Lecture 8
Symmetries, conserved quantities, and the labeling of states
Angular Momentum

Today's Program:

1. Symmetries and conserved quantities – labeling of states
2. Ehrenfest Theorem – the greatest theorem of all times (in Prof. Anikeeva's opinion)
3. Angular momentum in QM
4. Finding the eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$ - the spherical harmonics.

Questions you will by able to answer by the end of today's lecture

1. How are constants of motion used to label states?
2. How to use Ehrenfest theorem to determine whether the physical quantity is a constant of motion (i.e. does not change in time)?
3. What is the connection between symmetries and constant of motion?
4. What are the properties of "conservative systems"?
5. What is the dispersion relation for a free particle, why are ***E*** and ***k*** used as labels?
6. How to derive the orbital angular momentum observable?
7. How to check if a given vector observable is in fact an angular momentum?

References:

1. Introductory Quantum and Statistical Mechanics, Hagelstein, Senturia, Orlando.
2. Principles of Quantum Mechanics, Shankar.
3. http://mathworld.wolfram.com/SphericalHarmonic.html

Symmetries, conserved quantities and constants of motion – how do we identify and label states (good quantum numbers)

The connection between symmetries and conserved quantities:

In the previous section we showed that the Hamiltonian function plays a major role in our understanding of quantum mechanics using it we could find both the eigenfunctions of the Hamiltonian and the time evolution of the system.

What do we mean by when we say an object is symmetric? What we mean is that if we take the object perform a particular operation on it and then compare the result to the initial situation they are indistinguishable. When one speaks of a symmetry it is critical to state symmetric with respect to which *operation.*

How do symmetries manifest themselves in equations? Let us suppose that your system is symmetric with respect to translations in $\boldsymbol{x}$ that would imply that any physical property could not have an $\boldsymbol{x}$ dependence. In particular the energy would not have an explicit dependence on $\boldsymbol{x}$ thus:

$$\frac{\partial H(x,p)}{\partial x} = 0 = -\frac{dp}{dt} \Rightarrow p = const$$

The momentum in this case is called a constant of motion. **This illustrates a fundamental connection between symmetries and conserved quantities. In fact, every symmetry in a physical system implies an associated conserved quantity.**

In quantum mechanics the time evolution of an observable is describe by the following equation:

Ehrenfest Theorem:

$$\boxed{\begin{aligned} &\frac{d}{dt}\langle \hat{A}\rangle = \frac{1}{i\hbar}\left\langle \left[\hat{A},\hat{H}\right]\right\rangle + \left\langle \frac{\partial \hat{A}}{\partial t}\right\rangle \\ &\frac{d}{dt}\langle \psi(x)|\hat{A}|\psi(x)\rangle = \frac{1}{i\hbar}\langle \psi(x)|\left[\hat{A},\hat{H}\right]|\psi(x)\rangle + \langle \psi(x)|\frac{\partial \hat{A}}{\partial t}|\psi(x)\rangle \end{aligned}}$$

Consequently in order for a physical quantity to be a constant of motion the corresponding observable has to obey the following relationships:

$$\begin{cases} \dfrac{\partial \hat{A}}{\partial t} = 0 \\ \left[\hat{A},\hat{H}\right] = 0 \end{cases} \Rightarrow \frac{d}{dt}\langle \hat{A}\rangle = 0$$

States are labeled by specific values of their properties, which do not change with time – these properties are called constants of motion. We learned that in QM physical properties are represented by operators and that the values of properties obtained in measurements are eigenvalues of the corresponding operators. **Hence the eigenvalues are used as the labels.**

Conserved Quantities Example 0: Conservative Systems

The simplest example of a conserved quantity is Energy. Two lectures ago we have considered systems, where Hamiltonian does not depend on time explicitly. Obviously Hamiltonian commutes with itself and consequently energy is conserved and can be used as a label for a state.

