 2/3, corresponding to $\langle \ell_1 m_1; \ell_2 m_2 | JM \rangle = \langle 22; 10 | 32 \rangle = \sqrt{1/3}$ and $\langle 21; 11 | 32 \rangle = \sqrt{2/3}$, respectively. This is in agreement with equation (1) above.

The neighbouring column, headed J=2, M=+2, contains entries 2/3 and -1/3, corresponding to the Clebsch-Gordan coefficients $\langle 22; 10|22 \rangle = \sqrt{2/3}$ and $\langle 21; 11|22 \rangle = -\sqrt{1/3}$, respectively. This is in agreement with equation (2) above.

(d) The column headed J=1, M=-1 in the 2×1 table gives the state $|J,M\rangle=|1,-1\rangle$ as

$$|1, -1\rangle = \sqrt{\frac{1}{10}}|20\rangle|1, -1\rangle - \sqrt{\frac{3}{10}}|2, -1\rangle|10\rangle + \sqrt{\frac{3}{5}}|2, -2\rangle|11\rangle.$$
 (3)

(e) Expressing the operators \hat{L}_x and \hat{L}_y in terms of ladder operators as $\hat{L}_x = (1/2)(\hat{L}_+ + \hat{L}_-)$ and $\hat{L}_y = (1/2i)(\hat{L}_+ - \hat{L}_-)$, the scalar product $\hat{L}_1 \cdot \hat{L}_2$ can be written as

$$\hat{\boldsymbol{L}}_{1} \cdot \hat{\boldsymbol{L}}_{2} = (\hat{L}_{1})_{x}(\hat{L}_{2})_{x} + (\hat{L}_{1})_{y}(\hat{L}_{2})_{y} + (\hat{L}_{1})_{z}(\hat{L}_{2})_{z}
= \frac{1}{4}[(\hat{L}_{1})_{+} + (\hat{L}_{1})_{-}][(\hat{L}_{2})_{+} + (\hat{L}_{2})_{-}] - \frac{1}{4}[(\hat{L}_{1})_{+} - (\hat{L}_{1})_{-}][(\hat{L}_{2})_{+} - (\hat{L}_{2})_{-}] + (\hat{L}_{1})_{z}(\hat{L}_{2})_{z}.$$

This tidies up to give the result required:

$$\hat{\boldsymbol{L}}_1 \cdot \hat{\boldsymbol{L}}_2 = \frac{1}{2}(\hat{L}_1)_+(\hat{L}_2)_- + \frac{1}{2}(\hat{L}_1)_-(\hat{L}_2)_+ + (\hat{L}_1)_z(\hat{L}_2)_z.$$

To verify that the linear combination of product states on the right-hand side of equation (3),

$$|\psi\rangle \equiv \sqrt{\frac{1}{10}}|20\rangle|1,-1\rangle - \sqrt{\frac{3}{10}}|2,-1\rangle|10\rangle + \sqrt{\frac{3}{5}}|2,-2\rangle|11\rangle , \qquad (4)$$

truly is the total angular momentum state $|L, M\rangle = |1, -1\rangle$, we need to show that

$$(\hat{\boldsymbol{L}}_1 + \hat{\boldsymbol{L}}_2)^2 |\psi\rangle = L(L+1)\hbar^2 |\psi\rangle = 2\hbar^2 |\psi\rangle , \qquad (5)$$

$$((\hat{L}_1)_z + (\hat{L}_2)_z)|\psi\rangle = M\hbar|\psi\rangle = -\hbar|\psi\rangle.$$
 (6)

The second of these, equation (6), follows immediately from the general property

$$((\hat{L}_1)_z + (\hat{L}_2)_z)|\ell_1 m_1\rangle|\ell_2 m_2\rangle = (m_1 + m_2)\hbar|\ell_1 m_1\rangle|\ell_2 m_2\rangle ,$$

together with the fact that all terms on the right-hand side of equation (4) have $m_1 + m_2 = -1$

Equation (5) can be verified by writing $(\hat{\boldsymbol{L}}_1 + \hat{\boldsymbol{L}}_2)^2 = \hat{\boldsymbol{L}}_1^2 + \hat{\boldsymbol{L}}_2^2 + 2\hat{\boldsymbol{L}}_1 \cdot \hat{\boldsymbol{L}}_2$ as

$$(\hat{\boldsymbol{L}}_1 + \hat{\boldsymbol{L}}_2)^2 = \hat{\boldsymbol{L}}_1^2 + \hat{\boldsymbol{L}}_2^2 + (\hat{L}_1)_+ (\hat{L}_2)_- + (\hat{L}_1)_- (\hat{L}_2)_+ + 2(\hat{L}_1)_z (\hat{L}_2)_z$$

Since all three terms on the right-hand side of equation (4) have $\ell_1 = 2$, $\ell_2 = 1$, we have

$$\hat{\boldsymbol{L}}_1^2|\psi\rangle = \ell_1(\ell_1+1)\hbar^2|\psi\rangle = 6\hbar^2|\psi\rangle$$

$$\hat{\boldsymbol{L}}_2^2|\psi\rangle = \ell_2(\ell_2+1)\hbar^2|\psi\rangle = 2\hbar^2|\psi\rangle.$$

Using $(\hat{L}_1)_z(\hat{L}_2)_z|\ell_1 m_1\rangle|\ell_2 m_2\rangle = m_1 m_2 \hbar^2 |\ell_1 m_1\rangle|\ell_2 m_2\rangle$, the $(\hat{L}_1)_z(\hat{L}_2)_z$ contribution is

$$(\hat{L}_1)_z(\hat{L}_2)_z|\psi\rangle = -2\sqrt{\frac{3}{5}}\hbar^2|2,-2\rangle|11\rangle$$
.

