Quantum Two Body Problem

Consider the two body problem: Two point-like particles interacting with each other but not subject to any external forces. In quantum mechanics, this 2-body system is described by a Hamiltonian of the form

$$\hat{H} = \frac{\hat{\mathbf{P}}_1^2}{2M_1} + \frac{\hat{\mathbf{P}}_2^2}{2M_2} + V(\hat{\mathbf{X}}_1 - \hat{\mathbf{X}}_2). \tag{1}$$

For simplicity, we assume both particles are spinless. Note that the potential $V(\hat{\mathbf{X}}_1 - \hat{\mathbf{X}}_2)$ depends only on the *relative* position of the two particles but is invariant under simultaneous translations

$$\mathbf{X}_1 \to \mathbf{X}_1 + \mathbf{a}, \quad \mathbf{X}_2 \to \mathbf{X}_2 + \mathbf{a}, \quad \text{same shift } \mathbf{a} \text{ for both particles,} \tag{2}$$

and that's why the 2 particles interact with each other but are not subject to any external forces.

In quantum mechanics, the translational symmetries (2) are implemented by the unitary translation operators

$$\hat{T}_{\mathbf{a}} = \exp\bigl(-i\mathbf{a}\cdot\hat{\mathbf{P}}_{\text{net}}\bigr), \qquad \hat{\mathbf{P}}_{\text{net}} = \hat{\mathbf{P}}_1 + \hat{\mathbf{P}}_2 \tag{3}$$

which act in the coordinate basis as

$$\hat{T}_{\mathbf{a}}\,|\mathbf{X}_1, \mathbf{X}_2\rangle = |\mathbf{X}_1 + \mathbf{a}, \mathbf{X}_2 + \mathbf{a}\rangle\,. \tag{4}$$

It is easy to see that the 3 *generators* $\hat{P}^i_{\text{net}}$ $(i = x, y, z)$ of the translation symmetry commute with the Hamiltonian (1). Indeed, all 6 momentum operators $\hat{P}^i_{1,2}$ commute with each other, so the $\hat{P}^i_{\text{net}}$ commute with all functions of momenta such as the net kinetic energy operator (the first 2 terms in eq. (1)), which leaves with

$$\left[\hat{P}^i_{\rm net},\hat{H}\right]\;=\;\left[\hat{P}^i_{\rm net},\hat{V}\right]. \tag{5}$$

Furthermore,

$$\begin{aligned}
&\left[\hat{P}^i_{\rm net},\hat{V}\right]\;=\;\left[\hat{P}^i_1,\hat{V}\right]\;+\;\left[\hat{P}^i_2,\hat{V}\right]\;=\;-i\hbar\widehat{\frac{\partial V}{\partial X^i_1}}\;-\;i\hbar\widehat{\frac{\partial V}{\partial X^i_2}}\;=\;0\\
&\text{because}\quad\frac{\partial V}{\partial X^i_1}\;+\;\frac{\partial V}{\partial X^i_2}\;=\;0\quad\text{for}\quad V(\mathbf{X}_1-\mathbf{X}_2).
\end{aligned} \tag{6}$$

Altogether, we have the 3 generators $\hat{P}^i_{\rm net}$ and hence all the translation operators $\hat{T}_{\mathbf{a}}$ commuting with the Hamiltonian (1). Consequently, in the common eigenbasis of the net momenta operators $\hat{P}^i_{\rm net}$, all the translation operators are diagonal, and the Hamiltonian operator $\hat{H}$ should be block-diagonal.

To see how this works, we need linear redefinitions of the two particles' positions and momenta. On the position side we trade the $\hat{\mathbf{X}}_1$ and the $\hat{\mathbf{X}}_2$ operators for the

$$\begin{aligned}
\text{center of mass position}\quad\hat{\mathbf{X}}_{\rm cm}\;&=\;\frac{M_1}{M_1+M_2}\hat{\mathbf{X}}_1\;+\;\frac{M_2}{M_1+M_2}\hat{\mathbf{X}}_2\\
\text{and relative position}\quad\hat{\mathbf{X}}_{\rm rel}\;&=\;\hat{\mathbf{X}}_1\;-\;\hat{\mathbf{X}}_2\,,
\end{aligned} \tag{7}$$

while on the momentum side we trade the $\hat{\mathbf{P}}_1$ and the $\hat{\mathbf{P}}_2$ operators for the

$$\begin{aligned}
\text{net momentum}\quad\hat{\mathbf{P}}_{\rm net}\;&=\;\hat{\mathbf{P}}_1\;+\;\hat{\mathbf{P}}_2\\
\text{and reduced momentum}\quad\hat{\mathbf{P}}_{\rm red}\;&=\;\frac{M_2}{M_1+M_2}\hat{\mathbf{P}}_1\;-\;\frac{M_1}{M_1+M_2}\hat{\mathbf{P}}_2\,.
\end{aligned} \tag{8}$$

