Classical calculation of radiative lifetimes of atomic hydrogen in a homogeneous magnetic field

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Radiative lifetimes of hydrogenic atoms in a homogeneous magnetic field of moderate strength are calculated on the basis of classical radiation. The modifications of the Keplerian orbits due to the magnetic field are incorporated by classical perturbation theory. The model is complemented by a classical radiative decay calculation using the radiated Larmor power. A recently derived highly accurate formula for the transition rate of a field-free hydrogenic state is averaged over the angular momentum oscillations caused by the magnetic field. The resulting radiative lifetimes for diamagnetic eigenstates classified by n,m and the diamagnetic energy shift C compare well with quantum results.

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I. INTRODUCTION

The modeling of radiative cascades of even the simplest atoms such as hydrogen arises in the context of astrophysics and laboratory plasmas [1]. The fact that a classical model of the atom serves well in this context was proposed earlier [2] and has been developed in the literature [3,4]. Recently we have shown that the quantum-electrodynamics problem of hydrogenic spontaneous decay has a parallel in classical electrodynamics with classical lifetimes and branching ratios that match the quantum results accurately [5].

In the present work, we treat the radiative decay of a hydrogen atom in the presence of an external homogeneous magnetic field. This treatment is restricted to fields of small to moderate size, where the effect of the magnetic field can be treated as a perturbation to the field-free atom:

$$B < \frac{1 \text{ a.u.}}{n^3} = \frac{2.35 \times 10^5 \text{ T}}{n^3}. \tag{1}$$

Reference [6] gives a treatment of the classical hydrogen atom (without the inclusion of radiative decay) in this regime.

The classical and quantum descriptions of the atom both show conservation of energy E and of L_z (the component of angular momentum $\mathbf{L}$ along the direction of the magnetic field $B\hat{z}$). L^2 is not a conserved quantity in either description. In quantum mechanics the eigenstates are linear combinations of states with different L^2 eigenvalues, and these states can be labeled according to the value of their diamagnetic energy F [7,8]. In classical mechanics the value of L^2 oscillates in time.

The effect of the magnetic field on the classical elliptical orbits [6] is, first of all, to cause the orbital plane to precess, such that $\mathbf{L}(t)$ precesses about the direction of the magnetic field at the Larmor frequency $\Omega = eB/2\mu$. One can view the atom from within a frame of reference rotating at this frequency. The resulting Hamiltonian no longer contains the term linear in B which caused the precession, but only contains diamagnetic terms that are quadratic in B. In this frame of reference, without the inclusion of these quadratic terms, the classical orbit is a simple Kepler orbit in a fixed plane which is inclined at some fixed angle relative to the direction of the magnetic field.

For moderate B field magnitudes, the quadratic terms lead to a number of perturbing effects. First, the angle of this plane relative to $\mathbf{B}$ oscillates in time at a slow frequency of approximately Ω^2/ω, where ω is the orbital frequency of the Kepler orbit. Second, the eccentricity of the orbit varies in an oscillatory fashion at this same slow frequency. Since the semimajor axis remains constant, the orbital energy remains constant; however, the oscillating eccentricity results in an oscillating value for L^2. The value of L_z remains constant, as the effects on L_z of the changing orientation and the changing L^2 exactly cancel. An additional effect of the quadratic term is to slightly alter the precession frequency. Finally, the quadratic term causes the direction of the semimajor axis to vary within the orbital plane. This variation can be of two types, depending on the particular orbit considered (i.e., on the particular values of E, L_z, and F). In the first type, called librator states, the direction of the semimajor axis oscillates and thus is restricted to a limited range of angles. In the second type of orbit, called rotator states, this angle rotates through the full 360°.

At present, we treat the problem only to first order in the perturbations. We do not consider larger magnetic fields, where the problem becomes chaotic; nor do we treat the even larger magnetic fields where the magnetic field interactions dominate and the Coulomb interactions are perturbations on the cyclotron orbits.

