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# Excitation and ionization of a particle in a double quantum well by an extremely short light pulse

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The excitation and ionization of a particle in a double one-dimensional quantum well excited by an extremely short light pulse is considered theoretically. In the sudden perturbation approximation, analytical expressions for the population of bound states and the probability of ionization of the particle are obtained when the pulse duration is shorter than the characteristic time associated with the energy of the ground state of the particle. It is shown that the population of bound states and the ionization probability are determined by the ratio of the electrical area of the pulse to the value of its atomic scale, which is inversely proportional to the characteristic size of the system in the ground state. The results obtained demonstrate the possibility of controlling the ultrafast dynamics of electrons in heterostructures based on double quantum wells.

**Keywords:** unipolar pulses, electric pulse area, double quantum wells.

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## Introduction

Generation of electromagnetic impulses of femto- and attosecond duration made it possible to study and control the motion of wave packets in difference substances [1]. The results of recent experiments using attosecond impulses demonstrated the ability to study the response of the bound electrons in gas [2], to measure the delay in the time response in the dielectric [3]. Using attosecond impulses, it became possible to identify the impact of the bonding between the nuclei and electrons on the photoionization of the hydrogen molecule [4], to visualize the induced electron coherence in real time [5], to control the shape of the absorption line in the hydrogen molecule using XUV attosecond impulses [6] and to obtain other results that were important from the fundamental point of view. The significance of the conducted research was acknowledged by the recent Nobel Prize in physics for the experimental methods of light attosecond impulse generation to study the dynamics of electrons in the substance [7].

Usually the ultrashort impulses generated in practice from the regular sources, such as lasers with passive synchronization of modes or attosecond impulses in the units with the generation of high-order harmonics, contain several half-waves of the field intensity, i.e. are bipolar [1–6]. And their electric area

$$S_E \equiv \int_{-\infty}^{+\infty} E(t)dt$$

($E(t)$ — intensity of the electric field in the specified point of the space, $t$ — time) is always close to zero. The limit possibility for the reduction of the duration of laser impulses in the specified spectral range is the generation of unipolar impulses that contain the half-cycle of the single polarity field intensity oscillations and have the non-zero electric area [8].

Many papers [8–13] have been recently dedicated to the study of the possibility to generate such monopolar impulses and their interaction with the substance. These papers resulted in development of a new area in the contemporary optics — „optics of both unipolar and subcycle light" [9]. Unipolar impulses may quickly transmit the impulse to the charged particle in the same direction and, therefore, may be used for ultrafast and effective control of the quantum systems properties compared to the regular bipolar impulses, charge acceleration, holography with ultrahigh time resolution and other interesting applications [8–26].

Finally, if the impulse duration is less than the specific time related to the energy of the particle ground state (the period of electron rotation in the Bohr orbit), the standard Keldysh theory of photoionization [27] becomes inapplicable. In this case the impact of unipolar, half-cycle impulses on the microobjects is determined by the electric area of the impulse, and not its energy [8–26]. In such case in order to characterize the extent of impact of half-cycle impulses on the quantum systems, it is necessary to introduce a new value — atomic measure of area, which is inversely related to the specific size of the system in the ground state multiplied by the electron charge [16,19].

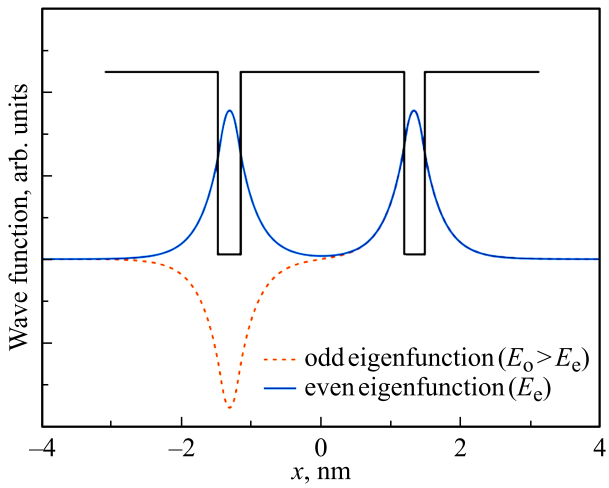


**Figure 1.** Double rectangular quantum wells and even and odd internal wave functions of the particle in them.

The results of the early theoretical studies show the possibility of using unipolar impulses with non-zero electric area for the effective and ultrafast control of atomic and molecular systems [9–19]. The papers [20–24] studied the impact of the shortest impulses on the particle in the one-dimensional potential well. Besides, a single rectangular quantum well was considered, which either had a very large depth (in the limit of the infinitely large), or a very small depth [20,23], when the well had only one energy level [22,24]. The case of the delta-shaped well (potential of zero radius) was considered in the paper [21]. The model of the one-dimensional rectangular potential well is widely used in the problems of interaction of ultrashort light impulses with various nanostructures, nanoparticles etc. [28–30].

