

THREE DIMENSIONAL AND QUANTUM ORBITS FROM ECE2:
LAGRANGIAN QUANTUM MECHANICS

by

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ABSTRACT

The Euler Lagrange theory of three dimensional and quantum orbits is developed using spherical polar coordinates. A new quantum mechanics of atoms and molecules is developed from the lagrangian, and shown to give the correct hydrogenic wavefunctions. The advantage of Lagrangian quantum mechanics is that it can be developed for all atoms and molecules in a straightforward way. This theory is the same for ECE2 and the standard model of physics.

Keywords: ECE2 theory, three dimensional and quantum orbits, Lagrangian quantum mechanics.

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1. INTRODUCTION

In recent papers of this series {1-12} the Lagrangian theory of the gyroscope has been developed in various ways. It has been shown that the Lagrangian theory is part of Cartan geometry and therefore of ECE2 generally covariant unified field theory. The spin connection of Cartan geometry has been defined for all coordinate systems in three dimensions, and the method can be developed in many ways. In Section 2 the method is applied to the theory of three dimensional orbits, and a new Lagrangian quantum mechanics developed and tested for correctness with the analytically known hydrogenic wave functions. Lagrangian quantum mechanics can be developed computationally for all atoms and molecules by solving sets of Euler Lagrange equations simultaneously with numerical methods. The theory is applied to spherical orbits, thus developing UFT270 ff. with numerical methods.

This paper is a short synopsis of extensive calculations found in the notes accompanying UFT371 on www.aias.us. Notes 371(1) to 371(3) define the spherical polar coordinates and Euler angles that can be used in the three dimensional theory of orbits. Note 371(4) defines a scheme of computation of spherical orbits using the spherical polar coordinates as the proper Lagrange variables. The three Euler Lagrange equations are solved simultaneously with Maxima and the results discussed in Section 3 of this paper. Note 371(5) defines the lagrangian for the planar orbit produced by ECE2 relativity. In this case there two proper Lagrange variables defined by the plane polar coordinates. Notes 371(6) to 371(8) develop Lagrangian quantum mechanics and show that the spherical orbits quantize to hydrogenic wavefunctions whose potential energy is defined by the attraction between a mass m orbiting a mass M in three dimensions.

2. LAGRANGIAN QUANTUM MECHANICS AND THREE DIMENSIONAL ORBITS

The lagrangian for three dimensional orbits is:

$$\mathcal{L} = \frac{1}{2} m \underline{v} \cdot \underline{v} - U(r) \quad - (1)$$

where m is the mass of an object orbiting a mass M , and where \underline{v} is its velocity. The potential energy of attraction between m and M is the gravitational potential:

$$U(r) = -\frac{mMg}{r} \quad - (2)$$

where G is Newton's constant and \underline{r} the vector joining m and M in the spherical polar coordinate system:

$$\begin{aligned} X &= r \sin\theta \cos\phi \\ Y &= r \sin\theta \sin\phi \\ Z &= r \cos\theta. \end{aligned} \quad - (3)$$

In this coordinate system the lagrangian (UFT270 ff) is:

$$\mathcal{L} = \frac{1}{2} m \left(\dot{r}^2 + r^2 (\dot{\theta}^2 + \dot{\phi}^2 \sin^2\theta) \right) + \frac{mMg}{r} \quad - (4)$$

and the proper Lagrange variables are r , θ and ϕ . There are three Euler

Lagrange equations:

$$\frac{\partial \mathcal{L}}{\partial r} = \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{r}} \right) \quad - (5)$$

$$\frac{\partial \mathcal{L}}{\partial \theta} = \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\theta}} \right) \quad - (6)$$

$$\frac{\partial \mathcal{L}}{\partial \phi} = \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}} \right) \quad - (7)$$

which must be solved simultaneously for the various orbits possible. This solution is carried out numerically using Maxima, and the results are described in Section 3, using graphical material. It is clear that an orbit must be three dimensional in general. Under certain circumstances it may seem to be planar, or it may have evolved to what seems to be a planar orbit. The existence of three dimensional orbits can be investigated using advanced astronomical methods. There are many more features of three dimensional orbits than of two dimensional orbits. Some of these have been discussed analytically in UFT270 to UFT276. However, the computational method allows many advances to be made. Some of these are described and graphed on Section 3.

