ANGULAR MOMENTUM & SPHERICAL TENSOR OPERATORS

The problem: In QM we need to evaluate many types of operators.

- some couple different particles, e.g. $\frac{1}{r_{12}}$, and can **transfer angular momentum** between particles.
- Some couple the system (e.g. an atom) to an external field e.g., $e\mathbf{r} \cdot \mathbf{E}$, and again **angular momentum is transferred**. If the field lacks spatial variation (the dipole approximation) only the **vector operator r** works on the atom.

The solution:

- Transform all operators to (combinations of) spherical tensor operators in order to be able to deal with arbitrary operators.
- The spherical tensor operators will then be a our operator basis.

ANGULAR MOMENTUM - REPETITION

Classically: $\mathbf{l} = \mathbf{r} \times \mathbf{p}$

- Conservation of angular momentum: An isolated system is invariant under the rotation of the whole system by an arbitrary angle $\rightarrow \sum_i \mathbf{l}_i = constant$

Quantum mechanically: $\mathbf{p} = -i\hbar\nabla$

$$\ell_x = -i\hbar \left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right), \ell_y = -i\hbar \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right),$$
$$\ell_z = -i\hbar \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial z} \right)$$

all the same if we replace $x \rightarrow y, y \rightarrow z, z \rightarrow x$

$$\rightarrow [\ell_x, \ell_y] = i\hbar\ell_z, [\ell_y, \ell_z] = i\hbar\ell_x, [\ell_z, \ell_x] = i\hbar\ell_y$$

GENERALIZATION

Generalize to an arbitrary operator

$$\mathbf{j} = j_x \hat{x} + j_y \hat{y} + j_z \hat{z} \tag{1}$$

and define it as an angular momentum operator if commutator relation holds:

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(last equation follows from the definition)

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(last equation follows from the definition) Find simultaneous eigenstates to $j_z, \mathbf{j}^2$ (now we use $\hbar = 1$)

$$\mathbf{j}^2 \Psi(\gamma, \mu, \mu_z) = \mu \Psi(\gamma, \mu, \mu_z) \tag{3}$$

$$j_z \Psi(\gamma, \mu, \mu_z) = \mu_z \Psi(\gamma, \mu, \mu_z). \tag{4}$$

With the the commutator relations we can in fact determine the spectra of $\mathbf{j}^2, j_z$.

LADDER OPERATORS

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$$j_+ j_- = (j_x + i j_y)(j_x - i j_y) = j_x^2 + j_y^2 + i\,[j_x, j_y] = \mathbf{j}^2 - jz^2 + j_z$$

$$\left[\mathbf{j}^2, j_\pm\right] = 0 \to \mathbf{j}^2 j_\pm \Psi(\mu, \mu_z) = \mu j_\pm \Psi(\mu, \mu_z)$$

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$$\left[\mathbf{j}^2, j_\pm\right] = 0 \rightarrow \mathbf{j}^2 j_\pm \Psi(\mu, \mu_z) = \mu j_\pm \Psi(\mu, \mu_z)$$

$$j_\pm j_z \Psi(\mu, \mu_z) = (j_z j_\pm - [j_z, j_\pm])\Psi(\mu, \mu_z) = (j_z j_\pm \mp j_\pm)\Psi(\mu, \mu_z) = \mu_z j_\pm \Psi(\mu, \mu_z)$$

$$j_z j_\pm \Psi(\mu, \mu_z) = (\mu_z \pm 1) j_\pm \Psi(\mu, \mu_z)$$

Ladder operators!

LADDER OPERATORS

For a given vale μ there must be a maximum μ_z and when we work on that state with J_+ we get zero, call the maximum j.

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Similarly: $(j - r)$ lowest eigenvalue of j_z

$$\begin{aligned} j_- \Psi(\mu, j-r) = 0 \ &\rightarrow j_+ j_- \Psi(\mu, j-r) = 0 \\ \mu - (j-r)^2 + (j-r) = j(j+1) - (j-r)^2 + (j-r) &= 0 \\ r^2 - r(2j-1) - 2j = 0 &\rightarrow r = 2j \end{aligned}$$

lowest eigenvalue $j - r = -j$.

LADDER OPERATORS

Thus we have for every $\mu = j(j+1)$, $2j+1$ eigenfunctions $\Psi(\mu, m)$, with $m = -j, -j+1, \dots j$. $2j$ must be an integer !

