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Quantization and Stable Attractors in a Dissipative Orbital Motion

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Abstract

We present a method for determining the motion of an electron in a hydrogen atom, which starts from a field Lagrangean foundation for non-conservative systems that can exhibit chaotic behavior. As a consequence, the problem of the formation of the atom becomes the problem of finding the possible stable orbital attractors and the associated transition paths through which the electron mechanical energy varies continuously until a stable energy state is reached.

Keywords: Stable Attractors, Non-Linear Dynamics, Non-Conservative Orbital Systems, Lagrangean Systems, Electron Capture in Hydrogen Atom

1. Introduction

In this paper we present a new method for dealing with quantization problems which is based, on the one hand, on the concept of a stable attractor associated with a non-linear differential equation from the usual chaos theory and, on the other hand, on the variational formulation of Quantum Mechanics introduced by E. Schrödinger in 1926 [1]. That is, our approach is not based in the current and well-known method of phase space representation in the semi-classical limit of quantum mechanics, usually known as "quantum chaos".

The theory of quantum chaos was pioneered by Einstein through his 1917 [2] paper, in which he made a connection between classical and (old) quantum mechanics. This theory was further improved by many authors, among which the works of Gutzwiller [3-7] and Ozorio de Almeida [8-11] have made major contributions. In particular, Gutzwiller obtained in 1967 [3] the exact wave functions for the bound states of the hydrogen atom, by performing a very complicated calculation using a phase integral approximation of a Green's function in momentum space.

We follow an alternative approach in this work, in which we show that it is possible to obtain the exact energy of the bound states of the hydrogen atom by searching for stable orbital attractors in a non-conservative Hamilton-Jacobi dynamics [12-14]. Thus, the quantization problem is solved by selecting, from all of the possible electron paths in which energy is dissipated, those that tend to stable closed paths in which bound states of motion are reached in the limit as time approaches infinity, that is, to stable orbital attractors. This is done in Section 2 where we are conducted from the well-known linear Schrödinger equation to a non-linear momentum equation. This equation will be shown to generate the dissipative dynamics and allow the existence of a set of stable attractors which prevent the collapse of the system. In Section 3 we solve the equations for the hydrogen atom obtaining the form of the dissipative energy function along the electron trajectory, in which the mechanical energy varies continuously until a stable attractor is reached, when it becomes finally constant.

2. The Equations of Motion

We start by considering the Hamiltonian function for an electron which is considered as an ordinary charged particle, whose motion is caused by a scalar potential energy function $V = -e^2/r$ and also that no vector potential is present, *i.e.*, $\boldsymbol{A} = 0$. That is

$$H = \frac{\boldsymbol{p}^2}{2m} + V, \tag{1}$$

where $\boldsymbol{p} = m\boldsymbol{v}$ is the electron linear momentum, $m = m_e m_p \left(m_e + m_p\right)^{-1}$ is the reduced mass and m_e and

m_p are the electron and proton masses, respectively.

Of course, since in general the system irradiates continuously, the Hamiltonian (1) *cannot be a constant of the motion*. Therefore, at first sight, the motion is always dissipative, the electron tending to fall into the proton, whose position may be called a collapsing attractor of the process. Hence, we shall search in this work for the possibility of non-collapsing stable attractor paths toward which the electron motion can tend asymptotically as time goes to infinity.

Since $V(r)$ is a spherically symmetric potential, this implies the conservation of the angular momentum vector $\boldsymbol{L} = r \times \boldsymbol{p}$ in the center of mass frame. Thus the motion should be plane, since $\boldsymbol{r}$ is always perpendicular to $\boldsymbol{L}$, from the initial moment until the stable motion is reached in the limit as time goes to infinity. Because $\boldsymbol{p}$ and $\boldsymbol{L}$ are mutually perpendicular vectors, and by using the linear momentum radial and polar components $p_r = m\dot{r}$ and $p_\varphi = mr\dot{\varphi}$, respectively, and the relationships $L_0 = |\boldsymbol{L}| = rp_\varphi = \text{constant}$ and $H = E = \text{constant}$, (1) assumes the form

$$E = \frac{1}{2}m\dot{r}^2 + \frac{L_0^2}{2mr^2} + V, \tag{2}$$

which defines a conservative or Hamiltonian system in Classical Mechanics.

