Lecture 7: Three Dimensions with Spherical Symmetry

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1 General Definition of Rotation in Quantum Mechanics

Our goal here to defined the concept of spherical symmetry in Quantum Mechanics. According to Correspondence Principle number 2 all the symmetries in the Classical Physics should be valid in Quantum Physics too. This is a general principle and we already learned that mathematical realization of this principle was that all the symmetry transformations of Classical Physics which was applied on r_i and p_i in Quantum Mechanics should be applied to the quantum state vector defined in the Hilbert Space.

Our definition of Spherical symmetry will be based on the above principle with the operator of rotation, $R(\hat{n}, \theta)$, being applied on the quantum state vector.

Classical Mechanics: In classical physics we defined the operator of rotation:

$$\hat{R}(\hat{n}, \theta), \tag{1}$$

where $\hat{R}$ means that it is an operator and $\hat{n}$ is the unit vector around which the rotation on θ angle takes a place. In classical physics $R(\hat{n}, \theta)$ is being acted on coordinate and momentum (building blocks of reality in classical mechanics). For example

$$\hat{R}(\hat{n}, \theta) : \vec{r} = \vec{r}' \quad \text{or in the matrix form} \quad r_i' = \sum_k R_{i,k}(\hat{n}, \theta) r_k, \tag{2}$$

where for infinitesimally small rotation $\theta = \epsilon$

$$\delta r_i = r_i' - r_i = \epsilon \sum_{i,j} \epsilon_{ijk} n_j, r_k = \epsilon \left[n \times r\right]_i . \tag{3}$$

Since the operator R is a contineous transformation (Li Group) one can define three component generator of rotation $\hat{J}_i$ defined such thath:

$$\hat{R}(\hat{n}, \epsilon) = e^{-i\hat{J}_i n_i \epsilon}, \tag{4}$$

where by repeating indices i one assumes a summation.

For the case when rotation was applied on the 3d vectors in the Euclidean space (such as vector r_i) we found that three generators of roations are (3×3) matrices in the form (see Lecture 2, Eq. (43))

$$(J_i)_{jk} = -\epsilon_{ijk}. \tag{5}$$

where ϵ_{jik} are Levi-Civita matrices and in the matrix form can be presented as:

$$J_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad J_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \quad J_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{6}$$

The important property of these generators of rotation is that they satisfy commutator relations

$$[J_i, J_j] = i \sum_k \epsilon_{ijk} J_k \tag{7}$$

which are generally referred to as Li Group Algebra. The important property of this algebra is that they are invariant with respect to the Group representation. What this mean in practice is that while the explicit form of the Generators of rotation depends on the object that is being rotated (for Eqs.(5,6) the rotated objects are 3d vectors in the Euclidian space) the expression of algebra in Eq.(7) is the same for any other kind of the objects that being rotated, such as fields, scalars, vectors in higher dimensional euclidean and non-euclidean spaces.

Quantum Mechanics: According to the Second Correspondence principle, in Quantum Mechanics the Symmetry transformation operator should now act on the "basic building block" of the quantum reality, which is the quantum state vector $\mid \psi\rangle$, i.e we should consider now:

$$\hat{R}(\hat{n}, \theta) \mid \psi\rangle. \tag{8}$$

For infinitesimally small rotations one can introduce the generator of rotation $\hat{J}_i$ in Quantum Mechanics and present the above transformation in the form:

$$\hat{R}(\hat{n}, \epsilon) \mid \psi\rangle = e^{-i \sum_i \hat{J}_i n_i \epsilon} \mid \psi\rangle = \mid \psi'\rangle. \tag{9}$$

Note that even if we don't know the exact form of $\hat{J}_i$ we know that due the invariance of the Algebra of generators it will satisfy the relation of Eq.(7).

1.1 Property of Generators of Rotation in Quantum Mechanics

Our starting point is the algebra of generators, Eq.(7). We will discuss following nine steps that allow us to elucidate the main properties of generators of rotation which are universal for any representation.

Step 1. We define the following operator (generally referred to as Casimir operator):

$$\hat{J}^2 = \sum_i \hat{J}_i \hat{J}_i = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 \tag{10}$$

which is a Hermitian operator because of $\hat{J}_i$ being Hermitian.

Step 2. We now show that operator $\hat{J}^2$ commutes with individual components of $\hat{J}_i$.

Using the relation:

$$[ab, c] = a\,[b, c] + [a, c]\,b \tag{11}$$

and Eq.(7) resulting in:

$$\left[\hat{J}^2, \hat{J}_j\right] = \sum_i \left[\hat{J}_i\hat{J}_i, \hat{J}_j\right] = \sum_i \hat{J}_i\left[\hat{J}_i, \hat{J}_j\right] + \sum_i \left[\hat{J}_i, \hat{J}_j\right]\hat{J}_i = i\sum_{ik}\epsilon_{ijk}\hat{J}_i\hat{J}_k + i\sum_{ik}\epsilon_{ijk}\hat{J}_k\hat{J}_i = 0, \tag{12}$$

where in the last part of the equation we used the algebra of Eq.(7) and the fact that for antisymmetric matrices like Levi-Civita, summation by any two identical vectors gives 0: $\sum_{ik}\epsilon_{ijk}J_kJ_i = 0$.

The above relations allows us to choose one of the $\hat{J}_i$ operators (usually $\hat{J}_z$) together with $\hat{J}^2$ and consider their common eigenstates $\mid \psi_{\lambda_{J^2},m}\rangle$ as follows:

$$\begin{aligned}\hat{J}^2 \mid \psi_{\lambda_{J^2},m}\rangle &= \lambda_{J^2} \mid \psi_{\lambda_{J^2},m}\rangle \\ \hat{J}_z \mid \psi_{\lambda_{J^2},m}\rangle &= m \mid \psi_{\lambda_{J^2},m}\rangle,\end{aligned} \tag{13}$$

where λ_{J^2} and m represent the eigenvalues of $\hat{J}^2$ and $\hat{J}_z$ operators respectively.

Step 3. We define the $\hat{J}_\pm$ operators as follows:

$$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y. \tag{14}$$

First using Eq.(12) one obtains:

$$\left[\hat{J}_\pm, \hat{J}^2\right] = 0 \tag{15}$$

then using the algebra of generators (7) one can show that:

$$\begin{aligned}\left[\hat{J}_z, \hat{J}_\pm\right] &= \left[\hat{J}_z, \hat{J}_x\right] \pm i\left[\hat{J}_z, \hat{J}_y\right] = i\sum_k \epsilon_{z,x,k}\hat{J}_k \mp \sum_k \epsilon_{z,y,k}\hat{J}_k = \\ &= i\epsilon_{z,x,y}\hat{J}_y \mp \epsilon_{z,y,x}\hat{J}_x = i\hat{J}_y \pm \hat{J}_x = \pm(\hat{J}_x \pm i\hat{J}_y) = \pm\hat{J}_\pm,\end{aligned} \tag{16}$$

where in the derivation we used the fact that Levi-Civita tensor is zero for identical indices, $\epsilon_{z,x,y} = -\epsilon_{z,y,x} = 1$. Applying the same algebra also gives:

$$\left[\hat{J}_+, \hat{J}_-\right] = 2\hat{J}_z \tag{17}$$

Step 4. We use several useful representations of operator $\hat{J}^2$ using Eq.(17):

$$\hat{J}^2 = \frac{1}{2}\left(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+\right) + \hat{J}_z^2 = \hat{J}_+\hat{J}_- - \hat{J}_z + \hat{J}_z^2 = \hat{J}_-\hat{J}_+ + \hat{J}_z + \hat{J}_z^2. \tag{18}$$

Step 5. We show that $\hat{J}_\pm$ represent rising and lowering operators for eigenstates of $\hat{J}_z$.

