Lecture 5: Quantum Mechanics with more than one degree of freedom

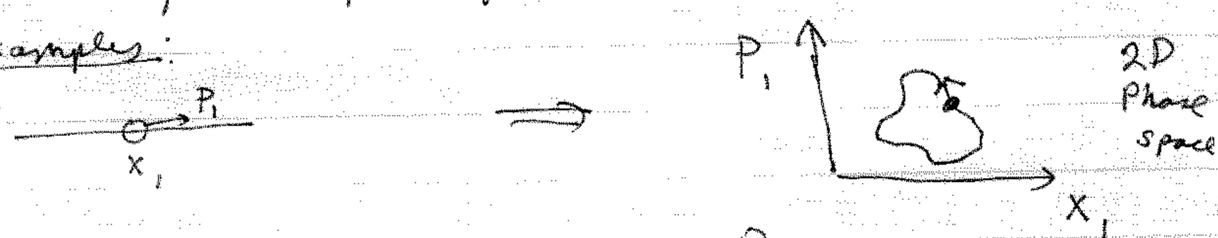
Up until now we have been considering only systems of a single structureless particle moving only in one dimension. Though this allowed us to explore various quantum phenomena such as tunnelling and quantum reflection, things get really interesting when we consider systems with more degrees of freedom. Phenomena which have no classical analog at all, such as entanglement, arise. We begin this exploration here and more deeply next semester.

Multiple Degrees of Freedom: The Classical Picture

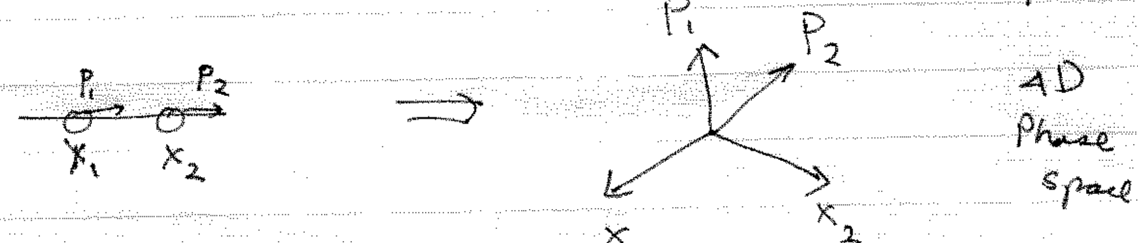
In classical physics, each "degree of freedom" (d.o.f) is assigned a pair of canonical coördinates: (x, p)

Examples:

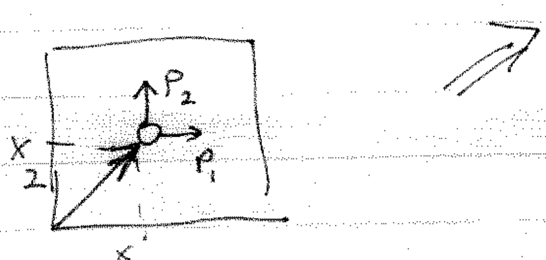
1 Particle in 1D



2 particles in 1D



1 particle in 2D



The phase space is said to be the "Cartesian product" of the canonical coördinates for each d.o.f

n-dof : $(x_1, x_2, \cdots x_n, p_1 p_2 \cdots p_n) = (x_1, p_1) \times (x_2, p_2)$

2n dim space $\cdots \times (x_n, p_n)$

The Hamiltonian generates the dynamics

$$H(x_1, x_2 \ldots x_n, p_1, p_2, \ldots p_n)$$

Example: 1 particle moving in the x-y plane with potential energy $V(x,y)$

$$H = \underbrace{\frac{p_x^2}{2m} + \frac{p_y^2}{2m}}_{\text{kinetic energy}} + V(x,y)$$

kinetic energy $\frac{|\vec{p}|^2}{2m} = \frac{p_x^2 + p_y^2}{2m}$

If $V(x,y) = V_x(x) + V_y(y)$

then $H = H_x(x, p_x) + H_y(y, p_y)$

where $H_x = \frac{p_x^2}{2m} + V_x(x)$, $H_y = \frac{p_y^2}{2m} + V_y(y)$

For such situations the Hamiltonian is said to be <u>separable</u> into motion along x and motion along y. The two degrees of freedom are completely independent and don't interact.