Finally, applying products of ladder operators gives the non-zero contributions

$$(\hat{L}_{1})_{+}(\hat{L}_{2})_{-}|2,-1\rangle|10\rangle = \sqrt{6}\sqrt{2}\hbar^{2}|20\rangle|1,-1\rangle$$

$$(\hat{L}_{1})_{+}(\hat{L}_{2})_{-}|2,-2\rangle|11\rangle = 2\sqrt{2}\hbar^{2}|2,-1\rangle|10\rangle$$

$$(\hat{L}_{1})_{-}(\hat{L}_{2})_{+}|20\rangle|1,-1\rangle = \sqrt{6}\sqrt{2}\hbar^{2}|2,-1\rangle|10\rangle$$

$$(\hat{L}_{1})_{-}(\hat{L}_{2})_{+}|2,-1\rangle|10\rangle = 2\sqrt{2}\hbar^{2}|2,-2\rangle|11\rangle.$$

Summing the various contributions above then establishes equation (5).

(f) For each table, the absolute values of the entries in each row or column (ie the moduli-squared of the Clebsch-Gordan coefficients) sum to unity. Also, remembering to take the signed square root of each table entry, each pair of rows in the table is orthogonal, as is each pair of columns. Hence each table corresponds to a unitary matrix of Clebsch-Gordan coefficients, $UU^{\dagger} = I$. In the standard convention, the Clebsch-Gordan coefficients are all real, so the matrix is in fact orthogonal: $UU^T = I$.

For the tables $(1/2) \otimes (1/2)$, $1 \otimes 1$, $(3/2) \otimes (3/2)$, $2 \otimes 2$, the coefficients in each column $|j,m\rangle$ are the same for the rows (m_1,m_2) and (m_2,m_1) , except possibly for a change in sign. The relative sign gives the symmetry of the $|j,m\rangle$ state under interchange $1 \leftrightarrow 2$. For $(1/2) \otimes (1/2)$, the states are symmetric for j = 1 and antisymmetric for j = 0.

For $1 \otimes 1$, the states are symmetric for j = 2, 0 and antisymmetric for j = 1.

For $(3/2) \otimes (3/2)$, the states are symmetric for j = 3, 1 and antisymmetric for j = 2, 0.

For $2 \otimes 2$, the states are symmetric for j = 4, 2, 0 and antisymmetric for j = 3, 1.

In general, the $j_1 \leftrightarrow j_2$ exchange symmetry is given by $(-1)^{J-j_1-j_2}$. This quantity appears in the box about half-way down the right-hand side of the page of Clebsch-Gordan coefficient tables.

Question e: Rotational symmetry Write down the Wigner-Eckart theorem for matrix elements of the form $\langle \alpha_1 j_1 m_1 | \hat{V}_m | \alpha_2 j_2 m_2 \rangle$, where the operators \hat{V}_m $(m = \pm 1, 0)$ are the spherical components of a vector operator \hat{V} , and the α_i represent any other quantum numbers needed to uniquely identify the total angular momentum eigenstates $|\alpha_i j_i m_i\rangle$ of the system.

(a) For the case $j_1 = 1$, $j_2 = 0$, identify the matrix elements $\langle \alpha_1 j_1 m_1 | \hat{V}_m | \alpha_2 j_2 m_2 \rangle$ which can be non-zero, and show that they are all equal. Hence show that the Cartesian components $(\hat{V}_x, \hat{V}_y, \hat{V}_z)$ of \hat{V} have matrix elements of the form

$$\langle \alpha_1 10 | (\hat{V}_x, \hat{V}_y, \hat{V}_z) | \alpha_2 00 \rangle = A(0, 0, 1)$$

 $\langle \alpha_1 1, \pm 1 | (\hat{V}_x, \hat{V}_y, \hat{V}_z) | \alpha_2 00 \rangle = \frac{A}{\sqrt{2}} (\mp 1, i, 0)$

where A is a constant.

(b) Verify this result explicitly for the matrix elements of the position operator $\hat{r} = (\hat{x}, \hat{y}, \hat{z})$ for a system such as the hydrogen atom for which the j = 0 and j = 1 angular momentum eigenstates $|\alpha jm\rangle$ are spatial wavefunctions of the form

$$|\alpha 00\rangle = R_{\alpha 0}(r)Y_{00}(\theta, \phi) ; \qquad |\alpha 1m\rangle = R_{\alpha 1}(r)Y_{1m}(\theta, \phi) .$$

[The $\ell=0$ and $\ell=1$ spherical harmonics $Y_{\ell m}(\theta,\phi)$ are

$$Y_{00} = \sqrt{\frac{1}{4\pi}}$$
, $Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta$, $Y_{1,\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi}$.

