

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

and

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

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.

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

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

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

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

# Solving TISE

The solutions we get will be the corresponding eigenstates

$\phi_n(x)$ ,  $\eta_m(y)$ , 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  $E_n, E_m$ , 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**

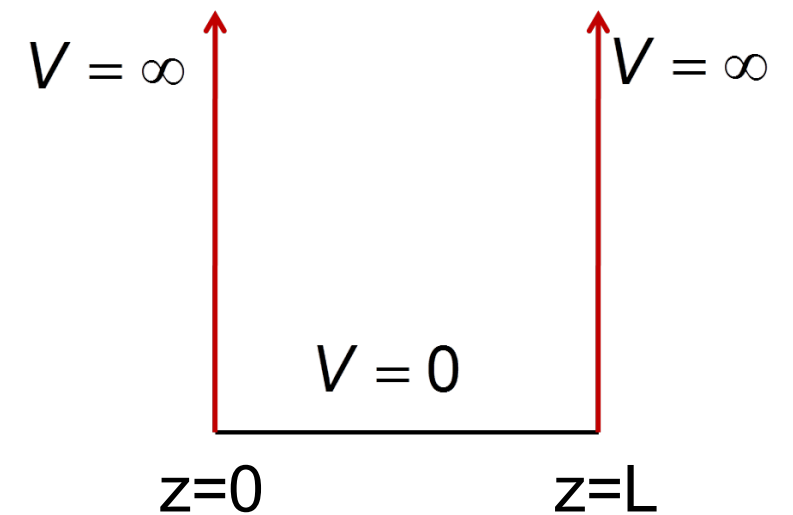
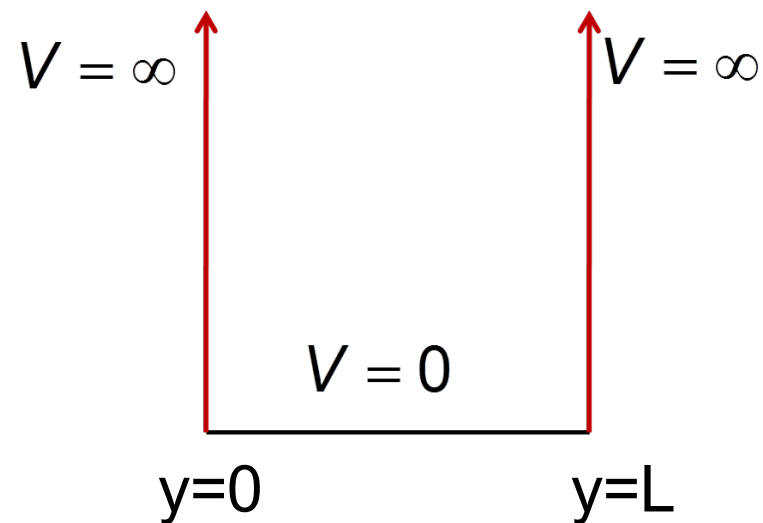
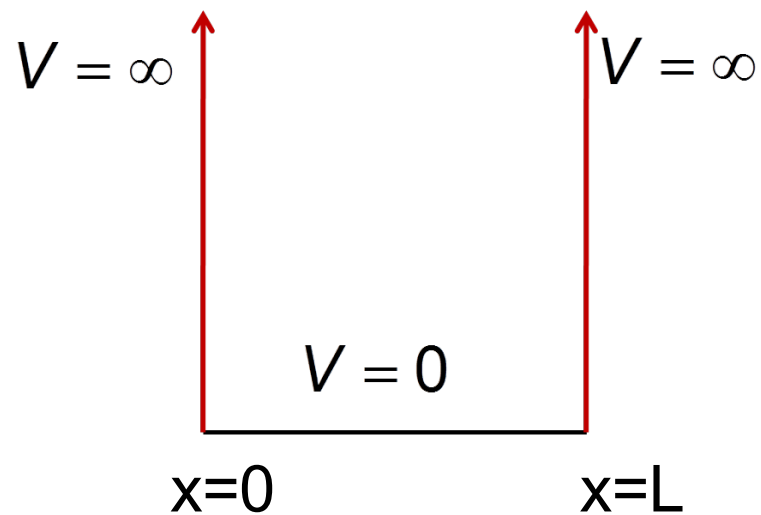
# Particle in an infinite 3D box

