Quantum Mechanics 2

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Chapter 1

Orbital Angular Momentum

1.1 Basics of QM

Let us recall some basic facts of quantum mechanics.

The expectation value of an observable $\mathcal{A}$ with an associated operator $\hat{A}$ is given by,

$$\left\langle \hat{A} \right\rangle = \langle\Psi|\, \hat{A}\, |\Psi\rangle = \int \Psi^* \hat{A} \Psi \, \mathrm{d}\mathbf{r}\,. \tag{1.1}$$

The fundamental position, momentum, and angular momentum operators are defined as follows,

Definition 1: Fundamental Operators

$$\hat{\mathbf{r}} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}} \tag{1.2}$$

$$\hat{p} = -i\hbar\boldsymbol{\nabla} \tag{1.3}$$

$$\hat{L}_i = \varepsilon_{ijk}\hat{r}_j\hat{p}_k \tag{1.4}$$

The Hamiltonian is defined,

Definition 2: Hamiltonian

$$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}, t). \tag{1.5}$$

We obtain the wavefunction Ψ by solving the TDSE,

Definition 3: Time Dependent Schrodinger Equation

$$i\hbar\frac{\partial\Psi(\mathbf{r}, t)}{\partial t} = \hat{H}\Psi(\mathbf{r}, t). \tag{1.6}$$

For the static case, this reduces to the TISE,

$$\hat{H}\Psi = E\Psi. \tag{1.7}$$

If $\Psi(\mathbf{r}, 0)$ is written in the energy eigenbasis, i.e., $\Psi(\mathbf{r}, 0) = \sum_i c_i |E_i\rangle$, then the time-dependent solution is trivial,

$$\Psi(\mathbf{r}, t) = \sum_i c_i |E_i\rangle \exp\left(\frac{-iE_i t}{\hbar}\right). \tag{1.8}$$

1.1.1 The Simple Harmonic Oscillator

The SHO has a Hamiltonian,

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2 x^2 \tag{1.9}$$

with energy eigenvalues,

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{1.10}$$

and has normalised Eigenfunctions,

$$\psi_n(x) = \left(\frac{1}{n!2^n a\sqrt{\pi}}\right) H_n\left(\frac{x}{a}\right) \exp\left(-\frac{x^2}{2a^2}\right) \tag{1.11}$$

where $a = \sqrt{\hbar/m\omega}$ and $H_n(x/a)$ is a Hermite polynomial.

1.1.2 Simple Perturbation Theory

In simple perturbation theory, we write the Hamiltonian as,

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{1.12}$$

where the Hamiltonian $\hat{H}_0$ is trivial and for which we already have obtained its eigenfunction ψ and eigenvalues $E_n^{(0)}$. We then use this to find the expectation value of the total Hamiltonian,

$$\left\langle \hat{H} \right\rangle = \langle\psi|\, \hat{H}_0 + \hat{V}\, |\psi\rangle = E_n^{(0)} + \Delta E. \tag{1.13}$$

Writing this more explicitly,

Definition 4: First Order Perturbation Theory

$$E_n = E_n^{(0)} + \langle\psi|\, \hat{V}\, |\psi\rangle \tag{1.14}$$

1.2 Particle in 2D SHO

The Hamiltonian of the 2D SHO is given by,

$$\hat{H}\psi(x,y) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{1}{2}m\omega(x^2+y^2)\psi(x,y) = E\psi(x,y) \tag{1.15}$$

We can separate this Hamiltonian into its x and y components,

$$\hat{H}_x = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega x^2 \qquad \hat{H}_y - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2}m\omega y^2. \tag{1.16}$$

We know the solution to the 1D SHO, as by eq. (1.10). We can intuit that the total solution of the 2D Hamiltonian will be a product of the two 1D wavefunctions. This comes from the fact that to add probabilities, we multiply the probability densities. So, we write,

$$\begin{aligned}
\hat{H}\psi_{n_x}(x)\psi_{n_y}(y) &= \left(\hat{H}_x + \hat{H}_y\right)\psi_{n_x}(x)\psi_{n_y}(y) \\
&= \left(\hat{H}_x\psi_{n_x}(x)\right)\psi_{n_y}(y) + \psi_{n_x}(x)\left(\hat{H}_y\psi_{n_y}(y)\right) \\
&= \left(n_x + \frac{1}{2}\right)\hbar\omega\psi_{n_y}(y) + \left(n_y + \frac{1}{2}\right)\hbar\omega\psi_{n_x}(x) \\
&= (n_x + n_y + 1)\,\hbar\omega\psi_{n_x}(x)\psi_{n_y}(y) \\
\implies E_{n_x,n_y} &= (n_x + n_y + 1)\hbar\omega.
\end{aligned} \tag{1.17}$$

1.2.1 Degeneracy

This is when there is more than one state with the same energy. The degeneracy D is the number of energy states that share the same energy. Non-degenerate states are those with $D = 1$.

