Quantum mechanics I : tutorial solutions

2021.11.11 / self-study pack 4

1) Show that the wave function given about 3 minutes in to the movie is an eigenfunction of the operator for total momentum, and find its (vector) eigenvalue.

- We look at the momentum operator in 3 DIMENSIONS which has the form:

$$\hat{\underline{P}} = -i\hbar \underline{\nabla}$$

$$= -i\hbar \left[\hat{x}\,\partial_x + \hat{y}\,\partial_y + \hat{z}\,\partial_z \right]$$

what are the eigenfunctions of this operator?

We show that the wavefunction

$$\psi(\underline{r}) = \psi(x,y,z) = \psi_x(x)\,\psi_y(y)\,\psi_z(z)$$

where

$$\psi_x(x) = A_x\, e^{ik_x x}$$

$$\psi_y(y) = A_y\, e^{ik_y y}$$

$$\psi_z(z) = A_z\, e^{ik_z z}$$

In order to do that, we apply $\hat{\underline{P}}$ on $\psi(\underline{r})$

NB these derivatives act only on the respective variables leaving $\psi(\underline{r})$ "intact"

$$\hat{\underline{P}}\,\psi(\underline{r}) = -i\hbar\,\underline{\nabla}\,\psi(\underline{r})$$

$$= -i\hbar \left[\hat{x}\,\partial_x + \hat{y}\,\partial_y + \hat{z}\,\partial_z \right] \psi_x(x)\,\psi_y(y)\,\psi_z(z)$$

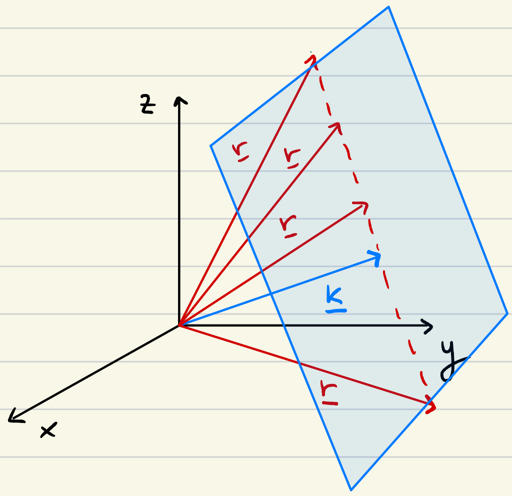
$$= -i\hbar \left[\hat{x}\,(ik_x) + \hat{y}\,(ik_y) + \hat{z}\,(ik_z) \right] \psi(\underline{r})$$

$$\hat{\underline{P}}\,\psi(\underline{r}) = \hbar \left[k_x\,\hat{x} + k_y\,\hat{y} + k_z\,\hat{z} \right] \psi(\underline{r})$$

this wave function $\psi(\underline{r})$, eigenfunction of $\hat{\underline{P}}$,

is a 3D PLANE WAVE $\Rightarrow$ let's see why "plane"

$$\psi(\underline{r}) = \psi_x(x)\,\psi_y(y)\,\psi_z(z)$$
$$= A_x A_y A_z \; e^{i(k_x x + k_y y + k_z z)}$$
$$= A \; e^{i\underline{k}\cdot\underline{r}}$$



The vector $\underline{k}$ is the constant momentum of the wave. We know that a wavefront is identified by a CONSTANT PHASE of the wave, therefore $\underline{k}\cdot\underline{r} = \text{const}$.

As shown in the picture, all the vectors $\underline{r}$ have the same projection along the WAVEFRONT $\perp$ $\underline{k}$, therefore constant phase. Note that the wavefront is a plane, therefore PLANE WAVE, in this case in 3D.

- What about the 3D Schrödinger equation?

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x,y,z)\right] u(x,y,z) = E\, u(x,y,z)$$

where $\nabla^2 = \underline{\nabla}\cdot\underline{\nabla} = \sum_i \partial_i^2$

LAPLACE OPERATOR

e.g. in 3D $\qquad \nabla^2 f = \dfrac{\partial^2 f}{\partial x^2} + \dfrac{\partial^2 f}{\partial y^2} + \dfrac{\partial^2 f}{\partial z^2}$

If the potential can be separated,

$$V(x,y,z) = V_1(x) + V_2(y) + V_3(z)$$

then we can find a solution to the equation of the form

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

2) Substitute the wave function $u(x,y,z)=X(x)Y(y)Z(z)$ into the Schrödinger equation to separate it out into three ordinary differential equations.

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x,y,z)\right] u(x,y,z) =$$

$$= \left[-\frac{\hbar^2}{2m}\underbrace{\nabla^2}_{\partial_x^2+\partial_y^2+\partial_z^2} + V_1(x) + V_2(y) + V_3(z)\right] X(x)\,Y(y)\,Z(z)$$

$$= -\frac{\hbar^2}{2m}\left[(\partial_x^2 X)\,YZ + X(\partial_y^2 Y)\,Z + XY(\partial_z^2 Z)\right] +$$

$$+ \left[V_1(x) + V_2(y) + V_3(z)\right] XYZ = E\,XYZ$$

divide everything by $u(x,y,z) = XYZ$

$$\rightarrow \quad E = \left(-\frac{\hbar^2}{2m}\frac{1}{X}\partial_x^2 X + V_1(x)\right) +$$

$$+ \left(-\frac{\hbar^2}{2m}\frac{1}{Y}\partial_y^2 Y + V_2(y)\right) +$$

$$+ \left(-\frac{\hbar^2}{2m}\frac{1}{Z}\partial_z^2 Z + V_3(z)\right)$$

therefore, the sum of these brackets has to be CONSTANT ($= E$).