Note that the net momentum is canonically conjugate to the center-of-mass position while the reduced momentum is conjugate to the relative position. In quantum terms, this means

$$\begin{aligned}
\left[\hat{X}^i_{\rm cm}, \hat{P}^j_{\rm net}\right] &= i\hbar\delta^{ij}, &\text{(a)}\\
\text{and}\quad \left[\hat{X}^i_{\rm rel}, \hat{P}^j_{\rm red}\right] &= i\hbar\delta^{ij}, &\text{(b)}\\
\text{but}\quad \left[\hat{X}^i_{\rm rel}, \hat{P}^j_{\rm net}\right] &= 0, &\text{(c)}\\
\text{and}\quad \left[\hat{X}^i_{\rm cm}, \hat{P}^j_{\rm red}\right] &= 0. &\text{(d)}
\end{aligned}$$

Indeed:

$$\begin{aligned}
\left[\hat{X}^i_{\rm cm}, \hat{P}^j_{\rm net}\right] &= \frac{M_1}{M_1+M_2}\left[\hat{X}^i_1, \hat{P}^j_1\right] + \frac{M_2}{M_1+M_2}\left[\hat{X}^i_2, \hat{P}^j_2\right]\\
&= \frac{M_1}{M_1+M_2}\times i\hbar\delta^{ij} + \frac{M_2}{M_1+M_2}\times i\hbar\delta^{ij} = 1\times i\hbar\delta^{ij}, \qquad \text{(a)}
\end{aligned}$$

$$\begin{aligned}
\left[\hat{X}^i_{\rm rel}, \hat{P}^j_{\rm red}\right] &= \frac{M_2}{M_1+M_2}\left[\hat{X}^i_1, \hat{P}^j_1\right] + \frac{M_1}{M_1+M_2}\left[\hat{X}^i_2, \hat{P}^j_2\right]\\
&= \frac{M_2}{M_1+M_2}\times i\hbar\delta^{ij} + \frac{M_1}{M_1+M_2}\times i\hbar\delta^{ij} = 1\times i\hbar\delta^{ij}, \qquad \text{(b)}
\end{aligned}$$

$$\begin{aligned}
\left[\hat{X}^i_{\rm rel}, \hat{P}^j_{\rm net}\right] &= +\left[\hat{X}^i_1, \hat{P}^j_1\right] - \left[\hat{X}^i_2, \hat{P}^j_2\right]\\
&= +i\hbar\delta^{ij} - i\hbar\delta^{ij} = 0, \qquad \text{(c)}
\end{aligned}$$

$$\begin{aligned}
\left[\hat{X}^i_{\rm cm}, \hat{P}^j_{\rm red}\right] &= +\frac{M_1M_2}{(M_1+M_2)^2}\left[\hat{X}^i_1, \hat{P}^j_1\right] - \frac{M_2M_1}{(M_1+M_2)^2}\left[\hat{X}^i_2, \hat{P}^j_2\right]\\
&= +\frac{M_1M_2}{(M_1+M_2)^2}\times i\hbar\delta^{ij} - \frac{M_2M_1}{(M_1+M_2)^2}\times i\hbar\delta^{ij} = 0. \qquad \text{(d)}
\end{aligned}$$

Similar to what we have in the homework#3 (problem 4(f)), eqs. (a–d) imply that in the $|\mathbf{X}_{\rm cm}, \mathbf{X}_{\rm net}\rangle$ coordinate basis, the net and the reduced momentum operators act on the wave-functions as

$$\hat{P}^i_{\rm net}\Psi(\mathbf{X}_{cm}, \mathbf{X}_{\rm rel}) = -i\hbar\frac{\partial\Psi}{\partial X^i_{\rm cm}}\,, \qquad \hat{P}^i_{\rm red}\Psi(\mathbf{X}_{cm}, \mathbf{X}_{\rm rel}) = -i\hbar\frac{\partial\Psi}{\partial X^i_{\rm rel}}\,. \qquad (9)$$

Consequently, the eigenstates of the net momentum operator have wave-function of the form

$$\Psi(\mathbf{X}_{cm},\mathbf{X}_{\rm rel}) \;=\; \exp\bigl(-i\mathbf{P}_{\rm net}\cdot\mathbf{X}_{\rm cm}/\hbar\bigr)\times\psi(\mathbf{X}_{\rm rel}) \tag{10}$$

where $\psi(\mathbf{X}_{\rm rel})$ is any 1-particle wave-function of the relative position. Thus, we see that all the eigenvalues of the net momentum are infinitely degenerate, and the eigenstate subspace for each eigenvalue is equivalent to the 1-particle Hilbert space.

