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Peculiarities of Excitation of a Particle in a Single-Level Quantum Well by an Extremely Short Attosecond Pulse

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Using the solution of the time-dependent Schrödinger equation, the features of the excitation of a bound state of a particle in a one-dimensional rectangular quantum well of small depth by an extremely short light pulse are studied. The case of a shallow well with only one energy level is considered. In this case, the system is excited by an attosecond pulse whose duration is shorter than the characteristic time associated with the energy of the bound state of the particle in the well. It is shown that in this case the population of the bound state and the ionization probability are determined by the ratio of the electric area of the pulse to its atomic scale, which is inversely proportional to the well width. The calculation results showed that unipolar subcycle pulses with nonzero electric area can excite the system faster and more efficiently than bipolar pulses with zero area. The possibility of using unipolar gamma-ray pulses of zeptosecond duration for deuteron excitation is discussed, and numerical estimates of the required duration and electric area of the pulse are given.

Keywords: extremely short pulses attosecond pulses, unipolar pulses, electric area of a pulse, atomic scale of electric area, one-dimensional quantum wells, nanostructures.

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Introduction

To date, the progress in reducing the duration of electromagnetic pulses has resulted in the possibility of getting the pulses whose duration is in the attosecond range ($1\,\text{as} = 10^{-18}\,\text{s}$) [1–5]. In the so-called cascade scheme, that was recently proposed, the duration of the generated pulses is able to reach the record values of 3 as [6]. And in the optical range, it is possible to generate the pulses with a duration of hundreds of attoseconds [7], which can be used to study the ultrafast dynamics of wave packets in various materials [7–11].

A further reduction in the duration of electromagnetic pulses inevitably leads to getting the already unipolar half-period pulses, which contain a half-wave of a field of the same polarity [12]. Unlike conventional bipolar multicycle pulses, the electric area of these pulses can be different from zero, which is defined as the integral of the electric field strength $\mathbf{E}$ with respect of time t at a given point in space [13]

$$\mathbf{S}_E(\mathbf{r}) = \int \mathbf{E}(\mathbf{r}, t)dt. \qquad (1)$$

The interest in obtaining unipolar pulses has increased sharply in recent years, see the review [12] and the cited publications. Recently, there have also been many papers that tackle various situations in which it is possible to obtaining such impulses, see, for example, [14–21]. Due to the unidirectional effect on micro-objects, they can be used for faster and more efficient excitation of quantum systems, acceleration of charges and other applications [12]. In point of fact, it was previously shown that if the duration of such a half-period pulse τ_p was shorter than the characteristic time associated with the ground state energy $T_g = 2\pi\hbar/E_1$ (where E_1 — the energy of the particle in the ground state), then they would be able to excite micro-objects faster and more efficiently, compared to bipolar multicycle pulses [22–27]. To quantify the degree of impact of such extremely short pulses (ESP) on micro-objects, a new physical quantity — atomic scale of electrical pulse area was previously introduced, which makes sense of the„of„intrinsic“ momentum of the system and is inversely proportional to the size of the system of interest [24,25].

Further, when $\tau_p < T_g$, the ESP impact on a quantum system, as shown by the results of the approximate solution and direct numerical integration of the time-dependent Schrödinger equation (TDSE), is determined by the ratio of the electrical area of the pulse to its atomic scale and not by the pulse energy [24–28]. This conclusion is universal for a wide class of quantum systems — atoms [24,25], molecules [23,26], ions [27] and nanostructures [28].

