DECOUPLING THE TWO-PARTICLE HAMILTONIAN


Shankar shows that, for a two-particle system, the state vector $|\psi\rangle$ is an element of the direct product space $V_1 \otimes V_2$. Its evolution in time is determined by the Schrödinger equation, as usual, so that

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = H |\psi\rangle = \left[ \frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2} + V(X_1, X_2) \right] |\psi\rangle \quad (1)$$

The method by which this equation can be solved (if it can be solved, that is) depends on the form of the potential $V$. If the two particles interact only with some external potential, and not with each other, then $V$ is composed of a sum of terms, each of which depends only on $X_1$ or $X_2$, but not on both. In such cases, we can split $H$ into two parts, one of which ($H_1$) depends only on operators pertaining to particle 1 and the other ($H_2$) on operators pertaining to particle 2. If the eigenvalues (allowed energies) of particle $i$ are given by $E_i$, then the stationary states are direct products of the corresponding single particle eigenstates. That is, in general

$$H |E\rangle = (H_1 + H_2) |E_1\rangle \otimes |E_2\rangle = (E_1 + E_2) |E_1\rangle \otimes |E_2\rangle = E |E\rangle \quad (2)$$

Thus the two-particle state $|E\rangle = |E_1\rangle \otimes |E_2\rangle$. Since a stationary state $|E_i\rangle$ evolves in time according to

$$|\psi_i(t)\rangle = |E_i\rangle e^{-iE_it/\hbar} \quad (3)$$

the compound two-particle state evolves according to

$$|\psi(t)\rangle = e^{-iE_1t/\hbar} |E_1\rangle \otimes e^{-iE_2t/\hbar} |E_2\rangle = e^{-i(E_1+E_2)t/\hbar} |E\rangle \quad (4)$$

$$= e^{-iEt/\hbar} |E\rangle \quad (5)$$

In this case, the two particles are essentially independent of each other, and the compound state is just the product of the two separate one-particle states.
If $H$ is not separable, which will occur if $V$ contains terms involving both $X_1$ and $X_2$ in the same term, we cannot, in general, reduce the system to the product of two one-particle systems. There are a couple of instances, however, where such a reduction can be done.

The first instance is if the potential is a function of $x_2 - x_1$ only, in other words, that the interaction between the particles depends only on the distance between them. Shankar shows that in this case we can transform the system to that of a reduced mass $\mu = m_1 m_2 / (m_1 + m_2)$ and a centre of mass $M = m_1 + m_2$. We’ve already seen this problem solved by means of separation of variables. The result is that the state vector is the product of a vector for a free particle of mass $M$ and of a vector of a particle with reduced mass $\mu$ moving in the potential $V$.

Another case where we can decouple the Hamiltonian is in a system of harmonic oscillators. We’ve already seen this system solved for two masses in classical mechanics using diagonalization of the matrix describing the equations of motion. The classical Hamiltonian is

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{m \omega^2}{2} \left[ x_1^2 + x_2^2 + (x_1 - x_2)^2 \right]$$  \hspace{1cm} (7)

The earlier solution involved introducing normal coordinates

$$x_I = \frac{1}{\sqrt{2}} (x_1 + x_2)$$ \hspace{1cm} (8)

$$x_{II} = \frac{1}{\sqrt{2}} (x_1 - x_2)$$ \hspace{1cm} (9)

and corresponding momenta

$$p_I = \frac{1}{\sqrt{2}} (p_1 + p_2)$$ \hspace{1cm} (10)

$$p_{II} = \frac{1}{\sqrt{2}} (p_1 - p_2)$$ \hspace{1cm} (11)

These normal coordinates are canonical as we can verify by calculating the Poisson brackets. For example
\[
\{x_I, p_I\} = \sum_i \left( \frac{\partial x_I}{\partial x_i} \frac{\partial p_I}{\partial p_i} - \frac{\partial x_I}{\partial p_i} \frac{\partial p_I}{\partial x_i} \right) = 1 \quad (12)
\]
\[
\{x_I, x_{II}\} = \sum_i \left( \frac{\partial x_I}{\partial x_i} \frac{\partial x_{II}}{\partial p_i} - \frac{\partial x_I}{\partial p_i} \frac{\partial x_{II}}{\partial x_i} \right) = 0 \quad (14)
\]
and so on, with the general result
\[
\{x_i, p_j\} = \delta_{ij} \quad (16)
\]
\[
\{x_i, x_j\} = \{p_i, p_j\} = 0 \quad (17)
\]
We can invert the transformation to get
\[
x_1 = \frac{1}{\sqrt{2}} (x_I + x_{II}) \quad (18)
\]
\[
x_2 = \frac{1}{\sqrt{2}} (x_I - x_{II}) \quad (19)
\]
and
\[
p_1 = \frac{1}{\sqrt{2}} (p_I + p_{II}) \quad (20)
\]
\[
p_2 = \frac{1}{\sqrt{2}} (p_I - p_{II}) \quad (21)
\]
Inserting these into (7) we get
\[
H = \frac{1}{4m} \left[ (p_I + p_{II})^2 + (p_I - p_{II})^2 \right] + \frac{m\omega^2}{2} \left[ (x_I + x_{II})^2 + (x_I - x_{II})^2 + 4x_{II}^2 \right] \quad (22)
\]
\[
= \frac{p_I^2}{2m} + \frac{p_{II}^2}{2m} + \frac{m\omega^2}{2} \left( x_I^2 + \frac{3}{2} x_{II}^2 \right) \quad (23)
\]
We can now substitute the usual quantum mechanical operators to get the quantum Hamiltonian:
\[
H = -\frac{\hbar^2}{2m} (P_I^2 + P_{II}^2) + \frac{m\omega^2}{2} \left( X_I^2 + \frac{3}{2} X_{II}^2 \right) \quad (25)
\]
In the coordinate basis, this is
DECOUPLING THE TWO-PARTICLE HAMILTONIAN

