FREE PARTICLE IN SPHERICAL COORDINATES

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Section 12.6.

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In solving the Schrödinger equation for spherically symmetric potentials, we found that we could reduce the problem to the equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2}\right]U_{El}=EU_{El} \tag{1}$$

where $U_{El}(r)$ is related to the radial function by

$$R_{El}(r)=\frac{U_{El}(r)}{r} \tag{2}$$

For a free particle, $V=0$ and $E>0$, so we have

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{l(l+1)\hbar^2}{2\mu r^2}\right]U_{El}=EU_{El} \tag{3}$$

Defining

$$k^2 \equiv \frac{2\mu E}{\hbar^2} \tag{4}$$

$$\rho \equiv kr \tag{5}$$

we convert the equation to

$$\left(-\frac{d^2}{d\rho^2}+\frac{l(l+1)}{\rho^2}\right)U_l=U_l \tag{6}$$

This equation can be solved by a method similar to that for the harmonic oscillator and its raising and lowering operators. The entire solution is fairly involved, so we'll start out here by showing how the new raising and lowering operators are defined.

We define

$$d_l \equiv \frac{d}{d\rho} + \frac{l+1}{\rho} \tag{7}$$

The adjoint is

$$d_l^\dagger = -\frac{d}{d\rho} + \frac{l+1}{\rho} \tag{8}$$

To see where the minus sign comes from on the RHS, we need to recall that the momentum operator is defined in one dimension as

$$P = -i\hbar \frac{\partial}{\partial x} \tag{9}$$

Since P is an observable, it is hermitian, so that $P^\dagger = P$. Under the hermitian operation $i \to -i$, so we must also have $\frac{\partial}{\partial x} \to -\frac{\partial}{\partial x}$. Thus the first derivative with respect to a position variable is anti-hermitian. If this doesn't convince you, you can also work out the integral:

$$\int_0^\infty \psi_2^* \frac{d}{d\rho} \psi_1 d\rho = \psi_2^* \psi_1 |_0^\infty - \int_0^\infty \psi_1 \frac{d}{d\rho} \psi_2^* d\rho \tag{10}$$

Under the usual assumption that $\psi \to 0$ at the limits, the integrated term is zero and we have

$$\begin{aligned} \int_0^\infty \psi_2^* \frac{d}{d\rho} \psi_1 d\rho &= -\int_0^\infty \psi_1 \frac{d}{d\rho} \psi_2^* d\rho && (11) \\ &= -\left[\int_0^\infty \psi_1^* \frac{d}{d\rho} \psi_2 d\rho \right]^* && (12) \end{aligned}$$

In bracket notation, this is

$$\left\langle \psi_2 \left| \frac{d}{d\rho} \psi_1 \right. \right\rangle = -\left\langle \frac{d}{d\rho} \psi_2 \left| \psi_1 \right. \right\rangle \tag{13}$$

which shows that $\frac{d}{d\rho}$ is an anti-hermitian operator.
Returning to 7 and 8, we have

$$\begin{aligned}
d_l d_l^\dagger U_l &= \left(\frac{d}{d\rho}+\frac{l+1}{\rho}\right)\left(-\frac{d}{d\rho}+\frac{l+1}{\rho}\right)U_l && (14)\\
&= \left(\frac{d}{d\rho}+\frac{l+1}{\rho}\right)\left(-U_l'+\frac{l+1}{\rho}U_l\right) && (15)\\
&= -U_l''-\frac{l+1}{\rho^2}U_l+\frac{l+1}{\rho}U_l'-\frac{l+1}{\rho}U_l'+\frac{(l+1)^2}{\rho^2}U_l && (16)\\
&= -U_l''+\frac{l(l+1)}{\rho^2}U_l && (17)
\end{aligned}$$

