Exact theory and numeric results for short pulse ionization of simple model atom in one dimension

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Abstract

Our exact theory for continuous harmonic perturbation of a one-dimensional model atom by parametric variations of its potential is generalized for the cases when a) the atom is exposed to short pulses of an external harmonic electric field and b) the forcing is represented by short bursts of different shape changing the strength of the binding potential. This work is motivated not only by the wide use of laser pulses for atomic ionization, but also by our earlier study of the same model which successfully described the ionization dynamics in all orders, i.e. the multi-photon processes, though being treated by the non-relativistic Schrödinger equation. In particular, it was shown that the bound atom cannot survive the excitation of its potential caused by any non-zero frequency and amplitude of the continuous harmonic forcing. Our present analysis found important laws of the atomic ionization by short pulses, in particular the efficiency of ionizing this model system and presumably real ones as well.

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We study a simple one-dimensional quantum system with the attractive potential, modeled by the \( \delta \)-function. This system is assumed to be in the bound state until at some initial time \( t = 0 \) a) it becomes exposed to an external harmonic electric field or b) the strength of the system binding potential gets time dependent. The perturbation after a short interval \( T \) is turned off and our objective is to study the time evolution of the bound state on the interval \( 0 < t < T \). The pulses of external electric field are modeling the application of laser beams for atomic ionization.

Excitation of the \( \delta \)-function atom was studied in [1-6] for a simpler case of harmonic parametric perturbation of its potential when \( T = \infty \), i.e. of infinite duration, and the main conclusion was the complete ionization for arbitrary frequency and amplitude of perturbation. Other results have shown a surprising similarity of main features of the process with observed experimentally and numerically in spite of simplicity of this model.

1. PROBLEM SET UP

As in [1] we start by considering the one-dimensional stationary system located at \( x = 0 \) with an unperturbed Hamiltonian

\[
H_0 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - g \delta(x), \quad g > 0, \quad -\infty < x < \infty,
\]  

(1)
which has a single bound state
\[ u_b(p, x) = \sqrt{p} e^{-p|x|}, \quad p = \frac{m}{\hbar^2} g. \] (2)

In the continuous spectrum the eigenfunctions are
\[ u(p, k, x) = \frac{1}{\sqrt{2\pi}} \left( e^{ikx} - \frac{p}{p + i|k|} e^{i|k|x} \right), \quad -\infty < k < \infty, \] (3)

with energies \( \hbar^2 k^2 / 2m \) while the bound state energy is \( W = -\hbar \omega_0 = -\hbar^2 p^2 / 2m. \) Functions \( u(p, k, x), u_b(p, x) \) are normalized to \( \delta(k - k') \) and to unity respectfully. Parameter \( m \) represents the mass of the bound charged particle.

On the interval \( 0 \leq t \leq T \) acts a perturbing potential which is described by adding in Eq.(1) a time dependent term \( V(x, t) \)
\[ V(x, t) = eEx\eta(t), \quad \text{or} \quad V(x, t) = R\delta(x)\eta(t), \quad t \in [0, T], \] (4)

where \( \eta_{\text{max}} = 1 \) and parameters \( E, R \) are responsible for the amplitude of perturbation. Thus we have to solve the time-dependent Schrödinger equation
\[ i\hbar \frac{\partial \psi(x, t)}{\partial t} = H_0 \psi(x, t) + V(x, t)\psi(x, t), \quad t \geq 0. \] (5)

After expanding \( \psi(x, t) \) in the complete set of functions \( u \):
\[ \psi(x, t) = \theta(t)u_b(p, x)e^{it} + \int_{-\infty}^{\infty} \Theta(k, t)u(k, x)e^{-it/k^2}dk, \quad t \geq 0, \] (6)

the survival of the bound state at time \( t \leq T \) can be evaluated by \( |\theta(t)|^2 \), if we assume the system to be initially in its bound state
\[ \theta(0) = 1, \quad \Theta(k, 0) = 0. \] (7)

It is more convenient [1] to proceed in dimensionless units \( (\hbar = 2m = g/2 = 1) \) and rewrite
\[ u_b(x) = e^{-|x|}, \quad W_b = -1, \quad u(k, x) = \frac{1}{\sqrt{2\pi}} \left( e^{ikx} - \frac{e^{i|k|x}}{1 + i|k|} \right), \] (8)

where \( W_b \) is the rescaled energy of the bound state. The energies of states \( u(k, x) \) are \( W(k) = k^2 \) with multiplicity two for \( k \neq 0 \). These functions are normalized to \( \delta(k - k') \), while the bound state \( u_b(x) \) to 1.