\[ H = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_{1I}^2} \right) + \frac{m\omega^2}{2} \left( x_1^2 + \frac{3}{2} x_{1I}^2 \right) \] (26)

The Hamiltonian is now decoupled and can be solved by separation of variables.

We could have arrived at this result by starting with (7) and promoting \( x_i \) and \( p_i \) to quantum operators directly, then made the substitution to normal coordinates. We would then start with

\[ H = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) + \frac{m\omega^2}{2} \left[ x_1^2 + x_2^2 + (x_1 - x_2)^2 \right] \] (27)

The potential term on the right transforms the same way as before, so we get

\[ \frac{m\omega^2}{2} \left[ x_1^2 + x_2^2 + (x_1 - x_2)^2 \right] \rightarrow \frac{m\omega^2}{2} \left( x_1^2 + \frac{3}{2} x_{1I}^2 \right) \] (28)

To transform the two derivatives, we need to use the chain rule a couple of times. To get the first derivatives:

\[ \frac{\partial \psi}{\partial x_1} = \frac{\partial \psi}{\partial x_I} \frac{\partial x_I}{\partial x_1} + \frac{\partial \psi}{\partial x_{1I}} \frac{\partial x_{1I}}{\partial x_1} \] (29)

\[ = \frac{1}{\sqrt{2}} \left( \frac{\partial \psi}{\partial x_I} + \frac{\partial \psi}{\partial x_{1I}} \right) \] (30)

\[ \frac{\partial \psi}{\partial x_2} = \frac{\partial \psi}{\partial x_I} \frac{\partial x_I}{\partial x_2} + \frac{\partial \psi}{\partial x_{1I}} \frac{\partial x_{1I}}{\partial x_2} \] (31)

\[ = \frac{1}{\sqrt{2}} \left( \frac{\partial \psi}{\partial x_I} - \frac{\partial \psi}{\partial x_{1I}} \right) \] (32)

Now the second derivatives:
\[ \frac{\partial^2 \psi}{\partial x_1^2} = \frac{\partial}{\partial x_I} \left( \frac{\partial \psi}{\partial x_I} \right) \frac{\partial x_I}{\partial x_1} + \frac{\partial}{\partial x_{II}} \left( \frac{\partial \psi}{\partial x_I} \right) \frac{\partial x_{II}}{\partial x_1} \] (33)

\[ = \frac{1}{2} \left[ \frac{\partial}{\partial x_I} \left( \frac{\partial \psi}{\partial x_I} + \frac{\partial \psi}{\partial x_{II}} \right) + \frac{\partial}{\partial x_{II}} \left( \frac{\partial \psi}{\partial x_I} + \frac{\partial \psi}{\partial x_{II}} \right) \right] \] (34)

\[ = \frac{1}{2} \left[ \frac{\partial^2 \psi}{\partial x_I^2} + \frac{2 \partial^2 \psi}{\partial x_I \partial x_{II}} + \frac{\partial^2 \psi}{\partial x_{II}^2} \right] \] (35)

\[ \frac{\partial^2 \psi}{\partial x_2^2} = \frac{\partial}{\partial x_I} \left( \frac{\partial \psi}{\partial x_2} \right) \frac{\partial x_I}{\partial x_1} + \frac{\partial}{\partial x_{II}} \left( \frac{\partial \psi}{\partial x_2} \right) \frac{\partial x_{II}}{\partial x_1} \] (36)

\[ = \frac{1}{2} \left[ \frac{\partial}{\partial x_I} \left( \frac{\partial \psi}{\partial x_I} - \frac{\partial \psi}{\partial x_{II}} \right) - \frac{\partial}{\partial x_{II}} \left( \frac{\partial \psi}{\partial x_I} - \frac{\partial \psi}{\partial x_{II}} \right) \right] \] (37)

\[ = \frac{1}{2} \left[ \frac{\partial^2 \psi}{\partial x_I^2} - \frac{2 \partial^2 \psi}{\partial x_I \partial x_{II}} + \frac{\partial^2 \psi}{\partial x_{II}^2} \right] \] (38)

Combining the two derivatives, we get

\[ \frac{\partial^2 \psi}{\partial x_1^2} + \frac{\partial^2 \psi}{\partial x_2^2} = \frac{\partial^2 \psi}{\partial x_I^2} + \frac{\partial^2 \psi}{\partial x_{II}^2} \] (39)

Inserting this, together with 28 into 27, we get 26 again.