DESCRIPTION OF SPIN ORBIT INTERACTION WITH x THEORY AND WITH ECKARDT QUANTIZATION.

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ABSTRACT

Spin orbit interaction and atomic fine structure in atomic hydrogen is described with two and three dimensional x theory, in which the extension of the non relativistic to the relativistic theory is achieved by transforming the elliptical description of the dynamics in x theory to a precessing elliptical description. A fully self consistent description requires a three dimensional lagrangian and hamiltonian expressed in spherical polar coordinates and relativistic quantum mechanics emerges when the angles of the spherical polar system are multiplied by the precession factor x. In Eckardt quantization this is an integer, the Eckardt quantum number.

Keywords: ECE theory, x theory spin orbit interaction, fine structure of atomic hydrogen.

UFT 268

1. INTRODUCTION

In recent papers of this series {1 - 10} the x theory has been developed to give a self consistent description of well known phenomena on all scales in physics and chemistry. These include planetary precession, electromagnetic deflection due to gravitation, photon mass theory, the gravitational time delay, gravitational red shift, the ubiquitous Thomas precession, and the Bohr and Sommerfeld theories of quantum mechanics. The origin of planetary precession has been shown to be ubiquitous Thomas precession, which occurs on all scales, from galactic to atomic. The parent ECE theory of x theory has been shown to give a satisfactory description of the basics of a whirlpool galaxy, notably its velocity curve and hyperbolic stellar orbits. All this has been achieved with a simple elliptical theory. The ellipse precesses when the angles of the spherical polar coordinate system are multiplied by the precession factor x. The latter has been analyzed in terms of the ubiquitous Thomas precession. Eckardt quantization is defined for integral x, a process which produces de Broglie wave structure superimposed on the ellipse. The precession and wave structure are examples of conical section theory with the angle multiplied by x. In previous papers of this series {1 - 10} on www.aias.us these patterns have been referred to as fractal conical sections. For x close to unity the ellipse precesses, but as it becomes larger the wave patterns appear. If x is defined as the integer n the number of waves superimposed on the ellipse is n. In the preceding paper the x theory was extended to Schroedinger quantization.

In Section 2 the x theory is applied to describe spin orbit coupling and the fine structure of atomic hydrogen (H). The background notes accompanying this paper should be read as an intrinsic part of the development of this paper. This paper itself (UFT268) gives a brief description of the main results. The first background note accompanying UFT268 on www.aias.us calculates the energy levels of the H atom by evaluating the expectation value of the hamiltonian for the first few hydrogenic wavefunctions using hand calculations and computer algebra. It is shown that expectation values of $\cos\phi$ and $\cos\theta$ are zero for all the hydrogenic wavefunctions, where ϕ and θ are the angles of the spherical polar coordinate system. The second background note 268(2) derives the elliptical orbit from the classical hamiltonian describing the interaction of an electron and proton using plane polar coordinates. This is an approximation to the three dimensional hamiltonian in which spherical polar coordinates are used. A fully consistent three dimensional theory is developed in note 268(9) and is described in Section 2 of this paper. The plane polar coordinates are sufficient for planetary orbits in a plane, but are clearly an approximation to the problem of orbitals in atomic hydrogen. The atomic orbitals are three dimensional and quantized. Planetary orbits are two dimensional, classical and planar. Various expectation values of relevance are computed for the first few hydrogenic wavefunctions and the results discussed in Section 3.

Note 268(3) begins the development of spin orbit interaction theory from x theory by first applying Schroedinger quantization to the classical non relativistic hamiltonian in a plane. There are two principal planes, defined by the two angles of the spherical polar coordinate system. Various relevant expectation values were found to be different for the two types of ellipse. The basic hypothesis of this paper is that relativistic quantum theory is defined by a precessing ellipse, arguing in analogy with the 1915 Sommerfeld theory of the atom, the first relativistic quantum theory described in immediately preceding UFT papers. The precessing ellipse produces a relativistic hamiltonian operator which is developed in this note. In note 268(4) expectation values are developed from the fermion equation {1 - 10}, the chiral Dirac equation of ECE theory, and prepared for comparison with note 268(3). Some details are given of the spin orbit hamiltonian and complete details in note 268(8) together with a description of the approximations used. Note 268(5) develops the theory further with a Bohr type quantization for the classical angular momentum. In a fully consistent theory, reached in Note 268(9), a Schroedinger type quantization is used with a three dimensional hamiltonian expressed in spherical polar coordinates.