For this let us take the eigenstate of operator $\hat{J}_z$ from Eq.(13) and act by $\hat{J}_+$. It will produce another state vector $\mid \phi_+\rangle$ in the Hilbert space:

$$\mid \phi_+\rangle = \hat{J}_+ \mid \psi_{\lambda_{J^2},m}\rangle. \tag{19}$$

Let us now check whether $\mid \phi\rangle$ is an eigenstate of $\hat{J}_z$:

$$\begin{aligned}\hat{J}_z \mid \phi_+\rangle &= \hat{J}_z\hat{J}_+ \mid \psi_{\lambda_{J^2},m}\rangle = (\hat{J}_+\hat{J}_z + \hat{J}_+) \mid \psi_{\lambda_{J^2},m}\rangle = \hat{J}_+(\hat{J}_z + 1) \mid \psi_{\lambda_{J^2},m}\rangle = \\ &= (m+1)\hat{J}_+ \mid \psi_{\lambda_{J^2},m}\rangle = (m+1) \mid \phi_+\rangle,\end{aligned} \tag{20}$$

where in the above derivation we used a relation $\hat{J}_z\hat{J}_+ = \hat{J}_+ + \hat{J}_+\hat{J}_z$ from Eq.(16). Thus from the above equation it follows that $\hat{J}_+$ is a step up operator on the eigenstate of $\hat{J}_z$ increasing its eigenvalue by one unit:

$$\hat{J}_+ \mid \psi_{\lambda_{J^2},m}\rangle \sim \mid \psi_{\lambda_{J^2},m+1}\rangle \tag{21}$$

With the very similar approach now using the relation $\hat{J}_z\hat{J}_- = -\hat{J}_- + \hat{J}_-\hat{J}_z$ one can show that $\hat{J}_-$ represents a step down operator on the eigenstate of $\hat{J}_z$ increasing decreasing its eigenvalue again by one unit: Indeed, if

$$\mid \phi_-\rangle = \hat{J}_- \mid \psi_{\lambda_{J^2},m}\rangle, \tag{22}$$

then,

$$\begin{aligned}\hat{J}_z \mid \phi_-\rangle &= \hat{J}_z\hat{J}_- \mid \psi_{\lambda_{J^2},m}\rangle = (\hat{J}_-\hat{J}_z - \hat{J}_-) \mid \psi_{\lambda_{J^2},m}\rangle = \hat{J}_-(\hat{J}_z - 1) \mid \psi_{\lambda_{J^2},m}\rangle = \\ &= (m-1)\hat{J}_+ \mid \psi_{\lambda_{J^2},m}\rangle = (m-1) \mid \phi_-\rangle.\end{aligned} \tag{23}$$

Thus

$$\hat{J}_- \mid \psi_{\lambda_{J^2},m}\rangle \sim \mid \psi_{\lambda_{J^2},m-1}\rangle. \tag{24}$$

Thus we proved that $\hat{J}_+$ and $\hat{J}_-$ operators create a ladder structure for the eigenstates of $\hat{J}_z$ operator with eigenvalues presenting a ladder with unit step up or unit step down.

Note that both sate vectors in Eq.(21) and (24) are still eigenstates of operator $\hat{J}^2$ with eigenvalue of λ_{J^2}.

Step 6. We now will demonstrate that above mentioned ladder has top and bottom, that is there are limiting states $\mid \psi_{\lambda_{J^2},m_{min}}\rangle$ and $\mid \psi_{\lambda_{J^2},m_{max}}\rangle$ below and above which one can not claim. To show this we consider the expectation value of the $\hat{J}_x^2 + \hat{J}_y^2$ operator which is by definition is positive definitive:

$$\langle\psi_{\lambda_{J^2},m} \mid \hat{J}_x^2 + \hat{J}_y^2 \mid \psi_{\lambda_{J^2},m}\rangle \geq 0. \tag{25}$$

Using Eq.(10) the above equation can be presented as follows:

$$\langle\psi_{\lambda_{J^2},m} \mid \hat{J}^2 - \hat{J}_z^2 \mid \psi_{\lambda_{J^2},m}\rangle = \lambda_{J^2} - m^2 \geq 0. \tag{26}$$

Where in the last step we used the relations of Eq.(13).

From the above equation it follows that

$$m^2 \leq \lambda_{J^2} \tag{27}$$

which means that eigenvalues of $\hat{J}_z$ operator bounded from below and above, i.e.

$$m_{min} \leq m \leq m_{max} \tag{28}$$

Step 7. Computation of the λ_{J^2} eigenvalues.

We now use Eq.(28) to calculate the value of λ_{J^2}. We first defined

$$\boxed{j \equiv m_{max}}, \tag{29}$$

and using Eq.(28) observe that

$$\hat{J}_+ \mid \psi_{\lambda_{J^2},j}\rangle = 0, \tag{30}$$

which is a mathematical statement that we reached the "top" eigenstate of $\hat{J}_z$ operator and can not step-up further. Multiplying Eq.(30) by $\hat{J}_-$ and using Eq.(18) one obtains:

$$\hat{J}_-\hat{J}_+ \mid \psi_{\lambda_{J^2},j}\rangle = (\hat{J}^2 - \hat{J}_z - \hat{J}_z^2 \mid \psi_{\lambda_{J^2},j}\rangle = \lambda_{J^2} - j - j^2 = \lambda_{J^2} - j(1+j) = 0. \tag{31}$$

From the above equation it follows that

$$\boxed{\lambda_{J^2} = j(j+1)} \tag{32}$$

where j was the maximal possible value of m.

We now want to evaluate the magnitude of m_{min} we For which we notice that:

$$\hat{J}_- \mid \psi_{\lambda_{J^2},j}\rangle = 0, \tag{33}$$

which is a mathematical statement that we reached the "bottom" eigenstate of $\hat{J}_z$ operator and can not step-down further. Multiplying Eq.(33) by $\hat{J}_+$ and using Eq.(18) one obtains:

$$\hat{J}_+\hat{J}_- \mid \psi_{\lambda_{J^2},j}\rangle = (\hat{J}^2 + \hat{J}_z - \hat{J}_z^2 \mid \psi_{\lambda_{J^2},j}\rangle = \lambda_{J^2} + m_{min} - m_{min}^2 = j(1+j) - m_{min}(m_{min}-1) = 0, \tag{34}$$

where in the last part of the derivation we used the previous result: $\lambda_{J^2} = j(j+1)$. The above equation has two solusions:

$$m_{min} = j+1 \quad \text{and} \quad m_{min} = -j. \tag{35}$$

Since by definition j was the highest possible magnitude of m, the only relevant solution will be the one:

$$m_{min} = -j \tag{36}$$

Thus we conclude that eigenvalue m has minimal and maximal value with equal absolute magnitude:

$$\boxed{-j \leq m \leq j} \tag{37}$$

In further considerations we will follow the convention in which whenever the eigenstate λ_{J^2} used as an index for the eigenstate it is denoted by j, i.e.

$$\mid \psi_{\lambda_{J^2},m}\rangle \equiv \mid \psi_{j,m}\rangle \tag{38}$$

Step 8. Allowed values of j.

