Adiabatic theory of ionization by intense laser pulses: Finite-range potentials

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The adiabatic theory of ionization of an electron, initially bound in a three-dimensional potential well, by an intense low-frequency laser pulse is developed. The general case of arbitrary time dependence and polarization of the laser field and arbitrary potential which can model an atom or a molecule in the single-active-electron approximation is treated, with the only restriction that the potential should not have a Coulomb tail. The asymptotics of the solution to the time-dependent Schrödinger equation and photoelectron momentum distribution in the adiabatic regime are obtained. Both the adiabatic and the rescattering parts of the wave function and ionization amplitude are considered. These asymptotics are expressed in terms of the Siegert state originating from the initial bound state in the presence of a static electric field and scattering states in the unperturbed potential. They are uniform in terms of the amplitude of the laser field and apply to weak underbarrier as well as strong overbarrier fields, provided the condition defining the region of validity of the adiabatic approximation is fulfilled. The theory is illustrated by calculations which confirm that the adiabatic results converge to the exact ones as the adiabatic parameter tends to zero.

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I. INTRODUCTION

An atom or molecule interacting with the field of an intense low-frequency laser pulse can be ionized. Driven by the field, the ionized electron returns and collides with the parent ion. As a result, it can be elastically rescattered, which generates high-energy photoelectrons [1], can radiatively recombine, which generates high-order harmonics [2], or can experience some other type of inelastic collision. These processes are currently being intensively studied experimentally [3–8]. The interest is fed by the wish to develop a technique for extracting the target structure information, hopefully even in a time-resolved way, which possibility has been predicted by calculations [9,10].

The main theoretical approach currently in use in this field has grown from an early paper by Keldysh [11]. A review of the initial period of the development of the Keldysh theory is given in Ref. [12]. The original Keldysh theory neglects the interaction of an active electron with the laser field, in the initial state, and with the target potential, in the final state. It was reformulated in terms of time-dependent perturbation theory by Faisal [13] and Reiss [14], which enabled one to account for the latter interaction perturbatively, and became known as the strong-field approximation. A review of this theory and its recent developments can be found in Ref. [15]. The Keldysh theory and its modifications certainly grasp one essential aspect of the problem: The motion of an ionized electron driven by the field can be described classically, which explains the success of the "simple-man theory" [16–18]. A classical trajectory is introduced into the theory through the action associated with a Volkov state. At the same time, the Keldysh theory suffers from an important drawback: It never becomes exact in the space of the target and laser parameters. In addition, it is restricted to weak underbarrier fields, much smaller than the atomic one, when ionization in the low-frequency regime occurs by tunneling.

Another approach to the problem was initiated in [19] and is currently being actively pursued [20,21]. It is based on the zero-range potential (ZRP) model, which allows a detailed analytical and numerical analysis [22–25], from which it develops as an effective range theory. A close relation to the ZRP model explains substantial analytical grounds of this theory, but also raises doubts on whether it can be extended to realistic atomic potentials with nontrivial scattering properties, let alone molecules.

Meanwhile, for low-frequency pulses of interest for applications, the problem contains a small parameter ϵ given by the ratio of the atomic and laser time scales. For example, for a typical wavelength of 800 nm ($\omega \approx 0.057$ a.u.) and neutral atoms in the ground state ($|E_0| \sim 0.5$ a.u.) one obtains $\epsilon \sim 0.1$. Thus, constructing the asymptotic solution of the problem for $\epsilon \to 0$ seems to be a sensible approach. This is the adiabatic theory. The development of this theory was initiated in Ref. [26] (to be referred to hereafter as "I"), where the simplest one-dimensional (1D) ZRP model was considered. In this paper we present a thorough development of the adiabatic theory in the three-dimensional (3D) case. Our treatment is restricted to potentials having no Coulomb tail in the asymptotic region. The extension of the theory to potentials with a Coulomb tail is possible, but the formulation from the very beginning is different, as is different the formulation of scattering theory for such potentials. Otherwise, we consider the most general case of arbitrary time dependence and polarization of the laser field and arbitrary target potential which can model an atom or a molecule in the single-active-electron approximation. We derive the asymptotics of the solution to the time-dependent Schrödinger equation (TDSE) and photoelectron momentum distribution (PEMD) for $\epsilon \to 0$. Although many steps in the derivation are based on ideas and techniques developed in I, the generalization of the theory to the 3D case is neither trivial nor straightforward. We feel that some interested readers may be unfamiliar with asymptotic methods [27,28], so we try to make our presentation self-contained. We omit unnecessary details, but some details are needed to make the results reproducible.

To implement the adiabatic theory one naturally needs to know some properties of the target. These properties are

represented by the Siegert state (SS) originating from the initial bound state in the presence of an external static electric field and scattering states in the unperturbed target potential. Whereas scattering states need no explanation, the SS is a less known object. In the general context of quantum mechanics, SSs are the regular solutions to the stationary Schrödinger equation satisfying the outgoing-wave boundary conditions. Such solutions were introduced by Gamow in his famous theory of α decay [29]. However, Siegert [30] was the first who formulated the corresponding eigenvalue problem and recognized the virtue of the complete set of its solutions as a basis for an alternative formulation of scattering theory. Therefore, such solutions now bear his name. So far, the theory of SSs is developed only for spherically symmetric finite-range potentials [30–40]. This theory was essentially advanced and made implementable in practical calculations by reformulating it in terms of Siegert pseudostates [41–44]. The properties of SSs in the presence of an electric field are much less studied. The approaches used in Refs. [30–44] do not apply in this case because of the difference in the asymptotic boundary conditions, and no more suitable approach is found yet. In particular, as far as we know, no results on the orthogonality and completeness properties of SSs in an electric field are available. Recently, we have developed the method of adiabatic expansion in parabolic coordinates to analyze and calculate individual SSs in an electric field, first for axially symmetric potentials (atoms and linear molecules aligned along the field) [45] and then for potentials without any symmetry (arbitrarily oriented molecules) [46]. This method is implemented in computer programs which enable one to calculate SSs for atoms [45] and molecules [47] in a wide range of the field strength. It is suitable also for constructing the analytical solution of the Siegert eigenvalue problem in the weak-field limit [46]. Without these preliminary developments the numerical implementation of the adiabatic theory would not be possible.

The paper is organized as follows. In Sec. II we formulate the problem, define the adiabatic regime where the present theory applies, and summarize basic equations on classical and quantum dynamics in a time-dependent electric field. In Sec. III we recall the definition of SSs in a static electric field. To illustrate the theory, we consider a model potential obtained by multiplying the Coulomb potential by a screening Gaussian factor. The ground $1s$ state in this potential is used as the initial state in the illustrative calculations. The properties of the corresponding SS required for implementing the adiabatic theory are discussed. The scattering states in this potential are discussed in Sec. IV. After these introductory sections, we turn to developing the theory. In Sec. V, the asymptotic solution of the TDSE for $\epsilon \to 0$ is constructed. In Sec. VI, this solution is used to obtain the asymptotics of the PEMD. These two sections present our main results. The quantitative performance of the theory is illustrated by calculations in Sec. VII. Section VIII summarizes the results and points out directions for further developments and applications of the theory. An alternative formal derivation of the asymptotic series for the adiabatic part of the wave function in operator form is given in Appendix A. In Appendix B, we show how the Keldysh approximation emerges in the weak-field limit of the adiabatic theory.

II. BASIC EQUATIONS

A. Formulation of the problem

We consider an electron interacting with an atomic potential and a laser field. The electron is assumed to be nonrelativistic, so the magnetic part of the Lorentz force is neglected, and its interaction with the electric field is treated in the dipole approximation. The TDSE in the length gauge reads (atomic units are used throughout)

$$i\,\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \left[-\frac{1}{2}\,\Delta + V(\mathbf{r}) + \mathbf{F}(t)\mathbf{r}\right]\psi(\mathbf{r},t). \tag{1}$$

We discuss atoms, but the potential $V(\mathbf{r})$ should not necessarily be spherically symmetric, so our treatment applies also to molecules in the single-active-electron approximation. For simplicity, we assume that $V(\mathbf{r})$ has a finite range,

$$V(\mathbf{r})|_{r>a} = 0. \tag{2}$$

However, our analysis remains valid also for potentials with sufficiently rapidly vanishing tail, whose effect on the dynamics can be neglected; potentials with the Coulomb tail are excluded by Eq. (2). We indicate points in the derivation where this assumption is essential. The electric field $\mathbf{F}(t)$ is taken in the most general form,

$$\mathbf{F}(t) = F_x(t)\mathbf{e}_x + F_y(t)\mathbf{e}_y + F_z(t)\mathbf{e}_z, \tag{3}$$

which enables us to consider the interaction simultaneously with several laser beams of arbitrary polarization. We distinguish three polarization cases: general polarization (GP), when all three Cartesian components of $\mathbf{F}(t)$ are independent functions; plane polarization (PP), which is the case for one or several generally polarized laser beams propagating in the same direction along the y axis, when $F_y(t) = 0$; and linear polarization (LP), which is the case for one or several laser beams linearly polarized along the z axis, when $F_x(t) = F_y(t) = 0$. The characteristic time scale and magnitude of $\mathbf{F}(t)$ are denoted by T_0 and F_0. Let us introduce notation:

$$F(t) = \left[F_x^2(t) + F_y^2(t) + F_z^2(t)\right]^{1/2}, \quad \mathbf{e}(t) = \frac{\mathbf{F}(t)}{F(t)}. \tag{4}$$

It is assumed that $F(t)$ is an analytic function of t; this requirement is essential since we need to consider $F(t)$ for generally complex values of t. For any vector $\mathbf{a}$ and a given moment t, the $\parallel$ and $\perp$ components of $\mathbf{a}$ with respect to $\mathbf{e}(t)$ are defined by

$$\mathbf{a} = a_\parallel \mathbf{e}(t) + \mathbf{a}_\perp, \quad a_\parallel = \mathbf{e}(t)\mathbf{a}. \tag{5}$$

The electric field is assumed to vanish in the remote past and future,

$$\mathbf{F}(t \to \pm\infty) = \mathbf{0}. \tag{6}$$

The initial condition for Eq. (1) is

$$\psi(\mathbf{r},t \to -\infty) = \phi_0(\mathbf{r})e^{-iE_0 t}, \tag{7}$$

where $E_0 < 0$ and $\phi_0(\mathbf{r})$ are the energy and normalized wave function of a bound state of the unperturbed atom,

$$\left[-\frac{1}{2}\,\Delta + V(\mathbf{r}) - E_0\right]\phi_0(\mathbf{r}) = 0, \quad \int \phi_0^2(\mathbf{r})\,d\mathbf{r} = 1. \tag{8}$$

The problem consists in finding observables defined by the coefficients in the expansion of the solution to Eqs. (1) and (7) in terms of the complete set of atomic states for $t \to \infty$.

B. Adiabatic regime

It is convenient to introduce $\varkappa$ defined by

$$\varkappa = \sqrt{2|E_0|}. \tag{9}$$

The reciprocal quantity $1/\varkappa$ gives the size of the initial bound state; for the outer shells of neutral atoms in the ground state $\varkappa \sim 1$. There are three characteristic energies in the problem: (1) the energy spacing between atomic levels E_a, which we assume to be of the order of the ionization potential $|E_0|$, (2) the energy associated with the laser field $E_f = 2\pi/T_0$, which for monochromatic pulses is equal to the photon energy ω, and (3) the energy of interaction of the bound electron with the laser field $E_{af} = F_0/\varkappa$. The following ratios of these energies give two independent dimensionless parameters characterizing the problem,

$$\epsilon = \frac{E_f}{E_a} = \frac{4\pi}{\varkappa^2 T_0}, \quad \xi = \frac{E_{af}}{E_a} = \frac{2F_0}{\varkappa^3}. \tag{10}$$

The third ratio coincides with the well-known Keldysh parameter [11],

$$\gamma = \frac{E_f}{E_{af}} = \frac{\epsilon}{\xi} = \sqrt{\frac{|E_0|}{2U_p}}, \quad U_p = \frac{F_0^2}{4\omega^2}. \tag{11}$$

In the present theory ϵ and ξ are primary parameters, while γ does not play any role. We note that the photon ω and ponderomotive U_p energies are well-defined quantities only for many-cycle almost monochromatic pulses; for few-cycle pulses of interest here it is more sensible to use the notion of the characteristic time T_0.

The adiabatic parameter ϵ gives the ratio of the atomic and laser time scales. It plays a key role in the following discussion. To uncover this parameter in Eq. (1), we assume that

$$\frac{d^n \mathbf{F}(t)}{dt^n} = O(\epsilon^n). \tag{12}$$

The validity of the adiabatic approximation requires $\epsilon \ll 1$. It is essential to realize the order of the various quantities in terms of ϵ as $\epsilon \to 0$. For example, the atomic properties do not depend on ϵ, so $a = O(\epsilon^0)$ and $\varkappa = O(\epsilon^0)$. The same holds for the amplitude of the laser field, $F_0 = O(\epsilon^0)$, but $T_0 = O(\epsilon^{-1})$. The parameter ξ characterizes the strength of the laser field. The adiabatic theory developed in this paper is the asymptotics defined by $\epsilon \to 0$ and $\xi = O(\epsilon^0)$. The latter condition means that this asymptotics is uniform in terms of ξ. In other words, the present theory applies to weak underbarrier, $\xi \ll 1$, as well as strong overbarrier, $\xi \gtrsim 1$, fields, provided that ϵ is sufficiently small. More specifically, it is shown below that the region of validity of the adiabatic approximation is defined by

$$\epsilon \ll \min(\xi^2, 1). \tag{13}$$

One can notice that the adiabatic regime $\epsilon \to 0$ corresponds to the tunneling regime $\gamma \to 0$ in terms of the Keldysh theory [11], since $\gamma = O(\epsilon^1)$. However, the Keldysh theory applies only to weak fields satisfying $\xi \ll 1$ [12], so the condition of applicability of this theory in the tunneling regime is $\epsilon \ll \xi \ll 1$, which differs from Eq. (13). Thus, the two theories are quite different. The results of the Keldysh theory will be duly recovered within the present theory in the region $\epsilon \ll \xi^2$, $\xi \ll 1$, where both theories apply.

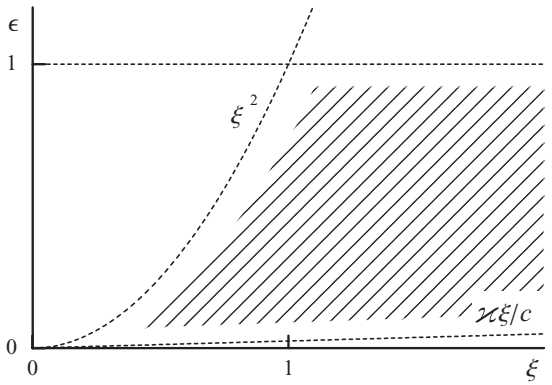

FIG. 1. The hatched area shows the region of applicability of the nonrelativistic version of the adiabatic theory. For comparison, the condition of applicability of the Keldysh theory in the tunneling regime is $\epsilon \ll \xi \ll 1$.

As a reply to Ref. [48], it is worthwhile to discuss the limitations of the adiabatic theory stemming from the nonrelativistic and dipole approximations. The validity of the nonrelativistic approximation requires

$$F_0 T_0 \ll c \quad \to \quad \epsilon \gg \frac{\xi \varkappa}{c}, \tag{14}$$

where $c \approx 137$ is the velocity of light. This condition must be compatible with Eq. (13). For $\xi \sim 1$, there always exists an interval $\varkappa/c \ll \epsilon \ll 1$ where conditions (13) and (14) are fulfilled. However, in the weak-field case, $\xi \ll 1$, the nonrelativistic version of the present theory does not have a region of applicability if $\xi \lesssim \varkappa/c$. Although this limitation does not seem to be important for applications of current interest, it should be emphasized that it is not intrinsic to the adiabatic approximation and can be eliminated by generalizing the following two sections to the relativistic case. The validity of the dipole approximation requires

$$1/\varkappa \ll T_0 c, \quad F_0 T_0^2 \ll T_0 c. \tag{15}$$

The first of these conditions amounts to $\epsilon \ll c/\varkappa$ and, taking into account Eq. (13), is not restrictive. The second one is equivalent to Eq. (14). Summarizing, the region of applicability of the present theory in the plane of the parameters ϵ and ξ is illustrated in Fig. 1.

C. Classical dynamics in a time-dependent electric field

It is well known that quantum dynamics in a homogeneous electric field can be described in purely classical terms [49]. Here we summarize formulas needed for the following. We consider an electron interacting only with an electric field $\mathbf{F}(t)$. Let us introduce a reference classical trajectory with the velocity $\mathbf{v}(t)$ and coordinate $\mathbf{r}(t)$ defined by

$$\dot{\mathbf{v}}(t) = -\mathbf{F}(t), \quad \dot{\mathbf{r}}(t) = \mathbf{v}(t), \tag{16a}$$

$$\mathbf{v}(t \to -\infty) = \mathbf{r}(t \to -\infty) = \mathbf{0}. \tag{16b}$$

Here and throughout, overdots denote differentiation with respect to time. We have

$$\mathbf{v}(t\to\infty)=\mathbf{v}_\infty,\quad \mathbf{r}(t\to\infty)=\mathbf{r}_\infty+\mathbf{v}_\infty t, \tag{17a}$$

where

$$\mathbf{v}_\infty=-\int_{-\infty}^{\infty}\mathbf{F}(t)\,dt, \tag{17b}$$

$$\mathbf{r}_\infty=\int_{-\infty}^{0}\mathbf{v}(t)\,dt+\int_{0}^{\infty}[\mathbf{v}(t)-\mathbf{v}_\infty]\,dt. \tag{17c}$$

It was argued [50] that a true laser pulse must satisfy $\mathbf{v}_\infty=\mathbf{r}_\infty=\mathbf{0}$. Even if so, these restrictions are not intrinsic to the present problem, so we do not impose them here; our theory applies to arbitrary values of $\mathbf{v}_\infty$ and $\mathbf{r}_\infty$. The velocity $\mathbf{u}(t)$ and coordinate $\mathbf{q}(t)$ for an arbitrary classical trajectory satisfy the same equations with different initial conditions,

$$\dot{\mathbf{u}}(t)=-\mathbf{F}(t),\quad \dot{\mathbf{q}}(t)=\mathbf{u}(t), \tag{18a}$$

$$\mathbf{u}(t_i)=\mathbf{u}_i,\quad \mathbf{q}(t_i)=\mathbf{q}_i. \tag{18b}$$

It is a property of the motion in a homogeneous electric field that any trajectory can be expressed in terms of the reference one,

$$\mathbf{u}(t)=[\mathbf{u}_i-\mathbf{v}(t_i)]+\mathbf{v}(t), \tag{19a}$$

$$\mathbf{q}(t)=[\mathbf{q}_i-\mathbf{r}(t_i)]+[\mathbf{u}_i-\mathbf{v}(t_i)](t-t_i)+\mathbf{r}(t). \tag{19b}$$

Hence, all classical quantities of interest can be expressed in terms of the functions $\mathbf{v}(t)$ and $\mathbf{r}(t)$.