$$\left.\begin{array}{c}\dfrac{\partial \hat{H}}{\partial t}=0\\ \left[\hat{H},\hat{H}\right]=0\end{array}\right\}\Rightarrow \frac{d}{dt}\langle \hat{H}\rangle=0\Rightarrow E=const\Rightarrow u_E(x)\Rightarrow \psi(x,t)=\sum_E u_E(x)e^{-i\frac{E}{\hbar}t}$$

Reminder:

Schrodinger's equation: $\left[-\frac{\hbar^2}{2m}\vec{\nabla}+V(\vec{r})\right]\psi(\vec{r},t)=i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)$

This type of differential equation is separable, i.e. we can look for a solution in the following form: $\psi(\vec{r},t)=\varphi(\vec{r})\xi(t)$. Let's substitute it into the Schrodinger's equation above:

$$\left[-\frac{\hbar^2}{2m}\vec{\nabla}+V(\vec{r})\right]\varphi(\vec{r})\xi(t)=i\hbar\frac{\partial}{\partial t}\varphi(\vec{r})\xi(t)$$

$$\frac{1}{\varphi(\vec{r})}\left\{\left[-\frac{\hbar^2}{2m}\vec{\nabla}+V(\vec{r})\right]\varphi(\vec{r})\right\}=\frac{1}{\xi(t)}i\hbar\frac{\partial}{\partial t}\xi(t)$$

Note that the left side of the equation only depends on position $\vec{r}$ and the right side of the equation only depends on time $\boldsymbol{t}$. This can only be true when both sides of the equation are constant $\boldsymbol{E}$ – for energy. Then the equation above splits into the following two equations:

$$(I)\quad i\hbar\frac{d}{dt}\xi(t)=E\xi(t)\Rightarrow \xi(t)=e^{-i\frac{E}{\hbar}}$$

$$(II)\quad \left[-\frac{\hbar^2}{2m}\vec{\nabla}^2+V(\vec{r})\right]\varphi(\vec{r})=E\varphi(\vec{r})\Rightarrow u_E(x),\quad E$$

Then the solutions to time-dependent Schrodinger's equation will have a form:

$$\psi_E(\vec{r},t)=u_E(\vec{r})\xi_E(t)=u_E(\vec{r})e^{-i\frac{E}{\hbar}t}$$

In general, since the Hamiltonian may have many eigenvalues and corresponding eigenfunctions, the solution for this system is a linear combination of all the possible solutions corresponding to different energies:

$\Psi(\vec{r},t)=\sum_E C_E u_E(\vec{r})e^{-i\frac{E}{\hbar}t}$, where $\boldsymbol{C_E}$ are the coefficients that can be determined from the initial and boundary conditions.

This is a very important result: If we know the special wavefunctions (Hamiltonian eigenfunctions) we can easily find time evolution of this conserveative system.

If we know *E* and $u_E(\vec{r})$ then we know $\Psi(\vec{r},t)$ at any time!

Conserved Quantities Example I: Particle in free space

Labeling of states is particularly important when the energy eigenvalues are degenerate such as in the case of the particle in free space:

$$\hat{H}\psi(x) = E\psi(x) \Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\psi(x) \Rightarrow u_E(x) = \begin{cases} e^{i\sqrt{\frac{2mE}{\hbar^2}}x} \\ e^{-i\sqrt{\frac{2mE}{\hbar^2}}x} \end{cases}$$

Using the energy as a "label" doesn't completely and uniquely specify a state.

What about momentum? – If momentum is a constant of motion then we can use it as an additional label to uniquely specify the eigenstate. We have shown earlier that the momentum operator commutes with free space Hamiltonian, and since it does not explicitly depend on time then momentum is indeed a constant of motion.

