VI V. ANGULAR MOMENTUM AND SPHERICALLY SYMMETRIC PROBLEMS

VI.1 V.1 The Orbital Angular Momentum Operator and Rotations

* Recall $\vec{L} = \vec{r} \times p$ is the (orbital) angular momentum operator. In coordinate representation: $\vec{L} = \vec{r} \times (-i\hbar \nabla_{\vec{r}})$

* We have

$$[L_x, L_y] = i\hbar L_z \;, \quad [L_y, L_z] = i\hbar L_x \;, \quad [L_z, L_x] = i\hbar L_y \qquad (\Delta)$$

$$[L^2, L_i] = 0 \qquad \text{with } i = x, y, z$$

Why? HW IX, [2]

$$(L^2 = L_x^2 + L_y^2 + L_z^2)$$

I.e. only one component of $\vec{L}$ can be measured at a time, but L^2 can be measured in addition!

* We also have

$$[L_i, r_j] = i\hbar\, \varepsilon_{ijk}\, r_k$$

generator of Galilei boosts

$$[L_i, K_j] = i\hbar\, \varepsilon_{ijk}\, K_k \qquad (\text{HW X})$$

$$[L_i, p_j] = i\hbar\, \varepsilon_{ijk}\, p_k$$

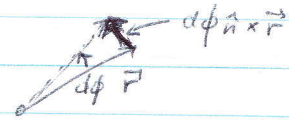
$i, j, k = 1, 2, 3$ (or x, y, z)

$$[L_i, T] = 0 \qquad (\text{HW III}, [3])$$

These relations complete the Galilei algebra, consisting of generators H, p_i, L_i, K_i $\quad (i=1,2,3)$.

* Recall from classical mechanics: an infinitesimal rotation by an angle $d\phi$ around an axis $\hat{n}$ maps a point $\vec{r}$ into

$$\vec{r} \mapsto \vec{r} + d\phi\, \hat{n} \times \vec{r}$$



We define $\vec{d\phi} = d\phi \cdot \hat{n}$.

For a wave ~~fct.~~ $\psi(\vec{r})$: $\quad \psi(\vec{r}) \mapsto \psi(\vec{r} + \vec{d\phi} \times \vec{r})$

$$= \psi(\vec{r}) + (\vec{d\phi} \times \vec{r}) \cdot \nabla\psi + \mathcal{O}(d\phi)^2$$

$\Rightarrow$ the infinitesimal change in wave fct. is

$$d\psi = (\vec{d\phi} \times \vec{r}) \cdot \nabla\psi = \vec{d\phi} \cdot (\vec{r} \times \nabla)\psi = \frac{i}{\hbar}\, \vec{d\phi} \cdot \vec{L}\, \psi \qquad (\square)$$

$\Rightarrow$ $D_{d\phi} = \mathbb{1} + \frac{i}{\hbar}\, d\phi\, \vec{L}$ ~~re~~represents rotations by $d\phi$,

and $\vec{L}$ is the generator for rotations as defined in I.12

A formal integration of $(\square)$ gives the rotation operator

$$D_\phi = e^{\frac{i}{\hbar} \vec{\phi} \cdot \vec{L}}$$

for arbitrary rotations $\vec{\phi}$.

VI.2 ~~V.2~~ Angular Momentum Eigenvalues

* There are other angular momentum operators besides orbital angular momentum $\vec{r} \times \vec{p}$! (e.g. spin) The defining property for a general angular momentum operator $\vec{J}$ is the set of equations (Δ) from V.1.

In this section we assume a general ang. momentum operator $\vec{J}$ with

$$[J_i, J_j] = i\hbar \, \varepsilon_{ijk} J_k \quad \text{and} \quad [J^2, J_i] = 0 \quad (i,j,k = 1,2,3)$$

We will discuss the joint eigenvalue spectrum of operators J^2 and J_z.

* Similar to the harm. osc. we define lowering and raising operators

$$J_\pm = J_x \pm i J_y \quad ; \quad \text{obviously} \quad J_+^\dagger = J_-$$

We have
$$[J_z, J_\pm] = \pm\hbar J_\pm$$
$$[J_+, J_-] = 2\hbar J_z$$
and
$$J^2 - J_z^2 = J_\pm J_\mp \mp \hbar J_z \qquad \text{(see HW X, [1])}$$

* The joint eigenvalue problem can be phrased as

$$J_z |\lambda m\rangle = m\hbar |\lambda m\rangle$$
$$J^2 |\lambda m\rangle = \lambda \hbar^2 |\lambda m\rangle$$

where we label common eigenstates by eigenvalues λ, m

Factors $\hbar, \hbar^2$ have been taken out to make λ, m dimensionless.

m will often be called the magnetic quantum number.