The paper [28], based on the TDSE solution, studied the ESP interaction with nanostructures, which were simulated using a one-dimensional model of a rectangular potential well with infinitely deep walls. However, this model is very approximate, and in practice it is more often necessary to deal with potential wells of finite sizes. Recently, there has

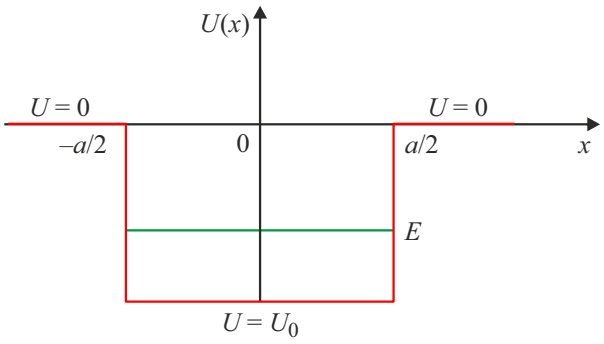

Figure 1. A one-dimensional rectangular potential well of finite depth in which there is only single energy level.

been considerable interest in the interaction of attosecond and femtosecond pulses not only with atomic systems, but also with various nanostructures, for instance, with spherical nanoparticles [29,30]. However, these studies use long bipolar pulses.

This paper, based on the approximate and numerical solution of the TDSE, studies the ESP interaction with a duration of $\tau_p < T_g$ with a one-dimensional nanostructure. The latter is simulated using a one-dimensional rectangular potential well of shallow depth, when there is only single energy level in the well (Fig. 1). It has been shown, that the level population and the probability of ionization are also determined by the ratio of the electrical area of the pulse to its atomic scale. In this paper is also discussed the use of unipolar zeptosecond pulses in nuclear physics for deuteron excitation.

Excitation of a particle in a one-dimensional shallow rectangular potential well by an extremely short light pulse

Let us consider a particle in a one-dimensional rectangular potential well of finite depth (one-dimensional nanostructure). The stationary Schrödinger equation has the form [31]

$$\psi'' + \frac{2m}{\hbar^2}(E - U(x))\psi = 0. \tag{2}$$

The potential energy of a particle in such a potential well is described by the expression

$$U(x) = \begin{cases} 0 & |x| < a/2, \\ U_0 & |x| > a/2, \end{cases} \tag{3}$$

where a — is the well width. Schematically, this well is shown in Fig. 1.

The problem of finding the stationary states of a particle in such a well can be easily solved analytically [31]. Below we are interested in the case of a shallow well in which there can be only single energy level (see Fig. 1). In this case, the expression for the particle energy looks like this [31]

$$E = U_0 - \frac{ma^2}{2\hbar^2}U_0^2. \tag{4}$$

The eigen function of the bound state can also be easily found. Omitting the detailed calculations (see [31]), let us provide expressions for the wave function of a particle inside the well and outside of it.

Inside the well at $|x| < a/2$:

$$\psi'' + \frac{2m}{\hbar^2}E\psi = 0 \rightarrow \psi = \alpha_1 \cos(kx), \;\; k^2 = \frac{2m}{\hbar^2}E.$$

Outside of the well at $x > a/2$:

$$\psi'' + \frac{2m}{\hbar^2}(E - U_0)\psi = 0 \rightarrow \psi = \alpha_2 \exp(-\kappa x),$$

$$\kappa^2 = \frac{2m}{\hbar^2}(U_0 - E).$$

The relationship between the constants α_1 and α_2 is found from the conditions for matching the wave functions and its first derivative at the boundary of the well. It is not difficult to show, that $\alpha_2 = \alpha_1 \cos(ka/2)\exp(\frac{\kappa a}{2})$.

It is not difficult to find the value α_1 from the wave function normalization condition $\int \psi_1^2(x)dx = 1$. It has the form

$$\alpha_1 = 1\Big/\left[\frac{a}{2} + \frac{\sin ka}{2k} + \frac{q^2}{\kappa}e^{-\kappa a}\right]^{1/2}.$$

To describe the system interaction with the ESP field, let us follow the same approach that was used earlier in the papers [22–28]. The interaction of a particle located in such a well with the ESP field is described by the time-dependent Schrödinger equation (TDSE) for the electron wave function $\Psi(x,t)$ [31]

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = [H_0 - qxE(t)]\Psi(x,t). \tag{5}$$

