Lecture 4: Solving the Schrödinger 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

\[ \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3 \otimes \cdots \otimes \mathcal{H}_N \]

where \( \mathcal{H}_i \) 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

\[ \hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_3 + \cdots \]

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

where \( \hat{H}_i \) acts on \( \mathcal{H}_i \)

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

\( \Rightarrow \exists \) simultaneous eigenstates of \( \sum \hat{H}_i \)

\( \Rightarrow \) Stationary states are separable:

\[ |\psi_{n_1, n_2, n_3, \ldots} \rangle = |\psi_{n_1} \rangle \otimes |\psi_{n_2} \rangle \otimes |\psi_{n_3} \rangle \otimes \cdots \]

\[ \hat{H} |\psi_{n_1, n_2, n_3, \ldots} \rangle = (E_{n_1} + E_{n_2} + \cdots + E_{n_N}) |\psi_{n_1, n_2, n_3, \ldots} \rangle \]
Time evolution of separable Hamiltonian

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

\[
\hat{U}(t) = e^{-i\frac{1}{2}\left(\sum_{i=1}^{N} \hat{A}_i^2\right)t} = \prod_{i} e^{-i\hat{A}_i t/\hbar} \quad \text{since} \quad [\hat{A}_i, \hat{A}_j] = 0
\]

\[
= e^{-i\hat{A}_1 t/\hbar} \otimes e^{-i\hat{A}_2 t/\hbar} \otimes e^{-i\hat{A}_3 t/\hbar} \otimes \ldots \otimes e^{-i\hat{A}_N t/\hbar}
\]

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

\[\Rightarrow \hat{U}(t) \text{ does not create entanglement between degrees of freedom}\]

**Example 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 later times it remains separable when it is separable.

Conversely, if $\hat{H}$ is not separable for d.o.f $\epsilon_i = \ldots N$, then the dynamics create entangled states.

Physically: If the Hamiltonian is separable, these d.o.f do not interact.
Examples:

For spinless particle in 2D potential

\[ \hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \hat{V}(x,y) \]

\[ = \hat{H}_x + \hat{H}_y \]

Separability in \( x \) and \( y \) depends on potential since kinetic energy separate in \( x \) and \( y \).

- 2D infinite "square" well

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

\[ \hat{V}_x(x) = \begin{cases} 0 & \text{if } 0 < x < L_x, \\ \infty & \text{elsewhere} \end{cases} \]

Eigenstates: \( |\psi_{n_x,n_y}\rangle = |U_{n_x}\rangle |U_{n_y}\rangle \)

Position rep:

\[ \psi_{n_x,n_y} = \langle x,y | \psi_{n_x,n_y} \rangle = U_{n_x}(x) U_{n_y}(y) \]

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

Energy eigenvalue

\[ E_{n_x,n_y} = E_{n_x} + E_{n_y} \]

\[ E_{n_x} = \left(\frac{\hbar k_{n_x}}{2m}\right)^2 = \hbar^2 \left(\frac{\pi^2 k_{n_x}^2}{2m L^2}\right) \]
2D Schrödinger Equation

\[ V(x, y) = \frac{1}{2} m a_x^2 \hat{x}^2 + \frac{1}{2} m a_y^2 \hat{y}^2 \]

\[ = V_x(x) + V_y(y) \]

\[ \Rightarrow \hat{H} = \hat{H}_x + \hat{H}_y \]

\[ \hat{H}_X = \hbar \omega_x (\hat{a}_x^\dagger \hat{a}_x + \frac{1}{2}) \quad \hat{a}_x = \frac{\hbar}{\sqrt{2 \omega_x}} (\hat{x}_c + i \hat{p}_x) \]

Eigenstates \( |n_x, n_y \rangle = |n_x \rangle \otimes |n_y \rangle \)

\[ \psi_{n_x n_y}(x, y) = U_{n_x}(x) U_{n_y}(y) e^{-\frac{1}{2} \left( x^2 + y^2 \right)} \]

\[ = \frac{1}{\sqrt{x_c y_c 2^{n_x + n_y} n_x! n_y!}} \sqrt{\frac{4}{n_x x_c}} \sqrt{\frac{4}{n_y y_c}} \psi_{n_x}(x) \psi_{n_y}(y) \]

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

Finite "Square Well" in 2D

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

\[ V(x, y) \neq V_x(x) + V_y(y) \]

\[ \Rightarrow \hat{H} \text{ not separable} \]

\[ \Rightarrow \text{There may be no bound state} \]
Whether a Hamiltonian is separable depends on which degrees of freedom we consider.

Example: Two coupled 1D SHO

\[ H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(x_1, x_2) \]

Choose \( m_1 = m_2 = m \)

\( \omega_1 = \omega_2 = \omega \)

Coupling spring: \( \omega_c^2 = \lambda \omega^2 \)

\[ V(x_1, x_2) = \frac{1}{2} m \omega^2 (x_1^2 + x_2^2) + \lambda m c \omega^2 (x_1 - x_2)^2 \]

Not separable is \( \dot{x}_1 \) and \( \dot{x}_2 \leftrightarrow \text{Coupled!} \)

However suppose we define:

\[ x_s = \frac{x_1 + x_2}{2} \] (center of mass coordinate)

\[ x_A = x_1 - x_2 \] (relative coordinate) \( \{x_s, x_A\} = 0 \)