Structures from double quantum wells comprising a pair of rectangular wells divided by a potential barrier are of specific interest [31]. Such structures and their properties are the subject of active research [32–35] in virtue of their multiple applications in different fields of science and engineering [28,31]. In the limit of the very narrow and deep well such system may be roughly approximated by two delta-shaped potential wells, i.e. the double zero radius potential (ZRP)

This paper, based on the solution of the Schrödinger's equation in the approximation of sudden disturbances, studies the interaction of the shortest impulses (SI) with the particle in the double quantum well, comprising two deep and narrow rectangular quantum wells separated by the barrier (Fig. 1). The impulse duration is deemed to be shorter than the specific time related to the energy of the particle in the ground state, therefore, the analysis applies the approximation of sudden disturbances [52–57]. It was shown that the populations of the bound states and the probability of ionization are determined by the ratio of the electric area of the impulse to its measure, which is inversely related to the specific size of such nanostructure.

## The considered system of double quantum wells

Let us consider the system of the double quantum well, comprising two one-dimensional rectangular quantum wells separated by a barrier (Fig. 1).

For simplicity of the analysis, we will consider the wells to be very deep and simultaneously narrow, which simplifies the analytical calculations, however, it does not interfere with the common nature of the conclusions made. In this case to simplify the calculations, we approximate this potential function by two delta-shaped potential wells (two-center ZRP). Wave functions and internal values of such system energy may easily be found [58].

The stationary Schrödinger's equation with such one-dimensional potential has the following form

$$\psi'' + \frac{2m}{\hbar^2}(E - U(x))\psi = 0, \quad (1)$$

where the electron potential energy profile is assumed as

$$U(x) = -V_0\delta\left(x - \frac{L}{2}\right) - V_0\delta\left(x + \frac{L}{2}\right), \quad (2)$$

where $V_0$ — „capacity“ of each well, $L$ — distance between the wells.

According to [58], such double well may either have even or odd internal states. They are schematically shown in Fig. 1. The expression for the wave function of even state has the following form

$$\psi_{\text{even}}(x) = \begin{cases} C_{\text{even}}\left(1 + e^{\kappa_0 L}\right) e^{\kappa_0(x+L/2)}, & x \le -L/2, \\ C_{\text{even}}\left(e^{\kappa_0(x+L/2)} + e^{-\kappa_0(x-L/2)}\right) \\ \quad = C_{\text{even}} e^{\kappa_0 L/2} \cosh \kappa_0 x, & -L/2 < x < L/2, \\ C_{\text{even}}(1 + e^{\kappa_0 L}) e^{-\kappa_0(x-L/2)}, & x \ge L/2, \end{cases}$$

where the normalization factor is indicated

$$C_{\text{even}} = \sqrt{\frac{\kappa_0}{2e^{\kappa_0 L}\left(e^{\kappa_0 L} + 1 + \kappa_0 L\right)}},$$

and the indicator of the exponent $\kappa_0$ is the solution to the equation

$$\kappa_0 L = \frac{mV_0 L}{\hbar^2}\left(1 + e^{-\kappa_0 L}\right). \quad (3)$$

Similarly, the wave function of the odd state has the following form

$$\psi_{\text{odd}}(x) = \begin{cases} C_{\text{odd}}\left(1 + e^{\kappa_1 L}\right) e^{\kappa_1(x+L/2)}, & x \le -L/2, \\ C_{\text{odd}}\left(e^{\kappa_1(x+L/2)} + e^{-\kappa_1(x-L/2)}\right) \\ = C_{\text{odd}} \sinh \kappa_1 x, & -L/2 < x < L/2, \\ C_{\text{odd}}\left(1 + e^{\kappa_1 L}\right) e^{-\kappa_1(x-L/2)}, & x \ge L/2, \end{cases}$$

