Propagation effect in atom excitation by ultrashort and intense laser pulses

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We study hydrogenlike target excitation by a traveling electromagnetic pulse. The spatial size of the pulse \( l = c \tau \) (\( c \) is the speed of light and \( \tau \) is the pulse duration) is assumed to be comparable or less than the characteristic size of the initially occupied atomic state. When propagating through the atom, the pulse is shown to transform the electron wave function "slice by slice." These transformations lead to electron transitions between states with \( \Delta m = \pm 1 \) which are forbidden in the dipole approximation. The case of linear polarization is considered. It is found that magnetic-level excitation probabilities are small for the hydrogen atom, but can be more significant for the hydrogenlike multicharged ions.

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I. INTRODUCTION

The field of laser-atom interactions has been intensively studied, both experimentally and theoretically, during the last two decades [1–9]. Many phenomena, such as above-threshold ionization, atomic stabilization, and high-order harmonic generation, have been discovered and understood. Twenty years ago researches used lasers which operated in the picosecond or subpicosecond time domain with relatively weak peak intensities up to \( \sim 10^{15} \) W/cm\(^2\). Modern-day lasers are capable of delivering unitary pulses [10] or trains of pulses [11] of duration up to a few hundred attoseconds (1 as = \( 10^{-18} \) s). Also, laser fields can now be significantly higher in magnitude than the characteristic atomic fields.

Electron processes in atoms occur in the attosecond time domain. Therefore attosecond pulses can be useful in experiments to directly investigate these processes. Though presently few such studies have been conducted [12,13], in the future they are expected to have a huge impact on different fields in physics and technology, such as nonlinear optics, extreme-ultraviolet optics technology, ultrashort high-power laser technology, intense laser-atom interactions, and coherent control of matter.

Our understanding of laser-atom interactions is based on solution of the time-dependent Schrödinger equation (only one-electron problems are considered here)

\[
i \frac{\partial}{\partial t} \psi(r, t) = \left[ \hat{H}_0 - A(r, t) \hat{p} + \frac{A^2(r, t)}{2} \right] \psi(r, t), \tag{1}\]

where \( \hat{H}_0 = \hat{p}^2/2 + V(r) \) is the unperturbed atomic Hamiltonian, \( \hat{p} = -i \nabla \) is the momentum operator, \( V(r) \) is the electron interaction potential with the ionic core, and \( A(r, t) \) is the vector potential of the field (\( E = -\partial A/\partial t \), where \( E \) is the electric-field strength). Atomic units are used throughout unless specified otherwise.

Equation (1) does not have an analytical solution. The numerical analysis of the three-dimensional problem with accounting of the spatial and time dependences of the electromagnetic field is very complicated [8,14]. Nevertheless, for a number of special cases, the problem can be significantly simplified and an approximate solution can be found, analytically or numerically. As an example the dipole approximation has the spatial dependence of the vector potential completely neglected,

\[
A(r, t) \approx A(0, t). \tag{2}\]

This approximation is justified when the carrier frequency \( \omega_c \) satisfies the relation

\[
\omega_c \ll 1, \tag{3}\]

where \( a \) is the characteristic size of the initially occupied atomic state and \( c \) is the speed of light.

The inequality (3) is well satisfied for the visible and ultraviolet spectral range provided that \( a \) is sufficiently small. For high frequencies Eq. (2) is no longer valid. Indeed, the nondipole corrections are known to be significant in photoionization for \( h \omega > 1 \) keV [15,16]. Moreover, nondipole effects are detectable even for extremely low photon energies \( h \omega < 15 \) eV [17]. With the use of attosecond laser technique, one can generate very short and dense bursts of photons with energies of \( \sim 100 \) eV. So one can expect that nondipole effects will also manifest themselves in electron processes initiated by attosecond laser pulses.

One of the ways to include nondipole effects is to retain the next term in the vector potential \( A(r, t) \) expansion. This approach was used by Va’zquez de Aldana and Roso [18] and Va’zquez de Aldana et al. [19] to study magnetic-field effects in atom-laser interaction for a model two-dimensional problem. The full three-dimensional problem was also considered by Bugacov et al. [20] and, recently, by Chirila et al. [21]. In these works \( A(r, t) \) was taken as

\[
A(r, t) \approx A(0, t) - \frac{\hat{k} \cdot r}{c} \frac{dA}{dt}(0, t), \tag{4}\]

where the unit vector \( \hat{k} \) determines the propagation direction. The second term on the right-hand side of Eq. (4) accounts for the electron drift in the direction \( \hat{k} \) induced by the magnetic-field component of the pulse. Bugacov et al. [20]...
show that this magnetic drift can cause breakdown of the atomic stabilization in an intense laser field. Also, it can result in significant modification of the photon emission spectra [21].

