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One-dimensional "atom" with zero-range potential perturbed by finite sequence of zero-duration laser pulses

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ABSTRACT

The exactly solvable model of a sequence of zero-duration electromagnetic kicks interacting with a 1D "atom" with short-range δ-potential is considered. This model can be applied to the real case when very short (a few attosecond) laser pulses follow one another separated by the time interval τ much bigger then the period of pulse.

Keywords: one-dimensional atom, pulse trains, ultra-short laser pulses

1. INTRODUCTION

Recent development of sources of intense XUV and X-ray radiation, such as free-electron lasers, generators of higher-order laser harmonics, novel undulator lines, offer significant prospects for different applications, e.g., in monitoring quantum processes with femto- and attosecond time resolution and coherent control of quantum dynamics[1] . Rigorous theories describing the atomic and molecular excitation/ionization by laser pulses finally lead to cumbersome and labor-consuming numerical calculations. For making estimates and clarifying the major physical mechanisms, simple approximate models are used. We can mention here the widely used strong field approximation (SFA) model (see, e.g.,[2,3] and references therein), the separable potential atomic model (SPAM) [4–6] , and the models making use of delta-potentials.

The first calculations of such kind with the 1D delta-potential were presented by Perelomov et al[7] . In this paper, the electric time-dependent field was described by a continuous function of time, and the model considered one pulse. Later on, the so-called kick-field model became popular [8–14] . In these papers the electric time-dependent field was presented as a sum of delta-functions, modelling the pulse shape as a train of localized kicks within its period.

Let us recall the basic ideas of the kick-field model .[13] The time-dependent Schrödinger equation (TDSE) of the model describing the interaction of the electromagnetic radiation with the atom in the dipole approximation reads as

$$i\frac{\partial}{\partial t}|\Psi >= H|\Psi > +V(t)|\Psi > . \tag{1}$$

Here H is the Hamiltonian of the 1D atom and

$$V(t) = x\sum_{n=0}^{N-1} A_n\delta(t-n\tau). \tag{2}$$

is the 1D dipole potential that describes the interaction of the atom with N kicks of the field, each having the amplitude A_n $(n = 0, ..., N-1)$, and separated by equal intervals τ. The amplitude $t_{f0}^{(N)}$ of the transition from the initial state of the atom into a certain final state takes the form

$$t_{f0}^{(N)} =< f|\prod_{n=0}^{N-1}[e^{-i\tau H}\ e^{-iA_n x}]|0 > . \tag{3}$$

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The corresponding transition probability density is

$$w_f^{(N)} = |t_{f0}^{(N)}|^2, \tag{4}$$

where the final state $< f|$ can be either the ground state, which is the only discrete state of the atom, $< 0|$, or a continuum state $< k|$ with the momentum k. We also define the total ionization probability

$$w_i^{(N)} = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\; w_k^{(N)}.$$

We could expect that such a model describes a one real laser pulse if the kicks in the train are sign-alternating, i.e., the adjacent amplitudes A_n have opposite signs. In this case the time period τ can be related to the field frequency ω as $\omega\tau = \pi$, and the total duration T of the pulse is $T = 2\pi(N-1)/\omega$, were $(N-1)$ is the number of optical cycles. Of course, a single kick ($N = 1$) has no physical meaning itself, but it presents the elementary base for describing the effect of multiple kicks.

Below we will see that the simplest physical case $N = 2$ (the model of one-cycle laser pulse) does not reproduce some well-known features of the real pulse with the continuous function $V(t)$. For example, for large τ (low frequency) the probability that the atom will stay in its ground state becomes exponentially small at the end of the pulse. This is not the case in this model. To our opinion, it can be applied to a train of very short (attosecond) real pulses, interacting with the atom. If the period of such pulse is T_0, then the condition $T_0 << \tau$ has to be satisfied. This application of the kick-field model seems to be more realistic. In this paper we combine the 1D delta-potential for the "atom" and the kick-train model of the electric dipole interaction in attempt to study the main mechanisms of the interaction between a train of attosecond pulses and an "atom", which can be a negative ion.

The atomic units are used.

