PH-107

Quantum Physics and Applications

Transition from One-Dimension to Higher-Dimensions

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From 1D to 2D and 3D

So far we have been discussing only one-dimensional problems. What happens when we venture out in higher dimensions (2D/3D)?

Life immediately becomes complicated! In 1D, we could move in only two directions: forward or backward.

In a 2D/3D, there are an infinite number of directions to choose from!

In 1D, bound motion is necessarily oscillatory. In 2D/3D, another type of bound motion becomes possible: Rotational motion!

From 1D to 2D and 3D

You can ask, *"Why are you so bothered by this notion of 2D/3D? We live in Euclidean space. The motion in x-direction is completely independent of the motion in y- (or z-)direction".*

True, if we have a problem which neatly separates itself into two/ three sub-problems: one each in *x*-, *y*-, and *z*-directions.

From 1D to 2D and 3D

That happens only when the potential can be written as the sum of two/three terms, i.e.,

$$V(x,y) = V(x) + V(y) \quad \text{(In 2D)}$$

and

$$V(x,y,z) = V(x) + V(y) + V(z) \quad \text{(In 3D)}$$

As an example, we consider the potential

$$\begin{aligned} V(x,y,z) &= \frac{1}{2}m\omega^2(x^2+y^2+z^2) \\ &= \frac{1}{2}m\omega^2x^2 + \frac{1}{2}m\omega^2y^2 + \frac{1}{2}m\omega^2z^2 \\ &= V(x) + V(y) + V(z) \end{aligned}$$

The problem neatly separates into 3 sub-problems.

From 1D to 2D and 3D

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and

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However, if we consider following

$$V(x,y,z) = -\frac{K}{\sqrt{x^2+y^2+z^2}}$$

$$V(x,y,z) \neq V(x) + V(y) + V(z)$$

From 1D to 2D and 3D

Now, let us solve the TISE for $V(x,y,z) = V(x) + V(y) + V(z)$

We first start by writing the TISE in 3D

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(x,y,z) + V(x,y,z)\Psi(x,y,z) = E\ \Psi(x,y,z)$$

$$= \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\Psi(x,y,z)$$

We try the same old trick of separation of variables, i.e., start with a trial solution

$$\Psi(x,y,z) = \phi(x)\ \eta(y)\ \zeta(z)$$

From 1D to 2D and 3D

So, we have

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(x)+V(y)+V(z)\right]\phi(x)\ \eta(y)\ \zeta(z)$$

$$= E\ \phi(x)\ \eta(y)\ \zeta(z)$$

Or

$$\left[\frac{\partial^2}{\partial x^2}+\frac{2m}{\hbar^2}V(x)\right]\phi\ \eta\ \zeta + \left[\frac{\partial^2}{\partial y^2}+\frac{2m}{\hbar^2}V(y)\right]\phi\ \eta\ \zeta$$

$$+ \left[\frac{\partial^2}{\partial z^2}+\frac{2m}{\hbar^2}V(z)\right]\phi\ \eta\ \zeta + \frac{2m}{\hbar^2}E\phi\ \eta\ \zeta = 0$$

From 1D to 2D and 3D

$$\left[\eta\ \zeta\frac{\partial^2\phi}{\partial x^2}+\frac{2m}{\hbar^2}V(x)\phi\eta\zeta\right] + \left[\phi\ \zeta\frac{\partial^2\eta}{\partial y^2}+\frac{2m}{\hbar^2}V(y)\phi\eta\zeta\right]$$

$$+ \left[\phi\ \eta\frac{\partial^2\zeta}{\partial z^2}+\frac{2m}{\hbar^2}V(z)\phi\eta\zeta\right] + \frac{2m}{\hbar^2}E\phi\ \eta\ \zeta=0$$

Let us divide above equation by $\phi\eta\zeta$

$$\left[\frac{1}{\phi}\frac{\partial^2\phi}{\partial x^2}+\frac{2m}{\hbar^2}V(x)\right] + \left[\frac{1}{\eta}\frac{\partial^2\eta}{\partial y^2}+\frac{2m}{\hbar^2}V(y)\right] + \left[\frac{1}{\zeta}\frac{\partial^2\zeta}{\partial z^2}+\frac{2m}{\hbar^2}V(z)\right]$$

$$=-\frac{2m}{\hbar^2}E$$

Since the RHS is a constant, each term in LHS should be equated to a constant. We can write as