Since the step-up and step-down operators change the value of m by one unit (changing it from -j to j), from Eq.(37) it follows that

$$j - (-j) = 2j = \text{integer} \tag{39}$$

thus we conclude that allowed values of j can be either integers or half integers.

$$\boxed{j = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, 2, \cdots} \tag{40}$$

Step 9. Matrix elements of $\hat{J}_\pm$ operators.

We now calculate the coefficients of proportionality in Eqs.(21) and (24) that we can define as:

$$\hat{J}_+ \mid \psi_{j,m}\rangle = a_{jm} \mid \psi_{j,m+1}\rangle \tag{41}$$

and

$$\hat{J}_- \mid \psi_{j,m}\rangle = b_{jm} \mid \psi_{j,m-1}\rangle. \tag{42}$$

For Eq.(41) calculating the inner product of the state $\mid \phi\rangle = a_{jm} \mid \psi_{j,m+1}\rangle$ one obtains

$$\langle\psi_{j,m+1} \mid a^*_{jm} a_{jm} \mid \psi_{j,m+1}\rangle = \mid a_{jm} \mid^2 = \langle\psi_{j,m} \mid \hat{J}^\dagger_+ \hat{J}_+ \mid \psi_{j,m}\rangle = \langle\psi_{j,m} \mid \hat{J}_- \hat{J}_+ \mid \psi_{j,m}\rangle \tag{43}$$

where in the last stage we used the relation $\hat{J}^\dagger_+ = \hat{J}_-$.

From Eq.(18) we can substitute $\hat{J}_-\hat{J}_+ = \hat{J}^2 - \hat{J}^2_z - \hat{J}_z$ into the above equation:

$$\mid a_{jm} \mid^2 = \langle\psi_{j,m} \mid \hat{J}^2 - \hat{J}^2_z - \hat{J}_z \mid \psi_{j,m}\rangle = j(j+1) - m(m+1) \tag{44}$$

Choosing phase factors such that a_{jm} to be real and using Eq.(41) one obtains:

$$\hat{J}_+ \mid \psi_{j,m}\rangle = a_{jm} \mid \psi_{j,m+1}\rangle = \sqrt{j(j+1) - m(m+1)} \mid \psi_{j,m+1}\rangle \tag{45}$$

With similar approach from Eq.(42) one obtains:

$$\langle\psi_{j,m-1} \mid b^*_{jm} b_{jm} \mid \psi_{j,m-1}\rangle = \mid b_{jm} \mid^2 = \langle\psi_{j,m} \mid \hat{J}^\dagger_- \hat{J}_- \mid \psi_{j,m}\rangle = \langle\psi_{j,m} \mid \hat{J}_+ \hat{J}_+ \mid \psi_{j,m}\rangle \tag{46}$$

where, now, in the last stage we used the relation $\hat{J}^\dagger_- = \hat{J}_+$. From Eq.(18) we can now substitute $\hat{J}_+\hat{J}_- = \hat{J}^2 - \hat{J}^2_z + \hat{J}_z$ into the above equation:

$$\mid b_{jm} \mid^2 = \langle\psi_{j,m} \mid \hat{J}^2 - \hat{J}^2_z + \hat{J}_z \mid \psi_{j,m}\rangle = j(j+1) - m(m-1) \tag{47}$$

Again, choosing phase factors such that b_{jm} to be real and using Eq.(42) one obtains:

$$\hat{J}_- \mid \psi_{j,m}\rangle = b_{jm} \mid \psi_{j,m+1}\rangle = \sqrt{j(j+1) - m(m-1)} \mid \psi_{j,m+1}\rangle. \tag{48}$$

Using Eq.(45) together with Eq.(41) we can calculate the matrix element of $\hat{J}_+$ operator as follows:

$$\langle\psi_{j,m'} \mid \hat{J}_+ \mid \psi_{j,m}\rangle = a_{jm}\ \delta_{m',m+1} = \sqrt{j(j+1) - m(m+1)}\ \delta_{m',m+1}. \tag{49}$$

With the similar approach Using Eq.(48) together with Eq.(42) we obtain:

$$\langle\psi_{j,m'} \mid \hat{J}_- \mid \psi_{j,m}\rangle = b_{jm}\delta_{m',m-1} = \sqrt{j(j+1) - m(m-1)}\ \delta_{m',m-1}. \tag{50}$$

Finally, for the future use we summarize the results of Eqs.(45) and (48) in the form

$$\boxed{\hat{J}_\pm \mid \psi_{j,m}\rangle = \sqrt{j(j+1) - m(m\pm 1)} \mid \psi_{j,m\pm 1}\rangle} \tag{51}$$

1.2 Generators of Rotation for Coordinate Wave Functions

Since we are discussing a rotation in the Euclidian space that is defined by space coordinates it is more convenient if we consider the above equation realize for coordinate wave function $\psi(r_i) \equiv \langle\psi_r \mid \psi\rangle$: where $\langle\psi_r \mid$, with r_i, $i = 1, 2, 3$ represents the eigenstate of coordnat operator $\hat{r}$. in 3d space of the reference frame where we are observing the given quantum state.

$$\langle\psi_r \mid \hat{R}(\hat{n},\epsilon) \mid \psi\rangle \approx \langle\psi_r \mid (I - i\hat{J}_i\hat{n}_i\epsilon) \mid \psi\rangle = \psi(r_i) - i\langle\psi_r \mid \hat{J}_i\hat{n}_i\epsilon \mid \psi\rangle = (1 - i\hat{L}_i\hat{n}_i\epsilon)\psi(r_i) = \psi'(r_i), \tag{52}$$

where by repeating indices i we assume a summation and where also we defined

$$\hat{L}_i\psi(r_i) = \langle\psi_r \mid \hat{J}_i \mid \psi\rangle. \tag{53}$$

In Eq.(52, $\psi'(r_i)$ describes the “rotated” (by ϵ angle around $\hat{n}$ axis) wave function observed in the same reference frame in which the quantum state was observed before the rotation. Now we recall the paradigm of “passive” and “active” transformations according to which the rotated by ϵ angle around $\hat{n}$ axis system is identical with the observation in which the reference frame is rotated by $-\epsilon$ around the same $\hat{n}$ axis. This result in a relation

$$\psi'(r_i) = \psi(r'_i), \tag{54}$$

where r_i' corresponds to the coordinates of wave function in the rotated (in the opposite direction) reference frame, thus:

$$r_i' = \hat{R}^{CL}(\hat{n}, -\epsilon)_{i,j} r_j, \tag{55}$$

where $\hat{R}^{CL}$ is the operator of rotation of euclidean vector in Classical Mechanics (see Eq.(54)). For rotation by $-\epsilon$ angle from Eq.(3) one has:

$$\delta r_i = r_i' - r_i = -\epsilon \sum_{i,j} \epsilon_{ijk} n_j, r_k = -\epsilon \left[n \times r\right]_i . \tag{56}$$

Comparing now Eqs.(52), (54) and (56) one obtains:

$$(1 - i\hat{L}_i \hat{n}_i \epsilon)\psi(r_i) = \psi(r_i') = \psi(r_i + \delta r_i). \tag{57}$$

Using the smallness of ϵ we can also expand the $\psi(r_i + \delta r_i)$ function into Taylor series keeping first order in ϵ

$$\psi(r_i + \delta r_i) \approx \psi(r_i) + \delta r_i \nabla_i \psi(r_i) = \psi(r_i) - \epsilon \left[n \times r\right]_i \nabla_i \psi(r_i), \tag{58}$$

where in the last part of the equation we used the relation of Eq.(56).