Multiple degrees of freedom: Quantum Picture

To "quantize" the system each pair of canonical coördinates becomes an operator

$$(x_j, p_j) \longrightarrow (\hat{x}_j, \hat{p}_j)$$

In the "position representation"

$$\hat{x}_j = x_j \qquad \Rightarrow \qquad [\hat{x}_j, \hat{p}_j] = i\hbar$$
$$\hat{p}_j = \frac{\hbar}{+i}\frac{\partial}{\partial x_j}$$

In general, for many degrees of freedom

$$\boxed{\begin{aligned} &[\hat{x}_j, \hat{x}_k] = 0 \qquad [\hat{p}_j, \hat{p}_k] = 0 \\ &[\hat{x}_j, \hat{p}_k] = i\hbar\,\delta_{jk} = \begin{cases} 0 & j \neq k \\ i\hbar & j = k \end{cases} \end{aligned}}$$

To see this last result $[\hat{x}_j, \hat{p}_k]\psi = \left(x_j \frac{\hbar}{+i}\frac{\partial \psi}{\partial x_k}\right. \left. - \left(\frac{\hbar}{+i}\frac{\partial}{\partial x_k} x_j \psi\right)\right)$

$$\Rightarrow [\hat{x}_j, \hat{p}_k]\psi = i\hbar\left(\frac{\partial}{\partial x_k} x_j\right) = \delta_{jk}$$

Thus, we see that observables associated with different dof commute and therefore we can specify simultaneous eigenstates of the observables. The <u>different degrees of freedom</u> have no uncertainty principle.

Schrödinger Equation:

The ~~S~~ T.D.S.E. is $\frac{\hbar}{i}\frac{\partial}{\partial t}\psi = \hat{H}\psi$

where $\hat{H} = H(\hat{x}_1, \dots \hat{x}_n, \hat{p}_1 \dots \hat{p}_n)$

for the n-degrees of freedom

As before the stationary states $\psi_E(\vec{x}, t) = u_E(\vec{x})\, e^{-\frac{iEt}{\hbar}}$

(here $\vec{x} = (x_1, x_2, \dots, x_n)$)

$\Rightarrow$ T.I.S.E $\quad \hat{H}u = Eu$

Suppose $\hat{H}$ is <u>separable</u>, e.g. 2 dof

$$\hat{H} = \hat{H}_1 + \hat{H}_2$$

$$\Longrightarrow \exists\, u(x_1, x_2) = u^{(1)}(x_1)\, u^{(2)}(x_2)$$

Proof $\quad \hat{H}\, u(x_1, x_2) = (\hat{H}_1 + \hat{H}_2)\, u^{(1)}(x_1)\, u^{(2)}(x_2)$

$$= u^{(2)}(x_2)\, \underbrace{\hat{H}_1 u^{(1)}(x_1)}_{E^{(1)} u^{(1)}(x_1)} + u^{(1)}(x_1)\, \underbrace{\hat{H}_2 u^{(2)}(x_2)}_{E^{(2)} u^{(2)}(x_2)}$$

$$= (E^{(1)} + E^{(2)})\, u^{(1)}(x_1)\, u^{(2)}(x_2)$$

$$\Rightarrow \boxed{\hat{H}u = E\, u(x_1, x_2) \quad \text{where } E = E^{(1)} + E^{(2)}}$$

In a separable system the energy eigenvalue is the sum of eigenvalues for each subsystem. The energy eigenfunction is the product of the eigenfunctions for each subsystem.

Separation of Variables and Separable Hamiltonians

Example: Free particle in 3D

$$\hat{H} = \frac{\hat{p}^2}{2m} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{\hat{p}_y^2}{2m}$$

Position rep: $\hat{\vec{p}} = \frac{\hbar}{i}\vec{\nabla} = \underbrace{\frac{\hbar}{i}\frac{\partial}{\partial x}}_{\hat{p}_x}\vec{e}_x + \underbrace{\frac{\hbar}{i}\frac{\partial}{\partial y}}_{\hat{p}_y}\vec{e}_y + \underbrace{\frac{\hbar}{i}}_{\hat{p}_y}\frac{\partial}{\partial z}\vec{e}_z$

$$\hat{p}^2 = |\hat{\vec{p}}|^2 = -\hbar^2\nabla^2 = -\hbar^2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial y^2}\right)$$

T.I.S.E. $\hat{H}\,u(x,y,z) = E\,u(x,y,z)$

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

$$\Rightarrow Y(y)Z(z)\left(\frac{\hat{p}_x^2}{2m}X(x)\right) + X(x)Z(z)\left(\frac{\hat{p}_y^2}{2m}Y(y)\right) + X(x)Y(y)\left(\frac{\hat{p}_z^2}{2m}Z(z)\right) = E\,XYZ$$

$$\Rightarrow \frac{1}{X(x)}\left(\frac{\hat{p}_x^2}{2m}X(x)\right) + \frac{1}{Y(y)}\left(\frac{\hat{p}_y^2}{2m}Y(y)\right) + \frac{1}{Z(z)}\left(\frac{\hat{p}_z^2}{2m}\hat{Z}(z)\right)$$

$$= E$$

Each of the terms on the left hand side is a separate function of x, y and z. They must always add to a constant E. Thus each term must be a constant.