* We have $\lambda \geq m^2$

Why? $\langle \lambda m | J^2 - J_z^2 | \lambda m \rangle = \langle \lambda m | J_x^2 + J_y^2 | \lambda m \rangle = \frac{1}{2} \langle \lambda m | J_+ J_- + J_- J_+ | \lambda m \rangle$

$$= \frac{1}{2} \left(\langle J_- \lambda m | J_- \lambda m \rangle + \langle J_+ \lambda m | J_+ \lambda m \rangle \right) \geq 0$$

(positive definiteness of scalar products)

$$\Rightarrow (\lambda - m^2) \hbar^2 \langle \lambda m | \lambda m \rangle \geq 0$$

$\square$

* The J_+, J_- are raising and lowering operators for m, i.e.

$$J_+ |\lambda m\rangle = N_+^{\lambda, m} \hbar | \lambda \; m+1 \rangle$$

$$J_- |\lambda m\rangle = N_-^{\lambda, m} \hbar | \lambda \; m-1 \rangle$$

$N_\pm^{\lambda, m}$ normalization factors

Why? $J_z (J_+ |\lambda m\rangle) = J_+ J_z |\lambda m\rangle + \hbar J_+ |\lambda m\rangle = (m+1)(J_+ |\lambda m\rangle)$

similar for J_-

$$J^2 (J_\pm |\lambda m\rangle) = J_\pm J^2 |\lambda m\rangle = \lambda \hbar^2 (J_\pm |\lambda m\rangle)$$

* Since $\lambda \geq m^2$ there should be a largest value j and smallest value j' of m, for which $J_+ |\lambda j\rangle = 0$, $J_- |\lambda j'\rangle = 0$; $j' \leq j$

$$\Rightarrow J_- J_+ |\lambda_j\rangle = (J^2 - J_z^2 - \hbar J_z) |\lambda_j\rangle = (\lambda - j^2 - j) \hbar^2 |\lambda_j\rangle \stackrel{!}{=} 0$$

$$\Rightarrow \lambda = j(j+1)$$

Similarly $\lambda = j'(j'-1)$

$\Rightarrow j = -j'$ or $j' = j+1$; second solution impossible because $j' \leq j$

It should be possible to go from $|\lambda j\rangle$ to $|\lambda \; {-j}\rangle$ by repeated application of J_- in steps of $\Delta m = -1$. $\Rightarrow 2j$ is integer $\Rightarrow j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$

half integer or integer.

* Conclusion: Common eigenstates of J^2, J_z can be parametrized by $j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$ and (for fixed j) $-j \le m \le j$, m integer.
The eigenvalues are $j(j+1)\hbar^2$ for J^2 and (for fixed) $-j\hbar, (-j+1)\hbar, \ldots, j\hbar$ for J_z.

j	m					
0			0			
$\frac{1}{2}$		$-\frac{1}{2}$		$+\frac{1}{2}$		
1		-1	0		$+1$	
$\frac{3}{2}$	$-\frac{3}{2}$	$-\frac{1}{2}$		$+\frac{1}{2}$	$+\frac{3}{2}$	
2	-2	-1	0	-1	-2	
⋮	- - - - - .					

* The normalization factors $N_{\pm}^{\lambda, m}$ are determined by

$$J_\pm |\lambda\, m\rangle = \sqrt{(j \mp m)(j \pm m + 1)}\, \hbar\, |\lambda\ m\pm 1\rangle$$

(see Merzbacher p. 240)

VI.3 V.3 Orbital Angular Momentum Eigenfunctions

* Recall that in polar coordinates r, θ, ϕ

$$\nabla = \hat{r}\frac{\partial}{\partial r} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta}$$

where $\hat{r}, \hat{\phi}, \hat{\theta}$ are the unit coordinate vectors.

Thus $\vec{L} = \vec{r} \times (-i\hbar\nabla)$ in polar coordinate representation is

$$L_x = -i\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$L_y = -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \sin\phi\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$L_z = -i\hbar\frac{\partial}{\partial\phi}$$

and $L^2 = -\hbar^2 \left[\frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta} \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) \right]$

Why? HW IX [2]

* We consider the joint eigenvalue problem

$$L_z Y(\theta,\phi) = m\hbar\, Y(\theta,\phi)$$

$$L^2\, Y(\theta,\phi) = \lambda\hbar^2 Y(\theta,\phi)$$

Summary of the solution: (derivations in HW IX, [1], [2])

The possible eigenvalues are $\lambda = \ell(\ell+1)$ with $\ell = 0, 1, 2, \ldots$ (integer)

and $-\ell \leq m \leq \ell$ integer. This is the same as in V.2, although, interestingly, half-integer values for ℓ, allowed by the general angular mom. algebra, are <u>not</u> realized for orbital angular momentum.