In note 268(6) the Bohr quantization is replaced by a Schroedinger quantization in the planar approximation using the phi ellipse (the ellipse in the angle ϕ of the spherical polar coordinate system). This model is compared with the experimental results for p orbital spin orbit splitting in atomic hydrogen and x found to be close to unity as in the theory of orbital precession. The origin of x is the ubiquitous Thomas precession, which is therefore a universal phenomenon occurring at all scales in the universe. This theory is described briefly in Section 2 of this paper but is still a rough approximation. It is developed further in Note 268(7) and some remarks given on Eckardt quantization in the context of this planar elliptical approximation. For ease of reference Note 268(8) gives a complete description of the derivation of the spin orbit hamiltonian from the fermion equation, a derivation that includes some very rough approximations made by Dirac and others but which produces a range of important results as is well known. These include the g factor of the electron without radiative corrections, the Landé factor, the Thomas half factor, ESR, NMR and MRI. Finally in Note 268(9) the completed three dimensional theory is developed, and it is shown that the relevant ellipse is the theta ellipse, which appears as a well defined part of the three dimensional theory.

2. DEVELOPMENT OF THE PLANAR PHI ELLIPTICAL APPROXIMATION AND THE THREE DIMENSIONAL THEORY.

As described in previous papers on x theory in the UFT section of www.aias.us the hamiltonian for the planar phi approximation to relativistic quantum mechanics is:

$$H\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{x^2 k}{r} + \frac{(x^2-1)L^2}{2mr^2} \right)\psi \quad -(1)$$

where $\hbar$ is the reduced Planck constant, m the mass of the electron, L the orbital angular momentum, r the distance between the electron and the proton in the H atom and ψ the hydrogenic wave function. The constant k is:

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

where -e is the charge on the electron and ϵ_0 the S. I. vacuum permittivity. The Schroedinger quantization:

$$L^2\psi = l(l+1)\hbar^2\psi \quad -(3)$$

is assumed a priori, although for Eq. (1) to be rigorously applicable a three dimensional theory is needed as developed later in this Section. As shown in all detail in Note 268(8) the hamiltonian from the fermion equation {1 - 10} of relativistic quantum mechanics is:

$$(E - mc^2)\psi = \left(-\frac{\hbar^2\nabla^2}{2m} - \frac{k}{r} + E_{so} \right)\psi \quad -(4)$$

so x can be found in this rough phi planar approximation by equating the right hand sides of

Eqs. (1) & (4). It follows that:

$$E_{so} = (x^2 - 1) V_{eff} \quad -(5)$$

where V_{eff} is the well known effective potential of the Schroedinger equation {1 - 10}:

$$V_{eff} = -\frac{e^2}{4\pi\epsilon_0 r} + \frac{\ell(\ell+1)\hbar^2}{2mr^2}. \quad -(6)$$

This phi planar theory is a first approximation but it is self consistent, because for

$$x = 1 \quad -(7)$$

the theory is non relativistic quantum mechanics, in which there is no spin orbit coupling:

$$E_{so} = 0 \quad -(8)$$

from Eq. (5). Therefore x can be calculated from:

$$\langle E_{so} \rangle = \frac{e^2\hbar^2}{8\pi\epsilon_0 m^2 c^2} \left(j(j+1) - \ell(\ell+1) - s(s+1) \right) \left\langle \frac{1}{r^3} \right\rangle$$

$$= (1 - x^2) \left(\frac{e^2}{4\pi\epsilon_0} \left\langle \frac{1}{r} \right\rangle - \frac{\ell(\ell+1)\hbar^2}{2m} \left\langle \frac{1}{r^2} \right\rangle \right). \quad -(9)$$

For self consistency the expectation values must be calculated numerically for each hydrogenic wavefunction using:

$$\left\langle \frac{1}{r^n} \right\rangle = \int \psi^* \frac{1}{r^n} \psi \, d\tau, \quad -(10)$$

$$\frac{1}{r} = \frac{1}{\alpha} \left(1 + \epsilon \cos(x\theta) \right). \quad -(11)$$

In these expressions the half right latitude and the ellipticity are given by:

$$\alpha = \frac{L^2}{mk} = \frac{4\pi\epsilon_0 \ell(\ell+1)\hbar^2}{me^2} \quad -(12)$$

and:

$$\epsilon^2 = 1 + \frac{2EL^2}{mk^2} = 1 - \frac{\ell(\ell+1)}{n^2}. \quad -(13)$$

Here n is the principal quantum number, and:

$$\ell = 0, 1, 2, \ldots, n-1. \quad -(14)$$

The j quantum number is defined by the Clebsch Gordan series:

$$j = \ell + s, \ell + s - 1, \ldots, |\ell - s| \quad -(15)$$

where s is the spin quantum number.

