

1) 59/6) Motion in a Coulomb Field, of Hydrogen Atom, and ECE Dem.  
(P.W. Atkins, "Molecular Quantum Mechanics", pp. 67 ff.)

The Schrödinger equation is used for this well known problem:

$$\hat{H}\psi = E\psi \quad \text{--- (1)}$$

where the Hamiltonian operator is:

$$\hat{H} = -\frac{\hbar^2}{2\mu} \nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} \quad \text{--- (2)}$$

where  $\mu$  is the reduced mass:

$$\mu = \frac{m_e m_p}{m_e + m_p} \quad \text{--- (3)}$$

These equations are written in SI units and  $m_e$  and  $m_p$  are the masses of the electron and proton respectively. The radial dependence of the wave-function can be obtained as is well known. The potential energy in eq. (2) is obtained from the Coulomb Law of the standard model:

$$\underline{\nabla} \cdot \underline{E} = \frac{\rho}{\epsilon_0} \quad \text{--- (4)}$$

where  $\rho$  is charge density,  $\underline{E}$  is electric field strength and  $\epsilon_0$  is the S.I. vacuum permittivity.

In the standard model:

$$\underline{E} = -\frac{\partial \underline{A}}{\partial t} - c \underline{\nabla} A^0 \quad \text{--- (5)}$$

2) For electrostatics:

$$\frac{\partial A}{\partial t} = 0 \quad - (6)$$

So eq. (4) is:

$$\underline{\nabla} \cdot \underline{\nabla} A^0 = -\frac{\rho}{\epsilon_0} \quad - (7)$$

In the standard model therefore the H atom spectrum is described by the Poisson equation (7) combined with the Schrödinger equation (1). This description is adequate for off-resonant situations, as when the separation of ECE theory is very small.

In ECE theory eq. (7) is replaced by:

$$\underline{\nabla} \cdot \underline{\nabla} A^{0a} + \frac{1}{c} \frac{\partial}{\partial t} (\underline{\nabla} \cdot \underline{A}^a) + \underline{\nabla} \cdot (\underline{\omega}^{0a} \underline{A}^b) - \underline{\nabla} \cdot (\underline{\omega}^a \underline{A}^{0b}) = -\mu_0 \tilde{J}^{0a} \quad - (8)$$

In a quasi-electrostatic approximation eq. (8) reduces (Notes 59(4)) to:

$$\nabla^2 A^{0a} - \underline{\omega}^a \cdot \underline{\nabla} A^{0b} - (\underline{\nabla} \cdot \underline{\omega}^a) A^{0b} = -\mu_0 \tilde{J}^{0a} \quad - (9)$$

i.e.

$$\boxed{\nabla^2 A^{0a} = -\mu_0 \tilde{J}^{0a} + (\underline{\omega}^a \cdot \underline{\nabla} A^{0b} + (\underline{\nabla} \cdot \underline{\omega}^a) A^{0b})} \quad - (10)$$

3) Comparison of eqn. (7) and (10) shows that the standard model Coulomb law is perturbed by the spin correction term  $\underline{\omega}^{ab} \cdot \underline{\nabla} A^{ob} + (\underline{\nabla} \cdot \underline{\omega}^{ab}) A^{ob}$ . If the charge density term  $\tilde{J}^{oa}$  is of the type:

$$\tilde{J}^{oa} = \tilde{J}^{oa}(0) \cos(\underline{k} \cdot \underline{r}) \quad - (11)$$

resonance may occur in the potential  $A^{oa}$  and if the potential energy in eq. (2). If this energy exceeds 13.6 eV, the H atom may break apart into an electron and a proton.

If the perturbation due to the spin correction is small the system may still be considered to be spherically symmetric as in the usual development of the H atom problem. In the usual development the Schrodinger equation is:

$$-\frac{\hbar^2}{2\mu} \nabla^2 \psi - \frac{e^2}{4\pi\epsilon_0 r} \psi = E \psi \quad - (12)$$

In spherical polar coordinates: - (13)

$$\frac{1}{r} \frac{d^2}{dr^2} r\psi + \frac{1}{r^2} \Lambda^2 \psi + \frac{\mu e^2}{2\pi\epsilon_0 \hbar^2 r} \psi = -\frac{2\mu E}{\hbar^2} \psi$$

The angular part of the solution are the spherical

4) harmonics  $Y(\theta, \phi)$ , so:

$$\psi(r, \theta, \phi) = R(r)Y(\theta, \phi) \quad - (14)$$

Now use:

$$\Lambda^2 Y = -l(l+1)Y \quad - (15)$$

$$\Rightarrow \frac{1}{r} \frac{d^2}{dr^2} rRY - \frac{1}{r^2} l(l+1)RY + \frac{\mu e^2}{2\pi\epsilon_0 \hbar^2 r} RY = - \frac{2\mu E}{\hbar^2} RY \quad - (16)$$

which is of the form:

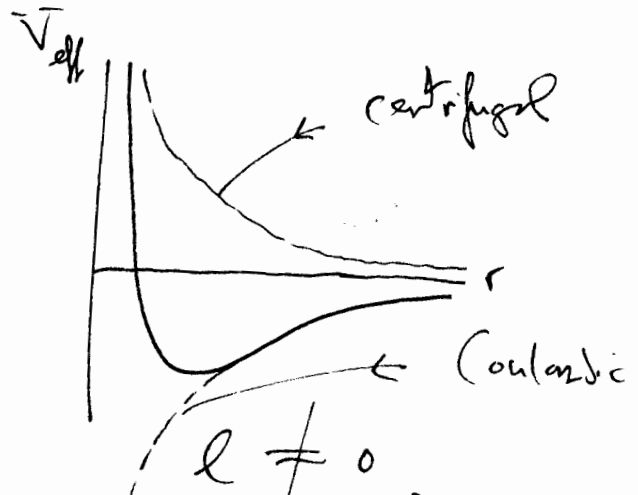
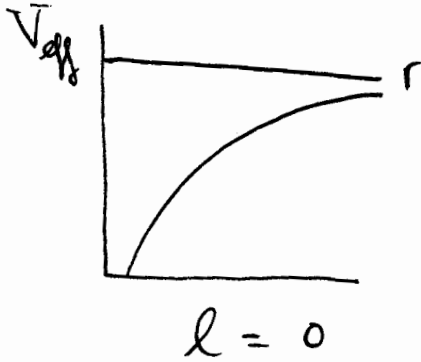
$$\frac{d^2 P}{dr^2} + \frac{2\mu}{\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0 r} - \frac{l(l+1)\hbar^2}{2\mu r^2} \right) P = - \frac{2\mu E}{\hbar^2} P \quad - (17)$$

This is equivalent to the use of an effective potential:

$$\boxed{V_{\text{eff}} = \frac{-e^2}{4\pi\epsilon_0 r} + \frac{l(l+1)\hbar^2}{2\mu r^2}} \quad - (18)$$

The first part of the RHS of eq. (18) is the attractive Coulombic force and the second part is the repulsive centrifugal force. For  $l=0$  the electron

5) has no angular momentum and there is no motion to send it away from the nucleus. For  $l \neq 0$  the centrifugal motion may dominate:



The solutions of the radial equation (17) are the associated Laguerre functions (Atkins p. 72). For bound states  $E$  is negative, for unbound states  $E$  is positive.

Therefore we wish to investigate the effect of resonance from eq. (10) in producing transitions from bound states to unbound states. This process frees the electron from the proton, i.e. dissociates the H atom. By substituting the radial wavefunctions of H into the radial equation (17) the energy levels of the H atom are given:

$$E = -\frac{\mu e^4}{32\pi^2 \epsilon_0^2 \hbar^2} \frac{1}{n^2} \quad (19)$$

6) Here  $n = 0, 1, 2, \dots$  is the principal quantum number of H. The energy depends only on  $n$ . As  $n \rightarrow \infty$ ,  $E \rightarrow 0$ . These features are true if and only if the Coulomb potential is used. With the use of resonance, the ECE theory these well known atomic spectral features of H may be affected.

The complete atomic orbitals of H are:

$$\psi_{nlm_l}(r, \theta, \phi) = R_{nl}(r) Y_{lm_l}(\theta, \phi) \quad (20)$$

Orbitals with  $l = 0$  are s orbitals, those with  $l = 1$  are p orbitals, those with  $l = 2$  are d orbitals, those with  $l = 3$  are f orbitals etc. These well known orbitals are all determined by the Coulomb law (7), and will all be changed by the ECE law (10). The

level corresponding to  $n$  is  $n^2$ -fold degenerate in H.

If a potential other than the Coulomb is used, this degeneracy is lifted. This is a way of investigating the effect of the spin correction on the H spectra.

The states in eqn. (20) are the bound states. The ionization energy of H is the

7) Difference between the lowest energy level,  $n=1$ , and the highest,  $n=\infty$ . This is:

$$\Delta E = \frac{\mu e^4}{32\pi^2 \epsilon_0^2 \hbar^2} = 2.2 \times 10^{-18} \text{ J} = 13.6 \text{ eV} \quad \text{--- (21)}$$

This corresponds to a potential energy of 13.6 eV for a bound electron to be removed to infinity. This is the ionization potential. If an electron is given more than that energy (e.g. by collision with a cosmic ray particle) its state is an unbound state. The unbound states of H correspond to an energy greater than  $\Delta E$  in eq. (21). These are the unquantized continuum states. In these unbound states ( $E > 0$ ):

$$R \sim \exp\left(\pm i \left(\frac{2\mu E}{\hbar^2}\right)^{1/2} r\right) \quad \text{--- (22)}$$

and there are travelling waves.

### Mathematical Task

This is to calculate the effect of the positive term  $\underline{\omega}^a \cdot \underline{\nabla} A^{ab} + (\underline{\nabla} \cdot \underline{\omega}^a) A^{ab}$  or the orbital of the H atom. At resonance the positive term dominates and the H atom breaks apart. There will be an extra positive term on the RHS of eqn. (18),

8) The ECE Coulomb Law is of the form:

$$\nabla \cdot \underline{E}^a = \epsilon \mu_0 \underline{J}^{oa} \quad (23)$$

but the presence of the positive terms on the RHS of eq. (10) (the repulsive spi connection terms) will change the Coulomb attraction into a Coulomb repulsion, thus breaking part of the H atom at resonance. The negative part of eq. (18) will become less negative but the analytical form of eq. (18) will remain the same to a first approximation. More generally the details of the H atom will depend on the analytical modelling of the spi connection and of the driving term  $-\mu_0 \underline{J}^{oa}$ .

The numerical problem is to solve eq. (10) simultaneously with eq. (1), deriving the Hamiltonian from eq. (10), and not from the usual eq. (7).

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