The eigenfcts. $Y_\ell^m(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}} \sqrt{\frac{(\ell-m)!}{(\ell+m)!}} (-1)^m P_\ell^m(\cos\theta)\, e^{im\phi}$ $(m \geq 0)$

are called spherical harmonics. $Y_\ell^m(\theta,\phi) = (-1)^m\, Y_\ell^{-m\,*}(\theta,\phi)$ $(m<0)$

The magnitude of the normalization factor is fixed by the orthonormality condition

$$\int_0^{2\pi}\int_0^{\pi} d\phi\, d\theta \sin\theta\; Y_\ell^{m\,*}(\theta,\phi)\, Y_{\ell'}^{m'}(\theta,\phi) = \delta_{\ell,\ell'}\,\delta_{m,m'}$$

(Phases of norm. factors convention) (Check!)

The $P_\ell^m(\xi)$ $(1-\xi^2)^{\frac{m}{2}} \frac{d^m}{d\xi^m} P_\ell(\xi)$

are the associated Legendre functions which solve the diff equation

$$\frac{d}{d\xi}\left((1-\xi^2)\frac{dP_\ell^m}{d\xi}\right) - \frac{m^2}{1-\xi^2}P_\ell^m + \lambda P_\ell^m = 0 \qquad \text{with } \lambda = \ell(\ell+1)$$

(Legendre's diff. equation)

The $P_\ell(\xi) = \frac{1}{2^\ell \ell!}\frac{d^\ell}{d\xi^\ell}(\xi^2-1)^\ell$

are the Legendre polynomials of degree ℓ, which form an orthogonal basis of $L^2([-1,1])$:

$$\int_{-1}^{1} d\xi\, P_\ell(\xi)\, P_{\ell'}(\xi) = \frac{2}{2\ell+1}\delta_{\ell\ell'}$$

* The first few spherical harmonics are

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta \qquad Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\, e^{\pm i\phi}\sin\theta$$

$\vdots$

* The spherical harmonics form a complete set of (orthonormal) basis functions on the sphere parameterized by θ, ϕ:

$$\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} Y_\ell^{m*}(\theta',\phi')\, Y_\ell^m(\theta,\phi) = \delta^{(\text{sph.})}(\hat{r}_{\theta,\phi} - \hat{r}_{\theta',\phi'}) \qquad \text{(closure relation)}$$

where the spherical δ-fct. is defined as

$$\int_0^{2\pi}\int_0^{\pi} d\phi \sin\theta\, d\theta\, \delta^{(\text{sph})}(\hat{r}_{\theta\phi} - \hat{r}_{\theta_0\phi_0})\, f(\theta,\phi) = f(\theta_0,\phi_0)$$

* The Y_ℓ^m have definite parity: $\Pi \, Y_\ell^m = (-1)^\ell \, Y_\ell^m$

Why? Recall $\vec{r} \mapsto -\vec{r}$, $\vec{p} \mapsto -\vec{p}$ under parity $\Rightarrow \vec{L} \mapsto \vec{L}$, in particular $[\Pi, \vec{L}] = 0$ as operators $\Rightarrow$ common eigenstates possible for L^2, L_z, Π.

Indeed: $\phi \mapsto \phi + \pi$, $\theta \mapsto \pi - \theta$ $\Rightarrow e^{im\phi} \mapsto (-1)^m e^{im\phi}$

$$P_\ell^m(\cos\theta) \mapsto (-1)^{\ell+m} P_\ell^m(\cos\theta)$$

$$\Rightarrow Y_\ell^m \mapsto (-1)^\ell \, Y_\ell^m$$

VI.4 V.4 Spherically Symmetric Potentials

* In this section we assume $H = \frac{\vec{p}^2}{2m} + V(r)$ in 3 dimensions where the pot. energy $V(r)$ only depends on $r = |\vec{r}|$ (central force problem).

$[T, \vec{L}]$ always, but for such $V(r)$ obviously $[V, \vec{L}]$ as well.

$\Rightarrow [H, \vec{L}]$ and we can choose common eigenfunctions for H, L^2 and L_z.