Comparing with 6 we see that

$$d_l d_l^\dagger U_l = U_l \quad (18)$$

We can also show that

$$\begin{aligned}
d_l^\dagger d_l U_l &= \left(-\frac{d}{d\rho}+\frac{l+1}{\rho}\right)\left(\frac{d}{d\rho}+\frac{l+1}{\rho}\right)U_l && (19)\\
&= \left(-\frac{d}{d\rho}+\frac{l+1}{\rho}\right)\left(U_l'+\frac{l+1}{\rho}U_l\right) && (20)\\
&= -U_l''+\frac{l+1}{\rho^2}U_l-\frac{l+1}{\rho}U_l'+\frac{l+1}{\rho}U_l'+\frac{(l+1)^2}{\rho^2}U_l && (21)\\
&= -U_l''+\frac{(l+1)^2+l+1}{\rho^2}U_l && (22)\\
&= -U_l''+\frac{(l+1)(l+2)}{\rho^2}U_l && (23)\\
&= d_{l+1}d_{l+1}^\dagger U_l && (24)
\end{aligned}$$

Starting from 18 we multiply on the left by $d_l^\dagger$ to get

$$d_l^\dagger d_l\left(d_l^\dagger U_l\right) = d_l^\dagger U_l \quad (25)$$

Comparing this with 24 we see that

$$d_l^\dagger U_l = c_l U_{l+1} \quad (26)$$

where c_l is a constant.

Thus $d_l^\dagger$ is a raising operator, in that it raises the angular momentum number l by 1 when it acts on U_l. By convention, $c_l = 1$ (any adjustments to the constant can be made when normalizing).

We can start the process by looking at 6 with $l = 0$ which is

$$\frac{d^2}{d\rho^2}U_l = -U_l \tag{27}$$

This has the two solutions

$$U_0^A(\rho) = \sin\rho \tag{28}$$
$$U_0^B(\rho) = -\cos\rho \tag{29}$$

The minus sign in front of $\cos\rho$ is just conventional. Since we require $U_0(0) = 0$, U_0^B is unacceptable if the region we're considering include $\rho = 0$, so we have

$$U_0(\rho) = \sin\rho \tag{30}$$

For the general case that excludes $\rho = 0$, we must include the cosine term as well.

From here, we can generate solutions for higher values of l by applying 26. Actually, the radial function that appears in the wave function is given by 2, so it is R_l that we really want. That is, we want

$$R_l = \frac{U_l}{r} = k\frac{U_l}{\rho} \tag{31}$$

As with the constant c_l in 26, we can absorb k into normalization to be done later, so we can generate functions

$$R_l = \frac{U_l}{\rho} \tag{32}$$

Applying 26 we have

$$\begin{aligned}
\rho R_{l+1} &= d_l^\dagger(\rho R_l) && (33)\\
&= \left(-\frac{d}{d\rho} + \frac{l+1}{\rho}\right)(\rho R_l) && (34)\\
&= -R_l - \rho R_l' + (l+1)R_l && (35)\\
&= -\rho R_l' + lR_l && (36)\\
R_{l+1} &= \left(-\frac{d}{d\rho} + \frac{l}{\rho}\right)R_l && (37)\\
&= -\rho^l \frac{d}{d\rho}\left(\frac{R_l}{\rho^l}\right) && (38)
\end{aligned}$$

We can convert this into a general formula by writing

$$\frac{R_{l+1}}{\rho^{l+1}} = \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)\frac{R_l}{\rho^l} \tag{39}$$

Starting at $l = 0$, we have

$$\frac{R_1}{\rho^1} = \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)\frac{R_0}{\rho^0} \tag{40}$$

For the next step, we have

$$\begin{aligned}
\frac{R_2}{\rho^2} &= \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)\frac{R_1}{\rho^1} && (41)\\
&= \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)\left(-\frac{1}{\rho}\frac{d}{d\rho}\right)\frac{R_0}{\rho^0} && (42)\\
&= \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^2\frac{R_0}{\rho^0} && (43)
\end{aligned}$$

Thus in general

$$\frac{R_{l+1}}{\rho^{l+1}} = \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^{l+1}\frac{R_0}{\rho^0} \tag{44}$$

Note that

$$\left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^{l+1} \neq \left(-\frac{1}{\rho}\right)^{l+1}\frac{d^{l+1}}{d\rho^{l+1}} \tag{45}$$

since the factor of $\frac{1}{\rho}$ has to be included when taking the derivative. We'll explore the nature of these solutions in the next post.