A different approach was recently employed by Va’zquez de Aldana and Roso [14]. They solved analytically a simple model for the strong-field approximation (SFA) case where the laser field is much stronger than the Coulomb field of the nucleus. They applied this model to estimate the influence of the field-induced local phase corrections on the initial state survival probability.

In this paper we consider an atom interacting with a traveling laser pulse. We assume that the pulse is very short so that its characteristic size \( l = c \tau \) is comparable or less than the characteristic size \( a \) of the initial atomic state. In this case expansion (4) is generally inapplicable for the whole space occupied by the atom. Instead, we use the approach similar to the one suggested by Va’zquez de Aldana and Roso [14].

In Sec. II we state the problem and derive an approximate solution of the Schrödinger equation (1) in the limit of a strong laser field. Numerical investigation of the propagation effect and its discussion are presented in Sec. III. Finally, Sec. IV is devoted to the conclusions.

II. THEORETICAL MODEL

We set the origin of the coordinate system to be at the nucleus. The target is subjected to a short electromagnetic pulse propagating along the \( x \) axis. Writing \( \eta = t - \alpha x \), we characterize the external field with a vector potential \( A(\eta) = (0, A_x(\eta), A_y(\eta)) \) (in what follows all capitalized vectors have zero \( x \) components). The components of the field have the following functional form \( A_x(\eta) = a_{f}(\eta) \sin(\omega \eta) \) and \( A_y(\eta) = a_{f}(\eta) \cos(\omega \eta) \) where \( f(\eta) \) is the pulse envelope and \( a_{f}(\alpha) \) is the magnitude of the \( y \) \( (z) \) component. The pulse duration is \( \tau \) and its characteristic length is \( l = c \tau \). The electromagnetic pulse arrives at the coordinate \( x_0 \) at the moment \( t_1 = x_0/c - \tau/2 \), and completely passes at \( t_2 = x_0/c + \tau/2 \), see Fig. 1. We also assume that the field is equal to zero outside the region of pulse localization.

Figure 1 shows the “space time” of the problem divided into three regions. Region I (III) is occupied by the electron wave function before (after) it is modified by the pulse. Region II corresponds to where the laser pulse is active. In what follows we will solve the Schrödinger equation in these three regions independently. This can be justified by the fact that the pulse propagates with the speed of light, and the regions I and III can be linked only by the continuity boundary conditions through the region II.

We will use the Schrödinger equation

\[
\frac{i}{\hbar}\frac{\partial}{\partial t} \psi(r,t) = \hat{H}_0 \psi(r,t)
\]

to describe evolution of the electronic wave function in the field-free space-time area (regions I and III in Fig. 1). The wave function in region I is

\[
\psi_I(r,t) = \sum_n a_n \phi_n(r) \exp[-i \epsilon_n t],
\]

where \( \phi_n \) and \( \epsilon_n \) are, respectively, eigenfunctions and eigenenergies of the Hamiltonian \( \hat{H}_0 \), and coefficients \( a_n \) are the mixing coefficients.

Assuming the SFA the action of the field on the electron wave function (region II) is described by the following equation:

\[
\frac{i}{\hbar} \frac{\partial}{\partial t} \psi_{II}(r,t) = \frac{1}{2} [\hat{p} - A(x,t)]^2 \psi_{II}(r,t),
\]

where the contribution of the atomic potential \( V(r) \) in Eq. (1) has been neglected. Solution of this equation can be found for the special case where \( A \) is independent of \( x \). It can be written as a linear combination of the Volkov functions,

\[
\psi_{II}(r,t) = \int dk \psi_I(k) e^{ik \cdot [r + \Delta R(t)]} 
\times \exp\left[-i \int_0^t [(k^2/2) + \epsilon_{osc}(t')] dt'\right],
\]

where \( \psi_I(k) \) is the initial wave function in the momentum space,

\[
\Delta R(t) = \int_0^t A(t) dt
\]

is the classical laser-induced electron displacement for time \( t \) of electron interaction with the field, and \( \epsilon_{osc}(t) = A^2(t)/2 \) is the electron “quiver energy.” We see that the effect of the spatially uniform field consists in electron wave-packet displacement by \( \Delta R \) from its original position. The phase factor \( \exp[-i \int_0^t \epsilon_{osc}(t') dt'] \) does not affect the integration.