For the 2p orbital of H:

$$j = 3/2 \text{ or } j = 1/2. \quad -(16)$$

If:

$$j = 3/2, \ \ell = 1, \ s = 1/2 \quad -(17)$$

then

$$\langle E_{so} \rangle_{3/2} = \frac{e^2\hbar^2}{8\pi\epsilon_0 m^2 c^2} \left\langle \frac{1}{r^3} \right\rangle \quad -(18)$$

and if:

$$j = 1/2,\ l = 1,\ s = 1/2 \quad -(19)$$

then:

$$\langle E_{so} \rangle = -\frac{e^2 \hbar^2}{4\pi \epsilon_0 m^2 c^2} \left\langle \frac{1}{r^3} \right\rangle. \quad -(20)$$

The observed splitting is therefore:

$$\langle E_{so} \rangle_{3/2} - \langle E_{so} \rangle_{1/2} = \frac{3}{8\pi} \frac{e^2 \hbar^2}{\epsilon_0 m^2 c^2} \left\langle \frac{1}{r^3} \right\rangle$$

$$= 7.25 \times 10^{-24}\ J = 0.365\ cm^{-1} \quad -(21)$$

where:

$$(1 - x^2)\left(\frac{e^2}{4\pi \epsilon_0} \left\langle \frac{1}{r} \right\rangle - \frac{\hbar^2}{m} \left\langle \frac{1}{r^2} \right\rangle \right) = 7.25 \times 10^{-24}. \quad -(22)$$

and:

$$\left\langle \frac{1}{r} \right\rangle = \int \psi_{2p}^* \frac{1}{\alpha} \left(1 + \epsilon \cos(x\phi)\right) \psi_{2p}\, d\tau \quad -(23)$$

with:

$$\left\langle \frac{1}{r^2} \right\rangle = \int \psi_{2p}^* \frac{1}{\alpha^2} \left(1 + \epsilon \cos(x\phi)\right)^2 \psi_{2p}\, d\tau. \quad -(24)$$

Eq. (21) is solved numerically in Section 3 to give x very close to unity. Clearly if x were exactly unity there would be no spin orbit splitting.

This result appears to suggest that x is a ubiquitous factor because its order of magnitude in planetary precession and the fine structure of atomic hydrogen is similar. This conclusion is consistent with the fact that x is due to the ubiquitous Thomas precession as shown in preceding papers on x theory. Despite this self consistent conclusion however a fully correct theory must be three dimensional, and this is developed next.

The classical hamiltonian is:

$$H = E = \frac{p^2}{2m} - \frac{k}{r} \quad -(25)$$

which in two dimensions for a planar orbit gives:

$$\frac{1}{r} = \frac{1}{\alpha}\left(1 + \epsilon\cos\phi\right) \quad -(26)$$

where:

$$\alpha = \frac{L^2}{mk}, \quad \epsilon^2 = 1 + \frac{2EL^2}{mk^2}. \quad -(27)$$

The Schroedinger quantization of Eq. (25) means

$$H\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{k}{r}\right)\psi. \quad -(28)$$

The Bohr radius is:

$$r_B = \frac{4\pi\epsilon_0\hbar^2 n^2}{me^2} \quad -(29)$$

so

$$E = \langle H \rangle = -\frac{\hbar^2}{2mr_B^2} \quad -(30)$$

and

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{r_B}. \quad -(31)$$

The ϕ ellipse gives the expectation values:

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{\alpha} \left\langle 1 + \epsilon \cos\phi \right\rangle = \frac{1}{\alpha} = \frac{1}{r_B} \quad -(32)$$

for all hydrogenic orbitals with:

$$\langle \cos\phi \rangle = 0 \quad -(33)$$

for all orbitals. Therefore:

$$\langle \alpha \rangle = \alpha = r_B \quad -(34)$$

for all orbitals. From Eqs. (27) and (34):

$$\langle L^2 \rangle = mk\, r_B = n^2 \hbar^2 \quad -(35)$$

for all orbitals. This means that:

$$\langle \epsilon^2 \rangle = 1 - \frac{k}{r_B} \frac{mk r_B}{mk^2} = 0 \quad -(36)$$

in the non relativistic planar phi ellipse approximation the classical ϵ^2 is non-zero in general but its expectation value is zero. The planar phi ellipse is a consequence of the planar kinetic energy, whereas the three dimensional kinetic energy is:

$$T = \frac{1}{2} m \left(\left(\frac{dr}{dt}\right)^2 + r^2 \left(\frac{d\theta}{dt}\right)^2 + r^2 \sin^2\theta \left(\frac{d\phi}{dt}\right)^2 \right) \quad -(37)$$

which originates from the fact that the linear velocity in spherical polar coordinates is:

$$\underline{v} = \dot{r}\, \underline{e}_r + r\dot{\theta}\, \underline{e}_\theta + r\sin\theta\, \dot{\phi}\, \underline{e}_\phi . \quad -(38)$$

So the lagrangian in three dimensions is:

$$\mathcal{L} = T - V = \frac{1}{2} m \left(\dot{r}^2 + r^2 \dot{\theta}^2 + r^2 \sin^2\theta \, \dot{\phi}^2 \right) + \frac{k}{r} \qquad -(39)$$

The lagrangian variables are r, θ and ϕ and there are three Euler Lagrange equations.