Comparing now Eqs.(57) and (58) one obtains:

$$\psi'(r_i) \approx (1 - i\hat{L}_i n_i \epsilon)\psi(r_i) = \psi(r_i) - \epsilon \left[n \times r\right]_i \nabla_i \psi(r_i) \tag{59}$$

which now can be solved for $\hat{L}_i$:

$$\hat{L}_i n_i = -i \left[n \times r\right]_i \nabla_i = -i \left[r \times \nabla\right]_i n_i \tag{60}$$

where we used a relation $[A \times B] \cdot C = [B \times C] \cdot A$ to express $[n \times r]_i \nabla_i = [r]_i n_i$. From above equation one obtains for the generator of rotation acted on the quant state:

$$\hat{L}_i = -i \left[r \times \nabla\right]_i \tag{61}$$

Remembering that this was the case of $\hat{J}_i$ acting on the state vector and projecting to the coordinate eigenstate wave one concludes that the expression for $\hat{L}_i$ acting on the quantum state in the Euclidean space will be:

$$\hat{L}_i = \frac{[\hat{r} \times \hat{p}]_i}{\hbar} \tag{62}$$

In the above equation we can introduce the operator of orbital angular momentum in the form:

$$\hat{L}_i^{QM} = \left[\hat{r} \times \hat{p}\right]_i \tag{63}$$

and conclude that the generator of rotations in Quantum Mechanics is related to the Orbital Angular Momentum operator as:

$$\hat{L}_i = \frac{\hat{L}_i^{QM}}{\hbar} \tag{64}$$

Note the interesting analogy that the generators of time and space translations $\hat{K}$ and $\hat{\mathbf{K}}_i$ were related the Hamiltonian and momentum operators in the form:

$$\hat{K} = \frac{\hat{H}}{\hbar} \qquad (65)$$
$$\hat{\mathbf{K}}_i = \frac{\hat{p}_i}{\hbar}$$

Going back to the generator of rotation $\hat{J}_i$, we notice that its particular representation in Eq.(62) is different from the representation in case of rotation of 3d-vector in Euclidean space Eq.(5). However due to the invariance of the algebra of generators, one still expects that generators of Eq.(62) to satisfy the relation:

$$[L_i, L_j] = i \sum_k \epsilon_{ijk} L_k \qquad (66)$$

Note: In the further discussions we adopt the notations in which we identify orbital orbital angular momentum operator with the generator of rotation in wave function representation, i.e.:

$$\hat{L}_i = \frac{\hat{L}^{QM}}{\hbar}. \qquad (67)$$

We will however distinguish it from $\hat{L}_i^{QM}$ which represents the "true" operator of orbital angular momentum.

1.3 General Definition of Spherical Symmetry in Quantum Mechanics

With the generator of rotation defined in Quantum Mechanics according to Eq.(62) we are able to give a formal definition of *Spherical Symmetry* in Quantum Mechanics.

Let us assume that we have a stationary quantum system that is characterize with Hamiltonion $\hat{H}$ such that :

$$\hat{H} \mid \psi\rangle = E \mid \psi\rangle \qquad (68)$$

where $\psi(r)$ is the wave function of the system in the considered reference frame.

Let us now rotate the quantum system around arbitrary $\hat{n}$ axis. Then for this rotated quantum system one has:

$$\hat{H} \mid \psi'\rangle = E' \mid \psi'\rangle \qquad (69)$$

We now state the Quantum System has a spherical symmetry if

$$\boxed{\mathrm{E} = \mathrm{E}'}. \qquad (70)$$

To see what are the mathematical consequence of the above relation we use the expression

$$\mid \psi'\rangle \approx (1 - i\hat{J}_i n_i \epsilon) \mid \psi\rangle \qquad (71)$$

in the LHS part of Eq.(69):

$$\hat{H} \mid \psi'\rangle = \hat{H}(1 - i\hat{J}_i n_i \epsilon) \mid \psi\rangle = E \mid \psi\rangle - i\hat{H}\hat{J}_i n_i \epsilon \mid \psi\rangle. \tag{72}$$

Applying now Eq.(71) to the RHS part of Eq.(69) and using condition of Eq.(70) one obtains:

$$E' \mid \psi'\rangle = E \mid \psi'\rangle = E(1 - i\hat{J}_i n_i \epsilon) \mid \psi\rangle = E \mid \psi\rangle - i\hat{J}_i n_i \epsilon \hat{H} \mid \psi\rangle. \tag{73}$$

where in the last part of the equation we moved E after $\hat{J}_i n_i \epsilon$ and used $E \mid \psi\rangle = \hat{H} \mid \psi\rangle$. Note that in the above expressions by the repeating indices of i we assume a summation: i.e. $\hat{J}_i n_i = \sum\limits_i \hat{J}_i n_i$

Subtracting now Eqs.(72) and (73) one obtains:

$$\left[\hat{H}, \hat{J}_i\right] = 0 \tag{74}$$

Thus we conclude that mathematical formulation of spherical symmetry in Quantum Mechanics is that the generator of rotation commutes with the Hamiltonian of quantum system.

If Eq.(74) is satisfied, one observes also the following commutator relation for $\hat{J}^2 = \sum_i \hat{J}_i \hat{J}_i$:

$$\left[\hat{J}^2 \hat{H}\right] = \hat{J}_i \hat{J}_i \hat{H} - H \hat{J}_i \hat{J}_i = H \hat{J}_i \hat{J}_i - H \hat{J}_i \hat{J}_i = 0 \tag{75}$$

Thus combining the above relation with Eqs.(7), (12) and (74) one obtains the following set of relations for Generators of Rotation in Quantum Mechanics,$\hat{J}_i$ and Hamiltonian $\hat{H}$.

$$[J_i, J_j] = i \sum_k \epsilon_{ijk} J_k, \quad [J^2, J_i] = 0, \quad \left[\hat{H}, \hat{J}_i\right] = 0, \quad \left[\hat{J}^2, \hat{H}\right] = 0. \tag{76}$$

The above relations indicate that there should be common eigenstates for operators $\hat{H}$, $\hat{J}^2$ and one of the components of $\hat{J}_i$ (Conventionally being chosen to be $\hat{J}_z$). The latter follows from the fact that operators $\hat{J}_i$ are mutually non-commutative, but each of them communicate with $\hat{J}$. Thus these eigenstates should satisfy simultaneously to the following relations:

$$\begin{aligned} \hat{H} \mid \psi_{E,j,m}\rangle &= E \mid \psi_{E,j,m}\rangle \\ \hat{J}^2 \mid \psi_{E,j,m}\rangle &= j(j+1) \mid \psi_{E,j,m}\rangle \\ \hat{J}_z \mid \psi_{E,j,m}\rangle &= m \mid \psi_{E,j,m}\rangle, \end{aligned} \tag{77}$$

where we used the result of Sec.1.1 according to which the eigenvalue of $\hat{J}^2$ operator is $j(j+1)$, where j is the maximal value of m.

