Lecture 4 : Solving the Schrodinger Equation with multiple degrees of freedom

Separability

Consider a system with N-degrees of freedom
(E.g. two spinless particles in 3D $\Rightarrow$ 6 d-o-f)

The Hilbert space for the composite is

$$\mathcal{H} = h_1 \otimes h_2 \otimes h_3 \otimes \cdots \otimes h_N$$

where h_i is the Hilbert space for d-o-f, i

Let $\hat{H}$ be the Hamiltonian acting on $\mathcal{H}$

$\hat{H}$ is said to be separable if

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_3 + \cdots$$

$$= \hat{H}_1 \otimes \hat{\mathbb{1}}_2 \otimes \cdots \hat{\mathbb{1}}_N + \hat{\mathbb{1}}_1 \otimes \hat{H}_2 \otimes \cdots \hat{\mathbb{1}}_N + \cdots$$

where $\hat{H}_i$ acts on h_i

Since $[\hat{H}_i, \hat{H}_j] = 0$

$\Rightarrow \exists$ simultaneous eigenstates of $\{\hat{H}_i\}$

$\Rightarrow$ Stationary states are separable:

$$|\Psi_{n_1, n_2, n_3 \ldots}\rangle = |u_{n_1}\rangle \otimes |v_{n_2}\rangle \otimes |w_{n_3}\rangle \cdots$$

$$\hat{H}\,|\Psi_{n_1, n_2, n_3 \ldots}\rangle = (E_{n_1} + E_{n_2} + \cdots + E_{n_N})\,|\Psi_{n_1, n_2 \ldots n_N}\rangle$$

Time evolution of separable Hamiltonian

Time evolution operator: $\hat{U}(t) = e^{-\frac{i}{\hbar}\hat{H}t}$

$$\Rightarrow \hat{U}(t) = e^{-\frac{i}{\hbar}\left(\sum_{i=1}^{N}\hat{H}_i\right)t} = \prod_i \otimes e^{-i\hat{H}_i t/\hbar} \quad \text{since } [\hat{H}_i, \hat{H}_j] = 0$$

$$= e^{\frac{-i\hat{H}_1 t}{\hbar}} \otimes e^{\frac{-i\hat{H}_2 t}{\hbar}} \otimes e^{\frac{-i\hat{H}_3 t}{\hbar}} \cdots \otimes e^{-i\hat{H}_N t/\hbar}$$

$$= \bigotimes_{i=1}^{N} \hat{U}_i(t) \Rightarrow \underline{\hat{U} \text{ factorized}}$$

$\therefore$ $\hat{U}(t)$ does not create <u>entanglement</u> between degrees of freedom

Eg $N=2$: suppose $|\Psi(0)\rangle = |\phi(0)\rangle \otimes |\chi(0)\rangle$

$$\Rightarrow |\Psi(t)\rangle = \hat{U}(t)\, |\phi(0)\rangle \otimes |\chi(0)\rangle$$

$$= \hat{U}_1(t)|\phi(0)\rangle \otimes \hat{U}_2(t)|\chi(0)\rangle$$

$$= |\phi(t)\rangle \otimes |\chi(t)\rangle$$

Thus if the state is initially separable at $t=0$, for latter times it remains separable when $\hat{H}$ is separable.

Conversely, if $\hat{H}$ is not separable for d-o-f $\{i=1,..N\}$ then the dynamics create <u>entangled states</u>

<u>Physically</u>: If the Hamiltonian is separable, these d-o-f do not <u>interact</u>.

Examples:

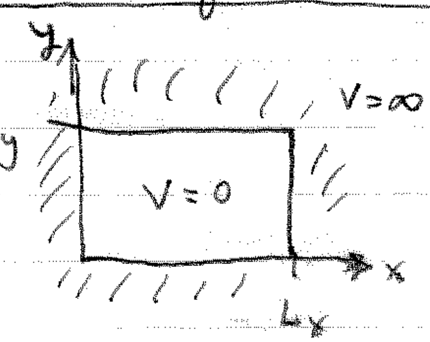
Spinless particle in 2D potential

$$\hat{H} = \frac{\hat{P}_x^2}{2m} + \frac{\hat{P}_y^2}{2m} + \hat{V}(x,y)$$

$$\stackrel{?}{=} \hat{H}_x + \hat{H}_y$$

Separability in x and y depends on potential since kinetic energy separate in x and y