Conjugate momenta:

\[ \hat{p}_s = \hat{p}_1 + \hat{p}_2 \]

\[ \hat{p}_A = \frac{1}{2} (\hat{p}_1 - \hat{p}_2) \]

\[ \{x_s, \hat{p}_A\} = \{x_A, \hat{p}_s\} = \frac{i}{\hbar} \]

\[ \{x_s, \hat{p}_A\} = \{x_A, \hat{p}_s\} = 0 \]

\[ H = \frac{\hat{p}_s^2}{2M} + \frac{\hat{p}_A^2}{2\mu} + \frac{1}{2} M \omega_s^2 x_s^2 + \frac{1}{2} \mu \omega_A^2 x_A^2 \]

where \( M = m_1 + m_2 = 2m \) total mass

\[ \mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{m}{2} \text{ reduced mass} \]
\[ \omega_s^2 = \omega^2, \quad \omega_A^2 = (1 + 4\lambda) \omega^2 \]

Normal modes: symmetric: \[ \text{symmetric} \]
anti-symmetric: \[ \text{anti-symmetric} \]

\[ \hat{H} = \hat{H}_5 + \hat{H}_A : \text{ separable in normal modes} \]

Eigenstates: \[ |\psi_{n_a n_s}\rangle = |n_a\rangle \otimes |n_s\rangle \]

\[ |\psi_{n_a n_s}\rangle = U_{n_a}(X_a) U_{n_s}(X_s) \]

Note: these eigenstates are entangled in \( X_1 \) and \( X_2 \)

**Degeneracy and Symmetry**

Consider the 2D as well:

\[ E_{n_x n_y} = \frac{\hbar^2}{2m} \left( (\frac{n_x}{L_x})^2 + (\frac{n_y}{L_y})^2 \right) = \frac{\hbar^2}{2mL_x^2} \left( n_x^2 + n_y^2 \left( \frac{L_x}{L_y} \right)^2 \right) = E_{1x}^{n_x} \]

If \( \frac{L_x}{L_y} = r \) is a rational \( \# \) then there are degenerate eigenstates.

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

"Accidental degeneracy!"
If \( L_x = L_y = L \) \( \Rightarrow \) \( E_{n_x, n_y} = E \left[ n_x^2 + n_y^2 \right] \)

Degeneracy, \( E_{n_x, n_y} = E_{n_y, n_x} \)

"Essential degeneracy" due to symmetry

Here reflection symmetry \( \hat{x} \Leftrightarrow \hat{y} \)

\[
\begin{array}{c}
0 \leftrightarrow 1 \\
\end{array}
\]

Potential is symmetric w.r.t. reflection through \( x = y \)

(kinetic also symmetric)

Consider 2D isotropic \( SL+O \) \( \omega_x = \omega_y = \omega \)

\[ V = \pm m \omega^2 (x^2 + y^2) \]

\[ E_{n_x, n_y} = \hbar \omega (n_x + n_y + 1) \]

depends only on sum \( n_x + n_y \)

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

\[ E_n = \hbar \omega (n + 1) \colon \text{Degeneracy factor} g_n \]

\( g_n = \text{All pairs which add to} \ n = n+1 \)

\( n=0 : \ n_x=0, \ n_y=0 \quad g_0 = 1 \)

\( n=1 : (n_x=1, \ n_y=0) \text{ or } (n_x=0, \ n_y=1) \quad g_1 = 2 \)

\( n=2 : (n_x=2, \ n_y=0) \text{ or } (n_x=1, \ n_y=1) \text{ or } (n_x=0, \ n_y=2) \quad g_2 = 3 \)
The degeneracy in the isotropic SHO is due to symmetry—this is an essential degeneracy. The isotropic SHO is rotational invariant about the z-axis. We see this the Hamiltonian in cylindrical coordinates.

\[
\hat{H} = \frac{\hat{p}_r^2}{2m} + \frac{1}{2}m\omega^2 r^2 \hat{\phi}^2 + V(\phi)
\]

Since the kinetic energy is rotationally invariant, the question of rotational symmetry depends on the potential energy. Since \( V \) depends only on \( \rho \), and not on \( \phi \), it is 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 \( \Rightarrow \hat{U}(\phi) \hat{A} \hat{U}(\phi) = \hat{A} \Rightarrow [\hat{A}, \hat{L}_z(\phi)] = 0 \)

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

\( \Rightarrow \) there exist common eigenstates of \( \hat{L}_z \) and the Hamiltonian.

\( \Rightarrow \hat{L}_z \) is conserved \( \Rightarrow \) eigenvalue of \( \hat{L}_z \) is a "good quantum number".

From elementary quantum mechanics, \( \hat{L}_z | m\rangle = m | m\rangle \), where \( m \) is an integer.

There are thus joint eigenstates \( | m, n\rangle \), where \( | m, n\rangle = (n+1)! \sqrt{n!} \langle n\rangle | m\rangle, \hat{L}_z | m, n\rangle = m | m, n\rangle \)

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

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

Generally, for \( N \)-degrees of freedom, a basis is formed by \( N \) mutually commuting operators such that in total they act on all d.o.f. If one of these is the Hamiltonian, then \( \hat{H}, \hat{A}_1, \hat{A}_2, \ldots, \hat{A}_N \) form a "complete set." The observables \( \hat{E}, \hat{J}, \hat{L}_z \) are conserved quantities. They are related to symmetries.