Here

$$H_0 = -\frac{\hbar^2}{2m} + U(x)$$

— the proper Hamiltonian of the system, $U(x)$ — potential energy of the particle described by the formula (3), m — electron mass q — electron charge, $\hbar$ — reduced Planck constant. If the pulse duration is shorter than T_g, then for the TDSE approximate solution in (4), as in the papers [22–28], we will use the approximation of sudden perturbations introduced by Migdal [32]. In this approximation, the expression for the electron wave function after the pulse has the form [22–28]

$$\Psi_+(x) = \psi_0(x)e^{i\frac{q}{\hbar}S_E x}, \tag{6}$$

where $\psi_0(x)$ is the wave function before the pulse arrival. If the particle was in a bound state with its eigen function $\psi_1(x)$ before the pulse arrival, then the amplitude of the

bound state a_1 is the projection of $\psi_1(x)$ onto the wave function of the system after the pulse $\Psi_+(x)$ (6) and is given by the expression

$$a_1 = \int_{-\infty}^{\infty} \psi_1^2(x) e^{i\frac{q}{\hbar}S_E x} dx. \qquad (7)$$

In this case, the population of the bound state is determined in terms of the square of the amplitude modulus a_1.

Using the (7) and the above expression for the intrinsic wave function of the bound state of a particle in the well, one can obtain the following expression for the amplitude of the bound state of the particle in the well:

$$a_1 = \frac{\sin(S_E/S_{0,QW})}{qS_E/\hbar} + \frac{\sin(ka + S_E/S_{0,QW})}{4k + 2qS_E/\hbar} + \frac{\sin(ka - S_E/S_{0,QW})}{4k - 2qS_E/\hbar} + 2\mathrm{Re}\left(\frac{-\kappa a + iaS_E/S_{0,QW}}{\kappa - iS_E/S_{0,QW}}\right). \qquad (8)$$

Here the $S_{0,QW} = 2\hbar/qa$ —is an atomic scale of the area for a quantum well inversely proportional to its width a. The corresponding probability of ionization is $w_i = 1 - |a_1|^2$. Thus, the population of the bound state of a particle in a rectangular well and the probability of ionization are determined by the ratio of the electric area of the pulse to its scale. This is consistent with the conclusions drawn earlier for atomic and molecular systems, and the particles in a well with infinitely high stacks [22–28].

Calculation results and analysis of the results obtained

In numerical calculations, the system was excited by the ESP of the Gaussian form $E_e(t) = E_0 e^{\frac{-t^2}{\tau_p^2}} \cos(\omega_p t)$, $\omega_p = 2\pi/T_p$, T_p — field period. For ESP the values ω_p and T_p have a conditional meaning. The well width had the value $a = 1.2$ nm. Pulse field amplitude $E_0 = 3 \cdot 10^8$ V/cm, frequency $\omega_p = 14 \cdot 10^{15}$ rad/s (wavelength $\lambda_a = 134.6$ nm, period $T_p = 2\pi/\omega_p = 448.8$ as). With the specified parameters, the time $T_g = 16$ fs.

To illustrate the population dependence $|a_1|^2$ after the passage of the pulse, we have calculated the dependence of $|a_1|^2$ on the parameters of the exciting pulses from the duration of exciting pulses τ_p (see fig. 2). The calculation was carried out using the approximation of sudden perturbations as per the analytical formula (7), which corresponds to the solid line in Fig. 2. Also, the population was calculated using the numerical solution of the TDSE by the Crank-Nicholson method [33]. The result of the numerical calculation is shown by a dotted line in Fig. 2.

It can be seen from the figure that the results of analytical and numerical calculations are qualitatively similar to each other in terms of the form. Similar results are obtained in the case of a deeper well, in which there are more levels.