- 2D infinite "square" well



$$\hat{V}(x,y) = \hat{V}_x(x) + \hat{V}_y(y)$$

$$\hat{V}_{x_i}(x_i) = \begin{cases} 0 & 0 < x_i < L_{x_i} \\ \infty & \text{elsewhere} \end{cases}$$

Eigenstates: $|\psi_{n_x,n_y}\rangle = |u_{n_x}\rangle |v_{n_y}\rangle$

Position rep: $\psi_{n_x,n_y} = \langle x,y|\psi_{n_x n_y}\rangle = u_{n_x}(x)\, v_{n_y}(y)$

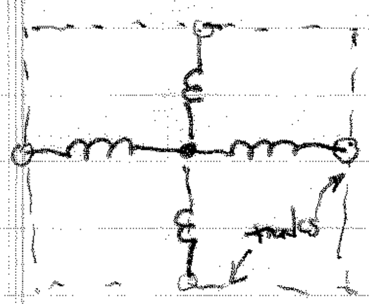
$$= \sqrt{\frac{2}{L_x}} \sin\left(\frac{n_x \pi x}{L_x}\right) \sqrt{\frac{2}{L_y}} \sin\left(\frac{n_y \pi}{L_y} y\right)$$

Energy eigenvalue

$$E_{n_x,n_y} = E_{n_x} + E_{n_y}$$

$$E_{n_{x_i}} = \frac{(\hbar k_{n_{x_i}})^2}{2m} = n_{x_i}^2 \left(\frac{\pi^2 \hbar^2}{2m L_{x_i}^2}\right)$$

• 2D SHO



$$\hat{V}(x,y) = \tfrac{1}{2} m\omega_x^2 \hat{x}^2 + \tfrac{1}{2} m\omega_y^2 \hat{y}^2$$
$$= V_x(\hat{x}) + V_y(\hat{y})$$
$$\Rightarrow \hat{H} = \hat{H}_x + \hat{H}_y$$

$$\hat{H}_{x_i} = \hbar\omega_{x_i}\left(\hat{a}_i^\dagger \hat{a}_i + \tfrac{1}{2}\right) \qquad \hat{a}_i = \tfrac{1}{\sqrt{2}}(\hat{X}_i + i\hat{P}_i)$$
$$x_c = \sqrt{\frac{\hbar}{m\omega_x}}, \quad y_c = \sqrt{\frac{\hbar}{m\omega_y}}$$

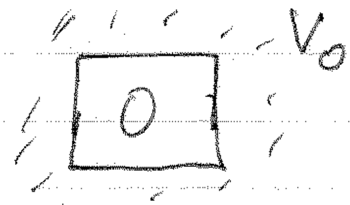
Eigenstates $|n_x, n_y\rangle = |n_x\rangle \otimes |n_y\rangle$

$$\psi_{n_x n_y}(x,y) = u_{n_x}(x)\, u_{n_y}(y)$$
$$= \frac{1}{\sqrt{x_c y_c 2^{n_x+n_y} n_x!\, n_y!}} H_{n_x}\!\left(\frac{x}{x_c}\right) H_{n_y}\!\left(\frac{y}{y_c}\right) e^{-\frac{1}{2}\left[\left(\frac{x}{x_c}\right)^2 + \left(\frac{y}{y_c}\right)^2\right]}$$

Eigenvalue: $E_{n_x,n_y} = \hbar\omega_x(n_x + \tfrac{1}{2}) + \hbar\omega_y(n_y + \tfrac{1}{2})$

• Finite "square well" in 2D

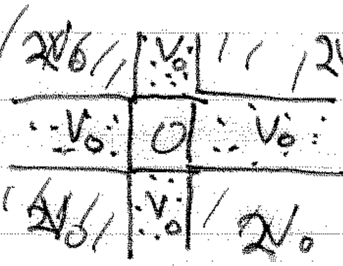
$$V(x,y) = \begin{cases} 0 & \begin{cases} 0 < x < L_x \\ 0 < y < L_y \end{cases} \\ V_0 & \text{elsewhere} \end{cases}$$



$$V(x,y) \neq V_x(x) + V_y(y)$$

$\Rightarrow$ $\hat{H}$ not separable

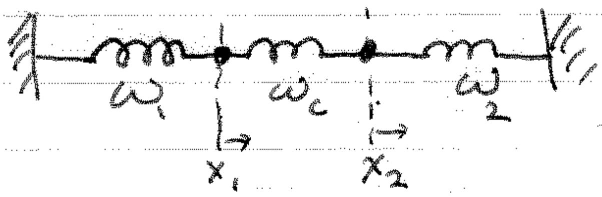
$\Rightarrow$ There may be no bound state!