2. DIPOLE FIELD PULSE PERTURBATION

Beginning at \( t = 0 \) a perturbing potential \( E\eta(t) \) is applied to the atom and it stops at \( t = T \). Here parameter \( E \) represents the electric field of the perturbation whose frequency is \( \omega \).

For solving Eq.(5) we use Eq.(6) and expand \( \psi(x, t) \) on the interval \( (0, T) \) in the complete set (8) of functions \( u \):
\[ \psi(x, t) = \theta(t)u_b(x)e^{it} + \int_{-\infty}^{\infty} \Theta(k, t)u(k, x)e^{-it/k^2}dk. \] (9)
Then using their orthonormality and assuming cutoff of the perturbation potential for large \(|x|\) reduce dimensionless form of Eq.(5) to the following set

\[
\dot{\theta}(t) = \frac{4E\eta(t)}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Theta(k,t) e^{-i(k^2+1)t} (k^2 + 1)^2 k dk; \quad (10a)
\]

\[
\Theta(k,t) = -\frac{4E\theta(t)e^{i(k^2+1)t} \sin \omega t}{\sqrt{2\pi(k^2 + 1)^2}} k.
\quad (10b)
\]

The evolution of \(\Theta(k,t)\) is determined in Eq.(10b) by \(\theta(t)\) only. Using Eq.(7), then integrating Eq.(10b) in time, and substituting the result into Eq.(10a) we obtain a single equation which describes the evolution of \(\theta(t)\)

\[
\dot{\theta}(t) = -\frac{(4E)^2}{2\pi} \eta(t) \int_0^t \theta(t') \eta(t') dt' \int_{-\infty}^{\infty} e^{-i(k^2+1)(t-t')} (k^2 + 1)^4 k^2 dk, \quad 0 < t < T. \quad (11)
\]

The ionization probability of the bound state is

\[
P(t) = 1 - |\theta(t)|^2, \quad \text{for } t \leq T,
\]

and it becomes constant \(P(T)\) for all later times \(t \geq T\). The internal integral over \(k\) in Eq.(11) can be expressed in terms of Fresnel’s integrals

\[
S(t-t') = \int_{-\infty}^{\infty} \frac{e^{-i(k^2+1)u}}{(k^2 + 1)^2} k^2 dk = \frac{3 - 4u^2}{48} A + iu \frac{3 + 4u^2 - 4iu}{24} B,
\]

where

\[
A = \pi[1 - \Phi(\sqrt{iu})], \quad B = e^{-iu} \sqrt{\pi/iu} - A, \quad u = t - t' \geq 0.
\]

**Numeric realization of ionizing by dipole pulses**

We solve Eq.(11) for \(\theta(t)\) by using the following technique, which is implied by a known method for the Volterra equations. The integral in time is approximated by the summation over discrete equal subintervals defined by equidistant points on the interval \([0,t]\): \(0, \delta, 2\delta, ..., N\delta = t\). As it is clear from Eqs.(7) and (11) \(\theta(0) = 1, \ \dot{\theta}(0) = 0\), then we have \(\theta(\delta) \approx \theta(0) + \delta \dot{\theta}(0) = 1\). In this way \(\theta(2\delta) = \theta(\delta) + \delta \dot{\theta}(\delta)\) where \(\dot{\theta}(\delta)\) is evaluated by the integral (11) without involving the end point at \(t = 2\delta\). And so on by consequent computations of \(\theta(j\delta)\) via the terms with numbers \(0, 1, 2, ..., j - 1\). This technique realizes an approximate quadrature of Eq.(11) and its precision becomes better when subintervals \(\delta\) get shorter. This approximation replaces Eq.(11) with the sum

\[
\dot{\theta}(n\delta) = -\frac{(4E)^2}{2\pi} \delta \eta(n\delta) \sum_{j=0}^{n} \theta(j\delta) \eta(j\delta) S((n-j)\delta), \quad (14)
\]

