

A NEW SCHROEDINGER EQUATION FROM THREE DIMENSIONAL ORBIT  
THEORY

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ABSTRACT

The theory of three dimensional orbits us used to produce a new type of Schroedinger equation that characterizes computational quantum physics and chemistry in an entirely new way. The new Schroedinger equation is derived from the beta conic section equivalent to the classical hamiltonian of three dimensional orbit theory in which the kinetic energy is described with spherical polar coordinates.

Keywords: EEC theory, 3D orbit theory, new Schroedinger equation.

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## 1. INTRODUCTION

Recently in this series of two hundred and seventy seven papers to date it has been shown that orbit theory is in general three dimensional {1 - 10}, requiring the use of spherical polar coordinates in the kinetic energy of the classical hamiltonian. The main result of the three dimensional orbit theory is that precession of the perihelion can be described classically without recourse to relativity. It has been shown that the classical hamiltonian is exactly equivalent to the three dimensional conic sections, which have far richer properties than the planar conic sections of the four hundred year old theory of orbits. In Section 2 the three dimensional conic sections are used to deduce a new Schroedinger equation for computational quantum physics and chemistry. This is a new fundamental equation which can be applied to any situation to which the traditional Schroedinger equation can be applied, so is of vast potential applicability. In Section three some discussion is given of the likely numerical methods needed to solve the new Schroedinger equation. This paper should be read in conjunction with notes 277(1) to 277(4) on [www.aias.us](http://www.aias.us), where more details are given.

## 2. THE NEW SCHROEDINGER EQUATION.

Consider the classical hamiltonian of three dimensional orbit theory:

$$H = E = \frac{p^2}{2m} + U(r) \quad - (1)$$

where:

$$\frac{p^2}{2m} = \frac{1}{2} m v^2 = \frac{1}{2} m (\dot{r}^2 + r^2 \dot{\beta}^2) \quad - (2)$$

and

$$U(r) = -\frac{k}{r} \quad - (3)$$

In these equations a mass  $m$  orbits a mass  $M$ . The attraction potential (3) gives the well known inverse square law of attraction. The momentum  $p$  and velocity  $v$  are defined by:

$$v^2 = \dot{r}^2 + r^2 \dot{\beta}^2 \quad - (4)$$

where  $r$  is the distance between  $m$  and  $M$ , and where

$$k = m M G \quad - (5)$$

where  $G$  is Newton's constant. The angle  $\beta$  is defined in terms of the spherical polar coordinate system  $(r, \theta, \phi)$  by:

$$\dot{\beta}^2 = \dot{\theta}^2 + \dot{\phi}^2 \sin^2 \theta. \quad - (6)$$

This hamiltonian can be transferred directly to atomic and molecular theory by redefining  $k$  as:

$$k = \frac{e^2}{4\pi \epsilon_0} \quad - (7)$$

where  $e$  is the charge on the proton and where  $\epsilon_0$  is the vacuum permittivity in S. I. units.

The quantization condition is:

$$-i \hbar \nabla \psi = p \psi \quad - (8)$$

where  $\hbar$  is the reduced Planck constant and  $\psi$  is the wavefunction. So the Schrodinger equation is:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi = (E - U) \psi = T \psi = \frac{1}{2} m (\dot{r}^2 + r^2 \dot{\beta}^2) \psi \quad - (9)$$

where  $T$  is the kinetic energy and where  $E$  is the total energy. Therefore the Schrodinger

equation is the well known equation:

$$\hat{H}\psi = E\psi \quad - (10)$$

where  $\hat{H}$  is the hamiltonian operator.

It has been shown in immediately preceding papers of this series {1 - 10} that the classical hamiltonian (  $\hat{H}$  ) is rigorously equivalent to the three dimensional conic sections:

$$r = \frac{\alpha}{1 + \epsilon \cos \beta} \quad - (11)$$

where  $\alpha$  is the half right latitude and  $\epsilon$  the eccentricity. These are defined by:

$$\alpha = \frac{L^2}{mk} \quad - (12)$$

and

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

where  $L$  is the magnitude of the total angular momentum. From a lagrangian analysis  $L$  is the constant of motion:

$$L = mr^2 \dot{\beta} = mr^2 \frac{d\beta}{dt} \quad - (14)$$

and is a conserved quantity. The other conserved quantity is the total energy  $E$ . Using:

$$\frac{dr}{dt} = \frac{dr}{d\beta} \frac{d\beta}{dt} \quad - (15)$$

the kinetic energy can be expressed as:

$$T = \frac{L^2}{2mr^4} \left( \left( \frac{dr}{d\beta} \right)^2 + r^2 \right) \quad - (16)$$

where:

$$\frac{dr}{d\beta} = -\frac{\epsilon r^2}{\alpha} \sin \beta \quad - (17)$$

from Eq. ( 11 ). It follows that the classical kinetic energy is:

$$T = \frac{1}{2} \frac{L^2}{md^2} (1 + \epsilon^2 + 2\epsilon \cos \beta) \quad - (18)$$

Eqs. ( 9 ) and ( 18 ) give an entirely new formulation of the Schrodinger equation:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi = (E - U) \psi = \frac{L^2}{2md^2} (1 + \epsilon^2 + 2\epsilon \cos \beta) \psi \quad - (19)$$

and a new computational quantum physics and chemistry.

