SCHRÖDINGER EQUATION FOR 2 PARTICLES - SEPARATION OF VARIABLES

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 5.1.

The Schrödinger equation that we've looked at so far involves the wave function for a single particle moving in a potential. To extend this to multi-particle systems, we need to make the wave function and the potential functions of the positions of all the particles and the time. Thus the Schrödinger equation for a system of n particles becomes

$$-\frac{\hbar^2}{2}\sum_{i=1}^{n}\frac{1}{m_i}\nabla_i^2\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_n,t)+ \tag{1}$$

$$V(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_n,t)\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_n,t)=i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_n,t) \tag{2}$$

Needless to say, finding solutions of this equation for even as few as 2 particles is extremely difficult. In one case, however, we can make some progress. In a 2-particle system, if the potential V is not time-dependent and depends only on the separation $\mathbf{r}\equiv\mathbf{r}_1-\mathbf{r}_2$ of the two particles, we can fiddle with it a bit and produce a simpler form.

First, we define the centre of mass

$$\mathbf{R}\equiv\frac{m_1\mathbf{r}_1+m_2\mathbf{r}_2}{m_1+m_2} \tag{3}$$

If we also introduce the reduced mass

$$\mu\equiv\frac{m_1m_2}{m_1+m_2} \tag{4}$$

then we get

$$\mathbf{r}_1=\mathbf{R}+\frac{\mu}{m_1}\mathbf{r} \tag{5}$$

$$\mathbf{r}_2=\mathbf{R}-\frac{\mu}{m_2}\mathbf{r} \tag{6}$$

In the coordinates $\mathbf{r}$ and $\mathbf{R}$, we can find the gradient operators. We use a dummy function f to give the gradient something to operate on. We'll consider the x component and use the chain rule (remember that $\mathbf{r}_1$ and $\mathbf{r}_2$ are independent vectors, each with 3 components, so there is a total of 6 independent position variables):

$$\frac{\partial f}{\partial r_{1_x}} = \frac{\partial f}{\partial r_x}\frac{\partial r_x}{\partial r_{1_x}} + \frac{\partial f}{\partial R_x}\frac{\partial R_x}{\partial r_{1_x}} \tag{7}$$

$$= \frac{\partial f}{\partial r_x}(1) + \frac{\partial f}{\partial R_x}\frac{m_1}{m_1+m_2} \tag{8}$$

$$= \frac{\partial f}{\partial r_x} + \frac{\partial f}{\partial R_x}\frac{\mu}{m_2} \tag{9}$$

$$\frac{\partial f}{\partial r_{2_x}} = \frac{\partial f}{\partial r_x}(-1) + \frac{\partial f}{\partial R_x}\frac{m_2}{m_1+m_2} \tag{10}$$

$$= -\frac{\partial f}{\partial r_x} + \frac{\partial f}{\partial R_x}\frac{\mu}{m_1} \tag{11}$$

The relations for the other two components are similar, so dropping the test function f , we get for the gradients:

$$\nabla_1 = \nabla_r + \frac{\mu}{m_2}\nabla_R \tag{12}$$

$$\nabla_2 = -\nabla_r + \frac{\mu}{m_1}\nabla_R \tag{13}$$

To get the Laplacian operators, we differentiate the x component expressions above.

$$\frac{\partial^2 f}{\partial r_{1_x}^2} = \left(\frac{\partial}{\partial r_x} + \frac{\mu}{m_2}\frac{\partial}{\partial R_x}\right)\left(\frac{\partial f}{\partial r_x} + \frac{\partial f}{\partial R_x}\frac{\mu}{m_2}\right) \tag{14}$$

$$= \frac{\partial^2 f}{\partial r_x^2} + \frac{\partial f}{\partial r_x \partial R_x}\frac{2m_1}{m_1+m_2} + \frac{\partial^2 f}{\partial R_x^2}\left(\frac{\mu}{m_2}\right)^2 \tag{15}$$

$$\frac{\partial^2 f}{\partial r_{2_x}^2} = \frac{\partial^2 f}{\partial r_x^2} - \frac{\partial f}{\partial r_x \partial R_x}\frac{2m_2}{m_1+m_2} + \frac{\partial^2 f}{\partial R_x^2}\left(\frac{\mu}{m_1}\right)^2 \tag{16}$$

The combination of these two expressions that appears in the Schrödinger equation is, after cancelling terms and putting the remaining terms over common denominators:

$$-\frac{\hbar^2}{2m_1}\frac{\partial^2 f}{\partial r_{1_x}^2}-\frac{\hbar^2}{2m_2}\frac{\partial^2 f}{\partial r_{2_x}^2}=-\frac{\hbar^2}{2(m_1+m_2)}\frac{\partial^2 f}{\partial R_x^2}-\frac{\hbar^2}{2\mu}\frac{\partial^2 f}{\partial r_x^2} \tag{17}$$

The calculations for the other two components are similar, so the final result is:

$$-\frac{\hbar^2}{2(m_1+m_2)}\nabla_R^2\psi-\frac{\hbar^2}{2\mu}\nabla_r^2\psi+V(\mathbf{r})\psi=E\psi \tag{18}$$

We can now try the usual technique of separation of variables, so we try

$$\psi=A(r)B(R) \tag{19}$$

We get, after substituting and dividing through by AB:

$$-\frac{\hbar^2}{2(m_1+m_2)B}\nabla_R^2 B-\frac{\hbar^2}{2\mu A}\nabla_r^2 A+V(\mathbf{r})=E \tag{20}$$

As usual, the terms involving each of the variables r and R must separately be equal to constants, so we get

$$-\frac{\hbar^2}{2(m_1+m_2)}\nabla_R^2 B=E_R B \tag{21}$$

$$-\frac{\hbar^2}{2\mu}\nabla_r^2 A+AV(\mathbf{r})=E_r A \tag{22}$$

The first equation is that of a free particle with mass m_1+m_2, while the second is that of a particle with mass μ moving in a potential V. Thus the system separates into one equation for a free particle with the total mass and a position at the centre of mass and another for a single particle with the reduced mass μ. The total energy is $E=E_R+E_r$.

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