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CLASSICAL INTERPRETATION OF SPONTANEOUS TRANSITIONS IN THE HYDROGEN ATOM

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ABSTRACT

Seidl and Lipas[1] have calculated the lifetime of the excited states of the hydrogen atom within an entirely classical framework, and obtained a good agreement with the corresponding quantum results. Here we propose a physical explanation for this good agreement and show that the agreement can be significantly improved by including the effects of the vacuum zeropoint electromagnetic fields in their classical model. Moreover, we show that the zeropoint electromagnetic radiation provides a physical mechanism for the atomic stability on classical grounds.

1. INTRODUCTION

Recent calculations[1] have shown that good numerical values for the lifetime of the excited states of the hydrogen can be obtained within an entirely classical framework. The classical lifetimes agree fairly well with the quantum calculations, through a wide range of order of magnitude, varying from 10^5 sec to 10^{-8} sec. In the present article, we propose a physical explanation for the good agreement between the classical and the quantum calculations. Moreover, we further refine this classical model for the hydrogen atom transitions by introducing the random zeropoint electromagnetic radiation characteristic of classical stochastic electrodynamics[2]. We will show that the zeropoint "vacuum" electromagnetic radiation provides a physical mechanism that accounts for the atomic stability on classical grounds[2,3].

Before we start our explanation, it is convenient to stress the differences of the classical and the quantum scenarios for the hydrogen atom. For this purpose, we briefly remind some historical steps of the transition from one scenario to the other. After all, even Niels Bohr, the author of the first (*ad hoc*) quantum model of the atom, was stunned by the constraints of this own theory. In a letter (September 1913) to a colleague of his, Bohr wrote[4]: "In the necessity of new assumption, I think that we agree; but do you think such horrid assumptions, as I have used, necessary?"

An important preliminary advance towards introducing quantum levels in atoms was the hypothesis of A. W. Conway (1907) that atoms should be altered in a *"disturbed state"*[5]. During the return of the atoms to their normal state, monochromatic alectromagnetic waves are emitted. This implies that an atom contributes to a single spectral line at a time. Without this assumption, each individual atom would radiate simultaneously all of the spectrum lines, and it would then possess a large number of degrees of freedom. This would imply an exceedingly large number of electrons per atom. Conway's hypothesis gained further support with the discovery of the Rydberg-Ritz combination rules, which were compatible with the existence of an enumerable set of "disturbed states".

In 1901, Perrin proposed a "nucleo planetary" model of the atom, a negative charge rotating around a positively charged nucleus. This model does not explain the atom stability, an important dynamical property of these microscopic assembly of charged constituents.

Within the framework of the nucleo-planetary atom, Nagaoka proposed in 1904 a model in which the electrons behave as uniformly charged rings, with a constant angular velocity (Saturnian model), which is a radiationless motion (see ref [5], chapter I). In this model the spectral lines correspond to the vibrational modes of the rotating ring. Moreover, the ring angular momentum (in this radiationless motion) would prevent the electron from collapsing into the nucleus. However, the spectrum produced by this model does not agree with the experimental facts.

Another attempt was made in 1911–1912 by Nicholson in a model that assumed an *ad hoc* quantization of the angular momentum of the orbiting electron[4,6]. The *"incapacity* (of an atom) *for radiating in a continuous way will secure the sharpness of the lines"*. However, in this model, the radiation frequencies are the classical frequencies of the rotating electron.

Finally, in 1913, Bohr proposed his nucleo planetary model of the atom that successfully reproduced the experimentally observed spectral lines of the hydrogen atom. This was possible due to the introduction of various *ad hoc* hypothesis, including the stability of the "ground" state and the instability of the "excited" states. The surprising feature of his model is that the radiated frequencies are not equal to the frequencies of the orbital motion of the electron as expected from classical electrodynamics.

As mentioned in the beginning of this introduction, we shall calculate the lifetime of excited states of the hydrogen atom, within a classical framework, taking into account the zeropoint electromagnetic radiation. We shall show that the zeropoint field improves the results of Seidl and Lipas[1] and provides the stability of the atom.

