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Temporal behavior and quantum Zeno time of an excited state of the hydrogen atom

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Abstract

The quantum "Zeno" time of the 2P-1S transition of the hydrogen atom is computed and found to be approximately 3.59×10^{-15} s (the lifetime is approximately 1.595×10^{-9} s). The temporal behavior of this system is analyzed in a quantum field theoretical framework and compared to the exponential decay law. © 1998 Published by Elsevier Science B.V.

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Unstable systems decay according to an exponential law. Such a law has been experimentally verified with very high accuracy on many quantum mechanical systems. Yet, its logical status is both subtle and delicate, because the temporal behavior of quantum systems is governed by unitary evolutions. The seminal work by Gamow [1] on the exponential law, as well as its derivation by Weisskopf and Wigner [2] are based on the assumption that a pole near the real axis of the complex energy plane dominates the temporal evolution of the quantum system. This assumption leads to a spectrum of the Breit-Wigner type [3] and to the Fermi golden rule [4]. However, it is well known that a purely exponential decay law can neither be expected for very short [5] nor for very long [6] times. The domain of validity of the exponential law is limited: The long-time power tails and the short-time quadratic behavior are unavoidable consequences of very general mathematical properties of the Schrödinger equation [7].

The short-time behavior [8], in particular, turns out to be very interesting, due to its apparently paradoxical consequences leading the so-called quantum Zeno effect. Recent theoretical and experimental work [9] has focused on the temporal behavior of a two-level system whose Rabi oscillations, induced by an r.f. field, are hindered by another, "measuring" field of different frequency. It should be noticed, however, that the idea of making use of an oscillating system to test the quantum Zeno effect is at variance with the original proposals, based on truly unstable systems [8]. For this reason, alternative schemes were recently proposed [10,11], that do not require any reinterpretation of the experimental data [12].

The purpose of this Letter is to investigate the characteristic features of the short-time nonexponential region of a *truly unstable system*. Our attention will be focused on a transition of the hydrogen atom: We shall

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endeavor to give an accurate estimate of the "Zeno" time for this system. Our general conclusions, however, will be valid for any two-level system interacting with a quantum field (as far as the theory is renormalizable).

Let us start by outlining the main features of the problem. Let $|\psi_0\rangle$ be the wave function of a given quantum system at time t=0. The evolution is governed by the unitary operator $U(t)=\exp(-\mathrm{i}Ht/\hbar)$, where H is the Hamiltonian. The "survival" or nondecay probability at time t is the square modulus of the survival amplitude,

$$P(t) = |\langle \psi_0 | e^{-iHt/\hbar} | \psi_0 \rangle|^2 = 1 - t^2 / \tau_Z^2 + \dots,$$
 (1)

$$\tau_{\rm Z}^{-1} \equiv \frac{\Delta H}{\hbar} = \frac{1}{\hbar} (\langle \psi_0 | H^2 | \psi_0 \rangle - \langle \psi_0 | H | \psi_0 \rangle^2)^{1/2}. \tag{2}$$

The short-time expansion is quadratic in t and therefore yields a vanishing decay rate for $t \to 0$. This quadratic behavior is in manifest contradiction with the exponential law that predicts an initial nonvanishing decay rate (the inverse of the lifetime). The quantity τ_Z will be referred to as "Zeno time" in the present Letter.

Unfortunately, when one considers quantum field theory, things do not work out that easily. In the above (naive) derivation, one assumes that all moments of H in the state $|\psi_0\rangle$ are finite and (implicitly) that $|\psi_0\rangle$ is normalizable and belongs to the domain of definition of H [13]. If the volume of the box containing the system is not finite, the spectrum of the Hamiltonian is continuous and the Zeno time turns out to be inversely proportional to some power of a frequency cut-off Λ : $\tau_Z \propto 1/\Lambda^{\alpha}$. This is a very general property, essentially due to the singular nature of the product of local observables when computed at short distances [14].