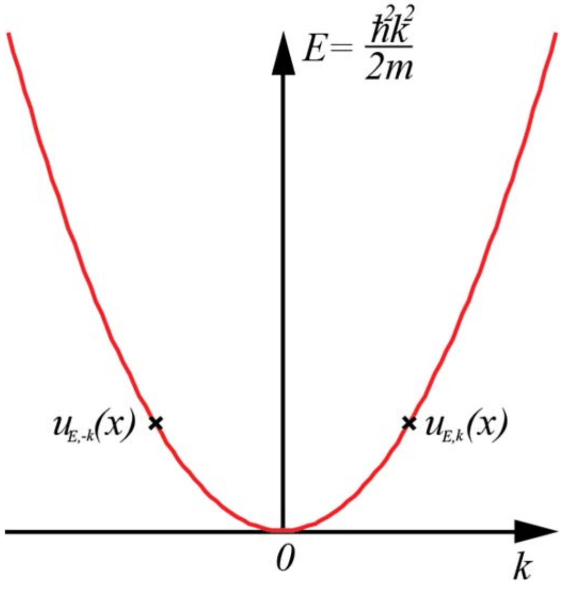
$$\left.\begin{array}{c} \hat{p} = -i\hbar\frac{\partial}{\partial x} \Rightarrow \frac{\partial \hat{p}}{\partial t} = 0 \\ \left[\hat{p}, \hat{H}\right] = 0 \end{array}\right\} \Rightarrow \frac{d}{dt}\langle \hat{p} \rangle = 0$$

Therefore the momentum is a conserved quantity and its eigenvalues can be used to label the states. Then the unique labels for the eigenfunctions above would be:

$$u_{E,k}(x) = e^{ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$u_{E,-k}(x) = e^{-ikx}$$

In fact we represent all the eigenfunctions (eigenstates) of the free space Hamiltonian and the momentum on the ***E*** vs ***k*** plot. Every point on this plot uniquely and completely specifies the state.



Conserved Quantities Example II: Parity operator and symmetric potentials

Definition of a parity operator: $\hat{\Pi}\psi(x)=\psi(-x)$

What are the eigenfunctions and eigenvalues of the parity operator:

$$\hat{\Pi}u(x)=\lambda u(x)\Rightarrow\hat{\Pi}\hat{\Pi}u(x)=\hat{\Pi}\lambda u(x)\Rightarrow\hat{\Pi}\hat{\Pi}u(x)=\lambda\hat{\Pi}u(x)\Rightarrow u(x)=\lambda^2u(x)\Rightarrow\lambda=\pm1$$

The eigenfunctions of the parity operator all are either odd or even.

f (−x)= f (x) even

f (−x)−= f (x) odd□

Does Hamiltonian for Simple Harmonic Oscillator commute with the parity operator?

$$\hat{H}(x)=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac{1}{2}m\omega^2x^2\Rightarrow\hat{H}(-x)=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial(-x)^2}+\frac{1}{2}m\omega^2(-x)^2=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac{1}{2}m\omega^2x^2=\hat{H}(x)$$

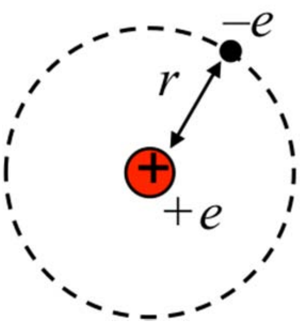
Let’s check the commutator:

$$\left[\hat{\Pi},\hat{H}\right]\psi(x)=\hat{\Pi}\hat{H}\psi(x)-\hat{H}\hat{\Pi}\psi(x)=\hat{\Pi}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac{1}{2}m\omega^2x^2\right)\psi(x)-\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac{1}{2}m\omega^2x^2\right)\psi(-x)=$$

$$=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial(-x)^2}+\frac{1}{2}m\omega^2(-x)^2\right)\psi(-x)-\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac{1}{2}m\omega^2x^2\right)\psi(-x)=0$$

This means that one can always find a set of eigenfunctions common to $\hat{H}$ and $\hat{\Pi}$. In fact, last lecture we have shown that SHO eigenfunctions are always even or odd.

