

ATOMIC AND MOLECULAR WAVE FUNCTIONS IN THE PRESENCE OF
GRAVITATION.

by

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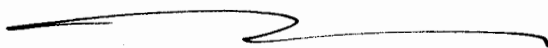
(www.aias.us, www.webarchive.org.uk, www.upitec.org, www.atomicprecision.com,

www.et3m.net)

ABSTRACT

The energy levels of the H atom are shown to be shifted by a constant amount due to the gravitational interaction between the proton of the atom and the earth's mass. The effect is about 1% of the electrostatic interaction between the proton and the electron. This constant shift has no effect on the atomic spectrum of the H atom because the spectrum is due to transitions in which the gravitational term cancels out. However, gravitation produces a set of novel wave functions which can be used to characterize any atom or molecule, or any material matter, thus introducing a new branch of computational quantum chemistry.

Keywords: ECE theory in the non relativistic quantum limit, novel wave functions in the presence of gravitation.

UFT 305


1. INTRODUCTION.

In recent papers of this series {1 - 10} it has been shown that the Planck / Einstein / de Broglie quantum theory (the "old quantum theory") predicts the experimentally discovered Evans / Morris shifts. The latter are colour changes produced by a sample in absorption or emission, and are describe in comprehensive detail on the blog of www.aias.us. So the Evans / Morris shifts provide a severe new test of the quantum theory. During the investigation of the Balmer $n = 2$ to $n = 3$ transitions of atomic H it was found that the energy degeneracy was lifted by the Evans / Morris effects, so that the single absorption line is split into several lines of different frequency. So it is of interest to try to investigate these shifts experimentally with high accuracy. In consequence of this interesting splitting of the H spectrum. Section 2 investigates the effect of gravitation on the H atom, in the first instance the effect of the earth's gravitational field. As usual this paper should be read in conjunction with its background notes posted with UFT305 on www.aias.us Section 3 gives a direct graphical comparison of the gravity affected radial wave functions with the usual radial wave functions of the H atom. The gravity affected wave functions are entirely new to science, despite being an outcome of the Schroedinger equation of the mid twenties.

2. GRAVITY AFFECTED RADIAL WAVE FUNCTIONS

The Schroedinger equation in the presence of the earth's gravitational field is:

$$\left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{4\pi \epsilon_0 r} + V_1 \right) \psi = E \psi \quad (1)$$

where

$$V_1 = -\frac{m_2 M G}{R} \quad (2)$$

is the gravitational potential between the proton of mass m_2 and the earth of mass M . Here R is the radius of the earth and G is Newton's constant. The gravitational effect on the electron is much smaller because the electron mass is much smaller than that of the proton. In the accompanying notes it is shown the gravitational effect of the electron on the proton is entirely negligible.

In Eq. (1), m is the mass of the electron, an excellent approximation to the reduced mass of electron and proton, e is the charge in the proton, ϵ_0 is the vacuum permittivity in S. I. units, and r is the distance between the electron and the proton. In Eq.

(1) ψ is the non relativistic wave function and E the total energy. On the classical level:

$$H = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} + V_1 \quad (3)$$

where H is the hamiltonian and \underline{p} the linear momentum. The transition from Eq. (3) to Eq.

(4) is made with the quantum postulate of Schroedinger:

$$\underline{p} \psi = -i\hbar \underline{\nabla} \psi \quad (4)$$

The expectation value of the total energy is defined by the Born method:

$$\begin{aligned} \langle E \rangle &= \int \psi^* E \psi d\tau \\ &= \int \psi^* \left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} + V_1 \right) \psi d\tau \\ &= - \left(\frac{m e^4}{32\pi^2 \epsilon_0^2 \hbar^2} \right) \frac{1}{n^2} - \frac{m_2 M G}{R} \quad (5) \end{aligned}$$

in which the integration is over the volume element $d\tau$.

Eq. (5) means that the gravitational interaction between the proton and the earth's mass produces a shift of about 1% in the well known energy levels of the H atom. So this is what is really being observed in a laboratory at sea level. This shift depends on altitude as measured by R and on the mass M. In supermassive stars of small radius it can be very large. However it does not affect the atomic spectrum of H because the spectrum depends on transitions between n, for example the n = 2 to n = 3 Balmer line of H studied in UFT304. In these transitions, the gravitational potential is constant and cancels out. So gravitation has no effect on the atomic spectrum. This result is a test of the quantum theory. An H spectrum in a satellite should be the same as an H spectrum on the earth's surface. The H spectrum is, however, affected by the fundamentally important Evans Morris shifts, of which the cosmological red shift is now known to be an example.

