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# Semi-analytical model of hydrogen ionization by strong laser pulse at low field frequencies

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**Abstract.** We consider the interaction of hydrogen atom with a very intense low frequency laser pulse. The Henneberger-Kramers representation of the time-dependent Schrödinger equation is the most appropriate one for this purpose. It is shown that in the case of very low frequencies, the quantum dispersion of the electron wave packet plays a dominant role in the dynamics of the atom.

## Introduction

Numerous theoretical and experimental research works on the interaction of quantum systems with an electromagnetic field have been performed lately. This is mainly due to recent advances in laser technologies allowing one to obtain very high intensities. However, in modern theories, the case of intense low frequency fields is still not very well described.

A quantum system exposed to an electromagnetic field can change its state by absorbing or emitting photons. Their energy corresponds in atomic units ( $\hbar = e = m_e = 1$ ) to the frequency  $\omega_0$  of the external field. In the case of low frequencies the period of laser pulse with  $N$  cycles  $T = (2\pi N)/\omega_0$  becomes really huge.

Usually one solves numerically the time-dependent Schrödinger equation (TDSE) with initial conditions by means of a finite difference grid method or a spectral method. This leads to a system of ordinary first order differential equations in time. However, such numerical approach is no longer tractable if the frequency of the laser pulse is very small and its intensity very high. Indeed, the amplitude of the quiver motion becomes so big that the size of the spatial grid or of the basis becomes prohibitively large making the numerical calculations impossible to perform even on supercomputers. In this case, we need mathematical and physically reliable models to understand deeply the interaction mechanisms. In this contribution, we consider such a model.



## Theory

The TDSE that describes the interaction of a pulsed electric field of period  $T$  with an hydrogenlike atom writes as follows:

$$\left[ i \frac{\partial}{\partial t} - \frac{1}{2} \left( -i \vec{\nabla} + \frac{1}{c} \vec{e} A(t) \right)^2 + \frac{Z}{r} \right] \tilde{\Psi}(\vec{r}, t) = 0, \quad \tilde{\Psi}(\vec{r}, 0) = \tilde{\varphi}_0(r) = \sqrt{\frac{Z^3}{\pi}} e^{-Zr}. \quad (1)$$

$Z$  designates the nuclear charge. The vector-potential associated to the electric field is given by  $1/c A(t) = -\omega_0^{-1} \sqrt{I/I_0} \sin^2(\pi \frac{t}{T}) \sin(\omega_0 t)$ ,  $0 \leq t \leq T$ , and  $\vec{e}$  is the field polarization vector. The electron wave packet satisfies the normalization condition:

$$\int d\vec{r} |\tilde{\Psi}(\vec{r}, t)|^2 = 1,$$

that guaranties the conservation of the total probability. In our numerical calculations, the peak intensity  $I = 1 \cdot 10^{14} \text{ W/cm}^2$  ( $I_0 = 3.5 \cdot 10^{16} \text{ W/cm}^2$  is the atomic unit of intensity), the photon frequency  $\omega_0 = 0.00228$  in atomic units, and  $N = 5$ . It is easy to see that for any fixed time  $t$ , the vector-potential vanishes like  $\omega_0^2$ , if  $\omega_0 \rightarrow 0$ .

The electromagnetic field is a gauge-invariant. Any gauge transformation of electromagnetic potentials can be compensated by a corresponding phase transformation of the wave function  $\tilde{\Psi}(\vec{r}, t)$ . In such a way, we obtain different gauge-equivalent forms of Eq. (1). For example, if we use the Henneberger-Kramers (HK) representation [1]

$$\tilde{\Psi}(\vec{r}, t) = \exp \left[ b(t) (\vec{e} \vec{\nabla}_r) - \frac{i}{2} \int_0^t dt' (1/c A(t'))^2 \right] \tilde{\Phi}_{HK}(\vec{r}, t), \quad b(t) = -\frac{1}{c} \int_0^t A(t') dt',$$

we obtain from (1)

$$\left[ i \frac{\partial}{\partial t} + \frac{1}{2} \Delta_r + \frac{Z}{|\vec{r} - \vec{e} b(t)|} \right] \tilde{\Phi}_{HK}(\vec{r}, t) = 0; \quad \tilde{\Phi}_{HK}(\vec{r}, 0) = \tilde{\varphi}_0(r). \quad (2)$$