We want this equation to be true for every x, y, z, therefore EACH bracket has to be a CONSTANT ITSELF.

$$E = \underbrace{\left(-\frac{\hbar^2}{2m}\frac{1}{X}\partial_x^2 X + V_1(x)\right)}_{E_1} +$$

(etc. for the others)

$$+ \left(-\frac{\hbar^2}{2m}\frac{1}{Y}\partial_y^2 Y + V_2(y)\right) +$$

$$+ \left(-\frac{\hbar^2}{2m}\frac{1}{Z}\partial_z^2 Z + V_3(z)\right)$$

$$= E_1 + E_2 + E_3$$

NB

An example of separable potential is the 3D box.

3) Find the energies and degeneracies of the low-lying excited states for the particle in a 3D cubic box, as specified about 21 minutes into the movie.

- the eigen energy of a particle in a 3D box is

$$E_{n_1,n_2,n_3} = \frac{\hbar^2 \pi^2}{8m} \left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2} \right)$$

Here, we consider the special case $a = b = c$

therefore

$$E_{n_1,n_2,n_3} = \frac{\hbar^2 \pi^2}{8ma^2} \left(n_1^2 + n_2^2 + n_3^3 \right)$$

If we set one of the $n_i = 2$ and fix the others to 1 we have:

$$n_1^2 + n_2^2 + n_3^2 = 6$$

$$\left.\begin{array}{ccc} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{array}\right\} \quad \text{DEG} = 3$$

therefore an energy equal to $E_{112} = E_{121} = E_{211} = \dfrac{6\hbar^2\pi^2}{8ma^2}$

3) $E_{n_1,n_2,n_3} = \dfrac{9\hbar^2\pi^2}{8ma^2}$ means that we have two energy levels $n_i = 2$ and one $n_j = 1$

$$n_1^2 + n_2^2 + n_3^2 = 9$$

$$\left.\begin{array}{ccc} 1 & 2 & 2 \\ 2 & 1 & 2 \\ 2 & 2 & 1 \end{array}\right\} \quad \text{DEG} = 3$$

for $$E_{n_1,n_2,n_3} = \frac{11\hbar^2\pi^2}{8ma^2}$$

$$n_1^2 + n_2^2 + n_3^2 = 11$$

$$\left.\begin{array}{ccc} 1 & 1 & 3 \\ 1 & 3 & 1 \\ 3 & 1 & 1 \end{array}\right\} \quad DEG = 3$$

for $$E_{n_1,n_2,n_3} = \frac{12\hbar^2\pi^2}{8ma^2}$$

$$n_1^2 + n_2^2 + n_3^2 = 12$$

$$\left.\begin{array}{ccc} 2 & 2 & 2 \end{array}\right\} \quad DEG = 1$$ (NO DEGENERACY)

for $$E_{n_1,n_2,n_3} = \frac{14\hbar^2\pi^2}{8ma^2}$$

$$n_1^2 + n_2^2 + n_3^2 = 14$$

$$\left.\begin{array}{ccc} 1 & 2 & 3 \\ 1 & 3 & 2 \\ 2 & 1 & 3 \\ 2 & 3 & 1 \\ 3 & 1 & 2 \\ 3 & 2 & 1 \end{array}\right\} \quad DEG = 6$$

4) Repeat this for a box that has a square section, but one dimension is different from the others (e.g. $a = b \neq c$). Look at both the cases $a > c$ and $a < c$ – the ordering of the states is different in the two cases.

if one dimension is different the energies are

$$E_{n_1, n_2, n_3} = \frac{\hbar^2 \pi^2}{8m} \left(\frac{n_1^2 + n_2^2}{a^2} + \frac{n_3^2}{c^2} \right)$$

$$= \frac{\hbar^2 \pi^2}{8m} \frac{(n_1^2 + n_2^2) c^2 + n_3^2 a^2}{a^2 c^2}$$

let's look at the first few states

$$E_{111} = \frac{\hbar^2 \pi^2}{8m} \left(\frac{2}{a^2} + \frac{1}{c^2} \right)$$

$$= \frac{\hbar^2 \pi^2}{8m} \left(\frac{2c^2 + a^2}{a^2 c^2} \right)$$

$$E_{112} = \frac{\hbar^2 \pi^2}{8m} \frac{2c^2 + 4a^2}{a^2 c^2}$$

$$E_{121} = E_{211} = \frac{\hbar^2 \pi^2}{8m} \frac{5c^2 + a^2}{a^2 c^2}$$

etc ...