with the normalization factor

$$C_{\text{odd}} = \sqrt{\frac{\kappa_1}{2e^{\kappa_1 L}\left(e^{\kappa_1 L} - 1 - \kappa_1 L\right)}},$$

and the indicator of the exponent $\kappa_1$ is the solution to the transcendental equation

$$\kappa_1 L = \frac{mV_0 L}{\hbar^2}\left(1 - e^{-\kappa_1 L}\right). \tag{4}$$

These expressions use the designation $\kappa = \frac{2m|E|}{\hbar^2}$, $E$ — particle energy in the bound state, which is found numerically. If $V_0 < \frac{\hbar^2}{mL}$, such well has always only one discrete level of energy, corresponding to the even wave function $\psi_{\text{even}}(x)$, which is the only solution to the equation (3). The equation (4) in this case does not have non-trivial material solutions. On the contrary, if $V_0 > \frac{\hbar^2}{mL}$, the well contains two discrete levels of energy, besides, the main level corresponds to the even wave function $\psi_{\text{even}}(x)$, and the excited one — to the odd one $\psi_{\text{odd}}(x)$ [58]. Accordingly, in this case the equation (3) and the equation (4) have the only solution for the values $\kappa_0$ and $\kappa_1$. Solutions with complex $\kappa_1$, compliant with the solid spectrum, are not considered by us.

## Theoretical consideration and discussion of results

Dynamics of the quantum system in the external field of SI is described by one-dimensional temporal Schrödinger's equation for the wave function of the electron $\Psi(x, t)$ [59]:

$$i\hbar\frac{\partial\psi}{\partial t} = [\hat{H}_0 + V(t)]\Psi.$$

Here $\hat{H}_0$ — internal Hamiltonian of the system, $\hbar$ — the reduced Planck's constant. $V(t) = -qxE(t)$ — energy of system interaction with the SI field in the dipole approximation, $q$ — electron charge.

The duration of the attosecond impulses currently generated may already be shorter than the specific intraatomic periods [60–67]. Therefore, to find the amplitudes of bound states after the impulse, we will consider that the duration of SI $\tau$ is shorter than the specific time related to the particle energy in the ground state, $T_g = 2\pi\hbar/E$, $\tau \ll T_g = 2\pi\hbar/E$.

When $\tau \ll T_g$, Keldysh theory of photoionization becomes inapplicable [19,27], therefore, to find amplitudes of bound states and probability of ionization, we will use the approximation of the sudden disturbances introduced by Migdal, Pauli and Schiff [52–54] and studied by other authors [15,55–57]

In the approximation of sudden disturbances the wave function of the particle after the impulse is recorded as [15,17–19,23,24]:

$$\Psi_e(x) = \psi_0(x)e^{i\frac{q}{\hbar}S_E x}. \tag{5}$$

After SI passage the wave function of the particle $\Psi_e(x)$ may be decomposed into internal functions of the non-disturbed Hamiltonian of the system (in our case these

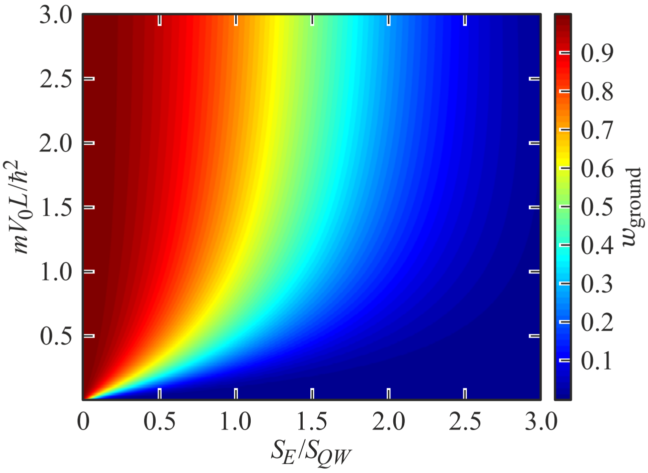


**Figure 2.** The population of the ground (even) state after the exposure of the medium to the shortest exciting impulse.

are states $\psi_{\text{even}}(x)$ and $\psi_{\text{odd}}(x)$, introduced in the previous section): $\Psi_e(x) = \sum_n a_n\psi_n(x)$. Here $a_n$ — amplitude of the bound state (index n complies with either the even or the odd state), expressions for which are recorded in the form of

$$a_n = \int_{-\infty}^{\infty} \psi_n^*(x)\psi_{\text{even}}(x)e^{i\frac{q}{\hbar}S_E x}dx. \tag{6}$$