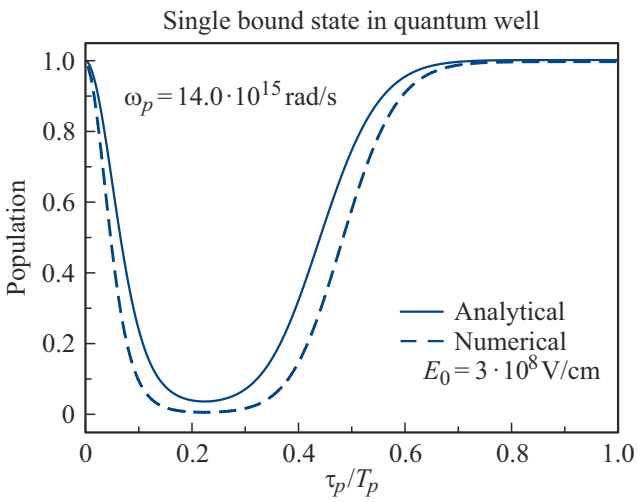

Figure 2. Population dependence of the bound state $|a_1|^2$ particles in a one-dimensional well from the pulse duration τ_p. The solid line — is a result of calculation in the approximation of sudden disturbances, the dashed line — is a result of numerical calculation using the TSE.

Despite some notable quantitative differences between the results of numerical and analytical calculations, the figure shows a trivial result — half-cyclepulses with a nonzero electrical area almost completely empty the bound state (in the range $\tau_p = 0.1T_p - 0.4T_p$), which leads to ionization of the particle from the well. When the pulse duration tends to the period of the field, its electric area tends to zero, and the population of the state $|a_1|^2$ tends to 1. That is, bipolar pulses with $S_E = 0$ have no effect on the system, which is consistent with the results of the previous studies [22–28].

Application of unipolar pulses in nuclear physics — deuteron excitation

The above model of a potential well containing only single energy level is used, for example, to describe the deuteron [34]. A deuteron consists of a proton and a neutron. They are connected by a force that is characterized by a rectangular potential well in which there is only single energy level [34]. This well radius is $r = 2.8 \cdot 10^{-13}$ cm. The binding energy between them $E = 2.23$ Me $= 3.57 \cdot 10^{-6}$ eng. Time $T_g = \frac{2\pi\hbar}{E} = 1.84 \cdot 10^{-21}$ s $= 1.84$ zs $= 0.0018$ as. The value of the area measure for the deuteron $S_{0,QW} = 2\hbar/qr \sim 1.56 \cdot 10^{-5}$ erg·s/cm·ESU. For comparison: for a hydrogen atom, this value is 5 orders of magnitude lower than $S_{0,H} \sim 10^{-10}$ erg·s/cm·ESU [24]. Thus, for effective excitation of deuterons, the X-ray and gamma-ray pulses in the zeptosecond duration range are needed (1 zs $= 10^{-21}$ s) [35]. The possibility of using unipolar gamma-quanta for effective control of nuclear reactions was also discussed in [16].

Conclusion

In this paper, we consider the problem of a particle excitation in a one-dimensional rectangular potential well, with a single energy level, using an ESP of attosecond duration, which is less than the time associated with the energy of the bound state, $\tau_p < T_g$. Such a model of a rectangular well with one energy level can describe nanostructures, nanoparticles with shallow potential wells [36–38], and is also used in nuclear physics, for example, to describe the deuteron [34].

Based on the approximate analytical solution of the time-dependent Schrödinger equation (TDSE), an expression is obtained for the amplitude of the bound state of a particle in such a well after the passage of a pulse. It has been shown that the population of the bound state is determined by the ratio of the electrical area of the pulse to its atomic scale. Once again this confirms the earlier conclusion that unipolar half-period pulses are able to excite the system more quickly than single-cycle pulses with zero area. The results of the population calculation obtained analytically are qualitatively consistent with the results of the calculation carried out on the basis of the numerical solution of the TDSE.

The results obtained can be used in the theoretical description of the excitation of nanoparticles, quantum dots, semiconductor nanostructures based on quantum wells by optical half-period attosecond pulses and in nuclear physics, for example, for the excitation of a deuteron using zeptosecond gamma and X-ray pulses.

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Conflict of interest

The authors declare that they have no conflict of interest.

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