DECOUPLING THE TWO-PARTICLE HAMILTONIAN

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 10, Exercise 10.1.3.

Shankar shows that, for a two-particle system, the state vector $|\psi\rangle$ is an element of the direct product space $\mathbb{V}_{1\otimes 2}$. Its evolution in time is determined by the Schrödinger equation, as usual, so that

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

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

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

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

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

the compound two-particle state evolves according to

$$\begin{aligned}
|\psi(t)\rangle &= e^{-iE_1t/\hbar}|E_1\rangle\otimes e^{-iE_2t/\hbar}|E_2\rangle &(4)\\
&= e^{-i(E_1+E_2)t/\hbar}|E\rangle &(5)\\
&= e^{-iEt/\hbar}|E\rangle &(6)
\end{aligned}$$

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 μ 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

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

The earlier solution involved introducing normal coordinates

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

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

and corresponding momenta

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

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

These normal coordinates are canonical as we can verify by calculating the Poisson brackets. For example

$$\{x_I, p_I\} = \sum_i \left(\frac{\partial x_I}{\partial x_i} \frac{\partial p_I}{\partial p_i} - \frac{\partial x_I}{\partial p_i} \frac{\partial p_I}{\partial x_i} \right) \tag{12}$$

$$= 1 \tag{13}$$

$$\{x_I, x_{II}\} = \sum_i \left(\frac{\partial x_I}{\partial x_i} \frac{\partial x_{II}}{\partial p_i} - \frac{\partial x_I}{\partial p_i} \frac{\partial x_{II}}{\partial x_i} \right) \tag{14}$$

$$= 0 \tag{15}$$

and so on, with the general result

$$\left\{x_i, p_j\right\} = \delta_{ij} \tag{16}$$

$$\left\{x_i, x_j\right\} = \left\{p_i, p_j\right\} = 0 \tag{17}$$

We can invert the transformation to get

$$x_1 = \frac{1}{\sqrt{2}} (x_I + x_{II}) \tag{18}$$

$$x_2 = \frac{1}{\sqrt{2}} (x_I - x_{II}) \tag{19}$$

and

$$p_1 = \frac{1}{\sqrt{2}} (p_I + p_{II}) \tag{20}$$

$$p_2 = \frac{1}{\sqrt{2}} (p_I - p_{II}) \tag{21}$$

Inserting these into 7 we get

$$H = \frac{1}{4m} \left[(p_I + p_{II})^2 + (p_I - p_{II})^2 \right] + \tag{22}$$

$$\frac{m\omega^2}{4} \left[(x_I + x_{II})^2 + (x_I - x_{II})^2 + 4x_{II}^2 \right] \tag{23}$$

$$= \frac{p_I^2}{2m} + \frac{p_{II}^2}{2m} + \frac{m\omega^2}{2} \left(x_I^2 + \frac{3}{2} x_{II}^2 \right) \tag{24}$$

We can now subsitute the usual quantum mechanical operators to get the quantum Hamiltonian:

$$H = -\frac{\hbar^2}{2m} \left(P_I^2 + P_{II}^2 \right) + \frac{m\omega^2}{2} \left(X_I^2 + \frac{3}{2} X_{II}^2 \right) \tag{25}$$

In the coordinate basis, this is

$$H=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_I^2}+\frac{\partial^2}{\partial x_{II}^2}\right)+\frac{m\omega^2}{2}\left(x_I^2+\frac{3}{2}x_{II}^2\right) \tag{26}$$

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

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

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

$$\frac{m\omega^2}{2}\left[x_1^2+x_2^2+(x_1-x_2)^2\right]\to\frac{m\omega^2}{2}\left(x_I^2+\frac{3}{2}x_{II}^2\right) \tag{28}$$

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

$$\begin{aligned}
\frac{\partial\psi}{\partial x_1} &= \frac{\partial\psi}{\partial x_I}\frac{\partial x_I}{\partial x_1}+\frac{\partial\psi}{\partial x_{II}}\frac{\partial x_{II}}{\partial x_1} && (29)\\
&= \frac{1}{\sqrt{2}}\left(\frac{\partial\psi}{\partial x_I}+\frac{\partial\psi}{\partial x_{II}}\right) && (30)\\
\frac{\partial\psi}{\partial x_2} &= \frac{\partial\psi}{\partial x_I}\frac{\partial x_I}{\partial x_2}+\frac{\partial\psi}{\partial x_{II}}\frac{\partial x_{II}}{\partial x_2} && (31)\\
&= \frac{1}{\sqrt{2}}\left(\frac{\partial\psi}{\partial x_I}-\frac{\partial\psi}{\partial x_{II}}\right) && (32)
\end{aligned}$$

Now the second derivatives:

$$\frac{\partial^2\psi}{\partial x_1^2} = \frac{\partial}{\partial x_I}\left(\frac{\partial\psi}{\partial x_1}\right)\frac{\partial x_I}{\partial x_1} + \frac{\partial}{\partial x_{II}}\left(\frac{\partial\psi}{\partial x_1}\right)\frac{\partial x_{II}}{\partial x_1} \tag{33}$$

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

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

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

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

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

Combining the two derivatives, we get

$$\frac{\partial^2\psi}{\partial x_1^2} + \frac{\partial^2\psi}{\partial x_2^2} = \frac{\partial^2\psi}{\partial x_I^2} + \frac{\partial^2\psi}{\partial x_{II}^2} \tag{39}$$

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