Consider the trajectory (19) in a finite interval of time $t_i\leqslant t\leqslant t_f$. Let $\mathbf{u}(t_f)=\mathbf{u}_f$ and $\mathbf{q}(t_f)=\mathbf{q}_f$. One can use $\mathbf{q}_f$, t_f, $\mathbf{q}_i$, and t_i as independent variables identifying the trajectory. In terms of these variables, the initial $\mathbf{u}_i$ and final $\mathbf{u}_f$ velocities are given by

$$\mathbf{u}_i(t_f,t_i,\Delta\mathbf{q})=\mathbf{u}_i(t_f,t_i)+\frac{\Delta\mathbf{q}}{t_f-t_i}, \tag{20a}$$

$$\mathbf{u}_f(t_f,t_i,\Delta\mathbf{q})=\mathbf{u}_f(t_f,t_i)+\frac{\Delta\mathbf{q}}{t_f-t_i}, \tag{20b}$$

where $\Delta\mathbf{q}=\mathbf{q}_f-\mathbf{q}_i$ and

$$\mathbf{u}_i(t_f,t_i)=\mathbf{v}(t_i)-\frac{\mathbf{r}(t_f)-\mathbf{r}(t_i)}{t_f-t_i}, \tag{21a}$$

$$\mathbf{u}_f(t_f,t_i)=\mathbf{v}(t_f)-\frac{\mathbf{r}(t_f)-\mathbf{r}(t_i)}{t_f-t_i}. \tag{21b}$$

The latter functions are the initial and final velocities for a closed trajectory which begins and ends at the same point; because of the homogeneity of the electric field, they depend only on the initial t_i and final t_f moments and do not depend on the point. We have

$$\frac{\partial\mathbf{u}_i(t_f,t_i,\Delta\mathbf{q})}{\partial t_f}=-\frac{\mathbf{u}_f(t_f,t_i,\Delta\mathbf{q})}{t_f-t_i}, \tag{22a}$$

$$\frac{\partial\mathbf{u}_i(t_f,t_i,\Delta\mathbf{q})}{\partial t_i}=-\mathbf{F}(t_i)+\frac{\mathbf{u}_i(t_f,t_i,\Delta\mathbf{q})}{t_f-t_i}, \tag{22b}$$

$$\frac{\partial\mathbf{u}_f(t_f,t_i,\Delta\mathbf{q})}{\partial t_f}=-\mathbf{F}(t_f)-\frac{\mathbf{u}_f(t_f,t_i,\Delta\mathbf{q})}{t_f-t_i}, \tag{22c}$$

$$\frac{\partial\mathbf{u}_f(t_f,t_i,\Delta\mathbf{q})}{\partial t_i}=\frac{\mathbf{u}_i(t_f,t_i,\Delta\mathbf{q})}{t_f-t_i}. \tag{22d}$$

The action accumulated along this trajectory between t_i and t_f is

$$\begin{aligned}\mathcal{S}(\mathbf{q}_f,t_f;\mathbf{q}_i,t_i)&=\int_{t_i}^{t_f}\left[\frac{1}{2}\,\mathbf{u}^2(t)-\mathbf{F}(t)\mathbf{q}(t)\right]dt\\&=\mathbf{v}(t_f)\mathbf{q}_f-\mathbf{v}(t_i)\mathbf{q}_i+\frac{[\mathbf{r}(t_f)-\mathbf{r}(t_i)-\Delta\mathbf{q}]^2}{2(t_f-t_i)}\\&\quad-\frac{1}{2}\int_{t_i}^{t_f}\mathbf{v}^2(t)\,dt.\end{aligned} \tag{23}$$

We have

$$\frac{\partial\mathcal{S}(\mathbf{q}_f,t_f;\mathbf{q}_i,t_i)}{\partial t_i}=\frac{1}{2}\,\mathbf{u}_i^2(t_f,t_i,\Delta\mathbf{q})+\mathbf{F}(t_i)\mathbf{q}_i, \tag{24a}$$

$$\frac{\partial\mathcal{S}(\mathbf{q}_f,t_f;\mathbf{q}_i,t_i)}{\partial t_f}=-\frac{1}{2}\,\mathbf{u}_f^2(t_f,t_i,\Delta\mathbf{q})-\mathbf{F}(t_f)\mathbf{q}_f. \tag{24b}$$

The same trajectory can be identified by different sets of independent variables. One can use $\mathbf{u}_i$ instead of $\mathbf{q}_i$. Then the final velocity $\mathbf{u}_f$ depends only on t_f, t_i, and $\mathbf{u}_i$ and is given by

$$\mathbf{u}_f(t_f,t_i,\mathbf{u}_i)=\mathbf{u}_i-\mathbf{v}(t_i)+\mathbf{v}(t_f). \tag{25}$$

Alternatively, one can use $\mathbf{q}_f$, t_f, and the asymptotic velocity $\mathbf{u}_\infty=\mathbf{u}(t\to\infty)$. Then $\mathbf{u}_i$ depends only on $\mathbf{u}_\infty$ and t_i and is given by

$$\mathbf{u}_i(t_i,\mathbf{u}_\infty)=\mathbf{u}_\infty-\mathbf{v}_\infty+\mathbf{v}(t_i). \tag{26}$$

The action as a function of $\mathbf{q}_f$ and t_f satisfies the Hamilton-Jacobi equation

$$\frac{\partial\mathcal{S}(\mathbf{q}_f,t_f)}{\partial t_f}+\frac{1}{2}\left(\frac{\partial\mathcal{S}(\mathbf{q}_f,t_f)}{\partial\mathbf{q}_f}\right)^2+\mathbf{F}(t_f)\mathbf{q}_f=0. \tag{27}$$

The particular solutions to this equation are defined by appropriate initial conditions through which they become dependent on some additional variables identifying the trajectory. Equation (23) gives one of the solutions. We need two other solutions defined by

$$\mathcal{S}(\mathbf{q}_f,t_f;\mathbf{u}_i,t_i)=\mathbf{u}_f(t_f,t_i,\mathbf{u}_i)\mathbf{q}_f-\mathcal{S}(t_f,t_i,\mathbf{u}_i), \tag{28a}$$

$$\mathcal{S}(t_f,t_i,\mathbf{u}_i)=\frac{1}{2}\int_{t_i}^{t_f}\mathbf{u}_f^2(t,t_i,\mathbf{u}_i)\,dt, \tag{28b}$$

$$\mathcal{S}(\mathbf{q}_f,t_f;\mathbf{u}_i,t_i)|_{t_f=t_i}=\mathbf{u}_i\mathbf{q}_f, \tag{28c}$$

and

$$\mathcal{S}(\mathbf{q}_f,t_f;\mathbf{u}_\infty)=\mathbf{u}_i(t_f,\mathbf{u}_\infty)\mathbf{q}_f-\mathcal{S}(t_f,\mathbf{u}_\infty), \tag{29a}$$

$$\mathcal{S}(t_f,\mathbf{u}_\infty)=\frac{1}{2}\,\mathbf{u}_\infty^2t_f-\frac{1}{2}\int_{t_f}^{\infty}\left[\mathbf{u}_i^2(t,\mathbf{u}_\infty)-\mathbf{u}_\infty^2\right]dt, \tag{29b}$$

$$\mathcal{S}(\mathbf{q}_f,t_f;\mathbf{u}_\infty)|_{t_f\to\infty}=\mathbf{u}_\infty\mathbf{q}_f-\frac{1}{2}\,\mathbf{u}_\infty^2t_f. \tag{29c}$$

The different actions are related by

$$\mathcal{S}(\mathbf{q}_f,t_f;\mathbf{q}_i,t_i)=\mathcal{S}(\mathbf{q}_f,t_f;\mathbf{u}_i,t_i)-\mathbf{u}_i\mathbf{q}_i \tag{30a}$$

$$=\mathcal{S}(\mathbf{q}_f,t_f;\mathbf{u}_\infty)-\mathcal{S}(\mathbf{q}_i,t_i;\mathbf{u}_\infty), \tag{30b}$$

where all the variables correspond to the same trajectory.

D. Quantum dynamics in a time-dependent electric field

Now we can introduce main objects describing quantum dynamics in a homogeneous electric field. The retarded Green's function is defined by

$$\left[i\frac{\partial}{\partial t}+\frac{1}{2}\Delta-\mathbf{F}(t)\mathbf{r}\right]G(\mathbf{r},t;\mathbf{r}',t')=\delta(t-t')\delta(\mathbf{r}-\mathbf{r}'), \tag{31a}$$

$$G(\mathbf{r},t;\mathbf{r}',t')|_{t<t'}=0. \tag{31b}$$

It can be expressed in terms of the action (23) [49],

$$G(\mathbf{r},t;\mathbf{r}',t')=\frac{e^{3i\pi/4}\theta(t-t')}{[2\pi(t-t')]^{3/2}}\,e^{i\mathcal{S}(\mathbf{r},t;\mathbf{r}',t')}. \tag{32}$$

The Volkov states satisfy

$$i\frac{\partial\Phi(\mathbf{r},t)}{\partial t}=\left[-\frac{1}{2}\Delta+\mathbf{F}(t)\mathbf{r}\right]\Phi(\mathbf{r},t). \tag{33}$$

The particular solutions to this equation are given by $\Phi(\mathbf{r},t)=\exp[i\mathcal{S}(\mathbf{r},t)]$, where $\mathcal{S}(\mathbf{r},t)$ is a solution to Eq. (27). We need two such solutions associated with the actions (28) and (29) and defined by

$$\Phi(\mathbf{r},t;\mathbf{u}_i,t_i)=e^{i\mathcal{S}(\mathbf{r},t;\mathbf{u}_i,t_i)}, \tag{34a}$$

$$\Phi(\mathbf{r},t;\mathbf{u}_i,t_i)|_{t=t_i}=e^{i\mathbf{u}_i\mathbf{r}}, \tag{34b}$$

and

$$\Phi(\mathbf{r},t;\mathbf{k})=e^{i\mathcal{S}(\mathbf{r},t;\mathbf{k})}, \tag{35a}$$

$$\Phi(\mathbf{r},t;\mathbf{k})|_{t\to\infty}=\exp\left[i\mathbf{k}\mathbf{r}-\frac{i}{2}\mathbf{k}^2t\right]. \tag{35b}$$

The first of them describes an electron with a given initial velocity $\mathbf{u}_i$ at the moment t_i; the second describes an electron with a given velocity $\mathbf{k}$ after the pulse is over.

E. Integral form of the time-dependent Schrödinger equation

Using Eq. (32), we rewrite Eq. (1) in the integral form

$$\psi(\mathbf{r},t)=\frac{e^{3i\pi/4}}{(2\pi)^{3/2}}\int d\mathbf{r}'\int_{-\infty}^{t}e^{i\mathcal{S}(\mathbf{r},t;\mathbf{r}',t')}V(\mathbf{r}')\psi(\mathbf{r}',t')\,\frac{dt'}{(t-t')^{3/2}}. \tag{36}$$

One could add any linear combination of the Volkov states to the rhs (throughout the paper, lhs and rhs stand for the left- and right-hand side, respectively) of this equation, the lhs will still satisfy Eq. (1). This means that all the solutions to the homogeneous integral equation (36) satisfy Eq. (1), but not vice versa. So it is worthwhile to make sure that the solution to Eq. (1) we seek, the one satisfying the initial condition (7), is among the solutions to Eq. (36). To this end, let us consider Eq. (36) for $t\to-\infty$. From Eqs. (6) and (23) one can see that the rhs of Eq. (32) for $t\to-\infty$ coincides with the retarded Green's function for a free particle. The homogeneous equation (36) in this case has nontrivial solutions of the form $\phi_n(\mathbf{r})e^{-iE_nt}$, where E_n and $\phi_n(\mathbf{r})$ are the energy and wave function corresponding to a bound state of the unperturbed atom, as in Eq. (7). Thus, the solution to Eqs. (1) and (7) is among the solutions to Eq. (36). To treat the solution to Eq. (1) with a scattering state in the initial condition (7), one would have to consider an inhomogeneous integral equation obtained by adding the corresponding Volkov state to the rhs of Eq. (36). We note that the step from Eq. (1) to Eq. (36) relies on the assumption (2). For potentials with the Coulomb tail, Eq. (36) requires a modification accounting for the logarithmic Coulomb phase.

Equation (36) is the starting point for developing the adiabatic theory. This equation was also used in theories treating the ZRP model [22–24]. However, there are two essential differences between these early works and the present theory. First, in Refs. [22–24], as well as in more recent studies [19–21], the authors focus on obtaining virtually exact analytical results for a very specific model, which is possible due to the simplicity of the model, while the adiabatic theory yields asymptotic results for $\epsilon\to0$ applicable to *any* potential satisfying Eq. (2). Second, the approaches developed in Refs. [22–24] are restricted to monochromatic fields and, as a consequence, are formulated in terms of quasienergy or Floquet states, while the adiabatic theory applies to fields with *arbitrary* dependence on time, including few-cycle pulses, and is formulated in terms of SSs. We expect that the SSs should emerge in the low-frequency limit from the Floquet states, but this issue has not been investigated yet.

III. SIEGERT STATES IN A STATIC ELECTRIC FIELD

In the following sections, the solution to Eq. (36) and observables are expressed in the adiabatic approximation in terms of an SS, the one which coincides with the initial bound state in the absence of the field, in a static electric field equal to the momentary value of $\mathbf{F}(t)$ at an appropriate saddle point. It can be said that the SS is the main brick in the building of the adiabatic theory. Therefore, before developing the theory it is worthwhile to recall the definition and discuss main properties of the SS.

The SSs in a static electric field $\mathbf{F}=F\mathbf{e}$, $F>0$, are the solutions to

$$\left(-\tfrac{1}{2}\Delta+V(\mathbf{r})+\mathbf{F}\mathbf{r}-E(\mathbf{F})\right)\phi(\mathbf{r};\mathbf{F})=0, \tag{37}$$

satisfying the regularity and outgoing-wave boundary conditions. For potentials satisfying Eq. (2), the outgoing-wave boundary condition can be formulated in the form [45,46]

$$\phi(\mathbf{r};\mathbf{F})|_{r_\parallel<-a}=\int A(\mathbf{k}_\perp;\mathbf{F})e^{i\mathbf{k}_\perp\mathbf{r}_\perp}g(r_\parallel,k_\perp;\mathbf{F})\frac{d\mathbf{k}_\perp}{(2\pi)^2}, \tag{38}$$

where the $\parallel$ and $\perp$ components of $\mathbf{r}$ and $\mathbf{k}$ are defined with respect to $\mathbf{e}$,

$$g(r_\parallel,k_\perp;\mathbf{F})=e^{-i\pi/12}2\pi^{1/2}(2F)^{-1/6}\,\mathrm{Ai}(\zeta), \tag{39a}$$

$$\zeta=\frac{2e^{-i\pi/3}}{(2F)^{2/3}}\left[E(\mathbf{F})-Fr_\parallel-\frac{1}{2}k_\perp^2\right], \tag{39b}$$

and $\mathrm{Ai}(z)$ is the Airy function [51]. The solution $\phi(\mathbf{r};\mathbf{F})$ decays as $r\to\infty$ in all directions except that opposite to $\mathbf{e}$. Equation (38) means that it contains only outgoing flux in the asymptotic region $r_\parallel\to-\infty$, with $A(\mathbf{k}_\perp;\mathbf{F})$ being the amplitude of the transverse momentum distribution (TMD) in the flux [45,46]. The regular solutions to Eqs. (37) and (38) exist only for a discrete set of generally complex values of

$E(\mathbf{F})$, so this is an eigenvalue problem. This problem can be reformulated as a homogeneous integral equation,

$$\phi(\mathbf{r};\mathbf{F}) = \int G(\mathbf{r},\mathbf{r}';E(\mathbf{F}),\mathbf{F})V(\mathbf{r}')\phi(\mathbf{r}';\mathbf{F})\,d\mathbf{r}', \quad (40)$$

where $G(\mathbf{r},\mathbf{r}';E,\mathbf{F})$ is the outgoing-wave solution to

$$\left(E + \tfrac{1}{2}\Delta - \mathbf{F}\mathbf{r}\right) G(\mathbf{r},\mathbf{r}';E,\mathbf{F}) = \delta(\mathbf{r}-\mathbf{r}'), \quad (41)$$

given by

$$G(\mathbf{r},\mathbf{r}';E,\mathbf{F}) = \frac{e^{3i\pi/4}}{(2\pi)^{3/2}} \int_0^\infty \exp\left[iEt + \frac{i(\mathbf{r}-\mathbf{r}')^2}{2t} - \frac{i}{2}\mathbf{F}(\mathbf{r}+\mathbf{r}')t - \frac{i}{24}\mathbf{F}^2t^3\right]\frac{dt}{t^{3/2}}. \quad (42)$$

The solutions to Eq. (37) depend on $\mathbf{F}$ as a parameter. The SS that coincides with the initial bound state of the unperturbed atom for $F = 0$ is indicated by a subscript 0. We have

$$E_0(\mathbf{F})|_{F\to 0} \to E_0, \quad \phi_0(\mathbf{r};\mathbf{F})|_{F\to 0} \to \phi_0(\mathbf{r}). \quad (43)$$

Its complex eigenvalue presented in the form

$$E_0(\mathbf{F}) = \mathcal{E}_0(\mathbf{F}) - \frac{i}{2}\Gamma_0(\mathbf{F}) \quad (44)$$

defines the energy $\mathcal{E}_0(\mathbf{F})$ and ionization rate $\Gamma_0(\mathbf{F})$ of the state. Its eigenfunction is normalized by

$$\int \phi_0^2(\mathbf{r};\mathbf{F})\,d\mathbf{r} = 1, \quad (45)$$

which coincides with the second of Eqs. (8) for $F = 0$. Note that the integral in Eq. (45) should be properly regularized, since the eigenfunction exponentially diverges as $r_\parallel \to -\infty$ [45,46]. Also note that there is no complex conjugation in Eq. (45), which is a general property of the theory of SSs [35–37,42–44]. Let us introduce a projection of the SS onto the initial bound state,

$$\Pi_0(\mathbf{F}) = \int \phi_0(\mathbf{r})\phi_0(\mathbf{r};\mathbf{F})\,d\mathbf{r}. \quad (46)$$

The functions $E_0(\mathbf{F})$, $A_0(\mathbf{k}_\perp;\mathbf{F})$, and $\Pi_0(\mathbf{F})$ are the main characteristics of the SS needed for the adiabatic theory. To implement the theory, one must be able to calculate these functions for a wide range of generally complex values of F. Recently, we have developed an efficient and accurate method to calculate SSs for axially symmetric potentials (atoms and linear molecules aligned along the field) [45] and potentials without any symmetry (arbitrarily oriented molecules) [46,47]. This method does not rely on Eq. (2) and works also for potentials with the Coulomb tail.

In this paper, we illustrate the theory by calculations for a model potential

$$V(r) = -\frac{\exp[-(r/10)^2]}{r}. \quad (47)$$

On the one hand, one can safely cut off the asymptotic tail of this potential at $r \sim 30$–40 in order to satisfy Eq. (2), without disturbing the dynamics. On the other hand, the width of the Gaussian screening factor in Eq. (47) is large enough so the energy of the ground $1s$ state $E_{1s} = -0.485\,483\,364$ is not too far from that in the purely Coulomb potential. This potential supports three s and two p bound states. The lowest

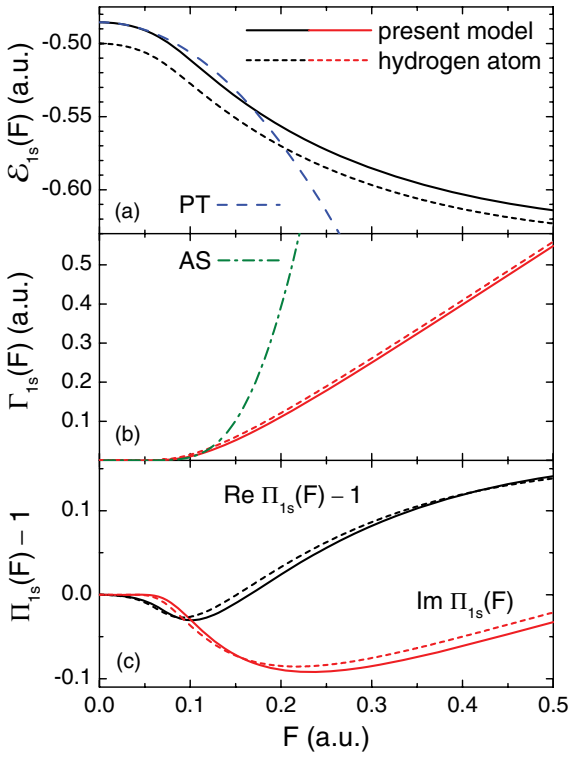

FIG. 2. (Color online) Energy (a), ionization rate (b), and projection (46) (c) for the SS that coincides with the ground $1s$ state for $F = 0$. Solid lines, the present model potential (47); dashed lines, the Coulomb potential, $V(r) = -1/r$. The perturbation theory (PT) and weak-field asymptotic theory (AS) results are obtained from Eqs. (48a) and (48b), respectively.

d state appears as a narrow shape resonance (the partial-wave potential still has a well) whose energy calculated by the SS method [44] is $E_d \approx 0.140 \times 10^{-2} - i\,0.366 \times 10^{-4}$. In addition, there is a broad f resonance (a well in the partial-wave potential has just disappeared) with energy $E_f \approx 0.262 \times 10^{-1} - i\,0.179 \times 10^{-1}$. Keeping in mind to use the $1s$ state as the initial state in the following numerical illustrations, we show in Figs. 2 and 3 the functions $E_{1s}(F)$, $\Pi_{1s}(F)$, and $A_{1s}(k_\perp;F)$ characterizing the corresponding SS for real F in the interval $0 \leqslant F \leqslant 0.5$. Because of the spherical symmetry

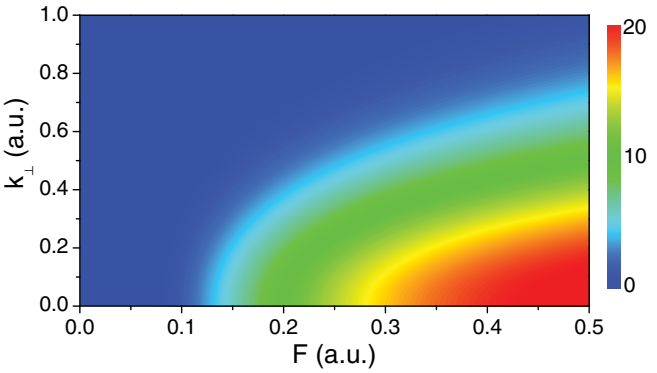

FIG. 3. (Color online) Transverse momentum distribution $|A_{1s}(k_\perp;F)|^2$ for the same SS as in Fig. 2 for the present model potential (47). The results for the Coulomb potential look very similar.

of the potential (47) and $1s$ state, these functions do not depend on the orientations of the electric field $\mathbf{F}$ and transverse momentum $\mathbf{k}_\perp$. For comparison, in Fig. 2 we also show similar results for the Coulomb potential. One can see that, apart from a shift of the energy of the state that is almost uniform in F, the Gaussian factor in Eq. (47) does not disturb very much the properties of this SS. The critical value of F indicating a boundary between the underbarrier and overbarrier regimes of ionization, estimated by requiring that the two turning points in parabolic coordinates coalescence [45,52], for the present model is $F_c \approx 0.12$. Indeed, one can see that the ionization rate $\Gamma_{1s}(F)$ acquires appreciable values for $F > F_c$. For weak fields, $F \ll F_c$, the energy of the SS can be found using perturbation theory [52], while the ionization rate and TMD amplitude can be evaluated using weak-field asymptotic theory [46,53]. One thus obtains

$$\mathcal{E}_{1s}(F)|_{F\to 0} = E_{1s} - \tfrac{1}{2}\alpha_{\rm st}F^2, \tag{48a}$$

$$\Gamma_{1s}(F)|_{F\to 0} = \int |A_{1s}(k_\perp;F)|^2 \frac{d\mathbf{k}_\perp}{(2\pi)^2} = \pi C^2 F \varkappa^{-2} \exp\left(-\frac{2\varkappa^3}{3F}\right), \tag{48b}$$

$$A_{1s}(k_\perp;F)|_{F\to 0} = e^{i\pi/4} 2\pi C \varkappa^{-1/2} \exp\left(-\frac{\varkappa^3}{3F} - \frac{\varkappa k_\perp^2}{2F}\right), \tag{48c}$$

where $\alpha_{\rm st} \approx 4.136$ is the static dipole polarizability in the $1s$ state, $C = re^{\varkappa r}\phi_{1s}(\mathbf{r})|_{r\to\infty} \approx 3.832$ is the asymptotic coefficient in the unperturbed wave function, and $\varkappa$ is related to E_{1s} by Eq. (9). However, it should be emphasized that these approximations are not intrinsic to the adiabatic theory. They work well only for very small F; for example, the error of Eq. (48b) reaches 10% already at $F = 0.01$. Therefore, Eqs. (48) are not suitable for a quantitatively predictive implementation of the theory even for moderate, let alone overbarrier values of the field. To treat strong fields, one must resort to exact numerical methods of calculating SSs like the one developed in [45–47].