1) The equation

$$\frac{\partial \mathcal{L}}{\partial r} = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{r}} \qquad -(40)$$

gives:

$$m\ddot{r} = mr \left(\dot{\theta}^2 + \sin^2\theta \, \dot{\phi}^2 \right) - \frac{k}{r^2} . \qquad -(41)$$

2) The equation

$$\frac{\partial \mathcal{L}}{\partial \theta} = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\theta}} \qquad -(42)$$

gives:

$$mr^2 \sin\theta \cos\theta \, \dot{\phi}^2 = \frac{d}{dt} \left(mr^2 \dot{\theta} \right) \qquad -(43)$$

and the angular momentum:

$$L_1 = mr^2 \dot{\theta} . \qquad -(44)$$

3) The equation:

$$\frac{\partial \mathcal{L}}{\partial \phi} = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\phi}} \qquad -(45)$$

gives

$$\frac{d}{dt} \left(mr^2 \dot{\phi} \sin^2\theta \right) = 0 \qquad -(46)$$

and the constant angular momentum:

$$L_2 = mr^2 \dot{\phi} \sin^2\theta. \quad -(47)$$

So the two angular velocities are:

$$\dot{\theta} = \frac{d\theta}{dt} = \frac{L_1}{mr^2} \quad -(48)$$

and

$$\dot{\phi} = \frac{d\phi}{dt} = \frac{L_2}{mr^2 \sin^2\theta} \quad -(49)$$

Therefore

$$m\frac{d^2 r}{dt^2} = \frac{L^2}{mr^3} - \frac{k}{r^2} \quad -(50)$$

where the total angular momentum is:

$$L^2 = L_1^2 + \frac{L_2^2}{\sin^2\theta} \quad -(51)$$

The total classical L^2 in three dimensions is quantized as:

$$L^2 \psi = \ell(\ell+1)\hbar^2 \psi \quad -(52)$$

as is well known.

Eq. (50) is now transformed into a Binet equation using:

$$\frac{d}{d\theta}\left(\frac{1}{r}\right) = -\frac{1}{r^2}\frac{dr}{d\theta} = -\frac{1}{r^2}\frac{dr}{dt}\frac{dt}{d\theta} \quad -(53)$$

in which $d\theta/dt$ is defined by Eq. (48):

$$\frac{dt}{d\theta} = \frac{mr^2}{L_1} \quad - (54)$$

So:

$$\frac{d}{d\theta}\left(\frac{1}{r}\right) = -\frac{m}{L_1}\frac{dr}{dt} \quad - (55)$$

and

$$\frac{d^2}{d\theta^2}\left(\frac{1}{r}\right) = -\frac{m}{L_1}\frac{d}{d\theta}\frac{dr}{dt}. \quad - (56)$$

Now use:

$$\frac{df}{d\theta} = \frac{dt}{d\theta}\frac{df}{dt} \quad - (57)$$

so:

$$\frac{d^2}{d\theta^2}\left(\frac{1}{r}\right) = -\frac{m^2}{L_1^2} r^2 \frac{d^2 r}{dt^2} \quad - (58)$$

and:

$$m\frac{d^2 r}{dt^2} = -\frac{L_1^2}{mr^2}\frac{d^2}{d\theta^2}\left(\frac{1}{r}\right). \quad - (59)$$

Eq. (44) therefore becomes the three dimensional Binet equation:

$$F = -\frac{k}{r^2} = -\frac{L_1^2}{mr^2}\left(\frac{d^2}{d\theta^2}\left(\frac{1}{r}\right) + \frac{1}{r}\right) - \frac{L_2^2}{mr^3 \sin^2\theta} \quad - (60)$$

The relevant ellipse is therefore:

$$\frac{1}{r} = \frac{1}{\alpha_1}\left(1 + \epsilon_1 \cos\theta\right) \quad - (61)$$

in which:

$$\alpha_1 = \frac{L_1^2}{mk}, \quad \epsilon_1^2 = 1 + \frac{2E_1 L_1^2}{mk^2} \quad - (62)$$

and:

$$E_1 = \frac{1}{2} m \left(\frac{dr}{dt} \right)^2 + \frac{L_1^2}{mr^3} \quad -(63)$$

The hamiltonian is:

$$\begin{aligned} H &= \frac{1}{2} m \left(\dot{r}^2 + r^2 \dot{\theta}^2 + r^2 \sin^2\theta \, \dot{\phi}^2 \right) - \frac{k}{r} \\ &= \frac{1}{2} m \dot{r}^2 + \frac{L_1^2}{2mr^2} + \frac{L_2^2}{2mr^2 \sin^2\theta} - \frac{k}{r} \\ &= \frac{p^2}{2m} - \frac{k}{r} \quad -(64) \end{aligned}$$

and upon quantization

$$H\psi = -\frac{\hbar^2}{2m} \nabla^2 \psi - \frac{k}{r} \psi \quad -(65)$$

where:

$$\nabla^2 \psi = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2 \psi}{\partial \phi^2} \quad -(66)$$