However, if the theory is renormalizable, this divergence can be tamed by introducing a *natural* cutoff for the system. In the present Letter we shall just concentrate our attention on such a situation: We will show that it is indeed possible to compute the value of τ_Z for the 2P–1S transition of the hydrogen atom. The result is finite. This confirms that a quantum Zeno region is not simply a phenomenon peculiar to the quantum mechanics of finite systems; rather, it is present even in the more general framework of quantum field theory, at least for a renormalizable theory.

We start from the total Hamiltonian ($\hbar = c = 1$)

$$H = H_{\text{atom}} + H_{\text{EM}} + H_{\text{int}}$$

$$= \sum_{i=1}^{2} E_{i} |i\rangle\langle i| + \sum_{\beta} \int_{0}^{\infty} d\omega \, \omega a_{\omega\beta}^{\dagger} a_{\omega\beta}$$

$$+ \sum_{\beta} \int_{0}^{\infty} d\omega [\varphi_{\beta}(\omega) a_{\omega\beta}^{\dagger} |1\rangle\langle 2|$$

$$+ \varphi_{\beta}^{*}(\omega) a_{\omega\beta} |2\rangle\langle 1|], \qquad (3)$$

where the first term is the free Hamiltonian of a two-level atom, the second term the Hamiltonian of the free EM field and the third term the interaction Hamiltonian. We considered only the linear part of the interaction (in the so-called rotating wave approximation) and expanded it in the energy-angular momentum basis for photons [15], with $\sum_{\beta} = \sum_{j=1}^{\infty} \sum_{m=-j}^{j} \sum_{\lambda=0}^{1}$, where $|i\rangle(i=1,2)$ are the atomic states (of energy E_i), λ defines the photon parity $P=(-1)^{j+1+\lambda}$, j is the total angular momentum (orbital + spin) of the photon, m its magnetic quantum number and

$$[a_{\omega jm\lambda}, a^{\dagger}_{\omega' j'm'\lambda'}] = \delta(\omega - \omega')\delta_{jj'}\delta_{mm'}\delta_{\lambda\lambda'}. \tag{4}$$

The quantities $\varphi_{\beta}(\omega)$ are the matrix elements of the interaction Hamiltonian between the states

$$|1; 1_{\omega\beta}\rangle \equiv |1\rangle \otimes |\omega, j, m, \lambda\rangle, |2; 0\rangle \equiv |2\rangle \otimes |0\rangle,$$
 (5)

where the first ket refers to the atom and the second to the photon. We now concentrate our attention on the 2P-1S transition of hydrogen, $|1\rangle \equiv |n_1 = 1, l_1 = 0, m_1 = 0\rangle, |2\rangle \equiv |n_2 = 2, l_2 = 1, m_2\rangle$. Conservation of angular momentum and parity ensures the validity of the selection rules $j = 1, m = m_2, \lambda = 1$. This reduces the sum over β in the interaction Hamiltonian to the single term $\bar{\beta} = (1, m_2, 1)$. In this case, the matrix elements were exactly evaluated by Moses [16] and Seke [17]

$$\varphi_{\beta}(\omega) = \langle 1, 1_{\omega\beta} | H_{\text{int}} | 2, 0 \rangle = \varphi_{\bar{\beta}}(\omega) \delta_{\beta\bar{\beta}}$$

$$= i(\chi \Lambda)^{1/2} \frac{(\omega/\Lambda)^{1/2}}{[1 + (\omega/\Lambda)^2]^2} \delta_{j1} \delta_{mm_2} \delta_{\lambda 1}, \tag{6}$$

with

$$\Lambda = \frac{3}{2} \alpha m_e \simeq 8.498 \times 10^{18} \text{ rad/s},$$

$$\chi = \frac{2}{\pi} \left(\frac{2}{3}\right)^9 \alpha^3 \simeq 6.435 \times 10^{-9},$$
(7)

where α is the fine structure constant and m_e the electron mass. Λ is the *natural* cut-off defining the atomic form factor and taking into account all retardation effects: in natural units, $\Lambda = 3/2a_0$, where a_0 is the Bohr radius, so that wavelengths shorter than a_0 do not contribute significantly to the interaction. The physical origin of Λ is ascribable to the exponential behavior of the atomic orbitals, which fall off like $\exp(-r/na_0)$ (where r is the radial coordinate and n the principal quantum number): for the 2P–1S transition, the orbitals overlap like $\exp(-r/a_0) \cdot \exp(-r/2a_0) = \exp(-r\Lambda)$. Notice that Λ is not put "by hand", like in analysis involving the dipole approximation, but naturally emerges from calculation [16,17].