which allows to find approximately \(\theta((n+1)\delta) = \theta(n\delta) + \delta \dot{\theta}(n\delta)\). We study in this work sometimes quite long pulses, they require for an acceptable precision long computing time as \(\delta\) should be very small. This can be helped by improving the transition from \(\theta(n\delta)\) to \(\theta((n+1)\delta)\) by involving two derivatives of \(\theta\):

\[
\theta((n+1)\delta) = \theta(n\delta) + \delta \dot{\theta}(n\delta) + \frac{\delta^2}{2} \ddot{\theta}(n\delta). \quad (15)
\]
Differentiating Eq.(11) we have

\[ \ddot{\theta}(t) = -\frac{(4E)^2}{2\pi} \left[ \eta(t) \int_0^t \dot{\theta}(t') \eta(t') dt' \int_{-\infty}^{\infty} \frac{e^{-i(k^2+1)(t-t')}}{(k^2 + 1)^3} k^2 \, dk \right] \]

\[ + \frac{5\pi}{128} \theta(t) \eta^2(t) - i\eta(t) \int_0^t \dot{\theta}(t') \sin \omega t' dt' \int_{-\infty}^{\infty} \frac{e^{-i(k^2+1)(t-t')}}{(k^2 + 1)^3} k^2 \, dk \]

By expressing the last integral over \( k \) in terms of Fresnel functions as

\[ V(u) = \int_{-\infty}^{\infty} e^{-iu(k^2+1)} \frac{k^2 \, dk}{(k^2 + 1)^3} = \pi \left[ 1 - \Phi(\sqrt{i}u) \right] \frac{1}{8} + e^{-iu} \frac{1}{4}, \]

Eq.(15) can be rewritten in the following form

\[ \theta((n+1)\delta) = \theta(n\delta) + \frac{8\delta^2 E^2}{\pi} \left\{ \frac{i\delta}{2} \eta(n\delta) \sum_{j=1}^{n} \theta(j\delta) \eta(j\delta) V((n-j)\delta) \right\} \]

\[ - \frac{5\pi}{256} \theta(n\delta) \eta^2(n\delta) - \left[ \eta(n\delta) + \frac{\delta}{dt} \eta(n\delta) \right] \sum_{j=1}^{n} \theta(j\delta) \eta(j\delta) S((n-j)\delta) \right\}, \]

convenient for numeric computation of the ionization probability.

**A. Sin-wave pulses \sin(\omega t)**

The ionization of our atom by the sin-wave electric field excitation, which models the laser pulses, means that \( \eta(t) = \sin(\omega t) \). For illustration everywhere in this work the ‘short’ harmonic pulses will have only five cycles, \( N = 5 \), this can be easily realized now by experimental techniques [7-10]. For \( \omega < 1 \) even 5 cycles of oscillations last a relatively long time, sometimes \( T > 100 \) and the use of \( \ddot{\theta}(t) \) is necessary. The results are exhibited in Fig.1, where time \( t \) is measured in numbers of cycles of perturbation.

![FIG.1. Ionization probability \( P(t) \) caused by harmonic pulses](image)
The plot structure shows that external frequency $\omega$ is doubled in the process, which is suggested in some measure by Eq.(11). When the electric field $E = 3$ the complete ionization occurs practically after the third cycle of the pulse.

All computations are done using Maple on the intervals $T = 5 \frac{2\pi}{\omega}$ with various $\omega$ and $E$, therefore $T = 78.54, 104.7, 157.1$ for $\omega = 0.4, 0.3, 0.2$ respectively. An acceptable precision requires $\delta \leq 0.04$, i.e. the sums in Eq.(17) will have up to 4000 terms and the computations is time consuming as the sum is of recursive nature.

Fig.2 confirms our observation that when $\omega$ is far from the resonance the total duration of the perturbation pulse can be more important than its frequency, experiments [7-9] confirm this effect in real systems. The same behavior is more visible in Fig.2b, where the electric field is smaller $E = 0.5$.