From 1D to 2D and 3D

$$\left[\frac{1}{\phi}\frac{\partial^2\phi}{\partial x^2}+\frac{2m}{\hbar^2}V(x)\right]=-\frac{2m}{\hbar^2}E_x$$

$$\left[\frac{1}{\eta}\frac{\partial^2\eta}{\partial y^2}+\frac{2m}{\hbar^2}V(y)\right]=-\frac{2m}{\hbar^2}E_y$$

$$\left[\frac{1}{\zeta}\frac{\partial^2\zeta}{\partial z^2}+\frac{2m}{\hbar^2}V(z)\right]=-\frac{2m}{\hbar^2}E_z$$

This was we are equating $E = E_x + E_y + E_z$

Therefore, the 3D TISE simplifies to three 1D sub-TISEs.

From 1D to 2D and 3D

Therefore, the 3D TISE simplifies to three 1D sub-TISEs.

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} + V(x)\phi = E_x\phi$$

$$-\frac{\hbar^2}{2m}\frac{d^2\eta}{dy^2} + V(y)\eta = E_y\eta$$

$$-\frac{\hbar^2}{2m}\frac{d^2\zeta}{dz^2} + V(z)\eta = E_z\zeta$$

We can solve each of them the way we did previously.

Solving TISE

The solutions we get will be the corresponding eigenstates

$\phi_n(x), \eta_m(y), \text{ and } \zeta_p(z),$ so that

$$\Psi_{n,m,p}(x,y,z) = \phi_n(x)\eta_m(y)\zeta_p(z)$$

and the corresponding eigenvalues $E_n, E_m, \text{ and } E_p$ add up to give the total energy of the particle, i.e.,

$$E = E_n + E_m + E_p$$

Now, let us solve a real problem: Particle in an infinite 3D box

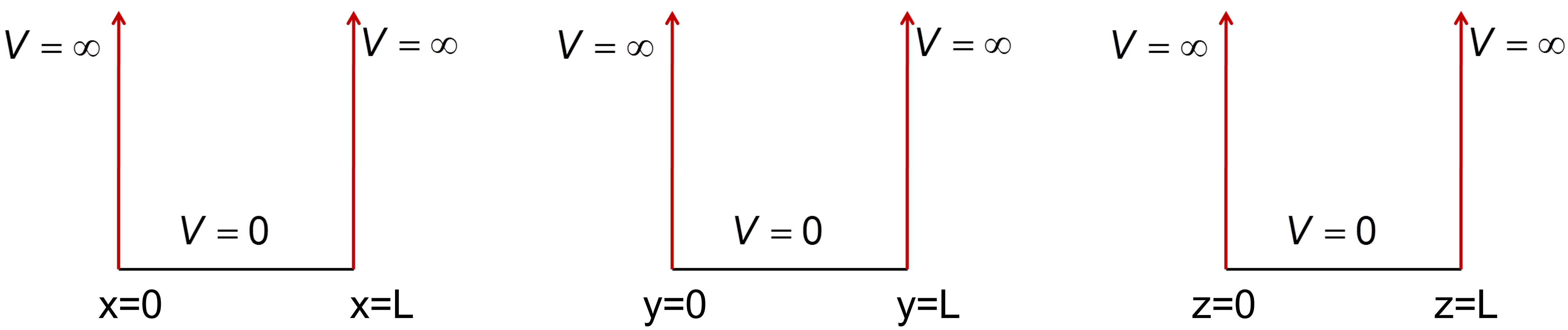
Particle in an infinite 3D box

$$V(x,y,z) = V(x) + V(y) + V(z)$$

Such that

$$V(x) = V(y) = V(z) = 0 \;\; \forall \, 0 \leq x,y,z \leq L$$

$$V(x) = V(y) = V(z) = \infty \;\; \text{otherwise}$$



Particle in an infinite 3D box

So, we have three identical equations to solve

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} = E_x\phi$$

$$-\frac{\hbar^2}{2m}\frac{d^2\eta}{dy^2} = E_y\eta$$

$$-\frac{\hbar^2}{2m}\frac{d^2\zeta}{dz^2} = E_z\zeta$$

The solution

$$\Psi_{n,m,p}(x,y,z) = \phi_n(x)\eta_m(y)\zeta_p(z)$$

is easy to guess.