When the field depends on the spatial coordinates the situation is more complicated. From the physical point of view it is associated with the fact that the electron also interacts with the magnetic field of the wave. This interaction depends on the electron velocity. For this reason different harmonics of
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where the initial wave packet will be affected differently. So the action of the magnetic field cannot be reduced to the wave-packet translation as a whole and one can expect distortion of the weight function $\psi_0(k)$ in Eq. (8) during the interaction.

To solve Eq. (7) with an $\eta(x)$-dependent vector potential $A(\eta)$ we introduce the following approximation. We assume that the term $\partial^2 \psi_\Pi/\partial x^2$ can be neglected in Eq. (7) when the effect of the Lorentz force is small. In this case the considered problem is effectively a two-dimensional problem since the electric field acts only in the plane orthogonal to the propagation direction. As a consequence, the term $\partial^2 \psi_\Pi/\partial x^2$ in Eq. (7) is not affected significantly by the field. It characterizes the $x$ component of the electron kinetic energy. For the wave packet (8) formed from the hydrogen wave function one can expect that $\partial^2 \psi_\Pi/\partial x^2$ is small in comparison with the field-dependent terms.

Let us specify the conditions when the magnetic-field effect is negligible. The Lorentz force can be estimated as follows [19,20]:

$$f_\ell(x,t) = \frac{\alpha}{2} \frac{d}{dt} A^2(x,t),$$

where $\alpha = 1/c$ ($c \approx 137$ a.u.) and $x$ is the coordinate of the $yz$ plane where the field is active. This force causes a shift in the $x$ component of the electron velocity $\Delta v_x \approx -\alpha A^2/2$ ($A$ is the magnitude of the vector potential) and, as a consequence, induces an additional electron displacement $\Delta x \approx \Delta v_x \tau$ along the propagation direction. Here we require that

$$\Delta v_x \ll \Delta v_y \quad \text{and} \quad \Delta x < a,$$

where $\Delta v_y = A$ characterizes the magnitude of the electron velocity shift due to the electric-field action. Inequalities (11) impose the following restrictions on the pulse magnitude and duration

$$A \ll 2c \quad \text{and} \quad \epsilon \tau \ll \epsilon/A^2,$$

where $\epsilon \approx 1/(2a)$ is the initial-state ionization energy.

In our case the SFA applies whenever $A \gg 1$. Taking $A \approx \sqrt{c}$ we have $\tau \ll \epsilon/\epsilon_i$. In addition, inequalities (12) need to be satisfied in order for $\partial^2 \psi_\Pi/\partial x^2$ to be neglected in Eq. (7), which we are now ready to solve.

When $\partial^2 \psi_\Pi/\partial x^2 = 0$, the operator on the right-hand side of Eq. (7) does not mix wave functions with different $x$ coordinates. For this reason $\psi_\Pi$ propagates from the initial point $(t_0(x_0),x_0)$ to the final point $(t_f(x_0),x_0)$ of region II (see Fig. 1), where the field is active. This determines the parametric dependence of the wave function $\psi_\Pi$ on the coordinate $x$. The solution of Eq. (7) can be found analytically. It is

$$\psi_\Pi(r,t) = \frac{1}{2\pi} \int dK \psi_\Pi(K,t_0) e^{-iK \cdot [R + \Delta R(x,t)]}$$

$$\times \exp \left[ -\frac{i}{2} \int_{t_0}^t \left[ K^2 + A(x,t')^2 \right] dt' \right].$$

where

$$\psi_\Pi(r,t) = \int \psi_\Pi(r,t) e^{-iK \cdot [R + \Delta R(x,t)]}$$

is the Fourier image of the initial wave function $\psi(r,t)$ from Eq. (6), $R$ is the projection of vector $r$ on the $yz$ plane ($r = \hat{x}x + \hat{y}y + \hat{z}z$), and

$$\Delta R(x,t) = \int_{t_0}^t A(x,t')dt'.$$

is the electron displacement in the $yz$ plane with coordinate $x$ at the moment $t (t \leq t \leq t_f)$.