We shall present our spiraling electron atomic model in section 2. The basic difference from the Seidl and Lipas description is the fact that the atom is immersed in the zeropoint electromagnetic radiation. The quantal transition rates are calculated within section 3. The summary of results is presented in section 4 where we stress the fundamental modifications due to the introduction of the zeropoint electromagnetic background. Our section 5 is devoted to a detailed justification of the physical mechanism underlying the agreement between the classical and the quantum calculations. Finally, a brief discussion of our conclusions is presented in section 6.

2. SPIRALING ELECTRON ATOMIC MODEL WITH ZEROPOINT RADIATION

From classical electrodynamics standpoint the hydrogen atom electron radiates energy at a rate given by the Larmor's equation

$$P_{\text{Larmor}} = \frac{2}{3}\frac{e^2}{c^3}\left(\ddot{x}_1^2 + \ddot{x}_2^2\right) \quad , \tag{1}$$

where $x_1(t)$ and $x_2(t)$ are the cartesian coordinates associated to the plane of the orbit and

$$r(t) = \sqrt{x_1^2 + x_2^2} \quad , \tag{2}$$

is the distance between the electron and the proton. In equation (1), e is the electron charge, and c is the velocity of light.

In the case of an attractive Coulomb force, an electron, moving in a circular orbit of radius r, has energy $\epsilon(r)$ given by

$$\epsilon(r) = -\frac{e^2}{2r} \quad . \tag{3}$$

The instantaneous angular frequency ω of the electron motion, which is also the frequency of the classically emitted radiation, is such that

$$\omega^2 = \frac{e^2}{mr^3} \quad , \tag{4}$$

where m is the electron mass.

Likewise Seidl and Lipas, we shall discuss only the particular case in which the electron orbit can be considered as almost circular. This special situation is simple enough and also corresponds to a well known regimen of the classical trajectory of the radiating electron. Due to the classical emission of radiation, any bounded orbit, which is initially elliptical, becomes almost circular while the electron is spiraling towards the nucleus (see for instance the text books by Jackson[7] and Landau[8]).

For a strictly circular motion, with angular frequency ω (see(4)), each component of the acceleration is such that

$$\ddot{x}_j + \omega^2 x_j = 0 \quad , \tag{5}$$

$j = 1, 2$. Here, however, we want to consider radiative corrections to equation (5) due to the fact that the electron is continuously emitting and absorbing radiation from the environment. In other words, we shall assume that a strictly isolated hydrogen atom does not exist. The atom is always immersed in a reservoir of random electromagnetic forces provided by the zeropoint radiation[2]. Therefore, a natural framework for our theoretical analysis is the so called classical stochastic electrodynamics, or simply SED[9,10]. This is the Lorentz's classical electron theory into which one introduces random electromagnetic radiation (classical zeropoint radiation) as the boundary conditions giving the homogeneous solution of Maxwell's equations. The theory contains one adjustable parameter setting the scale of random radiation, and this parameter is Planck's constant $h = 2\pi\hbar$. In accordance with the classical Wien law the energy density spectral distribution associated with a cavity at zero temperature is:

$$\rho_0(\omega) = \left(\frac{\omega^2}{\pi^2 c^3}\right) \frac{\hbar\omega}{2} \quad , \tag{6}$$

which corresponds to an average energy of $\hbar\omega/2$ per normal mode of angular frequency ω. Good and complementary reviews of SED are given by Boyer[2,11], Milonni[10] and de la Peña and Cetto[9].

Therefore, according to SED, the radiative corrections can be introduced into equation (5) which (in the dipole approximation) is modified to[2,11]

$$\ddot{x}_j + \omega^2 x_j \simeq \frac{2}{3}\frac{e^2}{mc^3}\,\dddot{x}_j + \frac{e}{m}E_j(t) \quad , \tag{7}$$

where the first term in the right hand side is the radiation reaction force. The second term is the contribution of the random electric field $E_j(t)$ in the dipole approximation. These radiative corrections are small and only modify the circular motion *slowly*, that is, one can consider that $\omega \simeq$ constant and $r \simeq$ constant (see (3) and (4)) for many periods $2\pi/\omega$ of oscillation. However, the stochastic forces $eE_j(t)$ produces a slow, but inevitable, diffusion of the circular orbit[9].