(c) What is the equivalent result to part (a) for the case $j_1 = j_2 = 0$?

Answer e: Rotational symmetry

The Wigner-Eckart theorem for a vector operator $\hat{\boldsymbol{V}}$, with spherical components \hat{V}_m , is

$$\langle \alpha_1 j_1 m_1 | \hat{V}_m | \alpha_2 j_2 m_2 \rangle = \langle \alpha_1 j_1 \parallel \hat{\mathbf{V}} \parallel \alpha_2 j_2 \rangle \langle 1 m; j_2 m_2 | j_1 m_1 \rangle .$$

The reduced matrix element $\langle \alpha_1 j_1 \| \hat{\boldsymbol{V}} \| \alpha_2 j_2 \rangle$ is a complex constant which is independent of the quantum numbers m_1 , m_2 and m. The Clebsch-Gordan coefficient $\langle 1m; j_2 m_2 | j_1 m_1 \rangle$ arises from angular momentum addition $1 \otimes j_2 = j_1$ and is independent of the vector operator $\hat{\boldsymbol{V}}$.

(a) The Clebsch-Gordan coefficient $\langle 1m; j_2m_2|j_1m_1\rangle$ vanishes unless $m_1=m+m_2$. Hence the matrix element $\langle \alpha_1j_1m_1|\hat{V}_m|\alpha_2j_2m_2\rangle$ vanishes unless $m_1=m+m_2$. For the case $j_1=1$

and $j_2 = 0$, with $m_1 = \pm 1, 0$ and $m_2 = 0$, the only matrix elements which can be non-zero are those with $m = m_1$:

$$\langle \alpha_{1}11|\hat{V}_{+1}|\alpha_{2}00\rangle = \langle \alpha_{1}1 \| \hat{V} \| \alpha_{2}0\rangle \langle 11;00|11\rangle$$

$$\langle \alpha_{1}1, -1|\hat{V}_{-1}|\alpha_{2}00\rangle = \langle \alpha_{1}1 \| \hat{V} \| \alpha_{2}0\rangle \langle 1, -1;00|1, -1\rangle$$

$$\langle \alpha_{1}10|\hat{V}_{0}|\alpha_{2}00\rangle = \langle \alpha_{1}1 \| \hat{V} \| \alpha_{2}0\rangle \langle 10;00|10\rangle.$$

The Clebsch-Gordan coefficients above derive from the "trivial" angular momentum addition $1\otimes 0=1$, and are all unity. Hence, for the spherical components \hat{V}_m , the non-vanishing matrix elements are all equal:

$$\overline{\langle \alpha_1 11 | \hat{V}_{+1} | \alpha_2 00 \rangle = \langle \alpha_1 1, -1 | \hat{V}_{-1} | \alpha_2 00 \rangle = \langle \alpha_1 10 | \hat{V}_0 | \alpha_2 00 \rangle = \langle \alpha_1 1 \parallel \hat{\boldsymbol{V}} \parallel \alpha_2 0 \rangle} .$$

The Cartesian components of \hat{V} are given in terms of the spherical components as

$$\hat{V}_x = \frac{1}{\sqrt{2}}(\hat{V}_{-1} - \hat{V}_{+1}) , \qquad \hat{V}_y = \frac{i}{\sqrt{2}}(\hat{V}_{-1} + \hat{V}_{+1}) , \qquad \hat{V}_z = \hat{V}_0 .$$

The matrix elements of the Cartesian components of \hat{V} are thus of the form

$$\langle \alpha_1 10 | (\hat{V}_x, \hat{V}_y, \hat{V}_z) | \alpha_2 00 \rangle = A(0, 0, 1)$$

 $\langle \alpha_1 1, \pm 1 | (\hat{V}_x, \hat{V}_y, \hat{V}_z) | \alpha_2 00 \rangle = \frac{A}{\sqrt{2}} (\mp 1, i, 0) ,$

where $A \equiv \langle \alpha_1 1 \| \hat{\mathbf{V}} \| \alpha_2 0 \rangle$ is a constant.

(b) For the position operator $\hat{\mathbf{V}} = \hat{\mathbf{r}} = (r \sin \theta \cos \phi, r \sin \theta \sin \phi, r \cos \theta)$, the matrix elements $\langle \alpha_1 1 m_1 | (x, y, z) | \alpha_2 00 \rangle$ can be evaluated explicitly. Starting with $|\alpha_1 10\rangle$, the z matrix element is

$$\langle \alpha_1 10 | z | \alpha_2 00 \rangle = \int \psi_{\alpha_1 10}^*(\mathbf{r}) \, r \cos \theta \, \psi_{\alpha_2 00}(\mathbf{r}) \, \mathrm{d}^3 r$$
$$= \int_0^\infty r^3 R_{\alpha_1 1}(r) R_{\alpha_2 0}(r) \, \mathrm{d}r \int_0^{2\pi} \int_{-1}^{+1} \cos \theta \, Y_{10}^* Y_{00} \, \mathrm{d} \cos \theta \, \mathrm{d}\phi \,.$$