It is known from UFT270 to UFT276 that the three dimensional orbit can be analyzed by defining the proper Lagrange variable β through the equation:

$$\dot{\beta}^2 = \dot{\theta}^2 + \dot{\phi}^2 \sin^2 \theta. \quad - (8)$$

The three dimensional lagrangian becomes:

$$\mathcal{L} = \frac{1}{2} m (\dot{r}^2 + r^2 \dot{\beta}^2) + \frac{mMG}{r} \quad - (9)$$

and there are two Euler Lagrange equations:

$$\frac{\partial \mathcal{L}}{\partial r} = \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{r}} \right) \quad - (10)$$

and

$$\frac{\partial \mathcal{L}}{\partial \beta} = \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\beta}} \right) \quad - (11)$$

giving the result:

$$r = \frac{d}{1 + \epsilon \cos \beta} \quad - (12)$$

which is a conic section in β . Here d is the half right latitude and ϵ is the eccentricity.

The Euler Lagrange equation (11) gives the result:

$$\dot{\beta} = \frac{L}{mr^2} \quad - (13)$$

where the angular momentum L is a constant of motion, i.e.:

$$\frac{dL}{dt} = 0. \quad - (14)$$

This theory can be applied to the quantum mechanics of atoms and molecules, for example the hydrogen atom in which the potential between the electron and the proton is the Coulomb potential (1 - 12):

$$U = -\frac{e^2}{4\pi\epsilon_0 r}. \quad - (15)$$

The magnitude of the charge on the electron of mass m is e and ϵ_0 is the vacuum permittivity in S. I. Units.

The classical velocity of the electron is:

$$v^2 = \left(\frac{dr}{dt}\right)^2 + r^2 \left(\frac{d\beta}{dt}\right)^2. \quad - (16)$$

Using:

$$\frac{dr}{dt} = \frac{dr}{d\beta} \frac{d\beta}{dt}, \quad - (17)$$

$$\frac{d\beta}{dt} = \frac{L}{mr^2} \quad - (18)$$

and Eq. (12) it is found as in Note 371(7) that:

$$p^2 = \frac{L^2}{a} \left(\frac{2}{r} - \frac{1}{a} \right) \quad - (19)$$

where p is the electron momentum. Here:

$$a = \frac{d}{1 - \epsilon^2} \quad - (20)$$

is the semi major axis of the conic section (12). Quantization is defined by the well known Schroedinger procedure:

$$-\hbar^2 \nabla^2 \psi = p^2 \psi \quad - (21)$$

Therefore the radial wavefunction $\psi(r)$ of Lagrangian quantum mechanics is defined

by:

$$\nabla^2 \psi = \frac{\partial^2 \psi}{\partial r^2} + \frac{2}{r} \frac{\partial \psi}{\partial r} = -\frac{L^2}{\hbar^2 a} \left(\frac{2}{r} - \frac{1}{a} \right) \psi \quad - (22)$$

Some results for $\psi(r)$ are graphed in Section 3.

The complete wavefunctions of the hydrogen (H) atom are :

$$\psi = \underbrace{\psi(r)}_{RY} \psi(\theta, \phi) \quad - (23)$$

where Y are the well known spherical harmonics {1-12}. The laplacian in spherical polar coordinates is:

$$\begin{aligned} \nabla^2 \psi &= \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\psi}{dr} \right) + \frac{1}{r^2 \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\psi}{d\theta} \right) \\ &+ \frac{1}{r^2 \sin^2 \theta} \frac{d^2 \psi}{d\phi^2} \quad - (24) \\ &:= \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\psi}{dr} \right) + \frac{1}{r^2} \Delta^2 \psi \end{aligned}$$

in which:

$$\Delta^2 Y = -l(l+1)Y \quad - (25)$$

where l is an integer, the angular momentum quantum number. It follows that Eq. (21)

can be developed as:

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) - \frac{l(l+1)}{r^2} R + \frac{2L^2}{2\pi^2 \epsilon_0 r} = \frac{L^2 R}{a_0^2 \hbar^2} \quad - (26)$$