II. CLASSICAL RADIATIVE DECAY

Previously, we have described the classical radiative decay of magnetic-field-free classical hydrogen-atom orbits due to classical radiation as described by the Larmor formula. A classical estimate of the lifetime is obtained by considering the Fourier components and polarization of this classical radiation [5]:

$$\frac{1}{\tau_{\text{cl}}^{B=0}} = \frac{2}{\tau_0} \sum_{k=1}^{\infty} k \left(J_k'^2(k\epsilon) + \frac{1-\epsilon^2}{\epsilon^2} J_k^2(k\epsilon) \right), \tag{2}$$

where the eccentricity of the classical orbit depends on the orbital energy E and angular momentum magnitude L according to

$$\epsilon = \sqrt{1 + \frac{2EL^2}{\kappa^2 \mu}}, \tag{3}$$

$$\kappa = \frac{Ze^2}{4\pi\epsilon_0}, \tag{4}$$

μ is the electron mass, and Z is the nuclear charge, and τ_0 can be written as

$$\tau_0 = \sqrt{\frac{\mu^3}{2|E|^5}} \frac{3\kappa^5}{8\hbar^4 Z^4 \alpha^5 c^2}. \tag{5}$$

To apply the classical approach to the case of an atom exposed to a magnetic field, we need to understand the variation of the Kepler orbit parameters with time. Since the classical radiation rate is independent of the orientation of the orbital plane and the orientation of the semimajor axis, we need only deal with the variation of L^2 with time. This variation is determined by the differential equation for $u = L^2$:

$$\dot{u}^2 = \frac{\Omega^4}{E^2}(u - u_{\min})(u_{\max} - u)(u_c - u), \tag{6}$$

where we have defined the quantities

$$u_{\min} = 2L_z^2 - \frac{4FE}{\Omega^2} - \sqrt{\left(2L_z^2 - \frac{4FE}{\Omega^2}\right)^2 + \frac{5L_z^2 \mu\kappa^2}{2E}}, \tag{7}$$

$$u_{\max} = \begin{cases} 2L_z^2 - \dfrac{4FE}{\Omega^2} + \sqrt{\left(2L_z^2 - \dfrac{4FE}{\Omega^2}\right)^2 + \dfrac{5L_z^2 \mu\kappa^2}{2E}}, & F < F_0, \\ \dfrac{2FE}{\Omega^2} + \dfrac{1}{4}\left(L_z^2 - \dfrac{5\mu\kappa^2}{2E}\right), & F > F_0, \end{cases} \tag{8}$$

$$u_c = \begin{cases} \dfrac{2FE}{\Omega^2} + \dfrac{1}{4}\left(L_z^2 - \dfrac{5\mu\kappa^2}{2E}\right), & F < F_0, \\ 2L_z^2 - \dfrac{4FE}{\Omega^2} + \sqrt{\left(2L_z^2 - \dfrac{4FE}{\Omega^2}\right)^2 + \dfrac{5L_z^2 \mu\kappa^2}{2E}}, & F > F_0, \end{cases} \tag{9}$$

with the critical value

$$F_0 = \left(2L_z^2 + \frac{\mu\kappa^2}{|E|}\right)\frac{\Omega^2}{16|E|}. \tag{10}$$

The following inequalities are satisfied:

$$L_z^2 \leqslant u_{\min} \leqslant u(t) \leqslant u_{\max} \leqslant \frac{\mu\kappa^2}{2|E|} < u_c. \tag{11}$$

The solution to Eq. (6) for the angular momentum magnitude oscillations can be obtained in terms of elliptic functions sn and $\mathbf{K}$ as

$$u(t) = u_{\min} + (u_{\max} - u_{\min})\mathrm{sn}^2\left(\frac{\mathbf{K}(\gamma)}{\pi}\Omega_u t, \gamma\right), \tag{12}$$

where the elliptic modulus is

$$\gamma = \sqrt{\frac{u_{\max} - u_{\min}}{u_c - u_{\min}}} \tag{13}$$

and the angular frequency of the oscillations is given as

$$\Omega_u = \frac{\pi\Omega^2\sqrt{u_c - u_{\min}}}{2|E|\mathbf{K}(\gamma)}. \tag{14}$$

The elliptic modulus $0 < \gamma < 1$ characterizes the shape of the angular momentum oscillations. For small γ the oscillations are approximately harmonic. In the limit of $\gamma \to 1$, which happens at the separatrix between the librator and rotator solutions, the period of oscillation goes to infinity and the oscillations become very anharmonic. Small-γ regimes occur for both small and large diamagnetic energies F.

