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Expectation of spherically symmetric 3D potential derivative

Exercise 1.1 Expectation of spherically symmetric 3D potential derivative. ([1] *pr. 5.16*)

1. For a particle in a spherically symmetric potential $V(r)$ show that
$$\left|\psi(0)\right|^2 = \frac{m}{2\pi\hbar^2} \left\langle \frac{dV}{dr} \right\rangle, \tag{1.1}$$
for all s-states, ground or excited.
2. Show this is the case for the 3D SHO and hydrogen wave functions.

Answer for Exercise 1.1

Part 1. The text works a problem that looks similar to this by considering the commutator of an operator A, later set to $A = p_r = -i\hbar\partial/\partial r$ the radial momentum operator. First it is noted that
$$0 = \left\langle {nlm} \right\rvert \left[H, A \right] \left\lvert {nlm} \right\rangle, \tag{1.2}$$
since H operating to either the right or the left is the energy eigenvalue E_n. Next it appears the author uses an angular momentum factoring of the squared momentum operator. Looking earlier in the text that factoring is found to be
$$\frac{\mathbf{p}^2}{2m} = \frac{1}{2mr^2}\mathbf{L}^2 - \frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \right). \tag{1.3}$$
With
$$R = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \right). \tag{1.4}$$
we have
$$\begin{aligned}
0 &= \left\langle {nlm} \right\rvert \left[H, p_r \right] \left\lvert {nlm} \right\rangle \\
&= \left\langle {nlm} \right\rvert \left[\frac{\mathbf{p}^2}{2m} + V(r), p_r \right] \left\lvert {nlm} \right\rangle \\
&= \left\langle {nlm} \right\rvert \left[\frac{1}{2mr^2}\mathbf{L}^2 + R + V(r), p_r \right] \left\lvert {nlm} \right\rangle \\
&= \left\langle {nlm} \right\rvert \left[\frac{-\hbar^2 l(l+1)}{2mr^2} + R + V(r), p_r \right] \left\lvert {nlm} \right\rangle.
\end{aligned} \tag{1.5}$$

Let's consider the commutator of each term separately. First

$$\begin{aligned}\left[V, p_r\right]\psi &= Vp_r\psi - p_rV\psi \\ &= Vp_r\psi - (p_rV)\psi - Vp_r\psi \\ &= -(p_rV)\psi \\ &= i\hbar\frac{\partial V}{\partial r}\psi.\end{aligned} \tag{1.6}$$

Setting $V(r) = 1/r^2$, we also have

$$\left[\frac{1}{r^2}, p_r\right]\psi = -\frac{2i\hbar}{r^3}\psi. \tag{1.7}$$

Finally

$$\begin{aligned}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}, \frac{\partial}{\partial r}\right] &= \left(\partial_{rr} + \frac{2}{r}\partial_r\right)\partial_r - \partial_r\left(\partial_{rr} + \frac{2}{r}\partial_r\right) \\ &= \partial_{rrr} + \frac{2}{r}\partial_{rr} - \left(\partial_{rrr} - \frac{2}{r^2}\partial_r + \frac{2}{r}\partial_{rr}\right) \\ &= -\frac{2}{r^2}\partial_r,\end{aligned} \tag{1.8}$$

so

$$\begin{aligned}\left[R, p_r\right] &= -\frac{2}{r^2}\frac{-\hbar^2}{2m}p_r \\ &= \frac{\hbar^2}{mr^2}p_r.\end{aligned} \tag{1.9}$$

Putting all the pieces back together, we've got

$$\begin{aligned}0 &= \langle nlm|\left[\frac{-\hbar^2 l(l+1)}{2mr^2} + R + V(r), p_r\right]|nlm\rangle \\ &= i\hbar\langle nlm|\left(\frac{\hbar^2 l(l+1)}{mr^3} - \frac{i\hbar}{mr^2}p_r + \frac{\partial V}{\partial r}\right)|nlm\rangle.\end{aligned} \tag{1.10}$$