Writing the radial integral above as K_r , this is

$$\langle \alpha_1 10 | z | \alpha_2 00 \rangle = K_r \sqrt{\frac{3}{4\pi}} \sqrt{\frac{1}{4\pi}} 2\pi \int_{-1}^{+1} \cos^2 \theta \, d \cos \theta = \frac{1}{\sqrt{3}} K_r.$$

The x and y matrix elements vanish:

$$\langle \alpha_1 10 | x | \alpha_2 00 \rangle \propto \int_0^{2\pi} \cos \phi \, d\phi = 0$$
, $\langle \alpha_1 10 | y | \alpha_2 00 \rangle \propto \int_0^{2\pi} \sin \phi \, d\phi = 0$.

Similarly, for $|\alpha_1 11\rangle$, the x matrix element is

$$\begin{split} \langle \alpha_1 11 | x | \alpha_2 00 \rangle &= \int \psi_{\alpha_1 11}^*(\boldsymbol{r}) \, r \sin \theta \cos \phi \, \psi_{\alpha_2 00}(\boldsymbol{r}) \, \mathrm{d}^3 r \\ &= \int_0^\infty R_{\alpha_1 1}(r) R_{\alpha_2 0}(r) r^3 \, \mathrm{d}r \int_0^{2\pi} \int_{-1}^{+1} \sin \theta \cos \phi \, Y_{11}^* Y_{00} \, \mathrm{d} \cos \theta \, \mathrm{d}\phi \\ &= -K_r \sqrt{\frac{3}{8\pi}} \sqrt{\frac{1}{4\pi}} \int_{-1}^{+1} \sin^2 \theta \, \mathrm{d} \cos \theta \int_0^{2\pi} \cos \phi \, e^{-i\phi} \, \mathrm{d}\phi = -\frac{1}{\sqrt{6}} K_r \; . \end{split}$$

The y matrix element is given similarly, but with a ϕ contribution $\int_0^{2\pi} \sin \phi \, e^{-i\phi} \, \mathrm{d}\phi = -i\pi$ in place of $\int_0^{2\pi} \cos \phi \, e^{-i\phi} \, \mathrm{d}\phi = \pi$, and hence with an extra factor of -i:

$$\langle \alpha_1 11 | y | \alpha_2 00 \rangle = \frac{i}{\sqrt{6}} K_r .$$

The matrix element for z vanishes:

$$\langle \alpha_1 11 | z | \alpha_2 00 \rangle \propto \int_0^{2\pi} e^{-i\phi} d\phi = 0$$
.

Finally, $|\alpha_1 1, -1\rangle$ is the same as $|\alpha_1 11\rangle$, but with $-e^{i\phi}$ instead of $e^{-i\phi}$.

The matrix elements of $(\hat{x}, \hat{y}, \hat{z})$ thus take the form expected from the Wigner-Eckart theorem, with the constant A (the reduced matrix element) given by

$$A = \frac{1}{\sqrt{3}} K_r = \frac{1}{\sqrt{3}} \int_0^\infty r^3 R_{\alpha_1 1}(r) R_{\alpha_2 0}(r) dr.$$

(c) For the case $j_1 = 0$, $j_2 = 0$ (and hence $m_1 = 0$, $m_2 = 0$), the Wigner-Eckart theorem gives

$$\langle \alpha_1 00 | \hat{V}_m | \alpha_2 00 \rangle = \langle \alpha_1 0 \| \hat{\boldsymbol{V}} \| \alpha_2 0 \rangle \langle 1m; 00 | 00 \rangle$$
.

The Clebsch-Gordan coefficients $\langle 1m; 00|00\rangle$ vanish for all $m=\pm 1, 0$ (because $1\otimes 0\neq 0$). Hence the matrix elements of all components of a vector operator $\hat{\boldsymbol{V}}$ taken between states with zero total angular momentum must vanish:

$$\boxed{\langle \alpha_1 00 | \hat{\boldsymbol{V}} | \alpha_2 00 \rangle = 0} .$$

Question g: Linear Stark effect

A hydrogen atom is placed in an external electric field of strength \mathcal{E} , resulting in shifts in the atomic energy levels which are large relative to atomic fine structure. The effect of the electric field on the level with principal quantum number n=3 is to be analysed using first-order degenerate perturbation theory, with a perturbation $\hat{H}' = e\mathcal{E}z$, and working in the basis of states $|n\ell m_{\ell}\rangle$ ordered as

$$|300\rangle, \quad |310\rangle, \quad |320\rangle, \quad |311\rangle, \quad |321\rangle, \quad |31,-1\rangle, \quad |32,-1\rangle, \quad |322\rangle, \quad |32,-2\rangle \ .$$

The reduced matrix elements for the electron position operator $\hat{\boldsymbol{r}}$ for n=3 are $\langle 3s \parallel \hat{\boldsymbol{r}} \parallel 3p \rangle = 9\sqrt{2}a_0$, and $\langle 3d \parallel \hat{\boldsymbol{r}} \parallel 3p \rangle = -(9/\sqrt{2})a_0$, where a_0 is the Bohr radius.