Without going into further detail, we mention that the different SSs are, in fact, different branches of the same solution to Eq. (37) whose eigenvalue $E(\mathbf{F})$ and eigenfunction $\phi(\mathbf{r};\mathbf{F})$ are multivalued analytic functions of F. These functions have an essential singular point at $F = 0$. Their Riemann surface has a complicated structure near this point, because of an infinite series of branch points converging to $F = 0$ [54]. Equations (48) hold only in a narrow sector near the positive real axis of F, which reveals another deficiency of these weak-field approximations.

IV. SCATTERING STATES

To describe rescattering of the ionized electrons, we need scattering states in the potential $V(\mathbf{r})$. They are defined by [52,55]

$$\left(-\tfrac{1}{2}\Delta + V(\mathbf{r}) - E\right)\varphi(\mathbf{r};\mathbf{k}) = 0, \quad E = \mathbf{k}^2/2, \tag{49a}$$

$$\varphi(\mathbf{r};\mathbf{k})|_{r\to\infty} = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\mathbf{k},\mathbf{n})\frac{e^{ikr}}{r}, \tag{49b}$$

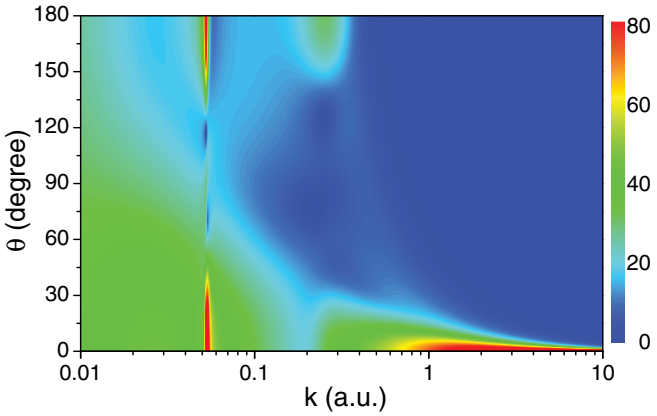

FIG. 4. (Color online) The absolute value of the scattering amplitude, $|f(k,\theta)|$, for the present model potential (47). The narrow d and broad f resonances are located at $k \approx 0.0529$ and 0.241, respectively.

where $f(\mathbf{k},\mathbf{n})$ is the scattering amplitude and $\mathbf{n} = \mathbf{r}/r$. For potentials satisfying Eq. (2), the scattering problem can be cast into the form of an integral equation,

$$\varphi(\mathbf{r};\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \int G(\mathbf{r}-\mathbf{r}';E)V(\mathbf{r}')\varphi(\mathbf{r}';\mathbf{k})\,d\mathbf{r}', \tag{50}$$

where $G(\mathbf{r};E)$ is the outgoing-wave Green's function for a free electron,

$$G(\mathbf{r};E) = \frac{e^{3i\pi/4}}{(2\pi)^{3/2}}\int_0^\infty \exp\left(iEt + \frac{i\mathbf{r}^2}{2t}\right)\frac{dt}{t^{3/2}} = -\frac{e^{ikr}}{2\pi r}. \tag{51}$$

This function can be obtained from Eq. (42) by substituting $\mathbf{F} = \mathbf{0}$.

For spherically symmetric potentials, the scattering amplitude depends only on $k = |\mathbf{k}|$ and the angle θ between $\mathbf{k}$ and $\mathbf{n}$ and is denoted by $f(k,\theta)$. Figure 4 shows the absolute value of $f(k,\theta)$ for the potential (47). The scattering properties of the present model considerably differ from that of the Coulomb potential. In the latter case $|f(k,\theta)| = [2k^2\sin^2(\theta/2)]^{-1}$, so the scattering amplitude diverges at $k = 0$ and $\theta = 0$. On the contrary, for finite-range potentials $f(k,\theta)$ remains finite for all values of its arguments. The scattering length for the present model is $-f(0,\theta) = 32.270\,451$. Another difference from the Coulomb case stems from the existence of two resonances mentioned in Sec. III. The narrow d resonance is clearly visible in Fig. 4, and the broad f resonance still can be recognized. Apart from the regions near $k = 0$ and $\theta = 0$ and resonances, the behavior of $|f(k,\theta)|$ for the present model resembles that for the Coulomb potential. In particular, for $k \gtrsim 0.5$ the scattering amplitude has a sharp peak in the forward direction.

V. ASYMPTOTIC SOLUTION OF THE TIME-DEPENDENT SCHRÖDINGER EQUATION

In this section we construct the asymptotic solution to Eq. (36) for $\epsilon \to 0$. Let us introduce some definitions. Functions $f(t)$ satisfying

$$\frac{d^n f(t)}{dt^n} = O(\epsilon^{\nu+n}) \tag{52}$$

are called "slow" functions of order ν; we write $f(t) = O(\epsilon^{\nu})$. For example, the electric field $\mathbf{F}(t)$ is a slow function of order 0 [see Eq. (12)]. From Eqs. (16) and (23) we have

$$\mathbf{v}(t) = O(\epsilon^{-1}), \quad \mathbf{r}(t) = O(\epsilon^{-2}), \tag{53}$$

and

$$\mathcal{S}(\mathbf{r},t;\mathbf{r}',t') = O(\epsilon^{-3}). \tag{54}$$

The solution to Eq. (36) is expressed in terms of "fast" functions having the form

$$g(t) = A(t)e^{iS(t)}, \quad A(t) = O(\epsilon^{\nu}), \quad S(t) = O(\epsilon^{\mu}), \tag{55}$$

where the amplitude $A(t)$ and action $S(t)$ are slow functions of orders $\nu \geqslant 0$ and $\mu < 0$. We deal with quantum actions of order -1 and classical actions of order -3; the examples are given by the exponents in Eqs. (7) and (36), respectively. The fact that $g(t)$ has the form (55) is denoted by $g(t) \sim (\nu,\mu)$.

Equations (53) and (54) provide the foundation for developing the adiabatic approximation. In the adiabatic regime, the integrand on the rhs of Eq. (36) is a rapidly oscillating function, so the main technique of the derivation is the steepest descent method [28]. The integral evaluated using this method is given by a sum of contributions from saddle points (SPs). Thus, our strategy is to analyze the different SPs, calculate their contributions, and collect together terms having the same action. For brevity, we use notation

$$\int_{-\infty}^{t} A(t')e^{iS(t')}\,dt'\Big|_{t'\in Z}, \tag{56}$$

which means that the integral is to be evaluated using the steepest descent method and only the contributions from SPs located in zone Z are to be taken into account.

A. Quasistationary zone

One can expect that in the adiabatic regime a bound electron adjusts its state to the momentary value of the electric field $\mathbf{F}(t)$ and adiabatically follows its variation in time. We show that this is indeed the case. However, there is some *retardation* because of finiteness of the electron's velocity, so the adiabatic approximation should break down at sufficiently large distance from the atom. An ionized electron moving in a static electric field equal to the value of $\mathbf{F}(t)$ at the moment of ionization recedes from the atom during the time Δt by a distance $\sim F(t)\Delta t^2$. The field can be treated as static for $\Delta t \lesssim T_0$. Therefore, the electron can recede from the atom before the field changes appreciably at most by a distance

$$R(t) \sim F(t)T_0^2 = O(\epsilon^{-2}). \tag{57}$$

The momentary quasistationary (QS) zone is defined by

$$\text{QS zone}: \quad r \ll R(t). \tag{58}$$

Inside this zone, retardation can be neglected and the electronic state evolves adiabatically. The concept of the QS zone is familiar from classical electrodynamics [56,57], where it is also known as the near-field zone. However, there is a difference: The size of the QS zone in the present problem depends on time and turns to zero at the moments when $F(t) = 0$. Thus, the adiabatic approximation breaks down outside the QS zone in space, and, in addition, near the zeros of $F(t)$ in time. An important consequence of Eq. (36) is that for potentials satisfying Eq. (2) the wave function $\psi(\mathbf{r},t)$ in the whole space is determined by its values in a finite region occupied by the potential. Thus, to find the observables it is sufficient to construct the solution to Eq. (36) in the region $r < a$. For this region to lie inside the QS zone for the most of time during the pulse, we require

$$a \ll R_0 \to \epsilon^2 \ll \frac{\xi}{\varkappa a}, \tag{59}$$

where $R_0 = F_0T_0^2 = O(\epsilon^{-2})$ is the characteristic value of $R(t)$. Taking into account Eq. (13), this condition is not restrictive, unless the range of the potential a becomes infinite.

In this section we consider Eq. (36) only in the QS zone (58). This is sufficient for finding the observables, provided that condition (59) is fulfilled. Following I, the solution to Eq. (36) is sought in the form of a sum of adiabatic and rescattering parts,

$$\psi(\mathbf{r},t) = \psi_a(\mathbf{r},t) + \psi_r(\mathbf{r},t), \tag{60}$$

where the two terms are identified by

$$\psi_a(\mathbf{r},t) \sim (0,-1), \tag{61a}$$

$$\psi_r(\mathbf{r},t) \sim (3/2,-3), \tag{61b}$$

and

$$\psi_a(\mathbf{r},t \to -\infty) = \phi_0(\mathbf{r})e^{-iE_0t}, \tag{62a}$$

$$\psi_r(\mathbf{r},t \to -\infty) = 0. \tag{62b}$$

Such representation of the solution is confirmed by the result. We reiterate that the adiabatic approximation and Eq. (60) hold only inside the QS zone.

B. Adiabatic part of the wave function

The adiabatic part $\psi_a(\mathbf{r},t)$ of the solution to Eq. (36) is sought in the form

$$\psi_a(\mathbf{r},t) = \phi_0(\mathbf{r};t)e^{-is_0(t)}, \tag{63}$$

where

$$s_0(t) = E_0t + \int_{-\infty}^{t} [E_0(t') - E_0]\,dt'. \tag{64}$$

Here $E_0(t)$ and $\phi_0(\mathbf{r};t)$ are slow functions of order 0, so $s_0(t) = O(\epsilon^{-1})$, in accordance with Eq. (61a). To satisfy the initial condition (62a), we require

$$E_0(t \to -\infty) = E_0, \quad \phi_0(\mathbf{r};t \to -\infty) = \phi_0(\mathbf{r}). \tag{65}$$

Substituting $\psi_a(\mathbf{r},t)$ for $\psi(\mathbf{r},t)$ into Eq. (36) and evaluating the time integral on the rhs, one should retain only SPs whose contributions have actions of order -1. Such SPs are located in the *adiabatic* zone A in the complex t' plane defined by

$$\text{zone } A: \quad |t' - t| \ll T_0. \tag{66}$$

Note that that there may exist other SPs located outside zone A which produce terms with actions of order -3 contributing

to $\psi_r(\mathbf{r},t)$ (see Sec. V D). Thus, we arrive at the equation

$$\phi_0(\mathbf{r};t) = \frac{e^{3i\pi/4}}{(2\pi)^{3/2}} \int d\mathbf{r}' \int_{-\infty}^{t} e^{iS_a(\mathbf{r},t;\mathbf{r}',t')} V(\mathbf{r}')\phi_0(\mathbf{r}';t') \times \frac{dt'}{(t-t')^{3/2}}\bigg|_{t'\in A}, \tag{67}$$

where

$$S_a(\mathbf{r},t;\mathbf{r}',t') = \mathcal{S}(\mathbf{r},t;\mathbf{r}',t') + \int_{t'}^{t} E_0(t'')\,dt''. \tag{68}$$

This equation defines the functions $E_0(t)$ and $\phi_0(\mathbf{r};t)$ introduced in Eqs. (63) and (64).

A simple way to proceed is to find all SPs located in zone A and calculate their individual contributions to the time integral in Eq. (67). The SPs for the action (68) are defined by

$$\frac{\partial S_a}{\partial t'} = \frac{1}{2}\mathbf{u}_i^2(t,t',\Delta\mathbf{r}) + \mathbf{F}(t')\mathbf{r}' - E_0(t') = 0, \tag{69}$$

where $\mathbf{u}_i(t,t',\Delta\mathbf{r})$ is given by Eq. (20a) and $\Delta\mathbf{r} = \mathbf{r} - \mathbf{r}'$. This equation has a transparent physical meaning. In the adiabatic regime, a transition can efficiently occur only when the energies of the initial and final states coincide; transitions associated with a change of the energy of the system are suppressed. In the initial state (63), the electron is bound by the potential and its energy is $E_0(t)$. In the final state, the electron is ionized and moves under the influence of the field. For the ionized electron emerging at the moment t' at the point $\mathbf{r}'$ to arrive at the moment t at the point $\mathbf{r}$ its initial velocity must be equal to $\mathbf{u}_i(t,t',\Delta\mathbf{r})$. Thus, Eq. (69) defines a moment of ionization t' in the adiabatic regime. The number and positions of SPs in zone A depend on $\mathbf{r}$, $\mathbf{r}'$, and t. Consider the region

$$r = O(\epsilon^0), \quad r' = O(\epsilon^0), \quad |t'-t| = O(\epsilon^0). \tag{70}$$

The first of these conditions is our temporary assumption, the second follows from Eq. (2), and the third indicates where the solutions to Eq. (69) are sought. Equation (69) has four solutions in this region to be denoted by $t_a^{(\pm,\pm)}$. Expanding all functions in Eq. (69) near $t' = t$, we find

$$t_a^{(\pm,\pm)} = t \pm \frac{i}{F(t)}\{\varkappa^2(\mathbf{r};t) \pm 2[\varkappa^2(\mathbf{r};t)\varkappa^2(\mathbf{r}';t) - \mathbf{F}^2(t)\Delta\mathbf{r}_\perp^2]^{1/2} + \varkappa^2(\mathbf{r}';t)\}^{1/2} + O(\epsilon^1), \tag{71}$$

where $\Delta\mathbf{r}_\perp$ is defined with respect to $\mathbf{e}(t)$ and

$$\varkappa(\mathbf{r};t) = \{2[\mathbf{F}(t)\mathbf{r} - E_0(t)]\}^{1/2}, \quad \varkappa(\mathbf{r};t\to-\infty) = \varkappa. \tag{72}$$

For $\Delta\mathbf{r}\to 0$, two of these solutions coalesce with t, while the two others stay at a finite distance from t; in I they were termed the *adiabatic* and *tunneling* SPs, respectively. In the case of general position, when $|\Delta\mathbf{r}| \sim r \sim r'$ and t is not too close to a zero of $\mathbf{F}(t)$, the SPs (71) indeed lie at a distance $O(\epsilon^0)$ from t, in accordance with the third of Eqs. (70). As r grows, they move away from t. When r approaches the boundary of the QS zone, that is, for $r \sim R(t)$, they approach the boundary of zone A, that is, $|t_a^{(\pm,\pm)} - t| \sim T_0$; in this case the error term in Eq. (71) becomes $O(\epsilon^{-1})$. Thus, as long as $\mathbf{r}$ is in the QS zone, there are four SPs in zone A given by Eq. (71).

The SPs (71) approach each other and coalesce with the singular point $t' = t$ of the integrand in Eq. (67) as $F(t)$ grows. The overall strength of the field is characterized by the parameter ξ [see Eqs. (10)]. For sufficiently large ξ, the contributions from these SPs cannot be considered independently. Thus, to obtain the asymptotic solution of Eq. (67), which is uniform in terms of ξ, the complex including all four SPs and the singular point must be treated as a whole. Such a uniform treatment generalizing the procedure developed in I is possible. Let us again consider the region (70). In this region,

$$S_a(\mathbf{r},t;\mathbf{r}',t') = \frac{\Delta\mathbf{r}^2}{2\delta} - \frac{1}{2}\mathbf{F}(t)(\mathbf{r}+\mathbf{r}')\delta - \frac{1}{24}\mathbf{F}^2(t)\delta^3 + E_0(t)\delta + \frac{1}{6}\dot{\mathbf{F}}(t)(\mathbf{r}+2\mathbf{r}')\delta^2 + \frac{1}{24}\mathbf{F}(t)\dot{\mathbf{F}}(t)\delta^4 - \frac{1}{2}\dot{E}_0(t)\delta^2 + O(\epsilon^2), \tag{73a}$$

$$\phi_0(\mathbf{r}';t') = \phi_0(\mathbf{r}';t) + \dot{\phi}_0(\mathbf{r}';t')\delta + O(\epsilon^2), \tag{73b}$$

where $\delta = t - t'$. The terms containing slow functions $\mathbf{F}(t)$, $E_0(t)$, and $\phi_0(\mathbf{r}';t)$ and their derivatives in these expansions have orders 0 and 1, respectively. Substituting Eqs. (73) into Eq. (67) and collecting together terms of the same order in ϵ, in the zeroth order using Eq. (42) we obtain

$$\phi_0(\mathbf{r};t) = \int G(\mathbf{r},\mathbf{r}';E_0(t),\mathbf{F}(t))V(\mathbf{r}')\phi_0(\mathbf{r}';t)\,d\mathbf{r}'. \tag{74}$$

This equation is equivalent to Eq. (40), so its solution is given by

$$E_0(t) = E_0(\mathbf{F}(t)), \quad \phi_0(\mathbf{r};t) = N(t)\phi_0(\mathbf{r};\mathbf{F}(t)), \tag{75}$$

where $N(t)$ is yet unknown normalization factor. To find this factor, one must proceed to the next order of the expansion. In the first order, we obtain

$$\int\left[\left(2\dot{\phi}_0(\mathbf{r}';t) + \phi_0(\mathbf{r}';t)\frac{d}{dt}\right)\frac{\partial G(\mathbf{r},\mathbf{r}';E,\mathbf{F}(t))}{\partial E}\bigg|_{E=E_0(t)} + \frac{1}{6}(\mathbf{r}-\mathbf{r}')\phi_0(\mathbf{r}';t)\frac{\partial^2 G(\mathbf{r},\mathbf{r}';E,\mathbf{F}(t))}{\partial E^2}\bigg|_{E=E_0(t)}\right] \times V(\mathbf{r}')\,d\mathbf{r}' = 0. \tag{76}$$

Multiplying this equation by $V(\mathbf{r})\phi_0(\mathbf{r};t)$, integrating over $\mathbf{r}$, and using Eq. (74), it can be shown (we omit the details) that Eq. (76) is equivalent to

$$\frac{d}{dt}\int \phi_0^2(\mathbf{r};t)\,d\mathbf{r} = 0. \tag{77}$$

Taking into account the normalization (8) and (45) and initial (65) conditions, we thus find

$$N(t) = 1. \tag{78}$$

This completes the construction of the leading-order term in the asymptotics of $\psi_a(\mathbf{r},t)$. The procedure can be continued; considering the next term in the expansion, one can obtain a correction to $\phi_0(\mathbf{r};t)$ of order $O(\epsilon^1)$, etc. An alternative derivation of this asymptotic series for $\phi_0(\mathbf{r};t)$ in operator form, including the first-order correction term, is presented in Appendix A.

The adiabatic part $\psi_a(\mathbf{r},t)$ of the wave function is the central object of the present theory from which all further results are derived. So it is important to specify the region of validity of Eq. (63), which determines that of the whole

theory. Expansions (73) hold for $\delta \ll T_0$, which explains the size of the adiabatic zone (66). For the SPs (71) to be located in this zone, two conditions must be fulfilled: (i) $r \ll R(t)$, which means that the region of validity of Eq. (63) in terms of r coincides with the QS zone; (ii) $|t_a^{(\pm,\pm)} - t| \sim \varkappa/F_0 \ll T_0$, which amounts to $\epsilon \ll \xi$. In addition, solving Eq. (67) we have expanded the exponential function. So the dotted terms in Eq. (73a) taken at the SPs, that is, for $\delta \sim \varkappa/F_0$, must be small compared not only with the leading-order terms, which leads to $\epsilon \ll \xi$, but also with unity [58], which requires $\epsilon \ll \xi^2$. We thus arrive at Eq. (13) as the condition of validity of the adiabatic approximation.

Summarizing, the leading-order term in the asymptotics of $\psi_a(\mathbf{r},t)$ for $\epsilon \to 0$ is given by Eqs. (63) and (64), where $E_0(t)$ and $\phi_0(\mathbf{r};t)$ are expressed in terms of the SS by Eqs. (75) and (78). Thus, in the presence of an external electric field, the initial bound state turns into a properly normalized SS which adiabatically follows a variation of the field. The integral term in Eq. (64) accounts for a difference between the eigenvalues. It describes the accumulation of an additional phase and decay of the initial state due to its interaction with the field. For weak fields, these effects can be approximately described in well-known terms of the second-order Stark shift and tunneling ionization rate given by Eqs. (48a) and (48b). The exact SS eigenvalue $E_0(\mathbf{F})$ arising in the present analysis makes Eq. (63) applicable to fields of arbitrary strength. The preexponential factor in Eq. (63) is the SS eigenfunction. Its difference from the initial bound state can be quantitatively characterized by a deviation of the projection (46) from unity (see Fig. 3); we show in Sec. VII A that this also leads to observable effects. We emphasize that the asymptotics (63) is uniform in terms of ξ. As shown in Appendix A, Eq. (63) does not rely on the assumption (2) and holds also for potentials with the Coulomb tail.