In the H atom:

$$\begin{aligned} -\frac{\hbar^2}{2m} \langle \nabla^2 \psi \rangle &= -\frac{\hbar^2}{2m} \int \psi^* \nabla^2 \psi \, d\tau \\ &= \frac{me^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} \quad -(67) \end{aligned}$$

and the total energy levels are:

$$E = \langle H \rangle$$
$$= \left\langle \frac{p^2}{2m} \right\rangle - \left\langle \frac{k}{r} \right\rangle \quad -(68)$$
$$= \frac{me^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} - \frac{me^4}{16\pi^2 \epsilon_0^2 \hbar^2 n^2}$$

In order to introduce relativistic effects the angle θ is changed to $x\theta$. The ellipse (61) becomes

$$\frac{1}{r} = \frac{1}{\alpha_1}\left(1 + \epsilon_1 \cos(x\theta)\right) \quad -(69)$$

and the energy levels are changed to:

$$E = -\frac{\hbar^2}{2m}\langle \nabla^2 \psi \rangle - k\left\langle \frac{1}{r} \right\rangle \quad -(70)$$

where:

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{\alpha_1}\left\langle 1 + \epsilon_1 \cos(x\theta) \right\rangle \quad -(71)$$

and
$$\langle \nabla^2 \psi \rangle = \int \psi^* \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial \psi}{\partial r} \right) d\tau$$
$$+ \int \psi^* \left(\frac{1}{r^2 \sin(x\theta)} \frac{\partial}{\partial (x\theta)} \left(\sin(x\theta) \frac{\partial \psi}{\partial (x\theta)} \right) \right) d\tau$$
$$+ \int \psi^* \left(\frac{1}{r^2 \sin^2(x\theta)} \frac{\partial^2 \psi}{\partial \phi^2} \right) d\tau \quad -(72)$$

in which:

$$\int \psi^* \left(\frac{1}{r^2 \sin(x\theta)} \frac{\partial}{\partial (x\theta)} \left(\sin(x\theta) \frac{\partial \psi}{\partial (x\theta)} \right) \right) d\tau$$
$$= \frac{1}{x^2} \int \frac{\psi^*}{r^2 \sin(x\theta)} \frac{\partial}{\partial \theta} \left(\sin(x\theta) \frac{\partial \psi}{\partial \theta} \right) d\tau \quad -(73)$$

It is also possible to evaluate the effect of x on Eq. (67):

$$\left\langle \frac{p^2}{2m} \right\rangle = \left\langle \frac{p_r^2}{2m} \right\rangle + \frac{L_1^2}{2m} \left\langle \frac{1}{r^2} \right\rangle + \frac{L_2^2}{2m} \left\langle \frac{1}{r^2 \sin^2\theta} \right\rangle \quad -(74)$$

by using:

$$\theta \rightarrow x\theta \quad -(75)$$

So:

$$\left\langle \frac{p_r^2}{2m} \right\rangle = -\frac{\hbar^2}{2m} \int \psi^* \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) d\tau ,$$

$$\left\langle \frac{1}{r^2} \right\rangle = -\frac{\hbar^2}{2m} \int \psi^* \frac{1}{r^2} \psi \, d\tau , \quad -(76)$$

$$\left\langle \frac{1}{r^2 \sin^2(x\theta)} \right\rangle = -\frac{\hbar^2}{2m} \int \psi^* \frac{1}{r^2 \sin^2(x\theta)} \psi \, d\tau$$

and:

$$\left\langle \frac{k}{r} \right\rangle = k \int \psi^* \frac{1}{r} \psi \, d\tau \quad -(77)$$

The final hydrogenic energy levels are changed to:

$$E = \left(\left\langle \frac{p^2}{2m} \right\rangle - \left\langle \frac{k}{r} \right\rangle \right)_x \quad -(78)$$

and can be compared with results from atomic fine structure such as spin orbit interaction.

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Description of spin orbit interaction with x theory and with Eckardt quantization

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3 Calculation of expectation values

The parameters of the ellipse, Eqs.(12,13), are in atomic units (with Schroedinger quantization):

$$\alpha = \frac{L^2}{mk} = l(l+1), \tag{79}$$

$$\epsilon = \sqrt{1 + \frac{2\,E\,L^2}{mk^2}} = \sqrt{1 - \frac{l(l+1)}{n^2}} \tag{80}$$

The elliptic orbits for the precessing ϕ and θ ellipse are:

$$r_\phi = \frac{\alpha}{1+\epsilon\cos(x\phi)}, \tag{81}$$

$$r_\theta = \frac{\alpha}{1+\epsilon\cos(x\theta)}. \tag{82}$$

The spin orbit splitting is given by Eq.(9) and is in a.u.:

$$\langle E_{so}\rangle = (1-x^2)\left(\left\langle\frac{1}{r}\right\rangle - \frac{l(l+1)}{2}\left\langle\frac{1}{r^2}\right\rangle\right). \tag{83}$$