Conserved Quantities Example II: Angular momentum and spherical symmetry



Consider a system with a spherical symmetry, such as Hydrogen atom:

Hydrogen atom consists of a proton with a positive charge $q = e = 1.6\times10^{-19}$ C an electron charge $-q = -e$. Consequently they are bound by a Coulombic potential:

$$V(r) = -\frac{q^2}{4\pi\varepsilon_0}\frac{1}{r} = -\frac{e^2}{r}$$

Where: $\varepsilon_0 = 8.85\times10^{-12}$ F/m is the permittivity of free space.

As you can notice this potential does not depend on the respective position of the proton and the electron but only on the distance between them, i.e. if electron revolves by a certain angle around the proton the potential will stay the same.

In the system with such spherical symmetry, i.e. independence of the Hamiltonian on the direction of the position vector just the length, the angular momentum is conserved – this is very important as we will use this conservation later to use it for labeling of the states associated with a spherically symmetric system.

But first let's just find out what is angular momentum in quantum mechanics, as usual we use the classical mechanics to build some intuition.

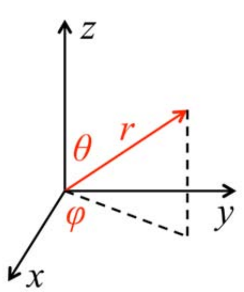
Classical angular momentum is a vector quantity defined as:

$$\vec{L} = \vec{r}\times\vec{p} = \begin{vmatrix} \hat{i}_x & \hat{i}_y & \hat{i}_z \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = \hat{i}_x\left(yp_z - zp_y\right) + \hat{i}_y\left(zp_x - xp_z\right) + \hat{i}_z\left(xp_y - yp_x\right) = \hat{i}_x L_x + \hat{i}_y L_y + \hat{i}_z L_z$$

In quantum mechanics we can define a corresponding observable (Hermitian operator):

$$\hat{\vec{L}} = \hat{\vec{r}}\times\hat{\vec{p}} = \begin{vmatrix} \hat{i}_x & \hat{i}_y & \hat{i}_z \\ x & y & z \\ -i\hbar\frac{\partial}{\partial x} & -i\hbar\frac{\partial}{\partial y} & -i\hbar\frac{\partial}{\partial z} \end{vmatrix} = \hat{i}_x\left(-i\hbar y\frac{\partial}{\partial z} + i\hbar z\frac{\partial}{\partial y}\right) + \hat{i}_y\left(-i\hbar z\frac{\partial}{\partial x} + i\hbar x\frac{\partial}{\partial z}\right) + \hat{i}_z\left(-i\hbar x\frac{\partial}{\partial y} + i\hbar y\frac{\partial}{\partial x}\right)$$

$$\hat{\vec{L}} = \hat{i}_x\hat{L}_x + \hat{i}_y\hat{L}_y + \hat{i}_z\hat{L}_z$$



While Descartes's coordinate system allows us to intuitively derive the components of the angular momentum operator, the spherical symmetry of the problem makes it more logical to move to the spherical coordinate system:

$$x = r\sin\theta\cos\varphi$$

$$y = r\sin\theta\sin\varphi$$

$$z = r\cos\theta$$

In spherical coordinates we can rewrite all the components of the angular momentum:

$$\hat{L}_x = \left(\hat{y}\hat{p}_z - \hat{z}\hat{p}_y\right) = i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right)$$

$$\hat{L}_y = \left(\hat{z}\hat{p}_x - \hat{x}\hat{p}_z\right) = i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} + \frac{\sin\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right)$$

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

$$\hat{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)$$

We call this operator the orbital angular momentum since it has a classical equivalent.
If one looks at the commutation relations of this operator one finds:

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z$$

$$\left[\hat{L}_y, \hat{L}_z\right] = i\hbar\hat{L}_x$$

$$\left[\hat{L}_z, \hat{L}_x\right] = i\hbar\hat{L}_y$$

Note: In QM there is another very important quantity, which is called spin. It turns out that this quantity also obeys the same commutation rules and is therefore also called an spin angular momentum. The spin angular momentum has no classical equivalent.

