WKB APPROXIMATION AND THE HYDROGEN ATOM

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 8.14.

As another example of applying the WKB approximation to a 3-d problem with a spherically symmetric potential, we'll look at the radial equation for the hydrogen atom.

The general wave function can be written as the product of a radial function $R(r)$ and a spherical harmonic $Y(\theta,\phi)$.

With the substitution $u(r) \equiv rR(r)$ the radial equation for hydrogen can be written

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\left(-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right)u=Eu \tag{1}$$

The effective potential is the term in parentheses:

$$V(r)=-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} \tag{2}$$

and has the form of a well with sloping sides on both sides, at points r_1 and r_2 defined by the roots of

$$E=-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} \tag{3}$$

In this case, the WKB equations satisfy the condition

$$\int_{r_1}^{r_2} p(r)\;dr=\left(n-\frac{1}{2}\right)\pi\hbar \tag{4}$$

Plugging in the formulas for the hydrogen atom we get

$$\int_{r_1}^{r_2} p(r)\;dr = \sqrt{2m}\int_{r_1}^{r_2}\sqrt{E+\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}-\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}}dr \tag{5}$$

$$=\sqrt{-2mE}\int_{r_1}^{r_2}\frac{1}{r}\sqrt{-r^2-\frac{e^2}{4\pi\epsilon_0 E}r+\frac{\hbar^2}{2mE}l(l+1)}dr \tag{6}$$

where we've factored out $-E$ (since for a bound state, $E<0$). We can simplify the notation by defining the positive quantities

$$
\begin{aligned}
B &\equiv -\frac{e^2}{4\pi\varepsilon_0 E} && (7)\\
C &\equiv -\frac{\hbar^2}{2mE}l(l+1) && (8)
\end{aligned}
$$

The turning points r_1 and r_2 can be found from the roots of the term inside the square root in 6:

$$
\begin{aligned}
r_1 &= \frac{B-\sqrt{B^2-4C}}{2} && (9)\\
r_2 &= \frac{B+\sqrt{B^2-4C}}{2} && (10)
\end{aligned}
$$

so we can factor the quadratic to get

$$
\begin{aligned}
\int_{r_1}^{r_2} p(r)\,dr &= \sqrt{-2mE}\int_{r_1}^{r_2}\frac{1}{r}\sqrt{(r-r_1)(r_2-r)}dr && (11)\\
&= \sqrt{-2mE}\frac{\pi}{2}\left(\sqrt{r_2}-\sqrt{r_1}\right)^2 && (12)\\
&= \sqrt{-2mE}\frac{\pi}{2}\left(r_1+r_2-2\sqrt{r_1 r_2}\right) && (13)\\
&= \sqrt{-2mE}\frac{\pi}{2}\left(B-2\sqrt{C}\right) && (14)\\
&= \sqrt{-2mE}\frac{\pi}{2}\left(-\frac{e^2}{4\pi\varepsilon_0 E}-2\sqrt{-\frac{\hbar^2}{2mE}l(l+1)}\right) && (15)\\
&= \frac{\pi}{2}\left(-\frac{e^2\sqrt{2m}}{4\pi\varepsilon_0\sqrt{-E}}-2\hbar\sqrt{l(l+1)}\right) && (16)\\
&= \left(n-\frac{1}{2}\right)\pi\hbar && (17)
\end{aligned}
$$

where we've used the integral given in Griffiths's question to get the second line, and the last line uses 4. Solving 16 for E gives the WKB energy levels:

$$E = -\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{m}{2\hbar^2\left(n-\frac{1}{2}+\sqrt{l\,(l+1)}\right)^2} \tag{18}$$

$$= \frac{-13.6 \text{ eV}}{\left(n-\frac{1}{2}+\sqrt{l\,(l+1)}\right)^2} \tag{19}$$

since the ground state of hydrogen is given by the Bohr formula

$$E_0 = -\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{m}{2\hbar^2} = -13.6 \text{ eV} \tag{20}$$