Second Year Quantum Mechanics - Lecture 21 QM in two dimensions

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1 Three dimensions

Generally, the basic changes in the quantities we use in going from 1D to 3D are as follows.

Position operator
$$\hat{x} \qquad \hat{r} = \hat{x}\boldsymbol{i} + \hat{y}\boldsymbol{j} + \hat{z}\boldsymbol{k}$$
Momentum operator
$$\hat{p} = -i\hbar\frac{d}{dx} \qquad \hat{p} = \hat{p}_x\boldsymbol{i} + \hat{p}_y\boldsymbol{j} + \hat{p}_z\boldsymbol{k} = -i\hbar\left(\frac{\partial}{\partial x}\boldsymbol{i} + \frac{\partial}{\partial y}\boldsymbol{j} + \frac{\partial}{\partial z}\boldsymbol{k}\right) = -i\hbar\nabla$$
Kinetic energy
$$\hat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \qquad \hat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) = -\frac{\hbar^2}{2m}\nabla^2$$
Potential energy
$$V(x) \qquad V(r)$$
Hamiltonian
$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \qquad \hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$$
Wavefunction
$$\psi(x,t) \qquad \psi(r,t)$$
Normalisation
$$\int |\psi(x,t)|^2 dx = 1 \qquad \int |\psi(r,t)|^2 dx \, dy \, dz = \int |\psi(r,t)|^2 d^3r = 1$$

There are two new effects we shall look at, degeneracy and angular momentum and we shall use the example of the 2D SHO to illustrate them.

2 The two dimensional SHO

Although to describe the real world we clearly need to work in three dimensions, we shall start by looking at two dimensions. This gives most of the extra QM effects compared to one dimension but mathematically, two dimensions is simpler than three.

We start by writing down the energy eigenstate equation, i.e. the TISE, of the 2D SHO

$$\hat{H}u = \left[-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + \frac{m\omega_x^2 x^2}{2} + \frac{m\omega_y^2 y^2}{2} \right] u = Eu$$

We will try using separation of variables, as we did for the time dependent Schrödinger equation where $\psi(x,t)$. Here we shall write

$$u(x,y) = X(x)Y(y)$$

so that the above equation becomes

$$-\frac{\hbar^2}{2m}\left(Y\frac{d^2X}{dx^2}+X\frac{d^2Y}{dy^2}\right)+\frac{m\omega_x^2x^2}{2}XY+\frac{m\omega_y^2y^2}{2}XY=EXY$$

Dividing throughout by XY gives

$$\left(-\frac{\hbar^2}{2m} \frac{1}{X} \frac{d^2 X}{dx^2} + + \frac{m \omega_x^2 x^2}{2} \right) + \left(-\frac{\hbar^2}{2m} \frac{1}{Y} \frac{d^2 Y}{dy^2} + \frac{m \omega_y^2 y^2}{2} \right) = E$$

The first set of terms depend on x only and the second set on y only, so these must be constants; let these be E_x and E_y , respectively. Note $E = E_x + E_y$ so only one of these is really independent. Using this, then

$$-\frac{\hbar^2}{2m} \frac{1}{X} \frac{d^2 X}{dx^2} + \frac{m\omega_x^2 x^2}{2} = E_x$$

SO

$$-\frac{\hbar^2}{2m}\frac{d^2X}{dx^2} + \frac{m\omega_x^2 x^2}{2}X = E_x X$$

and similarly for Y. However, the above is the one dimensional SHO energy eigenstate equation. Hence, the two dimensions act as independent one dimensional SHO systems. This means we immediately know the eigenvalues

$$E_x = \left(n_x + \frac{1}{2}\right)\hbar\omega_x, \qquad E_y = \left(n_y + \frac{1}{2}\right)\hbar\omega_y$$

and hence the total energy is

$$E = E_x + E_y = \left(n_x + \frac{1}{2}\right)\hbar\omega_x + \left(n_y + \frac{1}{2}\right)\hbar\omega_y$$

and the eigenstate is

$$u_{n_x n_y} = u_{n_x}(x)u_{n_y}(y)$$

where the u_n are the 1D states. We find the energy depends on two quantum numbers, n_x and n_y , rather than just one so we need to label the eigenstates $u_{n_x n_y}$. This is very general and is due to moving to 2D; it is not particular to the SHO. In 3D, this means we need three quantum numbers to label eigenstates, e.g. u_{nlm} , as we shall see in the later lectures.