Since s-states are those for which $l = 0$, this means

$$\begin{aligned}\left\langle\frac{\partial V}{\partial r}\right\rangle &= \frac{i\hbar}{m}\left\langle\frac{1}{r^2}p_r\right\rangle \\ &= \frac{\hbar^2}{m}\left\langle\frac{1}{r^2}\frac{\partial}{\partial r}\right\rangle \\ &= \frac{\hbar^2}{m}\int_0^\infty dr\int_0^\pi d\theta\int_0^{2\pi} d\phi r^2\sin\theta\psi^*(r,\theta,\phi)\frac{1}{r^2}\frac{\partial\psi(r,\theta,\phi)}{\partial r}.\end{aligned} \tag{1.11}$$

Since s-states are spherically symmetric, this is

$$\left\langle \frac{\partial V}{\partial r} \right\rangle = \frac{4\pi\hbar^2}{m} \int_0^\infty dr \psi^* \frac{\partial \psi}{\partial r}. \tag{1.12}$$

That integral is

$$\int_0^\infty dr \psi^* \frac{\partial \psi}{\partial r} = |\psi|^2\Big|_0^\infty - \int_0^\infty dr \frac{\partial \psi^*}{\partial r} \psi. \tag{1.13}$$

With the hydrogen atom, our radial wave functions are real valued. It's reasonable to assume that we can do the same for other real-valued spherical potentials. If that is the case, we have

$$2 \int_0^\infty dr \psi^* \frac{\partial \psi}{\partial r} = |\psi(0)|^2, \tag{1.14}$$

and

$$\boxed{\left\langle \frac{\partial V}{\partial r} \right\rangle = \frac{2\pi\hbar^2}{m} |\psi(0)|^2,} \tag{1.15}$$

which completes this part of the problem.

Part 2. For a hydrogen like atom, in atomic units, we have

$$\begin{aligned}
\left\langle \frac{\partial V}{\partial r} \right\rangle &= \left\langle \frac{\partial}{\partial r} \left(-\frac{Ze^2}{r} \right) \right\rangle \\
&= Ze^2 \left\langle \frac{1}{r^2} \right\rangle \\
&= Ze^2 \frac{Z^2}{n^3 a_0^2 \left(l + 1/2 \right)} \\
&= \frac{\hbar^2}{m a_0} \frac{2Z^3}{n^3 a_0^2} \\
&= \frac{2\hbar^2 Z^3}{m n^3 a_0^3}.
\end{aligned} \tag{1.16}$$

On the other hand for $n = 1$, we have

$$\begin{aligned}
\frac{2\pi\hbar^2}{m} |R_{10}(0)|^2 |Y_{00}|^2 &= \frac{2\pi\hbar^2}{m} \frac{Z^3}{a_0^3} 4 \frac{1}{4\pi} \\
&= \frac{2\hbar^2 Z^3}{m a_0^3},
\end{aligned} \tag{1.17}$$

and for $n = 2$, we have

$$
\begin{aligned}
\frac{2\pi\hbar^2}{m}|R_{20}(0)|^2|Y_{00}|^2 &= \frac{2\pi\hbar^2}{m}\frac{Z^3}{8a_0^3}4\frac{1}{4\pi} \\
&= \frac{\hbar^2 Z^3}{4ma_0^3}.
\end{aligned}
\tag{1.18}
$$

These both match the potential derivative expectation when evaluated for the s-orbital ($l = 0$).
For the 3D SHO I verified the ground state case in the Mathematica notebook sakuraiProblem5.16bSHO.nb
There it was found that

$$
\begin{aligned}
\left\langle \frac{\partial V}{\partial r} \right\rangle &= \frac{2\pi\hbar^2}{m}|\psi(0)|^2 \\
&= 2\sqrt{\frac{m\omega^3\hbar}{\pi}}
\end{aligned}
\tag{1.19}
$$

Bibliography

[1] Jun John Sakurai and Jim J Napolitano. *Modern quantum mechanics*. Pearson Higher Ed, 2014. 1.1