If before the arrival of the impulse the system was in the ground state, i.e. $\psi_{\text{even}}(x)$, then from (6) it is easy to produce the expression for the amplitude of the ground even state after impulse passage:

$$a_{\text{even}} = \int_{-\infty}^{\infty} \psi_{\text{even}}^2(x)e^{i\frac{q}{\hbar}S_E x}dx,$$

and for the odd state:

$$a_{\text{odd}} = \int_{-\infty}^{\infty} \psi_{\text{odd}}(x)\psi_{\text{even}}(x)e^{i\frac{q}{\hbar}S_E x}dx.$$

Populations of these states are determined by the square of the module of the corresponding amplitudes.

Let us introduce the following value:

$$S_{QW} = \frac{\hbar}{qL},$$

which we will call the specific measure of electric area for the double quantum well. This value is similar for other simplest quantum systems [16,18,19,21–24]. Then from the formulas (5),(6) we produce the following expressions for the population of the ground (even) state after the exposure of the medium to the shortest exciting impulse:

$$w_{\text{ground}} = C_{\text{even}}^4 L^2 e^{2\kappa_0 L} \left( \frac{8\kappa_0 L}{4\kappa_0^2 L^2 + S_E^2/S_{QW}^2} \right)^2$$
$$\times \left| (1 + e^{\kappa_0 L}) \cos \frac{S_E}{2S_{QW}} + \kappa_0 L \frac{2S_{QW}}{S_E} \sin \frac{S_E}{2S_{QW}} \right|^2 \qquad (7)$$

and for the population of the excited (odd) state:

$$w_{\text{excited}} = 4C_{\text{even}}^2 C_{\text{odd}}^2 L^2$$
$$\left| \left( \frac{(\kappa_0 + \kappa_1) L (2e^{(\kappa_0+\kappa_1)L} + e^{\kappa_1 L} - e^{\kappa_0 L})}{(\kappa_0 + \kappa_1)^2 L^2 + S_E^2/S_{QW}^2} \right. \right.$$
$$\left. + \frac{(\kappa_1 - \kappa_0) L (e^{\kappa_1 L} + e^{\kappa_0 L})}{(\kappa_1 - \kappa_0)^2 L^2 + S_E^2/S_{QW}^2} \right)$$
$$\times \sin \frac{S_E}{2S_{QW}} + \left( \frac{(e^{\kappa_1 L} - e^{\kappa_0 L})}{(\kappa_0 + \kappa_1)^2 L^2 + S_E^2/S_{QW}^2} \right.$$
$$\left. \left. + \frac{(e^{\kappa_0 L} - e^{\kappa_1 L})}{(\kappa_1 - \kappa_0)^2 L^2 + S_E^2/S_{QW}^2} \right) \cdot \frac{S_E}{S_{QW}} \cdot \cos \frac{S_E}{2S_{QW}} \right|^2. \qquad (8)$$

Remember that the odd state exists only if: $V_0 > \hbar^2/mL$.

Finally, the probability of ionization of the double quantum well may be produced as

$$w_{\text{ioniz}} = 1 - w_{\text{ground}} - w_{\text{excited}}. \qquad (9)$$

One can see that these populations and ionization are determined by the ratio of the electric area of the impulse to its atomic measure, which is proportionate to the well width, and not the energy of impulses, which is matched with the result of early studies for single quantum wells, atoms, molecules and other systems [16,18,19,21–24]. Note that the produced expressions are fair, when $\tau \ll T_g$. The calculation results of the populations in this approximation are matched with the results of the direct numerical solution to the Schrödinger's equation [18,22–24] for different systems, therefore the issue on the feasibility of this approximation in this paper is not considered (see some comments on its applicability in the Appendix).