3 Degeneracy

What happens if the two dimensions have the same potential, i.e. $\omega_x = \omega_y = \omega_0$? The potential takes the form

$$V(x,y) = \frac{m\omega_x^2 x^2}{2} + \frac{m\omega_y^2 y^2}{2} = \frac{m\omega_0^2 (x^2 + y^2)}{2} = \frac{m\omega_0^2 r^2}{2} = V(r)$$

and so becomes a central potential, i.e. it has circular symmetry. Also, the energies are given by

$$E = E_x + E_y = (n_x + n_y + 1) \hbar \omega_0$$

The ground state clearly has $n_x = n_y = 0$, for which $E_0 = \hbar \omega_0$. However, there are now two first excited states, given by $n_x = 1$, $n_y = 0$ and $n_x = 0$, $n_y = 1$, both of which have $E_1 = 2\hbar \omega_0$. This effect, whereby there is more than one eigenstate with the same eigenvalue, is called *degeneracy*. This clearly results from the symmetry of the potential, i.e. because the value of ω_0 is the same for x and y. This is a general result; a symmetry of the system gives rise to degeneracy in the eigenstates. In three dimensions, there is often spherical symmetry of potentials, e.g. in the hydrogen atom, and so we will see there is a lot of degeneracy of the energies in such systems.

There is one critical result which needs to be emphasised about degeneracy. For the two first excited states above, let u_{10} be the first and u_{01} the second. These satisfy

$$\hat{H}u_{10} = E_1 u_{10}, \qquad \hat{H}u_{01} = E_1 u_{01}$$

However, consider the superposition

$$\psi = \alpha u_{10} + \beta u_{01}$$

for any constants α and β , for which

$$\hat{H}\psi = \alpha \hat{H}u_{10} + \beta \hat{H}u_{01} = \alpha E_1 u_{10} + \beta E_1 u_{01} = E_1 (\alpha u_{10} + \beta u_{01}) = E_1 \psi$$

Hence any superposition of degenerate eigenstates is also a degenerate eigenstate. This means we can choose any relevant combinations that we wish, depending on the problem in hand. Note, this is true of degenerate eigenstates for any operator, not just the Hamiltonian.

4 Angular momentum

In two dimensions, there is only one component of angular momentum

$$L = xp_y - yp_x$$

so angular momentum is a scalar, rather than a vector, in two dimensions. However, it is clear this scalar is the equivalent of the L_z component in three dimensions. We want to look at the QM operator, which is

$$\hat{L} = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = -i\hbar x \frac{\partial}{\partial y} + i\hbar y \frac{\partial}{\partial x}$$

Let's see the effect of this operator on the u_{10} state for the case of $\omega_x = \omega_y$, when the potential is central and so we expect angular momentum to be conserved. A reminder that the 1D solutions are

$$u_0 = Ae^{-ax^2/2}, \qquad u_1 = Bxe^{-ax^2/2}$$

Hence, since $\omega_x = \omega_y$ then the a constant is the same for x and y so

$$u_{10} = \left(Bxe^{-ax^2/2}\right)\left(Ae^{-ay^2/2}\right) = ABxe^{-a(x^2+y^2)/2}$$

and similarly

$$u_{01} = ABye^{-a(x^2+y^2)/2}$$

For u_{10} , then

$$\frac{\partial u_{10}}{\partial x} = ABe^{-a(x^2+y^2)/2} - ABax^2e^{-a(x^2+y^2)/2}$$

while

$$\frac{\partial u_{10}}{\partial y} = -ABaxye^{-a(x^2+y^2)/2}$$

Hence

$$\hat{L}u_{10} = i\hbar ABax^2 y e^{-a(x^2+y^2)/2} + i\hbar ABy e^{-a(x^2+y^2)/2} - i\hbar ABax^2 y e^{-a(x^2+y^2)/2}
= i\hbar ABy e^{-a(x^2+y^2)/2} = i\hbar u_{01}$$

