8.1: Derivation of Radial Equation

Now, we have seen that the Cartesian components of the momentum, $\mathbf{p}$, can be represented as (see Section [s7.2])

$$p_i = -\mathrm{i}\,\hbar\,\frac{\partial}{\partial x_i} \tag{8.1.1}$$

for $i = 1, 2, 3$, where $x_1\equiv x$, $x_2\equiv y$, $x_3\equiv z$, and $\mathbf{r}\equiv(x_1, x_2, x_3)$. Likewise, it is easily demonstrated, from the previous expressions, and the basic definitions of the spherical coordinates [see Equations ([e8.21])–([e8zz])], that the radial component of the momentum can be represented as

$$p_r\equiv\frac{\mathbf{p}\cdot\mathbf{r}}{r} = -\mathrm{i}\hbar\frac{\partial}{\partial r} \tag{8.1.2}$$

Recall that the angular momentum vector, $\mathbf{L}$, is defined

$$\mathbf{L} = \mathbf{r}\times\mathbf{p} \tag{8.1.3}$$

[See Equation ([e8.0]).] This expression can also be written in the following form:

$$L_i = \epsilon_{ijk}\,x_j\,p_k. \tag{8.1.4}$$

Here, the ϵ_{ijk} (where i, j, k all run from 1 to 3) are elements of the so-called *totally anti-symmetric tensor* . The values of the various elements of this tensor are determined via a simple rule:

$$\epsilon_{ijk} = \left\{\begin{array}{ll}0&\mbox{if i, j, k not all different}\\ 1&\mbox{if i, j, k are cyclic permutation of $1, 2, 3$}\\ -1&\mbox{if i, j, k are anti-cyclic permutation of $1, 2, 3$}\end{array}\right. \tag{8.1.5}$$

Thus, $\epsilon_{123}=\epsilon_{231}=1$, $\epsilon_{321}=\epsilon_{132}=-1$, and $\epsilon_{112}=\epsilon_{131}=0$, et cetera. Equation ([e9.6]) also makes use of the *Einstein summation convention*, according to which repeated indices are summed (from 1 to 3) . For instance, $a_i\,b_i\equiv a_1\,b_1+a_2\,b_2+a_3\,b_3$. Making use of this convention, as well as Equation ([e9.7]), it is easily seen that Equations ([e9.5]) and ([e9.6]) are indeed equivalent.

Let us calculate the value of L^2 using Equation ([e9.6]). According to our new notation, L^2 is the same as $L_i\,L_i$. Thus, we obtain

$$L^2 = \epsilon_{ijk}\,x_j\,p_k\,\epsilon_{ilm}\,x_l\,p_m = \epsilon_{ijk}\,\epsilon_{ilm}\,x_j\,p_k\,x_l\,p_m. \tag{8.1.6}$$

Note that we are able to shift the position of ϵ_{ilm} because its elements are just numbers, and, therefore, commute with all of the x_i and the p_i. Now, it is easily demonstrated that

$$\epsilon_{ijk}\,\epsilon_{ilm}\equiv\delta_{jl}\,\delta_{km}-\delta_{jm}\,\delta_{kl}. \tag{8.1.7}$$

Here δ_{ij} is the usual *Kronecker delta*, whose elements are determined according to the rule

$$\delta_{ij} = \left\{\begin{array}{ll}1&\mbox{if i and j the same}\\ 0&\mbox{if i and j different}\end{array}\right. \tag{8.1.8}$$

It follows from Equations ([e9.8]) and ([e9.9]) that

$$L^2 = x_i\,p_j\,x_i\,p_j - x_i\,p_j\,x_j\,p_i. \tag{8.1.9}$$

Here, we have made use of the fairly self-evident result that $\delta_{ij}\,a_i\,b_j\equiv a_i\,b_i$. We have also been careful to preserve the order of the various terms on the right-hand side of the previous expression, because the x_i and the p_i do not necessarily commute with one another.

We now need to rearrange the order of the terms on the right-hand side of Equation ([e9.11]). We can achieve this goal by making use of the fundamental commutation relation for the x_i and the p_i:

$$[x_i, p_j] = \mathrm{i}\,\hbar\,\delta_{ij}. \tag{8.1.10}$$

[See Equation ([commxp]).] Thus,

$$\begin{aligned}L^2 &= x_i\,(x_i\,p_j - [x_i, p_j])\,p_j - x_i\,p_j\,\,(p_i\,x_j + [x_j, p_i])\\ &= x_i\,x_i\,p_j\,p_j - \mathrm{i}\,\hbar\,\delta_{ij}\,x_i\,p_j - x_i\,p_j\,p_i\,x_j - \mathrm{i}\,\hbar\,\delta_{ij}\,x_i\,p_j\\ &= x_i\,x_i\,p_j\,p_j - x_i\,p_i\,p_j\,x_j - 2\,\mathrm{i}\,\hbar\,x_i\,p_i.\end{aligned}$$

Here, we have made use of the fact that $p_j\,p_i = p_i\,p_j$, because the p_i commute with one another. [See Equation ([commpp]).] Next,

$$L^2 = x_i\,x_i\,p_j\,p_j - x_i\,p_i\,(x_j\,p_j - [x_j, p_j]) - 2\,\mathrm{i}\,\hbar\,x_i\,p_i. \tag{8.1.11}$$