The ensemble average of the random field $E_j(t)$ is such that $\langle E_j(t)\rangle = 0$ and the spectral density $\rho_0(\omega)$ is related to the correlation function $\langle E_j(t)\, E_j(0)\rangle$, namely[2]

$$\frac{3}{4\pi}\langle E_j(t)\, E_j(0)\rangle = \int_0^\infty d\omega\, \rho_0(\omega)\, \cos(\omega t) \quad , \tag{8}$$

where $\rho_0(\omega)$ is given by (6).

In what follows we shall assume that, for many periods, the random motion of the electron can be described by the equations (7). From the solutions $x_j(t)$ of Eq. (7) it is possible to show[2,3,9] that the electron absorbs energy from the background radiation. The average rate of absorption is such that[3]

$$P_{\rm abs} = e\langle \dot{x}_1\, E_1 + \dot{x}_2\, E_2\rangle = 2\langle \dot{x}_1\, E_1\rangle = \frac{2}{3}\frac{e^2}{mc^3}\hbar\omega^3 \quad , \tag{9}$$

in agreement with (6), (7) and (8). The frequency ω is given by (4).

Therefore, according to our proposal, the equation of motion for the spiral orbit of the electron will be:

$$-\frac{d\epsilon}{dt} = \frac{d}{dt}\left(\frac{e^2}{2r}\right) = P_{\rm Larmor} - P_{\rm abs} \quad , \tag{10}$$

where $P_{\rm abs}$ is given by (9) and $P_{\rm Larmor}$ can be obtained from (1), (4) and (5) in a first approximation.

This procedure will lead to the following differential equation for r

$$\frac{dr}{dt} = \dot{r} = -\frac{4}{3}\frac{e^2}{m^2c^3r^2}\left(1 - \sqrt{\frac{a_B}{r}}\right) \quad . \tag{11}$$

The constant a_B is the Bohr radius, namely

$$a_B \equiv \frac{\hbar^2}{me^2} \equiv \frac{1}{\alpha}\frac{\hbar}{mc} \quad , \tag{12}$$

where $\alpha = \frac{e^2}{\hbar c} = \frac{1}{137}$ is the fine structure constant.

Comparison of our equation (11) with equation (12) of Seidl and Lipas[1] shows that zeropoint electromagnetic radiation brings in the factor $\left(1 - \sqrt{a_B/r}\,\right)$.

Introducing the variable u

$$u \equiv \sqrt{\frac{r}{a_B}} - 1 \quad , \tag{13}$$

equation (11) becomes

$$(1+u)^6\frac{du}{u} = -\frac{2}{3}\alpha^5\frac{mc^2}{\hbar}dt \quad , \tag{14}$$

which can be easily integrated. The result can be written as

$$t(r) = \frac{3}{2}\frac{\hbar}{\alpha^5 mc^2}\,[\,F(u_0) - F(u(r))\,] \quad , \tag{15}$$

where

$$F(u) \equiv \ln u + 6u + \frac{15}{2}u^2 + \frac{20}{3}u^3 + \frac{15}{4}u^4 + \frac{6}{5}u^5 + \frac{u^6}{6} \quad , \tag{16}$$

and

$$u_0 \equiv \sqrt{\frac{r_0}{a_B}} - 1 \quad . \tag{17}$$

Here r_0 is value of the radius at $t = 0$.

Equations (13), (15) and (16) allow us to obtain the radius r as function of the time t. According to the result (11), the spiraling motion stops when r is approaching the Bohr radius a_B given by (12). This is a remarkable feature of SED[2,9].

In order to compare our numerical results with those obtained using the quantum approach, we shall consider the time $t(r_n^B)$ it takes for the electron to go from the initial distance r_0 (from the proton) to the Bohr radii,

$$r_n^B = a_B\, n^2 \equiv \frac{\hbar^2}{me^2}\, n^2 \quad , \tag{18}$$

where $n = 1, 2, 3...$. We shall define the "lifetime" of a state n, which is immersed in the zeropoint electromagnetic radiation, by

$$\tau_n^{ZP} \equiv t(r_n^B) - t\left(r_{n-1}^B\right) \quad . \tag{19}$$

This is the definition used by Seidl and Lipas[1] in the case without the zeropoint electromagnetic radiation.