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$$\begin{aligned}
j_{+} \mid jm\rangle &= \alpha \mid jm+1\rangle \\
(j_{+} \mid jm\rangle)^{*} &= \alpha^{*}\langle jm+1 \mid \\
\langle jm \mid j_{+}^{\dagger} &= \alpha^{*}\langle jm+1 \mid \\
\langle jm \mid j_{-} &= \alpha^{*}\langle jm+1 \mid \\
\rightarrow \langle jm \mid j_{-}\mathrm{J}_{+} \mid jm\rangle &=\mid \alpha \mid^{2} \\
\mid \alpha \mid^{2} &= j(j+1) - m(m+1)
\end{aligned}$$

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(j_+ \mid jm\rangle)^* &= \alpha^* \langle jm+1 \mid \\
\langle jm \mid j_+^\dagger &= \alpha^* \langle jm+1 \mid \\
\langle jm \mid j_- &= \alpha^* \langle jm+1 \mid \\
\rightarrow \langle jm \mid j_- \mathrm{j}_+ \mid jm\rangle &= \mid \alpha \mid^2 \\
\mid \alpha \mid^2 &= j(j+1) - m(m+1)
\end{aligned}
$$

Finally!

$$
\begin{aligned}
j_+ \mid jm\rangle &= (j(j+1) - m(m+1))^{1/2} \mid j\, m+1\rangle \\
j_- \mid jm\rangle &= (j(j+1) - m(m-1))^{1/2} \mid j\, m-1\rangle
\end{aligned}
$$

SPHERICAL TENSOR OPERATORS

Definition Operators that behave as angular momentum states when they are acted on by angular momentum operators.
$\mathbf{t}^k$, with components t_q^k

$$\left[j_z, t_q^k\right] = q t_q^k$$

$$\left[j_\pm, t_q^k\right] = \sqrt{k\left(k+1\right) - q\left(q \pm 1\right)}\ t_{q\pm1}^k$$

A basis for operators

COUPLING OF ANGULAR MOMENTUM
AND COUPLING OF OPERATORS

With two particles we may look at the sum of their angular momenta

$$\mathbf{J} = \mathbf{j}_1 + \mathbf{j}_2$$

- **J** will satisfies the same commutator relations as **j**

$$\mid (j_1 j_2)\, JM\rangle = \sum_{m_1, m_2} \mid j_1 m_1 j_2 m_2\rangle\langle j_1 m_1 j_2 m_2 \mid JM\rangle,\ M = m_1 + m_2$$

Used that eigenfunctions to an Hermitian operator form a complete set, i.e.

$$\sum_{m_1, m_2} \mid j_1 m_1 j_2 m_2\rangle\langle j_1 m_1 j_2 m_2 \mid = 1$$

$\langle j_1 m_1 j_2 m_2 \mid JM\rangle$ is a Clebsch-Gordan coefficient (possible to choose them to be real i.e. $\langle j_1 m_1 j_2 m_2 \mid JM\rangle = \langle JM \mid j_1 m_1 j_2 m_2\rangle$)

$3j$-SYMBOLS

An alternative, and more symmetric, quantity is the $3j$ symbol

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1-j_2-m_3} \frac{1}{\sqrt{2j_3+1}} \langle j_1 m_1 j_2 m_2 \mid j_3, -m_3 \rangle$$

non-zero only if $m_1 + m_2 + m_3 = 0$, and $\mid j_1 - j_2 \mid \leq j_3 \leq j_1 + j_2$
From the Clebsch-Gordan coefficients it follows that even permutations ($1 \rightarrow 2 \rightarrow 3$ etc.) does not change the $3j$-symbol and odd permutations introduce a factor $(-1)^{j_1+j_2+j_3}$. Also

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}$$

$3j$-SYMBOLS

MANY GOOD-TO-KNOW RELATIONS

Since

$$\sum_{m_1,m_2} \langle j_3' m_3' \mid j_1 m_1 j_2 m_2 \rangle \langle j_1 m_1 j_2 m_2 \mid j_3 m_3 \rangle = \delta(j_3, j_3')\delta(m_3, m_3')$$

$$\sum_{m_1,m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & m_3' \end{pmatrix} = \frac{1}{2j_3+1}\delta(j_3, j_3')\delta(m_3, m_3')$$

and

$$\sum_{j_3,m_3} (2j_3+1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1' & m_2' & m_3 \end{pmatrix} = \delta(m_1, m_1')\delta(m_2, m_2')$$

WIGNER-ECKART'S THEOREM

An operator that acts like an angular momentum can be *coupled* to the initial state to form the final state

$$t_q^k \mid \gamma_i j_i m_i\rangle = \sum_{j_f, m_f, \gamma_f} \mid j_f m_f\rangle\langle j_f m_f \mid kq, j_i m_i\rangle c\left(j_f, \gamma_f, j_i, \gamma_i\right)$$

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$$\begin{aligned} \langle \gamma_f j_f m_f \mid t_q^k \mid \gamma_i j_i m_i\rangle &= \langle j_f m_f \mid kq, j_i m_i\rangle c\left(j_f, \gamma_f, j_i, \gamma_i\right) \\ &= (-1)^{k-j_i+(m_f-j_f)+j_f} \sqrt{2j_f+1} \begin{pmatrix} k & j_i & j_f \\ q & m_i & -m_f \end{pmatrix} c\left(j_f, \gamma_f, j_i, \gamma_i\right) \end{aligned}$$

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$$= (-1)^{k-j_i+(m_f-j_f)+j_f} \sqrt{2j_f+1} \begin{pmatrix} k & j_i & j_f \\ q & m_i & -m_f \end{pmatrix} c\left(j_f, \gamma_f, j_i, \gamma_i\right)$$