(a) Show that the matrix representation of \hat{H}' in the basis above is block diagonal, with sub-matrices of the form

$$H_0' = \begin{pmatrix} 0 & a & 0 \\ a & 0 & b \\ 0 & b & 0 \end{pmatrix} , \qquad H_{+1}' = \begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix} , \qquad H_{-1}' = \begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix} ,$$

where a, b, c are constants such that $a = \sqrt{2}b = \sqrt{8/3}c$, and $c = -(9/2)ea_0\mathcal{E}$.

[You may find the $1 \otimes 1$ table of Clebsch-Gordan coefficients useful.]

- (b) Show that the electric field splits the n=3 level into five equally spaced levels with energy separation $(9/2)ea_0\mathcal{E}$. State the values of the quantum number m_ℓ associated with each of these five levels.
- (c) Show that, in the electric field, the n=3 level of highest energy corresponds to the zeroth-order eigenstate

$$|\psi\rangle = \sqrt{\frac{1}{3}}|300\rangle - \sqrt{\frac{1}{2}}|310\rangle + \sqrt{\frac{1}{6}}|320\rangle ,$$

and (optionally) determine the zeroth-order eigenstates for the other four levels.

Answer g: Linear Stark effect

(a) Matrix elements of the operator z taken between states $|n\ell m_{\ell}\rangle$ can only be non-zero if the states involved have $\Delta m_{\ell} = 0$ and opposite parity $(-1)^{\ell}$. For the n = 3 states of hydrogen, the only matrix elements $\langle n\ell' m'_{\ell}|\hat{H}'|n\ell m_{\ell}\rangle$ of the perturbation $\hat{H}' = e\mathcal{E}z$ that can possibly be non-zero are therefore

$$\langle 300 | \hat{H}' | 310 \rangle \equiv a \ ; \quad \langle 320 | \hat{H}' | 310 \rangle \equiv b \ ; \quad \langle 321 | \hat{H}' | 311 \rangle \equiv c \ ; \quad \langle 32, -1 | \hat{H}' | 31, -1 \rangle \equiv c' \ ,$$

together with their conjugates. In the basis of states $|n\ell m_{\ell}\rangle$ ordered as

$$|300\rangle$$
, $|310\rangle$, $|320\rangle$, $|311\rangle$, $|321\rangle$, $|31,-1\rangle$, $|32,-1\rangle$, $|322\rangle$, $|32,-2\rangle$,

the 9 × 9 matrix representation of \hat{H}' is therefore block-diagonal, with submatrices H'_{0} , H'_{+1} , H'_{-1} , $H'_{\pm 2}$ coming from the states with $m_{\ell} = 0$, $m_{\ell} = +1$, $m_{\ell} = -1$ and $m_{\ell} = \pm 2$:

$$H_0' = \begin{pmatrix} 0 & a & 0 \\ a^* & 0 & b^* \\ 0 & b & 0 \end{pmatrix} , \qquad H_{+1}' = \begin{pmatrix} 0 & c^* \\ c & 0 \end{pmatrix} , \qquad H_{-1}' = \begin{pmatrix} 0 & c'^* \\ c' & 0 \end{pmatrix} , \qquad H_{\pm 2}' = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} .$$

The reduced matrix elements are given to be

$$\langle 3s \| \hat{\boldsymbol{r}} \| 3p \rangle = 9\sqrt{2} a_0$$
, $\langle 3d \| \hat{\boldsymbol{r}} \| 3p \rangle = -(9/\sqrt{2}) a_0$.

Using the Wigner-Eckart theorem, the matrix elements a and b in H'_0 are

$$a = e\mathcal{E}\langle 300|\hat{z}|310\rangle = e\mathcal{E}\langle 3s \| \hat{r} \| 3p \rangle \langle 10; 10|00\rangle = 9\sqrt{2} e\mathcal{E}a_0 \times -\sqrt{\frac{1}{3}} = -9\sqrt{\frac{2}{3}}e\mathcal{E}a_0$$

$$b = e\mathcal{E}\langle 320|\hat{z}|310\rangle = e\mathcal{E}\langle 3d \| \hat{r} \| 3p \rangle \langle 10; 10|20\rangle = -9\sqrt{\frac{1}{2}}e\mathcal{E}a_0 \times \sqrt{\frac{2}{3}} = -9\sqrt{\frac{1}{3}}e\mathcal{E}a_0.$$

Similarly, the matrix elements c and c' in $H'_{\pm 1}$ are

$$c = e\mathcal{E}\langle 321|\hat{z}|311\rangle = e\mathcal{E}\langle 3d \| \hat{r} \| 3p \rangle \langle 10; 11|21\rangle = -9\sqrt{\frac{1}{2}} e\mathcal{E}a_0 \times \sqrt{\frac{1}{2}} = -\frac{9}{2}e\mathcal{E}a_0$$

$$c' = e\mathcal{E}\langle 32, -1|\hat{z}|31, -1\rangle = e\mathcal{E}\langle 3d \| \hat{r} \| 3p \rangle \langle 10; 1, -1|2, -1\rangle = -9\sqrt{\frac{1}{2}} e\mathcal{E}a_0 \times \sqrt{\frac{1}{2}} = -\frac{9}{2}e\mathcal{E}a_0$$