Particle in an infinite 3D box

The solution

$$\Psi_{n,m,p}(x,y,z)$$

$$= \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)\ \sqrt{\frac{2}{L}}\sin\left(\frac{m\pi}{L}y\right)\ \sqrt{\frac{2}{L}}\sin\left(\frac{p\pi}{L}z\right)$$

$$= \left(\frac{2}{L}\right)^{\frac{3}{2}}\sin\left(\frac{n\pi}{L}x\right)\ \sin\left(\frac{m\pi}{L}y\right)\ \sin\left(\frac{p\pi}{L}z\right)$$

and energy

$$E = E_n + E_m + E_p$$

$$E = \frac{\pi^2\hbar^2}{2mL^2}(n^2+m^2+p^2) \quad \text{with } n,m,p = 1,2,3...$$

Degeneracies

Energy

$$E = E_n + E_m + E_p$$

$$E = \frac{\pi^2 \hbar^2}{2mL^2}(n^2 + m^2 + p^2) \quad \text{with } n, m, p = 1, 2, 3...$$

So we can label the states as (n, m, p), i.e., (1,1,1), (2,1,1), (1,2,1), (1,1,2) etc.

We note that the state (1,1,1) is unique with energy $E_{111} = \frac{3\pi^2 \hbar^2}{2mL^2}$

The states (2,1,1) , (1,2,1) , (1,1,2) have the same energy

$$E_{211} = E_{121} = E_{112} = \frac{6\pi^2 \hbar^2}{2mL^2}$$

Degeneracies

$$E_{211} = E_{121} = E_{112} = \frac{6\pi^2\hbar^2}{2mL^2}$$

Thus we talk of **3-fold degeneracy** of the state with energy $\frac{6\pi^2\hbar^2}{2mL^2}$

This 3-fold degeneracy is characteristic of potentials with discrete symmetry $x \leftrightarrow y$, $y \leftrightarrow z$, $z \leftrightarrow x$, i.e., if we interchange the co-ordinates, we still have the same potential.

When this symmetry is lost, the degeneracy is also lost. For example, when the potential box is not cubic.

Degeneracies

Now if we have $V(x,y,z) = V(x) + V(y) + V(z)$

Such that

$$V(x) = 0 \;\; \forall \; 0 \leq x \leq L_x$$

$$V(y) = 0 \;\; \forall \; 0 \leq y \leq L_y$$

$$V(z) = 0 \;\; \forall \; 0 \leq z \leq L_z$$

$$V(x) = V(y) = V(z) = \infty \;\; \text{otherwise}$$

Then the total energy can be written as

$$E = \frac{\pi^2 \hbar^2}{2m}\left(\frac{n^2}{L_x^2} + \frac{m^2}{L_y^2} + \frac{p^2}{L_z^2}\right)$$

Degeneracies

Now we have

$$E = \frac{\pi^2\hbar^2}{2m}\left(\frac{n^2}{L_x^2} + \frac{m^2}{L_y^2} + \frac{p^2}{L_z^2}\right)$$

Then it is easy to see

$$E_{211} = \frac{\pi^2\hbar^2}{2m}\left(\frac{4}{L_x^2} + \frac{1}{L_y^2} + \frac{1}{L_z^2}\right)$$

$$E_{121} = \frac{\pi^2\hbar^2}{2m}\left(\frac{1}{L_x^2} + \frac{4}{L_y^2} + \frac{1}{L_z^2}\right)$$

$$E_{112} = \frac{\pi^2\hbar^2}{2m}\left(\frac{1}{L_x^2} + \frac{1}{L_y^2} + \frac{4}{L_z^2}\right)$$

$$\Longrightarrow E_{211} \neq E_{121} \neq E_{112}$$

Degeneracies: Harmonic Oscillator in 3D

We have $V(x,y,z) = \frac{1}{2}m\omega^2(x^2+y^2+z^2)$

It is easy to see that $V(x,y,z) = \frac{1}{2}m\omega^2x^2 + \frac{1}{2}m\omega^2y^2 + \frac{1}{2}m\omega^2z^2$

$$= V(x) + V(y) + V(z)$$

We can also write

$$\Psi_{000}(x,y,x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{3}{4}} e^{-\frac{m\omega}{2\hbar}(x^2+y^2+z^2)}$$

and

$$E_{nmp} = \left(n+m+p+\frac{3}{2}\right)\hbar\omega$$

Degeneracies: Harmonic Oscillator in 3D

We have $$E_{nmp} = \left(n + m + p + \frac{3}{2}\right)\hbar\omega$$

It is easy to see that $E_{000} = \frac{3}{2}\hbar\omega$ is unique.