It can immediately be seen that in this case (2) is a non-linear equation in both r and $\dot{r}$, so that Classical Mechanics is in its deepest grounds a non-linear theory. The closed paths that are solutions of Equation (2) are elliptic orbits which may be obtained by integrating it directly, through the chain rule $\dot{r} = \frac{\mathrm{d}r}{\mathrm{d}\varphi}\frac{L_0}{mr^2}$, as a function of the polar angle φ. Alternatively we may also observe that the only way that Equation (2) may be satisfied for any value of the continuous variable φ is by a composition of periodic sinusoidal functions of the form

$$\frac{1}{r} = \frac{1}{a}\left(1 + \varepsilon\cos\varphi\right), \tag{3}$$

which substituted into Equation (2), and with the help of the definition of the angular momentum, results respectively in the following inverse average radius and eccentricity formulae

$$a = \frac{L_0^2}{me^2},\ \varepsilon = \sqrt{1 + \frac{2aE}{e^2}} \tag{4}$$

A third way to address the Hamiltonian problem, which is followed in usual Lagrangian Classical Mechanics, is to make use of a variational procedure to transform the non-linear quadratic form given in (2) into an ordinary linear second-order differential equation in $1/r$, whose solution is given exactly by the function in (3) (see chap.2 of Ref. [15]). We shall follow a similar approach in this work.

It is a well known fact in Classical Mechanics that the motion in any path corresponding to (3) is unstable against energy loss by radiation, so that the electron in fact follows a decreasing spiral motion toward the proton position. In order to look for a stable orbital attractor, that is, an orbit in which the motion can be stable against a loss or gain of energy by emission or absorption of radiation, we allow the Hamiltonian function in (1) to vary along a virtual path and try to get a special state of motion in which a loss in energy in a region of space may be compensated by the absorption of energy in another region, producing a self-restoration effect in the Hamiltonian, so that, no net loss of energy occurs overall and, therefore, *the system becomes dynamically stable.*

Thus, we consider along the path given by the classical linear momentum $\boldsymbol{p}$, which is the solution of (1) with $H = E$, linear momentum variation vectors $\boldsymbol{p} \pm \delta\boldsymbol{p}$, which vary to the left or to the right of $\boldsymbol{p}$ by $\delta\boldsymbol{p}$, which is a solution of Equation (1) if $H \neq E$. This variation momentum must satisfy the asymptotic limit $\delta\boldsymbol{p} \to 0$, as $t \to \infty$, that define the stable attractors which we are looking for. At this limit, we get back to the $\boldsymbol{p}$ path at a matching point $r = r_a$, but with specific values for the parameters E and L_0 which determine the specific ellipses that make the system stable or self-restoring.

In order to accomplish this, we shall observe that, due to the emission of radiation, the finite difference

$$(\delta\boldsymbol{p})^2 - \boldsymbol{p}^2 = (\delta\boldsymbol{p} + \boldsymbol{p})\cdot(\delta\boldsymbol{p} - \boldsymbol{p}) = 2m(H - E) \tag{5}$$

must approach zero if $H > E$ as $t \to \infty$. Also, in the absorption process, Equation (5) must approach zero if $H < E$ as $t \to \infty$. In any case, (5) must be expressed as a quadratic form which is suitable for the variational procedure. This is made by introducing a variation function $\psi = \psi(r)$ through a transformation proposed originally by Schrödinger [1]:

$$\delta\boldsymbol{p} = \frac{\hbar}{\psi}\nabla\psi, \tag{6}$$

where $\hbar$ is the rationalized Planck's constant.

The Lagrangian density function we need is then obtained by considering ψ^2 times the difference between the Hamiltonian H and the energy attractor E. After substituting (6) into (5) and using (1) we obtain

$$Q \equiv (H - E)\psi^2 = \hbar^2(\nabla\psi)^2 + 2m(V - E)\psi^2. \tag{7}$$

Here, $Q = Q(\psi, \nabla\psi, r)$ is a quadratic form of the function ψ and its space derivatives, so that the variation of the volume integral of Q conducts to a partial linear differential equation, as expected in a Lagrange's variational problem.

We also need to impose the constraint that the function ψ must be square integrable or normalizable, because ψ^2 stands for an averaging weight function

$$\int_{space} \psi^2 \mathrm{d}V = 1, \tag{8}$$

where, for simplicity, the unity value for the normalization constant has been assumed.