1.3.1 Spherical Symmetry for the case of Coordinate Space Wave Functions

In Sec.1.2 we learned that rotation of coordinate wave functions are realized through the Angular Momentum operator defined as:

$$\hat{L}_i = \frac{[\hat{r}\times\hat{p}]_i}{\hbar}. \tag{78}$$

In analogy to Eq.(75) the spherical symmetry for the case of coordinate wave function will require the following condition to be satisfied:

$$\left[\hat{H},\hat{L}_i\right] = 0, \tag{79}$$

where now the Hamiltonian operator is defined as:

$$\hat{H} = -\frac{\hbar^2\nabla^2}{2m} + V(\vec{r}). \tag{80}$$

Before to check the condition of Eq.(79) it is useful to show that:

$$\begin{aligned}\left[\hat{p}_i,\hat{L}_j\right] &= i\sum_k \epsilon_{ijk}\hat{p}_k \\ \left[\hat{r}_i,\hat{L}_j\right] &= i\sum_k \epsilon_{ijk}\hat{r}_k.\end{aligned} \tag{81}$$

Using now Eq.(81) we can check the first part of the condition of Eq.(79):

$$\left[\frac{\hat{p}^2}{2m},\hat{L}_j\right] = \frac{1}{2m}\left[\hat{p}^2,\hat{L}_j\right] = \frac{1}{2m}\sum_i\left(\hat{p}_i\left[\hat{p}_i,\hat{L}_j\right] + \left[\hat{p}_i,\hat{L}_j\right]\hat{p}_i\right) = \frac{1}{2m}\sum_{ik}\left(\epsilon_{ijk}\hat{p}_i\hat{p}_k + \epsilon_{ijk}\hat{p}_k\hat{p}_i\right) = 0. \tag{82}$$

The last part is equal zero since the antisymmetric tensor ϵ_{ijk} couples with identical vectors p_k and p_i and there is a summation by i,k components.

To complete the proof of Eq.(79) one needs to show that

$$\left[V(\vec{r})),\hat{L}_j\right] = 0 \tag{83}$$

It can be shown (see appendix) that the above condition will be satisfied if the potential energy depends on the magnitude of r, i.e.

$$V(\vec{r}) = V(r). \tag{84}$$

In this case it is enough to show that

$$\left[\hat{r}^2,\hat{L}_j\right] = 0 \tag{85}$$

in order the condition of Eq.(83) to be satisfied. The proof of Eq.(85) proceeds similar to that of Eq.(82) using the relation for the commutator of $[\hat{r}_i,\hat{L}_j]$ from Eq.(81).

With this we conclude that in order the condition of Spherical Symmetry to be satisfied for the coordinate space wave function the condition is that the potential energy in the coordinate space representation of the Hamiltonian in Eq.(80) should depend on the magnitude of the coordinate r, (84).

With the spherical symmetry condition satisfied (Eq.(79) the analog of the Eq.(76) will be:

$$\left[\hat{L}_i, \hat{L}_j\right] = i \sum_k \epsilon_{ijk} \hat{L}_k, \quad \left[\hat{L}^2, \hat{L}_i\right] = 0, \quad \left[\hat{H}, \hat{L}_i\right] = 0, \quad \left[\hat{L}^2, \hat{H}\right] = 0. \tag{86}$$

and the one will have following system of eigenstate/eigenvalue equations:

$$\begin{aligned} \hat{H}\psi_{E,l,m}(r) &= E \cdot \psi_{E,l,m}(r) \\ \hat{L}^2\psi_{E,l,m}(r) &= l(l+1) \cdot \psi_{E,l,m}(r) \\ \hat{L}_z\psi_{E,l,m}(r) &= m \cdot \psi_{E,l,m}(r), \end{aligned} \tag{87}$$

where similar to Eq.(77) we denote the eigenvalue of $\hat{L}^2$ operator as $l(l+1)$ where l is the maximal value of m.

1.3.2 Calculating $\hat{L}^2$ and $\hat{L}_z$ Operators

$$\begin{aligned} \hbar^2 \hat{L}^2 &= \sum_i (\hat{r} \times \hat{p})_i (\hat{r} \times \hat{p})_i = \sum_i \sum_{jk} \epsilon_{ijk} \hat{r}_j \hat{p}_k \sum_{lm} \epsilon_{ilm} \hat{r}_l \hat{p}_m = \sum_i \sum_{jklm} \epsilon_{ijk}\epsilon_{ilm} \hat{r}_j \hat{p}_k \hat{r}_l \hat{p}_m \\ &= \sum_i \sum_{jklm} \epsilon_{ijk}\epsilon_{ilm} \hat{r}_j (\hat{r}_l \hat{p}_k - i\hbar\delta_{lk}) \hat{p}_m = \sum_{jklm} (\delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}) \hat{r}_j (\hat{r}_l \hat{p}_k - i\hbar\delta_{lk}) \hat{p}_m, \end{aligned} \tag{88}$$

were in the above derivations we used commutator relation:

$$[\hat{r}_l \hat{p}_k] = i\hbar\delta_{kl} \tag{89}$$

and sum rule relation for Levi-Civita matrices:

$$\sum_i \epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}. \tag{90}$$

Simplifying Eq.(88) further, one obtains:

$$\begin{aligned} \hbar^2 \hat{L}^2 &= \sum_{jklm} (\delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}) \hat{r}_j \hat{r}_l \hat{p}_k \hat{p}_m - i\hbar \sum_{jklm} (\delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}) \hat{r}_j \delta_{lk} \hat{p}_m = \\ &= \hat{r}^2 \hat{p}^2 - \sum_i \hat{r}_j (\sum_k \hat{r}_k \hat{p}_k) \hat{p}_j + 2i\hbar \sum_j \hat{r}_j \hat{p}_j. \end{aligned} \tag{91}$$

The above expression can be simplified further if we move from polar to cartesian coordinates. Using the derivative expression for the momentum operator, $\hat{p}_j = -i\hbar\frac{\partial}{\partial r_j}$ and relations of Eq.(**??**) one obtains

$$\sum_j \hat{r}_j \hat{p}_j = -i\hbar r \frac{\partial}{\partial r} \tag{92}$$

and

$$\sum_i \hat{r}_j (\sum_k \hat{r}_k \hat{p}_k) \hat{p}_j = -\hbar^2 r^2 \frac{\partial^2}{\partial r^2}. \tag{93}$$