We assume that the system is initially (at time t=0) in the eigenstate $|2,0\rangle$ of the unperturbed Hamiltonian $H_0=H_{\rm atom}+H_{\rm EM}$, whose eigenvalue is $\omega_0=E_2-E_1=\frac{3}{8}\alpha^2m_e\simeq 1.550\times 10^{16}~{\rm rad/s}$. We shall set $E_1=0$. It is now straightforward to compute the Zeno time, according to the definition (2),

$$\frac{1}{\tau_Z^2} = \langle 2, 0 | H_{\text{int}}^2 | 2, 0 \rangle$$

$$= \sum_{\beta} \int_{0}^{\infty} d\omega |\langle 2, 0 | H_{\text{int}} | 1, 1_{\omega\beta} \rangle|^2 = \int_{0}^{\infty} d\omega |\varphi_{\bar{\beta}}(\omega)|^2$$

$$= \chi \Lambda^2 \int_{0}^{\infty} dx \frac{x}{(1+x^2)^4} = \frac{\chi}{6} \Lambda^2. \tag{8}$$

Inserting the values (7) of Λ and χ we obtain

$$\tau_{\rm Z} = \sqrt{\frac{6}{\chi}} \frac{1}{\Lambda} = (3\pi)^{1/2} \left(\frac{3}{2}\right)^{7/2} \frac{1}{\alpha^{5/2} m_e}$$

$$\simeq 3.593 \times 10^{-15} \text{ s.}$$
(9)

This is our first result. It is an estimate of the duration of the Zeno region for a truly unstable system.

Observe that for hydrogen-like atoms of nuclear charge Z, the Zeno time scales (unfavorably) like Z^{-2} . This is because $\Lambda \propto Z/a_0$ and $\chi \propto Z^2\alpha^3$.

It is also worth stressing that the value of τ_Z , due to its very structure, would not be modified by the presence of counter-rotating terms in the Hamiltonian (3), whose contribution to Eq. (8) vanishes. Even

the introduction of additional atomic levels would not modify this result, within the framework of the rotating wave approximation [whose validity is discussed after Eq. (27)]. On the other hand, a straightforward but rather lengthy calculation shows that the introduction of the other atomic levels *and* of counter-rotating terms in the interaction Hamiltonian H'_{int} yields the following expression for the Zeno time,

$$\begin{split} \frac{1}{\tau_Z'^2} &= \langle 2, 0 | H_{\text{int}}'^2 | 2, 0 \rangle \\ &= \sum_{\nu,\beta} \int_0^\infty \mathrm{d}\omega \, |\langle 2, 0 | H_{\text{int}}' | \nu, 1_{\omega\beta} \rangle|^2 \simeq \frac{1.4210}{\tau_Z^2}, \end{split} \tag{10}$$

where ν is the set of atomic quantum numbers characterizing the intermediate state and matrix elements are computed as in Ref. [17]. Eq. (10) yields a -20% correction to the value of the Zeno time.

It is now interesting to look at the temporal behavior of our system at longer times. There is previous related work [18–22] on this subject. The survival amplitude and its Laplace transform read

$$y(t) = \langle 2, 0 | e^{-iHt} | 2, 0 \rangle,$$

$$\widetilde{y}(s) = \int_{0}^{\infty} dt e^{-st} y(t) = \langle 2, 0 | \frac{1}{s + iH} | 2, 0 \rangle.$$
(11)