Now, according to Equation ([e9.12]),

$$[x_j, p_j] \equiv [x_1, p_1] + [x_2, p_2] + [x_3, p_3] = 3\,\mathrm{i}\,\hbar. \tag{8.1.12}$$

Hence, we obtain

$$L^2 = x_i\,x_i\,p_j\,p_j - x_i\,p_i\,x_j\,p_j + \mathrm{i}\,\hbar\,x_i\,p_i. \tag{8.1.13}$$

When expressed in more conventional vector notation, the previous expression becomes

$$L^2 = r^{\,2}\,p^{\,2} - (\mathbf{r}\cdot\mathbf{p})^2 + \mathrm{i}\,\hbar\,\mathbf{r}\cdot\mathbf{p}. \tag{8.1.14}$$

Note that if we had attempted to derive the previous expression directly from Equation ([e9.5]), using standard vector identities, then we would have missed the final term on the right-hand side. This term originates from the lack of commutation between the x_i and p_i operators in quantum mechanics. Of course, standard vector analysis assumes that all terms commute with one another.

Equation ([e9.17]) can be rearranged to give

$$p^{\,2} = r^{\,-2}\left[(\mathbf{r}\cdot\mathbf{p})^2 - \mathrm{i}\,\hbar\,\mathbf{r}\cdot\mathbf{p} + L^2\right]. \tag{8.1.15}$$

Now,

$$\mathbf{r}\cdot\mathbf{p} = r\,p_r = -\mathrm{i}\,\hbar\,r\,\frac{\partial}{\partial r}, \tag{8.1.16}$$

where use has been made of Equation ([e9.4]). Hence, we obtain

$$p^{\,2} = -\hbar^{\,2}\left[\frac{1}{r}\,\frac{\partial}{\partial r}\left(r\,\frac{\partial}{\partial r}\right) + \frac{1}{r}\,\frac{\partial}{\partial r} - \frac{L^2}{\hbar^{\,2}\,r^{\,2}}\right]. \tag{8.1.17}$$

Finally, the previous equation can be combined with Equation ([e9.2]) to give the following expression for the Hamiltonian:

$$H = -\frac{\hbar^{\,2}}{2\,m}\left(\frac{\partial^{\,2}}{\partial r^{\,2}} + \frac{2}{r}\,\frac{\partial}{\partial r} - \frac{L^2}{\hbar^{\,2}\,r^{\,2}}\right) + V(r). \tag{8.1.18}$$

Let us now consider whether the previous Hamiltonian commutes with the angular momentum operators L_z and L^2. Recall, from Section [s8.3], that L_z and L^2 are represented as differential operators that depend solely on the angular spherical coordinates, θ and ϕ, and do not contain the radial coordinate, r. Thus, any function of r, or any differential operator involving r (but not θ and ϕ), will automatically commute with L^2 and L_z. Moreover, L^2 commutes both with itself, and with L_z. (See Section [s8.2].) It is, therefore, clear that the previous Hamiltonian commutes with both L_z and L^2.

According to Section [smeas], if two operators commute with one another then they possess simultaneous eigenstates. We thus conclude that for a particle moving in a central potential the eigenstates of the Hamiltonian are simultaneous eigenstates of L_z and L^2. Now, we have already found the simultaneous eigenstates of L_z and L^2—they are the spherical harmonics, $Y_{l,m}(\theta,\phi)$, discussed in Section [sharm]. It follows that the spherical harmonics are also eigenstates of the Hamiltonian. This observation leads us to try the following separable form for the stationary wavefunction:

$$\psi(r,\theta,\phi) = R(r)\,Y_{l,m}(\theta,\phi). \tag{8.1.19}$$

It immediately follows, from Equation ([e8.29]) and ([e8.30]), and the fact that L_z and L^2 both obviously commute with $R(r)$, that

$$\begin{aligned}L_z\,\psi &= m\,\hbar\,\psi,\\ L^2\,\psi &= l\,(l+1)\,\hbar^{\,2}\,\psi.\end{aligned}$$

Recall that the quantum numbers m and l are restricted to take certain integer values, as explained in Section [slsq].

Finally, making use of Equations ([e9.1]), ([e9.21]), and ([e9.24]), we obtain the following differential equation which determines the radial variation of the stationary wavefunction:

$$-\frac{\hbar^{2}}{2\,m}\left[\frac{d^{2}}{dr^{2}}+\frac{2}{r}\frac{d}{dr}-\frac{l\,(l+1)}{r^{2}}\right]R_{n,l}+V\,R_{n,l}=E\,R_{n,l}. \tag{8.1.20}$$

Here, we have labeled the function $R(r)$ by two quantum numbers, n and l. The second quantum number, l, is, of course, related to the eigenvalue of L^2. [Note that the azimuthal quantum number, m, does not appear in the previous equation, and, therefore, does not influence either the function $R(r)$ or the energy, E.] As we shall see, the first quantum number, n, is determined by the constraint that the radial wavefunction be square-integrable.

Contributors and Attributions

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