Thus the H' submatrices have the form

$$H_0' = \begin{pmatrix} 0 & a & 0 \\ a & 0 & b \\ 0 & b & 0 \end{pmatrix} , \qquad H_{+1}' = \begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix} , \qquad H_{-1}' = \begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix} ,$$

where the constants a, b, c are

$$a = \sqrt{2}b = -9\sqrt{\frac{2}{3}}e\mathcal{E}a_0 , \qquad c = -\frac{9}{2}e\mathcal{E}a_0 .$$

(b) In first-order degenerate perturbation theory, the energy shifts ΔE are obtained as the eigenvalues of the matrix H'. The energy shifts for the $m_{\ell} = 0$ states are given by the eigenvalues of the matrix H'_0 as

$$\Delta E = 0$$
, $\Delta E = \pm \sqrt{a^2 + b^2} = \pm 2c$.

Similarly, the eigenvalues of the matrices $H'_{\pm 1}$ give the $m_{\ell}=\pm 1$ energy shifts as $\Delta E=\pm c$. The states $|322\rangle$ and $|32,-2\rangle$ with $m_{\ell}=\pm 2$ have no energy correction at first-order: $\Delta E=0$.

Overall, we obtain energy shifts $\Delta E = 0, \pm c, \pm 2c$, and hence five equally spaced levels with energy separation $|c| = (9/2)e\mathcal{E}a_0$.

(c) The split state of highest energy has $\Delta E = 9e\mathcal{E}a_0$ and $m_{\ell} = 0$. The eigenvector of H'_0 corresponding to the eigenvalue ΔE is given by the solution of

$$-\frac{9}{\sqrt{3}}e\mathcal{E}a_0\begin{pmatrix}0&\sqrt{2}&0\\\sqrt{2}&0&1\\0&1&0\end{pmatrix}\begin{pmatrix}\alpha\\\beta\\\gamma\end{pmatrix}=9e\mathcal{E}a_0\begin{pmatrix}\alpha\\\beta\\\gamma\end{pmatrix}.$$

This gives the (normalised) zeroth-order eigenstate in the electric field as

$$|\psi\rangle = \sqrt{\frac{1}{3}} |300\rangle - \sqrt{\frac{1}{2}} |310\rangle + \sqrt{\frac{1}{6}} |320\rangle$$
.

Similarly, the eigenstate of H'_0 corresponding to the eigenvalue $\Delta E = -9e\mathcal{E}a_0$ is

$$|\psi\rangle = \sqrt{\frac{1}{3}} |300\rangle + \sqrt{\frac{1}{2}} |310\rangle + \sqrt{\frac{1}{6}} |320\rangle ,$$

and the eigenstate of H'_0 corresponding to $\Delta E = 0$ is

$$|\psi\rangle = \sqrt{\frac{1}{3}}|300\rangle - \sqrt{\frac{2}{3}}|320\rangle .$$

The eigenstates of H'_{+1} are

$$\Delta E = \mp \frac{9}{2} e \mathcal{E} a_0 \quad \Rightarrow \quad |\psi\rangle = \frac{1}{\sqrt{2}} (|311\rangle \pm |321\rangle) \ .$$

The eigenstates of H'_{-1} are

$$\Delta E = \mp \frac{9}{2} e \mathcal{E} a_0 \quad \Rightarrow \quad |\psi\rangle = \frac{1}{\sqrt{2}} (|31, -1\rangle \pm |32, -1\rangle) .$$

In summary (the final column contains the degeneracy g):

For completeness: to obtain the values of the reduced matrix elements given in the question, $\langle 3s \parallel \hat{r} \parallel 3p \rangle = 9\sqrt{2} \, a_0$ and $\langle 3d \parallel \hat{r} \parallel 3p \rangle = -(9/\sqrt{2}) \, a_0$, it is sufficient to evaluate explicitly a single relevant matrix element in each case, for example the matrix elements $\langle 300 | \hat{z} | 310 \rangle$ and $\langle 320 | \hat{z} | 310 \rangle$:

$$\langle 300 | \hat{z} | 310 \rangle = \langle 3s \| \hat{r} \| 3p \rangle \langle 10; 10 | 00 \rangle = -\langle 3s \| \hat{r} \| 3p \rangle \sqrt{(1/3)} , \qquad (7)$$

$$\langle 320|\hat{z}|310\rangle = \langle 3d \| \hat{r} \| 3p \rangle \langle 10; 10|20\rangle = \langle 3d \| \hat{r} \| 3p \rangle \sqrt{(2/3)} . \tag{8}$$

