Ex5a

Exercise 2

1 Relativistic Effects in the H-Atom

The Darwin term

$$\hat{H}_{\text{Darwin}} = -\frac{\hbar^2}{4m^2c^2} e\vec{E} \cdot \vec{\nabla}$$

describes a relativistic correction to the energy levels of the hydrogen atom due to the *Zitterbewegung*. Other corrections are the relativistic mass effect and the spin-orbit coupling.

(a) Specify the electric field $\vec{E}$ of a point-like charge and the nabla operator $\vec{\nabla}$ in spherical coordinates.

(b) Show using first order error propagation $\Delta E = \langle \Psi | \hat{H}_{\text{Darwin}} | \Psi \rangle$ that the energy shift is given by

$$\Delta E = \frac{\pi\hbar^2}{2m^2c^2} \frac{Ze^2}{4\pi\epsilon_0} |\Psi(0)|^2,$$

where Ψ is the solution of the undisturbed hydrogen Schrödinger equation.

(c) What is the consequence of the factor $|\Psi(0)|^2$? Which energy levels are shifted by the Darwin term?

Hints:
- Remember the separation of radial and angular coordinates.
- Which component is affected by the derivation of the Darwin term?
- Keep in mind that the wave functions are orthonormalized.
- $\frac{\partial}{\partial x} (f(x))^2 = 2f(x)\frac{\partial}{\partial x} f(x)$

2 Klein-Gordon and Dirac Equation

The Schrödinger equation uses the classical energy-momentum relation $E = \frac{\vec{p}^2}{2m} + V(\vec{x})$ and substitutes $\vec{p}$ and E for their respective momentum and energy operators $\hat{\vec{p}}$ and $\hat{H}$.

(a) Use the relativistic energy-momentum relation

$$E^2 = p^2c^2 + m^2c^4$$

to develop the Klein-Gordon equation in analogy to the Schrödinger equation.

(b) The Klein-Gordon equation treats time and space in the same manner by incorporating both as second derivatives. Paul Dirac tried to find an equation with first derivatives only. In 1928 he developed the Dirac equation

$$\hat{H}\Psi = (c\vec{\alpha} \circ \hat{\vec{p}} + \beta mc^2)\Psi.$$

Determine the constraints on $\vec{\alpha}$ and β so that the Dirac equation satisfies the relativistic energy-momentum relation by applying $\hat{H}$ a second time (see lecture).

(c) Show that these conditions cannot be fulfilled if α_i or β are simple complex numbers.

(d) We want $\hat{H} = \hat{H}^\dagger$ to be hermitian. Therefore α_i and β have to be hermitian. What are their eigenvalues?

(e) Show that α_i and β are traceless. What does this mean for their dimension?

3 Radial Expectation Values for Hydrogen

(a) By brute force, using generating functions for Laguerre polynomials, show that mean radius a one-electron atom in the hydrogenic orbital $|n, l, m\rangle$ is

$$\langle r \rangle_{nl} = n^2 \frac{a_0}{Z} \left[1 + \frac{1}{2}\left(1 - \frac{l(l+1)}{n^2}\right)\right] \text{ (independent of q-number } m \Big)$$

(b) For "circular" states (the ones with zero radial momentum, $n_r = 0$), and in the "correspondence limt" ($n \to \infty$) show that we retrieve Bohr's result,

$$\langle r \rangle \to n^2 \frac{a_0}{Z}$$

Though any expectation value can be calculated by tedious method in part (a), a trick to due Feyman and Hellman, saves a lot of work (note this was part of Feyman's undergrad thesis!). The radial Hamiltonian is a function of various "parameters", $m_e, e, l \equiv \xi$,

$$\hat{H}\,(m_e, e, l) = \frac{-\hbar^2}{2m_e}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2m_e r^2} - \frac{Ze^2}{r}$$

Mathematically, is well defined for arbitrary assignment or real numbers to any ξ.

(c) Defining the radial eigenstate as $\hat{H}(\xi)\,|n_r, \xi\rangle = E_{n_r}(\xi)\,|n_r, \xi\rangle = -\frac{1}{2(n_r+l+1)^2}\frac{Z^2me^4}{\hbar^2}\,|n_r, \xi\rangle$, show that $\left\langle n_r, \xi \left| \frac{\partial \hat{H}(\xi)}{\partial \xi} \right| n_r, \xi \right\rangle = \frac{\partial E_{n_r}(\xi)}{\partial \xi}$ (Feyman-Hellman theorem)

(d) Using the Feynman-Hellman theorem, show that

a) $\left\langle \frac{1}{r} \right\rangle_{n,l} = \frac{Z}{a_0 n^2}$ (use $\xi = e^2$). Relate this to the Viral Theorem.

b) $\left\langle \frac{1}{r^2} \right\rangle_{n,l} = \frac{Z^2}{a_0^2} \frac{1}{n^3 (l+1/2)}$ (use $\xi = l$).

c) $\left\langle \frac{1}{r^3} \right\rangle_{n,l} = \frac{Z}{a_0} \frac{1}{l(l+1)} \left\langle \frac{1}{r^2} \right\rangle_{n,l}$.

For this final case prove and then use the expectation value of the commutator,

$$\left\langle \left[\frac{d}{dr}, \hat{H}(\xi) \right] \right\rangle_{nl} = 0$$