The expectation values $\langle E_{so}\rangle$ have been calculated according to this equation for the ϕ and θ ellipse. The results with Hydrogen orbitals for the ϕ ellipse are given in Table 1. The corresponding values for the θ ellipse are highly complicated and not shown. As expected, there is no splitting for s states. The x dependence of the splitting has been graphed in Fig. 1 for 2p states of Hydrogen orbitals. The splitting is classified according to non-relativistic quantum numbers. The realistic range is a very small interval around $x = 1$ where the splitting is exactly zero due to the factor $1-x^2$ in the results. Eckardt quatization requires $x = 2, 3, ...$ which is completely out of spin orbit splitting range and is in the order of energy splitting of principal quantum numbers.

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As an example we compare the 2p 1/2 - 2p 3/2 splitting of Hydrogen with the experimental value and calculate the corresponding x value for this splitting. The experimental splitting is given by

$$\Delta E = 0.365 \text{ cm}^{-1} = 4.52542695 \cdot 10^{-5} \text{ eV}. \tag{84}$$

This is very small but detectable. We calculated the corresponding theoretical value first by standard theory and then by x theory. To obtain the value of Schroedinger/Dirac theory we used the first formula of Eq.(9) which involves the j quantum numbers and the expectation value $< 1/r^3 >$. For this expectation value we had to insert the usual r coordinate, not an ellipse. The result coincides with the above experimental value within 10^{-8} eV which is excellent agreement.

For computing the splitting with x theory we have to find the experimentally correct value of x. From Eq.(9) or (83), respectively, we obtain a function of $f(x)$ which must be equal to the experimental value, i.e. we have to solve

$$f(x) - \Delta E = 0 \tag{85}$$

which is a numerical root finding problem. The results for both ellipses are given in Table 2. The deviation from unity is of order 10^{-6} and extremely small, therefore not visible in Fig. 1. The values differ slightly according to ellipse and non-relativistic orbital type.

The other calculations refer to the relativistic effects introduced by the x factor in the total energy calculations from Eq.(70) onward. The r coordinate has to be replaced by the precessing ϕ or θ ellipse. The expectation value (71),

$$\left\langle \frac{1}{r} \right\rangle = \int \psi^* \frac{1}{r} \psi \, d\tau, \tag{86}$$

will be discussed later. In Eqs.(72,73) the kinetic energy operator has been decomposed according to its radial and angular parts:

$$\langle \nabla^2 \rangle = \langle (\nabla^2)_1 \rangle + \langle (\nabla^2)_2 \rangle + \langle (\nabla^2)_3 \rangle \tag{87}$$

with

$$\langle (\nabla^2)_1 \rangle = \int \psi^* \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) d\tau, \tag{88}$$

$$\langle (\nabla^2)_2 \rangle = \frac{1}{x^2} \int \psi^* \frac{1}{r^2 \sin(x\theta)} \frac{\partial}{\partial \theta} \left(\sin(x\theta) \frac{\partial \psi}{\partial \theta} \right) d\tau, \tag{89}$$

$$\langle (\nabla^2)_3 \rangle = \int \psi^* \frac{1}{r^2 \sin^2(x\theta)} \frac{\partial^2 \psi}{\partial \phi^2} \, d\tau. \tag{90}$$

The expectation values for the ϕ ellipse are given in Table 3. For the 1s state they vanish. The analytical solutions - although existing - are partially so complicated that it makes no sense to display them. The same data are presented for the θ ellipse in Table 4. They are even more complicated, and no analytical solutions exist for the θ and ϕ components of kinetic energy.

The last group of formula evaluations refers to the semi-classical results (74-78). For the ϕ ellipse, these are manageable, as far as analytical solutions exist (Table 5). For the θ ellipse they become more complicated again, see Table 6. The expectation values of $< k/r >$ which also appear in Eq.(70) as mentioned before, also depend on x as expected. For a non-precessing ellipse the result would simply be $1/\alpha_1$.

n	l	m_l	E_{so}
1	0	0	0
2	0	0	0
2	1	0,±1	$\left(1-x^2\right)\left(\frac{k\left(\frac{\sin(2\,\pi\,x)}{\sqrt{2}}+2\,\pi\,x\right)}{4\,\pi\,a_0\,x}-\frac{\hbar^2\left(\frac{\sin(4\,\pi\,x)}{2}+2^{\frac{5}{2}}\,\sin(2\,\pi\,x)+10\,\pi\,x\right)}{32\,\pi\,a_0^2\,m\,x}\right)$
3	0	0	0
3	1	0,±1	$\left(1-x^2\right)\left(\frac{k\left(\frac{\sqrt{7}\sin(2\,\pi\,x)}{3}+2\,\pi\,x\right)}{4\,\pi\,a_0\,x}-\frac{\hbar^2\left(\frac{7\sin(4\,\pi\,x)}{9}+\frac{8\,\sqrt{7}\sin(2\,\pi\,x)}{3}+\frac{100\,\pi\,x}{9}\right)}{32\,\pi\,a_0^2\,m\,x}\right)$