The well known quantized hamiltonian of the H atom is:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi - \frac{e^2}{4\pi \epsilon_0 r} \psi = E \psi \quad - (27)$$

which can be developed as:

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) - \frac{l(l+1)}{r^2} R + \frac{me^2}{2\pi^2 \epsilon_0 \hbar^2} \frac{R}{r} = -\frac{2mE}{\hbar^2} R \quad - (28)$$

It is seen that Eqs. (26) and (28) are the same provided that:

$$-2mE = \frac{L^2}{a_0} \quad - (29)$$

and

$$\frac{me^2}{2\pi^2 \epsilon_0} = \frac{2L^2}{a_0} \quad - (30)$$

The total energy E is negative valued so Eq. (29) is:

$$\frac{L^2}{a_0} = 2m|E| \quad - (31)$$

i.e.:

$$a_0 = \frac{a_0^2}{1-E^2} = \frac{L^2}{2m|E|} \quad - (32)$$

which is the definition of the semi minor axis of the ellipse (12):

$$b = \frac{a}{(1-e^2)^{1/2}} = \frac{L}{(2m|E|)^{1/2}} \quad - (33)$$

Q. E. D. So the analysis is rigorously self consistent.

Eq. (30) defines the constant of motion of Lagrangian quantum mechanics:

$$L^2 = \frac{dme^2}{4\pi\epsilon_0} \quad - (34)$$

Given this constant of motion, the hamiltonian and lagrangian both give the same well known hydrogenic wave functions, Q. E. D. The theory is rigorously self consistent.

Having proven the theory in this way it can be extended to give a new type of computational quantum chemistry based on the lagrangian (9), Euler Lagrange equations (10) and (11) and the general equation of quantization:

$$-\hbar^2 \nabla^2 \psi = m^2 (\dot{r}^2 + r^2 \dot{\beta}^2) \psi \quad - (35)$$

3. COMPUTATIONAL AND GRAPHICAL RESULTS

(Section by Dr. Horst Eckardt)

Three dimensional and quantum orbits from ECE2: Lagrangian quantum mechanics

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3 Computational and graphical results

3.1 Complete three-dimensional theory

The equations of motion of the Lagrangian (4) and the Lagrange equations (5-7) are:

$$\ddot{\theta} = -\frac{2\dot{r}\dot{\theta} - \dot{\phi}^2 r \cos(\theta) \sin(\theta)}{r}, \quad (36)$$

$$\ddot{\phi} = -\frac{2\dot{\phi}\dot{r} \cos(\theta)\dot{\theta} + 2\dot{\phi}\dot{r} \sin(\theta)}{r \sin(\theta)}, \quad (37)$$

$$\ddot{r} = \frac{r^3 \dot{\theta}^2 + \dot{\phi}^2 r^3 \sin^2(\theta) - GM}{r^2}. \quad (38)$$

In addition, β is defined by the first-order differential equation

$$\dot{\beta} = \sqrt{\dot{\theta}^2 + \dot{\phi}^2 \sin^2(\theta)}. \quad (39)$$

For a potential only depending on the radial coordinate r , a motion in a plane follows. For the initial conditions

$$\dot{\theta}(0) = 0, \quad (40)$$

$$\theta(0) = \pi/2 \quad (41)$$

we obtain a motion in the XY plane. In general, the constants of motion are the angular momenta

$$L = m r^2 \dot{\beta} = m r^2 \sqrt{\dot{\theta}^2 + \dot{\phi}^2 \sin^2(\theta)}, \quad (42)$$

$$L_\phi = m r^2 \dot{\phi} \sin^2(\theta). \quad (43)$$

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If the initial condition for $\dot{\theta}$ is different from zero, an oblique planar orbit appears. The results are graphed in Figs. 1-5. The periodicity in the graphs shows that we have a periodical motion, i.e. an ellipse. In particular, r oscillates between a minimal and maximal value (Fig. 2). From Fig. 3 it can be seen that the angle β is identical to ϕ for planar motion (β has been shifted by use of an initial value different from that of ϕ). This means that no additional information is obtained from β . This may be different for non-planar orbits.