– see section 3.2 of Rae

– understand figure 3.1

Is the order of the states dependent on the choice of a & c ?

$$E_{n_1, n_2, n_3} = \frac{\hbar^2 \pi^2}{8m} \left(\frac{n_1^2 + n_2^2}{a^2} + \frac{n_3^2}{c^2} \right)$$

$$E_{112} = \frac{\hbar^2 \pi^2}{8m} \left(\frac{2}{a^2} + \frac{4}{c^2} \right)$$

$$E_{121} = E_{211} = \frac{\hbar^2 \pi^2}{8m} \left(\frac{5}{a^2} + \frac{1}{c^2} \right)$$

$E_{112} > E_{121}$ if

$$\frac{2}{a^2} + \frac{4}{c^2} > \frac{5}{a^2} + \frac{1}{c^2}$$

$$\frac{3}{c^2} > \frac{3}{a^2} \Rightarrow \boxed{a > c}$$

Therefore, the order of the states changes wrt the choice of a & c.

for $a > c$ $E_{112} > E_{121} = E_{211}$

for $a < c$ $E_{112} < E_{121} = E_{211}$

5) Write down the wave functions for the 3D harmonic oscillator, and write down an expression for the energy.

Now, we consider a harmonic potential in 3D, that is the 3D harmonic oscillator.

$$V(x,y,z) = \frac{1}{2} m \left(\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2 \right)$$

We want to find a solution (in the form of wave function) to the following Schrödinger equation:

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi + \frac{1}{2} m \left(\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2 \right) \Psi = E \Psi$$

We know that, since the potential is SEPARABLE, we can try a separable solution of the form,

$$\Psi(x,y,z) = \varphi_x(x)\, \varphi_y(y)\, \varphi_z(z)$$

Dividing the Schrödinger eq. by Ψ we obtain three separate 1D harmonic oscillators.

$$-\frac{\hbar^2}{2m} \frac{1}{\Psi} \nabla^2 \Psi + \frac{1}{2} m \left(\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2 \right) = E$$

$$-\frac{\hbar^2}{2m} \frac{1}{\Psi} \partial_x^2 \varphi_x + \frac{1}{2} m \omega_1^2 x^2 \varphi_x +$$

$$-\frac{\hbar^2}{2m} \frac{1}{\Psi} \partial_y \varphi_y + \frac{1}{2} m \omega_1^2 y^2 \varphi_y +$$

$$-\frac{\hbar^2}{2m} \frac{1}{\Psi} \partial_z \varphi_z + \frac{1}{2} m \omega_1^2 z^2 \varphi_z = E_1 + E_2 + E_3 = E$$

We know that the solution of the 1D h.o. are the Hermite polynomials.

For x, for example,

$$\varphi_{x,0} = \left(\frac{\alpha_x}{\pi}\right)^{1/4} \exp\left(-\frac{x'^2}{2}\right)$$

$$\varphi_{x,1} = \left(\frac{4\alpha_x}{\pi}\right)^{1/4} x' \exp\left(-\frac{x'^2}{2}\right)$$

where $\alpha_x = \frac{m\omega_1}{\hbar}$ & $x' = \sqrt{\frac{m\omega}{\hbar}}\, x$

and similarly for the other variables.

In this way, the total ground state wave function is

$$\varphi_0 = \varphi_{x,0}\, \varphi_{y,0}\, \varphi_{z,0}$$

$$= \left(\frac{\alpha_x \alpha_y \alpha_z}{\pi^3}\right)^{1/4} \exp\left(-\frac{1}{2}\left(x'^2 + y'^2 + z'^2\right)\right)$$

while the energy is the sum of the single dimensional energies.

$$E = E_1 + E_2 + E_3 =$$

$$= \hbar\omega_1\left(n_1 + \frac{1}{2}\right) + \hbar\omega_2\left(n_2 + \frac{1}{2}\right) + \hbar\omega_3\left(n_3 + \frac{1}{2}\right)$$

6) For the special case in which all the omegas are equal, work out the energies and degeneracies of the ground state and the first five excited states.

If $\omega_1 = \omega_2 = \omega_3$ the energies are

$$E_{n_1, n_2, n_3} = \hbar\omega \left(n_1 + n_2 + n_3 + \frac{3}{2} \right)$$

$$E_{000} = \frac{3}{2} \hbar\omega$$

$$E_{100} = E_{010} = E_{001} = \frac{5}{2} \hbar\omega$$

$$E_{110} = E_{011} = E_{101} = E_{200} = E_{020} = E_{002} = \frac{7}{2} \hbar\omega$$

$$E_{111} = E_{210} = E_{201} = E_{102} = E_{120} = E_{012} = E_{021} = \frac{9}{2} \hbar\omega$$

$$E_{112} = E_{121} = E_{211} = \frac{11}{2} \hbar\omega$$

$$E_{122} = E_{212} = E_{221} = \frac{13}{2} \hbar\omega$$

tips

When we are dealing with a separable potential e.g. $V(x,y,z) = V_x(x)\, V_y(y)\, V_z(z)$, we have a separable solution $\psi(x,y,z) = \psi_x(x)\, \psi_y(y)\, \psi_z(z)$ and the eigenenergies will be the sum of the single energies , $E = E_x + E_y + E_z$