The eigenstates involved are $|300\rangle = R_{30}Y_{00}, |310\rangle = R_{31}Y_{10}, |320\rangle = R_{32}Y_{20}, \text{ where}$

$$R_{30}(r) = \left(\frac{1}{3a_0}\right)^{3/2} \left(1 - \frac{2r}{3a_0} + \frac{2r^2}{27a_0^2}\right) e^{-r/3a_0}$$

$$R_{31}(r) = \left(\frac{1}{3a_0}\right)^{3/2} \frac{4\sqrt{2}}{9} \left(1 - \frac{r}{6a_0}\right) \frac{r}{a_0} e^{-r/3a_0}$$

$$R_{32}(r) = \left(\frac{1}{3a_0}\right)^{3/2} \frac{4\sqrt{10}}{270} \left(\frac{r}{a_0}\right)^2 e^{-r/3a_0} ,$$

$$Y_{00} = \sqrt{\frac{1}{4\pi}}; \qquad Y_{10} = \sqrt{\frac{3}{4\pi}} \cos \theta; \qquad Y_{20} = \sqrt{\frac{5}{16\pi}} (3\cos^2 \theta - 1) .$$

With $\hat{z} = r \cos \theta$, the radial components of the matrix elements $\langle 300|\hat{z}|310 \rangle$ and $\langle 320|\hat{z}|310 \rangle$ are straightforwardly evaluated by repeated use of the standard integral $\int_0^\infty x^n e^{-x} \, \mathrm{d}x = n!$:

$$\int_0^\infty r^3 R_{30}(r) R_{31}(r) dr = -9\sqrt{2} a_0; \qquad \int_0^\infty r^3 R_{32}(r) R_{31}(r) dr = -\frac{9\sqrt{5}}{2} a_0.$$

The angular components are given by the integrals

$$\int \cos \theta \, Y_{00} Y_{10} \, d\Omega = \frac{1}{\sqrt{3}}; \qquad \int \cos \theta \, Y_{20} Y_{10} \, d\Omega = \sqrt{\frac{4}{15}}.$$

The product of the radial and angular components then gives the matrix elements required as

$$\langle 300 | \hat{z} | 310 \rangle = -9\sqrt{2} \, a_0 \sqrt{\frac{1}{3}} \, ; \qquad \langle 320 | \hat{z} | 310 \rangle = -\frac{9\sqrt{5}}{2} \, a_0 \sqrt{\frac{4}{15}} \, .$$

Question f: Identical particles

Two non-interacting, indistinguishable particles of mass m move in the one-dimensional potential V(x) given by

$$V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & \text{otherwise} \end{cases}.$$

Show that the energy of the system is of the form $E = (n_1^2 + n_2^2)\varepsilon$, where n_1 and n_2 are integers, and find an expression for ε .

Consider the state with $E = 5\varepsilon$ for each of the following three cases:

- (a) spin-zero particles;
- (b) spin-1/2 particles in a spin-singlet state;
- (c) spin-1/2 particles in a spin-triplet state.

In each case, state the symmetries of the spin and spatial components of the two-particle wavefunction. Write down the spatial wavefunction $\psi(x_1, x_2)$, and sketch the probability density $|\psi(x_1, x_2)|^2$ in the (x_1, x_2) plane.

Describe qualitatively how the energies of these states would change if the particles carried electric charge and hence interacted with each other.

Answer f: Identical particles

A single particle in the potential well has the (unnormalized) wavefunction $\psi_n(x) = \sin(n\pi x/L)$, and energy $E = (\hbar^2\pi^2/2mL^2)n^2 \equiv \epsilon n^2$. The wavefunction for a system of two indistinguishable particles must be either symmetric or antisymmetric under particle interchange $1 \leftrightarrow 2$, i.e.

$$\psi(x_1, x_2) = \sin(n_1 \pi x_1/L) \sin(n_2 \pi x_2/L) \pm \sin(n_2 \pi x_1/L) \sin(n_1 \pi x_2/L),$$

with energy $(n_1^2 + n_2^2)\epsilon$. If $E = 5\epsilon$, we must have $n_1 = 1$, and $n_2 = 2$ (or *vice versa*).

(a) Spin-zero particles are bosons and must have a symmetric wavefunction,

$$\psi(x_1, x_2) = \sin(\pi x_1/L) \sin(2\pi x_2/L) + \sin(2\pi x_1/L) \sin(\pi x_2/L)$$

= $2 \sin(\pi x_1/L) \sin(\pi x_2/L) [\cos(\pi x_1/L) + \cos(\pi x_2/L)]$.

This has zeros for $x_1 = 0$, $x_1 = L$, $x_2 = 0$, $x_2 = L$, and $x_1 + x_2 = L$.

- (b) Spin 1/2 particles are fermions and must have an antisymmetric wavefunction. In the singlet case, the spin wavefunction is antisymmetric, and hence the spatial wavefunction is symmetric, just as in (a).
- (c) In the triplet case, the spin wavefunction is symmetric, and hence the spatial wavefunction must be antisymmetric, i.e.

$$\psi(x_1, x_2) = \sin(\pi x_1/L) \sin(2\pi x_2/L) - \sin(2\pi x_1/L) \sin(\pi x_2/L)$$
$$= 2\sin(\pi x_1/L) \sin(\pi x_2/L) \left[\cos(\pi x_1/L) - \cos(\pi x_2/L)\right].$$

This has zeros for $x_1 = 0$, $x_1 = L$, $x_2 = 0$, $x_2 = L$, and $x_1 = x_2$.