Eq. (1), however, gives important new information about the H atom and indeed any atom or molecule in a gravitational field. This can be shown straightforwardly as follows.

Write the potential term in Eq. (1) as:

$$\frac{e^2}{4\pi\epsilon_0 r_1} = \frac{e^2}{4\pi\epsilon_0 r} + \sqrt{V_1} \quad - (6)$$

thus defining a new radial coordinate:

$$\frac{1}{r_1} = \frac{1}{r} + \alpha \quad - (7)$$

where:

$$\alpha = \frac{4\pi\epsilon_0 \cdot m_2 M G}{e^2 R} = 4.5346 \times 10^8 \text{ m}^{-1} \quad - (8)$$

using the earth's mass and radius. Therefore:

$$r_1 = \frac{r}{1 + \alpha r} \quad - (9)$$

Consider the Schrodinger equation in the coordinate system (r_1, θ, ϕ) . It is:

$$\left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{4\pi\epsilon_0 r_1} \right) \psi_{11} = E_1 \psi_{11} \quad (10)$$

so:

$$\langle E_1 \rangle = - \left(\frac{me^4}{32\pi^2 \epsilon_0^2 \hbar^2} \right) \frac{1}{n^2} \quad (11)$$

These are the well known energy levels of the H atom, where n is the principal quantum number.

The use of the coordinate system (r_1, θ, ϕ) produces the hydrogenic energy levels (11) in the presence of a gravitational field. The effect of gravitation has been subsumed into the electrostatic potential defined by Eq. (6).

The wavefunctions of Eq. (10) are:

$$\psi(r_1, \theta, \phi) = R(r_1) Y(\theta, \phi) \quad (12)$$

where Y are the spherical harmonics and where the radial wavefunctions are:

$$R_{nl}(r_1) = \left(\frac{2Z}{na} \right) \left[\frac{(n-l-1)!}{[2n(n+l)!]^3} \right] \rho_1^l L_{n+l}^{2l+1}(\rho_1) \exp\left(-\frac{\rho_1}{2}\right) \quad (13)$$

Here Z is the atomic number, a the Bohr radius:

$$a = \frac{4\pi\epsilon_0 \hbar^2}{me^2} = 5.29177 \times 10^{-11} \text{ m} \quad (14)$$

and L are the modified Laguerre polynomials. In Eq. (13):

$$\rho_1 = \left(\frac{2Z}{na} \right) r_1. \quad (15)$$

The energy expectation values in the coordinate system (r_1, θ, ϕ) are defined by:

$$\begin{aligned} \langle E_1 \rangle &= \int \psi_1^* E_1 \psi_1 d\tau \\ &= \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \int_{r_1=0}^{\infty} \psi_1^* E_1 \psi_1 r_1^2 \sin\theta dr_1 d\theta d\phi \quad (16) \end{aligned}$$

Therefore the effect of gravitation is to replace r of the usual Schrodinger equation:

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} - \frac{e^2}{4\pi\epsilon_0 r} \right) \psi = E \psi \quad (17)$$

by r_1 defined by Eq. (9). This procedure gives the same energy levels (11) from both Eq. (10) and Eq. (17), but the wave functions (ψ_1) are different. They are gravitationally affected wave functions. They are expressed in terms of r_1 in Eq. (13), but can be expressed in terms of r using Eq. (9). When expressed in terms of r the gravitationally affected wavefunctions can be compared with the usual radial wavefunctions from Eq. (17). The usual (or free) radial wavefunctions of the H atom are given by Eq. (13) with r_1 replaced by r . The gravitationally affected wave functions are given by Eq. (13) with r_1 replaced by $r / (1 + xr)$. They are compared directly in Section 3.

$$R_{nl}(r)$$

This finding initiates a new research area of gravitationally modified computational quantum chemistry, in which the gravitationally affected wave functions of

any atom or molecule can be computed using highly developed numerical methods and code packages.