Table 1: x-dependent spin orbit splitting for Hydrogen, ϕ ellipse.

exp. value of orbit	x
ϕ ellipse, $m_l = 0, \pm 1$	1.00000147920
θ ellipse, $m_l = 0$	1.00000158486
θ ellipse, $m_l = \pm 1$	1.00000123266

Table 2: x value for 2p 1/2 - 2 p 3/2 spin orbit splitting of Hydrogen.

n	l	m	$<(\nabla^2)_1>$	$<(\nabla^2)_2>$	$<(\nabla^2)_3>$
0	0	0	0	0	0
1	0	0	$-\frac{3\,(\sin(4\,\pi\,x)+8\sin(2\,\pi\,x)+12\,\pi\,x)}{16\,\pi\,\alpha_1^2\,x}$	0	0
1	1	0	$-\frac{\frac{\sin(4\,\pi\,x)}{2}+2^{\frac{5}{2}}\,\sin(2\,\pi\,x)+10\,\pi\,x}{16\,\pi\,\alpha_1^2\,x}$	no solution	0
1	1	±1	$\frac{\frac{\sin(4\,\pi\,x)}{2}+2^{\frac{5}{2}}\,\sin(2\,\pi\,x)+10\,\pi\,x}{16\,\pi\,\alpha_1^2\,x}$	no solution	no solution

Table 3: Contributions of energy expectation values for ϕ ellipse, Eqs.(70-73).

n	l	m	$<(\nabla^2)_1>$	$<(\nabla^2)_2>$	$<(\nabla^2)_3>$
0	0	0	0	0	0
1	0	0	$\frac{3\left(x^2\,\cos(2\,\pi\,x)-\cos(2\,\pi\,x)+16\,x^2\,\cos(\pi\,x)-4\cos(\pi\,x)-24\,x^4+47\,x^2-11\right)}{8\,\alpha_1^2\,(x-1)\,(x+1)\,(2\,x-1)\,(2\,x+1)}$	no solution	no solution
2	0	0	very complicated	no solution	no solution
2	1	0	very complicated	no solution	no solution
2	1	±1	very complicated	no solution	no solution

Table 4: Contributions of energy expectation values for θ ellipse, Eqs.(70-73).

n	l	m	$< p_r^2/2m >$
0	0	0	0
1	0	0	$\frac{3\,\hbar^2\,(\sin(4\,\pi\,x)+8\sin(2\,\pi\,x)+12\,\pi\,x)}{32\,\pi\,\alpha_1^2\,m\,x}$
1	1	0	$\frac{\hbar^2\,\left(\frac{\sin(4\,\pi\,x)}{2}+2^{\frac{5}{2}}\,\sin(2\,\pi\,x)+10\,\pi\,x\right)}{32\,\pi\,\alpha_1^2\,m\,x}$
1	1	±1	$\frac{\hbar^2\,\left(\frac{\sin(4\,\pi\,x)}{2}+2^{\frac{5}{2}}\,\sin(2\,\pi\,x)+10\,\pi\,x\right)}{32\,\pi\,\alpha_1^2\,m\,x}$
n	l	m	$< 1/r^2 >$
0	0	0	$-\frac{\hbar^2\,(\sin(4\,\pi\,x)+8\sin(2\,\pi\,x)+12\,\pi\,x)}{16\,\pi\,\alpha_1^2\,m\,x}$
1	0	0	$-\frac{\hbar^2\,(\sin(4\,\pi\,x)+8\sin(2\,\pi\,x)+12\,\pi\,x)}{16\,\pi\,\alpha_1^2\,m\,x}$
1	1	0	$-\frac{\hbar^2\,\left(\frac{\sin(4\,\pi\,x)}{2}+2^{\frac{5}{2}}\,\sin(2\,\pi\,x)+10\,\pi\,x\right)}{16\,\pi\,\alpha_1^2\,m\,x}$
1	1	±1	$-\frac{\hbar^2\,\left(\frac{\sin(4\,\pi\,x)}{2}+2^{\frac{5}{2}}\,\sin(2\,\pi\,x)+10\,\pi\,x\right)}{16\,\pi\,\alpha_1^2\,m\,x}$
n	l	m	$< 1/r^2\sin^2(x\theta) >$
0	0	0	no solution
1	0	0	no solution
1	1	0	no solution
1	1	±1	no solution
n	l	m	$< k/r >$
0	0	0	$\frac{k\,(\sin(2\,\pi\,x)+2\,\pi\,x)}{2\,\pi\,\alpha_1\,x}$
1	0	0	$\frac{k\,(\sin(2\,\pi\,x)+2\,\pi\,x)}{2\,\pi\,\alpha_1\,x}$
1	1	0	$\frac{k\,\left(\frac{\sin(2\,\pi\,x)}{\sqrt{2}}+2\,\pi\,x\right)}{2\,\pi\,\alpha_1\,x}$
1	1	±1	$\frac{k\,\left(\frac{\sin(2\,\pi\,x)}{\sqrt{2}}+2\,\pi\,x\right)}{2\,\pi\,\alpha_1\,x}$