The numerical values of τ_n^{ZP} will be compared with the values τ_n, obtained by Seidl and Lipas, and the values τ_n^{QM} which are the corresponding transition times calculated according to the Quantum Mechanics prescription[1,12].

3. THE QUANTAL TRANSITION RATES

If we consider two arbitrary states of energy ϵ_f and $\epsilon_i > \epsilon_f$, the transition times τ_{if} are calculated according to the following prescription[1,12]

$$\frac{1}{\tau_{if}} = \frac{4}{3}\,\alpha\,\frac{\omega_{if}^3}{c^2}|\langle f|\vec{r}|i\rangle|^2 \quad , \tag{20}$$

where $\alpha = 1/137$ and $|i\rangle$ and $|f\rangle$ are the corresponding H-atom states of energy ϵ_i and ϵ_f. The frequencies ω_{if} will be defined below. Assuming that the states are associated to circular orbits of radius r_n^B and r_{n-1}^B, namely, $|i\rangle = |n, n-1, n-1\rangle$ and $|f\rangle \equiv |n-1, n-2, n-2\rangle$ (see ref. [1] for more details), the frequencies ω_{if} can be written as

$$\hbar\omega_{if} = \frac{mc^2\alpha^2}{2}\left[\frac{1}{(n-1)^2} - \frac{1}{n^2}\right] \quad . \tag{21}$$

Therefore, according to (20) and (21), the quantum transition times $\tau_n^{QM} \equiv \tau_{if}$ are given by

$$\tau_n^{QM} = \frac{3}{2}\,\frac{\hbar}{\alpha^5 mc^2}\left[\frac{n^4(n-1)^2}{n-1/2}\right]\left[1 + \frac{1}{4n(n-1)}\right]^{2n} \quad . \tag{22}$$

The numerical values for τ_n^{QM} are shown in the last column of the TABLE presented in the next section.

4. SUMMARY OF RESULTS

The numerical results of τ_n^{ZP} (see (19) and (15)), τ_n^{QM} (see (22)) and the corresponding τ_n obtained by Seidl and Lipas are shown in the TABLE presented below. The values of the Bohr radii r_n^B are also shown.

From this TABLE we can see that taking into account the zeropoint radiation improves significantly the agreement between the classical and the quantum lifetimes. This improvement is specially significant in the case of small n values. For the transition $n = 3$ to $n = 2$, τ_3^{ZP} is approximately 8% larger than τ_3^{QM}, while the result without the zeropoint radiation (τ_3) is approximatcly 50% smaller than τ_3^{QM}. Even for the transition $n = 10$ to $n = 9$, τ_{10} is 15% smaller than τ_{10}^{QM} whereas τ_{10}^{ZP} presents only a discrepancy of 2% as compared to τ_{10}^{QM}. Notice, that the order of magnitude has changed from 10^{-8} sec to 10^{-5} sec in the above transitions.

TABLE

n	r_n^B (cm)	τ_n (sec)	τ_n^{ZP} (sec)	τ_n^{QM} (sec)
3	4.76×10^{-8}	1.03×10^{-8}	1.67×10^{-8}	1.55×10^{-8}
4	8.46×10^{-8}	0.52×10^{-7}	0.72×10^{-7}	0.73×10^{-7}
5	1.32×10^{-7}	1.79×10^{-7}	2.29×10^{-7}	2.35×10^{-7}
10	5.29×10^{-7}	0.73×10^{-5}	0.82×10^{-5}	0.84×10^{-5}
20	2.12×10^{-6}	2.64×10^{-4}	2.78×10^{-4}	2.84×10^{-4}
50	1.32×10^{-5}	2.78×10^{-2}	2.84×10^{-2}	2.86×10^{-2}
100	5.29×10^{-5}	9.11×10^{-1}	9.20×10^{-1}	9.24×10^{-1}
1000	5.29×10^{-3}	9.31×10^{4}	9.32×10^{4}	9.33×10^{4}