Substituting above equations into Eq.(92) one arrives at:

$$\hbar^2 \hat{L}^2 = r^2 \hat{p}^2 + \hbar^2 r^2 \frac{\partial^2}{\partial r^2} + 2\hbar^2 r \frac{\partial}{\partial r} = r^2 \left(\hat{p}^2 + \hbar^2 \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \right). \tag{94}$$

In the above derivation we used the fact that in the coordinate space representation $\hat{r}_i = r_i$. Now if we use the polar coordinate representation of $\hat{p}^2$ operator.

$$\hat{p}^2 = -\hbar^2 \nabla^2 = -\hbar^2 \left(\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} \left(\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \sin\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin\theta^2} \frac{\partial^2}{\partial \phi^2} \right) \right), \tag{95}$$

in Eq.(94) one obtains:

$$\boxed{\hat{L}^2 = -\left(\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \sin\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin\theta^2} \frac{\partial^2}{\partial \phi^2} \right)}. \tag{96}$$

To calculate the $\hat{L}_z$ operator one again use the polar coordinate representation of cartesian derivatives. Using the explicit form of the $\hat{L}_z$ operator and Eq.(156) one obtains

$$\hbar \hat{L}_z = (\hat{r} \times \hat{p})_z = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) = -i\hbar \frac{\partial}{\partial \phi} \tag{97}$$

From above relation one obtains

$$\boxed{\hat{L}_z = -i \frac{\partial}{\partial \phi}}. \tag{98}$$

As it follows from Eqs.(96) and (98), the remarkable properties of $\hat{L}^2$ and $\hat{L}_z$ operators are that they are independent of the radios r and fully defined by polar angle θ and ϕ for the case of $\hat{L}^2$ and only ϕ for the case of $\hat{L}_z$ operators.

1.4 Eigenstates and Eigenvalues of Orbital Angular Momentum Operators

Because of the relation

$$\left[\hat{L}_i, \hat{L}_j\right] = i \sum_k \epsilon_{ijk} \hat{L}_k, \quad \left[\hat{L}^2, \hat{L}_i\right] = 0 \tag{99}$$

one can choose a common eigenstate for $\hat{L}^2$ and for one of the $\hat{L}_z$ operators.

$$\hat{L}^2 Y_l^m(\theta,\phi) = l(l+1)\cdot Y_l^m(\theta,\phi), \tag{100}$$

and

$$\hat{L}_z Y_l^m(\theta,\phi) = m\cdot Y_l^m(\theta,\phi), \tag{101}$$

where eigenstates $Y_l^m(\theta,\phi)$ reflect the fact that $\hat{L}^2$ (Eq.(96)) and $\hat{L}_z$ (Eq.(98)) depend only on polar angles θ and ϕ.

The spherical wave functions are normalized as follows:

$$\int Y_{l'}^{m'}(\theta,\phi)^\dagger Y_l^m(\theta,\phi) d\Omega = \delta_{l',l}\delta_{m',m} \tag{102}$$

1.4.1 Eigenstates and Eigenvalues of the $\hat{L}_z$ Operator

We first consider the solution of Eq.(101). Using Eq.(98) on obtains

$$\hat{L}_z Y_l^m(\theta,\phi) = -i\frac{\partial}{\partial\phi} Y_l^m(\theta,\phi) = m\cdot Y_l^m(\theta,\phi). \tag{103}$$

The above equation is a simple first order differential equation depending only on ϕ which indicates that we can look for the solution in the form in which θ and ϕ arguments are separated:

$$Y_l^m(\theta,\phi) = \Theta_{l,m}(\theta)\Phi_m(\phi). \tag{104}$$

Inserting this expression into Eq.(103) one obtains:

$$-i\frac{\partial}{\partial\phi}\Phi_m(\phi) = m\Phi_m(\phi), \tag{105}$$

whose solution has a form:

$$\Phi_m(\phi) = Ce^{im\phi}. \tag{106}$$

One can find the normalization constant and gain some idea about the magnitude of m by considering the orthonormality condition:

$$\int_0^{2\pi} \Phi_{m'}^\dagger(\phi)\Phi_m(\phi)d\phi = \delta_{m'm}. \tag{107}$$

For $m' = m$ one obtains

$$C^2 2\pi = 1 \quad \rightarrow \quad C = \frac{1}{\sqrt{2\pi}}. \tag{108}$$

Thus one obtains for the eigenstate of $\hat{L}_z$ operator:

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi} \tag{109}$$

Possible values of m: To evaluate the magnitude of m one first observes that, if $m' \neq m$ from Eq.(107) one obtains:

$$\frac{1}{2\pi(m'-m)} e^{(m'-m)2\pi} = 0 \tag{110}$$

which indicates that

$$m' - m = \text{integer}. \tag{111}$$

This result is in agreement with the Step.8 of Sec.1.1. However, mathematically the above relation does not indicate whether m is integer of half-integer.

However if one requires a singlevaluedness of the function, which will constrains the solution of Eq.(109) requiring that it reproduces itself after rotation by azimuthal angle 2π, i.e. $\phi \to \phi + 2\pi$ one arrive to the integer values for m.

Thus the requirement that the eigenstates of $\hat{L}_z$ operators are single valued results in a condition that eigenvalues of orbital angular momentum operators are integers.

1.4.2 Eigenvalues of Eigenstates of the $\hat{L}^2$ Operator

From the observation from the above subsection that that m should have integer value to satisfy singlevaluedness of eigenstate $\Phi_m(\phi)$ we conclude that l too should have an integer value.

To obtain the eigenstate of $\hat{L}^2$ operator, we use Eqs.(100,96) and Eq.(104) to obtain

$$\hat{L}^2\Theta_{l,m}(\theta)\Phi_m(\phi) = -\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin\theta^2}\frac{\partial^2}{\partial\phi^2}\right)\Theta_{l,m}(\theta)\Phi_m(\phi) = l(l+1)\Theta_{l,m}(\theta)\Phi_m(\phi). \tag{112}$$

Now using Eq.(101) the above equation reduces to the following differential equation:

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \left(l(l+1) - \frac{m^2}{\sin\theta^2}\right)\right]\Theta_{lm}(\theta) = 0. \tag{113}$$

Introducing a variable $z = \cos\theta$, the above equation can be presented in the form:

$$(1-z^2)\frac{d^2}{dz^2}\Theta_{l,m}(z) - 2z\frac{d}{dz}\Theta_{l,m}(z) + \left(l(l+1) - \frac{m^2}{(1-z^2)}\right)\Theta_{l,m}(z) = 0. \tag{114}$$

We can solve the above differential equation considering first the case $m = 0$, which reduces the above equation to the Legandre's equation"

$$(1-z^2)\frac{d^2}{dz^2}\Theta_{l,0}(z) - 2z\frac{d}{dz}\Theta_{l,0}(z) + l(l+1)\Theta_{l,0}(z). \tag{115}$$

Thus one can relate $\Theta_{l,0}(z)$ to the Legandre polinomials $P_l(z)$ which are solutions of the above equation.