C. Formation zone

Let the electric field $\mathbf{F}(t)$ have a simple zero at $t = t_F$,

$$\mathbf{F}(t_F) = \mathbf{0}, \quad \dot{\mathbf{F}}(t_F) \neq \mathbf{0}. \tag{79}$$

In the GP and PP cases, such a zero can appear only accidentally and can be eliminated by a small variation of the function $\mathbf{F}(t)$. However, not so in the LP case: The zeros of the electric field are a generic property of linearly polarized pulses. Since linearly polarized pulses are frequently used in applications, consequences of Eq. (79) must be discussed.

One of the consequences has already been mentioned in Sec. V A. The adiabatic approximation breaks down near t_F, because the radius of the momentary QS zone (58) turns to zero. Taking into account that $\dot{\mathbf{F}}(t_F) = O(\epsilon^1)$, the condition $a \ll R(t)$ is violated inside a region $|t - t_F| = O(\epsilon^1)$. This does not cause any problem because the electric field in this region is very weak, $\mathbf{F}(t) = O(\epsilon^2)$, so the interaction with it can be neglected.

Another consequence can be seen from Eq. (71). As t approaches t_F, the SPs $t_a^{(\pm,\pm)}$ depart from t. The analysis of the previous section does not apply if they leave the adiabatic zone (66). Thus, the validity of Eq. (63) for t in a vicinity of t_F requires special consideration. Following I, let us introduce the *formation* zone defined by

$$\text{zone } F: \quad |t - t_F| = O(\epsilon^{-1/2}). \tag{80}$$

In this zone $\mathbf{F}(t) = O(\epsilon^{1/2})$ and $R(t) = O(\epsilon^{-3/2})$. For $r = O(\epsilon^0)$, $r' = O(\epsilon^0)$, and $t \in F$, Eq. (69) has six solutions: Two of them (adiabatic SPs) are located near $t \pm i|\mathbf{r} - \mathbf{r}'|/\varkappa$, and four others (tunneling SPs) lie at a distance $\sim\varkappa/F(t) = O(\epsilon^{-1/2})$ from t, which is still inside the adiabatic zone (66). Evaluating the contributions from these SPs, it can be shown (this analysis is similar to that presented in I, so we skip the details) that the asymptotic solution to Eq. (67) in zone F is given by Eqs. (63) and (64), where $\phi_0(\mathbf{r};t)$ is to be substituted by the unperturbed initial state $\phi_0(\mathbf{r})$ and $E_0(t)$ by the weak-field approximations (48a) and (48b) for the SS eigenvalue. In other words, the solution is given by the weak-field approximation to Eqs. (63) and (64), as one would expect. We thus conclude that the asymptotics (63) remains valid throughout zone F and hence is uniform in terms of t.

The third consequence of Eq. (79) is the appearance of rescattering trajectories and a new type of SPs associated with them. In zone F, these new SPs coincide with two of the four tunneling SPs mentioned above. Their contribution to the time integral in Eq. (67) is a seed from which the rescattering term in Eq. (60) grows up as t passes through zone F. Thus, zone F is where the formation of $\psi_r(\mathbf{r},t)$ takes place, which explains the terminology.

D. Rescattering part of the wave function

Substituting Eq. (63) for $\psi(\mathbf{r},t)$ into the rhs of Eq. (36) and calculating the contribution to the time integral from the adiabatic zone (66), one obtains a term with action of order -1. This term is compensated by the adiabatic part $\psi_a(\mathbf{r},t)$ of the wave function on the lhs of the equation (see Sec. V B). In this section we show that, under a certain condition, the asymptotics of the rhs of Eq. (36) contains terms with actions of order -3. This leads to the appearance of the rescattering part $\psi_r(\mathbf{r},t)$ on the lhs of the equation.

Let $\psi_r^{(a)}(\mathbf{r},t)$ denote a function obtained by substituting $\psi_a(\mathbf{r},t)$ for $\psi(\mathbf{r},t)$ into the rhs of Eq. (36) and omitting the contribution to the time integral from zone A. We have

$$\psi_r^{(a)}(\mathbf{r},t) = \frac{e^{3i\pi/4}}{(2\pi)^{3/2}} \int d\mathbf{r}' \int_{-\infty}^{t} e^{iS_r(\mathbf{r},t;\mathbf{r}',t')} V(\mathbf{r}')\phi_0(\mathbf{r}';t') \times \frac{dt'}{(t-t')^{3/2}}\bigg|_{t'\notin A}, \tag{81}$$

where

$$S_r(\mathbf{r},t;\mathbf{r}',t') = \mathcal{S}(\mathbf{r},t;\mathbf{r}',t') - s_0(t'). \tag{82}$$

One could expect that $\psi_r^{(a)}(\mathbf{r},t)$ coincides with $\psi_r(\mathbf{r},t)$, which is sought, but this is not so; we show that the latter function satisfies an inhomogeneous integral equation where the former one acts as a source term. In the following, we first discuss the condition of the appearance of the rescattering term in Eq. (60), then find $\psi_r^{(a)}(\mathbf{r},t)$ by reducing the rhs of Eq. (81) to an integral over the transverse momentum of an ionized electron, then solve the integral equation for $\psi_r(\mathbf{r},t)$, and finally integrate over the transverse momentum.

The SPs for the action (82) are defined by

$$\frac{\partial S_r}{\partial t'} = \frac{1}{2}\,\mathbf{u}_i^2(t,t',\Delta\mathbf{r}) + \mathbf{F}(t')\mathbf{r}' - E_0(t') = 0. \tag{83}$$

This equation coincides with Eq. (69) and hence defines a moment of ionization t' in the adiabatic regime. However, now we are interested in the solutions lying in a different region of the complex t' plane. The SPs responsible for appearing on the rhs of Eq. (81) terms with actions of order -3 lie at a distance $O(\epsilon^{-1})$ from t. We need to consider only SPs which are located sufficiently close to the real axis; otherwise their contribution is negligible. Let us analyze when such solutions to Eq. (83) exist. Similar to Eqs. (70), consider the region

$$r = O(\epsilon^0), \quad r' = O(\epsilon^0), \quad |t'-t| = O(\epsilon^{-1}). \tag{84}$$

In the case of general position in this region $\mathbf{u}_i(t,t',\Delta\mathbf{r}) = O(\epsilon^{-1})$, so the first term in Eq. (83) is $O(\epsilon^{-2})$, while the other two terms are $O(\epsilon^0)$. We also have $\mathbf{u}_i(t,t',\Delta\mathbf{r}) = \mathbf{u}_i(t,t') + O(\epsilon^1)$, where $\mathbf{u}_i(t,t') = O(\epsilon^{-1})$ [see Eqs. (20a) and (21a)]. Therefore, the solutions to Eq. (83) should be sought near the zeros of $\mathbf{u}_i(t,t')$. This argumentation justifies the frequently heard assertion that an ionized electron emerges after tunneling through the potential barrier with zero initial velocity, which is usually taken for granted. The vanishing of $\mathbf{u}_i(t,t')$ means that a classical trajectory starting with zero initial velocity at the moment t' at any point returns at the moment t to the same point. Such trajectories were termed in I closed rescattering trajectories (CRTs). The requirement $\mathbf{u}_i(t,t') = \mathbf{0}$ is unnecessarily too strong for the 3D case. An important difference of the present 3D problem from the 1D model considered in I is that at the moment of ionization the electron can have a nonzero transverse momentum $\mathbf{k}_\perp = O(\epsilon^0)$ [see Eq. (38)], which can compensate for the transverse component of $\mathbf{u}_i(t,t')$. This enables us to slightly extend the definition of CRTs by including closed trajectories with not quite zero initial velocity. The CRTs in the 3D case are associated with the solutions to

$$\mathbf{e}(t')\mathbf{u}_i(t,t') = 0 \quad \rightarrow \quad t' = t_i(t), \tag{85a}$$

$$\mathbf{u}_{i\perp}(t,t_i(t)) = O(\epsilon^0), \tag{85b}$$

where the $\perp$ component is defined with respect to $\mathbf{e}(t_i(t))$. This definition includes the case $\mathbf{u}_{i\perp}(t,t_i(t)) = \mathbf{0}$. Equations (85) may have several solutions corresponding to the different CRTs ending at the same moment t. Equation (85a) defines the initial moment $t_i(t)$ of a CRT, and Eq. (85b) ensures that the corresponding solutions to Eq. (83) are located sufficiently close to the real axis. Indeed, it can be shown that for each CRT Eq. (83) has two solutions $t_r^{\pm}$ lying at a distance $O(\epsilon^0)$ from $t_i(t)$. The existence of CRTs critically depends on the polarization. In the GP case, they may appear only accidentally. In the PP case, they can exist only for some isolated values of t. However, CRTs are a generic property of linearly polarized pulses. The analysis of CRTs in I fully applies to the present problem in the LP case. It was shown that for the existence of CRTs for a given t the electric field $\mathbf{F}(t')$ must have zeros in the interval $-\infty < t' < t$, and a new CRT appears when t passes through a zero of $\mathbf{F}(t)$. The appearance of a new CRT is accompanied by the appearance of a new pair of the solutions $t_r^{\pm}$ to Eq. (83), which explains the role of the formation zone discussed in the end of the previous section. Thus, the condition of appearance of the rescattering term in Eq. (60) is the existence of the solutions to Eqs. (85), that is, CRTs ending at the moment t. In such a general form, this condition applies to all polarization cases.

We turn to calculating $\psi_r^{(a)}(\mathbf{r},t)$. Using Eq. (37), the integration over $\mathbf{r}'$ in Eq. (81) can be performed by parts. The volume integral in the result consists of two terms where the integrand in Eq. (81) is multiplied by $(t-t')^{-1} = O(\epsilon^1)$ and the derivative (83), respectively. These terms are of higher order in ϵ than the surface integral and should be neglected in the leading-order approximation. We thus obtain

$$\psi_r^{(a)}(\mathbf{r},t) = \frac{e^{-3i\pi/4}}{(2\pi)^{3/2}} \int_{-\infty}^{t} \int_{\Sigma'} \mathbf{j}(\mathbf{r},t;\mathbf{r}',t')\, d\boldsymbol{\Sigma}' \frac{dt'}{(t-t')^{3/2}}\bigg|_{t'\notin A}, \tag{86}$$

where

$$\mathbf{j}(\mathbf{r},t;\mathbf{r}',t') = \frac{-i}{2}[e^{iS_r(\mathbf{r},t;\mathbf{r}',t')}\nabla'\phi_0(\mathbf{r}';t') - \phi_0(\mathbf{r}';t')\nabla' e^{iS_r(\mathbf{r},t;\mathbf{r}',t')}]. \tag{87}$$

The spatial integration in Eq. (86) goes over $\mathbf{r}' \in \Sigma'$, where Σ' is any surface enclosing the region occupied by the atomic potential, for example, a sphere of radius $r' > a$, $d\boldsymbol{\Sigma}' = \mathbf{n}' d\Sigma'$, and $\mathbf{n}'$ is the external unit normal vector to Σ'. We first calculate the surface integral. Let $\mathbf{r}' = r'_\parallel \mathbf{e}(t') + \mathbf{r}'_\perp$, where the components are defined with respect to the momentary polarization vector $\mathbf{e}(t')$. We deform Σ' into a plane $r'_\parallel = \text{const} < -a$ perpendicular to $\mathbf{e}(t')$. This is possible because $\phi_0(\mathbf{r}';t')$ vanishes as $r' \to \infty$ in all directions except that opposite to $\mathbf{e}(t')$, where the ionization flux goes. On this plane, $\phi_0(\mathbf{r}';t')$ can be substituted in the form (38). Then the integral over Σ' can be calculated exactly using

$$\int e^{iS_r(\mathbf{r},t;\mathbf{r}',t')+i\mathbf{k}_\perp\mathbf{r}'_\perp}\, d\mathbf{r}'_\perp = 2i\pi(t-t')e^{i\tilde{S}_r(\mathbf{r},t;r'_\parallel,\mathbf{k}_\perp,t')}, \tag{88}$$

where

$$\tilde{S}_r(\mathbf{r},t;r'_\parallel,\mathbf{k}_\perp,t') = \mathcal{S}(\mathbf{r},t;\mathbf{u}_i,t') - u_{i\parallel}r'_\parallel - s_0(t'), \tag{89a}$$

$$\mathbf{u}_i = u_{i\parallel}\mathbf{e}(t') + \mathbf{k}_\perp, \quad u_{i\parallel} = u_{i\parallel}(t,t') + \frac{\Delta r_\parallel}{t-t'}, \tag{89b}$$

and $\mathcal{S}(\mathbf{r},t;\mathbf{u}_i,t')$ is defined by Eqs. (28). Now we calculate the time integral. The SPs for the action (89a) are defined by

$$\frac{\partial \tilde{S}_r}{\partial t'} = \frac{1}{2}\,\mathbf{u}_i^2 + F(t')r'_\parallel - E_0(t') = 0. \tag{90}$$

Consider this equation in the region (84). Near each solution $t_i(t)$ to Eqs. (85), there exist two solutions to Eq. (90) to be denoted by $\tilde{t}_r^{\pm}$. Expanding all functions in Eq. (90) near $t' = t_i(t)$, we find

$$\tilde{t}_r^{\pm} = t_i(t) \pm i\,\frac{[\varkappa^2(\mathbf{r}',t_i(t)) + \mathbf{k}_\perp^2]^{1/2}}{F(t_i(t))} + O(\epsilon^1). \tag{91}$$

These two SPs coalesce as ξ grows. Thus, to obtain the asymptotics of $\psi_r^{(a)}(\mathbf{r},t)$, which is uniform in terms of ξ, the complex including both SPs must be treated as a whole. This can be done by expanding the action (89a) near some suitable reference point inside the complex [59]. In the case of general position, when $F(t_i(t)) = O(\epsilon^0)$, the distance between the SPs

is $O(\epsilon^0)$, so they both contribute to the integral. Then the moment $t_i(t)$ lying between $\tilde{t}_r^+$ and $\tilde{t}_r^-$ is a suitable reference point. However, the case when $t_i(t)$ is located close to a zero t_F of $\mathbf{F}(t)$ causes a difficulty. This happens when t has just passed through t_F and a new solution $t_i(t)$ to Eqs. (85) has appeared. It can be shown that when t is still in the formation zone (80), $t_i(t)$ is also located in the formation zone on the other side of t_F, and the distances between the SPs $\tilde{t}_r^{\pm}$ as well as between each of them and $t_i(t)$ are $O(\epsilon^{-1/2})$. In this case, only one SP $\tilde{t}_r^+$ located in the upper half of the complex time plane contributes to the integral. Hence, the reference point must be chosen somewhere near $\tilde{t}_r^+$; the moment $t_i(t)$ is not suitable for this role anymore. Let us introduce $t_i^{\pm}(t,\mathbf{k}_\perp)$ defined by

$$\tfrac{1}{2}u_{i\parallel}^2(t,t') + \tfrac{1}{2}\,\mathbf{k}_\perp^2 - E_0(t') = 0 \quad \rightarrow \quad t' = t_i^{\pm}(t,\mathbf{k}_\perp). \tag{92}$$

We have left here terms of two leading orders in the formation zone from Eq. (90). The solutions to this equation lie at a distance $O(\epsilon^0)$ from the solutions to Eq. (90) uniformly in t, including the case when t is in the formation zone. Thus, choosing $t_i^+(t,\mathbf{k}_\perp)$ instead of $t_i(t)$ as the reference point for expanding the action (89a) resolves the above-mentioned difficulty and enables one to obtain the asymptotics of $\psi_r^{(a)}(\mathbf{r},t)$, which is uniform in terms of t. For brevity, in the following we omit the arguments in $t_i^+(t,\mathbf{k}_\perp)$. In the region $\delta = t' - t_i^+ = O(\epsilon^0)$ we have

$$\begin{aligned}&\tilde{S}_r(\mathbf{r},t;r'_\parallel,\mathbf{k}_\perp,t')\\ &\quad= \tilde{S}_r(\mathbf{r},t;r'_\parallel,\mathbf{k}_\perp,t_i^+) + F(t_i^+)r'_\parallel\delta\\ &\qquad- \tfrac{1}{2}F(t_i^+)u_{i\parallel}(t,t_i^+)\delta^2 + \tfrac{1}{6}F^2(t_i^+)\delta^3 + O(\epsilon^1).\end{aligned} \tag{93}$$

Substituting this expansion into the rhs of Eq. (88), one can calculate the time integral in Eq. (86). The result is expressed in terms of an Airy function whose argument differs from that of the other Airy function, the one which originates from $\phi_0(\mathbf{r}';t_i^+)$ substituted in the form (38), by a factor $e^{-2i\pi/3}$. The flux (87) taken at the plane Σ' reduces to the Wronskian of the two Airy functions, which eliminates the dependence on $r'_\parallel$ defining the position of the plane. Omitting further details, the result is

$$\begin{aligned}\psi_r^{(a)}(\mathbf{r},t) = \sum_i \int \frac{A_0(\mathbf{k}_\perp;t_i^+)}{[(t-t_i^+)F(t_i^+)]^{1/2}}\,\Phi(\mathbf{r},t;\mathbf{u}_i^+,t_i^+)\\ \times\,\exp\left[-is_0(t_i^+) - \frac{iu_{i\parallel}^3(t,t_i^+)}{3F(t_i^+)}\right]\frac{d\mathbf{k}_\perp}{(2\pi)^2},\end{aligned} \tag{94}$$

where $A_0(\mathbf{k}_\perp;t) \equiv A_0(\mathbf{k}_\perp;\mathbf{F}(t))$. Here

$$\Phi(\mathbf{r},t;\mathbf{u}_i^+,t_i^+) = e^{i\mathbf{u}_f^+\mathbf{r} - i\mathcal{S}(t,t_i^+,\mathbf{u}_i^+)} \tag{95}$$

is the Volkov state defined by Eqs. (28) and (34), $\mathbf{u}_i^+$ and $\mathbf{u}_f^+$ are shorthand notation for the initial velocity of an electron at the moment of ionization t_i^+,

$$\mathbf{u}_i^+(t,\mathbf{k}_\perp) = u_{i\parallel}(t,t_i^+)\mathbf{e}(t_i^+) + \mathbf{k}_\perp = O(\epsilon^0), \tag{96a}$$

and its final velocity at the moment of rescattering t [see Eq. (25)],

$$\mathbf{u}_f^+(t,\mathbf{k}_\perp) = \mathbf{u}_i^+(t,\mathbf{k}_\perp) - \mathbf{v}(t_i^+) + \mathbf{v}(t) = O(\epsilon^{-1}), \tag{96b}$$

and the summation runs over the different (for the same t and $\mathbf{k}_\perp$) solutions to Eq. (92). All the components here are defined with respect to $\mathbf{e}(t_i^+)$.

We now turn to the derivation of $\psi_r(\mathbf{r},t)$. The superscript in $\psi_r^{(a)}(\mathbf{r},t)$ indicates that this contribution to $\psi_r(\mathbf{r},t)$ comes directly from the adiabatic term in Eq. (60). A key moment in the derivation consists of recognizing the fact that there exist other terms on the rhs of Eq. (36) which have the same actions as individual terms in the sum in Eq. (94). Indeed, let us substitute $\psi_r^{(a)}(\mathbf{r},t)$ for $\psi(\mathbf{r},t)$ into the rhs of Eq. (36) and calculate the contribution to the time integral from the adiabatic zone (66). The result is given by a sum of terms with the same actions as in Eq. (94), but different amplitudes. Substituting it for $\psi(\mathbf{r},t)$ into the rhs of Eq. (36) and again calculating the contribution from the adiabatic zone, one obtains yet another sum of terms with the same actions, etc. The function $\psi_r(\mathbf{r},t)$ is given by the sum of the series of all such terms on the rhs of Eq. (36). As follows from the construction, this function satisfies the inhomogeneous integral equation

$$\begin{aligned}\psi_r(\mathbf{r},t) = \psi_r^{(a)}(\mathbf{r},t) + \frac{e^{3i\pi/4}}{(2\pi)^{3/2}}\int d\mathbf{r}'\\ \times\int_{-\infty}^{t} e^{i\mathcal{S}(\mathbf{r},t;\mathbf{r}',t')}V(\mathbf{r}')\psi_r(\mathbf{r}',t')\,\frac{dt'}{(t-t')^{3/2}}\bigg|_{t'\in A}.\end{aligned} \tag{97}$$

We solve this equation under the condition

$$\tfrac{1}{2}\,\mathbf{u}_f^{+2} \gg \max[E_0(t),F(t)a] = O(\epsilon^0). \tag{98}$$

Taking into account Eq. (96b), this condition is fulfilled in the adiabatic regime for all values of t except for small intervals near the moments where $\mathbf{u}_f^+$ turns zero, if any. At such moments tunneling recombination occurs, which is the inverse process to tunneling ionization (for more details, see I). Thus, excluding the recombination zones from the consideration, we seek the solution to Eq. (97) in the form

$$\begin{aligned}\psi_r(\mathbf{r},t) = \sum_i \int \frac{A_0(\mathbf{k}_\perp;t_i^+)}{[(t-t_i^+)F(t_i^+)]^{1/2}}\,\Psi_r(\mathbf{r},t,\mathbf{k}_\perp)\\ \times\,\exp\left[-i\mathcal{S}(t,t_i^+,\mathbf{u}_i^+) - is_0(t_i^+) - \frac{iu_{i\parallel}^3(t,t_i^+)}{3F(t_i^+)}\right]\\ \times\,\frac{d\mathbf{k}_\perp}{(2\pi)^2}.\end{aligned} \tag{99}$$

Substituting this into Eq. (97) and expanding the actions in the integral term near $t' = t$ using

$$\frac{\partial}{\partial t}[\mathcal{S}(t,t_i^+,\mathbf{u}_i^+) + s_0(t_i^+)] = \frac{1}{2}\,\mathbf{u}_f^{+2}, \tag{100}$$

we obtain an equation for $\Psi_r(\mathbf{r},t,\mathbf{k}_\perp)$,

$$\begin{aligned}\Psi_r(\mathbf{r},t,\mathbf{k}_\perp) = e^{i\mathbf{u}_f^+\mathbf{r}} + \int G\big(\mathbf{r}-\mathbf{r}';\tfrac{1}{2}\,\mathbf{u}_f^{+2}\big)V(\mathbf{r}')\\ \times\,\Psi_r(\mathbf{r}',t,\mathbf{k}_\perp)\,d\mathbf{r}',\end{aligned} \tag{101}$$

where $G(\mathbf{r};E)$ is defined by Eq. (51). This equation coincides with Eq. (50), so the solution is given by

$$\Psi_r(\mathbf{r},t,\mathbf{k}_\perp) = \varphi(\mathbf{r};\mathbf{u}_f^+), \tag{102}$$

where $\varphi(\mathbf{r};\mathbf{k})$ is a scattering state introduced in Sec. IV. Thus, the effect of the integral term in Eq. (97) amounts to replacing the incident plane wave factor in the Volkov state (95) with the scattering state.