Table 5: Contributions to classical expectation values for ϕ ellipse, Eqs.(76-78).

n	l	m	$< p_r^2/2m >$
0	0	0	0
1	0	0	$-\frac{3\,\hbar^2\left(x^2\cos(2\,\pi\,x)-\cos(2\,\pi\,x)+16\,x^2\cos(\pi\,x)-4\cos(\pi\,x)-24\,x^4+47\,x^2-11\right)}{16\,\alpha_1^2\,m\,(x-1)\,(x+1)\,(2\,x-1)\,(2\,x+1)}$
1	1	0	very complicated
1	1	± 1	very complicated
n	l	m	$< 1/r^2 >$
0	0	0	$\frac{\hbar^2\left(x^2\cos(2\,\pi\,x)-\cos(2\,\pi\,x)+16\,x^2\cos(\pi\,x)-4\cos(\pi\,x)-24\,x^4+47\,x^2-11\right)}{8\,\alpha_1^2\,m\,(x-1)\,(x+1)\,(2\,x-1)\,(2\,x+1)}$
1	0	0	$\frac{\hbar^2\left(x^2\cos(2\,\pi\,x)-\cos(2\,\pi\,x)+16\,x^2\cos(\pi\,x)-4\cos(\pi\,x)-24\,x^4+47\,x^2-11\right)}{8\,\alpha_1^2\,m\,(x-1)\,(x+1)\,(2\,x-1)\,(2\,x+1)}$
1	1	0	very complicated
1	1	± 1	very complicated
n	l	m	$< 1/r^2 \sin^2(x\theta) >$
0	0	0	no solution
1	0	0	no solution
1	1	0	no solution
1	1	± 1	no solution
n	l	m	$< k/r >$
0	0	0	$-\frac{k\left(\cos(\pi\,x)-2\,x^2+3\right)}{2\,\alpha_1\,(x-1)\,(x+1)}$
1	0	0	$-\frac{k\left(\cos(\pi\,x)-2\,x^2+3\right)}{2\,\alpha_1\,(x-1)\,(x+1)}$
1	1	0	$-\frac{k\left(\frac{3\,x^2\cos(\pi\,x)}{\sqrt{2}}-\frac{9\cos(\pi\,x)}{\sqrt{2}}-2\,x^4+\frac{3\,x^2}{\sqrt{2}}+20\,x^2-\frac{9}{\sqrt{2}}-18\right)}{2\,\alpha_1\,(x-3)\,(x-1)\,(x+1)\,(x+3)}$
1	1	± 1	$\frac{k\left(\frac{9\cos(\pi\,x)}{\sqrt{2}}+2\,x^4-20\,x^2+\frac{9}{\sqrt{2}}+18\right)}{2\,\alpha_1\,(x-3)\,(x-1)\,(x+1)\,(x+3)}$

Table 6: Contributions to classical expectation values for θ ellipse, Eqs.(76-78).

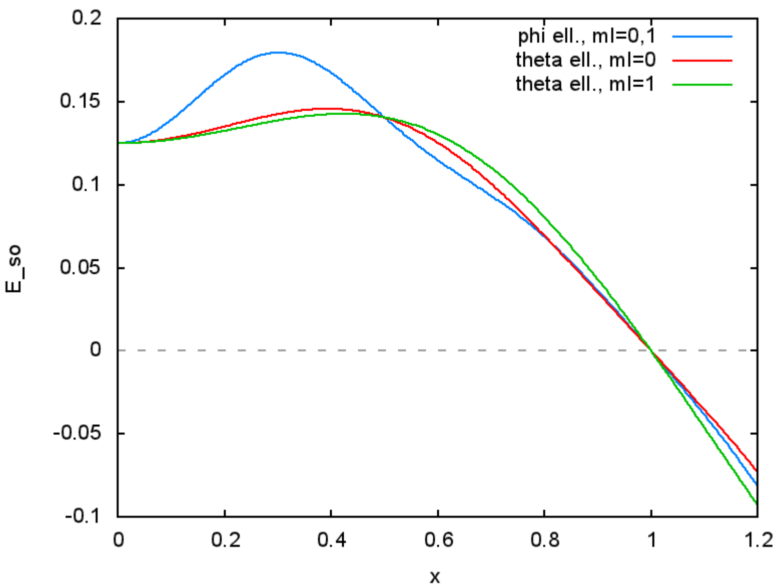

Figure 1: Spin orbit splitting of Hydrogen 2p orbitals for ϕ and θ ellipse (a.u.).