2. STATIONARY SOLUTIONS AND BASIC TRANSITION MATRIX ELEMENTS

The Shrödinger equation for one-dimensional atom with zero-range potential is of the form

$$\left[\frac{1}{2}\frac{\partial^2}{\partial x^2} + E + Z\delta(x)\right]\psi(x) = 0, \quad Z > 0. \tag{5}$$

The normalized ground state wave function ($E_0 = -Z^2/2$) is

$$\psi_0(x) = \sqrt{Z}e^{-Z|x|}. \tag{6}$$

The continuum wave functions ($E = k^2/2$) are expressed as

$$\psi^{(+)}(k,x) = e^{ikx} - \frac{Z}{Z + i|k|}e^{i|k||x|}, \quad \psi^{(-)}(k,x) = \psi^{(+)*}(k,-x). \tag{7.1}$$

In the momentum space

$$\varphi_0(p) = \frac{2Z^{3/2}}{Z^2+p^2}, \quad \varphi^{+}(k,p) = (2\pi)\delta(k-p) - \frac{i|k|Z}{Z+i|k|}\,\frac{1}{E-(p^2/2)+i0}, \quad \text{and } \varphi^{-*}(k,p) = \varphi^{+}(k,p). \tag{7.2}$$

These eigenfunctions satisfy the orthogonality and completeness conditions

$$\int\limits_{-\infty}^{\infty} dx\psi^*(k',x)\psi(k,x) = 2\pi\delta(k'-k), \qquad \int\limits_{-\infty}^{\infty} dx\psi^*(k',x)\psi_0(x) = 0,$$

$$\int\limits_{-\infty}^{\infty} \frac{dk}{2\pi}\psi(k,x')\psi^*(k,x) + \psi_0(x')\psi_0(x) = \delta(x'-x).$$

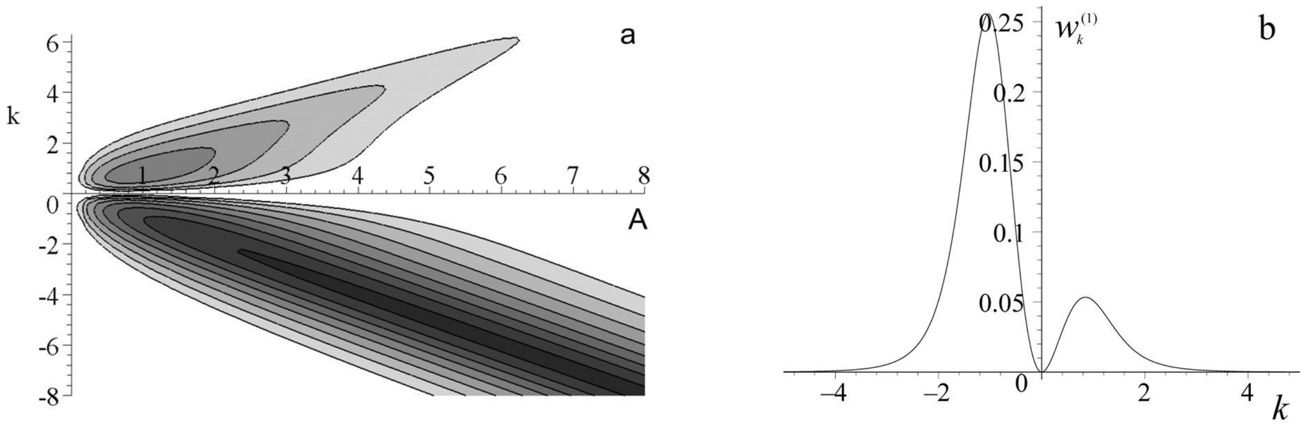

Figure 1. (a) Plot of the ionization probability density $w_k^{(1)}$ at $Z = 1$ versus the intensity A and the momentum k. The intensities of the isolines are (white) 0.004, 0.008, 0.016, 0.032, 0.064, 0.128, 0.256, 0.512 (dark/grey); (b) The ionization probability $w_k^{(1)}$ at $A = 1$, $Z = 1$ versus the momentum k.

2.1 Single kick: $N = 1$

For definiteness we put $A > 0$. The amplitude of the probability for the "atom" to stay in the ground state $t_{00}^{(1)}$

$$t_{00}^{(1)} = e^{iZ^2\tau/2} \, \frac{4Z^2}{4Z^2 + A^2} \tag{8}$$

and the amplitude of ionization $t_{k0}^{(1)}$

$$t_{k0}^{(1)} = 2Z^{3/2} \left[\frac{1}{Z^2 + (k+A)^2} - \left(\frac{Z - i|k|}{Z + i|k|} \right) \frac{1}{(Z - i|k|)^2 + A^2} \right] \, e^{-ik^2\tau/2} \tag{9}$$

are simply calculated with Eq. (3), and some results are presented in Fig. 1. It is obvious from the completeness condition that

$$w_0^{(1)} + w_i^{(1)} = 1.$$

We see that the electrons after the kick leave our "atom" in the direction opposite to the polarization vector (negative k), which follows from (9).