A remarkable similarity between the SED and the QM approach is that spiral orbit becomes stable for r equal to the Bohr radius $\hbar^2/me^2$ (see (12) and (18)). This is shown, in FIGURES 1 and 2, by the solid line. The dashed line corresponds to the solution of equation (11) with $a_B = 0$, or $\hbar = 0$. In this case the electron spiral is inevitably associated with the collapse of the atom. In the FIGURE 3 we show the solution for an initial radius $r_0 < a_B$. In this case the electron absorbs more energy from the zeropoint background radiation than it is lost by emission, that is, the last term in equations (10) and (11) is dominant. Therefore, the solution (15) leads to a stationary orbit (stable) of radius equal to the Bohr radius.

5. PHYSICAL MECHANISM UNDERLYING THE AGREEMENT BETWEEN THE CLASSICAL AND THE QUANTUM CALCULATIONS

The standard quantum mechanical expression for the instantaneous power of the electromagnetic radiation, associated to the transition $|i\rangle \to |f\rangle$, and the consequent emission of radiation with frequency ω_{if}, is (see (20))

$$P(\omega_{if}) \equiv \frac{\hbar\omega_{if}}{\tau_{if}} = \frac{4}{3}\frac{e^2}{c^3}\omega_{if}^4 \,|\langle f|\vec{r}|i\rangle|^2 \quad . \tag{23}$$

This formula can also be written as

$$P(\omega_{if}) = \frac{4}{3}\frac{e^2}{c^3}\,|\langle f|\ddot{\vec{r}}|i\rangle|^2 \quad , \tag{24}$$

if we consider that the approximate equality, namely

$$\ddot{\vec{r}} = -\frac{e^2}{mr^3}\vec{r} \simeq -\omega_{if}^2\,\vec{r} \tag{25}$$

is valid for the transitions associated to the "circular"[1] states $|i\rangle = |n, n-1, n-1\rangle$ and $|f\rangle = |n-1, n-2, n-2\rangle$ used in section 3. A related observation is that (for $n \gg 1$) we can write equation (21) in the form

$$\omega_{if}^2 \simeq \left(\frac{mc^2\alpha^2}{2\hbar}\right)^2 \frac{4}{n^6} = \frac{e^2}{m(r_n^B)^3} \quad , \tag{26}$$

where r_n^B is the Bohr radius introduced in equation (18). This approximate result (26) is, therefore, equivalent to our previous equation (4).

An important remark should be made at this point. Let us consider the expectation value of the Larmor formula, introduced by Dalibard, Dupont-Roc and Cohen Tannoudji[13] within the Quantum Electrodynamics (QED) context, namely

$$\begin{aligned} P_{\text{Larmor}}^{\text{QED}} &= \frac{2}{3}\frac{e^2}{c^3}\,|\langle i|\ddot{\vec{r}}|i\rangle|^2 \equiv \\ &\equiv \frac{2}{3}\frac{e^2}{c^3}\sum_f \langle i|\ddot{\vec{r}}|f\rangle\langle f|\ddot{\vec{r}}|i\rangle \quad , \end{aligned} \tag{27}$$

which is entirely analogous to the Larmor formula of classical radiation theory. The identity in the second expression in (27) follows from the fact that $\sum_f |f\rangle\langle f| = 1$.

Within the QED approach the electron also absorbs energy from the vacuum electromagnetic fluctuations. According to the authors of reference [13] the rate of absorption is such

$$\begin{aligned} P_{\text{abs}}^{\text{QED}} &= \frac{2}{3}\frac{e^2}{c^3}\left[\sum_{f(\epsilon_f>\epsilon_i)} \langle i|\ddot{\vec{r}}|f\rangle\langle f|\ddot{\vec{r}}|i\rangle + \right. \\ &\left. - \sum_{f(\epsilon_f<\epsilon_i)} \langle i|\ddot{\vec{r}}|f\rangle\langle f|\ddot{\vec{r}}|i\rangle\right] \quad . \end{aligned} \tag{28}$$

The first term contains the *upward* transitions $|i\rangle \to |f\rangle$ induced by the zeropoint radiation with spectral distribution $\rho_0(\omega)$ as given by (6). The second term is associated to *downward* transitions $|i\rangle \to |f\rangle$ *stimulated* by the same zeropoint radiation. The

derivation of these results for the motion in the Coulomb field is rather lengthy[13]. However, a more simple derivation can be obtained in the case of a harmonic oscillator[14].

