Discussion 11: Quantum Mechanics in 3D Part 1: Cartesian coords and linear momentum

Quantum Mechanics in 3D: examples + basics

In some ways, the transition from 1D QM to 3D is simple and painless. The state space goes from the space of complex-valued continuous functions $\psi(x)$ to the same, but over 3d space, $\psi(x,y,z)$. The complete set of position states $|x\rangle$ is replaced by a complete set

$$|\vec{r}\rangle = |x, y, z\rangle$$

of eigenstates of the position operators $\hat{x}, \hat{y}, \hat{z}$. Normalization means

$$\langle\psi|\psi\rangle = 1 \iff \int d^3x \, |\psi(x,y,z)|^2 = 1$$

There are now three momentum operators, $\hat{p}_x \; \hat{p}_y \; \hat{p}_z$. The probability of locating the particle within a volume V is:

$$\text{Prob}(\text{in } V) = \iiint_V dx\,dy\,dz \, |\psi(x,y,z)|^2$$

However, there is something new in 2d and 3d not present in 1d: continuous rotational symmetry and the concept of angular momentum. We'll examine this next week, and focus ~~and~~ on the "painless" part today.

problems:

$\boxed{1}$ Let $\psi(x,y,z)$ describe the state of a particle at a certain moment. Write an expression for the probability of measuring its position to be:

x ~~with~~ between x_0 and $x_0 + dx$

y between y_0 and $y_0 + dy$

z anything

at that moment.

$\boxed{2}$ Same as part 1, except write the probability of finding it within a distance R of the origin. Write the integral in spherical coordinates.

$\boxed{3}$ Using the position representations

$$\hat{x} \longrightarrow x \qquad p_x \longrightarrow -i\hbar \frac{\partial}{\partial x}$$

$$\hat{y} \longrightarrow y \qquad p_y \longrightarrow -i\hbar \frac{\partial}{\partial y}$$

$$\hat{z} \longrightarrow z \qquad p_z \longrightarrow -i\hbar \frac{\partial}{\partial z}$$

of the position & momentum operators, determine all commutators between all pairs of operators. (You don't need to write them all if you can explain the pattern).

4 Let

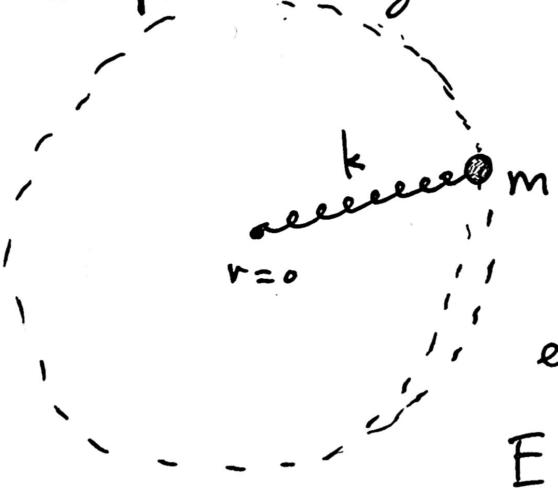
$$\psi(x,y,z) = N e^{-(x^2+y^2+z^2)/2a}$$

where a, N are some positive constants.

(a) Normalize the state.

(b) Compute the expectation value $\langle r \rangle \equiv \langle \sqrt{x^2+y^2+z^2} \rangle$ of the particle's distance to the origin.

5 Let's solve the simple harmonic oscillator in 3d. I promise you can do it!



A 3d <u>classical</u> harmonic oscillator is just a mass on the end of a spring which can move in any direction. Its energy is

$$E = \frac{1}{2} m \vec{v}^{\,2} + \frac{1}{2} k \vec{r}^{\,2}$$

$$= \frac{1}{2} \frac{p_x^2}{m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + \frac{1}{2} k \left(x^2+y^2+z^2\right)$$

The quantum Hamiltonian just makes these into <u>operators</u>:

$$\hat{H} = \frac{1}{2m}\left(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2\right) + \frac{1}{2} k \left(\hat{x}^2 + \hat{y}^2 + \hat{z}^2\right)$$

The TISE is:

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

where I've used $k = m\omega^2$ and $\hat{p}_j \to -i\hbar \frac{\partial}{\partial r_j}$.

By using seperation of variables with guess

$$\psi(x,y,z) = X(x)\, Y(y)\, Z(z)$$

Find ~~the~~ the equation satisfied by $X(x)$, $Y(y)$, $Z(z)$ and "Solve" it to find the energies and eigenfunctions. [Hint: Feel free to re-use the solution to the 1d problem without working through it]. What are the allowed energies of the 3d system. What are the degeneracies of the 4 lowest energies?