We also express the continuum-continuum transition amplitude as ($\varepsilon \to \pm i0$)

$$e^{ik^2\tau/2} \, t_{kp}^{(1)} = (2\pi)\delta(k - p - A) - \frac{Z}{(Z - i|p|)} \, \frac{2i|p|}{(\varepsilon + i|p|)^2 + (A+k)^2} + \frac{Z}{(Z + i|k|)} \, \frac{2i|k|}{(\varepsilon - i|k|)^2 + (A-p)^2}$$
$$+ \frac{Z^2}{(Z + i|k|)(Z - i|p|)} \, \frac{2i(|p| - |k|)}{(\varepsilon + i|p| - i|k|)^2 + A^2}. \tag{10}$$

2.2 Two kicks: $N = 2$

The amplitude of the transition into the state $< f|$ in the case of two laser pulses with the amplitudes A_0 and A_1, separated by the interval τ, takes the form

$$t_{f0}^{(2)} = e^{-iE_f\tau} \sum_{\nu} < f|e^{-iA_1x}|\nu > e^{-iE_\nu\tau} < \nu|e^{-iA_0x}|0 >, \tag{11}$$

The simplest calculation can be executed for the amplitude (and the probability) for the case when the "atom" itself remains in the ground state under the impact of two kicks with equal absolute values and opposite directions $A_0 = -A_1 = A$. In this particular case

$$t_{00}^{(2)} = e^{iZ^2\tau/2} \left[e^{iZ^2\tau/2} < 0|e^{iAx}|0 >< 0|e^{-iAx}|0 > + \int_{-\infty}^{\infty} \frac{dp}{2\pi} < 0|e^{iAx}|p > e^{-ip^2\tau/2} < p|e^{-iAx}|0 > \right]$$

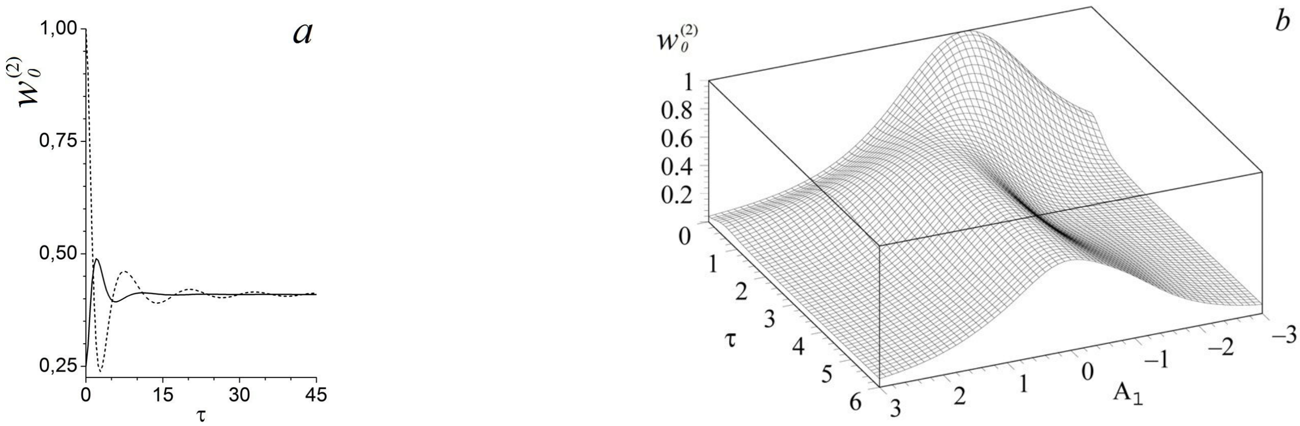

Figure 2. (a)The ground state probability $w_0^{(2)}$ versus the period τ. Solid line: $A_0 = A_1 = 1$, dotted line: $A_0 = -A_1 = 1$, $Z = 1$; (b) The ground state probability $w_0^{(2)}$ versus the period τ for two different kicks, the intensity of the first kick is $A_0 = 1$.