For a very qualitative comparison with experimental results we note that in the case of Cs atoms, whose external orbitals have radii about 2 Angstroms, where the electric field is about 30 $GV/m$. When we rescale $|W_{Cs}| = 3.89$ eV to $|W_b| = 1$ this would correspond in Eq.(14) to $E \sim 8$ in the dimensionless units, therefore our $E = 0.5$ means roughly about 2 $GV/m$, which is a very high electric field in laser pulses, but reachable for present techniques. The case with the field strength $E = 0.2$ (in physical units this corresponds $E \sim 0.8$ $GV/m$ for Cs or $\sim 1.6$ $GV/m$ for Tungsten with $|W| = 7.86$ eV) was computed too: $P(T) \approx 0.053$ for $\omega = 0.2$ and $0.027$ for $\omega = 0.3$ while the shape of curves $P(t)$ is similar to plots in Fig.2. These results are only for orientation and clearly should be considered as qualitative due to the limitations of our model. It looks that for smaller $E$ the value of $P(T)$ becomes proportional to $\sim E^2$ in agreement with Eq.(17).

B. Pulsed dipole forcing

Here we consider electric bursts acting on the model atom: rectangular $\eta(t) = 1$ and bell-shaped $\eta(t) = 4(t/T - t^2/T^2)$ on the interval $0 \leq t \leq T$. Though the bell-shaped pulse has the same amplitude as the rectangular one, but its ionization efficiency is much lower in Fig.3 because its total energy is smaller and more importantly it does not have high frequency harmonics. The ionization probability $P(t)$ is an oscillating function but there is an important
difference between plots in Figs.3a and 3b. While the ionization probability by a rectangular pulse of duration $t_1$ is given by $P(t_1)$ in Fig.3a, the ionization evolution for bell-shaped pulses is presented by Fig.3b, but only for the pulse of length 10, i.e. if $T = t_1$ function $P(t_1)$ in Fig.3b does not represent the final probability and the corresponding computation should be performed namely for $T = t_1$ because $\delta = \delta(T)$. Our calculation with $E = 0.2$ and the bell-shaped pulse is not plotted in Fig.3b because the curve $P(t)$ runs very low: its maximum $P(4) \sim 0.013$ and $P(10)$ is less than 0.002.

Our approach is modified below for studying the ionization caused by the parametric modulations of the binding potential. Though this is hardly achievable in practice but, as we already mentioned, it exhibits some illuminating features of the ionization by short pulses which are quite universal.

### 3. PULSED MODULATION OF BINDING POTENTIAL.

Here we consider short pulse bursts of the potential strength which has to be studied by a different computations technique. Eq.(5) now has the following form

\[
i \frac{\partial \psi(x,t)}{\partial t} = H_0 \psi(x,t) + R\delta(x)\eta(t)\psi(x,t), \quad \eta(t) = 0 \text{ when } t \notin [0,T], \quad t \geq 0, \tag{18}
\]

with the initial conditions given by Eq.(7). Using the expansion (6) in terms of the stationary eigen-functions and the methods developed in [1] yields a simple equation for the function $\theta(t)$

\[
\theta(t) = 1 + 2i \int_0^t Y(t') dt', \tag{19}
\]

where $Y(t)$ is defined by the following integral equation

\[
Y(t) = R\eta(t) \left\{ 1 + \int_0^t [2i + M(t - t')Y(t')] dt' \right\}. \tag{20}
\]

The function $M(s)$ in (20), see [1], is

\[
M(s) = \frac{2i}{\pi} \int_0^\infty \frac{u^2 e^{-isu(1+u^2)}}{1 + u^2} du = -i + \sqrt{i \pi} e^{-is} + i\Phi(\sqrt{s}). \tag{21}
\]
It behaves as $\sqrt{i/\pi}s - i$ when $s \to 0$ and is proportional to $s^{-3/2}e^{-is}$ when $s \to \infty$.

A. Case of rectangular pulse $\eta(t) = 1$.

For approximate evaluation of the function $\theta(t)$ in this set up we have to solve numerically the integral equation (20) that can be done if there is an effective way of computing $M(s)$ for not very large values of $s$ as our pulses are not long. Using [11] equation for the integral in Eq.(21) can be written in terms of gamma functions

$$\int_0^\infty \frac{\sqrt{x}e^{-isx}}{1+x} \, dx = e^{is}\Gamma\left(\frac{3}{2}\right) \Gamma\left(-\frac{1}{2}, is\right),$$

and then one can apply the power series expansion for the confluent hypergeometric function and present $M(s)$ in a rapidly convergent form

$$M(s) = -i - \sqrt{\frac{i}{\pi s}} \sum_{n=0}^{\infty} \frac{(-is)^n}{(2n-1) \, n!},$$

For a given pulse duration $T$ the upper limit in the sum (22) can be only slightly larger than $\epsilon T$ to give a good precision for $M(s)$.