The 3D orbit is plotted in Fig. 4, showing an ellipse rotated against the XY plane. Fig. 5 shows the constants of motion L and L_ϕ computed from the resulting orbit. They are constant as expected, and for an orbit in the XY plane follows

$$L = L_\phi \tag{44}$$

as expected. So far we have arrived at a consistent state of the numerical calculation.

3.2 Angular-dependent potentials

Non-planar orbits are obtained from angle-dependent potentials. First we use a potential dependent on the polar angle:

$$U_1 = -\frac{mMG}{r} \sin(\theta). \tag{45}$$

This leads to the orbit graphed in Fig. 6. The orbit oscillates in height. The constants of motion are impacted, the modulus of angular momentum (42) is no more a constant of motion as seen from Fig. 7. The motion around the Z axis, however, conserves angular momentum L_ϕ as before.

Finally we introduce an additional ϕ dependence of the potential:

$$U_2 = -\frac{mMG}{r} \sin(\theta) \cos(\phi). \tag{46}$$

Then a difference between ϕ and β appears (Fig. 8). The orbit is not periodic but the orbiting mass falls into the centre where the motion ends, at the upper left end in Fig. 9. Both angular momenta are no more a constant of motion as can be seen from Fig. 10.

3.3 Solution of the radial Schroedinger equation

The Schrödinger-like radial Equation (22) has been solved numerically. The standard method in computational physics is to integrate the equation for a grid of energy values (here represented by L , α and a) and find non-diverging solutions for $r \rightarrow \infty$. These are the radial eigen states. Here we used the direct integration with Maxima for some pre-defined parameters. It can be seen that the solutions diverge in general.

In Fig. 11 and Fig. 12 two solutions for $L = 1$ and $L = 5$ are shown. These (arbitrary) values correspond roughly to the number of extrema of ψ , representing the angular momentum eigen state, as is the case for the physical, convergent solutions obtained with other, more elaborate methods.

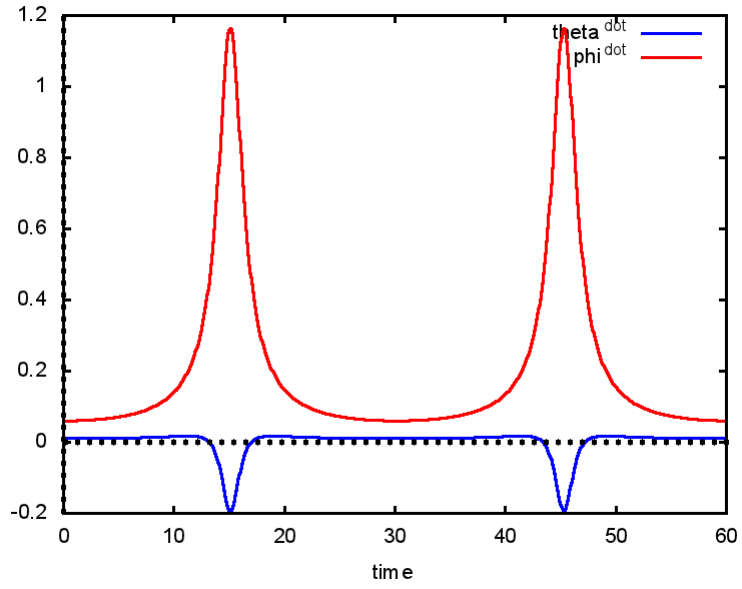


Figure 1: Trajectories $\dot{\theta}(t), \dot{\phi}(t)$.

