329(3): Evaluation of the Quantum Relativistic Hamiltonian in the First Approximation

The Hamiltonian is:

$$H_0 = H - mc^2 = \frac{p^2 c^2}{(p^2c^2 + m^2c^4)^{1/2} + mc^2} + U \quad -(1)$$

i.e.:

$$\langle H_0 \rangle = -\hbar^2 c^2 \int \frac{\psi^* \nabla^2 \psi \, d\tau}{(p^2c^2 + m^2c^4)^{1/2} + mc^2} + \int \psi^* U \psi \, d\tau \quad -(2)$$

In this equation:

$$p_0^2 = 2m(H_0 - U) \quad -(3)$$

in the denominator of the first term on the right hand side of eq. (2). Eq. (3) is the non-relativistic first approximation, in which:

$$U = -\frac{e^2}{4\pi\epsilon_0 r}. \quad -(4)$$

The classical hamiltonian H_0 is a constant of motion.

Now use:

$$(p^2c^2 + m^2c^4)^{1/2} + mc^2 = (\gamma + 1) mc^2 \quad -(5)$$

where:
$$\gamma = \left(1 - \frac{p_0^2}{m^2c^2}\right)^{-1/2} \quad -(6)$$

Therefore:
$$\langle H_0 \rangle = -\hbar^2 c^2 \int \frac{\psi^* \nabla^2 \psi \, d\tau}{\left(2 + \frac{p_0^2}{2m^2c^2}\right) mc^2} + \int \psi^* U \psi \, d\tau \quad -(7)$$
where the following approximation has been used:
$$\left(1 - \frac{p_0^2}{m^2c^2}\right)^{-1/2} \sim 1 + \frac{1}{2}\frac{p_0^2}{m^2c^2}. \quad -(8)$$
Therefore:
$$\langle H_0 \rangle = -\hbar^2 \int \frac{\psi^* \nabla^2 \psi \, d\tau}{\left(2 + \frac{H_0 - U}{mc^2}\right) m} + \int \psi^* U \psi \, d\tau \quad -(9)$$
$$\xrightarrow[H_0 - U \ll mc^2]{} -\frac{\hbar^2}{2m} \int \psi^* \nabla^2 \psi \, d\tau + \int \psi^* U \psi \, d\tau,$$
the non-relativistic result from the Schroedinger equation. This is:
$$H_0 = \frac{-me^4}{32\pi^2 \epsilon_0^2 \hbar^2} \frac{1}{n^2} \quad -(10)$$
for the energy levels of the hydrogen atom,

) where n is the principal quantum number.

More accurately:

$$\langle H_0 \rangle = -\frac{\hbar^2}{m}\int \phi^* \nabla^2 \left(\left(2 + \frac{H_0 - U}{mc^2} \right)^{-1} \phi \right) d\tau$$

$$+ \int \phi^* U \phi \, d\tau \quad -(11)$$

where

$$U = -\frac{e^2}{4\pi\epsilon_0 r} \quad -(12)$$

Now use:

$$\frac{1}{2 + \frac{H_0 - U}{mc^2}} = \frac{1}{2}\left(\frac{1}{1 + \frac{H_0 - U}{2mc^2}} \right) \sim \frac{1}{2}\left(1 - \frac{H_0 - U}{2mc^2} \right) \quad -(13)$$

if

$$H_0 - U \ll 2mc^2 \quad -(14)$$

So:

$$\langle H_0 \rangle = -\frac{\hbar^2}{2m}\int \phi^* \nabla^2 \phi \, d\tau + \int \phi^* U \phi \, d\tau$$

$$+ \frac{\hbar^2}{4m^2c^2}\int \phi^* \nabla^2 \left((H_0 - U)\phi \right) d\tau \quad -(15)$$

4) i.e.

$$\langle H_0 \rangle = \frac{-me^4}{32\pi^2\epsilon_0^2\hbar^2n^2} + \frac{\hbar^2}{4m^2c^2}\int \psi^* \nabla^2\left((H_0 - U)\psi\right) d\tau \qquad -(16)$$

There is a shift in the energy levels of the H atom which is different for each n.