Note, that at any time  $t$ , the wave packet is normalized to unity

$$\int d\vec{r} |\tilde{\Phi}_{HK}(\vec{r}, t)|^2 = 1.$$

Here, we analyze the amplitude  $\mathcal{A}_0$  which determines the probability for the atom to stay in its ground state. For this purpose, we define

$$\langle \varphi_0 | \tilde{\Phi}_{HK}(t) \rangle = e^{i(Z^2/2)t} \mathcal{A}_0(t)$$

and obtain from (2)

$$\frac{\partial}{\partial t} \mathcal{A}_0(t) = -iZ e^{-i(Z^2/2)t} \langle \varphi_0 | \left[ \frac{1}{r} - \frac{1}{|\vec{r} - \vec{e} b(t)|} \right] \tilde{\Phi}_{HK}(t) \rangle, \quad \mathcal{A}_0(0) = 1. \quad (3)$$

In this particular case the integration volume is always limited by  $r \sim Z^{-1}$ .

Near  $t \leq t_0 \sim 0$  ( $\sqrt{I/I_0} \omega_0 / (2N)^2 t_0^3 \ll 1$ ), the amplitude is still vanishingly small. But the value  $b(t)$  being proportional to  $\omega_0^{-2}$  grows quickly in a course of time, and the ionization begins. A further quick growth of  $b(t)$  leads to the disappearance of the term  $1/|\vec{r} - \vec{e} b(t)|$  in (3). The electron leaves the vicinity of the nucleus, follows the field oscillation and simultaneously

undergoes the free evolution (dispersion). At the root-point  $t_1$ , the  $b(t_1)$  is zero again (see Fig. 1 left), and the amplitude stays constant during very short time around  $t \sim t_1$ . Afterward, the term  $1/|\vec{r}' - \vec{e}b(t)|$  disappears again.

For  $t \geq t_0$  the free solution of Eq. (2) can be written in the form

$$\tilde{\Phi}_{HK}(\vec{r}, t) = \int d^3r' G_0(\vec{r} - \vec{r}', t - t_0) \tilde{\Phi}_{HK}(\vec{r}', t_0) \quad (4)$$

with

$$G_0(\vec{r}, t) = \int \frac{d^3k}{(2\pi)^3} \exp \left[ i\vec{k} \cdot \vec{r} - i\frac{k^2}{2}t \right] \theta(t).$$

Inserting (4) in (3) we obtain

$$\begin{aligned} \mathcal{A}_0(t) &\approx \mathcal{A}_0(t_0) - iZe^{-i(Z^2/2)t_0} \int_0^{t-t_0} d\xi e^{-i(Z^2/2)\xi} \int d^3r' \int \frac{d^3r}{r} \varphi_0(r) G_0(\vec{r} - \vec{r}', \xi) \tilde{\Phi}_{HK}(\vec{r}', t_0) = \\ &\mathcal{A}_0(t_0) - \left(\frac{Z}{\pi}\right)^{5/2} e^{-i(Z^2/2)t_0} \int d^3k \frac{1 - \exp[-i(k^2/2 + Z^2/2)(t - t_0)]}{(Z^2 + k^2)^2} \Phi_{HK}(\vec{k}, t_0). \end{aligned} \quad (5)$$

where  $\Phi_{HK}(\vec{k}, t_0)$  is a Fourier transform of  $\tilde{\Phi}_{HK}(\vec{r}', t_0)$ . We write approximately

$$\Phi_{HK}(\vec{k}, t_0) \approx \frac{8\sqrt{\pi Z^5}}{(k^2 + Z^2)^2} e^{i(Z^2/2)t_0}$$

In this case for  $t > t_0$  we have

$$\mathcal{A}_0(t) \approx \frac{8Z^5}{\pi^2} e^{-i(Z^2/2)(t-t_0)} \int d^3k \frac{\exp[-i(k^2/2)(t - t_0)]}{(Z^2 + k^2)^4}, \quad \mathcal{A}_0(t_0) \approx 1 \quad (6)$$