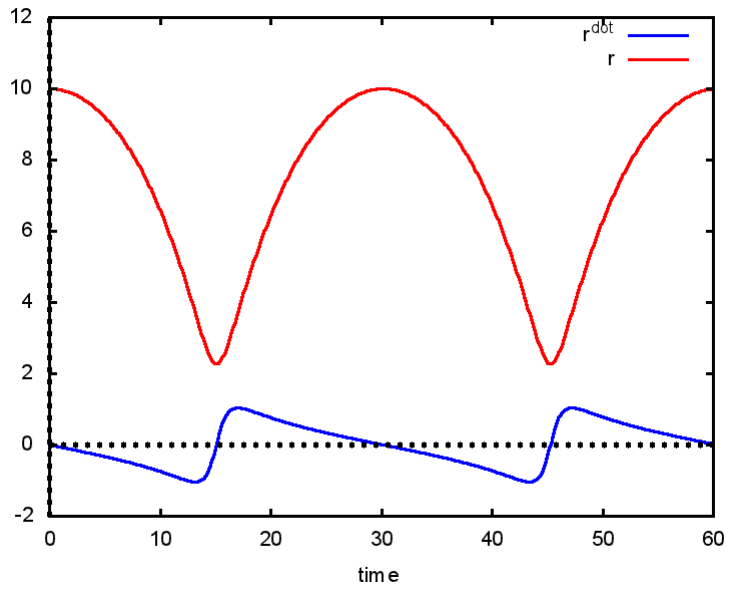


Figure 2: Trajectories of $\dot{r}(t), r(t)$.

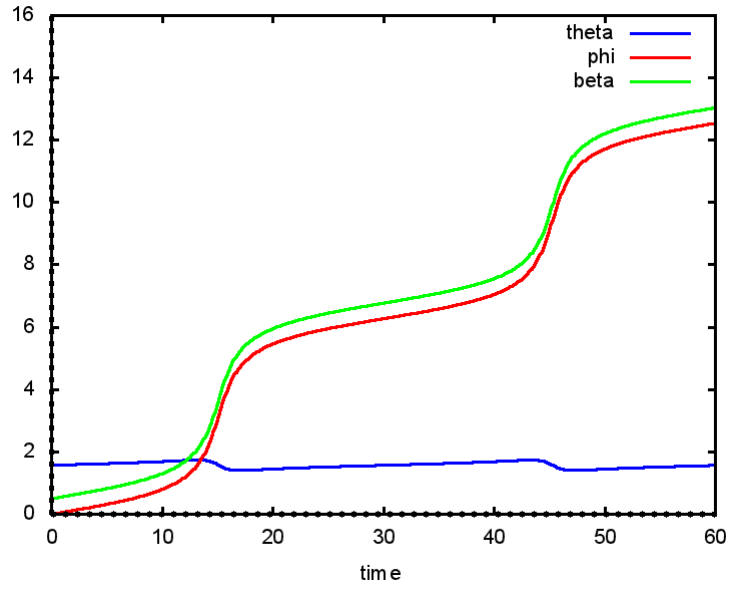


Figure 3: Trajectories $\theta(t), \phi(t), \beta(t)$.

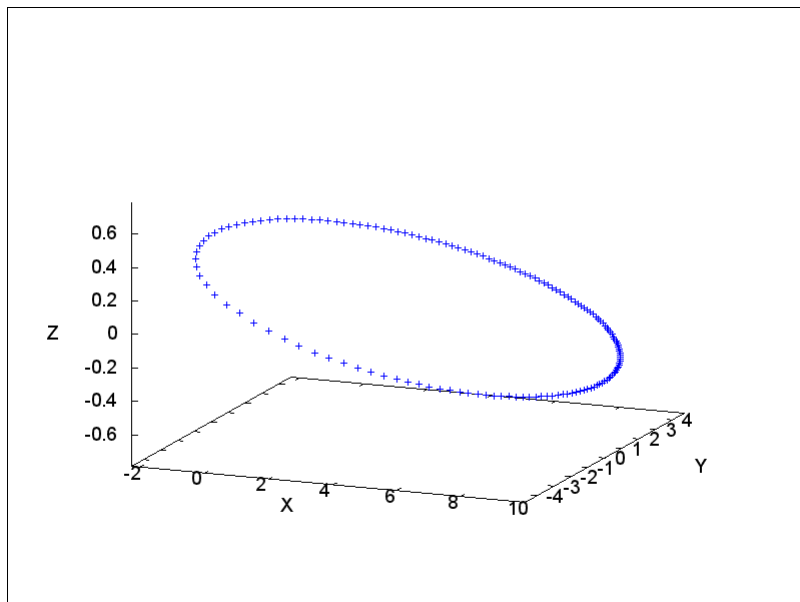


Figure 4: Orbit $r(X, Y, Z)$.