Equation (99) is a fork in the derivation. A further simplification of this intermediate result by performing the integration over the transverse momentum depends on the properties of the scattering state (102). For potentials with the Coulomb tail, the scattering amplitude contained in $\varphi(\mathbf{r};\mathbf{u}_f^+)$ diverges in the forward direction, which requires a special treatment. Keeping this circumstance in mind for future generalizations, we proceed with the derivation for finite-range potentials.

The action in Eq. (99) depends on $\mathbf{k}_\perp$ through the term $-\frac{1}{2}[\mathbf{k}_\perp - \mathbf{u}_{i\perp}(t,t_i^+)]^2(t-t_i^+)$. In the case of general position $t-t_i^+ = O(\epsilon^{-1})$, so one can think of calculating the integral over $\mathbf{k}_\perp$ by the steepest descent method. The corresponding SP is given by $\mathbf{k}_\perp = \mathbf{u}_{i\perp}(t,t_i^+)$. For this value of the transverse momentum of an electron ionized at the moment t_i^+, its trajectory returns to the initial point at the moment t. Thus, the dominant contribution to the integral in Eq. (99) comes from closed trajectories. The width of the region around the SP contributing to the integral is $\sim|t-t_i^+|^{-1/2} = O(\epsilon^{1/2})$, while the widths of the TMD amplitude and the scattering state as functions of $\mathbf{k}_\perp$ are $O(\epsilon^0)$ (this is where the Coulomb tail causes a problem). In this case, the integral indeed can be evaluated using the steepest descent method. The result is

$$\psi_r(\mathbf{r},t) = \frac{-i}{2\pi}\sum_i \frac{A_0(\mathbf{u}_{i\perp}^+(t);t_i^+)}{[(t-t_i^+)^3F(t_i^+)]^{1/2}}\,\varphi(\mathbf{r};\mathbf{u}_f^+(t)) \times \exp\left[-i\mathcal{S}(t,t_i^+,\mathbf{u}_i^+(t)) - is_0(t_i^+) - \frac{iu_{i\parallel}^{+3}(t)}{3F(t_i^+)}\right]. \tag{103}$$

Here $t_i^+ = t_i^+(t)$ is the moment of ionization and $\mathbf{u}_i^+(t)$ and $\mathbf{u}_f^+(t)$ are the initial and final velocities for the closed trajectory obtained by substituting into Eqs. (92), (96a), and (96b) the SP value of $\mathbf{k}_\perp$ and explicitly defined in terms of functions (21) by

$$\tfrac{1}{2}\mathbf{u}_i^2(t,t') - E_0(t') = 0 \quad\rightarrow\quad t' = t_i^\pm(t), \tag{104}$$

and

$$\mathbf{u}_i^+(t) \equiv \mathbf{u}_i(t,t_i^+(t)), \quad \mathbf{u}_f^+(t) \equiv \mathbf{u}_f(t,t_i^+(t)). \tag{105}$$

The $\perp$ and $\parallel$ components of $\mathbf{u}_i^+(t)$ in Eq. (103) are defined with respect to $\mathbf{e}(t_i^+(t))$. This completes the construction of $\psi_r(\mathbf{r},t)$.

Summarizing, the existence of CRTs defined by Eqs. (85) leads to the appearance of the rescattering part of the wave function in Eq. (60). The leading-order term in the asymptotics of $\psi_r(\mathbf{r},t)$ for $\epsilon\to 0$ is given by Eq. (103). This asymptotics is uniform in terms of ξ and holds for all values of t excluding small intervals near the recombination points, where the electron's velocity at the moment of rescattering $\mathbf{u}_f^+(t)$ turns zero.

The asymptotics of $\psi_r(\mathbf{r},t)$ given by Eq. (103) holds in the case of general position, that is when $t-t_i^+(t) = O(\epsilon^{-1})$, as well as in the formation zone, when $t-t_i^+(t) = O(\epsilon^{-1/2})$. In the former case Eq. (103) can be simplified further. To make this result more transparent, it is instructive to discuss its simplification. Using $t_i(t)$ defined by Eqs. (85) as a reference point for expanding the action (89a) and repeating the derivation, we obtain

$$\psi_r(\mathbf{r},t) = \frac{-i}{2\pi}\sum_i \frac{A_0(\mathbf{u}_{i\perp}(t);t_i)}{[(t-t_i)^3F(t_i)]^{1/2}}\,\varphi(\mathbf{r};\mathbf{u}_f(t)) \times \exp[-i\mathcal{S}(t,t_i,\mathbf{u}_i(t)) - is_0(t_i)], \tag{106}$$

where $t_i = t_i(t)$ and

$$\mathbf{u}_i(t) \equiv \mathbf{u}_i(t,t_i(t)), \quad \mathbf{u}_f(t) \equiv \mathbf{u}_f(t,t_i(t)). \tag{107}$$

Note that from Eq. (85a) we have $u_{i\parallel}(t) = 0$, so $\mathbf{u}_{i\perp}(t) = \mathbf{u}_i(t)$, where the components are defined with respect to $\mathbf{e}(t_i(t))$. Equation (106) is the simplified form of Eq. (103) mentioned above. The rhs of Eq. (106) is expressed in terms of the initial moment $t_i(t)$ of a CRT, which is real and completely determined by classical mechanics, while $t_i^+(t)$ in Eq. (103) is generally complex and depends on the properties of the SS [see Eq. (104)]. The different terms in the sum correspond to the different CRTs arriving for rescattering at the moment t. Each term is a scattering state $\varphi(\mathbf{r};\mathbf{u}_f(t))$ multiplied by appropriate amplitude. The incident velocity $\mathbf{u}_f(t)$ is equal to the final velocity on the corresponding CRT. We note that the incident velocities in Eqs. (103) and (106) are related by

$$\mathbf{u}_f^+(t) = \mathbf{u}_f(t) + \left[\frac{1}{2}\mathbf{u}_i^2(t) - E_0(t_i)\right]\frac{\mathbf{F}(t_i)}{(t-t_i)F^2(t_i)} + O(\epsilon^2), \tag{108}$$

where the second term on the rhs is $O(\epsilon^1)$. The amplitude consists of factors describing the following stages in the evolution of the electron prior to the rescattering event: (i) staying in the adiabatic SS (63) until the moment t_i [the quantum action $s_0(t_i)$], (ii) ionization at the moment t_i with the transverse momentum $\mathbf{u}_{i\perp}(t)$ [the TMD amplitude $A_0(\mathbf{u}_{i\perp}(t);t_i)$], and (iii) traveling along a CRT and returning to the initial point at the moment t [the classical action $\mathcal{S}(t,t_i,\mathbf{u}_i(t))$]. From Eqs. (85) we obtain

$$\frac{u_{f\parallel}(t)}{t-t_i} = -F(t_i)\frac{dt_i}{dt} + O(\epsilon^1). \tag{109}$$

Using this relation, it can be shown that the denominator in Eq. (106) ensures conservation of the flux (for more details, see I). Such an interpretation of Eq. (106) is quite in the spirit of a naive picture of the ionization dynamics known as the "simple-man theory" [16–18]. However, the fact that Eqs. (103) and (106) express $\psi_r(\mathbf{r},t)$ in terms of the adiabatic SS (63) instead of the unperturbed initial state (7) and the presence in the former equation of the quantum $t_i^+(t)$ instead of classical $t_i(t)$ moment of ionization show that the true quantitatively predictive theory is not that simple. From Eq. (106) one can clearly see the necessity of condition (85b); indeed, because of a rapid decay of the TMD amplitude at large transverse momenta, contributions from CRTs for which this condition is not fulfilled are negligible. Since the first CRT appears not earlier than the first zero of $\mathbf{F}(t)$, Eq. (106) satisfies the initial condition (62b). Because of the factor $(t-t_i)^{-3/2}$, the amplitude in Eq. (106) is $O(\epsilon^{3/2})$, in accordance with Eq. (61b). One can notice that in the present analysis we have taken into account only one-loop CRTs, using the terminology of I. The contributions to $\psi_r(\mathbf{r},t)$ from many-loop CRTs with

several rescattering events are generally of higher order in ϵ and are neglected in the leading-order approximation.

VI. PHOTOELECTRON MOMENTUM DISTRIBUTION

Having constructed the asymptotic solution to Eqs. (1) and (7) for $\epsilon \to 0$, we can calculate the observables. For example, the leading-order term in the probability to find the system in the initial bound state as a function of time is determined by the projection of $\psi_a(\mathbf{r},t)$ onto $\phi_0(\mathbf{r})$ and given by

$$P_0(t) = |\Pi_0(t)|^2 \exp\left[-\int_{-\infty}^{t} \Gamma_0(t')\,dt'\right], \qquad (110)$$

where $\Pi_0(t) \equiv \Pi_0(\mathbf{F}(t))$ and $\Gamma_0(t) \equiv \Gamma_0(\mathbf{F}(t))$. The survival probability is

$$P_0 = P_0(t \to \infty) = \exp\left[-\int_{-\infty}^{\infty} \Gamma_0(t)\,dt\right]. \qquad (111)$$

The probabilities of transitions to other bound states can be obtained in a standard way [60–62]. This, however, requires to analyze the Riemann surface and branch points of the solution to Eq. (37) as a multivalued analytic function of F. We postpone this analysis to future studies. In this work, we restrict our treatment to calculating the PEMD.

A. Exact expressions

The PEMD $P(\mathbf{k})$ can be expressed in terms of the exact solution to Eqs. (1) and (7) in several different ways. We begin with the derivation of a formula which is most convenient for the present purposes. By definition,

$$P(\mathbf{k}) = |I(\mathbf{k})|^2, \quad P_{\rm ion} = \int P(\mathbf{k})\,\frac{d\mathbf{k}}{(2\pi)^3}, \qquad (112)$$

where the ionization amplitude $I(\mathbf{k})$ for potentials satisfying Eq. (2) is given by

$$I(\mathbf{k}) = \int e^{-i\mathbf{k}\cdot\mathbf{r}+iEt}(1-\hat{P}_b)\psi(\mathbf{r},t)d\mathbf{r}\Big|_{t\to\infty}, \qquad (113)$$

and $P_{\rm ion}$ is the total ionization probability. Here $E = \mathbf{k}^2/2$ and $\hat{P}_b$ is the projector onto the subspace of bound states of the unperturbed atom. Substituting Eq. (36) into the first term on the rhs of Eq. (113), we obtain

$$I(\mathbf{k}) = \left[-i\int_{-\infty}^{t} dt' \int e^{-i\mathcal{S}(\mathbf{r},t';\mathbf{k})}V(\mathbf{r})\psi(\mathbf{r},t')d\mathbf{r} - \int e^{-i\mathbf{k}\mathbf{r}+iEt}\hat{P}_b\psi(\mathbf{r},t)d\mathbf{r}\right]_{t\to\infty}, \qquad (114)$$

where the action $\mathcal{S}(\mathbf{r},t;\mathbf{k})$ is defined by Eqs. (29). Using $V(\mathbf{r})(1-\hat{P}_b)\psi(\mathbf{r},t)|_{t\to\infty} = 0$, it can be shown that

$$\int e^{-i\mathbf{k}\cdot\mathbf{r}+iEt}\hat{P}_b\psi(\mathbf{r},t)d\mathbf{r}\Big|_{t\to\infty} = i\int_{t}^{\infty} dt' \int e^{-i\mathcal{S}(\mathbf{r},t';\mathbf{k})}V(\mathbf{r})\psi(\mathbf{r},t')d\mathbf{r}\Big|_{t\to\infty}, \qquad (115)$$

and hence

$$I(\mathbf{k}) = -i\int_{-\infty}^{\infty} dt \int e^{-i\mathcal{S}(\mathbf{r},t;\mathbf{k})}V(\mathbf{r})\psi(\mathbf{r},t)d\mathbf{r}. \qquad (116)$$

Using Eq. (1) and integrating by parts, we obtain yet another representation for $I(\mathbf{k})$,

$$I(\mathbf{k}) = \int_{-\infty}^{\infty} dt \int_{\Sigma} \mathbf{j}(\mathbf{r},t)d\boldsymbol{\Sigma}, \qquad (117)$$

where

$$\mathbf{j}(\mathbf{r},t) = \frac{-i}{2}[e^{-i\mathcal{S}(\mathbf{r},t;\mathbf{k})}\nabla\psi(\mathbf{r},t) - \psi(\mathbf{r},t)\nabla e^{-i\mathcal{S}(\mathbf{r},t;\mathbf{k})}]. \qquad (118)$$

The spatial integration here goes over $\mathbf{r} \in \Sigma$, where Σ is again any surface enclosing the region occupied by the atomic potential, $d\boldsymbol{\Sigma} = \mathbf{n}d\Sigma$, and $\mathbf{n}$ is the external unit normal vector to Σ. Formulas (113), (116), and (117) are equally exact, but differ in implementation. The last formula is most convenient for calculating PEMD within the adiabatic theory. We note that it relies on the assumption (2) and does not hold for potentials with the Coulomb tail. For real $\mathcal{S}(\mathbf{r},t;\mathbf{k})$, the exponential factor in Eqs. (116) and (118) coincides with the complex conjugate of the Volkov state (35). However, this is not so if t is complex; therefore, we refrain from using notation $\Phi^*(\mathbf{r},t;\mathbf{k})$.

Similarly to Eq. (54), we have

$$\mathcal{S}(\mathbf{r},t;\mathbf{k}) = O(\epsilon^{-3}), \qquad (119)$$

so the time integral in Eq. (117) can be evaluated using the steepest descent method. This is consistent with the asymptotic solution of Eq. (36) and does not introduce any additional approximation. Substituting Eq. (60) into Eq. (118), the ionization amplitude (117) can be presented in the form

$$I(\mathbf{k}) = I_a(\mathbf{k}) + I_r(\mathbf{k}), \qquad (120)$$

where the two terms correspond to the two terms in Eq. (60). We calculate these two terms separately. As before, our strategy is to analyze contributions from the different SPs and collect together terms having the same action.

B. Adiabatic part of the ionization amplitude

The adiabatic part $I_a(\mathbf{k})$ of the ionization amplitude is defined by Eqs. (117) and (118), where $\psi(\mathbf{r},t)$ is to be substituted by $\psi_a(\mathbf{r},t)$ given by Eq. (63). The corresponding action is

$$S_a(\mathbf{r},t;\mathbf{k}) = -\mathcal{S}(\mathbf{r},t;\mathbf{k}) - s_0(t). \qquad (121)$$

The SPs for this action are the solutions to

$$\frac{\partial S_a}{\partial t} = \frac{1}{2}\mathbf{u}_i^2(t,\mathbf{k}) + \mathbf{F}(t)\mathbf{r} - E_0(t) = 0. \qquad (122)$$

Similarly to Eq. (69), this equation defines a moment of ionization t in the adiabatic regime, now as a function of the point $\mathbf{r}$, where the ionization occurs, and the asymptotic velocity $\mathbf{k}$ of an ionized electron. Equation (122) implies that after ionization the electron interacts only with the field; thus, $I_a(\mathbf{k})$ represents the direct (without rescattering) part of the ionization amplitude.

The number and positions of the solutions to Eq. (122) in the complex t plane depend on $\mathbf{r}$ and $\mathbf{k}$. Let us specify the region in the space of these variables where the solutions are sought. As for $\mathbf{r}$, its length is restricted by $r > a$, which follows from $\mathbf{r} \in \Sigma$ [see Eq. (117)], and $r \ll R_0 = O(\epsilon^{-2})$, which is required for the applicability of Eq. (63). We satisfy both conditions by assuming that $r = O(\epsilon^0)$. The region of

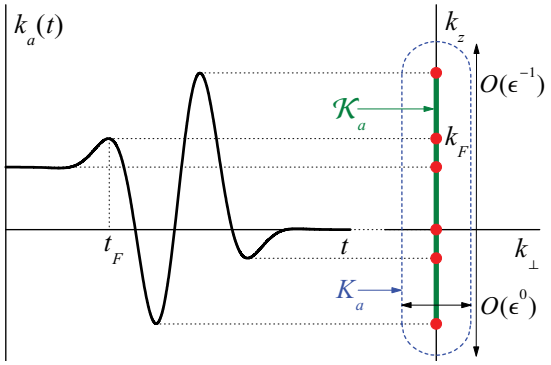

FIG. 5. (Color online) Illustration of the function $\mathbf{k}_a(t) = k_a(t)\mathbf{e}_z$ and the corresponding classical $\mathcal{K}_a$ and quantum K_a supports of the adiabatic part of the PEMD for a few-cycle linearly polarized laser pulse. Solid circles show the classical boundaries of the PEMD.

interest in the $\mathbf{k}$ space coincides with the support of the function $I_a(\mathbf{k})$. In the adiabatic regime it is determined by the following consideration. In the case of general position $\mathbf{u}_i(t,\mathbf{k}) = O(\epsilon^{-1})$, so the first term in Eq. (122) is $O(\epsilon^{-2})$, while the other two terms are $O(\epsilon^0)$. Hence, the solutions to Eq. (122) should be sought near the zeros of $\mathbf{u}_i(t,\mathbf{k})$. This situation is similar to the one we met in the analysis of Eq. (83). Let us introduce $\mathbf{k}_a(t)$ defined by

$$\mathbf{u}_i(t,\mathbf{k}) = 0 \quad \rightarrow \quad \mathbf{k} = \mathbf{k}_a(t) = \mathbf{v}_\infty - \mathbf{v}(t). \tag{123}$$

Let $\mathcal{K}_a$ denote a curve in the $\mathbf{k}$ space traced by the end of $\mathbf{k}_a(t)$ as t varies along the real axis. In the extreme adiabatic limit $\epsilon \to 0$, which corresponds to classical mechanics, possible values of the asymptotic velocity of an ionized electron are restricted to $\mathcal{K}_a$, so $\mathcal{K}_a$ is the classical support of the adiabatic part of the PEMD. The curve $\mathcal{K}_a$ begins at $\mathbf{k}_a(-\infty) = \mathbf{v}_\infty$ and ends at $\mathbf{k}_a(+\infty) = \mathbf{0}$, being closed if $\mathbf{v}_\infty = \mathbf{0}$. The shape of $\mathcal{K}_a$ depends on the polarization. In the GP case, $\mathcal{K}_a$ is a 3D curve; in the PP case, $\mathcal{K}_a$ is a 2D curve lying in the $k_x k_z$ plane; in the LP case, $\mathcal{K}_a$ is an interval of the k_z axis (see Fig. 5). The function $\mathbf{k}_a(t)$ parameterizes $\mathcal{K}_a$ by time. In the GP case, there is a one-to-one correspondence between the points of $\mathcal{K}_a$ and moments on the real-time axis. In the PP case, $\mathcal{K}_a$ generally has self-intersection points. There is only one moment corresponding to each generic point of $\mathcal{K}_a$, but there are two moments corresponding to each self-intersection point. In the LP case, $\mathcal{K}_a$ is multiply traced by $\mathbf{k}_a(t)$, so there generally are several moments corresponding to each point of $\mathcal{K}_a$ (see Fig. 5). The electric field $\mathbf{F}(t)$ is tangential to $\mathcal{K}_a$ at the point $\mathbf{k}_a(t)$. The curve $\mathcal{K}_a$ has cusps where $\mathbf{F}(t) = \mathbf{0}$. For any polarization, the ends of $\mathcal{K}_a$ are the cusp points [see Eq. (6)]. The existence of internal cusps in $\mathcal{K}_a$ is an accident in the GP and PP cases, but is a generic property of $\mathcal{K}_a$ in the LP case. The cusp points are also called the classical boundaries of the PEMD. The length of $\mathcal{K}_a$ is $O(\epsilon^{-1})$. Let K_a denote the neighborhood of $\mathcal{K}_a$ in the $\mathbf{k}$ space of size $O(\epsilon^0)$ (see Fig. 5). This quasi-1D set is a quantum counterpart of $\mathcal{K}_a$; we show shortly that in the adiabatic regime $I_a(\mathbf{k})$ rapidly vanishes outside K_a. Thus, we are interested in the solutions to Eq. (122) in the region

$$r = O(\epsilon^0), \quad \mathbf{k} \in K_a. \tag{124}$$

The classical boundaries divide $\mathcal{K}_a$ and K_a into segments. Let us consider one of the segments. We first assume that $\mathbf{k}$ is located in its main part, that is, sufficiently far from its ends. Each $\mathbf{k}$ in this region can be presented in the form

$$\mathbf{k} = \mathbf{k}_a(t_i(\mathbf{k})) + \Delta\mathbf{k}_\perp, \quad \Delta\mathbf{k}_\perp = O(\epsilon^0), \tag{125}$$

where the moment $t_i(\mathbf{k})$ is defined by

$$\mathbf{e}(t)\mathbf{u}_i(t,\mathbf{k}) = 0 \quad \rightarrow \quad t = t_i(\mathbf{k}), \tag{126}$$

and $\Delta\mathbf{k}_\perp$ is perpendicular to $\mathcal{K}_a$ at the point $\mathbf{k}_a(t_i(\mathbf{k}))$. One can see that $t_i(\mathbf{k})$ is the inverse function to $\mathbf{k}_a(t)$ for $\mathbf{k} \in \mathcal{K}_a$. Equation (122) has two solutions in this region to be denoted by $t_a^\pm$. Expanding all functions in Eq. (122) near $t = t_i(\mathbf{k})$, we find

$$t_a^\pm = t_i(\mathbf{k}) \pm i\frac{[\varkappa^2(\mathbf{r},t_i(\mathbf{k})) + \Delta\mathbf{k}_\perp^2]^{1/2}}{F(t_i(\mathbf{k}))} + O(\epsilon^1). \tag{127}$$