$$= e^{iZ^2\tau/2}\left[e^{iZ^2\tau/2}w_0^{(1)} + \int_{-\infty}^{\infty}\frac{dp}{2\pi}w_p^{(1)}e^{-ip^2\tau/2}\right]. \tag{12}$$

However, Eq. (11) allows also calculating the case $A_0 = A_1 = A$ without significant numerical difficulties. The results of computing the probability $w_0^{(2)}$ are presented in Fig. 2a. As follows from the Figure, at large τ the probabilities for the cases of co- and contra-directed kicks tend to one limit. This fact follows from Eq. (12), since the second term in the square brackets decreases with the growth of τ, and $t_{00}^{(1)}$ is independent of the sign of A. In turn, this circumstance indicates the fact that the "atom" after the impact of two field kicks well separated in time is stabilized in the ground state with the probability $w_0^{(2)} = | < 0|e^{iA_0x}|0 >< 0|e^{iA_1x}|0 > |^2$. A part of the "atoms" is ionized with the probability $w_i^{(2)} = 1 - w_0^{(2)}$. Both probabilities are already independent of τ. For small periods τ, the probability $w_0^{(2)}$ is already not a constant, which is illustrated in Fig. 2b.

2.3 Train of N kicks

Here for numerical calculations it is convenient to use recurrence relations. Let us denote a certain current number in the product (3) by $n = s$. Then

$$t_{k0}^{(s+1)} =< k|\prod_{n=0}^{s} e^{-i\tau H}e^{-iA_nx}|0 >, \tag{13.1}$$

and

$$t_{00}^{(s+1)} =< 0|\prod_{n=0}^{s} e^{-i\tau H}e^{-iA_nx}|0 > . \tag{13.2}$$

Here $0 \le s < N - 2$. Then

$$t_{k0}^{(s+2)}=e^{-i\tau k^2/2}\left[< k|e^{-iA_{s+1}x}|0 > \ t_{00}^{(s+1)}+\int_{-\infty}^{\infty}\frac{dp}{2\pi}\ < k|e^{-iA_{s+1}x}|p > \ t_{p\,0}^{(s+1)}\right], \tag{14.1}$$

and

$$t_{00}^{(s+2)}=e^{i\tau Z^2/2}\left[< 0|e^{-iA_{s+1}x}|0 > \ t_{00}^{(s+1)}+\int_{-\infty}^{\infty}\frac{dp}{2\pi}\ < 0|e^{-iA_{s+1}x}|p > \ t_{p\,0}^{(s+1)}\right]. \tag{14.2}$$

The completeness condition must be valid for any s

$$w_0^{(s+1)} + \int_{-\infty}^{\infty}\frac{dp}{2\pi}\ w_p^{(s+1)} = 1. \tag{14.3}$$