* Recall the Laplace operator in spherical coordinates

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \phi^2}$$

$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) - \frac{L^2}{\hbar^2 r^2}$$

$$\Rightarrow H = -\frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{L^2}{2mr^2} + V(r)$$

* The separation of r-derivatives from L^2 in H suggests a separation ansatz $\psi(r,\theta,\phi) = R(r)\, Y_\ell^m(\theta,\phi)$

Then automatically $L^2 \psi(\vec{r}) = \ell(\ell+1)\hbar^2 \psi(\vec{r})$

$$L_z \psi(\vec{r}) = m\hbar\, \psi(\vec{r})$$

and we obtain the radial equation

$$\left[-\frac{\hbar^2}{2mr^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{\ell(\ell+1)\hbar^2}{2mr^2} + V(r)\right] R(r) = E\, R(r)$$

for $R(r)$.

V.4.1 The Free Particle Case

* We already know solutions to the free Schrödinger equation to be plane waves $\phi(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}$.
They are eigenstates of $H = -\frac{\hbar^2}{2m}\Delta$ together with $\vec{p} = (p_x, p_y, p_z)$
Now we look for eigenstates of H together with L^2, L_z.

* The radial equation for the free particle, $V=0$, is Bessel's equation:

$$\frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} + \left[1 - \frac{\ell(\ell+1)}{\rho^2}\right] R = 0$$

with the dimensionless variable $\rho = \frac{r}{\hbar}\sqrt{2mE}$

with solutions $j_\ell(\rho) = \frac{\rho^\ell}{2^{\ell+1}\ell!}\int_{-1}^{+1} e^{i\rho s}(1-s^2)^\ell ds$

(integral representation of the spherical Bessel functions)

Why? HW X, [3]

* Thus the free particle eigenstates with definite L^2 and L_z are

$$\psi(r,\theta,\phi) = C_{\ell,m}\, j_\ell\left(\frac{r}{\hbar}\sqrt{2mE}\right) Y_\ell^m(\theta,\phi)$$

($C_{\ell,m}$ = normalization constant). They form an orthonormal basis, thus plane waves $(H,\vec{p})$-eigenstates can be written in terms of (H, L^2, L_z) eigenstates, i.e.

$$e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} a_{\ell,m}\, j_\ell\Big(\underbrace{\frac{pr}{\hbar}}_{\sqrt{2mE}=p}\Big) Y_\ell^m(\theta,\phi)$$

* For a plane wave in z-direction ($\vec{p} = p\hat{e}_z$) in particular

$$e^{\frac{i}{\hbar}pr\cos\theta} = \sum_{\ell=0}^{\infty}(2\ell+1)\, i^\ell\, j_\ell\left(\frac{pr}{\hbar}\right)P_\ell(\cos\theta)$$

Why? HW X, [3]; note that ϕ does not appear on the l.h.s. thus $m=0$ on the r.h.s.

This is a very useful formula in scattering theory

V.4.2 Particle in a Coulomb Field

* We consider a potential energy $\propto \frac{1}{r}$ similar to the potential energy $V(r) = -\frac{Ze^2}{r}$ of an electron in the field of a nucleus of charge Ze. We only discuss bound states, i.e. $E<0$ here.

* In order to solve the radial equation it is customary to explicitly separate out the asymptotic behavior for $r \to 0$ and $r \to \infty$ and write $R(\rho) = \rho^{\ell} \; e^{-\rho} \, w(\rho)$ where $\rho = \underbrace{\frac{r}{\hbar}\sqrt{-2mE}}_{=:kr}$ is again a dimensionless variable.

Why? – for $r \to 0$ centrifugal term $\frac{\ell(\ell+1)}{r^2}$ dominates over $\frac{Ze^2}{r}$ (for $\ell \neq 0$)

$$\Rightarrow \left[r^2 \frac{d^2}{dr^2} + 2r\frac{d}{dr} - \ell(\ell+1)\right] R = 0 \Rightarrow R \propto r^{\ell} \propto \rho^{\ell} \text{ for small } r \text{ or } \rho.$$

(a second singular solution is not admissable)

– for $r \to \infty$ centrifugal, potential terms vanish

$$\Rightarrow \left[\frac{d^2}{dr^2} + \underbrace{\frac{2}{r}}_{\substack{\downarrow \\ r\to\infty}}\frac{d}{dr} - k^2\right] R = 0 \Rightarrow R \propto e^{-kr} \propto e^{-\rho}$$

* The reduced radial equation for $w(\rho)$ is

$$\left(\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2 \frac{d}{d\rho}\right) + \frac{\ell(\ell+1)}{\rho^2} + \frac{V}{E}\right) R(\rho) = 0$$

$$\Rightarrow \frac{d^2 w}{d\rho^2} + 2\left(\frac{\ell+1}{\rho} - 1\right)\frac{dw}{d\rho} + \left[\frac{V}{E} - \frac{2(\ell+1)}{\rho}\right] w = 0$$

(check algebra!)

