Evolution of the 2-particle state vector

Schrödinger equation:

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle = \left(\frac{\hat{P}_1^2}{2m_1} + \frac{\hat{P}_2^2}{2m_2} + \hat{V}(\hat{X}_1, \hat{X}_2)\right)|\psi(t)\rangle$$

$$\longleftrightarrow |\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi(0)\rangle$$

Two classes of problems

(A) $\hat{H}$ is separable, i.e. $\hat{H} = \frac{P_1^2}{2m_1} + \hat{V}(\hat{X}_1) + \frac{\hat{P}_2^2}{2m_2} + \hat{V}(\hat{X}_2) = \hat{H}_1 + \hat{H}_2$

(B) $\hat{H}$ is not separable, i.e. $\hat{V}(\hat{X}_1, \hat{X}_2) \neq \hat{V}_1(\hat{X}_1) + \hat{V}(\hat{X}_2) \Rightarrow \hat{H} \neq \hat{H}_1 + \hat{H}_2$

(Note: $\hat{X}_1, \hat{X}_2$ need not be the positions of the particle, but could be linear compinations $\rightarrow$ recall case of 2 coupled harmonic oscillators which can be decoupled by $X_1 = \frac{1}{2}(x_1+x_2), X_2 = x_1 - x_2$)

Class A – separable Hamiltonians:

Classically $\mathcal{H} = \mathcal{H}_1(x_1, p_1) + \mathcal{H}_2(x_2, p_2)$ $\rightarrow$ particles move independently of each other

In quantum theory:

For a stationary state

$|\psi(t)\rangle = e^{-iEt/\hbar}|E\rangle$

the S-Eq. reduces to the eigenvalue equation

$$[\hat{H}_1(\hat{X}_1, \hat{P}_1) + \hat{H}_2(\hat{X}_2, \hat{P}_2)]|E\rangle = E|E\rangle \qquad (*)$$

Since $[\hat{H}_1, \hat{H}_2] = 0$, they have simultaneous eigenstates $|E_1\rangle \in \mathbb{V}_1$, $|E_2\rangle \in \mathbb{V}_2$, and the eigenstates of $\hat{H}$ are $|E_1\rangle \otimes |E_2\rangle = |E_1 E_2\rangle \in \mathbb{V}_{1\otimes 2}$:

$$\left.\begin{aligned} \hat{H}_1 |E_1 E_2\rangle &= E_1 |E_1 E_2\rangle \\ \hat{H}_2 |E_1 E_2\rangle &= E_2 |E_1 E_2\rangle \end{aligned}\right\} \quad \begin{aligned} \hat{H}|E\rangle &= (\hat{H}_1 + \hat{H}_2)|E_1\rangle \otimes |E_2\rangle = (E_1 + E_2)|E_1\rangle \otimes |E_2\rangle \\ &= (E_1 + E_2)|E\rangle \equiv E|E\rangle \end{aligned}$$

$$\Rightarrow \boxed{E = E_1 + E_2} \text{ for the eigenvalues of } \hat{H}.$$

Hence
$$|\psi(t)\rangle = e^{-iEt/\hbar}|E\rangle = e^{-i(E_1+E_2)t/\hbar}|E_1\rangle \otimes |E_2\rangle$$
$$= \left(e^{-iE_1 t/\hbar}|E_1\rangle\right) \otimes \left(e^{-iE_2 t/\hbar}|E_2\rangle\right)$$

is the direct product of stationary states of $\hat{H}_1$ and $\hat{H}_2$.

Let's go through this exercise a second time, using the coordinate representation:

$$|E\rangle \longrightarrow \langle x_1 x_2 | E\rangle = \psi_E(x_1, x_2)$$

The eigenvalue eq. (*) becomes a differential equation:

$$\left[-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} + V_1(x_1) - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2^2} + V_2(x_2)\right]\psi_E(x_1, x_2) = E\psi_E(x_1, x_2)$$

Separation of variables: $\psi_E(x_1, x_2) = \psi_{E_1}(x_1)\,\psi_{E_2}(x_2)$

Plug this in and divide by ψ_E:

$$\underbrace{\frac{1}{\psi_{E_1}(x_1)}\left(-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} + V_1(x_1)\right)\psi_{E_1}(x_1)}_{=E_1} + \underbrace{\frac{1}{\psi_{E_2}(x_2)}\left(-\frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2^2} + V_2(x_2)\right)\psi_{E_2}(x_2)}_{=E_2} = E$$

$\Rightarrow$ 3 equations: $\quad E = E_1 + E_2$

$$\left(-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} + V_1(x_1)\right)\psi_{E_1}(x_1) = E_1\psi_{E_1}(x_1)$$

$$\left(-\frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2^2} + V_2(x_2)\right)\psi_{E_2}(x_2) = E_2\psi_{E_2}(x_2)$$

$$\Rightarrow \psi_E(x_1,x_2,t) = \psi_E(x_1,x_2)e^{-iEt/\hbar}$$

$$= \left(e^{-iE_1t/\hbar}\psi_{E_1}(x_1)\right)\cdot\left(e^{-iE_2t/\hbar}\psi_{E_2}(x_2)\right)$$

This is the x-representation of our formal solution above.