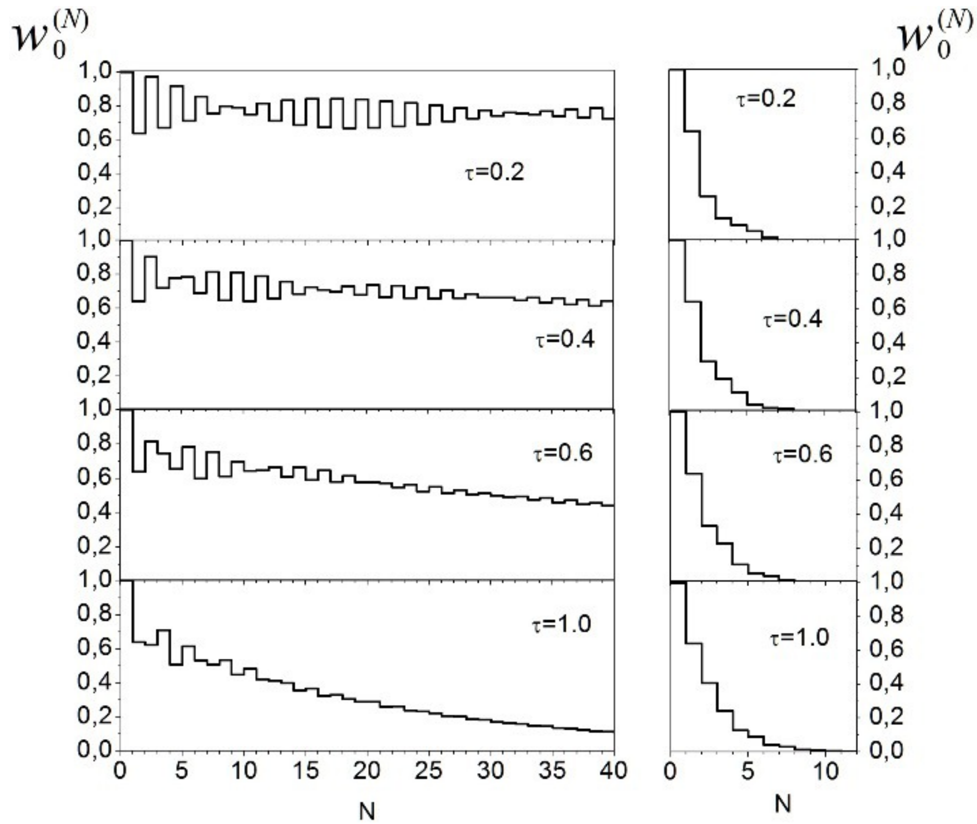

Figure 3. Ground state probability $w_0^{(N)}$ for different short periods τ versus the number of kicks N in the case of alternating-sign kicks $A_s = (-1)^s$ (left-hand column) and the identical kicks $A_s = 1$ (right-hand column) at $Z = 1$.

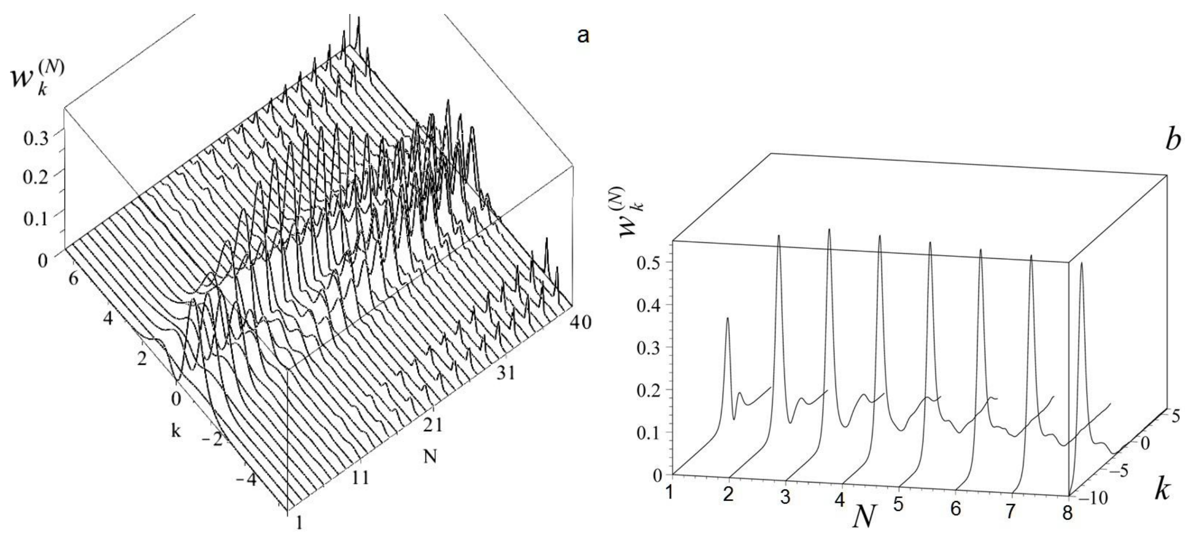

Figure 4. Ionization probability density $w_k^{(N)}$ at $Z = 1$ for short period τ versus the number of kicks N and momentum k in the case of (a) alternating-sign kicks $A_s = (-1)^s$, $\tau = 0.2$ and (b) identical kicks $A_s = 1$, $\tau = 0.3$.

