

326(3) : Quantization of the Sommerfeld Hamiltonian using the Schrödinger/Dirac Procedure

First review the Dirac quantization procedure, which is also the semi classical quantization

Consider the relativistic momentum:

$$\underline{p} = \gamma m \underline{v}_N \quad - (1)$$

where γ is the Lorentz factor and \underline{v}_N the Newtonian velocity. Eq. (1) can be rewritten as the Einstein energy equation:

$$E^2 = c^2 p^2 + m^2 c^4 \quad - (2)$$
$$= \gamma^2 m c^2$$

where E is the total kinetic energy. It follows that:

$$E^2 - c^2 p^2 = (E - mc^2)(E + mc^2) = c^2 p^2 \quad - (3)$$

so

$$E - mc^2 = \frac{c^2 p^2}{E + mc^2} \quad - (4)$$

The Hamiltonian of special relativity is:

$$H = E + U \quad - (5)$$

and is a constant of motion. Therefore:

$$E \rightarrow E + U \quad - (6)$$

2) in the presence of a potential energy U . The latter is

$$U = e\phi \quad - (7)$$

where ϕ is the potential. Therefore:

$$\boxed{E \rightarrow H - U} \quad - (8)$$

It follows that:

$$(H - U)^2 = c^2 p^2 + m^2 c^4 \quad - (9)$$

is Sol. the Sommerfeld and Dirac atoms. Therefore:

$$\begin{aligned} c^2 p^2 &= (H - U)^2 - m^2 c^4 \\ &= (H - U - mc^2)(H - U + mc^2) \end{aligned} \quad - (10)$$

So eq. (4) is modified to:

$$H - mc^2 - U = \frac{c^2 p^2}{H + mc^2 - U} \quad - (11)$$

$$= \frac{c^2 p^2}{E + mc^2}$$

where

$$E = \gamma mc^2 \quad - (12)$$

The classical Hamiltonian is written as:

$$3) \quad H - mc^2 = \frac{c^2 p^2}{E + mc^2} + U \quad - (13)$$

Eq. (11) was solved by Dirac and contemporaries using various approximations which are apparently justified by experimental data. The first approximation is to assume that:

$$U \ll E \quad - (14)$$

so $H \sim E. \quad - (15)$

Then eq. (11) becomes:

$$H - mc^2 \sim \frac{c^2 p^2}{E + mc^2 - U} + U \quad - (16)$$

The second approximation is to assume that:

$$v \ll c \quad - (17)$$

so: $E = \gamma mc^2 \sim mc^2. \quad - (18)$

Then $H - mc^2 \sim \frac{c^2 p^2}{2mc^2 - U} + U \quad - (19)$

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

4) i.e

$$H - mc^2 \sim \frac{p^2}{2m} \left(1 + \frac{U}{2mc^2} \right) + U \quad (20)$$

This quantizes to

$$\left(-\frac{\hbar^2 \nabla^2}{2m} \left(1 + \frac{U}{2mc^2} \right) + U \right) \psi = (H - mc^2) \psi \quad (21)$$

which reduces when:

$$U \ll 2mc^2 \quad (22)$$

to the Schrödinger equation:

$$\left(-\frac{\hbar^2 \nabla^2}{2m} + U \right) \psi = E \psi \quad (23)$$

where

$$E := H - mc^2 \quad (24)$$

is the classical total energy. In the H atom:

$$U = -\frac{e^2}{4\pi\epsilon_0 r} \quad (25)$$

The Sommerfeld quantization therefore results in a rearrangement of eq. (21) to give shifted energy levels as follows:

$$\left(-\frac{\hbar^2 \nabla^2}{2m} + U\right) \psi = \left(E + \frac{\hbar^2 U \nabla^2}{4m^2 c^2}\right) \psi \quad (26)$$

where E in eq. (26) is defined by eq. (24).

Therefore

$$\langle E \rangle \rightarrow \langle E \rangle + \left\langle \frac{\hbar^2 U \nabla^2}{4m^2 c^2} \right\rangle \quad (27)$$

where

$$\left\langle \frac{\hbar^2 U \nabla^2}{4m^2 c^2} \right\rangle = - \int \psi^* \frac{\hbar^2 e^2}{16\pi \epsilon_0 m^2 r} \nabla^2 \psi \quad (28)$$

To a first approximation the hydrogenic orbitals can be used in eq. (28). The result is a small shift in the energy levels of the H atom, but there is no spin orbit coupling because the $SU(2)$ basis has not been used.

The Sommerfeld wavefunctions are found by solving eq. (21) for ψ .