Eq. (6) is valid for the time period  $t_0 \leq t < t_1$ . In a very narrow time-period near  $t \sim t_1$  we can fix  $\mathcal{A}_0(t) \approx \mathcal{A}_0(t_1)$  from (6). For  $t > t_1$  (second half-period of the first optical cycle) we can repeat the scheme (4) - (6), but instead of (5) we obtain

$$\mathcal{A}_0(t > t_1) = \mathcal{A}_0(t_1) - \left(\frac{Z}{\pi}\right)^{5/2} e^{-i(Z^2/2)t_1} \int d^3k \frac{1 - \exp[-i(k^2/2 + Z^2/2)(t - t_1)]}{(Z^2 + k^2)^2} \Phi_{HK}(\vec{k}, t_1), \quad (7)$$

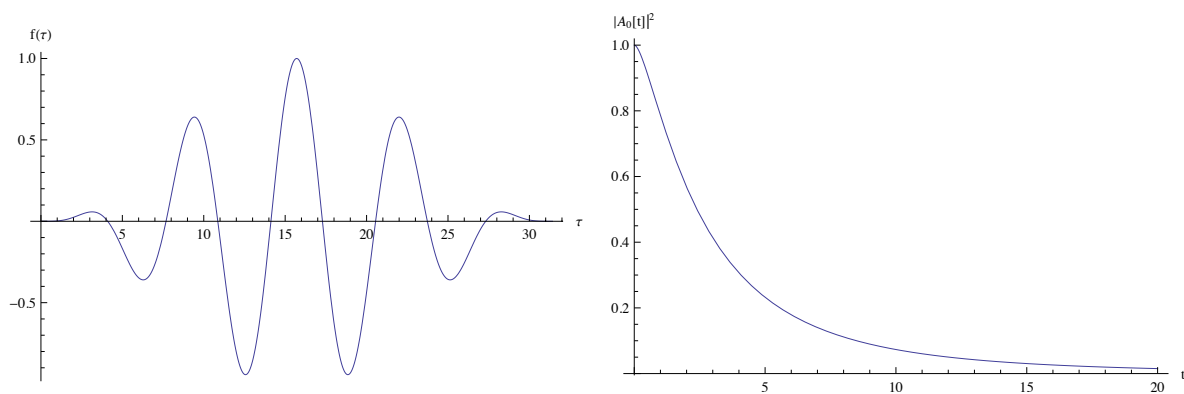
etc. The amplitude  $\mathcal{A}_0(t_1)$  is very small and continues to decrease at  $t > t_1$ . At the end of pulse after 5 optical cycles we obtain  $|\mathcal{A}_0(T)|^2 = 5 \times 10^{-11}$ .

## Conclusion

What is the physical picture implied? Two distinct physical processes determine the motion of the bound electron in the oscillating electric field. First, the quiver motion of this electron. In the absence of Coulomb potential, the electron oscillates in the field with an amplitude given by the ratio of the peak electric field and the square of the frequency in atomic units. In the present case, this amplitude is very large, of the order of 30 000 atomic units. The second process is the dispersion of the electron wave packet. For low frequencies, the dispersion time is extremely long. After each half cycle, the electrons that go back to the nucleus interact only weakly and during a rather short time with the nucleus so that the probability to stay in the ground state is hardly affected. So, at very small frequencies, the only role of the field is to push out the electron from its stationary state at the very beginning of the process. Afterward, the electron wave packet freely disperses. By contrast, for higher frequencies and shorter pulse durations, the role of the field becomes more and more dominant, while dispersion is much less important.

## References

- [1] H. A. Kramers, Les particules elementaires, Report to the Eighth Solvay Conference (Editions Stoops, Brussels, 1950); W. C. Henneberger, Phys. Rev. Lett. **21**, 838 (1968).



**Figure 1.** On the rhs: x-axis,  $\tau = \omega_0 t$ , y-axis, the reduced  $b(t) = \omega_0^{-2} \sqrt{I/I_0} f(\tau)$ .  $|A_0(t)|^2$  from (6) on the lhs. In this time scale  $t_0 \approx 0$ .