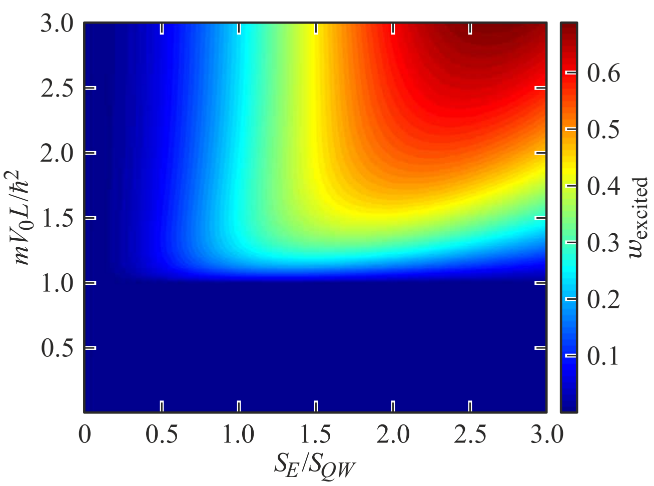


**Figure 3.** The population of the excited (odd) state after the exposure of the medium to the shortest exciting impulse.

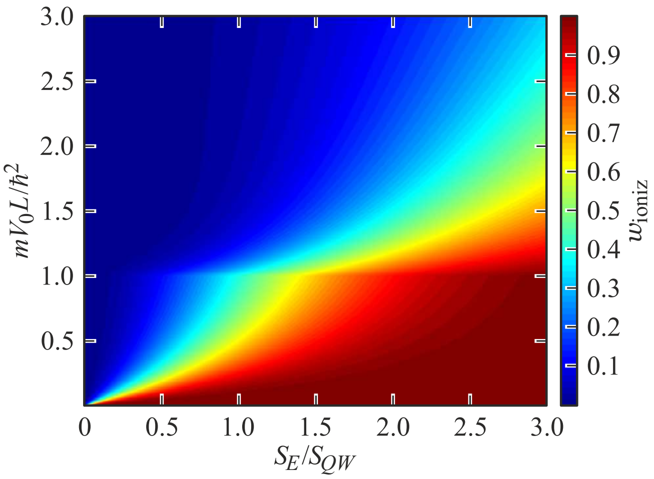


**Figure 4.** The probability of electron ionization in the double quantum well upon exposure of the medium to the shortest exciting impulse.

Dependences of the excitation probabilities of both levels and the probability of ionization on the parameters of the well and the electric area of the exposing impulse are demonstrated in Fig. 2–4.

It is seen clearly from these figures that in case of electric area close to zero the system remains in the ground (even) state. The second excited state is not populated, no ionization takes place. This circumstance is quite evident, since the electric area of the impulse has the sense of the transmitted mechanical impulse to the system, which in this case is equal to 0.

As the electric area grows, when it becomes comparable or exceeds the measure $S_{QW}$, the population of the second state and the probability of ionization increase. It is evident that in this case the half-cycle impulse of the field quickly transmits the mechanical impulse to the system that is already comparable to its measure $S_{QW}$, which results in its quick excitation and ionization. The produced results show the possibility of ultrafast control of electron dynamics in the double quantum wells, which opens the new opportunities for the studies in this area using half-cycle impulses.

## Conclusion

This paper, based on the approximated solution to the Schrödinger's equation in the approximation of sudden disturbances, produced analytical expressions for the populations of the even and odd states and probability of particle ionization in the double rectangular quantum well, excited by a single SI with duration of shorter than the specific time, related to the particle energy in the ground state, $T_g = 2\pi\hbar/E$. The wells are assumed to be deep and narrow, which makes it possible to approximate them with delta-shaped wells. However, it does not interfere with the common nature of the conclusions made.

The produced expressions show that in this case the value of populations and probability of ionization is determined as the ratio of the electric area of the impulse to its atomic measure. This conclusion is compliant with the early studies of authors for the atomic, molecular systems and single quantum wells, both one- and three-dimensional ones [16–26]. These results show that the half-cycle impulses with non-zero electric area make it possible to provide noticeable and quick excitation and ionization of electrons in the double quantum wells in contrast to the bipolar impulses with the area close to zero.

The produced results may be used in analysis of electron excitation in the heterostructures based on double quantum wells by shortest impulses. The conducted research shows the new opportunities in using half-cycle impulses for ultrafast excitation of the quantum wells on the basis of double quantum wells and therefore opens new directions for research in the optics of unipolar light and physics of heterostructures.

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### Conflict of interest

The authors declare that they have no conflict of interest.