We make use of the identity

$$\frac{1}{s+iH} = \frac{1}{s+iH_0} - i\frac{1}{s+iH_0} H_{int} \frac{1}{s+iH_0} - \frac{1}{s+iH_0} H_{int} \frac{1}{s+iH_0} H_{int} \frac{1}{s+iH}$$
(12)

and by introducing a complete orthonormal set of eigenstates of the unperturbed Hamiltonian H_0 (note that the interaction Hamiltonian $H_{\rm int}$ has nonvanishing matrix elements only between the states (5)), we easily obtain

$$\widetilde{y}(s) = \frac{1 - Q(s)\widetilde{y}(s)}{s + i\omega_0} \Rightarrow \widetilde{y}(s) = \frac{1}{s + i\omega_0 + Q(s)},$$
(13)

$$Q(s) \equiv \int_{0}^{\infty} dk |\varphi_{\bar{\beta}}(k)|^{2} \frac{1}{s + ik}.$$
 (14)

By inverting the transform we get

$$y(t) = \frac{1}{2\pi i} \int_{R} ds \frac{e^{sAt}}{s + i(\omega_0/\Lambda) + \chi \bar{Q}(s)},$$
 (15)

$$\bar{Q}(s) \equiv \frac{1}{\chi \Lambda} Q(s\Lambda) = -i \int_{0}^{\infty} dx \frac{x}{(1+x^2)^4} \frac{1}{x-is},$$
(16)

where B is the so-called Bromwich path, i.e. a vertical line at the right of all the singularities of $\tilde{y}(s)$, and we used Eq. (6). Notice that Q and \bar{Q} are self-energy contributions. It is straightforward to integrate Eq. (16) to get

$$\bar{Q}(s) = \frac{-15\pi i - (88 - 48\pi i)s - 45\pi i s^2 + 144s^3}{96(s^2 - 1)^4} + \frac{15\pi i s^4 - 72s^5 - 3\pi i s^6 + 16s^7 - 96s \log s}{96(s^2 - 1)^4}.$$
(17)

The quantity $\bar{Q}(s)$ has a logarithmic branch cut extending from 0 to $-i\infty$, and no singularities on the first Riemann sheet (physical sheet). Indeed, the fourth order zeros of the denominator $s=\pm 1$ are also zeros of the numerator and $\bar{Q}(\pm 1)=(\pm 32-5\pi i)/256$. On the second Riemann sheet the function $\bar{Q}(s)$ becomes

$$\bar{Q}_{II}(s) = \bar{Q}(se^{-2\pi i}) = \bar{Q}(s) + 2\pi i \frac{s}{(s^2 - 1)^4},$$
 (18)

where the additional term represents the discontinuity across the cut. It is easy to show that $\tilde{y}(s)$ has a pole on the second Riemann sheet. From the denominator in Eq. (15), by expanding $\bar{Q}_{\rm II}(s)$ around $-{\rm i}(\omega_0/\Lambda)-0^+=-{\rm i}(\alpha/4)-0^+$, we get a power series whose convergence radius is $\alpha/4$, because of the branching point at the origin. Therefore

$$s_{\text{pole}} = -i\frac{\alpha}{4} - \chi \bar{Q}_{\text{II}} \left(-i\frac{\alpha}{4} - 0^{+} \right) + O(\chi^{2})$$

$$= -i\frac{\alpha}{4} - \chi \bar{Q} \left(-i\frac{\alpha}{4} + 0^{+} \right) + O(\chi^{2})$$

$$\equiv -i\frac{\alpha}{4} + i\frac{\Delta E}{4} - \frac{\gamma}{24},$$
(20)

because $\bar{Q}_{\rm II}(s)$ is the analytical continuation of $\bar{Q}(s)$ below the branch cut. By Eq. (16) we get

$$\gamma = 2\pi |\varphi_{\bar{\beta}}(\omega_0)|^2 + O(\chi^2)
= 2\pi \chi \frac{\omega_0}{[1 + (\alpha/4)^2]^4} + O(\chi^2)
\simeq 6.268 \times 10^8 \text{ s}^{-1},$$
(21)

$$\Delta E = P \int_{0}^{\infty} d\omega |\varphi_{\bar{\beta}}(\omega)|^{2} \frac{1}{\omega - \omega_{0}} + O(\chi^{2}) \simeq 0.5 \chi \Lambda,$$
(22)