Let us consider now the calculation of the volume integral $I = \int_{space} Q\mathrm{d}V$ over all space. If there is a finite loss or gain of energy due to radiation, $H - E$ is a finite quantity too. In order to avoid collapse of the system I must be a finite constant. In order to assure that, it is enough that Q is limited at the origin and tend to zero as the space volume tends to infinity. Therefore, in order to allow the existence of stable attractors, we shall impose that I must have an extreme value near zero[1] so that its variation vanishes, namely

$$\delta \int_{space} Q\mathrm{d}V = 0. \tag{9}$$

It will be seen in what follows that only trajectories which tend to a closed path as time goes to infinity will satisfy the variational problem, reaching a stable attractor path. Equation (9) cannot be satisfied if we consider either the free electron motion or the motion in a scattering process, since such motions are remarkably unbound, and therefore cannot satisfy (8).

Now, by introducing the Lagrangian density, (7), into (9), we get

$$\int_{space} \left[\frac{\hbar^2}{2m} \Delta\psi + (E - V)\psi \right] \delta\psi \mathrm{d}V + \frac{\hbar^2}{2m} \int_{surface} \nabla\psi \cdot \mathrm{d}\boldsymbol{F} \delta\psi = 0 \tag{10}$$

In the calculation of the variations, usual integration by parts has been made and $\mathrm{d}\boldsymbol{F}$ is the surface element vector. In order to satisfy (10), it is sufficient to require that the integrand in the volume integral and the surface integral vanish separately, namely

$$\hbar^2 \Delta\psi + 2m(E - V)\psi = 0 \tag{11}$$

and

$$\int_{surface} \nabla\psi \cdot \mathrm{d}\boldsymbol{F} \delta\psi = 0. \tag{12}$$

Equation (11) is the variational form of the Schrödinger equation and (12) is automatically satisfied by the requirement that the variation $\delta\psi$ vanishes at infinity, where the surface integral is calculated, although it would also be asked to vanish on a finite surface[2]. This is guaranteed by the constraint (8), which implies that ψ as well as $\delta\psi$ vanish at infinity.

Now, from (11), we can obtain an equation for the varied linear momentum of the electron through (6) and the identity

$$\nabla \cdot \left(\frac{\nabla\psi}{\psi} \right) = \frac{\Delta\psi}{\psi} - \left(\frac{\nabla\psi}{\psi} \right)^2, \tag{13}$$

which substituted into Equation (11) results in

$$(\delta \boldsymbol{p})^2 + \hbar \nabla \cdot \delta \boldsymbol{p} + 2m(E - V) = 0. \tag{14}$$

From this non-linear momentum variation equation for a non-conservative system, which is analogous to (2) for a conservative system, the electron trajectories resulting in the stable attractor mentioned above will be obtained. Thus, Equation (11) is the linear differential equation associated with the non-linear momentum equation, (14).

3. Determination of the Electron Path Functions in the Formation of a Hydrogen Atom

We can now perform the reduction of both the equations of motion, (11) and (14). Starting with the former, we consider a variation in path with a constant angular momentum[3] $L_0 = \ell\hbar$, so that $\delta L = 0$. This value assigned to L is provisory because the actual value will come from the specific orbits to be found. Thus, $\psi(r)$ depends only on the radius and hence (11) becomes

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}\psi}{\mathrm{d}r} + \left[\frac{2m}{\hbar^2} \left(E_\ell + \frac{e^2}{r} \right) - \frac{\ell^2}{r^2} \right] \psi = 0, \tag{15}$$

where the numeric factor ℓ will be determined later.

The radial variation may be obtained through (6) as

$$\delta p_r = \frac{\hbar}{\psi} \frac{\mathrm{d}\psi}{\mathrm{d}r}. \tag{16}$$

Now, we remember that the divergence of a vector $\boldsymbol{u}$ in polar coordinates is

$$\nabla \cdot \boldsymbol{u} = \frac{\partial u_r}{\partial r} + \frac{1}{r} u_r + \frac{1}{r^2} \frac{\partial u_\varphi}{\partial \varphi}, \tag{17}$$

through which we can reduce (14) to its radial form, namely

$$(\delta p_r)^2 + \hbar \left(\frac{\mathrm{d}(\delta p_r)}{\mathrm{d}r} + \frac{\delta p_r}{r} \right) - \frac{\ell^2 \hbar^2}{r^2} + 2m \left(E_\ell + \frac{e^2}{r} \right) = 0, \tag{18}$$

[1]It would be exactly zero for a Hamiltonian system, since in this case $H = E$ always.