## Appendix

### On compliance with the results, produced within the standard theory of disturbances and approximation of sudden disturbances

We would like to note that in the limit of the weak field the results produced with the help of approximation of sudden disturbances reduce to the result produced within the regular theory of disturbances. This corresponds to the case when the intensity of the exciting field is much less than the intraatomic field in the system and the duration of the exciting impulse is much less than the specific time of the internal dynamics of the quantum system.

In this case it is easy to show that the approximated solution to the Schrödinger's equation using the standard theory of disturbances and the approximated solution to the Schrödinger's equation using the approximation of sudden disturbances match precisely. This issue was previously discussed in [15]. Below this circumstance was considered in detail.

Indeed, the solution to the Schrödinger's equation in the approximation of the sudden disturbance has the following form

$$\psi(\bar{r}, t) = \psi(\bar{r}, -\infty) \cdot e^{\frac{iq}{\hbar}\bar{r} \int_{-\infty}^{t} \bar{E}(t')dt'}, \qquad (\Pi 1)$$

where it is assumed that the exciting impulse starts acting at the moment of time $t = -\infty$.

In the standard theory of disturbances, which is fair for the small amplitudes of exciting field, the population of the bound n-state of the quantum well is provided as the expression

$$w_n = \frac{d_{kn}^2}{\hbar^2} \left| \int_0^t E(t') e^{i\omega_{kn}t'} dt' \right|^2. \qquad (\Pi 2)$$

First we will assume that initially the system was in $k$-th state, $d_{kn}$ — dipole moment of transition between $k$-th and $n$-th energy level, $\omega_{kn}$ — frequency of this transition.

Approximation of the sudden disturbances is used, when the duration of the exposure is shorter than the specific time of the system:

$$\omega_{kn}\tau_p \ll 1. \qquad (\Pi 3)$$

(see Schrödinger's equation (2), where you can neglect the internal Hamiltonian, $\hat{H}_0$ for the time of exposure, see also [68]). Physically it means that for the time of impulse exposure the electron will not manage to shift noticeably in the orbit. However, the field should not be so strong to remove the electron from the orbit, which imposes certain limitations on the amplitude of excitation impulses as well (see in more detail the applicability of approximations of sudden disturbances in [69,70]).

In this case the population of the state with the number from the expression (P1) is determined in the following manner:

$$w_n = \left| \int_R \psi_k(\bar{r}) \cdot e^{\frac{iq}{\hbar}\bar{r} \int_0^t \bar{E}(t')dt'} \psi_n(\bar{r}) d\bar{r} \right|^2. \qquad (\Pi 4)$$

When the field amplitude is small, the exponent under the integral sign may be decomposed in the following series:

$$e^{\frac{iq}{\hbar}\bar{r} \int_0^t \bar{E}(t')dt'} \approx 1 + \frac{iq}{\hbar}\bar{r} \int_0^t \bar{E}(t')dt'. \qquad (\Pi 5)$$

Then, using the condition of orthogonality of the system wave functions, we get for the populations in approximation of the sudden disturbances

$$w_n = \left| \int\limits_{\bar{R}} \psi_k(\bar{r}) \cdot \left( 1 + \frac{iq}{\hbar} \bar{r} \int\limits_0^t \bar{E}(t')dt' \right) \psi_n(\bar{r}) d\bar{r} \right|^2$$

$$= \left| \int\limits_{\bar{R}} \psi_k(\bar{r}) \cdot \frac{iq}{\hbar} \bar{r} \int\limits_0^t \bar{E}(t')dt' \cdot \psi_n(\bar{r}) d\bar{r} \right|^2$$

$$= \frac{q^2}{\hbar^2} \left| \int\limits_{\bar{R}} \psi_k(\bar{r}) \cdot \bar{r} \cdot \psi_n(\bar{r}) d\bar{r} \right|^2 \cdot \left| \int\limits_0^t \bar{E}(t')dt' \right|^2$$

$$= \frac{d_{kn}^2}{\hbar^2} \left| \int\limits_0^t \bar{E}(t')dt' \right|^2, \qquad k \neq n. \qquad (\Pi 6)$$

The expression produced in this manner in approximation of the sudden disturbances in the approximation of the weak field matches the expression (P2) for the populations within the standard theory of disturbances, where one can neglect the exponent under the integral as a result of meeting the condition $\omega_{kn}\tau_p \ll 1$.

Therefore, this analysis illustrates that at small amplitude of the exciting impulse the calculation results of the populations in the approximation of the sudden disturbances reduce to the results produced within the standard theory of disturbances.

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