According to Dalibard et al.[13] the total rate of variation of the energy ϵ_i is given by (see our equation (10) for comparison)

$$-\frac{d\epsilon_i}{dt} \equiv P^{\rm QED}_{\rm Larmor} - P^{\rm QED}_{\rm abs} \quad . \tag{29}$$

Using (27) and (28) we get

$$-\frac{d\epsilon_i}{dt} = +\frac{4}{3}\frac{e^2}{c^3} \sum_{f(\epsilon_f<\epsilon_i)} \langle i|\ddot{\vec{r}}|f\rangle\langle f|\ddot{\vec{r}}|i\rangle = \sum_{f(\epsilon_f<\epsilon_i)} P\left(\omega_{if}\right) \quad , \tag{30}$$

where $P(\omega_{if})$ is given by equation (24).

6. DISCUSSION

The result (30) is very suggestive and deserves a few comments. According to Dalibard, Dupont-Roc and Cohen Tannoudji[13]. "Such a result is extremely simple and exactly coincides with that found in classical radiation theory. The rate of radiation of electromagnetic energy is proportional to the square of the acceleration of the radiating charge, the proportionality coefficient being just the one appearing in (24). We note also that, if self reaction was alone, the atomic ground state would not be stable, since the square of the acceleration (see (27)) has a non zero average value in such a state".

According to Dalibard et al.[13]: "The previous discussion clearly shows that the (atomic) ground state cannot be stable in the absence of vacuum fluctuations which exactly balance the energy loss due to self reaction. ... . When applied to the case of an atomic electron interacting with the vacuum field, such a procedure gives results in complete agreement with the usual picture associated with vacuum fluctuations and self reaction. All self reaction effects, which are independent of $\hbar$, are strictly identical to those derived from classical radiation theory. All vacuum fluctuation effects, which are proportional to $\hbar$, can be interpreted by considering the vibration of the electron induced by a random field having a spectral power density equal to $\hbar\omega/2$ per mode". Similar conclusions were reached, more recently, by França, Marshall and Santos[15] which have described classicaly the modifications in the spontaneous

emission observed in the excited ("circular") states of Cesium atoms passing between two parallel mirrors[16].

Finally we would like to stress that the present approach can shed some light on the difficult (not solved yet in a satisfactory manner[17]) problem of the stability of the H-atom when immersed in thermal radiation. In this case our equation (9) is modified to

$$P_{\rm abs} = \frac{2}{3}\frac{e^2}{mc^3}\hbar\,\omega^3 \left[1 + \frac{2}{\exp\left(\frac{\hbar\omega}{kT}\right) - 1}\right] \quad , \tag{31}$$

where T is the temperature, and k is the Boltzmann constant. A calculation related to this problem, and based on our equations (10) and (31), is in progress.