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

Such that

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

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



# 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

$$\begin{aligned}\Psi_{n,m,p}(x, y, z) &= \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \sqrt{\frac{2}{L}} \sin\left(\frac{m\pi}{L}y\right) \sqrt{\frac{2}{L}} \sin\left(\frac{p\pi}{L}z\right) \\ &= \left(\frac{2}{L}\right)^{\frac{3}{2}} \sin\left(\frac{n\pi}{L}x\right) \sin\left(\frac{m\pi}{L}y\right) \sin\left(\frac{p\pi}{L}z\right)\end{aligned}$$

and energy

$$E = E_n + E_m + E_p$$

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

# Degeneracies

Energy

$$E = E_n + E_m + E_p$$

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

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 coordinates, 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

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

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

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

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

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

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

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

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

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

# 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

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

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

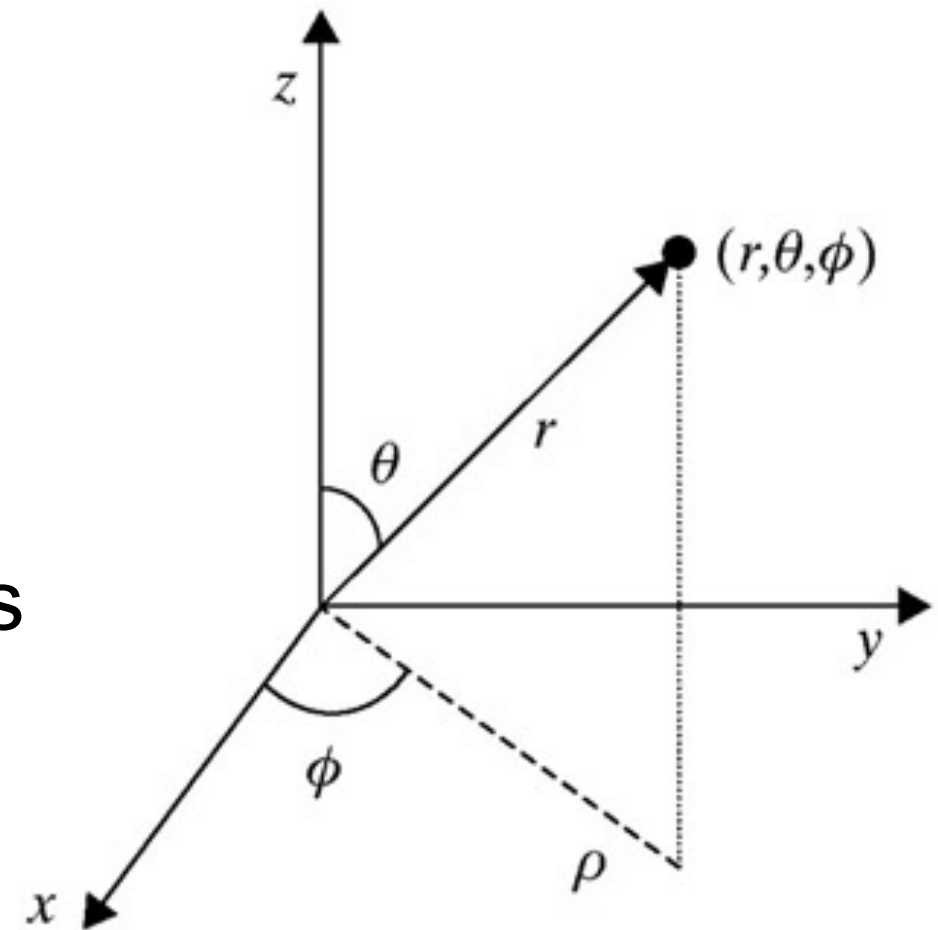
If we write  $V(x, y, z) = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2)$

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  
 $\theta$  and  $\phi$  :

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

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

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

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