Now consider the two-particle Hamiltonian operator (1). Since it commutes with the net momenta, it must be block-diagonal the basis of net momentum eigenstates. In terms of the wave functions (10), this means

$$\begin{aligned} \textbf{for}\quad \Psi(\mathbf{X}_{cm},\mathbf{X}_{\rm rel}) \;&=\; \exp\bigl(-i\mathbf{P}_{\rm net}\cdot\mathbf{X}_{\rm cm}/\hbar\bigr)\times\psi(\mathbf{X}_{\rm rel}),\\ \hat H\Psi(\mathbf{X}_{cm},\mathbf{X}_{\rm rel}) \;&=\; \exp\bigl(-i\mathbf{P}_{\rm net}\cdot\mathbf{X}_{\rm cm}/\hbar\bigr)\times\hat H(\text{block }\mathbf{P}_{\rm net})\psi(\mathbf{X}_{\rm rel}) \end{aligned} \tag{11}$$

where $\hat H(\text{block }\mathbf{P}_{\rm net})$ — the diagonal block of $\hat H$ for a particular value of the net momentum — acts only on the 1-particle wave function $\psi(\mathbf{X}_{\rm rel})$, so we may interpret it as some kind of a 1-particle Hamiltonian.

Moreover, all the $\hat H(\text{block }\mathbf{P}_{\rm net})$ for different net momenta are completely similar to each other apart from constant terms. To see how this works, let's re-express the net kinetic energy in terms of the net and the reduced momenta:

$$\hat K_{\rm net} \;=\; \frac{\hat{\mathbf{P}}_1^2}{2M_1}\;+\;\frac{\hat{\mathbf{P}}_2^2}{2M_2}\;=\;\frac{\hat{\mathbf{P}}_{\rm net}^2}{2M_{\rm net}}\;+\;\frac{\hat{\mathbf{P}}_{\rm red}^2}{2M_{\rm red}}\,, \tag{12}$$

where

$$M_{\rm net} \;=\; M_1\;+\;M_2 \quad\text{and}\quad M_{\rm red}\;=\;\frac{M_1M_2}{M_1+M_2}\,. \tag{13}$$

Consequently, the net 2-particle Hamiltonian becomes

$$\hat H \;=\; \frac{\hat{\mathbf{P}}_{\rm net}^2}{2M_{\rm net}}\;+\;\frac{\hat{\mathbf{P}}_{\rm red}^2}{2M_{\rm red}}\;+\;V(\hat{\mathbf{X}}_{\rm rel}), \tag{14}$$

and when we restrict it to an eigenspace of the net momentum, we get

$$\hat{H}(\text{block }\mathbf{P}_{\text{net}}) \;=\; \left(\text{constant }\frac{\mathbf{P}_{\text{net}}^2}{2M_{\text{net}}}\right) \;+\; \hat{H}_{\text{red}}\,, \tag{15}$$

with the same reduced Hamiltonian

$$\hat{H}_{\text{red}} \;=\; \frac{\hat{\mathbf{P}}_{\text{red}}^2}{2M_{\text{red}}} \;+\; V(\hat{\mathbf{X}}_{\text{rel}}) \tag{16}$$

for all eigenvalues of the net momentum. This reduced Hamiltonian governs the relative motion of the two particles, which looks like the motion of a single particle of reduced mass M_{red} in the external potential $V(\mathbf{X})$. In the wave-function language, it acts only on the $\psi(\mathbf{X}_{\text{rel}}$ factor of the 2-particle wave-function (10) as

$$\hat{H}_{\text{red}}\psi(\mathbf{X}_{\text{rel}}) \;=\; -\frac{\hbar^2}{2M_{\text{red}}}\nabla^2\psi(\mathbf{X}_{\text{rel}}) \;+\; V(\mathbf{X}_{\text{rel}})\times\psi(\mathbf{X}_{\text{rel}}). \tag{17}$$

Altogether, we have reduced the 2-particle problem to a 1-particle problem in an external potential. Indeed, once we diagonalize the reduced Hamiltonian (16) and find its eigenvalues E_n^{red} and eigenwaves $\psi_n(\mathbf{X}_{\text{rel}})$,

$$\hat{H}_{\text{red}}\psi_n(\mathbf{X}_{\text{rel}}) \;=\; E_n^{\text{red}}\psi_n(\mathbf{X}_{\text{rel}}), \tag{18}$$

the eigenstates of the net 2-particle Hamiltonian $\hat{H}$ obtain as $|\mathbf{P}_{\text{net}};n\rangle$ with wave-functions

$$\Psi(\mathbf{X}_{cm},\mathbf{X}_{\text{rel}}) \;=\; \exp\bigl(-i\mathbf{P}_{\text{net}}\cdot\mathbf{X}_{\text{cm}}/\hbar\bigr)\times\psi_n(\mathbf{X}_{\text{rel}}) \tag{19}$$

and energies

$$E(\mathbf{P}_{\text{net}};n) \;=\; \frac{\mathbf{P}_{\text{net}}^2}{2M_{\text{net}}} \;+\; E_n^{\text{red}}\,. \tag{20}$$