Similarly

$$\hat{L}u_{01} = -i\hbar u_{10}$$

This means neither u_{10} nor u_{01} are eigenstates of \hat{L} , even though we would expect L to be conserved classically. This seems to contradict our expectations. However, the above can be written as

$$\hat{L}u_{10} = i\hbar u_{01}, \qquad i\hat{L}u_{01} = \hbar u_{10}$$

Hence, adding these two equations gives

$$\hat{L}u_{10} + i\hat{L}u_{01} = \hbar u_{10} + i\hbar u_{01}$$

$$\hat{L}(u_{10} + iu_{01}) = \hbar(u_{10} + iu_{01})$$

Hence, $u_{10}+iu_{01}$ is an eigenstate of \hat{L} with eigenvalue \hbar . Similarly, by subtracting the equations, we get

$$\hat{L}(u_{10} - iu_{01}) = -\hbar(u_{10} - iu_{01})$$

which means this combination is an eigenstate with eigenvalue $-\hbar$. Remember, these states are linear combinations of the u_{01} and u_{10} and so because of degeneracy are therefore also eigenstates of energy. Hence, there are states which are indeed eigenstates of both energy and angular momentum, as we would expect, and this means the two operators must be compatible. It must be the case that $[\hat{H}, \hat{L}] = 0$ when $\omega_x = \omega_y$, as can be shown by direct calculation.

It is illustrative to look at this in terms of plane (circular) polar coordinates. For these, then

$$x = r\cos\phi, \qquad y = r\sin\phi$$

Consider $\partial/\partial\phi$, which is found by a standard calculation

$$\frac{\partial}{\partial \phi} = \frac{\partial x}{\partial \phi} \frac{\partial}{\partial x} + \frac{\partial y}{\partial \phi} \frac{\partial}{\partial y} = -r \sin \phi \frac{\partial}{\partial x} + r \cos \phi \frac{\partial}{\partial y} = -y \frac{\partial}{\partial x} + x \frac{\partial}{\partial y}$$

Hence

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

This looks intuitive; for the (linear) coordinate x, the (linear) momentum operator associated with it is $\hat{p} = -i\hbar\partial/\partial x$, while we have just found that for the angular coordinate ϕ , the associated angular momentum operator is $\hat{L} = -i\hbar\partial/\partial\phi$. The eigenstates and eigenvalues of angular momentum are easily found, exactly as for the linear momentum. Writing the eigenstate equation as

$$-i\hbar \frac{d\psi}{d\phi} = m_l \hbar \psi$$

so

$$\frac{d\psi}{\psi} = im_l \phi$$

SO

$$\psi = C(r)e^{im_l\phi}$$

where C(r) is any function of the radial coordinate r; it appears as the equivalent of a constant of integration as it is not a function of ϕ .

Unlike for the momentum case, there is a boundary condition, namely that the eigenstate has to be single-valued, i.e. adding 2π to ϕ must give the same state, so $\psi(\phi + 2\pi) = \psi(\phi)$. This means

$$e^{im_l(\phi+2\pi)} = e^{im_l\phi}e^{im_l2\pi} = e^{im_l\phi}$$

so

$$e^{im_l 2\pi} = 1$$

so this restricts m_l to be an integer, which can be either positive or negative. This means angular momentum eigenstates are discrete, not continuous.

The \hat{L} eigenstates $u_{10}\pm iu_{01}$ found above had eigenvalues of $\pm\hbar$ and therefore must correspond to $m_l=\pm 1$. Explicitly

$$u_{10} \pm iu_{01} = AB(x \pm iy)e^{-a(x^2+y^2)/2} = AB(r\cos\phi \pm ir\sin\phi)e^{-ar^2/2}$$

= $ABr(\cos\phi \pm i\sin\phi)e^{-ar^2/2} = ABre^{-ar^2/2}e^{\pm i\phi}$

which is exactly the form we found for $m_l=\pm 1.$

Finally, let's put in the time dependence explicitly; for an angular momentum eigenstate

$$C(r)e^{im_l\phi}e^{-iEt/\hbar} = C(r)e^{i(\hbar m_l\phi - Et)/\hbar} = C(r)e^{i(L\phi - Et)/\hbar}$$

The r part does not depend on time and so is constant. The ϕ part looks just like our previous travelling wave $e^{i(px-Et)/\hbar}$ except it is travelling in ϕ not x, i.e. it is going round in a circle, either in the positive ϕ direction if $m_l > 0$ or the negative ϕ direction if $m_l < 0$. Hence, it physically corresponds to waves circulating around the origin and hence to angular momentum.