The single-kick transition amplitudes for the kick A_{s+1} are determined by Eqs. (8)–(10). One can expect that the integral in Eq. (14.2) would decrease with the growth of the period τ. Then the probability amplitude for the "atom" to stay in the ground state after a series of N kicks is equal to

$$t_{00}^{(N)}|_{\tau\to\infty} \approx e^{i\tau Z^2/2} < 0|e^{-iA_{N-1}x}|0 > \ t_{00}^{(N-1)} = ... = e^{iN\tau Z^2/2} \prod_{n=0}^{N-1} < 0|e^{-iA_n x}|0 > . \tag{15}$$

For equal-magnitude kicks (of arbitrary signs) we obtain from Eqs. (15) and (8)

$$w_0^{(N)} \approx e^{-2N\ln(1+A^2/4Z^2)}. \tag{16}$$

For smaller τ the probabilities $w_0^{(N)}$ and density of ionization probabilities $w_k^{(N)}$ are presented in Fig. 3 and Fig. 4. We do not display the corresponding total ionization probabilities $w_i^{(N)}$, because they connected with probabilities $w_0^{(N)}$ by relation $w_i^{(N)} = 1 - w_0^{(N)}$.

It is interesting to note that while for the kicks of one sign the probability $w_0^{(N)}$ decreases with the growing number of kicks rather quickly for relatively small τ, for the kicks of alternating sign this decrease is strongly suppressed even for 40 kicks. The probability beats are observed that are clearly expressed at $\tau = 0.2$. These observations still require physical interpretation.

The results of calculations of the ionization probability density $w_k^{(N)}$ versus the number of kicks N and momentum k for the short period τ between identical ($A_s = 1$) and opposite ($A_s = (-1)^s$) kicks are presented in Fig.4. From this figure one can see that in the case of the kicks of alternating sign the maximum of the probability density $w_k^{(N)}$ oscillates with increasing the number of kicks N, and its distribution slowly fades away with respect to momentum k between negative and positive values of the momentum in an increasing domain. For given parameters $Z = 1$ and $|A| = 1$ this domain even for 40 kicks is restricted by $k \in (-12; 12.02478213)$.

In the case of the kicks of one sign maximum of the probability density $w_k^{(N>2)}$ slowly decreases and its distribution with respect to momentum k locates in increasing interval of k toward to negative values from zero. From view point of solving TDSE with respect to spatial variable the wave packet fades away but in the first case it oscillates around the origin of spatial axis, i.e. covers the region of effective radius of the short-range interaction potential, while in the second case it goes out from this region. It means that total ionization probability $w_i^{(N)}$ slowly increases in the first case and quickly increases in the second one. This fact explains why in the first case we have stabilization of probability $w_0^{(N)}$ of atom to remain in the ground state of the discrete spectrum and greater ionization probability $w_i^{(N)}$ in the second one that have been shown in Fig. 3.

2.4 Computational details

For the sequence of $N \geq 3$ kicks the integration over p in Eqs (14.1), (14.2) was executed using the Gaussian quadrature formula with six nodes in each of the subintervals $[p_i, p_{i+1} = p_i + 0.07928971]$, $i = 0, 1, ..., 302$, $p_0 = -12$, $p_{302} = 12.02478213$ of the interval $p \in (-12, 12.02478213)$. This provided the accuracy ϵ_0 of the results presented in Figs. 3 and 4 not worse than $\sim 10^{-3}$ at $\tau N \leq T = 64$ and $|A_n| = 1$. The fact of localization of the wave packet in the chosen integration interval at each kick was checked by the discrepancy of the completeness condition (14.3) within the given accuracy ϵ_0.

Thus, to calculate the integrals in a wider range of the parameters A_n, τ, and N one should use the method of integration of fast-oscillating functions.[15,16] The corresponding calculations aimed at analysing the problem in more detail and comparing the results with those for a train of kicks in a wider range of parameters are in progress.

3. ALTERNATIVE APPROACH

To consider the 1D model of a single laser pulse having a continuous envelope with the delta-"atom"[7], we solve the 1D TDSE

$$\left[i\frac{\partial}{\partial t} + \frac{1}{2}\frac{\partial^2}{\partial x^2} - b''(t)x\right]\tilde{\Phi}_L(x,t) = -Z\delta(x)\tilde{\Phi}_L(x,t), \quad \tilde{\Phi}_L(x,0) = \tilde{\varphi}_0(x) = \sqrt{Z}e^{-Z|x|},\ \varepsilon_0 = -\frac{Z^2}{2}. \tag{17}$$

In Eq. (17) the function $b''(t)$ is the time-dependent part of the dipole electric alternating field. This part can be either the sum of delta-functions like in Eq.(2), or a continuous function, for example,

$$b''(t) = \sqrt{\frac{I}{I_0}}\sin^2(\pi\frac{t}{T})\sin(\omega t).$$

Here $0 \le t \le T = (2\pi N)/\omega$, I is the intensity, $I_0 = 3.5 \cdot 10^{16}\ W/cm^2$, and ω is the field frequency.

