Radial equation: an alternative view

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Now I would like to present a complementary perspective on the radial equation, one which carries a bit more physical intuition. Working in terms of $u(r)$ led us to an equation that seemed easier to solve based on our 1d experience, but devoid of physical intuition. So rather than working in terms of $u(r)$, let's stick with the differential equation satisfied by $R(r)$ – after all, this is truly what determines the radial form of energy eigenstates. We have simply

$$-\frac{\hbar^2}{2mr^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\left[V(r)+\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]R(r)=ER(r)$$

How should we think about the term with derivatives? Well, let's first ask a related question: what is the operator corresponding to momentum in the radial direction? You might be tempted to say that it's the radial component of $\vec{p}=-i\hbar\vec{\nabla}$ expressed in spherical polar coordinates. Since

$$\vec{p}=-i\hbar\left(\hat{r}\frac{\partial}{\partial r}+\hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta}+\hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\right)$$

in spherical polar coordinates, that would simply be $\frac{\partial}{\partial r}$. We could extract it from $\vec{p}$ by taking $\hat{r}\cdot\vec{p}$.

But now there is a problem. $\hat{r}\cdot\vec{p}$ is not a Hermitian operator:

$$(\hat{r}\cdot\vec{p})^\dagger=\vec{p}\cdot\hat{r}\neq\hat{r}\cdot\vec{p}$$

Why are these unequal? Well, remember

$$\vec{p}\cdot\hat{r}=\vec{p}\cdot\frac{\vec{r}}{r}=\vec{p}\cdot\left(\frac{x\hat{x}}{r}+\frac{y\hat{y}}{r}+\frac{z\hat{z}}{r}\right)=p_x x/r+p_y y/r+p_z z/r$$

and so the momentum operator must be commuted past all of these to give $\hat{r}\cdot\vec{p}$, and these commutators are nonzero. So $\hat{r}\cdot\vec{p}$ is not Hermitian, and can't correspond to an observable in quantum mechanics.

But we can clearly define radial momentum as $\hat{r} \cdot \vec{p}$ in classical mechanics, so it had better be the case that we can define a Hermitian operator corresponding to a quantum mechanical observable that reproduces this in the classical limit. The natural choice is to combine $\hat{r} \cdot \vec{p}$ and $\vec{p} \cdot \hat{r}$, defining

$$p_r \equiv \frac{1}{2}\left(\hat{r} \cdot \vec{p} + \vec{p} \cdot \hat{r}\right) = -\frac{i\hbar}{2}\left(\frac{1}{r}\vec{r} \cdot \nabla + \nabla \cdot (\vec{r}/r)\right)$$

We can simplify this further by noticing that

$$r\frac{\partial}{\partial r} = x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} + z\frac{\partial}{\partial z} = \vec{r} \cdot \nabla$$

hence

$$p_r = -\frac{i\hbar}{2}\left(\frac{\partial}{\partial r} + \frac{3}{r} - \frac{r}{r^2} + \frac{\partial}{\partial r}\right) = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$$

Now it is easy to show that r and p_r have a canonical commutation relation,

$$[r, p_r] = -i\hbar\left[r, \frac{\partial}{\partial r}\right] = i\hbar$$

Having defined an operator corresponding to momentum in the radial direction, we can consider its square, which as you will confirm on the problem set reduces to

$$p_r^2 = -\frac{\hbar^2}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)$$

Thus we see that the differential equation satisfied by R is of the form

$$\left[\frac{p_r^2}{2m} + V(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}\right]R = ER$$

This looks like an operator equation telling us that the total energy for an energy eigenstate in a spherically symmetric potential is given by the kinetic energy in the radial direction plus the effective potential. This is a far more intuitive framing of the differential equation satisfied by the radial part of the energy eigenstates for spherically symmetric potentials.

It is useful to think of the LHS of the above equation as a sort of radial Hamiltonian acting on the radial wavefunction. Of course, there is a different "radial

Hamiltonian" for every value of the nonnegative integer ℓ, so let's call these Hamiltonians H_ℓ. In this sense the radial wavefunction satisfies an eigenvalue equation

$$H_\ell R_\ell = E R_\ell$$

where

$$H_\ell \equiv \frac{p_r^2}{2m} + V(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}$$

From a practical perspective, when we are pursuing analytic solutions to the TISE, it is still easier to work in terms of $u(r)$, in which case the differential equation involves fewer terms. However, it is still harder than solving 1d problems due to the presence of the centrifugal term. On the other hand, we can also consider *algebraic* solutions to the TISE, much as we did for the harmonic oscillator in 1d. From this perspective, the TISE satisfied by R is a better starting point, since it involves Hermitian operators p_r and r. As we will see, such algebraic solutions are incredibly powerful in three dimensions.

Before moving on, let's summarize what we have learned: for spherically symmetric potentials $V(\vec{r}) = V(r)$, the energy eigenstates are labeled by energies E_n, and the spatial parts of these eigenstates are separable into the product of a radial wavefunction and a spherical harmonic, which are further labeled by integers ℓ, m:

$$\psi_{n,\ell,m}(r,\theta,\phi) = R_\ell(r) Y_\ell^m(\theta,\phi)$$

Here I am taking care to attach the explicit labels ℓ, m to the functions in which they appear.