Our next step is express this function by a power series using the behavior of $Y(t)$ near zero,

$$Y(t) = \sum_{m=0} c_m t^{m/2}, \quad 0 < t < T, \tag{23}$$

and substitute Eqs.(22) and (23) into the integral equation (20). The result reads

$$R^{-1} \sum_{m=0} c_m t^{m/2} = 1 + i \sum_{m=0} c_m \frac{t^{1+m/2}}{1+m/2} + \sum_{k,n=0} B\left(\frac{k}{2} + 1, n + \frac{1}{2}\right) c_k a_n t^{n+m/2},$$

where $B(x,y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the $\beta$-function [11]. Thus we obtain equations for finding coefficients $c_*$:

$$c_0 = R, \quad c_1 = B\left(1, \frac{1}{2}\right) Ra_0 c_0 = 2R^2 \sqrt{\frac{i}{\pi}}, \tag{24}$$

$$c_m = \frac{2iR}{m} c_{m-2} + R \sum_{n=0}^{\lfloor m/2 \rfloor} B\left(m+1, n + \frac{1}{2}\right) a_n c_{m-2n-1}, \quad m \geq 2.$$

The symbol $\lfloor x \rfloor$ as usual means the integer part of $x$, and coefficients $c_m$ in (24) can be calculated consequently as they are expressed in terms of $c_*$ evaluated earlier. Clearly we will keep in (22) and (23) only finite numbers of terms.

By combining Eqs.(19), (23), and (12) we find the ionization probability as a function of the pulse duration $T$

$$P(T) = 1 - \left| 1 + 4i \sum_{m=0} \frac{c_m}{m+2} t^{1+m/2}\right|^2. \tag{25}$$

The results of computation by Eqs.(22-25), where we keep about 80 terms in sums, are presented in Figs.4 which show this probability for different values
of pulse amplitude $R$ and $T \leq 10$. Left Fig.4 shows also that a very short attractive pulse with $R = -0.5$, $T \approx 0.9$ is more effective for ionization than longer pulses of the same amplitude.

![Graph of ionization probability $P(T)$ for rectangular pulses](image)

**FIG.4** Plots of ionization probability $P(T)$ for rectangular pulses

In agreement with the common sense when the external pulse decreases the binding energy, $R > 0$ in (4), the ionization rate is larger. There is always an intermediate pulse duration corresponding to maximum of ionization and for longer positive pulses the ionization rate approaches to a constant. Right Fig.4 exhibits the ionization probability caused by the attractive positive pulse whose amplitude is one half of the binding energy and duration $T \leq 4.5$. One can see the resonances and quite a high probability 0.32 when $T = 0.55$ because the pulse fronts have infinite slopes and thus introduce very high harmonics though the total pulse energy is limited. Note also that $R$ should be compared with $g = 2$ in our units, $|R| = 1$ is the largest considered here.

**B. Bell-shaped pulse** $\eta(t) = 4(t/T - t^2/T^2)$

On the interval $0 < t < T$ we consider a pulse, symmetric about $t = T/2$, whose maximum amplitude is $R$, see Eq.(4). In this case the same approach as before converges slower and one needs more terms in Eqs.(22) and (23), we used up to 400-500 of them.

A straightforward analysis of Eq.(20) shows that the power series expansion for $Y(t)$ has the following form

$$Y(t) = \sum_{m=0}^\infty c_m t^{1+m/2}, \quad 0 < t < T. \tag{26}$$

By substituting (26) into Eq.(20) and using Eq.(22) we solve Eq.(26) and find the coefficients which define $Y(t)$

$$\frac{T_{c_0}}{4R} = 1, \quad c_1 = 0, \quad \frac{T_{c_2}}{4R} = -\frac{1}{T}, \quad \frac{T_{c_3}}{4R} = a_0 c_0 B \left(\frac{1}{2}, \frac{5}{2}\right), \quad \frac{T_{c_4}}{4R} = i \frac{c_0}{2} + a_0 c_1 B \left(\frac{1}{2}, \frac{1}{2}\right),$$