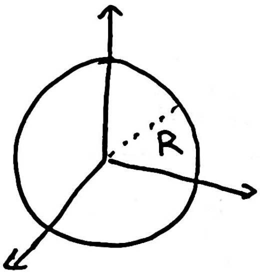
Solutions

1

$$\text{Prob}\left(\begin{matrix} x_0 < x < x_0 + dx \\ y_0 < y < y_0 + dy \\ z = \text{anything} \end{matrix} \right) = \left[\int_{-\infty}^{\infty} dz \, |\psi(x_0, y_0, z)|^2 \right] dx_0 \, dy_0$$

2

$$\text{Prob}(r < R) = \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \int_0^{R} dr \; r^2 \sin\theta \; |\psi(r, \theta, \varphi)|^2$$



3

$$\boxed{[\hat{x}, \hat{y}] = [\hat{x}, \hat{z}] = [\hat{y}, \hat{z}] = 0}$$

because numbers commute:

$$[\hat{x}, \hat{y}] \psi(x,y,z) = xy\psi(x,y,z) - yx\psi(x,y,z) = 0$$

Next,

$$\boxed{[\hat{p}_x, \hat{p}_y] = [\hat{p}_x, \hat{p}_z] = [\hat{p}_y, \hat{p}_z] = 0}$$

because partial derivatives commute (on smooth functions):

$$[\hat{p}_x, \hat{p}_y] \psi(x,y,z) = (-i\hbar)^2 \frac{\partial^2 \psi}{\partial x \, \partial y} - (-i\hbar)^2 \frac{\partial^2 \psi}{\partial y \, \partial x} = 0$$

Finally, we already have seen that:

$$[\hat{x}, \hat{p}_x]\psi = -i\hbar \, x \frac{\partial}{\partial x}\psi - (-i\hbar) \frac{\partial}{\partial x}(x\psi)$$

$$= -i\hbar \left[x\psi' - \psi - x\psi' \right]$$

$$= i\hbar \psi$$

so

$$\boxed{[\hat{x}, \hat{p}_x] = i\hbar}$$

The others are no different so

$$\boxed{[\hat{y}, \hat{p}_y] = i\hbar} \qquad \boxed{[\hat{z}, \hat{p}_z] = i\hbar}$$

Lastly, the mixed position-momentum commutators are zero:

$$[\hat{x}, \hat{p}_y]\psi = (-i\hbar)\left[x \frac{\partial}{\partial y}\psi - \frac{\partial}{\partial y} x \psi\right]$$

But $\frac{\partial}{\partial y} x = 0$ so the expression vanishes.

$$\boxed{\begin{gathered}[\hat{x}, \hat{p}_y] = [\hat{x}, \hat{p}_z] = [\hat{y}, \hat{p}_x] = [\hat{y}, \hat{p}_z] = 0 \\ [\hat{z}, \hat{p}_x] = [\hat{z}, \hat{p}_y] = 0\end{gathered}}$$

$\boxed{4}$

(a) Require that $\langle\psi|\psi\rangle = 1$, In position basis:

$$\iiint dx\,dy\,dz \; |N|^2 \left|e^{-(x^2+y^2+z^2)/2a}\right|^2 = 1$$

This breaks into 3 integrals:

$$= |N|^2 \int_{-\infty}^{\infty} dx\; e^{-x^2/a} \int_{-\infty}^{\infty} dy\; e^{-y^2/a} \int_{-\infty}^{\infty} dz\; e^{-z^2/a}$$

$$= |N|^2 \sqrt{\pi a}\sqrt{\pi a}\sqrt{\pi a}$$

Conclude that $\boxed{N = (\pi a)^{-3/4}}$

(b) Work in spherical coords. where $\sqrt{x^2+y^2+z^2} = r$.

$$\langle r \rangle = \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \int_0^{\infty} dr \; r^2 \sin\theta \;\; r \; |\psi(r,\theta,\varphi)|^2$$

The angular integrals give 4π (ψ is a function of r only). Then:

$$\langle r \rangle = 4\pi \int_0^\infty dr\ r^3 e^{-r^2/a} (\pi a)^{-3/2}$$

$$= 4\pi \frac{a^2}{2} (\pi a)^{-3/2}$$

$$\boxed{\langle r \rangle = 2\sqrt{\frac{a}{\pi}}}$$

check units: $[a] = (\text{length})^2$ because $e^{-r^2/a} \Rightarrow [r^2] = [a]$. ✓