which are the Fermi "golden rule" (yielding the lifetime $\tau_{\rm E} = \gamma^{-1} \simeq 1.595 \times 10^{-9} \, {\rm s}$) and the second order correction to the level energy E_2 . Notice that ΔE is not the Lamb shift, but only the shift of the 2P level due to its interaction with the ground state [23,17]. Observe that for hydrogen-like atoms of nuclear charge Z, $\tau_{\rm E} \propto (\chi \omega_0)^{-1}$ scales like Z^{-4} , so that the ratio τ_Z/τ_E has the favorable scaling Z^2 . This might be important for experimental observation of the Zeno region.

The exponential law is readily obtained by deforming the original Bromwich path into a new contour $C = C_1 + C_2$, composed of a small circle C_1 turning anticlockwise around the simple pole s_{pole} on the second Riemann sheet and a path C_2 starting from $-\infty$ on the second sheet, turning around the branch point s = 0 and extending back to $-\infty$ on the first sheet. We get

$$y(t) = y_{\text{pole}}(t) + y_{\text{cut}}(t), \tag{23}$$

where

$$y_{\text{pole}}(t) = \mathcal{Z}e^{-(\gamma/2)t}e^{-i(\omega_0 - \Delta E)t + i\zeta}, \tag{24}$$

$$\mathcal{Z}e^{i\zeta} \equiv \frac{1}{1 + \chi \bar{Q}'_{II}(s_{\text{nole}})} = 1 + O(\chi), \qquad (25)$$

and the prime denotes the derivative. Notice that $\chi = O(\alpha^3)$ and $\zeta \simeq -2.02 \times 10^{-8}$. As is well known, the exponential law is obtained by neglecting the contribution arising from the branch cut. Let us estimate the latter. From Eq. (15),

$$y_{\text{cut}}(t) = \frac{1}{2\pi i} \int_{C_{2}} ds \, e^{sAt} \left(\frac{1}{s + i(\omega_{0}/\Lambda) + \chi \bar{Q}(s)} \right)$$

$$= \chi x_{0}^{2} \int_{0}^{\infty} d\xi [\xi e^{-\xi} (\xi^{2} x_{0}^{2} - 1)^{-4}]$$

$$\times \left[\left(\xi x_{0} - i \frac{\omega_{0}}{\Lambda} - \chi \bar{Q}(-\xi x_{0}) \right) \right]^{-1}, \qquad (26)$$

where $x_0 = 1/t\Lambda$. At times $t \gg \Lambda^{-1}$ (so that $x_0 \to 0$),

$$y_{\text{cut}}(t) \sim \chi x_0^2 \frac{\int_0^\infty d\xi \, \xi e^{-\xi}}{\left[-i(\omega_0/\Lambda) - \chi \bar{\mathcal{Q}}(0)\right]^2}$$
$$= -\chi \frac{\mathcal{C}}{(\omega_0 t)^2}, \tag{27}$$

$$C \equiv \left(1 - \frac{5}{8}\pi \frac{\chi}{\alpha}\right)^{-2} = 1 + \mathcal{O}(\chi). \tag{28}$$

Expressions (17)–(28) are robust against the introduction of counter-rotating terms in the Hamiltonian (3), which can be shown to contribute only first order corrections in $\chi = O(\alpha^3)$ in Eq. (17) and therefore second order corrections in Eqs. (20), (25) and (28).

Summarizing, the general expressions (valid $\forall t \ge 0$) for the survival amplitude y(t) and survival probability $P(t) = |y(t)|^2$ are, respectively,

$$y(t) = \mathcal{Z}e^{-(\gamma/2)t}e^{-i(\omega_0 - \Delta E)t + i\zeta}$$

$$-\chi \frac{\mathcal{C}}{(\omega_0 t)^2}h(t)e^{i\eta(t)}, \qquad (29)$$

$$P(t) = \mathcal{Z}^2e^{-\gamma t} + \chi^2 \frac{\mathcal{C}^2}{(\omega_0 t)^4}h^2(t) - 2\chi \frac{\mathcal{C}\mathcal{Z}}{(\omega_0 t)^2}$$