For nonzero $\tau$ the wave function displacement is accompanied with wave-packet spreading. One can expect that the spreading is insignificant for small interaction times $\tau$. If this is the case Eq. (13) can be transformed, see the Appendix, to the following expression:

$$\psi_\Pi(r,t) \approx \psi_\Pi(r + \Delta R(x,t),t_0) \exp \left[ -\frac{i}{2} \int_{t_0}^t A^2(x,t')dt' \right].$$

One can show that this $\psi_\Pi$ satisfies the requirement that $\partial^2 \psi_\Pi/\partial x^2$ is small in comparison with the field-dependent terms.

As $\psi_\Pi$ propagates with time $t$ it accumulates a phase which is a function of $x$. The influence of this phase factor on the probability of the atom remaining in its initial state was recently considered by [14]. In our case of a traveling electromagnetic pulse, the phase factor can be shown to be independent of $x$ at $t = t_f(x)$ and can be omitted in the calculations of the transition probabilities.

As for region I, in region III of Fig. 1, the wave function develops according to Eq. (5) and is written as

$$\psi_\Pi(r,t) = \sum_n b_n \phi_n(r) \exp[-i\epsilon_n t],$$

where summation over $n$ also includes integration over the target continuum. The unknown coefficients $b_n$ in Eq. (17) can be found from the continuity of the wave function

$$|\psi_\Pi(r,t)|_{t = t_f(x)} = |\psi_\Pi(r,t)|_{t = t_f(x)}$$

at $t = t_f(x) = \alpha \epsilon + \pi/2$. By multiplying Eq. (18) by $\phi_n^*(r)\exp[i\epsilon_n t_f(x)]$ and integrating over the whole space one gets the following matrix equation:

$$\sum_{n'} \langle n'| \exp[i\omega_{nn'}^{\pi}]|n'\rangle b_{n'} = \langle n'| \exp[i\epsilon_n^{\pi}]|\psi_\Pi(t_f)\rangle,$$

where $\omega_{nn'} = \epsilon_n - \epsilon_n'$, $\langle n'| \hat{\mathcal{O}}|n'\rangle = \int \phi_n^*(r)\hat{\mathcal{O}}\phi_n(r) dr$ and $\phi_n^*$ is a complex conjugate of $\phi_n$. By expanding the exponential on the left-hand side of Eq. (19) in a series of $\alpha$ an approximate solution for coefficients $b_n$ can be found. Up to the first order in $\alpha$. 

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\[
 b_n = \sum_{n'} \left[ b_{n,n'}^{(0)}(\Delta R) - i \alpha b_{n,n'}^{(1)}(\Delta R) \right] a_{n'} e^{i_0 n' \tau},
\]
(20)
where \( \Omega_{n'n} = \epsilon_n + \epsilon_{n'} \).

\[
 b_{n,n'}^{(0)}(\Delta R) = \int \phi_n^* (r) \phi_{n'}(r + \Delta R) dr,
\]
(21)
and
\[
 b_{n,n'}^{(1)}(\Delta R) = \int dr \phi_n^* (r) \left[ V(r) - V(r + \Delta R) \right] \phi_{n'}(r + \Delta R),
\]
(22)
and where \( \Delta R = \Delta R(x, t_f(x)) \). To derive Eqs. (21) and (22) we used the completeness of the hydrogen wave-function set. Equation (21) could also be obtained directly from Eq. (19) by replacing \( \alpha \) with 0 in \( t_f(x) \).

The \( b_{n,n'}^{(0)} \) is the transition amplitude which can be derived in the framework of the dipole approximation. It can be shown with the use of the sudden perturbation approximation [22] where the perturbation \( V_L \) is the electron-laser interaction potential taken in the velocity gauge form \( [V_L = -A(t) \hat{p}] \). The \( b_{n,n'}^{(1)} \) is a nondipole correction which also takes into account the effect of pulse propagation.

### III. RESULTS AND DISCUSSION

In this section we give a numerical investigation of the ultrashort laser-pulse effect on a hydrogenlike target. Without loss of generality, we start with the atomic hydrogen and assume that the electromagnetic field is linearly polarized. In this case the \( b_{n,n'}^{(0)} \) are nonzero if the magnetic quantum numbers of the wave functions \( \phi_n \) and \( \phi_{n'} \) in Eqs. (21) are equal to each other. The selection rule for the \( b_{n,n'}^{(1)} \) allows transitions only for those states for which the magnetic quantum number difference has \( \Delta m = \pm 1 \). It was shown in Sec. II that the transition probabilities depend on the field parameters through \( \Delta R(x, t_f(x)) \). For this reason we present the calculated matrix elements as functions of \( \Delta R_f = [\Delta R(x, t_f(x))] \).