separable

Whether a Hamiltonian is separable depends on which degrees of freedom we consider

Example: Two coupled 1D SHO



Choose $m_1 = m_2 = m$

$\omega_1 = \omega_2 = \omega$

Coupling spring: $\omega_c^2 = \lambda \omega^2$

$$\hat{H} = \frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m} + V(\hat{x}_1, \hat{x}_2)$$

$$\Rightarrow V(\hat{x}_1, \hat{x}_2) = \frac{1}{2} m\omega^2 (\hat{x}_1^2 + \hat{x}_2^2) + \lambda m\omega^2 (\hat{x}_1 - \hat{x}_2)^2$$

Not separable is $\hat{x}_1$ and $\hat{x}_2$ $\Longleftrightarrow$ Coupled!

However suppose we define:

$$\hat{x}_S = \frac{\hat{x}_1 + \hat{x}_2}{2} \quad \text{(center of mass coordinate)}$$

$$\hat{x}_A = \hat{x}_1 - \hat{x}_2 \quad \text{(relative coordinate)}, \quad [\hat{x}_S, \hat{x}_A] = 0$$

Conjugate momenta: $\hat{P}_S = \hat{p}_1 + \hat{p}_2$, $\hat{P}_A = \frac{1}{2}(\hat{p}_1 - \hat{p}_2)$

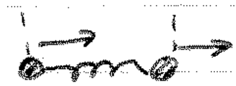
$$\Rightarrow [\hat{x}_S, \hat{P}_S] = [\hat{x}_A, \hat{P}_A] = i\hbar \qquad [\hat{x}_S, \hat{P}_A] = [\hat{x}_A, \hat{P}_S] = 0$$

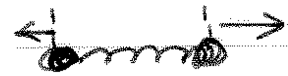
$$\Rightarrow \hat{H} = \frac{\hat{P}_S^2}{2M} + \frac{\hat{P}_A^2}{2\mu} + \frac{1}{2} M\omega_S^2 \hat{x}_S^2 + \frac{1}{2}\mu\omega_A^2 \hat{x}_A^2$$

where $M = m_1 + m_2 = 2m$ total mass

$$\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{m}{2} \quad \text{reduced mass}$$

$$\omega_S^2 = \omega^2 , \qquad \omega_A^2 = (1+4\lambda)\,\omega^2$$

Normal modes: symmetric: 

anti-symmetric: 

$$\hat{H} = \hat{H}_S + \hat{H}_A$$: <u>separable in normal modes</u>

Eigenstates $|\psi_{n_A n_S}\rangle = |n_A\rangle \otimes |n_S\rangle$

$$\psi_{n_A, n_S} = u_{n_A}(x_A)\, u_{n_S}(x_S)$$

Note: these eigenstates are entangled in x_1 and x_2

<u>Degeneracy and Symmetry</u>

Consider the 2D ∞ well:

$$E_{n_x n_y} = \frac{\pi^2\hbar^2}{2m}\left(\left(\frac{n_x}{L_x}\right)^2 + \left(\frac{n_y}{L_z}\right)^2\right) = \underbrace{\frac{\pi^2\hbar^2}{2mL_x^2}}_{\equiv E_{1x}} \left(n_x^2 + n_y^2\left(\frac{L_x}{L_y}\right)^2\right)$$

If $\frac{L_x}{L_y} = r$ is a <u>rational</u> # then there are degenerate eigenstates

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

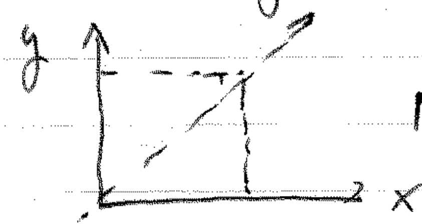
"Accidental degeneracy"