The first few radial wavefunctions from Eq. (10) are as follows. In the H. atom the atomic number Z is unity.

For the 1s orbital, $n = 1, l = 0$:

$$R_{10}(r) = \left(\frac{1}{a}\right)^{3/2} \exp\left(-\frac{\rho_1}{2}\right) \quad - (18)$$

where:

$$\rho_1 = \frac{2Z}{na} \left(\frac{r}{1+\alpha r}\right) \quad - (19)$$

For the 2s orbital, $n = 2, l = 0$:

$$R_{20}(r) = \left(\frac{1}{a}\right)^{3/2} \left(\frac{1}{2\sqrt{2}}\right) (2 - \rho_1) \exp\left(-\frac{\rho_1}{2}\right) \quad - (20)$$

For the 2p orbital, $n = 2, l = 1$:

$$R_{21}(r) = \left(\frac{1}{a}\right)^{3/2} \left(\frac{1}{2\sqrt{6}}\right) \rho_1 \exp\left(-\frac{\rho_1}{2}\right) \quad - (21)$$

For the 3s orbital, $n = 3, l = 0$:

$$R_{30}(r) = \left(\frac{1}{a}\right)^{3/2} \left(\frac{1}{9\sqrt{3}}\right) (6 - 6\rho_1 + \rho_1^2) \exp\left(-\frac{\rho_1}{2}\right) \quad - (22)$$

For the 3p orbital, $n = 3, l = 1$:

$$R_{31}(r) = \left(\frac{1}{a}\right)^{3/2} \left(\frac{1}{9\sqrt{6}}\right) (4 - \rho_1) \rho_1 \exp\left(-\frac{\rho_1}{2}\right) \quad - (23)$$

For the 3d orbital, $n = 3, l = 2$:

$$R_{32}(r) = \left(\frac{1}{a}\right)^{3/2} \left(\frac{1}{9\sqrt{30}}\right) \rho_1^2 \exp\left(-\frac{\rho_1}{2}\right) \quad - (24)$$

Atomic and molecular wave functions in the presence of gravitation

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3 Graphical comparison of gravitationally affected and free radial orbitals of H

The hydrogenic wave functions (18-24) have been calculated with the coordinate ρ_1 defined in Eq.(15) which contains the correction due to gravitational effects. For convenience we use atomic units where for example the Bohr radius is unity. Then of Eq.(8) amounts to

$$x = 4.53 \cdot 10^8 \text{ m}^{-1} = 0.024 \text{ a.u.} \quad (25)$$

The inverse of x is 41.7 Bohr radii which is only slightly above atomic dimensions. Therefore the effects are clearly visible in the graph of the wave functions. In Figs. 1-3 the 3s, 3p and 3d radial wave functions are graphed. The undistorted wave functions are those for $x = 0$. The gravitational field contribution of the proton leads to a significant broadening of wave functions ($x = 0.024$). The other two examples ($x = 0.07$, $x = 0.18$) lead to a qualitatively different behaviour, there is no asymptotic convergence to the zero line, i.e. the wave functions are not normalizable and no valid solutions of the Schrödinger equation anymore. Even for small x , the normalization must be computed anew. This is only possible numerically because the normalization integrals with r_1 are not analytically solvable.

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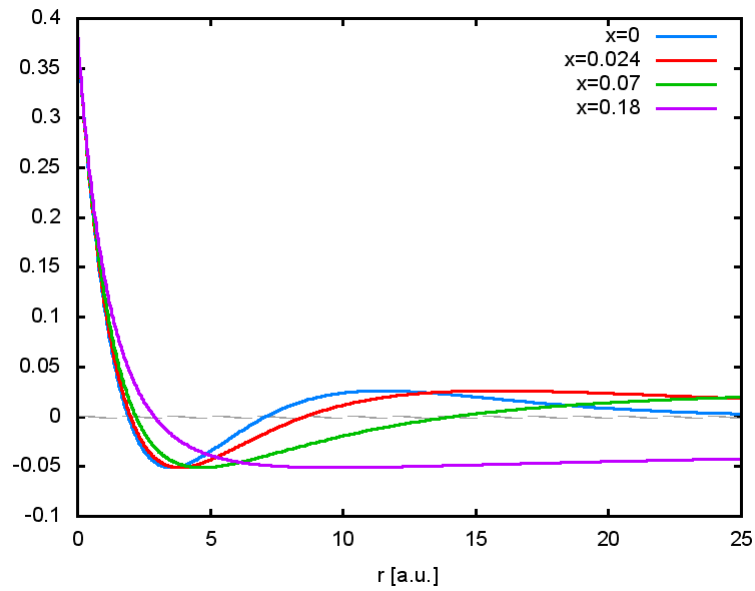


Figure 1: Hydrogenic wave function with different gravitational distortions x , state $3s$.