Before examining the numerical results we consider how displacement \( \Delta R_f \) depends on the electromagnetic field parameters. Since the vector potential \( A \) is an integral field characteristic \( (A = -\int E \, dt) \) we will characterize the pulse with its electric-field strength \( E \). Specifically, let \( E \) be defined by

\[
 E(\eta) = \begin{cases} 
 \frac{\eta E \cos^2(\eta \pi / \tau) \sin(\omega \eta + \phi)}{2} & \text{if } |\eta| < \pi/2, \\
 0 & \text{otherwise},
\end{cases}
\]
(23)
where \( E, \tau, \omega, \) and \( \phi \) are the magnitude, pulse duration, carrier frequency, and phase, respectively.

In this work we consider the case where both the electric component and the vector potential of the wave vanish when the pulse completely passes through some \( yz \) plane \( (\eta = \pi/2) \). So, in Eq. (23) we put \( \phi = 0 \) to ensure the pulse to be without dc components for \( \eta > \pi/2 \). Also, \( \omega \) is taken to be equal to \( 2 \pi / \tau \) to fix the form of the pulse irrespective of the pulse duration \( \tau \). In this case the vector potential \( A(\eta) \) and the electron displacement \( \Delta R(\eta) \) can be written as

\[
 A(\eta) = A \cos(\pi \eta / \tau)^4,
\]
(24)
and

\[
 \Delta R(\eta) = \Delta R_f \left[ \frac{1}{2} + \frac{\eta}{\tau} + \frac{2}{3} \sin \frac{2\pi \eta}{\tau} + \frac{1}{12\pi} \sin \frac{4\pi \eta}{\tau} \right],
\]
(25)
where \( A = E \pi/(2\pi) \) is the vector potential magnitude and \( \Delta R_f = 3E \pi^2/(16\pi) \) is the maximum displacement reached at \( \eta = \pi/2 \).

The applicability limits of our theory are defined by inequalities (12). They restrict the possible values of \( A \) and \( \tau \). Taking into account that our theory applies for \( 1 < A < 2e \) we can assume, without loss of generality, that \( A = \sqrt{\epsilon} \). Then, with the use of Eq. (12) we have

\[
 \tau < 1/e_1,
\]
(26)
with increase in ns in some initial states. We see from Fig. 2(c) that this is also true for excitation from the 3s initial state (note that the term \( |b^{(0)}_{3s3s}|^2 \) is excluded from \( \Sigma_{l_f=0}^{n-1} |b^{(0)}_{n,l_f,0,3s}|^2 \) for \( n = 3 \)).

Figures 3–7 present the calculated matrix elements \( b_{i_f}^{(1)} \) as functions of the laser-induced displacement \( \Delta R_f \) for the initial states being 1s, 4s, 6s, 6p, and 6d, respectively. For simplicity of presentation we only consider excitation of \( p \) states with \( m = 1 \). Figure 3 depicts \( b_{2p,1s}^{(1)} \) where \( n \) takes the values from 2 to 6. One can see that the magnitude of the calculated matrix elements decreases with increasing \( n \) for \( 0 < \Delta R_f < 10 \). Thus, in this region, the transition from 1s to 2p dominates over the transitions to higher excited levels. One can also see from Fig. 3 that as \( n \) increases the matrix elements decrease generally.

Figure 4 demonstrates the \( \Delta R_f \) dependence of the matrix elements \( b_{1p,1s}^{(1)} \). We see that the magnitude of the propagation effect for transitions from highly excited s states can be several times bigger than for transitions from the 1s state. So, for example, the maximum value of \( b_{2p,1s}^{(1)} \) is about 0.05 while the maximum value of \( b_{2p,1s}^{(1)} \) is about 0.016. However, to get this value of \( b_{2p,1s}^{(1)} \) one needs to have five times larger \( \Delta R_f \) or, in other words, to apply a five times stronger field.

Figures 5–7 show the transition matrix elements calculated for the initial states being, respectively, 6s, 6p, and 6d, and as \( \Delta R_f \) increases leading to excitation of predominantly higher \( n \) states. We see from Fig. 2(c) that this is also true for excitation from the 3s initial state (note that the term \( |b^{(0)}_{3s3s}|^2 \) is excluded from \( \Sigma_{l_f=0}^{n-1} |b^{(0)}_{n,l_f,0,3s}|^2 \) for \( n = 3 \)).
6d. Comparing with the dependencies shown in Figs. 3 and 4, we see that the absolute values of the matrix elements \( b_{np,6s}^{(1)} \) are maximal for larger \( \Delta R_f \). These values are of the same order of magnitude as for the case \( n_i = 4 \) shown in Fig. 4. For \( b_{np,6p}^{(1)} \) and \( b_{np,6d}^{(1)} \) we see that their maximal absolute values are slightly larger than those of \( b_{np,4s}^{(1)} \).