If the particles were charged, they would repel each other through the Coulomb interaction. Therefore, in the spin 1/2 case, the triplet state would have the lower energy, because the particles tend to be further apart. This is an example of the exchange interaction, and is a simplified model of what happens in the Helium atom.

Question a: Aharonov-Bohm effect A ring-shaped semiconductor device is fabricated from a high mobility two-dimensional electron gas (Fig.1), and cooled in a cryostat to 0.3 K. On the figure, the lighter grey is the conducting region.

A voltage is applied across the ring (between points at the bottom and the top of the image) and the current flow is measured as a function of a magnetic field applied perpendicular to the plane of the ring.

Explain why the oscillations in conductance occur, account for their periodicity, and obtain a value for the average diameter of the ring. (1 Tesla = 10^4 Gauss.)

Answer a: Aharonov Bohm effect Electron wavefunctions that pass on either side of the ring produce constructive/destructive interference that is periodic in the flux BS passing through the ring, where S is the area of the hole in the ring.

Following the discussion of the Aharanov-Bohm effect in lectures, the phase difference is

$$\Delta \phi = \frac{e}{\hbar} BS \; ,$$

, and so a period 2π in the phase translates to a flux of $2\pi\hbar/e = h/e$.

The interference leads to oscillations in the conductance with field B, with period

$$\Delta B = \frac{h}{eS} \ .$$

Hence the area S and diamater d of the ring are given by

$$S = \frac{h}{e(\Delta B)} = \pi (d/2)^2$$
, $d = 2\sqrt{\frac{h}{\pi e(\Delta B)}}$.

From the graph, there are 12.5 oscillations in $400 \,\mathrm{Gauss}$ (= 0.04 T), which gives

$$\Delta B = 3.2 \times 10^{-3} \,\text{T/osc.}$$
, $d = 2\sqrt{\frac{h}{\pi e(\Delta B)}} = 1.28 \times 10^{-6} \,\text{m}$.

The results agree reasonably well with the value 0.65×10^{-6} m for the radius of the ring quoted in the paper.

43. CLEBSCH-GORDAN COEFFICIENTS, SPHERICAL HARMONICS, AND d FUNCTIONS

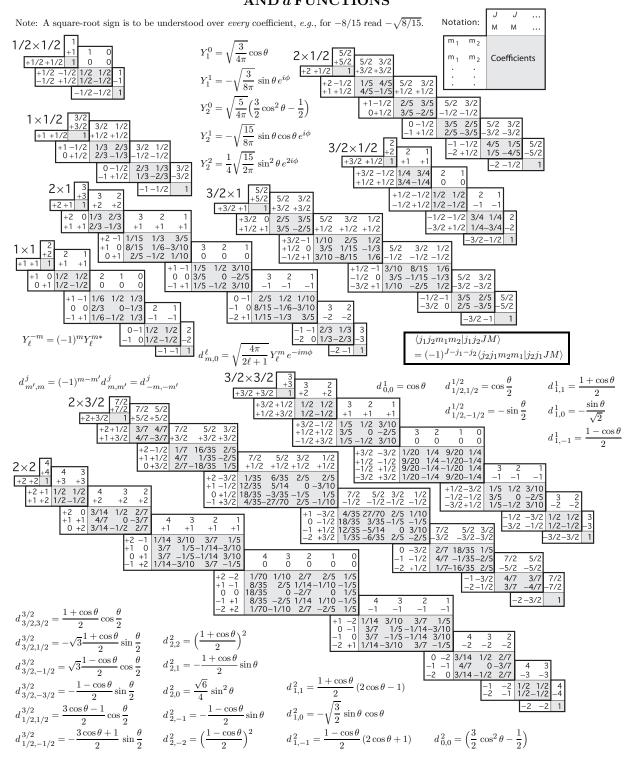


Figure 43.1: The sign convention is that of Wigner (*Group Theory*, Academic Press, New York, 1959), also used by Condon and Shortley (*The Theory of Atomic Spectra*, Cambridge Univ. Press, New York, 1953), Rose (*Elementary Theory of Angular Momentum*, Wiley, New York, 1957), and Cohen (*Tables of the Clebsch-Gordan Coefficients*, North American Rockwell Science Center, Thousand Oaks, Calif., 1974).

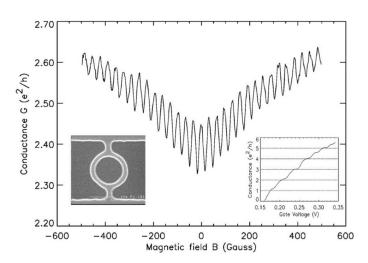


Figure 1: Aharonov-Bohm effect in a semiconductor quantum ring. [From S. Pedersen $\it et~al.,$ Phys. Rev. B $\it 61~(2000)~5457.]$