RADIAL FUNCTION FOR SMALL R

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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

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

We've looked at some properties of U_{El} (which Griffiths calls u) for the hydrogen atom, but we can also try to extract some information about U_{El} in the more general case where we don't need to specify the potential V precisely. Here we'll examine what happens as $r\to0$.

The quantity in the square brackets in 1 is an operator which will call $D_l(r)$:

$$D_l(r)\equiv-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2} \tag{3}$$

If we require D_L to be hermitian, this results in the condition that, for two functions U_1 and U_2,

$$U_1^*\frac{dU_2}{dr}\bigg|_0^\infty-U_2\frac{dU_1^*}{dr}\bigg|_0^\infty=0 \tag{4}$$

If we require U_{El} to be normalizable then it must satisfy either

$$U_{El}\underset{r\to\infty}{\longrightarrow}0 \tag{5}$$

which is valid for bound states where $E>V$ as $r\to\infty$, or

$$U_{El}\underset{r\to\infty}{\longrightarrow}e^{ikr} \tag{6}$$

where

$$k=\sqrt{\frac{2\mu E}{\hbar^2}} \tag{7}$$

if $E>V$ as $r\to\infty$. In the latter case, we're using the definition of normalization for an oscillating function. If $U_{El}\underset{r\to\infty}{\longrightarrow}0$ then 4 is 0 at the upper limit. Using the normalization condition for oscillating functions, if $U_{El}\underset{r\to\infty}{\longrightarrow}e^{ikr}$ then 4 is also zero (on average) at the upper limit. Thus in order for D_l to be Hermitian, we must have

$$U_1^*\frac{dU_2}{dr}\bigg|_0-U_2\frac{dU_1^*}{dr}\bigg|_0=0 \tag{8}$$

at the lower limit as well.

One way of satisfying this condition is if

$$U_{El}\underset{r\to 0}{\longrightarrow}c \tag{9}$$

Because the actual radial function is given by 2, a value of $c\neq 0$ would give

$$R\sim\frac{U}{r}\sim\frac{c}{r} \tag{10}$$

Such a function is still square integrable because an integral over all space introduces a factor of r^2 in the volume element:

$$\int R^2r^2\sin\theta dr\,d\theta\,d\phi \tag{11}$$

Thus the integrand is still finite at $r=0$ so the integral itself can be finite.

The problem with $c\neq 0$ is that the Laplacian of $\frac{1}{r}$ gives a delta function:

$$\nabla^2\frac{1}{r}=-4\pi\delta^3(\mathbf{r}) \tag{12}$$

Unless the potential V has a delta function at the origin (which would be quite unusual), the ∇^2 in the Schrödinger equation can't be allowed to generate a delta function there, so we must have $c=0$.

So far, everything is true for any potential. If we now assume that V is less singular than $\frac{1}{r^2}$ (that is, $V\underset{r\to 0}{\longrightarrow}\frac{1}{r^a}$ where $a<2$), the centrifugal barrier term in 1 will dominate as $r\to 0$, so for small r, 1 reduces to the differential equation

$$U_l''\simeq\frac{l(l+1)}{r^2}U_l \tag{13}$$

The E in the suffix of U has been dropped because the term involving E in 1 is negligible compared to the centrifugal barrier for $r \to 0$. This equation has solutions

$$U_l \sim r^\alpha \tag{14}$$

Plugging this into 13 we get

$$\alpha(\alpha - 1) = l(l+1) \tag{15}$$

This is a quadratic equation in α which has the two solutions

$$\alpha = -l, l+1 \tag{16}$$

If we are to have $U_{El} \to 0$ as $r \to 0$, then we must discard the solution $U_l \sim r^{-l}$, so we have that

$$U_{El} \sim r^{l+1} \tag{17}$$

All of this works only if $l \neq 0$ since in the case where $l = 0$ (zero angular momentum), there is no centrifugal barrier and we must look at the form of the potential. Shankar notes that the problems he considers in his book are such that 17 is also valid for $l = 0$.