These two SPs coalesce as ξ grows. For obtaining the asymptotics of $I_a(\mathbf{k})$ which is uniform in terms of ξ, the complex including both SPs must be treated as a whole. To this end, we need to find a suitable reference point inside the complex for expanding the action (121) [59]. In the main part of the segment $F(t_i(\mathbf{k})) = O(\epsilon^0)$, the distance between the SPs (127) is $O(\epsilon^0)$, so they both contribute to the time integral in Eq. (117). In this case, the moment $t_i(\mathbf{k})$ lying between t_a^+ and t_a^- is a suitable reference point. Let now $\mathbf{k}$ be located near one of the ends of the segment. Let t_F be the corresponding zero of $\mathbf{F}(t)$. As $\mathbf{k}$ approaches $\mathbf{k}_F = \mathbf{k}_a(t_F)$, $t_i(\mathbf{k})$ approaches t_F (see Fig. 5), so $F(t_i(\mathbf{k}))$ vanishes and Eq. (127) ceases to hold. It can be shown that in the region $\mathbf{k} - \mathbf{k}_F = O(\epsilon^0)$ the distances between the SPs $t_a^\pm$ as well as between each of them and $t_i(\mathbf{k})$ become $O(\epsilon^{-1/2})$. In this case, only one SP t_a^+ located in the upper half of the complex time plane contributes to the integral, and the moment $t_i(\mathbf{k})$ cannot be used as a reference point anymore. This difficulty is similar to the one discussed in Sec. V D, so its remedy is known. Let us introduce $t_i^\pm(\mathbf{k})$ defined by

$$\tfrac{1}{2}\,\mathbf{u}_i^2(t,\mathbf{k}) - E_0(t) = 0 \quad \rightarrow \quad t = t_i^\pm(\mathbf{k}). \tag{128}$$

The solutions to this equation lie at a distance $O(\epsilon^0)$ from the solutions to Eq. (122) uniformly in $\mathbf{k} \in K_a$, including the regions near the classical boundaries of the PEMD. Thus, choosing $t_i^+(\mathbf{k})$ instead of $t_i(\mathbf{k})$ as the reference point for expanding the action (121) we obtain the asymptotics of $I_a(\mathbf{k})$, which is uniform in terms of $\mathbf{k}$. In the rest of this section, we omit the argument in $t_i^+(\mathbf{k})$ and all the components are defined with respect to $\mathbf{e}(t_i^+)$. Each $\mathbf{k} \in K_a$ can be presented in the form

$$\mathbf{k} = \mathbf{k}_a(t_i^+) + \Delta\mathbf{k}, \quad \Delta\mathbf{k} = \Delta k_\parallel \mathbf{e}(t_i^+) + \Delta\mathbf{k}_\perp = O(\epsilon^0). \tag{129}$$

In the region $\delta = t - t_i^+ = O(\epsilon^0)$ we have

$$S_a(\mathbf{r},t;\mathbf{k}) = S_a(\mathbf{r},t_i^+;\mathbf{k}) + F(t_i^+)r_\parallel\delta - \tfrac{1}{2}\,F(t_i^+)\Delta k_\parallel\delta^2 + \tfrac{1}{6}\,F^2(t_i^+)\delta^3 + O(\epsilon^1). \tag{130}$$

This expansion enables one to calculate the time integral in Eq. (117). The result is expressed in terms of an Airy function. To calculate the surface integral over $\mathbf{r} \in \Sigma$ we substitute $\mathbf{r} = r_\parallel\mathbf{e}(t_i^+) + \mathbf{r}_\perp$ and deform Σ into a plane $r_\parallel = \text{const} < -a$ perpendicular to $\mathbf{e}(t_i^+)$. On this plane, $\phi_0(\mathbf{r};t)$ can be substituted

in the form Eq. (38). Then the integral can be calculated, which results in the appearance of another Airy function. The flux (118) taken at the plane Σ reduces to the Wronskian of the two Airy functions, which eliminates the dependence on $r_\parallel$. We thus obtain

$$I_a(\mathbf{k}) = e^{i\pi/4}(2\pi)^{1/2}\sum_i \frac{A_0(\Delta\mathbf{k}_\perp;t_i^+)}{F^{1/2}(t_i^+)} \times \exp\left[i\mathcal{S}(t_i^+,\mathbf{k}) - is_0(t_i^+) - \frac{i\Delta k_\parallel^3}{3F(t_i^+)}\right], \quad (131)$$

where the summation runs over the different (for the same $\mathbf{k}$) solutions to Eq. (128), and the vector $\Delta\mathbf{k}$ depends on the summation index via Eq. (129). Summarizing, Eq. (131) gives the leading-order term in the asymptotics of the adiabatic part $I_a(\mathbf{k})$ of the ionization amplitude. This asymptotics is uniform in terms of ξ and $\mathbf{k} \in K_a$.

Two comments regarding this result are in order here. First, since the TMD amplitude $A(\Delta\mathbf{k}_\perp;t_i^+)$ rapidly decays as $\Delta k_\perp$ grows [45], and the solutions to Eq. (128) rapidly move deep into the complex time plane as $\Delta k_\parallel$ grows, function (131) rapidly vanishes outside the region K_a, in agreement with what was stated above. Second, the number of terms in Eq. (131) depends on the polarization. In the GP and PP cases, there is only one term for each $\mathbf{k}$ in the main part of K_a, and there are two such terms near the classical boundaries of the PEMD and self-intersection points of $\mathcal{K}_a$, if any, where the different segments of K_a overlap. However, in the LP case, there generally are several terms for each $\mathbf{k} \in K_a$, provided that $\mathbf{F}(t)$ has zeros. This means that, in the adiabatic regime, PEMDs typically have a rich interference structure in the LP case, but are smooth function of $\mathbf{k}$ in the GP and PP cases.

Another comment concerns the Keldysh approximation [11]. We now can show how it emerges within the present theory. As can be seen from Eqs. (43), $\psi_a(\mathbf{r},t)$ converges to the unperturbed initial state (7) as $\xi \to 0$. Hence, in this limit $I_a(\mathbf{k})$ coincides with the ionization amplitude in the Keldysh approximation $I_{\rm K}(\mathbf{k})$ (see Appendix B). For $I_a(\mathbf{k})$ to preserve its meaning, the limit $\xi \to 0$ must be taken within the adiabatic regime, that is, condition (13) must be fulfilled. We thus conclude that $I_{\rm K}(\mathbf{k})$ is a weak-field approximation to $I_a(\mathbf{k})$ that holds in the region $\epsilon \ll \xi^2$, $\xi \ll 1$. Physically, the difference between $I_a(\mathbf{k})$ and $I_{\rm K}(\mathbf{k})$ accounts for the interaction with the laser field in the initial state, which is neglected in the Keldysh approximation. This interaction leads, in particular, to the Stark shift and depletion of the initial state. It was shown in I that, because of these effects, the Keldysh approximation becomes qualitatively wrong for sufficiently long and/or intense laser pulses.

The asymptotics of $I_a(\mathbf{k})$ given by Eq. (131) holds in the main part of K_a as well as near classical boundaries of the PEMD. In the former case it can be simplified. As shown above, in this case one can use $t_i(\mathbf{k})$ defined by Eq. (126) as a reference point for expanding the action (121). Then, repeating the derivation, we obtain

$$I_a(\mathbf{k}) = e^{i\pi/4}(2\pi)^{1/2}\sum_i \frac{A_0(\Delta\mathbf{k}_\perp;t_i)}{F^{1/2}(t_i)} \exp[i\mathcal{S}(t_i,\mathbf{k}) - is_0(t_i)], \quad (132)$$

where $t_i = t_i(\mathbf{k})$ and $\Delta\mathbf{k}_\perp = \mathbf{k} - \mathbf{k}_a(t_i)$. Equation (132) could be also obtained from Eq. (131) by expanding all the functions in $t_i^+(\mathbf{k}) - t_i(\mathbf{k})$ and retaining only the leading-order terms. Note that the moment $t_i(\mathbf{k})$ is real and determined by classical mechanics, while $t_i^+(\mathbf{k})$ is complex and depends on the properties of the SS [see Eq. (128)]. Such an expansion is not possible when $t_i(\mathbf{k})$ is close to a zero of $F(t)$, that is when $\mathbf{k}$ is close to a classical boundary of the PEMD, which explains the advantage of Eq. (131) over Eq. (132).

C. Rescattering part of the ionization amplitude

We begin with classical consideration of rescattering. Being ionized at the moment $t_i(t)$ defined by Eqs. (85), an electron moves along the CRT and returns for rescattering at moment t with velocity $\mathbf{u}_f(t)$. In order to fly away with the asymptotic momentum $\mathbf{k}$, its velocity after rescattering must be equal to $\mathbf{u}_i(t,\mathbf{k})$ (we consider only trajectories with one rescattering). From the conservation of energy in the rescattering event, we have

$$\mathbf{u}_i^2(t,\mathbf{k}) = \mathbf{u}_f^2(t) \quad \to \quad t = t_r(\mathbf{k}). \quad (133)$$

This equation defines the moment of rescattering $t_r(\mathbf{k})$ as a function of $\mathbf{k}$. Let $\mathcal{K}_r$ denote a set in the $\mathbf{k}$ space where Eq. (133) has real solutions. This is the classical support of the rescattering part of the PEMD. At the boundary of $\mathcal{K}_r$ the different solutions to Eq. (133) coalesce, which results in a caustic in $I_r(\mathbf{k})$. The neighborhood of $\mathcal{K}_r$ of size $O(\epsilon^0)$ including this caustic is denoted by K_r. We show shortly that $I_r(\mathbf{k})$ rapidly vanishes outside K_r, so K_r is the quantum support of the rescattering part of the PEMD. Since in the illustrative calculations we focus on K_a, we do not describe the structure of K_r in more detail here.

The rescattering part $I_r(\mathbf{k})$ of the ionization amplitude is defined by Eqs. (117) and (118), where $\psi(\mathbf{r},t)$ is to be substituted by $\psi_r(\mathbf{r},t)$ given by Eq. (103). To calculate the spatial integral in Eq. (117), we choose the surface Σ to be a sphere of radius r satisfying $a < r \ll R(t)$; these two conditions are required for the applicability of Eqs. (117) and (103), respectively. Taking into account Eqs. (57) and (98), for $\epsilon \to 0$ it is always possible to choose a sufficiently large r in the specified interval such that the scattering state in Eq. (103) on the surface Σ can be substituted by its asymptotics (49b). We thus obtain

$$I_r(\mathbf{k}) = \frac{-i}{2\pi}\int_{-\infty}^{\infty} dt \sum_i \frac{A_0(\mathbf{u}_{i\perp}^+;t_i^+)}{[(t-t_i^+)^3F(t_i^+)]^{1/2}} \times \exp\left[iS_r^+(t,\mathbf{k}) - \frac{iu_{i\parallel}^{+3}}{3F(t_i^+)}\right] \times \frac{1}{2}\int_\Sigma \left\{[\mathbf{u}_f^+ + \mathbf{u}_i]e^{i\mathbf{u}_f^+\mathbf{r}} + [u_f^+\mathbf{n} + \mathbf{u}_i]f(\mathbf{u}_f^+,\mathbf{n})\frac{e^{iu_f^+r}}{r}\right\} \times e^{-i\mathbf{u}_i\mathbf{r}}\,d\boldsymbol{\Sigma}, \quad (134)$$

where

$$S_r^+(t,\mathbf{k}) = \mathcal{S}(t,\mathbf{k}) - \mathcal{S}(t,t_i^+,\mathbf{u}_i^+) - s_0(t_i^+). \quad (135)$$

Here $\mathbf{n} = \mathbf{r}/r$ and we have omitted the arguments in $t_i^+(t)$, $\mathbf{u}_i^+(t)$, $\mathbf{u}_f^+(t)$, and $\mathbf{u}_i(t,\mathbf{k})$. The SPs for the action (135) are

defined by

$$\frac{\partial S_r^+}{\partial t} = \frac{1}{2}\,\mathbf{u}_i^2(t,\mathbf{k}) - \frac{1}{2}\,\mathbf{u}_f^{+2}(t) = 0 \quad \rightarrow \quad t = t_r^+(\mathbf{k}). \tag{136}$$

We recall that $\mathbf{u}_f^+(t)$ is the incident velocity of an electron ionized at moment $t^+(t)$ and arriving for rescattering at moment t. So this equation is nothing but the energy conservation condition for the rescattering event and its solution $t_r^+(\mathbf{k})$ is the quantum counterpart of $t_r(\mathbf{k})$ defined by Eq. (133). The integration over Σ in Eq. (134) can be performed with the help of the relation [63]

$$e^{i\mathbf{k}\cdot\mathbf{r}}|_{r\to\infty} = \frac{2\pi}{ikr}\left[e^{ikr}\,\delta\left(\frac{\mathbf{r}}{r} - \frac{\mathbf{k}}{k}\right) - e^{-ikr}\,\delta\left(\frac{\mathbf{r}}{r} + \frac{\mathbf{k}}{k}\right)\right]. \tag{137}$$

The first term in the curly brackets vanishes at the SP, and we obtain

$$I_r(\mathbf{k}) = e^{i\pi/4}(2\pi)^{1/2}\sum_{ir}\frac{A_0(\mathbf{u}_{i\perp}^+(t_r^+);t_i^+)}{[(t_r^+ - t_i^+)^3 F(t_i^+) S_r^{+\prime\prime}]^{1/2}} \times f\left(\mathbf{u}_f^+(t_r^+), \frac{\mathbf{u}_i(t_r^+,\mathbf{k})}{u_i(t_r^+,\mathbf{k})}\right) \times \exp\left[iS_r^+(t_r^+,\mathbf{k}) - \frac{iu_{i\parallel}^{+3}(t_r^+)}{3F(t_i^+)}\right], \tag{138}$$

where

$$S_r^{+\prime\prime} = \left.\frac{\partial^2 S_r^+}{\partial t^2}\right|_{t=t_r^+} = \mathbf{F}(t_r^+)[\mathbf{u}_f^+(t_r^+) - \mathbf{u}_i(t_r^+,\mathbf{k})] + \frac{\mathbf{u}_f^{+2}(t_r^+)}{t_r^+ - t_i^+}. \tag{139}$$

Here $t_i^+ = t_i^+(t_r^+(\mathbf{k}))$ and $t_r^+ = t_r^+(\mathbf{k})$ are the quantum moments of ionization and rescattering defined by Eqs. (104) and (136), respectively. The summation in Eq. (138) runs over the different (for the same $\mathbf{k}$) solutions to Eqs. (104) and (136). Equation (138) gives the leading-order term in the asymptotics of $I_r(\mathbf{k})$. Since the moments t_i^+ and t_r^+ go deep into the complex plane as $\mathbf{k}$ leaves the set $\mathcal{K}_r$, $I_r(\mathbf{k})$ rapidly vanishes outside K_r. This asymptotics is uniform in terms of ξ and $\mathbf{k} \in K_r$. We note that the exact scattering state appears in Eq. (103) and, as a consequence, exact scattering amplitude appears in Eq. (138).

Let us return to the comment on the integration over the transverse momentum of an ionized electron made in a paragraph following Eq. (102). On the step from Eq. (99) to Eq. (103) this integral has been calculated using the steepest descent method. As a result, $I_r(\mathbf{k})$ given by Eq. (138) is proportional to the scattering amplitude $f(\mathbf{k},\mathbf{n})$ taken at appropriate values of its arguments. For potentials with the Coulomb tail, this amplitude diverges in the forward direction. This indicates that in the Coulomb case the integration in Eq. (99) should be performed differently.

Without further details, we give a simplified form of Eq. (138) similar to Eq. (132). Using Eq. (108), we obtain

$$I_r(\mathbf{k}) = e^{i\pi/4}(2\pi)^{1/2}\sum_{ir}\frac{A_0(\mathbf{u}_{i\perp}(t_r);t_i)}{[(t_r - t_i)^3 F(t_i) S_r^{\prime\prime}]^{1/2}} \times f\left(\mathbf{u}_f(t_r), \frac{\mathbf{u}_i(t_r,\mathbf{k})}{u_i(t_r,\mathbf{k})}\right)\exp\left[iS_r(t_r,\mathbf{k})\right], \tag{140}$$

where

$$S_r(t,\mathbf{k}) = \mathcal{S}(t,\mathbf{k}) - \mathcal{S}(t,t_i,\mathbf{u}_i(t)) - s_0(t_i), \tag{141}$$

and

$$S_r^{\prime\prime} = \left.\frac{\partial^2 S_r}{\partial t^2}\right|_{t=t_r} = \mathbf{F}(t_r)[\mathbf{u}_f(t_r) - \mathbf{u}_i(t_r,\mathbf{k})] + \frac{\mathbf{u}_f^2(t_r)}{t_r - t_i}. \tag{142}$$

Here $t_i = t_i(t_r(\mathbf{k}))$ and $t_r = t_r(\mathbf{k})$ are the classical moments of ionization and rescattering defined by Eqs. (85) and (133), respectively. Equation (140) does not hold in the regions of K_r where t_i lies near a zero of $F(t)$, while Eq. (140) holds uniformly in K_r.

VII. ILLUSTRATIVE CALCULATIONS

In this section we illustrate the theory by numerical calculations. Although the theory is developed for arbitrary polarization of laser field, here we consider only linearly polarized pulses; testing the theory against exact numerical solution of the TDSE for more general polarizations is much more laborious and left for future studies. The target potential used in the calculations is given by Eq. (47). The initial state is chosen to be the ground $1s$ state. We consider pulses with the Gaussian envelope,

$$\mathbf{F}(t) = F_0 e^{-\tau^2} f(\tau)\mathbf{e}_z, \quad \tau = 2t/T, \tag{143}$$

where $f(\tau)$ defines the internal shape of the pulse. In the LP case, only the z components of the velocity $\mathbf{v}(t)$ and coordinate $\mathbf{r}(t)$ for the reference trajectory defined by Eqs. (16) differ from zero, so it is convenient to slightly modify notation. Let $\mathbf{v}_\infty = v_\infty\mathbf{e}_z$, $\mathbf{k}_a(t) = k_a(t)\mathbf{e}_z$, and $\mathbf{k} = \mathbf{k}_\perp + k_z\mathbf{e}_z$. Because of spherical symmetry of the potential (47), the PEMD $P(\mathbf{k})$ does not depend on the orientation of $\mathbf{k}_\perp$ and is denoted by $P(k_\perp,k_z)$. The set $\mathcal{K}_a$ is an interval of the k_z axis of length $O(\epsilon^{-1})$ whose boundaries are denoted by $k_z^{\min}$ and $k_z^{\max}$. The set K_a is a neighborhood of $\mathcal{K}_a$ of size $O(\epsilon^0)$, as shown in Fig. 5.

We wish to clearly specify the role of the illustrative calculations in the present study. Our goal is to test the performance of the adiabatic theory and thus demonstrate its validity at a quantitative level rather than discuss some physical properties of the particular system under consideration or the corresponding spectra. We plan to turn to the analysis of various interesting features of PEMDs in the adiabatic regime on the basis of the present theory in future publications; in this work, we focus on establishing the theory. We therefore consider only simplest half- and one-cycle pulses, which is *necessary* and *sufficient* for testing the accuracy of the adiabatic and rescattering parts of the wave function (60) and ionization amplitude (120). The adiabatic parameter ϵ for the present pulse (143) is inversely proportional to T. Thus, our goal is to demonstrate that the adiabatic results converge to the exact ones as the pulse length T grows and this convergence is uniform with respect to the pulse amplitude F_0. The "exact" results reported below are obtained by solving Eq. (1) with the initial condition (7) and calculating the spectrum numerically using a program described in [64]. These results are fully converged with respect to all parameters of the numerical scheme. The maximum values of F_0 and T considered are limited by our computational resources available for the exact

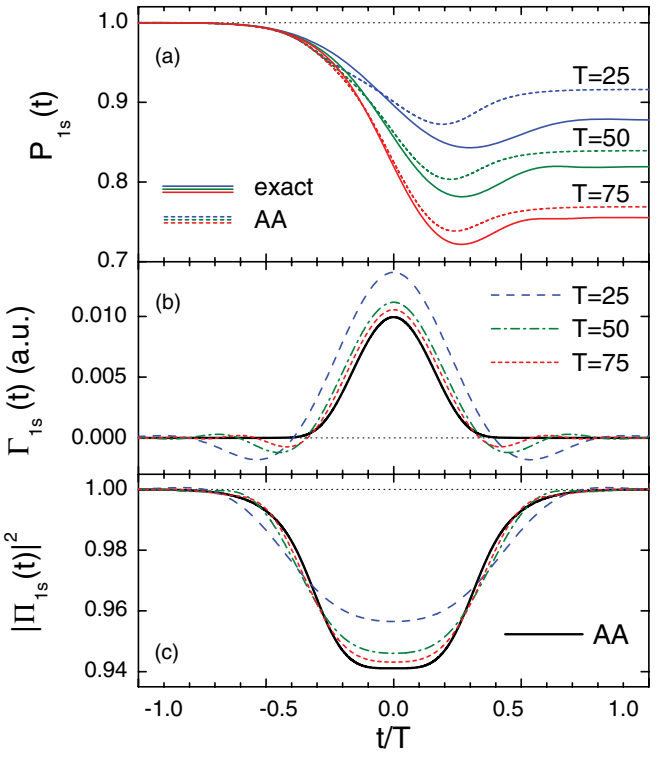

FIG. 6. (Color online) Exact results and adiabatic approximation (AA) for (a) time-dependent probability to survive in the initial $1s$ state, (b) ionization rate, and (c) projection factor for three half-cycle pulses [Eqs. (143) and (144)] with $F_0 = 0.1$. The adiabatic results in (a) are obtained from Eq. (110). The "exact" results in (b) and (c) are reconstructed from the exact $P_{1s}(t)$ using Eqs. (145).