For moderate-sized magnetic fields, where Ω_u is much smaller than the orbital frequency ω, the classical radiation given off by $B \neq 0$ orbits can be obtained by averaging the known radiation given off by the $B = 0$ orbits, for which L^2 (and thus ϵ) are static, over one cycle of variation of $u = L^2$. Thus,

$$\frac{1}{\tau_{\mathrm{cl}}^{B\neq 0}} = \frac{\Omega_u}{2\pi}\int_0^{2\pi/\Omega_u} \frac{dt}{\tau_{\mathrm{cl}}^{B=0}}, \tag{15}$$

where $\tau_{\mathrm{cl}}^{B=0}$ is given by Eq. (2) and varies in time since ϵ [given by Eq. (3)] depends on $u = L^2$ [given by Eq. (12)].

Using Eq. (6), time can be changed to u as the integration variable. The integral can be further simplified by using the approximation obtained in Ref. [9], where it is shown that the infinite series of Bessel functions of Eq. (2) can be approximated to better than 100 ppm by

$$\tau_{\mathrm{cl,approx}}^{B=0} = \frac{\tau_0(1-\epsilon^2)}{1 + \frac{19}{88}\left[\left(\frac{1}{\epsilon^2} - 1\right)\ln(1-\epsilon^2) + 1 - \frac{\epsilon^2}{2} - \frac{\epsilon^4}{40}\right]}. \tag{16}$$

Thus, a very accurate (better than 100 ppm) estimate of the classical lifetime in a magnetic field is

$$\frac{1}{\tau_{\mathrm{cl}}^{B\neq 0}} \approx \frac{\sqrt{u_c - u_{\min}}}{2\mathbf{K}(\gamma)} \times \int_{u_{\min}}^{u_{\max}} \frac{du}{\tau_{\mathrm{cl,approx}}^{B=0}\sqrt{(u - u_{\min})(u_{\max} - u)(u_c - u)}}, \tag{17}$$

which can easily be solved numerically (e.g., using MAPLE).

A second and less accurate approximation to Eq. (2), which is good to 10%, is given in Ref. [3]:

$$\tau_{\mathrm{cl}}^{B=0} \approx \tau_0(1 - \epsilon^2). \tag{18}$$

The relationship of this approximation to the exact classical result has been explained recently [9]. It represents a small-ϵ approximation to Eq. (16) with deviations beginning at order

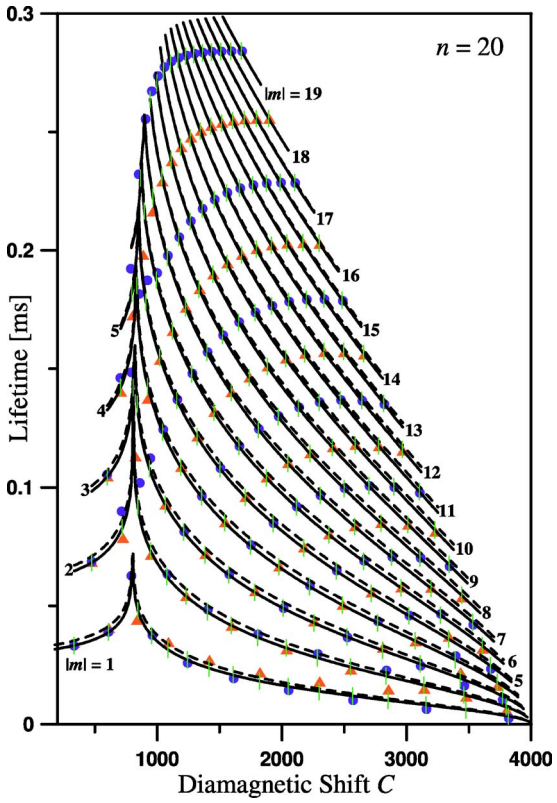

FIG. 1. (Color online) Lifetimes of neutral hydrogen versus the dimensionless diamagnetic energy shift C shown for $n=20$, $|L_z|/\hbar = |m| = 1,2,\ldots,19$. Quantum-mechanical results are shown as circles for odd-parity and as triangles for even-parity states. The solid lines are the present classical results of Eq. (17); the dashed lines are the approximate closed-form classical results of Eq. (19). The short vertical tick marks show the values of C predicted according to semiclassical quantization.