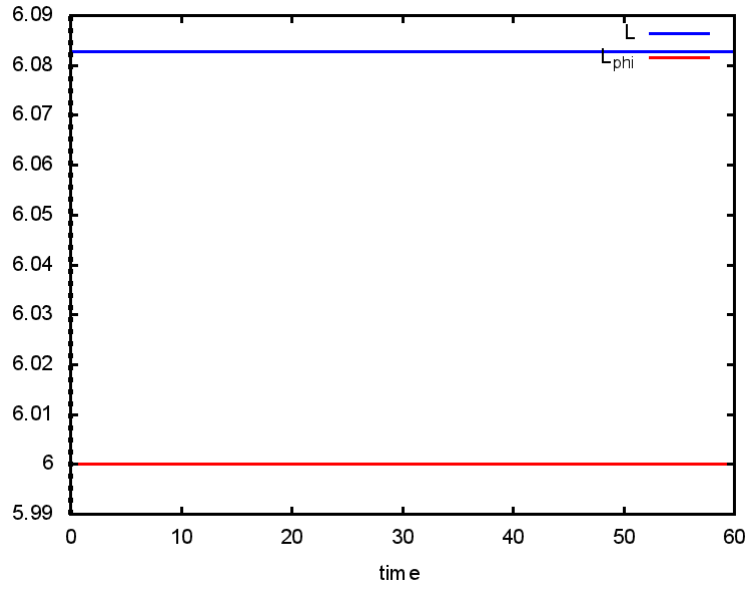


Figure 5: Constants of motion L and L_ϕ .

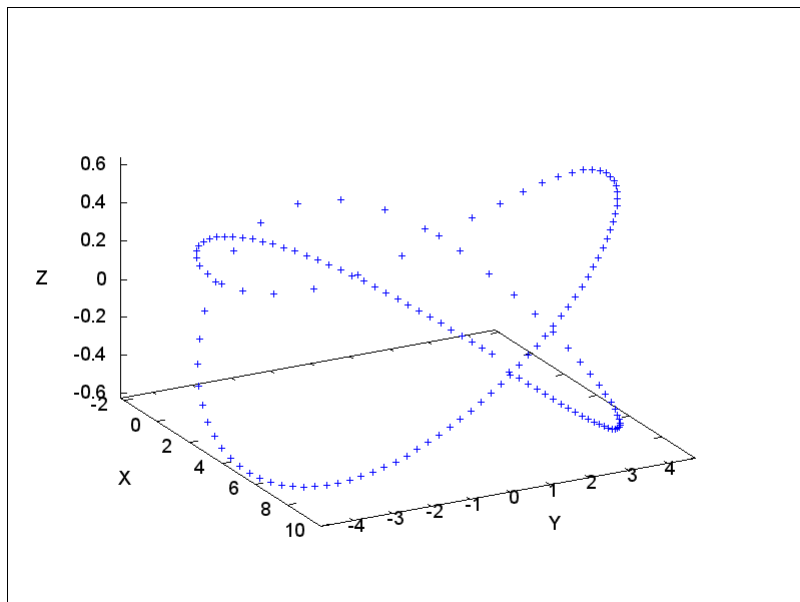


Figure 6: Orbit $r(X, Y, Z)$ for potential (45).

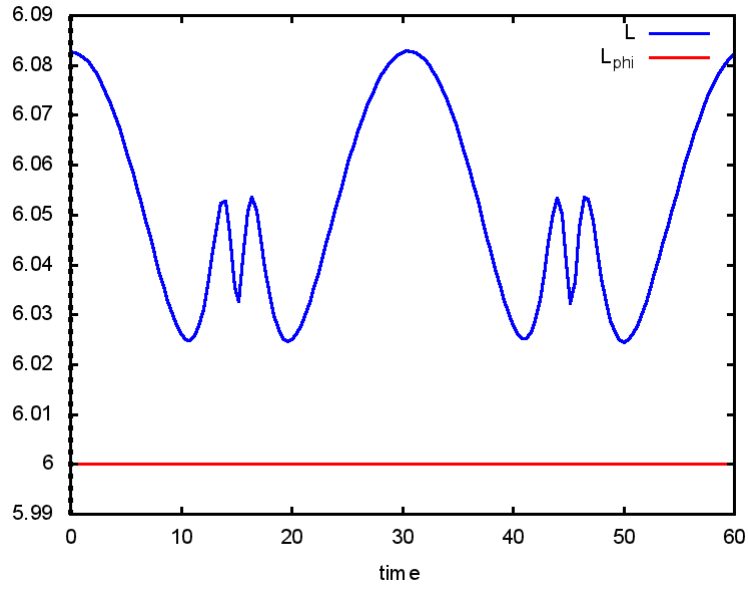


Figure 7: Angular momenta L and L_ϕ for potential (45).