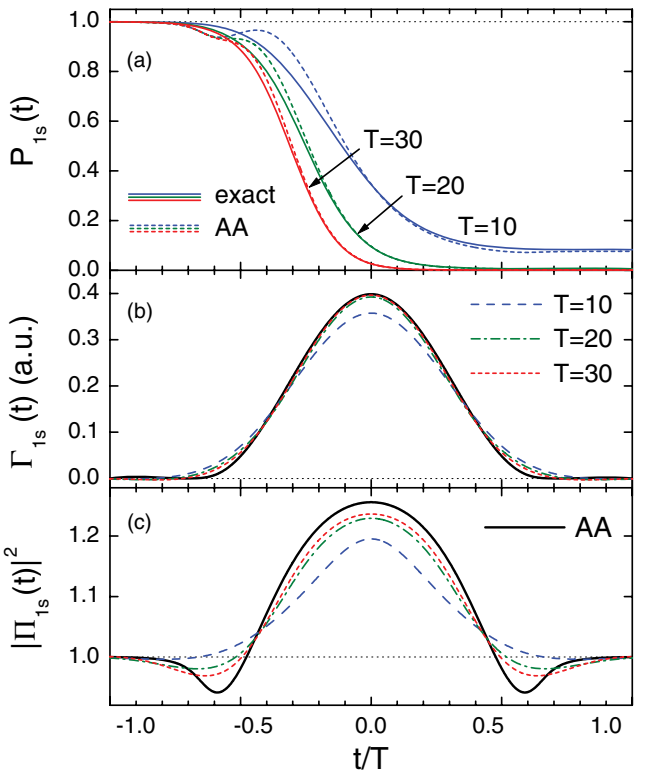

FIG. 7. (Color online) Same as in Fig. 6, but for $F_0 = 0.4$.

calculations. The adiabatic results are obtained by finding the SPs and implementing formulas (131) and (138), as prescribed in Secs. V and VI. The implementation of the adiabatic theory is restricted only by the ability of our program to calculate the SS [45] and can be extended to $F_0 \gtrsim 1$ and arbitrarily large T.

A. Half-cycle pulse: Testing the adiabatic part

The overall accuracy of the present theory is determined by that of the adiabatic parts of the wave function and ionization amplitude; the rescattering parts are derived from them. So our first goal is to scrutinize the quality of $\psi_a(\mathbf{r},t)$ and $I_a(\mathbf{k})$ given by Eqs. (63) and (131), respectively. To this end, we consider a half-cycle pulse with,

$$f(\tau) = -1. \tag{144}$$

The electric field $\mathbf{F}(t)$ in this case does not have zeros; hence, no rescattering occurs and $\psi_r(\mathbf{r},t) = I_r(\mathbf{k}) = 0$. Although this model for $\mathbf{F}(t)$ is far from realistic laser pulses, it is quite suitable for testing the performance of the adiabatic approximation. The dependence of the total probability of ionization of hydrogen by Gaussian pulses on the pulse length for rather weak amplitudes $F_0 \leqslant 0.06$ was analyzed in Ref. [65].

We consider two series of pulses with underbarrier, $F_0 = 0.1$, and overbarrier, $F_0 = 0.4$, amplitudes and growing length T. The characteristic time T_0 in this case coincides with T, so the onset of the adiabatic regime defined by $\epsilon = 1$ is $T = 4\pi$. To illustrate the quality of $\psi_a(\mathbf{r},t)$ as an approximate solution to Eq. (1), we consider the time-dependent probability to survive in the initial state $P_{1s}(t)$. The exact and adiabatic results for this function for pulses with $F_0 = 0.1$ and 0.4 are shown in Figs. 6(a) and 7(a), respectively. The final survival probabilities are given in Table I. For both values of F_0, the adiabatic results do converge to the exact ones as T grows, and for the stronger field this convergence is faster, in accordance with condition (13).

The behavior of $P_{1s}(t)$ shown in Figs. 6(a) and 7(a) deserves a more detailed discussion. In simple models of tunneling ionization it is generally believed that the time-dependent survival probability is given by Eq. (110) with the preexponential factor omitted. This would result in a monotonic decay of $P_0(t)$ with time. However, as is seen from Fig. 6(a),

TABLE I. Probability to survive in the initial $1s$ state. The results of the adiabatic approximation (AA) are obtained from Eq. (111). $a[b] = a \times 10^b$.

$F_0 = 0.1$			$F_0 = 0.4$		
T	Exact	AA	T	Exact	AA
			Half-cycle pulses		
25	0.878	0.916	10	0.834[−1]	0.765[−1]
50	0.819	0.839	20	0.602[−2]	0.585[−2]
75	0.755	0.769	30	0.452[−3]	0.448[−3]
			One-cycle pulses		
50	0.729	0.783	20	0.770[−3]	0.900[−3]
75	0.656	0.693	30	0.229[−4]	0.270[−4]
100	0.587	0.613	40	0.691[−6]	0.810[−6]

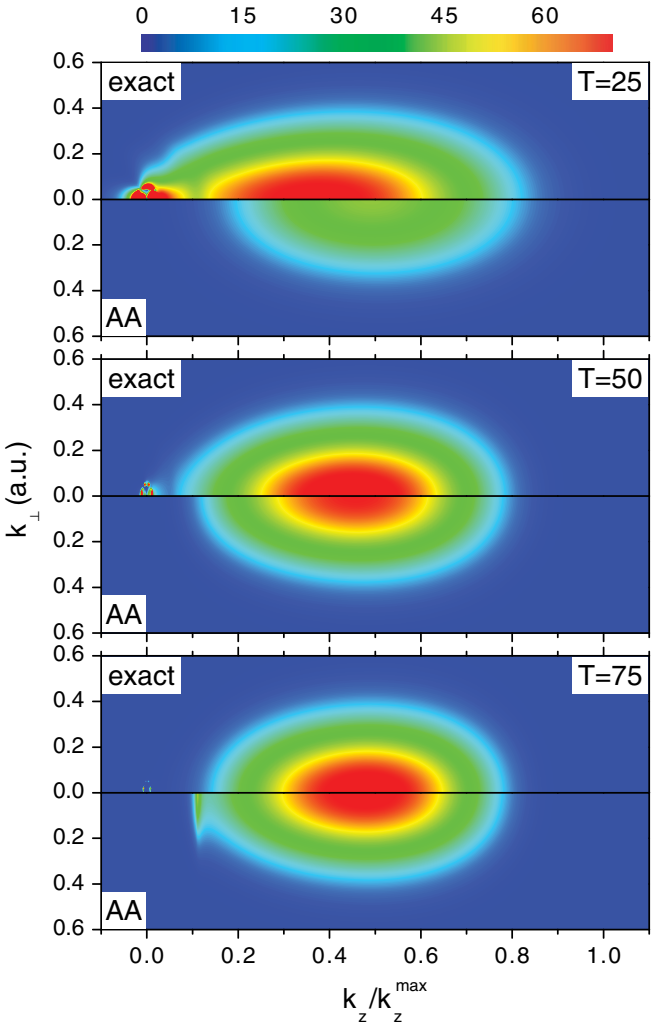

FIG. 8. (Color online) Exact results and adiabatic approximation (AA) for PEMDs $P(k_\perp,k_z)$ produced by three half-cycle pulses with $F_0 = 0.1$ (see Fig. 6). The upper classical boundaries of the PEMD $k_z^{\max}$ for these pulses are 2.22, 4.43, and 6.65, respectively.

there are situations when function $P_{1s}(t)$ is nonmonotonic. A similar nonmonotonic behavior of the ionization yield related to the survival probability by unitarity was observed experimentally [66]. Such a behavior in the adiabatic regime cannot be explained without invoking the preexponential factor in Eq. (110). A remarkable property of Eq. (110) is that this equation enables one to *reconstruct* the ionization rate $\Gamma_0(t)$ and projection factor $|\Pi_0(t)|^2$ from $P_0(t)$. Indeed, for the present pulse $F(t) = F(-t)$, so both $\Gamma_0(t)$ and $|\Pi_0(t)|^2$ are even functions of t. Then they can be found from the even and odd parts of the logarithmic derivative of $P_0(t)$, respectively,

$$\Gamma_0(t) = -\frac{1}{2}\left[\frac{\dot{P}_0(-t)}{P_0(-t)} + \frac{\dot{P}_0(t)}{P_0(t)}\right], \tag{145a}$$

$$|\Pi_0(t)|^2 = \sqrt{\frac{P_0(-t)P_0(t)}{P_0}}. \tag{145b}$$

Assuming that the exact $P_{1s}(t)$ has the form (110) and using Eqs. (145), we can reconstruct the corresponding "exact" $\Gamma_{1s}(t)$ and $|\Pi_{1s}(t)|^2$; the results are shown in the bottom two

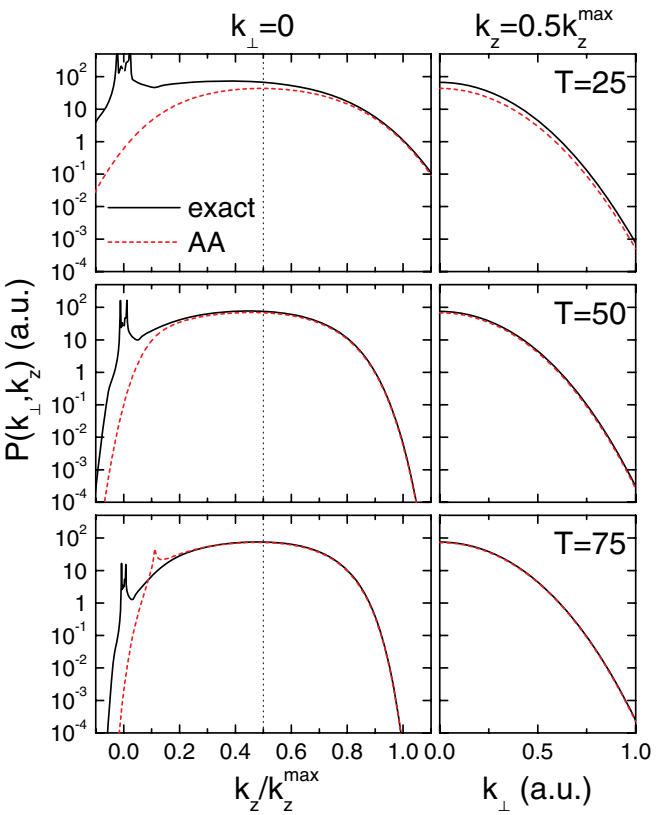

FIG. 9. (Color online) The cuts of $P(k_\perp,k_z)$ shown in Fig. 8 at $k_\perp = 0$ (left) and $k_z = 0.5k_z^{\max}$ (right). All panels have the same vertical scale.

panels in Figs. 6 and 7. In the adiabatic approximation, these functions for a given F_0 depend only on the ratio t/T, so the adiabatic results in Figs. 6 and 7 for all three pulses are represented by the same curves. One can see that the reconstructed "exact" results converge to the adiabatic ones as T grows. Their comparison with the predictions of the adiabatic theory provides a much more stringent test of the accuracy of $\psi_a(\mathbf{r},t)$ than the comparison of $P_{1s}(t)$ alone. The behavior of $\Gamma_{1s}(t)$ and $|\Pi_{1s}(t)|^2$ in Figs. 6 and 7 is explained by the properties of the SS shown in Figs. 2(b) and 2(c). We note that while the ionization rate is a standard and commonly used characteristic, the projection factor in Eq. (110) is a more subtle quantity. For $F_0 = 0.1$ its effect on $P_{1s}(t)$ is within 6%, but for $F_0 = 0.4$ replacing this factor by unity would cause a more considerable error of 25%. Thus, not only $\Gamma_{1s}(t)$ defined by the SS eigenvalue, but also $|\Pi_{1s}(t)|^2$ defined by its eigenfunction can be extracted from the observable $P_{1s}(t)$. We emphasize that this is true also in the overbarrier regime, when the SS does not seem to have any physical meaning as an individual state. Equations (145) hold for any even $F(t)$, for spherically symmetric potentials (atoms), and even $\mathbf{F}(t)$, for general potentials (molecules). The reconstructed functions $\Gamma_0(t)$ and $|\Pi_0(t)|^2$ present an additional with respect to $P_0(t)$ information on the ionization dynamics, which may be found useful in applications. For example, Eqs. (145) were used in Ref. [67] for the analysis of tunneling ionization dynamics of a model diatomic molecule.

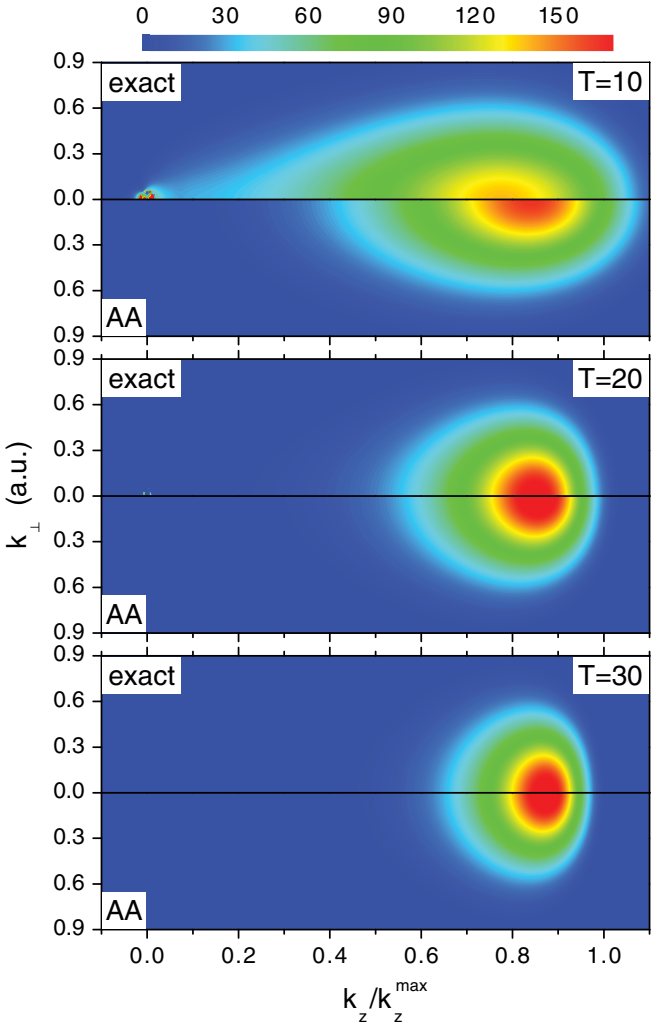

FIG. 10. (Color online) Same as in Fig. 8, but for half-cycle pulses with $F_0 = 0.4$ (see Fig. 7). The values of $k_z^{\max}$ for these pulses are 3.54, 7.09, and 10.63, respectively.

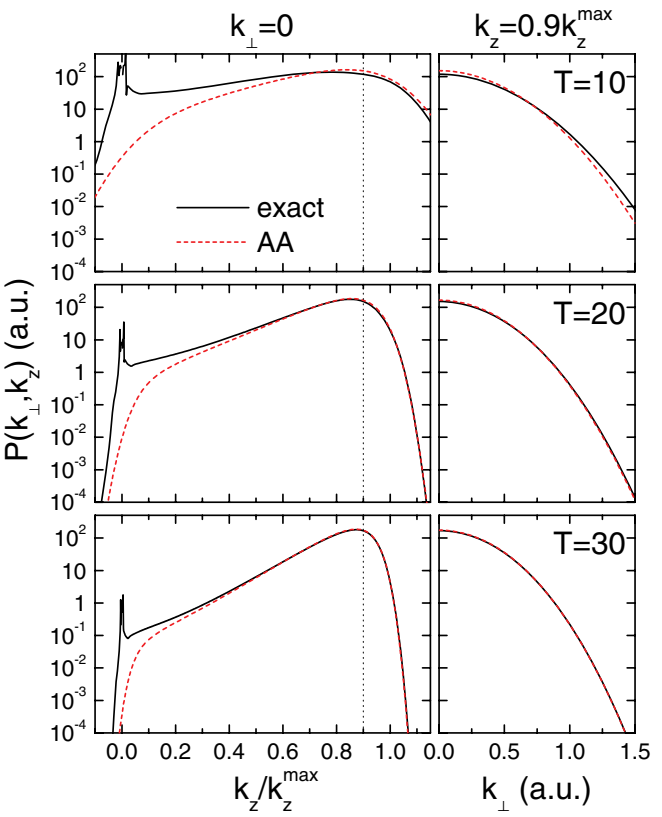

FIG. 11. (Color online) The cuts of $P(k_\perp,k_z)$ shown in Fig. 10 at $k_\perp = 0$ (left) and $k_z = 0.9k_z^{\max}$ (right). All panels have the same vertical scale.

The PEMDs for the same pulses are shown in Figs. 8–11. Figures 8 and 10 present 2D distributions $P(k_\perp,k_z)$ for $F = 0.1$ and 0.4, respectively; Figs. 9 and 11 show their cuts at $k_\perp = 0$ and some value of k_z near the maximum of $P(k_\perp,k_z)$. The adiabatic results are obtained from Eq. (131), where the moment of ionization $t_i^+(\mathbf{k})$ is found by solving Eq. (128). For the present pulse shape, $k_a(t)$ monotonically decreases from $v_\infty = \frac{\sqrt{\pi}}{2} F_0 T$, at $t \to -\infty$, to 0, at $t \to \infty$, so $\mathcal{K}_a$ consists of a single segment bounded by $k_z^{\min} = 0$ and $k_z^{\max} = v_\infty$, which are the classical boundaries of the PEMD. The PEMDs are shown in a region corresponding to K_a. For each $\mathbf{k}$ in this region, there is only one solution to Eq. (128), and hence only one term in Eq. (131).

Let us first focus on the differences between the adiabatic and exact results. The first feature to be noticed is the d resonance mentioned in Sec. III and seen in Fig. 4. This resonance state reveals itself in exact spectra near $\mathbf{k} = \mathbf{0}$. Its excitation proceeds via a nonadiabatic transition [60–62], so its contribution to the spectrum rapidly decreases as T grows. This excitation mechanism is not (but can be) accounted for by the present theory. Another difference stems from a feature seen in the adiabatic results for $F = 0.1$ and $T = 75$ near $k_z = 0.1k_z^{\max}$. This feature arises from a branch point of the function $E_{1s}(F)$ encountered by the moment of ionization $t_i^+(\mathbf{k})$ in complex time plane as $\mathbf{k}$ varies within K_a. Such branch points provide a path to excitation. As T grows further, $t_i^+(\mathbf{k})$ passes closer to the real axis, the branch point is not encountered anymore, and the feature indicated disappears. These two features are peculiar to the present atomic model. The main difference is localized near $\mathbf{k} = \mathbf{0}$, as can be seen from the cuts shown in Figs. 9 and 11. This part of the spectra corresponds to electrons ionized by the tail of the pulse. The difference here decreases as T grows, but very slowly. The failure of the adiabatic approximation in this case seems to have a general origin; a similar difference was observed in I.

Apart from these rather minor differences, it is clear that the agreement between the adiabatic and exact results in Figs. 8–11 rapidly improves as T grows. For the longest pulses considered, the agreement (excluding the region near $\mathbf{k} = \mathbf{0}$) is virtually perfect. This is true for both pulse amplitudes, including the overbarrier case, when almost complete ionization occurs (see Table I). Again, for the stronger field a good agreement is achieved at smaller T, in accordance with Eq. (13). The results shown in Figs. 8–11 establish the validity of Eq. (131). It is worth noting that they are very far from the predictions of the first-order perturbation theory: The spectrum in this approximation is an even function of k_z, which is obviously not the case. We also note that the Keldysh approximation [Eq. (B2)] does not account for depletion of the

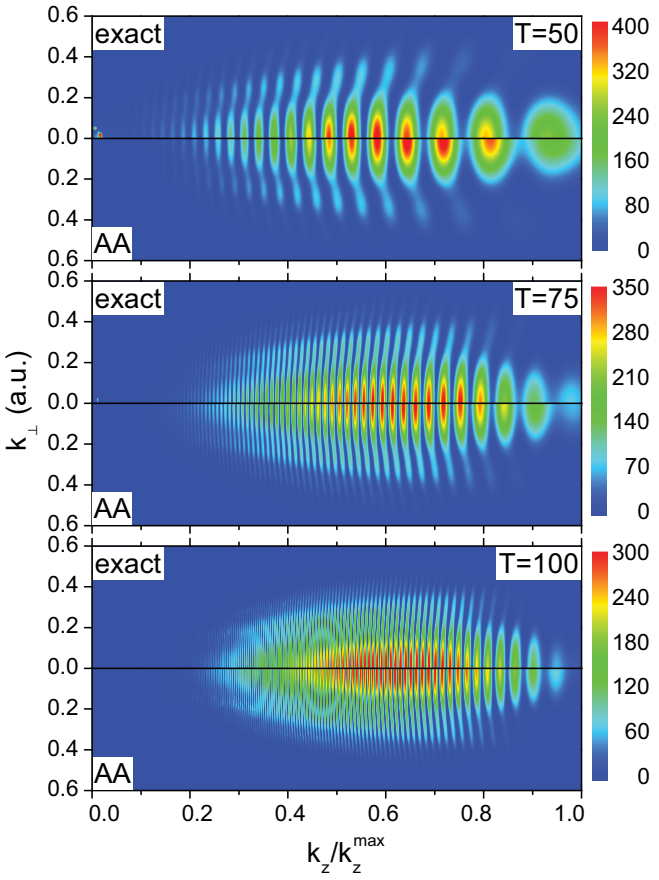

FIG. 12. (Color online) Exact results and adiabatic approximation (AA) for PEMDs $P(k_\perp,k_z)$ produced by three one-cycle pulses [Eqs. (143) and (146)] with $F_0 = 0.1$. The values of $k_z^{\max}$ for these pulses are 2.91, 4.37, and 5.83, respectively.