One can show that: $\left[\hat{L}^2, \hat{L}_z\right] = 0$

Therefore we now that one can fin d a set of eigenfunctions common to $\hat{L}^2$ and $\hat{L}_z$:

$$\hat{L}_z Y_l^m(\theta,\varphi) = m\hbar Y_l^m(\theta,\varphi)$$

$$\hat{L}^2 Y_l^m(\theta,\varphi) = \hbar^2 l(l+1) Y_l^m(\theta,\varphi)$$

Where:

$$Y_l^m(\theta,\varphi) = \begin{cases} (-1)^m\sqrt{\dfrac{2l+1}{4\pi}\dfrac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\varphi}, & m \geq 0 \\ \sqrt{\dfrac{2l+1}{4\pi}\dfrac{(l+m)!}{(l-m)!}}P_l^{-m}(\cos\theta)e^{im\varphi}, & m < 0 \end{cases}$$

Since the wave function needs to be continuous at 2π, ***m*** is an integer. One can show that ***l*** also needs to be an integer and that $-l \leq m \leq l$. $l \geq 0$. $P_l^m(\cos\theta)$ are Legendre polynomials and the eigenfunctions $Y_l^m(\theta,\varphi)$ are called spherical harmonics:

$$Y_0^0(\theta,\varphi)=\frac{1}{\sqrt{4\pi}}$$

$$Y_1^0(\theta,\varphi)=\sqrt{\frac{3}{4\pi}}\cos\theta$$

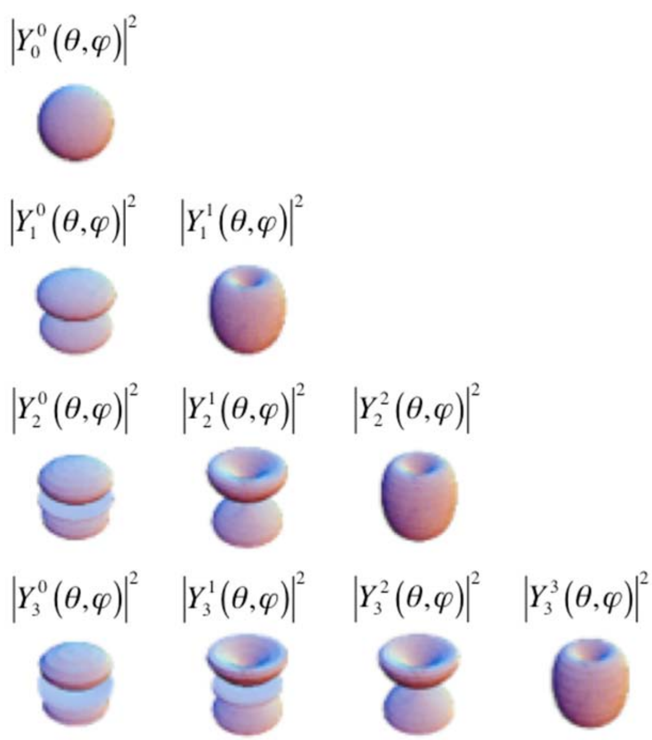
$$Y_1^{\pm1}(\theta,\varphi)=\mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\varphi}$$

$$Y_2^0(\theta,\varphi)=\sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta-1\right)$$

$$Y_2^{\pm1}(\theta,\varphi)=\mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{\pm i\varphi}$$

$$Y_2^{\pm2}(\theta,\varphi)=\sqrt{\frac{15}{32\pi}}\sin^2\theta e^{\pm 2i\varphi}$$

Below are the plots of first several spherical harmonics:



Weisstein, Eric W. "Spherical Harmonic." From *MathWorld* - A Wolfram Web Resource. Used with permission.

3.024 Electronic, Optical and Magnetic Properties of Materials
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