$$\frac{1}{X(x)}\left(\frac{\hat{p}_x^2}{2m} X(x)\right) = E_x \leftarrow \text{(separation constant)}$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} X(x) = E_x X(x)$$

etc. ... $$-\frac{\hbar^2}{2m}\frac{d^2}{dy^2} Y(y) = E_y Y(y)$$

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

We thus have three separate 1D T.I.S.E. for a free particle along $x, y,$ and z

$$X(x) = \frac{1}{\sqrt{2\pi}} e^{ik_x x}, \quad Y(y) = \frac{1}{\sqrt{2\pi}} e^{ik_y y}, \quad Z(z) = \frac{1}{\sqrt{2\pi}} e^{ik_z z}$$

$$E_x = \frac{(\hbar k_x)^2}{2m}, \quad E_y = \frac{(\hbar k_y)^2}{2m}, \quad E_z = \frac{(\hbar k_z)^2}{2m}$$

$$\Rightarrow \boxed{\begin{array}{l} \psi_E(x,y,z) = \dfrac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{x}} \\ E = \dfrac{(\hbar \vec{k})^2}{2m} \end{array}} \leftarrow \text{plane waves in 3D}$$

where $\vec{k} = k_x \vec{e}_x + k_y \vec{e}_y + k_z \vec{e}_z \leftarrow \frac{\vec{p}}{\hbar}$ = Wave vector

$$|\vec{k}|^2 = k_x^2 + k_y^2 + k_z^2$$

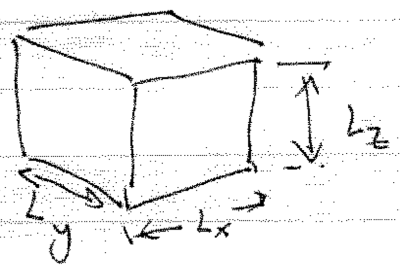
Example: Infinite well in 3D (particle in a box)

We consider a rectangular box with infinitely high walls.

$$V = \begin{cases} 0 & \text{inside the box} \\ \infty & \text{outside} \end{cases}$$

Let the dimensions of the box be:

$$-\frac{L_x}{2} < x < \frac{L_x}{2}, \quad -\frac{L_y}{2} < y < \frac{L_y}{2}, \quad -\frac{L_z}{2} < z < \frac{L_z}{2}$$



(origin at corner of box)

This potential is separable:

$$V(x,y,z) = V_x(x) + V_y(y) + V_z(z)$$

where $V_x(x) = \begin{cases} 0 \\ \infty \end{cases}$

$V_y(y)$ and $V_z(z)$ similar

$\Rightarrow$ Energy eigenvalues:

$$E(n_x,n_y,n_z) = \frac{(\hbar k(n_x,n_y,n_z))^2}{2m}, \quad n_x\, n_y\, n_z = 1,2,3,\ldots$$

$$\vec{k}(n_x,n_y,n_z) = \frac{\pi}{L_x}\vec{e}_x + \frac{\pi}{L_y}\vec{e}_y + \frac{\pi}{L_z}\vec{e}_z$$

$$\Rightarrow E(n_x,n_y,n_z) = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)$$

The corresponding stationary state

$$u_{n_x,n_y,n_z}(x,y,z) = u_{n_x}(x)\, u_{n_y}(y)\, u_{n_y}(z)$$

where $u_{n_x}(x) = \sqrt{\frac{2}{L_x}} \sin\left(\frac{n_x \pi}{L_x} x\right)$

etc.

$$\Rightarrow \boxed{u_{n_x n_y n_z}(\vec{x}) = \frac{2^{3/2}}{\sqrt{V}} \sin\left(\frac{n_x \pi}{L_x} x\right) \sin\left(\frac{n_y \pi}{L_y} y\right) \sin\left(\frac{n_z \pi}{L_x} z\right)}$$

where $V = L_x L_y L_z$ = Volume of box

Typically, we use a short hand and label the stationary states by the indecies n_x, n_y, n_z

$$\Rightarrow |n_x, n_y, n_z\rangle \doteq u_{n_x,n_y,n_z}(x,y,z)$$

These states form a basis for the Hilbert Space

$$|\psi\rangle = \sum_{n_x,n_y n_z} c_{n_x,n_y,n_z} |n_x, n_y, n_z\rangle$$

Expansion coefficients $c_{n_x n_y n_z} = \langle n_x, n_y, n_z | \psi\rangle$

$$= \int d^3x\, u^*_{n_x n_y n_z}(\vec{x})\, \psi(\vec{x})$$

where $d^3x = dx\, dy\, dz$

Example: Finite square well in 2D

Unlike the infinite well, the finite square well is not separable. Consider the 2D problem