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FIGURES AND FIGURES CAPTION

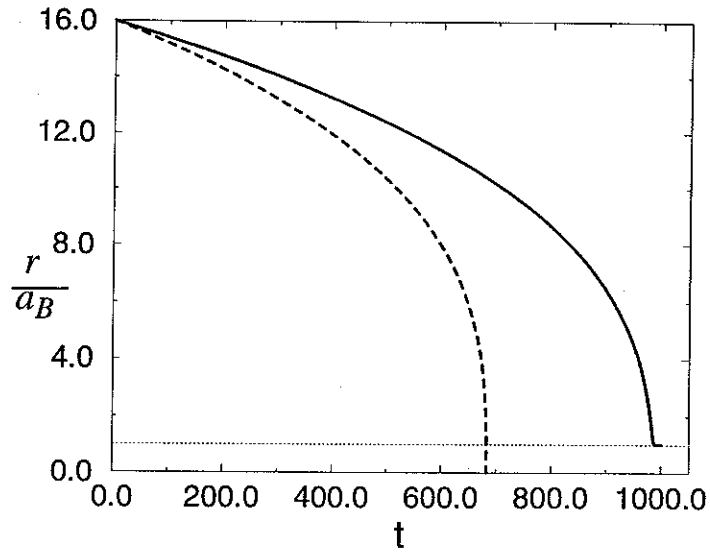

Figure 1: Spiraling motion starting at $r_0 = r_4^B$ (see equation(18)). Solid line: classical model including the zeropoint electromagnetic radiation. Dashed line: Seidl and Lipas[1] classical model (without the zeropoint electromagnetic radiation). The dotted line is $r/a_B = 1.0$. The time unit is $\frac{3}{2}\frac{\hbar}{mc^2\alpha^5}$.

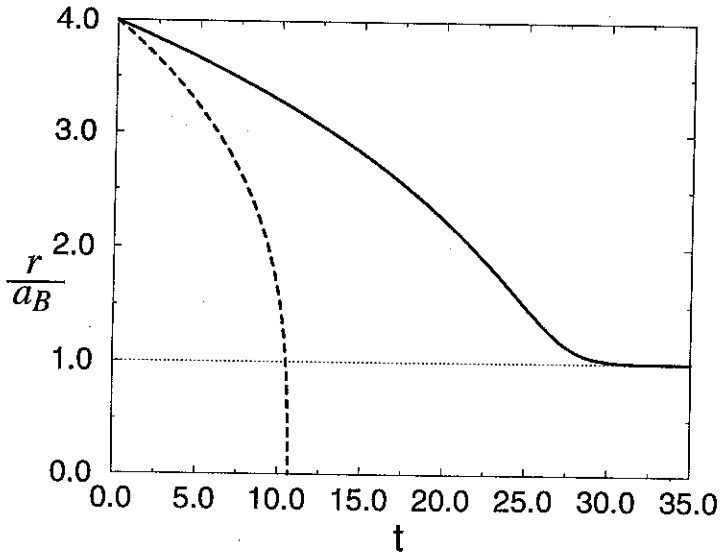

Figure 2: Illustrating the atom stability due to the inclusion of the zeropoint electromagnetic radiation (solid line). The dashed line is the spiraling motion using the model of Seidl and Lipas. Initial condition: $r_0 = r_2^B$. When $r_0 > a_B$ the spiraling motion is inward in both models. The time unit is the same of figure 1. The dotted line corresponds to $r = a_B$.

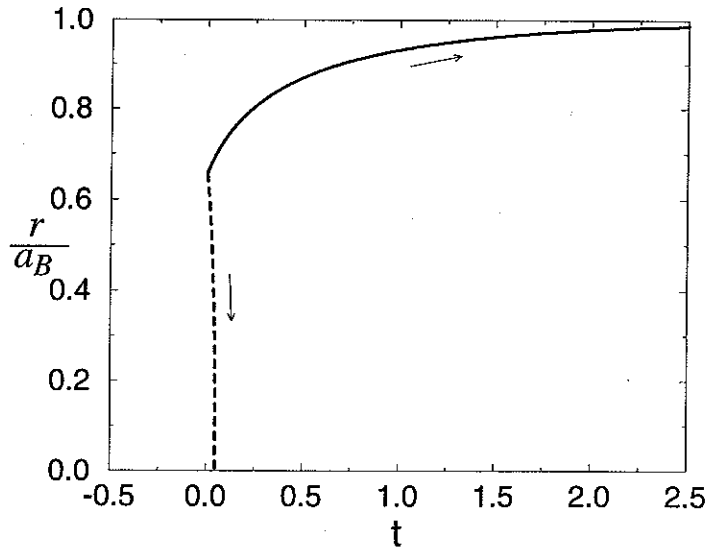

Figure 3: Spiraling motion of the electron for $r_0 < a_B$. The electron spirals outward in the case with the zeropoint electromagnetic radiation (solid line) while in the case of the model of Seidl and Lipas the spiraling is inward (dashed line). The time unit is the same of figure 1.