As one can see from Eq. (20) the transition probabilities \( |b_n|^2 \) are affected by the parameter \( \alpha \). If the target is initially in some pure state then one has the factor \( \alpha^2 \approx 0.5 \times 10^{-4} \) in the magnetic-level excitation probabilities. For example, with accounting of this factor the transition probabilities are of the same order of magnitude as for the case \( n_i = 4 \) shown in Fig. 4. For mixed initial states the transition probabilities can be of the order of \( \alpha \) due to the effect of quantum interference. Another difference between the cases of pure and mixed initial states is in the dependence of the transition probabilities on the pulse duration \( \tau \). Equation (20) shows that, for pure initial states, the transition probabilities \( |b_n|^2 \) depend on \( \tau \) only through the laser-induced displacement \( \Delta R_f \). This is not the case for mixed initial states since the terms \( e^{i\Omega_n \tau} \) are not factored out from \( |b_n|^2 \).

As indicated above, the excitation probabilities of the magnetic sublevels are small due to the factor \( \alpha^2 \). A stronger propagation effect is expected for laser excitation of hydrogen-like multicharged ions. To see this we may redefine the parameter \( \alpha \) and displacement \( \Delta R_f \) in Coulomb units by \( \alpha \rightarrow Z \alpha \) and \( \Delta R_f \rightarrow \Delta R_f / Z \), where \( Z \) is the nuclear charge. Hence, the propagation effect becomes more pronounced with increasing \( Z \).

The propagation effect demands special consideration in the case of Rydberg atoms interacting with ultrashort laser pulses or trains of pulses. Modern experimental methods allow engineering of Rydberg states with principal quantum numbers \( n_i \approx 400 \) [23]. In this case the smallness of the transition probabilities can be compensated by a large number of states involved through the propagation effect mechanism. To avoid the Rydberg atom ionization we suggest to use a scheme where the atom is subjected to two ultrashort laser pulses with opposite effects on the atomic electron.

IV. CONCLUSIONS

The hydrogenlike target excitation by an ultrashort electromagnetic pulse traveling in space has been considered for the first time to the best of our knowledge. We have outlined the propagation effect mechanism that leads to magnetic-sublevel excitation, which is forbidden in the dipole approximation. This effect is not related to the action of the magnetic-field component of the pulse. The problem has been studied numerically subject to the strong-field approximation with a linearly polarized pulse. We considered the case where the field vector potential \( \textbf{A} \) is zero outside the space-time region where the field is active. The transition probabilities are small for hydrogen, but increase with \( Z \) for hydrogen-like ions.

The propagation effect is not uniquely attributed to the SFA case. For weak fields one should take into consideration the competitive action of the atomic Hamiltonian on the electron evolution. This is currently under investigation. Also, more work is needed to include relativistic effects if sufficiently highly charged ions are considered.

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APPENDIX

To derive Eq. (16) we neglected the wave-packet spreading and put \( \exp[-iK^2(t-t_f(x))/2] = 1 \) in Eq. (13). Here we specify the condition where the error introduced by this approximation is small.

The integrand in Eq. (13) is highly peaked for \( K < \sqrt{2\varepsilon_i} \). For such \( K \), utilizing \( \varepsilon_i \tau \ll 1 \) we have

\[
\exp[-iK^2(t-t_f(x))/2] \approx 1 - iK^2/2(t-t_f(x)) + \cdots
\]

\[
\approx 1 - i\varepsilon_i \tau \approx 1.
\]  

For \( K > \sqrt{2\varepsilon_i} \), this expansion is not applicable. Nevertheless, one can show that the contribution of the region with large \( K \) in the integral (13) is insignificant almost for all values of coordinates.

The expansion (A1) cannot be generally used at \( x = 0 \) where the integrand of Eq. (13) decays by the power law in \( K \). Our numerical calculations of \( \psi_{\text{II}} \) according to Eqs. (13) and (16) showed that the relative error takes the maximum value at \( r = -\Delta R \). For small \( \tau \ll 1/10e_i \), the volume occupied by this peak is small in comparison with the atomic volume.