But, once again $E_{100} = E_{010} = E_{001}$

and $E_{110} = E_{011} = E_{101}$ and so on.

The degeneracy is lost if $V(x, y, z) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$

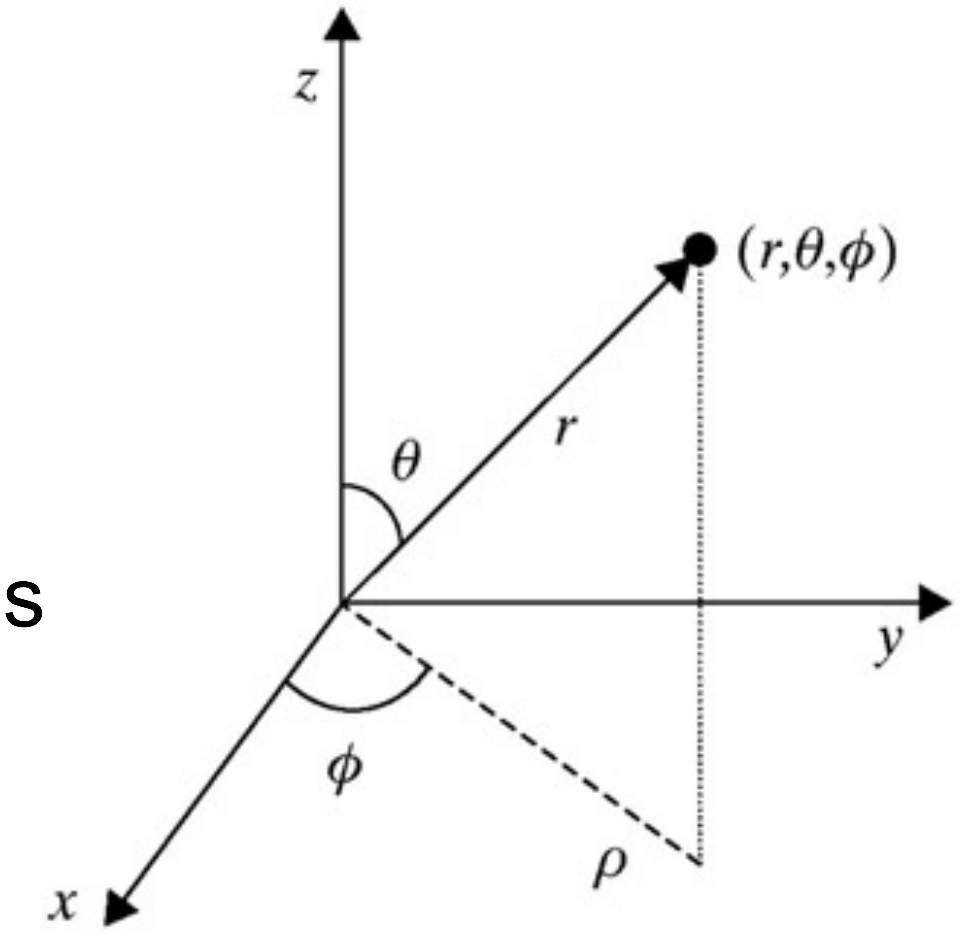
i.e., if the symmetry $x \leftrightarrow y$, $y \leftrightarrow z$, $z \leftrightarrow x$ is broken.

Symmetry and Degeneracy

If we write $V(x,y,z) = \frac{1}{2}m\omega^2(x^2+y^2+z^2)$

in spherical polar coordinates, we find

$$V(r,\theta,\phi) = \frac{1}{2}m\omega^2 r^2$$



The potential does not depend on the angles

θ and ϕ :

i.e., it possesses **spherical symmetry**.

Symmetry and Degeneracy

For a **spherically symmetric potential**, the problem may become more tractable by going to spherical co-ordinates. For example if

we have $V(x,y,z) = -\dfrac{K}{\sqrt{x^2+y^2+z^2}}$

there is no way to write $V(x,y,z) = V(x) + V(y) + V(z)$

However, in spherical co-ordinates $V(r,\theta,\phi) = -\dfrac{K}{r}$

You recognize that the chosen potential is like that of the hydrogen atom, where we can use the trick of separation of variables.

Symmetry and Degeneracy

But only after writing out the TISE in spherical co-ordinates.

The TISE in spherical co-ordinate is

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\Psi+V\Psi=E\Psi$$

Note that $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, and $z = r\cos\theta$.

Recommended Readings

Quantum Mechanics in Three Dimensions, Chapter 8