Case B – two interacting particles:

$$\mathcal{H} = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(x_1,x_2) \quad \text{with} \quad V(x_1,x_2) \neq V_1(x_1) + V_2(x_2)$$

This cannot be reduced to two independent single-particle problems except in special cases. The most prevalent one is that the interaction is only between the particles and depends only on their distance $|x_1 - x_2|$:

$$V(x_1,x_2) = V(x_1 - x_2)$$

In this case we can transform to relative and CM coordinates:

$$x = x_1 - x_2$$

$$x_{CM} = \frac{m_1x_1 + m_2x_2}{m_1+m_2} \Rightarrow p_{CM} = M\dot{x}_{CM} = m_1\dot{x}_1 + m_2\dot{x}_2\ , \ p = \mu\dot{x}$$

$$\left(\mu = \frac{m_1m_2}{m_1+m_2} = \frac{m_1m_2}{M}\right)$$

This allows to rewrite

$$\mathcal{H} = \underbrace{\frac{p_{CM}^2}{2M}}_{\mathcal{H}_{CM}(x_{CM},\, p_{CM})} + \underbrace{\frac{p^2}{2\mu} + V(x)}_{\mathcal{H}_{rel}(x,\, p)}$$

The new variables are again Cartesian and canonical, hence the quantization rules are

$$[\hat{X}_{CM}, \hat{P}_{CM}] = i\hbar \hat{\mathbb{1}} \underbrace{\{x_{CM}, p_{CM}\}}_{=1} = i\hbar \hat{\mathbb{1}}$$

$$[\hat{X}, \hat{P}] = i\hbar \hat{\mathbb{1}} \underbrace{\{x, p\}}_{1} = i\hbar \hat{\mathbb{1}}$$

(all other commutators are zero), and therefore

$$\hat{H} = \frac{\hat{P}_{CM}^2}{2M} + \frac{\hat{P}^2}{2\mu} + \hat{V}(\hat{X}) = \hat{H}_{CM} + \hat{H}_{rel}$$

and the eigenfunctions factorize:

$$\psi_E(x_{CM}, x) = \frac{e^{i p_{CM} x_{CM}/\hbar}}{\sqrt{2\pi\hbar}} \psi_{E_{rel}}(x); \quad E = \frac{p_{CM}^2}{2M} + E_{rel}$$

The interesting part of the dynamics is described by $\psi_{rel}(x)$; the CM motion is trivial, so one usually eliminates it by going to the CM frame.

N particles in one dimension

All $N=2$ results can be generalized to $N>2$, except those from the last subsection: Even if the interaction depends only on the distance between particles, the problem cannot be reduced to independent one-particle problems.

10.2 More particles in more dimensions

Usually the particles we will try to describe live in 3 dimensions. For a single particle the position eigenkets are

$$|x\,y\,z\rangle = |x\rangle \otimes |y\rangle \otimes |z\rangle \equiv |\vec{r}\rangle, \qquad \langle \vec{r}\,'|\vec{r}\rangle = \delta^{(3)}(\vec{r}-\vec{r}\,') = \delta(x-x')\,\delta(y-y')\,\delta(z-z')$$

momentum eigenkets are

$$|p_x\,p_y\,p_z\rangle \equiv |\vec{p}\rangle, \qquad \langle \vec{p}\,'|\vec{p}\rangle = \delta^{(3)}(\vec{p}-\vec{p}\,')$$

Two particles in 3 dimensions are described by states that can be expanded in position eigenstates

$$|\vec{r}_1\,\vec{r}_2\rangle = |\vec{r}_1\rangle \otimes |\vec{r}_2\rangle, \qquad \langle \vec{r}_1{}'\,\vec{r}_2{}'|\vec{r}_1\,\vec{r}_2\rangle = \delta^{(3)}(\vec{r}_1-\vec{r}_1{}')\,\delta^{(3)}(\vec{r}_2-\vec{r}_2{}')$$

or in momentum eigenstates

$$|\vec{p}_1\,\vec{p}_2\rangle, \qquad \langle \vec{p}_1{}'\,\vec{p}_2{}'|\vec{p}_1\,\vec{p}_2\rangle = \delta^{(3)}(\vec{p}_1-\vec{p}_1{}')\,\delta^{(3)}(\vec{p}_2-\vec{p}_2{}')$$

For example, a single particle in a 3-d cubic box of length L and Volume L^3 has normalized eigenstates (see Exercise 10.2.1, p.259)

$$|E_{\vec{n}}\rangle = |n_x\rangle \otimes |n_y\rangle \otimes |n_z\rangle = |n_x\,n_y\,n_z\rangle \qquad (n_i>0)$$

with eigenenergies $E_{\vec{n}} = \dfrac{\hbar^2\pi^2}{2ML^2}\,\vec{n}^{\,2} = \dfrac{\hbar^2\pi^2}{2ML}\left(n_x^2+n_y^2+n_z^2\right)$

whose wavefunctions in x-representation are given by

$$
\begin{aligned}
\langle \vec{r}\,|E_n\rangle = \psi_{\vec{n}}(\vec{r}) &= \Big(\underbrace{\langle x|}_{\in \mathbb{V}_x} \otimes \underbrace{\langle y|}_{\in \mathbb{V}_y} \otimes \underbrace{\langle z|}_{\in \mathbb{V}_z}\Big)\Big(\underbrace{|n_x\rangle}_{\in \mathbb{V}_x} \otimes \underbrace{|n_y\rangle}_{\in \mathbb{V}_y} \otimes \underbrace{|n_z\rangle}_{\in \mathbb{V}_z}\Big) \\
&= \langle x|n_x\rangle \langle y|n_y\rangle \langle z|n_z\rangle \\
&= \psi_{n_x}(x)\, \psi_{n_y}(y)\, \psi_{n_z}(z) \\
&= \left(\sqrt{\frac{2}{L}} \sin\left(\frac{n_x \pi x}{L}\right)\right) \cdot \left(\sqrt{\frac{2}{L}} \sin\left(\frac{n_y \pi y}{L}\right)\right) \cdot \left(\sqrt{\frac{2}{L}} \sin\left(\frac{n_z \pi z}{L}\right)\right)
\end{aligned}
$$

if the box sits at $0 \leq x, y, z \leq L$.