The solution takes the following general form[7]

$$\tilde{\Phi}_L(x,t) = \int_{-\infty}^{\infty} \frac{dp}{2\pi}\ \chi_L(x,p;t)\left[\varphi_0(p) + iZ\int_0^t\ d\xi\ \chi_L^*(0,p;\xi)\tilde{\Phi}_L(0,\xi)\right]. \tag{18}$$

In (18) the Volkov wave in the length gauge (L-gauge) is

$$\chi_L(x,p;t) = e^{iP(t)x - iS(p,t)}, \quad \text{and} \quad \varphi_0(p) = \frac{2Z^{3/2}}{Z^2+p^2}, \quad P(t) = p - b'(t),\ S(p,t) = \frac{1}{2}\int_0^t P^2(\xi)d\xi.$$

We denote solution $\tilde{\Phi}_L(0,t)$ at $x = 0$ in the terms of unknown $\phi(t)$,

$$\tilde{\Phi}_L(0,t) = e^{-i\zeta(t)}\phi(t), \quad \zeta(t) = \frac{1}{2}\int_0^t\ (b'(\xi))^2 d\xi$$

and get the integral equation for $\phi(t)$ from Eq.(18)

$$\phi(t) = F(t) + iZ\int_0^t\ d\xi\ K(t,\xi)\phi(\xi). \tag{19}$$

Here kernel $K(t,\xi)$ and inhomogeneous term $F(t)$ are given in the analytical form

$$K(t,\xi) = \int_{-\infty}^{\infty} \frac{dp}{2\pi}\ e^{-i(p^2/2)(t-\xi)+ip[b(t)-b(\xi)]} = \frac{e^{-i\pi/4}}{\sqrt{2\pi(t-\xi)}}\exp\{i[b(t)-b(\xi)]^2/2(t-\xi)\}, \tag{20}$$

and

$$F(t) = \int_{-\infty}^{\infty} \frac{dp}{2\pi}\ e^{-i(p^2/2)t+ipb(t)}\varphi_0(p) = \frac{Z^{3/2}}{\pi}\int_{-\infty}^{\infty} \frac{dp}{Z^2+p^2}\ e^{-i(p^2/2)t+ipb(t)} = \frac{\sqrt{Z}}{2}e^{itZ^2/2}[R_+(t)+R_-(t)]. \tag{21}$$

In Eq. (21) the functions $R_\pm(t)$ are expressed by means of the error function erfc(t)

$$R_\pm(t) = e^{\pm Zb(t)}\mathrm{erfc}\left(e^{i\pi/4}Z\sqrt{t/2} \pm e^{-i\pi/4}\frac{b(t)}{\sqrt{2t}}\right).$$

In the momentum space after the Fourier transformation we get

$$\Phi_L(P(t),t) = e^{-iS(p,t)}\left[\varphi_0(p) + iZ\int_0^t\ d\xi\ e^{i(p^2/2)\xi - ipb(\xi)}\phi(\xi)\right]. \tag{22}$$

To get the probability amplitudes for the atom to stay in the ground state or to be ionized, we have to project the wave packet (22) at the end of the pulse ($b''(T) = b'(T) = b(T) = 0$) onto the proper final state, given in Sec.2.

In this approach we have to solve the Volterra equation of the second type (19). This equation strongly resembles the one considered in Ref.[4] In this paper the "atom" with also one bound state was considered, but the potential was separable (nonlocal). The corresponding calculations and comparison with the train of kicks for short values of τ are in a progress.

4. CONCLUSION

We apply the earlier considered model[13] , in which the train of zero-duration electromagnetic kicks interacts with a 1D "atom" with δ-potential, to the sequence of rather short (attosecond) laser pulses separated by relatively large time-intervals τ. This train of pulses interacts with the 1D "atom". It was found that while for the kicks of similar sign the probability $w_0^{(N)}$ decreases with the increasing number of kicks rather quickly for relatively small τ, for the kicks of alternating sign this decrease is strongly suppressed even for 40 kicks. The beats of the probability are observed that are clearly expressed at $\tau = 0.2$. For large time intervals τ in both cases the probability decrease is exponential and independent on the kick signs. The considered model can be useful for studies of the problem of coherent control of quantum dynamics[1] .

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