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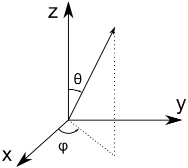
$$= (-1)^{j_f-m_f} \begin{pmatrix} j_f & k & j_i \\ -m_f & q & m_i \end{pmatrix} \langle\gamma_f j_f \,||\, \mathbf{t}^k \,||\, \gamma_i j_i\rangle$$

- the reduced matrix element independent of all the magnetic quantum numbers

EXAMPLE: DIPOLE OPERATOR

- Length gauge: $e\mathbf{r}\cdot\mathbf{E}$, assume $\mathbf{E}$ independent of r.



$$\mathbf{r} = (x, y, z) = r\left(\frac{x}{r}, \frac{y}{r}, \frac{z}{r}\right) = r\left(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta\right)$$

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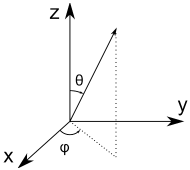

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$$\frac{z}{r} = \cos\theta = \sqrt{\frac{4\pi}{3}}Y_{10}\left(\theta,\phi\right) = C^1_0$$

$$\frac{1}{r}\frac{x \pm iy}{\sqrt{2}} = \frac{\sin\theta\cos\phi \pm i\sin\theta\sin\phi}{\sqrt{2}} = \sqrt{\frac{4\pi}{3}}Y_{1\pm1}\left(\theta,\phi\right) = C^1_{\pm1}$$

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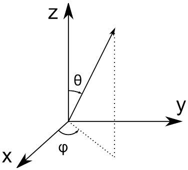

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- Spherical tensor operator of rank one: components $t^{k=1}_{q=-1,0,1}$
- C^1_0 interaction with linearly polarized light (along z-axis).
- $C^1_{\pm1}$ with circularly polarized light (in the xy-plane).

EXAMPLE: DIPOLE OPERATOR

$$\langle n'\ell' m' \mid z \mid n\ell m\rangle\, E_z = (-1)^{\ell'-m'} \begin{pmatrix} \ell' & 1 & \ell \\ -m' & 0 & m \end{pmatrix} \langle n'\ell' \,||\, \mathbf{r} \,||\, n\ell\rangle\, E_z$$

Selection rules:

- $m = m'$, triangle condition $\mid \ell - \ell' \mid \leq 1 \leq \ell + \ell'$, from the three-j symbol
- $\ell + \ell' + 1 =$ even comes from the reduced matrix element

$$\langle n'\ell' \,||\, \mathbf{r} \,||\, n\ell\rangle = \langle \ell' \,||\, \mathbf{C}^1 \,||\, \ell\rangle \int P_{n'\ell'}(r)\ \ r\ P_{n\ell}(r)\, dr$$

REDUCED MATRIX ELEMENTS OF C-TENSORS

Since the reduced matrix element is *m*- independent we can pick any *m* and *q*:

$$\begin{aligned}\langle \ell' 0 \mid C^k_0 \mid \ell 0 \rangle &= \frac{4\pi}{2k+1} \int Y_{\ell',0}(\theta,\phi)\, Y_{k,0}(\theta,\phi)\, Y_{\ell,0}(\theta,\phi) \sin\theta d\theta d\phi \\ &= (-1)^{\ell} \langle \ell' \,||\, \mathbf{C}^k \,||\, \ell \rangle \begin{pmatrix} \ell' & k & \ell \\ 0 & 0 & 0 \end{pmatrix}\end{aligned}$$

Addition theorem for Spherical Harmonics gives

$$\langle \ell' \,||\, \mathbf{C}^k \,||\, \ell \rangle = (-1)^{\ell} \sqrt{(2\ell+1)(2\ell'+1)} \begin{pmatrix} \ell' & k & \ell \\ 0 & 0 & 0 \end{pmatrix}$$

EXAMPLE: SPONTANEOUS PHOTON EMISSION

$$\text{transition rate} \sim \sum_{n'\ell'm'} |\, \langle n'\ell'm' \mid \mathbf{r} \mid n\ell m\rangle \,|^2$$

$$\langle n'\ell'm' \mid \mathbf{r} \mid n\ell m\rangle = \int P_{n'\ell'}(r)\ \ r\ P_{n\ell}(r)\, dr\ \langle \ell'm' \mid \mathbf{C}^1 \mid \ell m\rangle$$

vector with three components C_q^1

$$\sum_{m'} |\, \langle \ell'm' \mid \mathbf{C}^1 \mid \ell m\rangle \,|^2 = \sum_{q,m'} \begin{pmatrix} \ell' & 1 & \ell \\ -m' & q & m \end{pmatrix}^2 \times |\, \langle \ell' \,\|\, \mathbf{C}^1 \,\|\, \ell\rangle \,|^2$$

$$= \frac{|\, \langle \ell' \,\|\, \mathbf{C}^1 \,\|\, \ell\rangle \,|^2}{2\ell+1}$$

- independent of m

EXERCISES

- Time to do all from Chapter 2 (except 2.19 which we haven't got to yet)