$\boxed{5}$ Insert $X(x)Y(y)Z(z) = \psi(x,y,z)$ into the TISE:

$$-\frac{\hbar^2}{2m}\left(X''YZ + XY''Z + XYZ''\right) + \frac{1}{2}m\omega^2(x^2+y^2+z^2)XYZ = EXYZ$$

Divide through by $\psi = XYZ$:

$$\Rightarrow -\frac{\hbar^2}{2m}\left(\frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z}\right) + \frac{1}{2}m\omega^2(x^2+y^2+z^2) = E$$

$$\Rightarrow \underbrace{\left[-\frac{\hbar^2}{2m}\frac{X''}{X} + \frac{1}{2}m\omega^2 x^2\right]}_{f(x)} + \underbrace{\left[-\frac{\hbar^2}{2m}\frac{Y''}{Y} + \frac{1}{2}m\omega^2 y^2\right]}_{g(y)} + \underbrace{\left[-\frac{\hbar^2}{2m}\frac{Z''}{Z} + \frac{1}{2}m\omega^2 z^2\right]}_{h(z)} = E$$

We have three functions of independent variables summing to a constant. The only way this is possible is if each function is a constant; call them E_x, E_y, E_z:

$$f(x) = E_x \qquad g(y) = E_y \qquad h(z) = E_z$$

Then our system of equations is :

$$\begin{cases} -\frac{\hbar^2}{2m}\frac{X''}{X} + \frac{1}{2}m\omega^2 x^2 = E_x \\ -\frac{\hbar^2}{2m}\frac{Y''}{Y} + \frac{1}{2}m\omega^2 y^2 = E_y \\ -\frac{\hbar^2}{2m}\frac{Z''}{Z} + \frac{1}{2}m\omega^2 z^2 = E_z \\ E_x + E_y + E_z = E \end{cases}$$

Take the X-equation, multiply through by X:

$$-\frac{\hbar^2}{2m}X'' + \frac{1}{2}m\omega^2 x^2 X = E_x X$$

But this is just the TISE for a 1D Harmonic oscillator! So the solutions to it are:

$$X(x)_n = \phi_n(x) \qquad E_{x,n} = \hbar\omega(n + \tfrac{1}{2})$$

for $n = 0, 1, 2, \ldots$ where ϕ_n is the n^{th} HO energy eigenfunction. Similarly, the Y and Z equations have solutions

$$Y(y)_m = \phi_m(y) \qquad E_{y,m} = \hbar\omega(m + \tfrac{1}{2})$$

$$Z(z)_\ell = \phi_\ell(z) \qquad E_{z,\ell} = \hbar\omega(\ell + \tfrac{1}{2})$$

for $m, \ell = 0, 1, 2, 3, \ldots$. The full solutions are:

$$\boxed{\Psi_{n,\ell,m}(x,y,z) = \phi_n(x)\,\phi_m(y)\,\phi_\ell(z)}$$

for a triplet (n, m, ℓ) of integers $n, \ell, m = 0, 1, 2, 3, \ldots$

The energies are:

$$\boxed{E_{n,m,\ell} = \hbar\omega\left(n+m+\ell+\frac{3}{2}\right)}$$

The energies are now <u>degenerate</u>, since for instance $(1,0,0)$, $(0,1,0)$, and $(0,0,1)$ all give the same energy $\left(\frac{5}{2}\hbar\omega\right)$. The first few are:

$n+m+\ell \equiv$ "N"	E_N	degeneracy	list of (n,m,ℓ)
0	$\frac{3}{2}\hbar\omega$	1	$(0,0,0)$
1	$\frac{5}{2}\hbar\omega$	3	$(1,0,0)$, $(0,1,0)$, $(0,0,1)$
2	$\frac{7}{2}\hbar\omega$	6	$(2,0,0)$, $(0,2,0)$, $(0,0,2)$ $(1,1,0)$, $(1,0,1)$, $(0,1,1)$
3	$\frac{9}{2}\hbar\omega$	10	$(3,0,0)$, $(0,3,0)$, $(0,0,3)$ $(2,1,0)$, $(1,2,0)$, $(0,2,1)$ $(0,1,2)$, $(1,0,2)$, $(2,0,1)$ $(1,1,1)$
4	$\frac{11}{2}\hbar\omega$	left as exercise ☺	