[2]This will be considered in a future work concerning discrete transitions.

[3]We will consider a variable angular momentum in a future work in connection with the transition between energy levels.

where ℓ is the above-mentioned parameter.

Since (18) is non-linear, it is not a simple task to obtain its solution directly. Instead of this, we shall employ the radial solutions of the linear (15), and generate solutions for the (18), through (16). In its simplest form the solutions for (15) that are regular at the origin and at infinity can be written as [16]

$$R_\ell(r) = r^\ell e^{-r/n_{0\ell}}, \tag{19}$$

which, after substitution into (15) and equating coefficients in the same power, yields

$$E_\ell = -\frac{\mathrm{E_B}}{\left(\ell+\frac{1}{2}\right)^2}, \tag{20}$$

where $E_B = \frac{e^2}{2a_B} = \frac{\hbar^2}{2ma_B^2} \cong 13.6$ eV is the ionization or Bohr energy of the hydrogen atom. We see immediately that the only possible values for the parameter ℓ which make the above expression for the energy levels to agree with the experiment are the half-integers[4]:

$\ell = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \cdots$

Thus, the solution of (18) obtained through (19) becomes

$$\delta p_r = \ell\hbar\left(\frac{1}{r} - \frac{1}{r_{0\ell}}\right). \tag{21}$$

Therefore the simplest stable attractor condition is given by $\delta p_r(r_{0\ell}) = 0$ and the possible stable attractor radii are given by

$$r_{0\ell} = \ell\left(\ell+\frac{1}{2}\right)a_B, \tag{22}$$

where $a_B = \frac{\hbar^2}{me^2} \cong 0.53$ Å, is the Bohr radius. The plot of Equation (21) for $\ell = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$ is shown in **Figure 1**, in which $r_{0\ell}$ assumes the values 0.5, 3.0 and 7.5 a.u., respectively. We note that for $r > r_{0\ell}$, we have $\delta p_r < 0$ so that the three curves correspond to decreasing spirals toward $r_{0\ell}$. On the other hand, for $r < r_{0\ell}$, we have $\delta p_r > 0$, so that the three curves correspond to increasing spirals also toward $r_{0\ell}$, therefore illustrating the workings of the self-restoring effect. Thus $r_{0\ell}$ is really an asymptotically stable orbital point, *i.e.* a stable attractor.

By considering now the solution (21) of the non-linear equation (18) and again comparing coefficients in the same power, we obtain the same energy levels specified by (20). And from the radii given in (22) we can calcu

[4]These half-integers will be connected with periodic wave conditions in a future work.

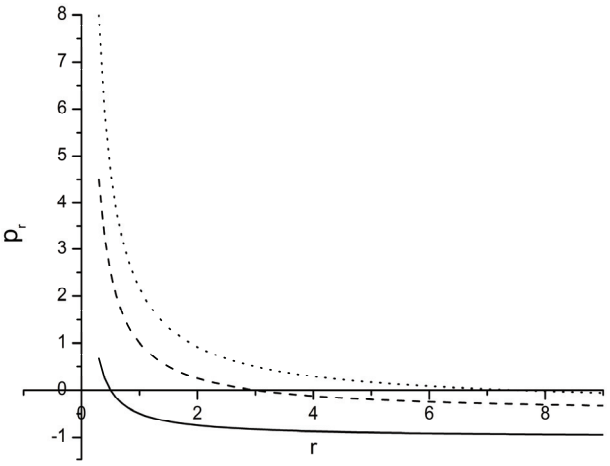

Figure 1. The radial varied linear momenta $\delta p_r(r)$, where r is in a.u., for $\ell = \frac{1}{2}$ (solid line), $\ell = \frac{3}{2}$ (dashed line) and $\ell = \frac{5}{2}$ (dotted line).

late the values of the derivative of the variation of the radial component of the linear momentum

$$\left.\frac{\mathrm{d}(\delta p_r)}{\mathrm{d}r}\right|_{r_{o\ell}} = -\frac{\ell\hbar}{r_{o\ell}^2}, \tag{23}$$

which, once inserted into Equation (18), yields the conservative form

$$V(r_{o\ell}) + \ell(\ell+1)\frac{\hbar^2}{2mr_{o\ell}^2} = E_\ell. \tag{24}$$

We see that, for $p_r(r_{0\ell}) = 0$ and with $L_0' = \sqrt{\ell(\ell+1)}\,\hbar \equiv \ell'\hbar$, (24) has the same classical conservation form as (2), which is consequently the actual value of the angular momentum. Therefore, the resulting conservative orbit is described in phase space by the twofold function

$$p_r = \pm\sqrt{2m\left(E_\ell + \frac{e^2}{r}\right) - \frac{\ell(\ell+1)\hbar^2}{r^2}}. \tag{25}$$

The plot of (25) together with the radial variation (21) are shown in **Figure 2** for $\ell = \frac{1}{2}$, from which we can note that $r_{0\ell}$ (= 0.5 a.u.) is the intersection point of the paths because it is their only common root.