$O(\epsilon^4)$. Although this second approximation is less accurate, it has the distinct advantage of allowing for an analytic solution to the integral of Eq. (17):

$$\tau_{\rm cl}^{B\neq 0} \approx \left(\frac{\tau_0 2|E|}{\mu\kappa^2}\right)\frac{u_{\rm min}\mathbf{K}(\gamma)}{\mathbf{\Pi}(1-u_{\rm max}/u_{\rm min},\gamma)}, \tag{19}$$

where $\mathbf{\Pi}$ is the complete elliptic integral of the third kind.

III. COMPARISON OF QUANTUM AND CLASSICAL LIFETIMES

In Fig. 1, we demonstrate the usefulness of the classical decay calculations by comparing the classically derived lifetimes of Sec. II to the quantum-mechanical lifetimes for the $n=20$ state of neutral hydrogen. The x axis of the plot is a dimensionless diamagnetic shift

$$C = \frac{F}{\lambda}, \tag{20}$$

where

$$\lambda = \frac{B^2e^2\hbar^2}{64\mu^2|E|}. \tag{21}$$

Whereas classical mechanics allows for continuous values of E, L_z, and C, quantum mechanics restricts the allowed values to

$$E = -Z^2\mathcal{R}/n^2 \quad (n=1,2,\ldots), \tag{22}$$

$$L_z = m\hbar \quad (m=-n+1,-n+2,\ldots,n-2,n-1), \tag{23}$$

as well as allowing for only discrete values of C for each value of n and m.

Figure 1 shows the classical lifetime estimates obtained by both Eq. (17) (solid black line) and the more approximate Eq. (19) (dashed black line) for $E=-\mathcal{R}/20^2$ and for quantum-mechanically allowed values of L_z. Note that the lifetimes are identical for corresponding positive and negative values of L_z. Equations (17) and (19) fail for $L_z=0$ since Eq. (2) is not valid for $L^2=0$ states. Also shown on the plot are the quantum-mechanical lifetimes (circles for odd-parity states, triangles for even-parity states). The fact that the quantum-mechanical lifetimes lie almost directly on the classically derived curves shows the correspondence between classical and quantum physics for this radiating system.

The bulk of the states show excellent agreement between the classical estimates and the quantum-mechanical lifetimes. For over 80% of the $n=20$ states the agreement is better than 1%, and a similar level of agreement is found for other n values. Even the analytic approximation of Eq. (19) (the dashed curve in Fig. 1) gives a good approximation to the quantum-mechanical lifetimes (within 10% for 90% of the states).

There are two regions where the agreement between the classical and quantum-mechanical values is somewhat worse, and both result from physics that is not present in the classical treatment. The first region is at low $|m|$, where the classical result is nearly halfway between the quantum results for odd-parity (circles) and even-parity (triangles) wave functions. The classical result cannot reproduce the separation between odd- and even-parity wave functions, since this concept of parity is not present in classical physics. In quantum mechanics the odd-parity $m=1$ states, for example, have some p-state character and are therefore shorter lived than the even-parity states that do not have any admixture of the short-lived p state. For $m=2$ the situation is reversed, since $l=2,4,\ldots$, and $l=3,5,\ldots$ are mixed in this case for even and odd parities, respectively.

The second region where the agreement is somewhat worse is near $C=C_0$, where

$$C_0 = \frac{F_0}{\lambda} = 2(n^2+m^2) \tag{24}$$

separates the classical librator states at low C from the classical rotator states at higher C and leads to the cusps seen in Fig. 1. In this regime, quantum physics allows for tunneling, whereas classical physics demands firm turning points for the librations.