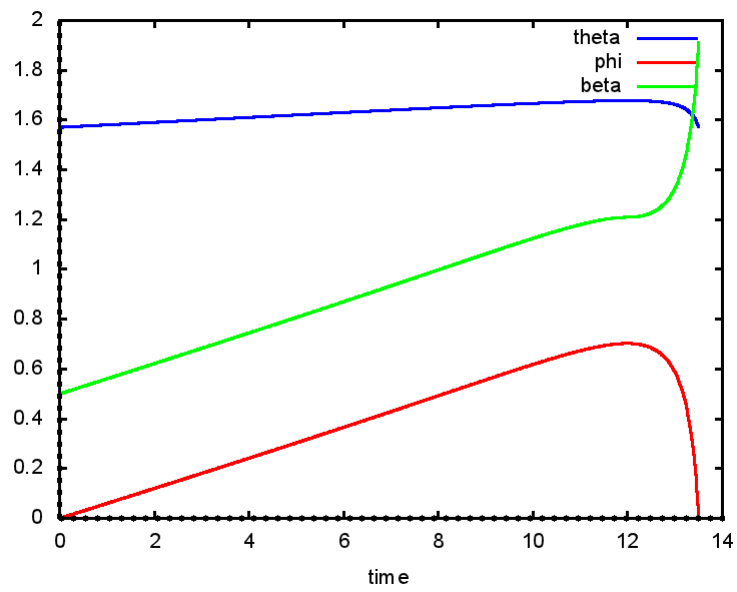


Figure 8: Trajectories $\theta(t)$, $\phi(t)$, $\beta(t)$ for potential (46).

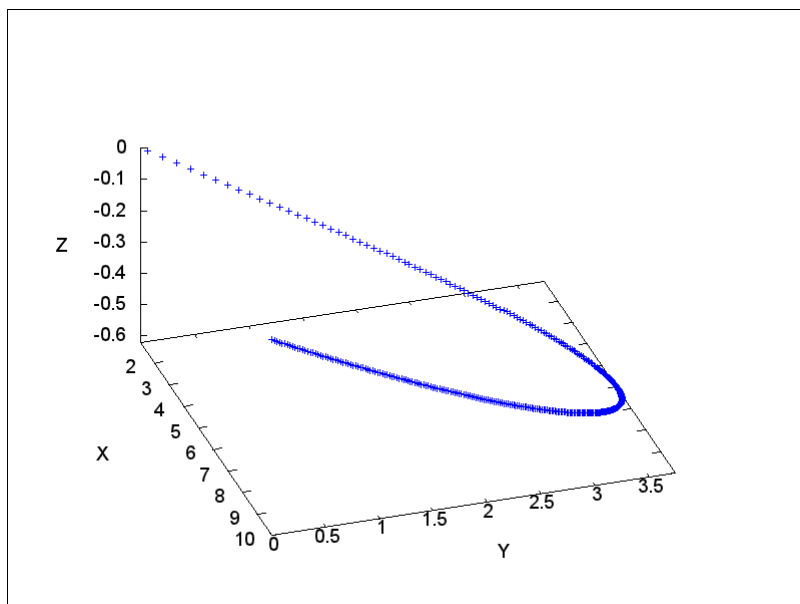


Figure 9: Orbit $r(X, Y, Z)$ for potential (46).