$$\frac{T_{c_5}}{4R} = \frac{2 c_1}{5} + a_0 c_2 B \left(\frac{1}{2}, \frac{3}{2}\right) + a_1 c_0 B \left(\frac{3}{2}, \frac{5}{2}\right) - \frac{1}{T} a_0 c_0 B \left(\frac{1}{2}, \frac{1}{2}\right). \tag{27}$$
\( Tc_m = \frac{2ic_{m-4}}{m} \frac{2ic_{m-6}}{T(m-2)} + a_0c_{m-3}B\left(\frac{1}{2}, \frac{m+1}{2}\right) \)
\[ + \sum_{n=0}^{\frac{m-5}{2}} c_m-2n-5 \left( \frac{2n+1}{m} a_n+1 - \frac{a_n}{T} \right) B\left(n + \frac{1}{2}, \frac{m-1}{2} - n\right), \quad m \geq 6. \]

One can see again that as in Eqs.(24) each coefficient \( c_\ast \) is defined via corresponding ones found earlier.

\[
P(T) = 1 - |\theta(T)|^2 = 1 - \left| 1 + 4i \sum_{m=0}^\infty \frac{c_m}{m + 4} t^{2+m/2} \right|^2, \quad (28)
\]

where all \( c_k, \ k = 0, 1, ... \) depend on \( T \).

\( P(T) \) in Fig.5a is the ionization probability at the end of the corresponding pulse with \( R = -0.5 \) and length \( T \), but the plot for maximum \( Max(P) \) which occurs at an intermediate time \( 0 < t < T \) and for longer pulses it is much larger than \( P(T) \). Fig.5b shows \( P(t) \) behavior in the case \( T = 2.5 \) when the pulse amplitudes are \( R = \pm 0.5 \). Positive pulses are more effective as before: \( P(T) = 0.13 \) is close to \( Max(P) \) when \( T = 2.5 \) while \( P(T) \) and \( Max(P) \) are 0.139 and 0.147 respectively for \( T = 3 \). This probably means that change of sign of the external force plays an important role and might suggest that more realistic perturbation (a harmonic one with some envelope) can be more efficient.

One can see that the system can be ionized before the end of perturbation pulse, i.e. the value of \( Max(P) \) is interesting.

C. Short sin-wave pulses \( \eta(t) = \sin(\omega t) \)
Our pulse exists on the interval $0 \leq t \leq T$ and as in Part 2 its length has always an integer number $N = 5$ of cycles, $T = 2\pi N/\omega$. We assume in computations that the frequency of principal harmonic of $Y(t)$ is $\omega$ and choose an integer $K$ of harmonics sufficient for modeling $Y(t)$. Then using the Galerkin [12] method for solving Eq.(20) the function $Y(t)$ is approximated by the following sum

$$Y(t) = \sum_{k=-K}^{K} a_k f_k(t), \quad \text{where } f_k(t) = e^{i\omega kt}.$$  \hfill (29)

The solution method requires the discrepancy of using the approximation (29) in Eq.(20) be orthogonal to all functions $f_k$. This procedure creates the linear algebraic system for coefficients $a_k$

$$\sum_{k=-K}^{K} a_k \int_0^T dt \tilde{f}_m(t) \left\{ f_k(t) - R\eta(t) \int_0^t [2i + M(t')] f_k(t - t') dt' \right\} = R \int_0^T \eta(t) \tilde{f}_m(t) dt, \quad -K \leq m \leq K. \hfill (30)$$

By substituting Eq.(29) into (30) this system can be rewritten in the standard form

$$\sum_{k=-K}^{K} C_{k,m} a_k = B_m, \hfill (31)$$

where all coefficients with $k \neq m \pm 1$ defined by the following relations:

$$C_{k,m} = A_{k-m} + \frac{R}{2\omega} \left( \frac{M_{-k} - M_{1-m}}{k-m+1} - \frac{M_{-k} - M_{1-m}}{k-m-1} \right). \hfill (32)$$

For $k = m - 1$ and $k = m + 1$ we have respectively

$$C_{m-1,m} = \frac{R}{4\omega} [(1 + 2i\omega T) M_{1-m} - M_{1-m} - 2i\omega \overline{M}_{1-m}], \hfill (33)$$

$$C_{m+1,m} = \frac{R}{4\omega} [(1 - 2i\omega T) M_{1-m} - M_{1-m} + 2i\omega \overline{M}_{1-m}].$$