$$\Theta_{l,0}(z) = C_{l,0}P_l(z) \tag{116}$$

where with $C_{l,0}$) we denote the constant of proportionality. For future application we may use the Rodrigues' representation of the Legandre polynomials in the form:

$$P_l(z) = \frac{1}{2^l l!}\frac{d^l}{dz^l}(z^2-1)^l. \tag{117}$$

Let us now consider Eq.(115) with Legandre Polinomials $P_l(z)$ and differentiate it m times: One obtains:

$$(1-z^2)\frac{d^2}{dz^2}u(z) - 2z(m+1)\frac{d}{dz}u(z) - (l-m)(l+m+1)u(z) = 0, \tag{118}$$

where

$$u(z) \equiv \frac{d^m}{dz^m}P_l(z). \tag{119}$$

We define now a new function referred to as Associated Legandre Functions

$$P_l^m(z) \equiv (1-z^2)^{\frac{m}{2}}u(z) = (1-z^2)^{\frac{m}{2}}\frac{d^m}{dz^m}P_l(z). \tag{120}$$

Using the above definition the Eq.(118) can be written as:

$$(1-z^2)\frac{d^2}{dz^2}P_l^m(z) - 2z\frac{d}{dz}P_l^m(z) + \left(l(l+1) - \frac{m^2}{(1-z^2)}\right)P_l^m(z) = 0. \tag{121}$$

Comparing the above equation with Eq.(114) we conclude that:

$$\Theta_{l,m} = C_{l,m}P_l^m(\cos\theta), \tag{122}$$

where $C_{l,m}$ is a normalization constant which can be fixed using the relation (need to be derived in the project)

$$\int\limits_0^\pi P_{l'}^m(\cos\theta)P_l^m(\cos\theta)d\cos\theta = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{l'l}. \tag{123}$$

Using the above equation for $\Theta_{l,m}$ function that is normalized to unity one obtains:

$$\Theta_{l,m}(\theta) = (-1)^m i^l \sqrt{\frac{(2l+1}{2}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta), \tag{124}$$

here $(-1)^m i^l$ is a phase factor that does not change the overall answer however is conventional in characterizing states with given orbital angular momentum and its projection in z direction.

The above derivation is made for $m \geq 0$. However we know that $-l \leq m \leq l$, thus m also have negative values symmetric to its positive magnitudes. The $-m$ cases of eigenstates can be obtained from the above solution if one assume that we changed the direction of $\hat{z}$ in the opposite direction.

In this case l will not change thus $P_l(\cos(\theta))$ should not change too, but $\frac{d}{dz}$ should change to $-\frac{d}{dz}$, which according to Eq.(119) will result in:

$$\Theta_{l,-m}(\theta) = (-1)^m \Theta_{l,|m|}(\theta). \tag{125}$$

Using Eqs.(124,125) together with Eq.(109) one arrives to the final expression for $Y_l^m(\theta, \phi)$

$$Y_l^m(\theta, \phi) = (-1)^{\frac{m+|m|}{2}} i^l \sqrt{\frac{(2l+1}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}} P_l^{|m|}(\cos\theta) e^{im\phi}. \tag{126}$$

The above functions generally referred to as Spherical Harmonics, with orthonormality conditions defined in Eq.(102).

One important property of Spherical Harmonics that frequently used is its space inversion property. If one replaces $\vec{r} \to -\vec{r}$, in the polar coordinates it corresponds to $r \to r$, $\theta \to \pi - \theta$ and $\phi \to \phi + \pi$. Using the properties of $\Phi_m(\phi)$ and $P_l^m(\cos\theta)$ functions, from Eq.(109) (117) and (120) one can show that:

$$Y_l^m(\pi - \theta, \phi + \pi) = (-1)^l Y_l^m(\theta, \phi) \tag{127}$$

2 Radial Part of the Schroedinger Wave Function Equation

Recall that we are considering a solution for Schroedinger wave equation:

$$\left(-\frac{\hbar^2 \nabla^2}{2m} + V(r) \right) \Psi_E(\vec{r}) = E \Psi_E(\vec{r}) \tag{128}$$

for spherically symmetric potential $V(r) \equiv V(|r|)$.

Using Eq.(95) for $-\hbar^2\nabla^2$ and Eq.(96 for $\hat{L}^2$ operators, the expression Eq.(128) can be written as:

$$-\frac{\hbar^2}{2m} \left(\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{\hat{L}^2}{r^2} \right) \Psi_{E,l,m}(r, \theta, \phi) + V(r) \Psi_{E,l,m}(r, \theta, \phi) = E \Psi_{E,l,m}(r, \theta, \phi), \tag{129}$$

where we also expressed the wave function in the polar coordinates. We can further separate the spherical part from the wave function in the form

$$\Psi_{E,l,m}(r, \theta, \phi) = R_{E,l,m}(r) Y_l^m(\theta, \phi), \tag{130}$$

where $R_{E,l,m}$ represents the radial part of the wave function. Substituting Eq.(130) back into Eq.(129) and using the fact that spherical part of the wave function is the eigenstate of the $\hat{L}^2$ operator (Eq.(100)) for Eq.(129) one obtains:

$$-\frac{\hbar^2}{2mr^2} \left[\left(\frac{d}{dr} r^2 \frac{d}{dr} - l(l+1) \right) + V(r) \right] R_{E,l}(r) = E R_{E,l}(r). \tag{131}$$

As it follows from the above equation it does not depend on eigenvalues of $\hat{L}_z$ operator m but depends on l. Thus one expects that the energy of the quantum particle under such potential will depend only on l. Since for any given l one has $2l+1$ different ms $(-l \leq m \leq l)$ one concludes that for spherical symmetric potentials there is a degeneracy in m in the order of $2l+1$.

Now we would like to analyze the general properties of the radial part of the wave function.

First, we notice from Eq.(131) that the radial part does not depend on m. Furthermore, for bound and unbound systems the normalization conditions for the total wave function are as follows:

$$\begin{aligned} &\text{for bound} \quad \int \mid \Psi_{E,l,m}(r,\theta,\phi) \mid^2 d^3r = 1 \\ &\text{for unbound} \quad \int \Psi^{\dagger}_{E',l,m}(r,\theta,\phi)\Psi_{E,l,m}(r,\theta,\phi) d^3r = \delta(E'-E). \end{aligned} \tag{132}$$

Using now the relation $d^3r = r^2 d\Omega$ and the normalization condition for the spherical harmonics (Eq.(102)) for the normalization condition of radial wave functions one obtains:

$$\begin{aligned} &\text{for bound} \quad \int \mid R_{E,l}(r) \mid^2 r^2 dr = 1 \\ &\text{for unbound} \quad \int R^{\dagger}_{E',l}(r) R_{E,l}(r) r^2 dr = \delta(E'-E). \end{aligned} \tag{133}$$

For the proceeding discussion we express the radial wave function through the new function $u_{E,l}(r)$ in the form:

$$R_{E,l}(r) \equiv \frac{u_{E,l}(r)}{r}, \tag{134}$$

for which the normalization conditions now become:

$$\begin{aligned} &\text{for bound} \quad \int \mid u_{E,l}(r) \mid^2 2dr = 1 \\ &\text{for unbound} \quad \int u^{\dagger}_{E',l}(r) u_{E,l}(r) dr = \delta(E'-E). \end{aligned} \tag{135}$$

One **general** property of $u_{E,l}(r)$ function is that, in order $R_{E,l}(r)$ to be finite at the origin

$$\lim_{r\to 0} u_{E,l}(r) \to r^{1+\beta} \to 0, \quad \text{with} \quad \beta \geq 0, \tag{136}$$

otherwise radial wave function in Eq.(134) will not be finite at the origin.