In addition, $r_{0\ell}$ is not the only root of (24) or for the condition $p_r = 0$ in (25); the other root being

$$r_{0\ell}' = (\ell+1)\left(\ell+\frac{1}{2}\right)a_B, \tag{26}$$

so that $r_{0\ell}$ and $r_{0\ell}'$ become respectively the semiminor and semimajor axes of the ellipse

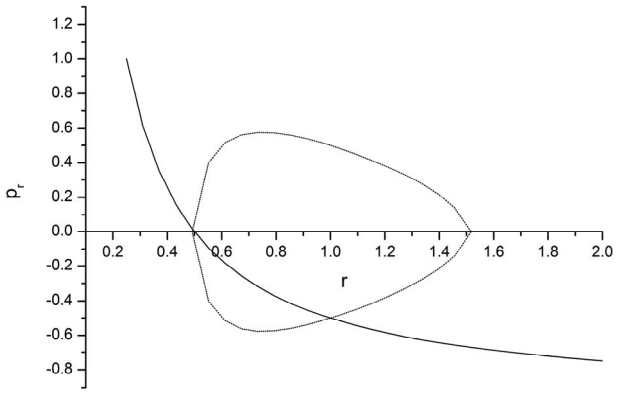

Figure 2. The electron radial momenta: classical (dotted line) and varied (solid line) for $\ell = \frac{1}{2}$.

$$\frac{1}{r} = \frac{1}{a'}\left(1 + \varepsilon' \cos\varphi\right), \tag{27}$$

which satisfy (25) and, thus, it is the orbital stable attractor searched for, where

$$a' = \frac{L_0^2}{me^2} = a_B \ell\left(\ell + 1\right) \text{ and}$$
$$\varepsilon' = \sqrt{1 + \frac{2a'E_\ell}{e^2}} = \sqrt{1 - \frac{\ell\left(\ell+1\right)}{\left(\ell + \frac{1}{2}\right)^2}} \tag{28}$$

The corresponding average electron position for a circular motion is given by the average value of the ellipse semi-axes, which agrees with the Bohr model:

$$r_{av} = \frac{1}{2}\left(r_{o\ell} + r'_{o\ell}\right) = \left(\ell + \frac{1}{2}\right)^2 a_B .$$

In order to obtain the actual electron trajectory we must integrate the varied radial linear momentum together with the constant angular momentum,

$$\delta p_r = m\frac{\mathrm{d}r}{\mathrm{d}t} = \frac{\mathrm{d}r}{\mathrm{d}\varphi}\frac{L'_0}{r^2}, \tag{29}$$

$$\int \frac{\mathrm{d}r}{r^2 \delta p_r} = \frac{1}{\ell' \hbar}\int \mathrm{d}\varphi, \tag{30}$$

from which we readily obtain the equation for the electron trajectory

$$r\left(\varphi\right) = \frac{r_{o\ell}}{1 \pm C_\pm \mathrm{e}^{-\varphi/\sqrt{1+1/\ell}}}, \quad \varphi \geq 0 \tag{31}$$

whose corresponding integration constant is undetermined, since the followed trajectory depends on the initial conditions. This means that if we consider for example $r_{0\ell} < r\left(0\right) < \infty$, we would have $0 < C_- < 1$ and the path, Equation (31), would become a decreasing spiral. On the other hand, for $0 < r\left(0\right) < r_{0\ell}$ we would have $0 < C_+ < \infty$ and the path, (31), would become an increasing spiral. In both cases they converge toward the stable attractor $r = r_{o\ell}$. The plot of the ellipse, (27), and the spirals, (31), is shown in **Figure 3** for $\ell = \frac{1}{2}$.

