Physics 5646

Quantum Mechanics B

Problem Set VI

Due: Tuesday, Mar 6, 2018

6.1 Useful Hydrogen Atom Expectation Values I

The radial equation for the hydrogen atom is,

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

where u(r) = rR(r). Last semester, we solved this equation using the power series method, and found that normalizable solutions occurred when

$$E = -\frac{e^2}{2a_0} \frac{1}{(p+l+1)^2}, \quad p = 0, 1, 2, \dots$$

where n = p + l + 1 is then the usual n quantum number for hydrogen.

If we imagine adding a perturbation

$$V = \frac{\lambda}{\hat{r}^2}$$

to the hydrogen atom, it is easy to see that the radial equation will be modified as follows,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - \frac{e^2}{r} + \frac{\hbar^2 l(l+1)}{2mr^2} + \frac{\lambda}{r^2}\right)u(r) = Eu(r).$$
(1)

(a) Show that the radial equation for the perturbed problem (1) can be rewritten,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - \frac{e^2}{r} + \frac{\hbar^2 l'(l'+1)}{2mr^2}\right)u(r) = Eu(r),$$

where l' is a function of λ .

(b) The power series analysis applied to the perturbed problem will yield the same result for the quantized energy levels we obtained last semester, but with l replaced by l'. The resulting exact energy levels can then be expanded in powers of λ as follows,

$$E = -\frac{e^2}{2a_0} \frac{1}{(p+l'+1)^2} = E^0 + \lambda E^1 + \lambda^2 E^2 + \cdots$$

Here λE^1 is the first order energy shift due to the perturbation $V = \frac{\lambda}{\hat{r}^2}$. Use that fact, and the fact that

$$\lambda E^1 = \lambda \frac{dE}{d\lambda} \bigg|_{\lambda=0} = \lambda \frac{dE}{dl'} \bigg|_{l'=l} \frac{dl'}{d\lambda} \bigg|_{\lambda=0},$$

To show that the expectation value of $1/\hat{r}^2$ in a hydrogen-atom energy eigenstate is

$$\left\langle \frac{1}{\hat{r}^2} \right\rangle = \frac{1}{a_0^2 n^3 (l + \frac{1}{2})}.$$

- 6.2 Useful Hydrogen Atom Expectation Values II
 - (a) Show that the operator (in position representation using spherical coordinates),

$$\hat{p}_r = \frac{\hbar}{i} \left(\frac{\partial}{\partial r} + \frac{1}{r} \right),\,$$

has the property that

$$\hat{p}_r^2 = -\hbar^2 \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r},$$

and, hence, the Hamiltonian for the hydrogen atom can be expressed (again in position representation),

$$H = \frac{\hat{p}_r^2}{2m} + \frac{1}{2mr^2}\vec{L}^2 - \frac{e^2}{r}.$$

where

$$\vec{L}^2 = \frac{1}{\sin^2 \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$$
 (2)

Here \hat{p}_r is the operator corresponding to the radial component of the momentum. In what follows you may use the fact that $[\hat{p}_r, \vec{L}^2] = 0$ which follows trivially from the fact that \vec{p}_r acts only on r and \vec{L}^2 acts only on θ and ϕ .

(b) Show that for any operator O,

$$\langle [H, O] \rangle = 0,$$

if the expectation value is taken in a hydrogen-atom energy eigenstate.

(c) Evaluate $[H, \hat{p}_r]$. Show that when the result is combined with what you proved in Part (b) you find that,

$$\left\langle \frac{1}{\hat{r}^3} \right\rangle = \frac{1}{a_0} \frac{1}{l(l+1)} \left\langle \frac{1}{\hat{r}^2} \right\rangle.$$

Finally, using the result from Problem 6.1, show that

$$\left\langle \frac{1}{\hat{r}^3} \right\rangle = \frac{1}{a_0^3} \frac{1}{n^3 l(l + \frac{1}{2})(l+1)}.$$

6.3 Heisenberg equations of motion for a charged particle.

The Hamiltonian for a particle of mass m and charge e moving in the presence of a magnetic and electric field is

$$H = \frac{1}{2m} \left(\hat{\vec{p}} - \frac{e}{c} \vec{A} \right)^2 + e\phi,$$

where \vec{A} and ϕ are the vector and scalar potentials corresponding to magnetic and electric fields $\vec{B} = \vec{\nabla} \times \vec{A}$ and $\vec{E} = -\vec{\nabla} \phi$. Here we assume \vec{A} and ϕ do not depend on time.

(a) Show that the Heisenberg equation of motion for $\hat{\vec{r}}$ is

$$\frac{d\hat{\vec{r}}}{dt} = \frac{1}{i\hbar} [\hat{\vec{r}}, H] = \frac{1}{m} (\hat{\vec{p}} - \frac{e}{c} \vec{A}) \equiv \frac{1}{m} \vec{\Pi}.$$

Here $\vec{\Pi} = \hat{\vec{p}} - \frac{e}{c}\vec{A}$ is the gauge invariant kinematical momentum.

(b) Show that

$$[\Pi_i, \Pi_j] = i \frac{\hbar e}{c} \sum_k \epsilon_{ijk} B_k,$$

where the indices run over x,y, and z in the usual way.

(c) Show that the Heisenberg equation of motion for $\vec{\Pi}$ is

$$\frac{d\vec{\Pi}}{dt} = \frac{1}{i\hbar}[\vec{\Pi}, H] = e\vec{E} + \frac{1}{2c} \left(\frac{\vec{\Pi}}{m} \times \vec{B} - \vec{B} \times \frac{\vec{\Pi}}{m} \right).$$

Hint: You can use the result from Part (b) and the fact that $H = \frac{\vec{\Pi}^2}{2m} + e\phi$.

(d) Combining your result from Parts (a) and (c), show that

$$m\frac{d^2\hat{r}}{dt^2} = e\vec{E} + \frac{1}{2c} \left(\frac{d\hat{r}}{dt} \times \vec{B} - \vec{B} \times \frac{d\hat{r}}{dt} \right).$$

(e) Argue that if you form a wave packet, and if \vec{E} and \vec{B} are smooth enough functions of \vec{r} that they can be treated as being approximately constant over the size of this wave packet, then the wave packet will follow the usual Lorentz force law of a charged particle moving through an electric and magnetic field.