1.3 Orbital Angular Momentum

The angular momentum in given direction in a classical system is given by,

$$L_i = \varepsilon_{ijk} r_j p_k. \tag{1.18}$$

The angular momentum operator in quantum mechanics is thus,

$$\hat{L}_i = \varepsilon_{ijk} \hat{r}_j \hat{p}_k. \tag{1.19}$$

We are particularly interested in the case where $i = z$, in which case the operator becomes,

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = -i\hbar \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right). \tag{1.20}$$

Let us consider this operator in plane polar coordinates, (r, θ). We have,

$$x = r\cos\theta \qquad\qquad y = r\sin\theta \tag{1.21}$$

Let us consider the following,

$$\begin{aligned} \frac{\partial}{\partial\theta} &= \frac{\partial x}{\partial\theta}\frac{\partial}{\partial x} + \frac{\partial y}{\partial\theta}\frac{\partial}{\partial y} = -r\sin\theta\frac{\partial}{\partial x} + r\cos\theta\frac{\partial}{\partial y} \\ &= -y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y}. \end{aligned} \tag{1.22}$$

So, in plane polars,

Definition 5: Angular Momentum Operator in Z

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\theta}. \tag{1.23}$$

1.3.1 Eigenfunctions and Eigenvalues of $\hat{L}_z$

We wish to consider the following,

$$\hat{L}_z\Theta(\theta) = L_z\Theta(\theta). \tag{1.24}$$

So,

$$-i\hbar\frac{\mathrm{d}\Theta}{\mathrm{d}\theta} = L_z\Theta \tag{1.25}$$

which we can solve trivially,

$$\Theta(\theta) = Ae^{\frac{L_z\theta}{\hbar}} \tag{1.26}$$

where $A = \frac{1}{\sqrt{2\pi}}$ is a normalisation constant. We require a cyclic boundary condition, such that $\Theta(\theta) = \Theta(\theta + 2\pi)$. So,

$$\begin{aligned} Ae^{\frac{iL_z(\theta+2\pi)}{\hbar}} &= Ae^{\frac{iL_z\theta}{\hbar}} \\ e^{\frac{iL_z 2\pi}{\hbar}} &= 1. \end{aligned} \tag{1.27}$$

Not all values of L_z satisfy the eq. (1.27), so we have to impose the following restriction,

$$L_z = \hbar m, \quad m \in \mathbb{Z} \tag{1.28}$$

and thus, we can write the angular momentum eigenfunction as,

Definition 6: Angular Momentum Eigenfunction

$$\Theta_m(\theta) = \frac{1}{\sqrt{2\pi}}e^{im\theta} \tag{1.29}$$

1.3.2 Angular Momentum of the 2D SHO

We wish to express eigenfunctions of the 2D SHO as eigenfunctions of angular momentum. we will find that we require a combination of all degenerate eigenfunctions for a givevn D in order to represent angular momentum eigenfunction. Observing the ground state,

$$\Psi_{00}(x,y) = e^{-\frac{x^2}{2a^2}} \cdot e^{-\frac{y^2}{2a^2}} = e^{-\frac{r^2}{2a^2}}, \qquad a^2 = \frac{\hbar}{2m}. \tag{1.30}$$

Applying the angular momentum operator we find,

$$\hat{L}_z \Psi_{00} = 0 \cdot \Psi_{00} \tag{1.31}$$

which holds, as 0 is an allowed value of m. The first excited states of $D = 2$ are given by,

$$\Psi_{10} = xe^{-\frac{x^2}{2a^2}} \cdot e^{-\frac{y^2}{2a^2}} \qquad\qquad \Psi_{01} = e^{-\frac{x^2}{2a^2}} \cdot ye^{-\frac{y^2}{2a^2}} \tag{1.32}$$

which we combine to form,

$$\begin{aligned} \Psi_\pm &= \Psi_{10} \pm i\Psi_{01} \\ &= [r\cos\theta \pm ir\sin\theta]\, e^{-\frac{r^2}{2a^2}} = re^{\pm i\theta} e^{-\frac{r^2}{2a^2}}. \end{aligned} \tag{1.33}$$

Applying $\hat{L}_z$ to eq. (1.33),

$$\hat{L}_z \Psi_\pm = \pm\hbar\Psi_\pm \tag{1.34}$$

$\implies \Psi_\pm$ is an eigenfunction of $\hat{L}_z$ with eigenvalues $\pm\hbar$. Furthermore, $\Psi_\pm$ is an eigenfunction of $\hat{H}$, so $\hat{H}$ and $\hat{L}_z$ commute. This allows for the 2D SHO to be described by *good quantum numbers*. These satisfy the following,

1. Can be known simultaneously,
2. Fully and uniquely specify the state of a system.

For the 2D SHO, its good quantum numbers are (n, m), where $n = n_x + n_y$. n specifies the energy of the system (as by $E_n = (n+1)\hbar\omega$), and m specifies the angular momentum of the system (as by $L_z = m\hbar$).

1.3.3 3D Angular Momentum

Definition 7: Angular Momentum Commutation Relation

$$\left[\hat{L}_i, \hat{L}_j\right] = \epsilon_{ijk} i\hbar \hat{L}_k \tag{1.35}$$

where i, j, k indicate orthogonal directions.

The above definition indicates that components of $\hat{L}_i$ do not commute in different directions, however it can be shown that,

$$\left[\hat{L}^2, \hat{L}_i\right] = 0. \tag{1.36}$$

Proof.

$$\begin{aligned} \hat{L}^2 &= \sum_j \hat{L}^2 \\ \left[\hat{L}^2, \hat{L}_i\right] &= \sum_j \left[\hat{L}_j^2, \hat{L}_i^2\right] \\ &= \sum_j \left(\hat{L}_j \left[\hat{L}_j, \hat{L}_i\right] + \left[\hat{L}_j, \hat{L}_i\right] \hat{L}_j\right) \\ &= i\hbar \sum_{j,l} \left(\hat{L}_j \varepsilon_{ijk} \hat{L}_k + \underbrace{\hat{L}_k \varepsilon_{ijk} \hat{L}_j}_{-\varepsilon_{ijk}\hat{L}_j\hat{L}_k}\right) \\ &= \sum_{j,l} \left(\hat{L}_j \hat{L}_k - \hat{L}_j \hat{L}_k\right) = 0 \end{aligned} \tag{1.37}$$

□

Eigenvalues and eigenfunctions of Angular Momentum

It can be shown that the angular momentum operators in the 3 cardinal directions expressed in polar coordinates are given by,

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi} \tag{1.38}$$