If $L_x = L_y = L \Rightarrow E_{n_x,n_y} = E_1[n_x^2 + n_y^2]$

Degeneracy $E_{n_x,n_y} = E_{n_y,n_x}$

"Essential degeneracy" due to symmetry

Here reflection symmetry $\hat{x} \Leftrightarrow \hat{y}$



potential is symmetry w.r.t. reflection through $x=y$ (kinetic also symmetric)

- Consider 2D isotropic SHO $\omega_x = \omega_y = \omega$

$$\Rightarrow \hat{V} = \tfrac{1}{2} m\omega^2 (x^2 + y^2)$$

$$E_{n_x,n_y} = \hbar\omega(n_x + n_y + 1)$$ depends only on sum $n_x + n_y$

Label eigenstates by single integer $n = 0, 1, 2, \ldots$

$E_n = \hbar\omega(n+1)$: Degeneracy factor g_n

g_n = All pairs which add to n $= n+1$

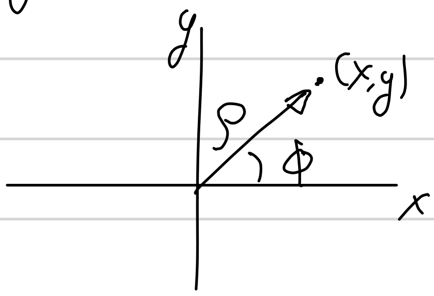
$n=0$: $n_x = 0$, $n_y = 0$ $\qquad g_0 = 1$

$n=1$: $(n_x=1, n_y=0)$ or $(n_x=0, n_y=1)$ $\qquad g_1 = 2$

$n=2$: $(n_x=2, n_y=0)$ or $(n_x=1, n_y=1)$ or $(n_x=0, n_y=2)$

$g_2 = 3$

The degeneracy in the isotropic SHO is due to symmetry – this is an <u>essential</u> degeneracy. The isotropic SHO is rotational invariant about the z-axis. We see this the Hamiltonian in cylindrical coordinates.



$$\hat{H} = \frac{\hat{P}^2}{2m} + \underbrace{\frac{1}{2} m\omega^2 \hat{\rho}^2}_{V(\hat{\rho})}$$

Since the kinetic energy is rotationally invariant, the question of rotational symmetry depends on the potential energy. Since V depends only on ρ, and not on φ, it in rotationally invariant. Formally, the rotation operator around the z-axis is generated by the (orbital) angular momentum operator component $\hat{L}_z$

$$\hat{U}(\phi) = e^{-i\phi \hat{L}_z/\hbar}$$

(Azimuthal) rotational symmetry $\Rightarrow$ $\hat{U}^\dagger(\phi)\,\hat{H}\,\hat{U}(\phi) = \hat{H} \Rightarrow [\hat{H}, \hat{U}(\phi)] = 0$

This symmetry is associated with a conserved quantity, $\hat{L}_z$: $[\hat{H}, \hat{L}_z] = 0$

$\Rightarrow$ There exist common eigenstates of $\hat{L}_z$ and the Hamiltonian.

$\Rightarrow$ L_z is conserved $\Rightarrow$ eigenvalue of L_z is a "good quantum number"

From elementary quantum mechanics, $\hat{L}_z|m\rangle = m\hbar|m\rangle$, where m is an integer

There are thus joint eigenstates $\{|n,m\rangle\}$, where $\hat{H}|n,m\rangle = (n+1)\hbar\omega|n\rangle$, $\hat{L}_z|n,m\rangle = m|n,m\rangle$

There are, in fact, $n+1$ diffrent values of m (L_z angular momentum) given n quanta of vibration (see homework) $\Rightarrow$ Degeneracy $g_n = n+1$

We say that $\{\hat{H}, \hat{L}_z\}$ form a complete set of mutually commuting operators, in that a state is completely specified by the eigenvectors of these two operators.

<u>Generally</u>: Given N-degrees of freedom, a basis is formed by N mutually commuting Hermitian operators such that in total they act on all d.o.f. If one of those is the Hamiltonian, then $\{\hat{H}, \hat{A}_1, \hat{A}_2, \ldots \hat{A}_{N-1}\}$ form a "complete set." The observables $\{\hat{A}_j\}$ are <u>conserved quantities</u>. They are related to <u>symmetries</u>