Other terms in Eqs.(31-33) are

$$A_{k-m} = \begin{cases} 0, & k \neq m, \\ T, & k = m, \end{cases} \quad B_m = \frac{R}{2i} [A_{1-m} - A_{1-m}], \hfill (34)$$

$$M_n = \int_0^T [2i + M(t)] e^{i\omega t} dt, \quad \overline{M}_n = \int_0^T [2i + M(t)] te^{i\omega t} dt.$$

Our computation by Eqs.(31-34) for the cases when $T = 5$, $R = 0.2$, $0.4$, and the pulse consisting of 5 cycles (therefore $\omega = 2\pi N/T \approx 6.3 > \omega_0$) are shown in Fig.6:
One can see that with pulse amplitude 0.4 the ionization is quite effective. We used only five harmonics, \( K = 5 \), in computations but checked the precision by taking \( K = 10 \) which produced the curves \( P(t) \) almost identical to ones in Fig.4. The roughly linear time dependence of the ionization probability is caused by the fact that \( \omega \) is significantly larger than \( \omega_0 \), i.e. the energy of ionizing photons in Fig.4 exceeds the binding energy of the model atom and thus we observe the first order effect. In reality this process might be compared with the soft X-ray ionization.

For solving Eq.(20) this method of approximation \( Y(t) \) by Eq.(29) and the routine defined by Eqs.(31-34) becomes inefficient when \( \omega \) is much smaller because the interval \( T \) is too long in this case and oscillations of \( M(s) \) are not well modeled by harmonics of \( \eta(t) \). We use the special properties of the Volterra Eq.(20) to model function \( Y(t) \) by a set of its discrete points. When the ionization is provided by at least two photons and \( \omega = 0.6 \), 5 cycles of sin wave make \( T > 60 \), and thus one needs about \( N = 10^4 \) points for a decent approximation of \( Y(t) \). Denoting temporarily \( F(s) = 2i + M(s) \) the integral equation (20) is replaced by the following one, where we keep the integral term in the interval of divergent behavior of \( M(s) \)

\[
R^{-1}Y(t_n) = \eta(t_n) + \eta(t_n) \left[ \Delta \sum_{m=1}^{n-1} F(t_n - t_m)Y(t_m) + \int_0^\Delta F(s)Y(t_n - s)ds \right].
\]

Here \( t_n = n\Delta, n \) runs from 1 to \( N \) and \( \Delta = T/N \). The integral in Eq.(35) is approximated using Eq.(22) for \( M(s) \) when \( s \) is small and only the linear term of \( Y(t) \)-dependence on the interval \( (t_{n-1}, t_n) \):

\[
F(s) \approx i + \sqrt{\frac{i}{\pi s}} \left[ 1 + is + \frac{s^2}{6} - i\frac{s^3}{30} \right], \quad Y(t_n - s) \approx Y(t_n) + \frac{Y(t_{n-1}) - Y(t_n)}{\Delta}s.
\]

Near small \( s \) we keep more terms in singular \( F(s) \) than in \( Y(t_n - s) \) because \( Y(t) \) has a regular behavior there. By evaluating the integral in Eq.(35) we come to the recurrent equation for computing the set \( Y(t_n) \) consequently starting from...
\[ n = 2. \]

\[ Y(t_n) = \frac{R\eta(t_n)}{1 - B - i\Delta/2} \bigg[ 1 + \Delta \sum_{m=1}^{n-1} F(t_n - t_m)Y(t_m) + (A + i\Delta/2)Y(t_{n-1}) \bigg], \]

\[ A = \sqrt{\frac{i\Delta}{\pi}} \left( \frac{2}{3} + \frac{2i\Delta}{5} + \frac{\Delta^2}{21} - \frac{i\Delta^3}{135} \right), \]

\[ B = \sqrt{\frac{i\Delta}{\pi}} \left( \frac{4}{3} + \frac{4i\Delta}{15} + \frac{2\Delta^2}{105} - \frac{2i\Delta^3}{945} \right). \]

Here we will neglect terms of the order \( \Delta^6 \) and higher.