Substituting Eq.(134) in Eq.(131) on now obtains:

$$\begin{aligned} &-\frac{\hbar^2}{2mr^2}\left(\frac{d}{dr}r^2\frac{d}{dr}\right)\frac{u_{E,l}(r)}{r} + \frac{\hbar^2}{2mr^2}l(l+1)\frac{u_{E,l}(r)}{r} + V(r)\frac{u_{E,l}(r)}{r} = \\ &-\frac{\hbar^2}{2mr^2}\left(\frac{d}{dr}(u'_{E,l}r - u_{E,l})\right) + \left(\frac{\hbar^2}{2mr^2}l(l+1) + V(r)\right)\frac{u_{E,l}(r)}{r} \\ &-\frac{\hbar^2}{2mr}u''_{E,l}(r) + \left(\frac{\hbar^2}{2mr^2}l(l+1) + V(r)\right)\frac{u_{E,l}(r)}{r} = E\frac{u_{E,l}(r)}{r} \end{aligned} \tag{137}$$

where by $'$ we defined the $\frac{d}{dr}$ derivatives. Cancelling the $\frac{1}{r}$ parts in the last part of the above equation, one arrives at:

$$-\frac{\hbar^2}{2m}u''_{E,l}(r) + V_{eff}(r)u_{E,l}(r) = Eu_{E,l}(r), \tag{138}$$

where

$$V_{eff} \equiv \frac{\hbar^2}{2mr^2}l(l+1) + V(r). \tag{139}$$

The most striking result of Eq.(138) is that it analytically identical with the one dimensional Schroedinger equation:

$$-\frac{\hbar^2}{2m}\psi(x) + V(x)\psi(x) = E\psi(x) \tag{140}$$

with differences such as: (a) $0 \leq r \leq \infty$ while $-\infty \leq x \leq \infty$, (b) It is only required that $\psi(x)$ to be finite at any x, while for the radial wave function, $u_{E,l}$ in addition of finiteness it should be zero at the origin (see Eq.(136). (c) Finally instead of potential energy $V(x)$ for the radial case one has $V_{eff}(r)$ defined according to Eq.(139). The additional term in V_{eff} can be associated with the centrifugal motion.

We now consider Eq.(138) to obtain several asymptotic values for the radial wave function in the $r \to \infty$ and $r \to 0$ limits.

First, we consider $r \to \infty$ limit assuming:

$$\lim_{r\to\infty} V(r) \sim \frac{const}{r^\alpha} \to 0 \quad \text{with} \quad \alpha > 1. \tag{141}$$

At this limit Eq.(138) becomes:

$$-\frac{\hbar^2}{2m}u''_{E,l}(r) = Eu_{E,l}(r). \tag{142}$$

For the case of $\boxed{E > 0}$ the above equation has two solutions

$$u_+(r) = Ae^{ikr} \quad \text{and} \quad u_-(r) = Be^{ikr} \tag{143}$$

that corresponds to diverging and converging radial waves for function $R_{E,l}(r)$:

$$R_+(r) = A\frac{e^{ikr}}{r} \quad \text{and} \quad R_-(r) = B\frac{e^{ikr}}{r} \tag{144}$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$ and A and B are constants.

For the case of $\boxed{E < 0}$ Eq.(142) has the two following solutions:

$$u_+(r) = Ce^{\kappa r} \quad \text{and} \quad u_-(r) = De^{-\kappa r}, \tag{145}$$

resulting in:

$$R_+(r) = C\frac{e^{\kappa r}}{r} \quad \text{and} \quad R_-(r) = D\frac{e^{-\kappa r}}{r} \tag{146}$$

where $\kappa = \sqrt{\frac{-2mE}{\hbar^2}}$, with C and D being constant. Here we observe that $R_+(r)$ solution is not finite at infinity thus is not physical and can be discarded. This results in the final expression of the asymptotic form of the radial wave function:

$$R_-(r) = D\frac{e^{-\kappa r}}{r}, \tag{147}$$

which is exponentially decreasing function with the distance that is characteristic to the bound system.

First, we consider $r \to 0$ limit assuming that potential is such thath

$$\lim_{r\to 0} V(r)r^2 = 0, \tag{148}$$

that it has slower than $\frac{1}{r^2}$ dependence at the origin. In this case one can neglect by the potential energy in Eq.(**??**) but keep the centrifugal part, i.e.:

$$-\frac{\hbar^2}{2m}u''_{E,l}(r) + \frac{\hbar^2}{2mr^2}l(l+1)u_{E,l}(r) = Eu_{E,l}(r). \tag{149}$$

Since we consider finite values for energy E and according to Eq.(136) one expects $u_{E,l}(r)$ to disappear at the origin, in the above equation one can also neglect the $Eu_{E,l}(r)$ part of the equation compare to centrifugal as well as derivative parts of the equation arriving at:

$$-\frac{\hbar^2}{2m}u''_{E,l}(r) + \frac{\hbar^2}{2mr^2}l(l+1)u_{E,l}(r) = 0. \tag{150}$$

The solution for the above equation one can look in the form of:

$$u_{E,l}(r) \approx const r^{\alpha}. \tag{151}$$

Inserting the above form in Eq.(150) one obtains:

$$\alpha(\alpha-1)\frac{u_{E,l}}{r^2} = l(l+1)\frac{u_{E,l}}{r^2} \quad \to \quad \alpha(\alpha-1) = l(l+1). \tag{152}$$

The RHS part of the equation has two solutions:

$$\text{(a)} \quad \alpha = l+1 \quad \text{and} \quad \text{(b)} \quad \alpha = -l. \tag{153}$$

Since one expects the $u_{E,l}(r)$ function to disappear at the origin one concludes that only (a) represents the physical solutions. Therefor one obtains:

$$u_{E,l} = const \cdot r^{l+1} \quad \text{and} \quad R_{E,l}(r) \equiv \frac{u_{E,l}(r)}{r} = const \cdot r^l. \tag{154}$$

The above result indicates that quantum states with high orbital angular momentum approach to zero at the origin faster while for the case of $l = 0$ the radial function can be finite at the origin.

3 Appendix A

$$\begin{aligned}
\frac{\partial}{\partial x} &= \sin\theta\cos\phi\frac{\partial}{\partial r} + \cos\theta\cos\phi\frac{1}{r}\frac{\partial}{\partial\theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi} \\
\frac{\partial}{\partial y} &= \sin\theta\sin\phi\frac{\partial}{\partial r} + \cos\theta\sin\phi\frac{1}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi} \\
\frac{\partial}{\partial z} &= \cos\theta\frac{\partial}{\partial r} - \sin\theta\frac{1}{r}\frac{\partial}{\partial\phi}
\end{aligned} \tag{155}$$