Introducing $\rho_0 = \rho \frac{V}{E} = \frac{Ze^2}{\hbar}\sqrt{\frac{2m}{|E|}}$

$$\Rightarrow \quad \rho \frac{d^2 w}{d\rho^2} + 2(\ell+1-\rho)\frac{dw}{d\rho} + [\rho_0 - 2(\ell+1)]\, w = 0 \qquad (\square)$$

* Since we removed the leading power behavior for $r \to 0$ we can employ a power series $\quad w(\rho) = \sum_{j=0}^{\infty} a_j \rho^j$

In $(\square)$:

$$(j+1)j\, a_{j+1} \rho^j + 2(\ell+1)(j+1)\, a_{j+1} \rho^j - 2j \rho^j + [\rho_0 - 2(\ell+1)]\, a_j \rho^j = 0$$

$$\Rightarrow a_{j+1} = \frac{2(\ell+j+1)-\rho_0}{(j+1)(j+2\ell+2)}\, a_j \qquad \text{recursive solution of } (\square)$$

One can show that w diverges faster than $e^{+2\rho}$ and thus $R(r)$ would not be square-integrable unless the power series terminates and w is a polynomial.

For that $\rho_0 = 2(N+\ell+1)$ with some integer $N \geq 0$.

We define $\boxed{n = N+\ell+1}$ as the principal quantum number of the system. Since $\rho_0 > 0$ $\;n$ integer with $n \geq 1 \Rightarrow \ell+1 \leq n$

Furthermore $\quad E_n = -\frac{2m Z^2 e^4}{\hbar^2 \rho_0^2} = -\frac{Z^2 m e^4}{2\hbar^2 n^2} \qquad$ allowed energy eigenvalues

* Summary of the eigenvalue spectrum

principal qu. number n	orb. ang. mom. qu. number ℓ	magnetic qu. number m
1	0	$-\ell \leq m \leq \ell$
2	0, 1	⋮
3	0, 1, 2	⋮
4	0, 1, 2, 3	⋮
⋮		

The energy is only determined by n, not by ℓ or m.

The degeneracy of a state with fixed n is $\sum_{\ell=0}^{n-1} (2\ell+1) = n^2$

* The polynomials defined by the recursion

$$a_{j+1} = \frac{2(j-N)}{(j+1)(j+2\ell+2)} a_j$$

are called associated Laguerre polynomials $L^{2\ell+1}_{n-\ell-1}(2\rho)$ ← note factor 2 in argument

They are defined as $(\alpha, \beta \in \mathbb{N})$

$$L^{\beta}_{\alpha-\beta}(\rho) = (-1)^{\beta} \frac{d^{\beta}}{d\rho^{\beta}} L_{\alpha}(\rho)$$

where $L_{\alpha}(\rho) = e^{\rho} \frac{d^{\alpha}}{d\rho^{\alpha}} \left(e^{-\rho} \rho^{\alpha} \right)$ is a Laguerre polynomial

* Note: sometimes, there is an additional factor $\frac{1}{\alpha!}$ in the normalization

Laguerre polynomials form an orthonormal basis on $[0, \infty]$

with respect to the scalar product $\langle f, g \rangle = \int_0^{\infty} f(x)\, g(x)\, e^{-x}\, dx$

For the associated Laguerre polynomials

$$\int_0^{\infty} L^{\beta}_{\alpha}(\rho)\, L^{\beta}_{\alpha'}(\rho)\, \rho^{\beta} e^{-\rho}\, d\rho = \frac{(\alpha+\beta)!^{3}}{\alpha!} \delta_{\alpha\alpha'}$$

Why? w/o proof here, but cf. Merzbacher p. 270f.

* The stationary states of the Coulomb problem with well-defined angular momentum are

$$\psi_{n\ell m}(r,\theta,\phi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n\,(n+\ell)!^3}}\; e^{-\rho}\,(2\rho)^{\ell}\, L^{2\ell+1}_{n-\ell-1}(2\rho)\, Y^{m}_{\ell}(\theta,\phi)$$

where $a_0 = \frac{\hbar^2}{Z m e^2}$ is the Bohr radius.