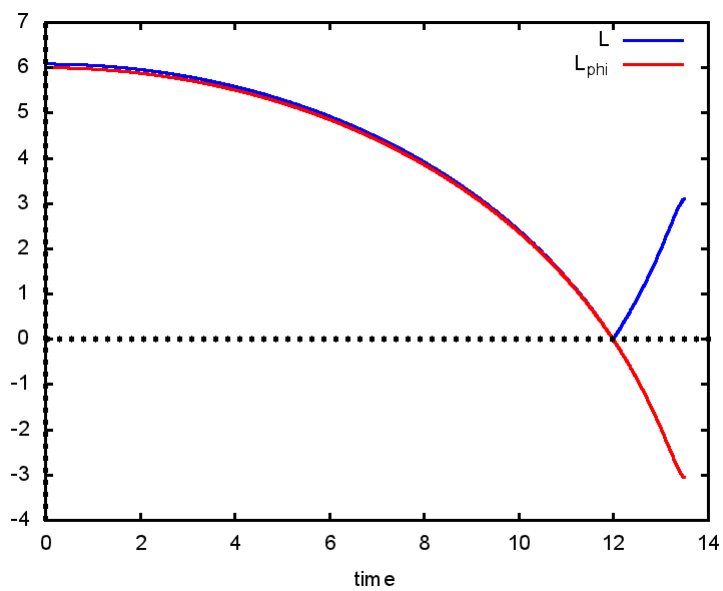


Figure 10: Angular momenta L and L_ϕ for potential (46).

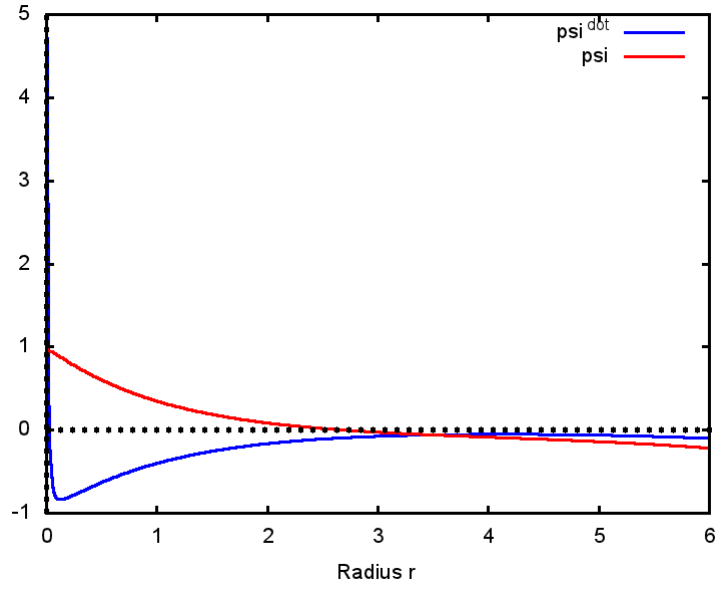


Figure 11: Radial wave function $\dot{\psi}(r), \psi(r)$ for parameter $L = 1$.

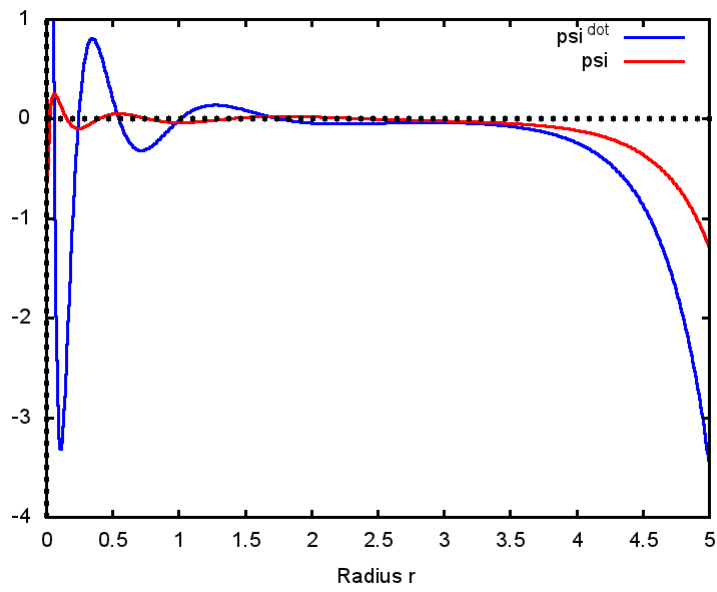


Figure 12: Radial wave function $\dot{\psi}(r), \psi(r)$ for parameter $L = 5$.

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