It is clear that \( Y(0) = 0 \) and for approximating \( Y(t_1) \) by a polynomial with the same precision we substitute \( Y(\Delta - s) \) into Eq.(20) and using Eqs.(36,37) obtain the following relation

\[ \sum_{k=0}^{10} c_k \Delta^{1+k/2} = R \left( \omega \Delta - \frac{\omega^3\Delta^3}{3!} + \frac{\omega^5\Delta^5}{5!} \right) \left\{ 1 + \sum_{n=0}^{6} c_n \left[ i\Delta^{2+n/2} + \sqrt{\frac{i}{\pi}} H_n(\Delta) \right] \right\}, \]

where \( H_n(\Delta) = \)

\[ \Delta^{2+n/2} \left[ B \left( \frac{4+n}{2}, \frac{1}{2} \right) + i\Delta B \left( \frac{4+n}{2}, \frac{3}{2} \right) + \frac{\Delta^2}{6} B \left( \frac{4+n}{2}, \frac{5}{2} \right) - \frac{i\Delta^3}{30} B \left( \frac{4+n}{2}, \frac{7}{2} \right) \right]. \]

These equations are sufficient to evaluate \( c_k, \ k = 0, \ldots, 10 \) and find \( Y(t_1) = Y(\Delta) \). We applied Eqs.(35-38) to compute the ionization by the five cycle pulses of lower than in Fig.6 frequency \( \omega = 0.6 \) and amplitudes \( R = 0.2, \ R = 0.4 \).

The dynamics of the process is shown in Fig.7. One can see that the ionization probability is higher than in the case of \( \omega \approx 6 \) in Fig.6. This result is probably caused by a much longer (more than in order) action of the perturbation while its average force (determined by \( R \)) roughly the same. The sin-wave pulses appeared to be quite efficient for ionization and \( P(T) \) seems to be proportional to \( R^2 \) for smaller \( R \) like for the laser pulse perturbation. The time of perturbation in Fig.5 is measured in the number of harmonic cycles, the pulse ends when \( N = 5 \) and \( T \approx 52.4 \).

In the dimensionless units when the atomic ionization energy is 1 our results can be tentatively mapped onto real system again, say Tungsten W and Cesium.
Cs with binding energies 7.86 eV and 3.89 eV respectively. It is easy to see that \( \omega = 0.6 \) would correspond the wavelength about 260 nm for W and 530 nm for Cs in our cases. In experiments often are used \( \sim 4 - 10 \) fsec laser pulses of \( \lambda = 800 - 830 \) nm, [7-10], and having in mind a qualitative application of our theory we perform a somewhat less precise computation for smaller \( \omega = 0.4 \) and 0.2 respectively when the pulse time \( T \) is longer.

![Graph](image1)

**FIG.8.** Ionization by short pulse harmonic waves of \( \omega = 0.2 \)

The results presented in Figs.8 and 9 confirm the importance of total pulse duration. As before our pulses have only 5 cycles, the time of their action is \( T = 157 \) dimensionless units when \( \omega = 0.2 \) in Fig.6 and twice shorter when \( \omega = 0.4 \) in Fig.9. Fig.8 roughly imitates the Cesium ionization when \( R = 0.1 \) and 0.2 while \( \lambda \sim 800 - 830 \) nm. The amplitude \( R = 0.2 \) is sufficient for almost complete ionization even at the pulse beginning.

Fig.9 gives a hint of the Tungsten ionization (keeping in mind the same \( \lambda \sim 800 \) nm).

![Graph](image2)

**FIG.9.** Short pulse ionization when atomic binding energy is larger

The ionization level is lower than in case of Cs though the wave length is twice
shorter. This clearly agrees with greater binding energy in W atoms.

As the parametric perturbation acts directly on the binding energy it is more efficient in Figs.7-9 than the more realistic perturbation by the external harmonic electric field in Part 2. These results show that the ionization of our model atom in some measure describes qualitative behavior of real systems.

4. SUMMARY

The atomic ionization by short pulses of external forces is studied on a simple one-dimensional model which allows to construct an exact theory of the process and realize its conclusions by several methods of numerical computations. This creates a basis for comparison with approximate solutions of more realistic models, simulations, and experiments. Our main results include the observation that for external frequencies, much lower than the resonance ones, the total duration of the pulse is more important for effective ionization than its frequency. When the ionization level is substantially far from the complete one it is increasing approximately linearly in time and has resonances as a function of pulse duration. For ionization caused by the dipole electric field the frequency of these resonances is twice larger than the frequency of external forcing.

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