Now use the fact that H_0 is a constant of motion. Therefore:

$$\langle H_0 \rangle = \frac{-me^4}{32\pi^2\epsilon_0^2\hbar^2n^2} + \frac{\hbar^2 H_0}{4m^2c^2}\int \psi^* \nabla^2 \psi \, d\tau$$

$$- \frac{\hbar^2}{4m^2c^2}\int \psi^* \nabla^2 (U\psi) \, d\tau \qquad -(17)$$

In the first approximation eq (10) can be used for H_0 on the right hand side of eq. (17), so:

$$\langle H_0 \rangle = \frac{-me^4}{32\pi^2\epsilon_0^2\hbar^2n^2}\left(1 + \frac{\hbar^2}{4m^2c^2}\int \psi^* \nabla^2 \psi \, d\tau\right)$$

$$- \frac{\hbar^2}{4m^2c^2}\int \psi^* \nabla^2 (U\psi) \, d\tau$$

$$-(18)$$

2) The shift in the energy levels can be worked out using the hydrogenic wavefunctions for ϕ. Note that:

$$\nabla^2 (U\phi) = \underline{\nabla} \cdot \underline{\nabla} (U\phi)$$
$$= \underline{\nabla} \cdot (\phi \underline{\nabla} U + U \underline{\nabla} \phi) \quad -(19)$$

using the Leibnitz Theorem. Similarly:

$$\underline{\nabla} \cdot (\phi \underline{\nabla} U + U \underline{\nabla} \phi) = \underline{\nabla} \phi \cdot \underline{\nabla} U + \phi \nabla^2 U$$
$$+ \underline{\nabla} U \cdot \underline{\nabla} \phi + U \nabla^2 \phi \quad -(20)$$
$$= \phi \nabla^2 U + U \nabla^2 \phi + 2 \underline{\nabla} \phi \cdot \underline{\nabla} U.$$

So:

$$\langle H_0 \rangle = -\frac{me^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} \left(1 + \frac{\hbar^2}{4m^2c^2} \int \phi^* \nabla^2 \phi \, d\tau \right)$$
$$- \frac{\hbar^2}{4m^2c^2} \left[\int \phi^* \nabla^2 U \phi \, d\tau + \int \phi^* U \nabla^2 \phi \, d\tau \right. \quad -(21)$$
$$\left. + 2 \int \phi^* \underline{\nabla} U \cdot \underline{\nabla} \phi \, d\tau \right]$$

<u>So there are several types of shift.</u>

As in UFT266 in the non-relativistic limit:

6)

$$\langle H_0 \rangle = -\frac{\hbar^2}{2m}\int \psi^* \nabla^2 \psi \, d\tau + \int \psi^* U \psi \, d\tau$$

$$= \frac{e^2}{8\pi\epsilon_0 r} - \frac{e^2}{4\pi\epsilon_0 r} = -\frac{e^2}{8\pi\epsilon_0 r} \quad -(22)$$

where

$$r = \frac{4\pi\epsilon_0 n^2 \hbar^2}{m e^2} \quad -(23)$$

is the Bohr radius.

Comparison with the Dirac Approximation

In the Dirac approximation eq. (1) is written as:

$$H_0 = H - mc^2 = \frac{p^2 c^2}{H - U + mc^2} = \frac{p^2 c^2}{\underbrace{E \quad}_{} + mc^2} \quad -(24)$$

Dirac assumed that:

$$H \sim E \sim mc^2 \quad -(25)$$

i.e

$$U << E \sim mc^2 \quad -(26)$$

So

$$H_0 \sim \frac{p^2 c^2}{2mc^2 - U} + U \quad -(27)$$

$$= \frac{p^2}{2m}\left(1 - \frac{U}{2mc^2}\right)^{-1} + U$$

$$\sim \frac{p^2}{2m}\left(1 + \frac{U}{2mc^2}\right) + U$$

1) From this approximation:

$$\langle H_0 \rangle = -\frac{\hbar^2}{2m}\int \psi^* \nabla^2 \psi \, d\tau + \int \psi^* U \psi \, d\tau$$

$$-\frac{\hbar^2}{4m^2c^2}\int \psi^* \nabla^2 (U\psi) \quad -(28)$$

$$= \frac{-me^4}{32\pi^2\epsilon_0^2\hbar^2 n^2} - \frac{\hbar^2}{4m^2c^2}\int \psi^* \nabla^2 (U\psi)$$

Comparison of eqns (21) and (28) shows that the Dirac approximation misses the term:

$$\boxed{\langle H_0 \rangle_1 = -\frac{me^4}{32\pi^2\epsilon_0^2\hbar^2 n^2}\left(\frac{\hbar^2}{4m^2c^2}\int \psi^* \nabla^2 \psi \, d\tau\right)} \quad -(29)$$

$$= -\frac{e^4}{128\pi^2\epsilon_0^2 mc^2 n^2}\int \psi^* \nabla^2 \psi \, d\tau$$

and this could be evaluated by computer algebra and looked for spectroscopically.