We can immediately write the electron energy function, (1), in polar coordinates as

$$H\left(\varphi\right) = \ell^2\left[\frac{1}{r} - \frac{1}{\ell^2\left(\ell + 1/2\right)^2}\right]^2 - \frac{2}{r} + \frac{\ell\left(\ell+1\right)}{r^2}, \tag{32}$$

where $H\left(\varphi\right)$ is in Ry and $r\left(\varphi\right)$ is in a.u. The plot of $H\left(\varphi\right)$ is shown in **Figure 4** for $\ell = \frac{1}{2}$ (first attractor or fundamental energy) and $\ell = \frac{3}{2}$ (second attractor or first excited energy) of the hydrogen atom. For each value of ℓ, the self-restoring process of the stable attractor is quite clear: in the emission range, $r_{0\ell} < r < \infty$, $H\left(\varphi\right)$ converges monotonically to the energy attractors if $H > E$ as $\varphi \to \infty$. On the other hand, in the absorption range, $0 < r < r_{0\ell}$, $H\left(\varphi\right)$ first decreases from its starting energy to a point of minimum, and then it increases converging to the energy attractors if $H < E$ as $\varphi \to \infty$.

4. Conclusions

In this paper we have introduced a different chaotic approach in which we show that it is possible to obtain the exact energy of the bound states of the hydrogen atom by looking for stable orbital attractors in a non-conservative Hamilton-Jacobi dynamics. In it, a variable energy process tends asymptotically toward an energy stable attractor

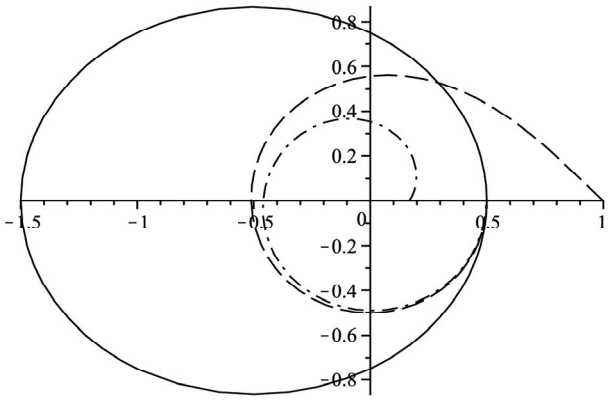

Figure 3. The electron trajectories in polar coordinates for $\ell = \frac{1}{2}$, $C_- = \frac{1}{2}$ and $C_+ = 2$: ellipse (solid line), decreasing spiral (dashed line) and increasing spiral (dot-dashed line).

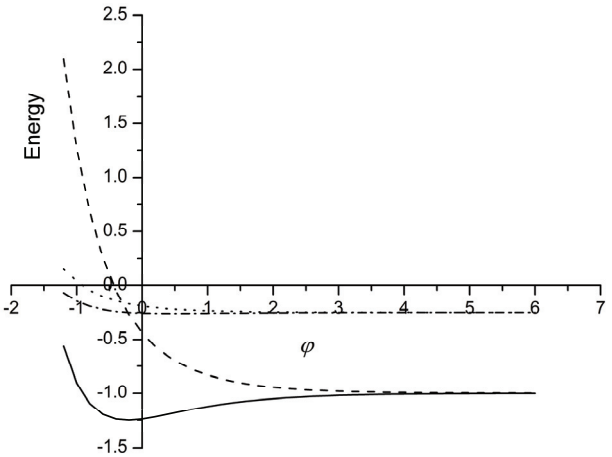

Figure 4. The energy function, $H(\varphi)$, in Ry with φ in radians, for the electron trajectories corresponding to the ground state of the hydrogen atom $\left(\ell=\frac{1}{2}\right)$ in the absorption range (solid line) and in the emission range (dashed line); also for the first excited state $\left(\ell=\frac{3}{2}\right)$ in the absorption range (dot-dashed line) and in the emission range (dotted line).

as time approaches infinity. The stable orbital attractor is found to be a self-restoring process in which energy is absorbed or emitted as the electron is displaced away from the equilibrium orbit, hence immediately returning the electron to the equilibrium orbit. Therefore, the energy is constant. The variation in the mechanical energy is due to the continuous irradiation of energy in the form of electromagnetic waves which carry energy away from or toward the mechanical system, while the electron moves through space. The determination of the attractors was made through a variational procedure, starting from the work done by E. Schrödinger in 1926 [1], which yielded a linear partial differential equation in an auxiliary action function. This equation allowed obtaining a solution for the non-linear equations that govern the variation of the electron linear and angular momenta during the process of electron capture by a proton.

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