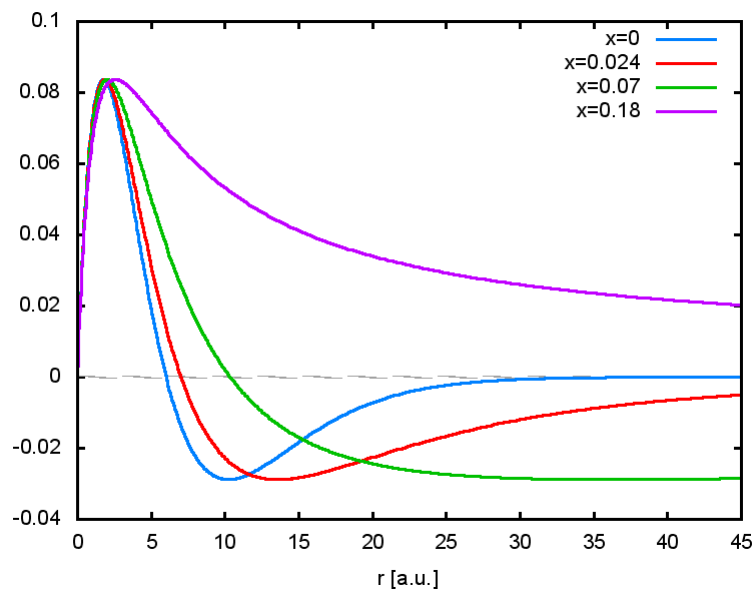


Figure 2: Hydrogenic wave function with different gravitational distortions x , state $3p$.

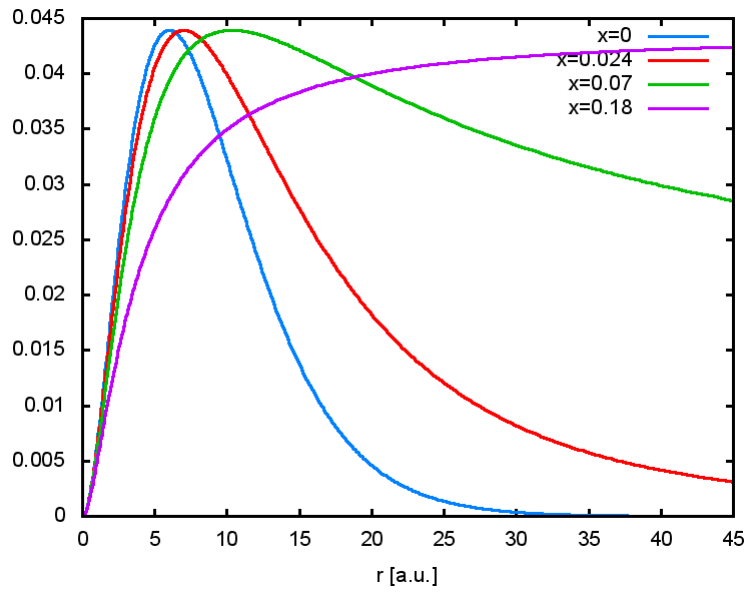


Figure 3: Hydrogenic wave function with different gravitational distortions x , state 3d.

3. GRAPHICAL COMPARISON OF GRAVITATIONALLY AFFECTED AND FREE RADIAL ORBITALS OF H

Section by Dr. Horst Eckardt

ACKNOWLEDGMENTS

The British Government is thanked for a Civil List Pension, and the staff of AIAS for many interesting discussions. Dave Burleigh is thanked for posting, Alex Hill for translation and broadcasting, and Robert Cheshire for broadcasting.

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