In atoms and molecules:

$$\alpha = \frac{L^2}{m\hbar} = \frac{4\pi \epsilon_0 L^2}{me^2} \quad - (20)$$

and particular examples of Eq. ( 19 ) can be discussed as follows. The particle on a sphere is given by:

$$U = 0, \quad \epsilon = 0, \quad \alpha = r \quad - (21)$$

so Eq. ( 19 ) reduces to:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi = E \psi = \frac{L^2}{2md^2} \psi \quad - (22)$$

which can be written as:

$$-\frac{\hbar^2}{r^2} \Delta^2 \psi = \frac{L^2}{r^2} \psi \quad (23)$$

where  $\Delta^2$  is the laplacian. The latter operates on the spherical harmonics  $Y$  as follows:

$$\Delta^2 Y = -l(l+1)Y \quad (24)$$

Using:

$$r = a \quad (25)$$

and

$$\Delta^2 \psi = -l(l+1)\psi \quad (26)$$

it follows that:

$$L^2 = l(l+1)\hbar^2 \quad (27)$$

which is the well known expression for the square of orbital angular momentum in quantum theory. Therefore the particle on a sphere is generated from the spherical conic section in which the ellipticity vanishes. There is no potential energy in the particle on a sphere. It is a hypothetical exercise which shows the origin of Eq. ( 27 ) in the three dimensional conic sections.

The Bohr atom is generated by:

$$E = 0, \quad U = -\frac{k}{r} \quad (28)$$

and is therefore generated from the spherical conic section with the Coulomb law between

proton and electron. In the Bohr atom:

$$\alpha = r \quad - (29)$$

and the Bohr quantization is:

$$L = n\hbar \quad - (30)$$

where  $n$  is the Bohr quantum number. This is related to Schrodinger quantization by:

$$n^2 = l(l+1) \quad - (31)$$

In general, Eq. (19) is:

$$\begin{aligned} -\frac{\hbar^2}{2m} \nabla^2 \psi &= (E - U) \psi \\ &= \frac{me^4}{32\pi^2 \epsilon_0^2 L^2} (1 + \epsilon^2 + 2\epsilon \cos\beta) \psi \end{aligned} \quad - (32)$$

Therefore the energy levels of the H atom are given by:

$$\hat{H}\psi = E\psi = \left[ \frac{me^4 (1 + \epsilon^2 + 2\epsilon \cos\beta)}{32\pi^2 \epsilon_0^2 L^2} - \frac{\hbar^2}{r} \right] \psi \quad - (33)$$

It follows that:

$$\left\langle \frac{me^4 (1 + \epsilon^2 + 2\epsilon \cos\beta)}{32\pi^2 \epsilon_0^2 L^2} \right\rangle = \frac{me^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} \quad - (34)$$

where  $n$  in Eq. (34) denotes the principal quantum number. Therefore:

$$\langle L^2 \rangle = \frac{n^2 \hbar^2}{1 + \epsilon^2 + 2\epsilon \cos \beta} \quad - (35)$$

and when:

$$\epsilon = 0 \quad - (36)$$

Eq. (35) reduces to the Bohr quantization:

$$\langle L^2 \rangle = n^2 \hbar^2 \quad - (37)$$

so the principal quantum number  $n$  can be identified in this limit with the Bohr quantum number. Conversely the Bohr quantization is generalized to Eq. (35), which is a completely new expression of the Schroedinger equation.

In general the new computation quantum physics and chemistry are characterized by the expectation value:

$$\langle \cos \beta \rangle = \int \psi^* \cos \beta \psi \, d\tau \quad - (38)$$

where

$$\begin{aligned} \cos \beta &= \frac{\cos \phi}{\left( \cos^2 \phi + \left( \frac{L_z}{L} \right)^2 \sin^2 \phi \right)^{1/2}} \\ &= \left( 1 - \left( \frac{1}{1 - \left( \frac{L_z}{L} \right)^2} \right) \cos^2 \theta \right)^{1/2} \quad - (39) \end{aligned}$$

Here  $L_z$  is the Z component of L. Computational methods are needed to evaluate these expectation values and this is discussed further in Section 3.



### 3. COMPUTATIONAL METHODS

By Dr. Horst Eckardt.

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