The classically allowed values of C are shown by the extent of each of the solid curves in Fig. 1. They range from

$$C_{\min} = 4|m|(\sqrt{5}n - 2|m|) \tag{25}$$

to

$$C_{\max} = 2(5n^2 - 3m^2). \tag{26}$$

The quantum-mechanically allowed values of C are discrete values within the classically allowed range. The allowed values can be obtained by diagonalizing the Hamiltonian for the system or, of course, by measuring the diamagnetic shifts of the states. Useful approximate values for the allowed C values come from semiclassical quantization (cf. Ref. [6]) which demands that

$$-\frac{1}{2} + \frac{m^2\hbar}{4\pi r}\int_{u_{\min}}^{u_{\max}} \frac{\hbar^2(C/2 - n^2 - m^2)[n^2\hbar^2 - u^2/(m^2\hbar^2)] - 4(n^2\hbar^2 - u)^2}{(n^2\hbar^2 - u)(u - m^2\hbar^2)\sqrt{(u - u_{\min})(u_{\max} - u)(u_c - u)}} du \tag{27}$$

be an integer, where

$$r = \begin{cases} 1, & C < C_0, \\ 1/2, & C > C_0. \end{cases} \tag{28}$$

The integral can be expressed as

$$-\frac{1}{2} + \frac{(C/2 - n^2 + 3m^2)\mathbf{K}(\gamma) - (C/2 - n^2 - m^2)W(n^2\hbar^2) - (C/2 - 5n^2 + 3m^2)W(m^2\hbar^2)}{2\pi r\sqrt{u_c - u_{\min}}/\hbar}, \tag{29}$$

where we have defined

$$W(u) = \frac{u}{u - u_{\min}}\mathbf{\Pi}\left(\frac{u_{\max} - u_{\min}}{u - u_{\min}}, \gamma\right). \tag{30}$$

Here $\mathbf{K}$ and $\mathbf{\Pi}$ are complete elliptic integrals of the first and third kinds, respectively. These expressions are simpler than those obtained from uniform semiclassical quantization using group-theoretical methods [10].

Delos *et al.* [6] show that for $m \geq n/\sqrt{5}$ the classically allowed values of C are all greater than C_0, indicating that only rotator states are possible in this case. The classically allowed range of C leads to $n-m$ possible integer values in Eq. (29), thus defining the $n-m$ allowed values of C. For $m < n/\sqrt{5}$, things are more complicated, since both librator and rotator states are possible. In this case, each value of $C > C_0$ which leads to an integer in Eq. (29) corresponds to one quantum state, while each value of $C < C_0$ which leads to an integer corresponds to two degenerate states, due to the motion of the librator states in a double-well potential (cf. Ref. [11]). Sometimes this leads to one fewer or one extra state compared to the expected $n-m$ quantum states. In these cases, the correct number of states can be obtained by adding a state at $C = C_0$ or removing one state by counting the highest $C < C_0$ as a single state rather than a degenerate pair.

Figure 1 shows these semiclassical quantization allowed values of C as vertical tick marks centered on the solid curves. The fact that the vertical tick marks fall at almost exactly the same values of C as the triangles and circles shows that semiclassical quantization [as represented by Eq. (29)] does very well in estimating the quantum-mechanically allowed values of C. It should be stressed that semiclassical quantization is not necessary for demonstrating the excellent correspondence between classical and quantum predictions for the decay rates, since that is already demonstrated by the fact that the quantum-mechanical lifetimes fall on the solid curves of Fig. 1. The semiclassical quantization simply allows one to use a simple analytic formula [Eq. (29)] to approximate the quantum-mechanically allowed values of C.

To summarize, we have shown a close correspondence between classical and quantum physics for calculated radiative lifetimes. We have shown that the classical rates agree with the quantum-mechanical rates to within 1% for the bulk of the states. We have given an analytic approximate form for the classical rates and have also provided an analytic form for the semiclassical quantization which can be used to accurately estimate the quantum-mechanically allowed diamagnetic shifts. These formulas allow for a very simple calculation of the lifetimes of hydrogenic states in a moderate-sized magnetic field.

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