$$\times e^{-(\gamma/2)t}h(t)\cos[(\omega_0 - \Delta E)t + \eta(t) - \zeta], \qquad (30)$$

where h(t) and $\eta(t)$ are real functions satisfying

$$\lim_{t \to 0} \frac{h(t)}{(\omega_0 t)^2} = \frac{\sqrt{1 + Z^2 - 2Z \cos \zeta}}{\chi C},$$

$$\lim_{t \to \infty} h(t) = 1,$$

$$\eta(0) = \arctan\left(\frac{Z \sin \zeta}{Z \cos \zeta - 1}\right),$$

$$\lim_{t \to \infty} \eta(t) = 0. \tag{31}$$

Notice the presence of an oscillatory term in Eq. (30). Physically, this represents an interesting (fully quantum mechanical) interference effect between the cut and the pole contribution to the survival amplitude (29).

For short and long times, Eq. (30) yields

$$P(t) \sim 1 - \frac{t^2}{\tau_Z^2} \quad (t \ll \tau_Z)$$
 (32)

$$P(t) \sim \mathcal{Z}^2 e^{-\gamma t} + \chi^2 \frac{\mathcal{C}^2}{(\omega_0 t)^4} - 2\chi \frac{\mathcal{C}\mathcal{Z}}{(\omega_0 t)^2}$$
$$\times e^{-(\gamma/2)t} \cos[(\omega_0 - \Delta E)t - \zeta] \quad (t \gg \Lambda^{-1}). \tag{33}$$

Numerical investigation of Eq. (30) shows that the "long-time" expansion is already valid for rather short times $t \gtrsim 2 \times 10^{-17}$ s. For even shorter times, the system undergoes a rapid initial oscillation, of duration about $200 A^{-1} \simeq 2.3 \times 10^{-17}$ s, and then quickly relaxes towards the asymptotic expression (33). The initial convexity of the curve is given by Eq. (32), which agrees extremely well with the numerical investigation.

The above analysis clarifies an important point: In contrast with a widespread, naive expectation, the short time behavior, yielding a vanishing decay rate, is nothing but the first of a series of oscillations, whose amplitude vanishes exponentially with time, eventually leading to a power law. The asymptotic frequency of the oscillations is essentially ω_0 (see Eq. (33)): Any correction (like our ΔE , or the total Lamb shift, or fine structure effects, not considered in our analysis) is at most of order $10^{-6}\omega_0$. The transition to a power law occurs when the two summands in Eq. (29) are comparable, so that $(\omega_0 t)^2 e^{-(\gamma/2)t} \approx \chi$, namely for $t \simeq 98$ lifetimes [19–21,18].

The above conclusions, derived for the hydrogen atom in interaction with the EM field, are generally valid for a renormalizable (or superrenormalizable) theory: Any interaction Hamiltonian of the type (3), which does *not* contain derivative couplings in the fields, yields similar results. One should notice, however, that the evaluation of the duration of the Zeno region depends on the frequency cut-off: In general, one expects a dependence on some inverse power of

 Λ [14]; for example, in our case $\tau_Z = O(\Lambda^{-1})$, as in Eq. (9). An accurate estimate of Λ can in general pose a difficult problem.

An interesting problem is to understand whether the initial quadratic behavior (32) is experimentally observable. This is an experimentally challenging task, that raises interesting theoretical and experimental questions about the problem of state preparation. The time scales involved are very small, so that a sharp initial state preparation, even by modern pulsed-laser techniques, appears to be difficult. On the other hand, state preparation by means of *indirect* excitation processes, e.g. by electron or ion collision, seems more realistic.

It is also worth stressing that the problem of sharply defining the initial moment of excitation might be circumvented: Close scrutiny of Eqs. (29)–(33) suggests that experimental observation of the probability oscillations would not only provide direct evidence of the cut contribution to the survival amplitude, but also an indirect, yet convincing, proof of the presence of the Zeno region, in the light of the discussion following Eq. (33).

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