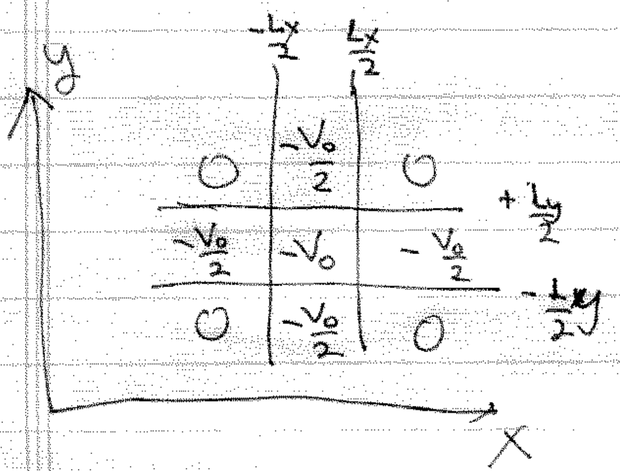
$$V(x,y) = \begin{cases} -V_0 & \text{inside} \\ 0 & \text{outside} \end{cases}$$

We might be tempted to try $V(x,y) = V_x(x) + V_y(y)$

where $V_x(x) = \begin{cases} -V_0/2 & -\frac{L_x}{2} \le x \le L_x/2 \\ 0 & \text{otherwise} \end{cases}$

$$V_y(y) = \begin{cases} -V_0/2 & -\frac{L_y}{2} \le y \le L_y/2 \\ 0 & \text{otherwise} \end{cases}$$

However $V_x(x) + V_y(y) = \begin{cases} -V_0 & \text{inside box} \\ -\frac{V_0}{2} & |x| < L_x/2,\ |y| > \frac{L_y}{2} \\ & |x| > L_x/2,\ |y| < \frac{L_y}{2} \\ 0 & \text{otherwise} \end{cases}$



: This is $V_x(x) + V_y(y)$

Thus, solving for the stationary states of the 2D finite well involves a 2D PDE – very messy!

Degeneracies:

Unlike problems with 1 dof, in higher dimensions there ~~are~~ are often degeneracies in the energy spectrum, i.e. different stationary states with the same energy eigenvalue.
These come ~~in~~ two classes: "accidental" and "essential"

Consider the infinite square well in 2D

$$E(n_x, n_y) = n_x^2 \frac{\pi^2\hbar^2}{2mL_x^2} + n_y^2 \frac{\pi^2\hbar^2}{2mL_y^2}$$

$$= \frac{\pi^2\hbar^2}{2mL_x^2}\left(n_x^2 + n_y^2\left(\frac{L_x}{L_y}\right)^2\right)$$

If $\frac{L_x}{L_y}$ = rational number, there there are degeneracies

e.g. $\frac{L_x}{L_y} = \frac{1}{2} \Rightarrow E(n_x=2, n_y=2) = E(n_x=1, n_y=4)$
$$= 5\, E_{1x}$$

This is an accidental degeneracy, i.e.

not due to any essential symmetry

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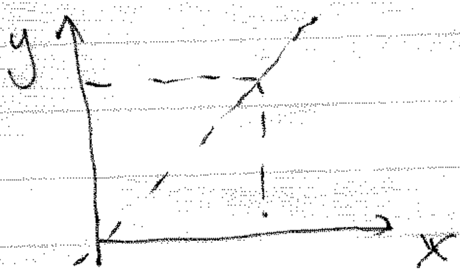
In contrast, suppose $L_x = L_y \equiv L$

$$\Rightarrow E(n_x^2+n_y^2) = \frac{\pi^2\hbar^2}{2mL^2}(n_x^2+n_y^2)$$

$$\Rightarrow \text{Degeneracy} \quad E_{n_x,n_y} = E_{n_y,n_x}$$

"Essential degeneracy" due to symmetry

Here reflections $x \Leftrightarrow y$



$V(x,y)$ is invariant under $x \Leftrightarrow y$

Example: Free particle

$E = \frac{\hbar |\vec{k}|^2}{2m}$: Infinitely degenerate. ~~Dependent~~

Depends only on $|\vec{k}|$ and not the direction of $\vec{k}$

Essential degeneracy: Rotation symmetry