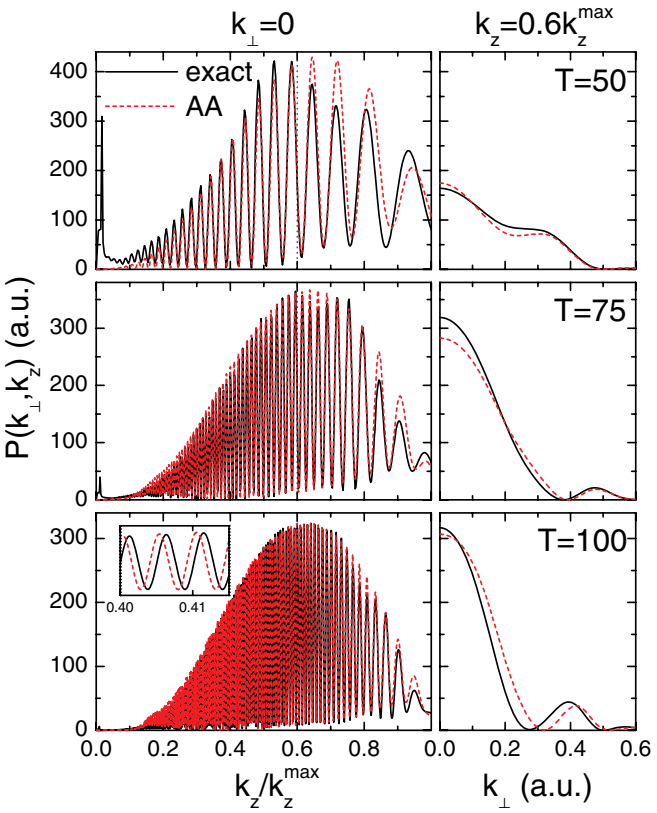

FIG. 13. (Color online) The cuts of $P(k_\perp,k_z)$ shown in Fig. 12 at $k_\perp = 0$ (left) and $k_z = 0.6k_z^{\max}$ (right).

initial state and hence fails qualitatively for sufficiently large F_0 and T, as demonstrated in I.

Figures 8–11 illustrate the quantitative performance of the adiabatic theory. To close this section, let us give an example of a qualitative analysis of PEMDs which can be done on the basis of this theory. For the present pulse, there is only one contribution to $I_a(\mathbf{k})$ for each $\mathbf{k} \in K_a$, so there is a one-to-one correspondence between photoelectron momentum $\mathbf{k}$ and the moment of ionization $t_i^+(\mathbf{k})$. In this case, $P(k_\perp,k_z)$ is a smooth function exhibiting no interference structure. The PEMDs are localized in the region K_a, as predicted. The vanishing of $P(k_\perp,k_z)$ near the classical boundaries of K_a results from smaller values of $F(t)$ at the moment of ionization, and hence smaller ionization rate $\Gamma_{1s}(t)$ (see Figs. 6 and 7). For the weaker field, depletion is not very important. The distributions $P(k_\perp,k_z)$ in this case are more or less symmetric with respect to the center of $\mathcal{K}_a$, which results from the evenness of $F(t)$. For the stronger field, the PEMDs are localized near the upper boundary $k_z^{\max}$ of K_a. This is explained by depletion: Almost complete ionization occurs on the rising part of the pulse, which contributes to the region near $k_z^{\max}$. The dependence of $P(k_\perp,k_z)$ on $k_\perp$ essentially reproduces the shape of the TMD, see Fig. 3, for F equal to the value of $F(t)$ at the moment of ionization. This explains why PEMDs for the stronger field are broader in the transverse direction.

B. One-cycle pulse: Testing the rescattering part

In the LP case, rescattering appears only after the electric field $\mathbf{F}(t)$ passes through a zero. Each zero of $f(\tau)$ in Eq. (143) leads to the appearance of new CRTs, and each such CRT produces a contribution to the rescattering part $I_r(\mathbf{k})$ of the ionization amplitude. To be able to focus on a single CRT and its individual contribution to the PEMD, we consider a one-cycle pulse with only one zero of $f(\tau)$ defied by

$$f(\tau) = -\sqrt{2e}\,\tau. \tag{146}$$

The coefficient here is chosen to satisfy $\max_t F(t) = F_0$. For this pulse $v_\infty = 0$, $k_z^{\min} = 0$, and $k_z^{\max} = \sqrt{2e}F_0T/4$. Function $k_a(t)$ traces the set $\mathcal{K}_a$ twice, once per each half-cycle. Hence, there are two contributions to $I_a(\mathbf{k})$ originating from each of the two half-cycles and given by Eq. (131). The moments of ionization $t_i^+(t_r^+(\mathbf{k}))$ and rescattering $t_r^+(\mathbf{k})$ needed to implement Eq. (138) are found by solving Eqs. (104) and (136). These equations have solutions describing rescattering trajectories originating only in the first half-cycle. There are two such trajectories for each $\mathbf{k} \in K_r$. In a smaller region $K_a \in K_r$, they correspond to rescattering in almost forward and backward directions, respectively. The contribution from the backward rescattering trajectory to $I_r(\mathbf{k})$ is suppressed by small values of the scattering amplitude (see Fig. 4). Thus, focusing on the region K_a enables us to retain only the forward rescattering trajectory and, hence, to single out the only contribution to $I_r(\mathbf{k})$ to be tested. In the following, we restrict our consideration of PEMDs to the region K_a.

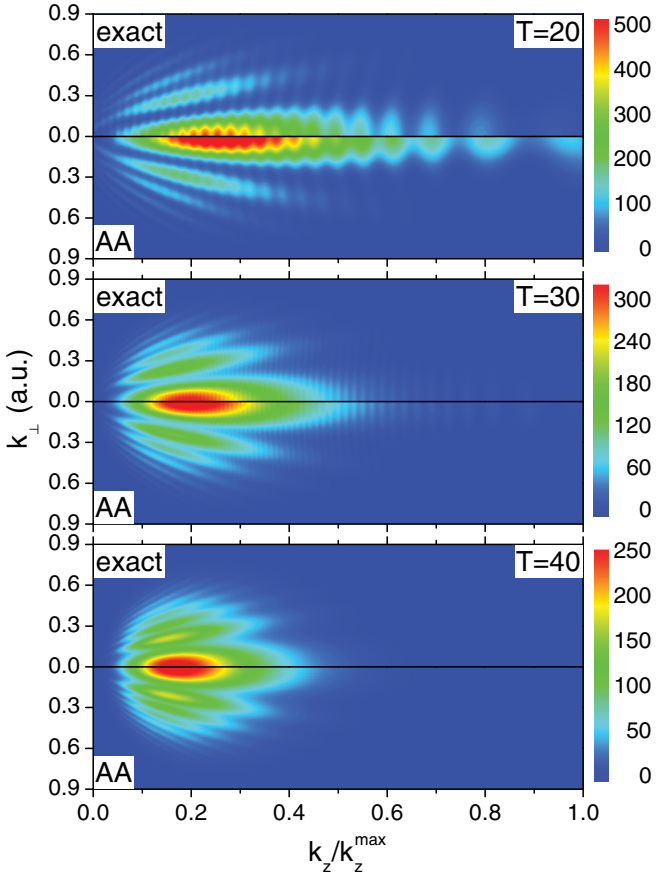

FIG. 14. (Color online) Same as in Fig. 12, but for $F_0 = 0.4$. The values of $k_z^{\max}$ for these pulses are 4.66, 6.99, and 9.33, respectively.

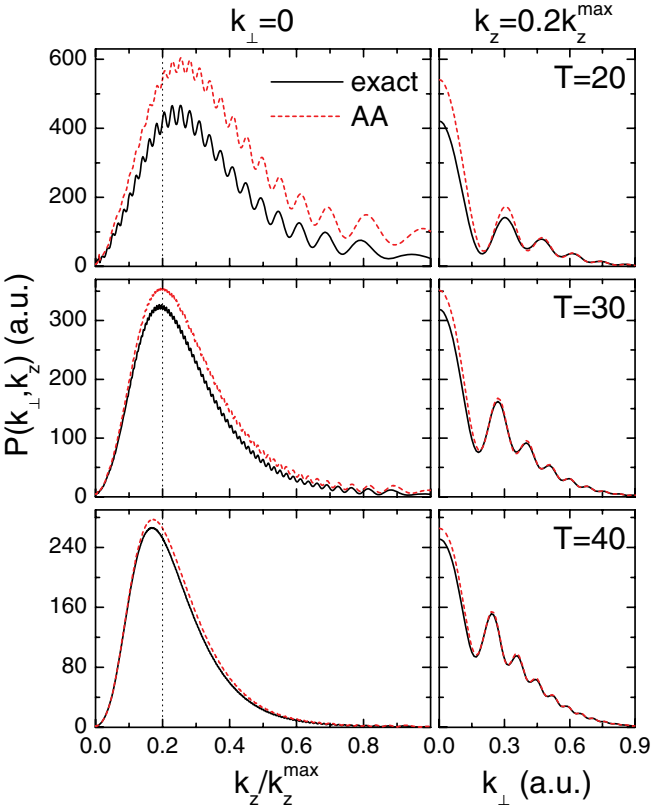

FIG. 15. (Color online) The cuts of $P(k_\perp,k_z)$ shown in Fig. 14 at $k_\perp = 0$ (left) and $k_z = 0.2k_z^{\max}$ (right).

We again consider two series of pulses with $F_0 = 0.1$ and 0.4 and growing length T. The characteristic time T_0 in this case estimated as the duration of each of the two half-cycles coincides with T, so the onset of the adiabatic regime remains the same. The probabilities to survive in the initial state are given in Table I. For $F_0 = 0.1$, the relative error of the adiabatic results decreases as T grows, as it should, but for $F_0 = 0.4$ it does not change and remains on the level of 17% for all three pulses considered. Given very small values of the survival probabilities in this case, it is difficult to say whether the difference comes from an imperfection of our numerical calculations or results from some physical mechanism, such as excitation, not accounted for by the present theory.

The PEMDs for these pulses are shown in Figs. 12–15. Figures 12 and 14 present 2D distributions $P(k_\perp,k_z)$ for $F = 0.1$ and 0.4, respectively, and Figs. 13 and 15 show their cuts. Note that the cuts are now plotted in a linear scale. The agreement between the exact and adiabatic results rapidly improves as T grows, and for the stronger field the convergence is faster, as predicted. For the longest pulses considered, the agreement is very good. There remains a small difference in the amplitude and a tiny phase shift between the interference fringes (see the insert for $T = 100$ in Fig. 13), which should disappear as T grows further. However, even the level of accuracy already achieved is certainly sufficient for the majority of applications. We note that the present pulse can be approximated by one cycle of a monochromatic field with period $2T$, so $T = 50$, for example, corresponds to the wavelength of 800 nm. Since the adiabatic part of the ionization amplitude has been already tested, these results establish the validity of Eq. (138) defining the rescattering part. Because of the existence of several different contributions to the ionization amplitude, the PEMDs in the present case exhibit rich interference structures. Similar structures were recently observed experimentally [68]. Their analysis on the basis of the adiabatic theory will be presented elsewhere.

VIII. SUMMARY AND PERSPECTIVES

In this paper, the adiabatic theory of ionization of an electron, initially bound in a potential well, by an intense low-frequency laser pulse in the 3D case is developed. The theory is developed for arbitrary time dependence and polarization of the laser field and arbitrary (without any symmetry) finite range potential. The asymptotics of the solution of the TDSE and PEMD for $\epsilon \to 0$ are obtained. The main results are given by the asymptotics of the adiabatic [Eq. (63)] and rescattering [Eq. (103)] parts of the wave function and the corresponding adiabatic [Eq. (131)] and rescattering [Eq. (138)] parts of the ionization amplitude. These asymptotics are expressed in terms of the SS originating from the initial bound state in the presence of an external static electric field and scattering states in the unperturbed target potential. They are uniform in terms of ξ, that is, they apply to weak underbarrier as well as strong overbarrier fields and hold in the adiabatic regime defined by Eq. (13). In comparison with the Keldysh theory [11,12] and the strong-field approximation [13–15], the adiabatic theory

is based on different physical assumptions and has a different region of applicability (see Sec. II B), so the two approaches are complimentary. The Keldysh approximation [11] is shown to emerge in the weak-field limit of the adiabatic theory.

The target potential may have arbitrary shape and hence can model an atom or a molecule in the single-active-electron approximation. The only limitation of the present formulation of the theory stems from the assumption that the potential has no Coulomb tail. The generalization to potentials with a Coulomb tail is the most important direction for further development of the theory.

In terms of applications, it should be emphasized that the adiabatic theory does not deal with one particular phenomenon, like photoionization, but can treat all kinds of phenomena in the adiabatic regime. The calculations presented in this work are aimed only at validating the theory. They can be extended to realistic few-cycle pulses and to the entire region of localization of the photoelectron spectrum, including the backward rescattering ridge [9,10]. The adiabatic theory can be used to calculate and analyze spectra produced by pulses with the wavelength, amplitude, and polarization beyond the capability of current computational resources to solve the TDSE. The excitation of other bound and resonance states via nonadiabatic transitions [60–62] also can be included into the theory. Finally, the adiabatic asymptotics of the high-order harmonic spectrum can be obtained on the basis of the present theory, as it was demonstrated for the 1D ZRP model in Ref. [69]. All these extensions and applications of the theory are subjects for future studies.

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APPENDIX A: FORMAL DERIVATION OF THE ADIABATIC APPROXIMATION

The derivation of the adiabatic part of the wave function in Sec. V B is specific to the present problem and may seem to be essentially based on the knowledge of the exact Green's function (32). To emphasize the generality of the result (63), it is instructive to reproduce the derivation in more general operator form. We begin with the time-dependent retarded Green's function defined by

$$\left[i\frac{\partial}{\partial t} - H(\epsilon t)\right] G(t,t') = \delta(t-t'), \quad G(t,t')|_{t<t'} = 0, \quad \text{(A1)}$$

where the operators $H(\epsilon t)$ and $G(t,t')$ are understood as matrices with discrete or continuous indices representing spatial coordinates, and we have explicitly introduced the adiabatic parameter $\epsilon \to 0$. Let us introduce new time variables,

$$T = t - t', \quad \tau = \epsilon t. \quad \text{(A2)}$$

In terms of these variables Eq. (A1) reads

$$\left[i\epsilon\frac{\partial}{\partial \tau} + i\frac{\partial}{\partial T} - H(\tau)\right] G(T,\tau) = \delta(T), \quad G(T,\tau)|_{T<0} = 0. \quad \text{(A3)}$$

Substituting

$$G(T,\tau) = \int G(E,\tau) e^{-iET}\frac{dE}{2\pi}, \quad \text{(A4)}$$

we obtain

$$\left[i\epsilon\frac{\partial}{\partial \tau} + E - H(\tau)\right] G(E,\tau) = 1. \quad \text{(A5)}$$

We seek the solution in the form of the expansion

$$G(E,\tau) = \sum_{n=0}^{\infty} \epsilon^n G^{(n)}(E;\tau). \quad \text{(A6)}$$

In the zeroth order we find

$$G^{(0)}(E;\tau) = [E - H(\tau) + i0]^{-1}. \quad \text{(A7)}$$

This is the stationary outgoing-wave Green's function for the Hamiltonian $H(\tau)$; it depends on slow time τ as a parameter. It can be readily seen that

$$G^{(n)}(E;\tau) = \left[-iG^{(0)}(E;\tau)\frac{\partial}{\partial \tau}\right]^n G^{(0)}(E;\tau) \quad \text{(A8)}$$

and

$$G(E,\tau) = \left[1 + i\epsilon G^{(0)}(E;\tau)\frac{\partial}{\partial \tau}\right]^{-1} G^{(0)}(E;\tau). \quad \text{(A9)}$$

Let us now consider a nonstationary problem associated with Eq. (A1),

$$\left[i\frac{\partial}{\partial t} - H(\epsilon t) - V\right]\psi(t) = 0, \quad \text{(A10)}$$

where the operator V does not depend on time and $\psi(t)$ is understood as a column vector. We refrain from using Dirac's notation because $\langle\psi(t)|$ means transpose *and* complex conjugate of $|\psi(t)\rangle$, while we will never need complex conjugation. We assume that $H(\epsilon t)$ becomes independent of time for $t \to -\infty$, and

$$\psi(t)|_{t\to-\infty} = \phi_0 e^{-iE_0 t}, \quad \text{(A11)}$$

where E_0 and ϕ_0 are the eigenvalue and eigenvector corresponding to one of the bound states of the initial Hamiltonian $H(-\infty) + V$. Equation (A10) with the initial condition (A11) is equivalent to

$$\psi(t) = \int G(t,t')V\psi(t')\,dt'. \quad \text{(A12)}$$

We seek the solution in the form

$$\psi(t) = \phi_0(\tau)\exp\left[-\frac{i}{\epsilon}\left(E_0\tau + \int_{-\infty}^{\tau}[E_0(\tau') - E_0]d\tau'\right)\right], \quad \text{(A13)}$$

where $\tau = \epsilon t$ [see Eqs. (A2)] and the functions $E_0(\tau)$ and $\phi_0(\tau)$ are to be found. The equation for $\phi_0(\tau)$ reads

$$\phi_0(\tau) = \int G(T,\tau)\exp\left[\frac{i}{\epsilon}\int_{\tau-\epsilon T}^{\tau} E_0(\tau')\,d\tau'\right] \times V\phi_0(\tau - \epsilon T)\,dT. \quad \text{(A14)}$$

Substituting here

$$\phi_0(\tau) = \sum_{n=0}^{\infty}\epsilon^n\phi_0^{(n)}(\tau), \quad \text{(A15)}$$

and expanding the right-hand side in powers of ϵ using Eq. (A6), in the zeroth order we obtain

$$\phi_0^{(0)}(\tau) = G^{(0)}(E_0(\tau);\tau)V\phi_0^{(0)}(\tau). \tag{A16}$$

Thus, $\phi_0^{(0)}(\tau)$ is an eigenvector of the momentary Hamiltonian $H(\tau)+V$ satisfying outgoing-wave boundary conditions and $E_0(\tau)$ is the corresponding eigenvalue; in other words, the solution of Eq. (A16) is an adiabatic SS. This state depends on slow time τ as a parameter. In order to satisfy Eq. (A11) we require $E_0(-\infty)=E_0$ and $\phi_0^{(0)}(-\infty)=\phi_0$, which means that the SS of interest is the one that coincides with the initial bound state for $\tau\to-\infty$. This explains the subscript 0 in notation $\phi_0(\tau)$ and $E_0(\tau)$. Note that at this stage of the derivation the normalization of $\phi_0^{(0)}(\tau)$ remains undefined. In the first order we obtain

$$\begin{aligned}&\left[\left(G^{(1)}(E;\tau)+\frac{i}{2}\,\dot{E}_0(\tau)\frac{\partial^2 G^{(0)}(E;\tau)}{\partial E^2}\right)V\phi_0^{(0)}(\tau)\right.\\&\qquad\left.+i\,\frac{\partial G^{(0)}(E;\tau)}{\partial E}\,V\dot{\phi}_0^{(0)}(\tau)\right]_{E=E_0(\tau)}\\&\quad=[1-G^{(0)}(E_0(\tau);\tau)V]\phi_0^{(1)}(\tau),\end{aligned} \tag{A17}$$

where the dots denote differentiation with respect to τ. Multiplying this equation from the left by $\phi_0^{(0)T}(\tau)V$, where the superscript T stands for transpose, and using Eqs. (A8), (A16), and the relation

$$\frac{\partial G^{(0)}(E;\tau)}{\partial E} = -[G^{(0)}(E;\tau)]^2, \tag{A18}$$

which follows from Hilbert's identity [63],

$$G^{(0)}(E;\tau)G^{(0)}(E';\tau) = -\frac{G^{(0)}(E;\tau)-G^{(0)}(E';\tau)}{E-E'}, \tag{A19}$$

one can see that Eq. (A17) reduces to

$$\frac{d}{d\tau}\left[\phi_0^{(0)T}(\tau)\phi_0^{(0)}(\tau)\right]=0. \tag{A20}$$

The expression in the square brackets is the norm of the adiabatic SS, and the equation means that this norm should not depend on τ and hence should coincide with the norm $\phi_0^T\phi_0$ of the initial bound state. Equation (A20) completes the derivation of $\phi_0^{(0)}(\tau)$. We can proceed to higher-order terms in the expansion (A15). For example, from Eq. (A17) we find

$$\phi_0^{(1)}(\tau) = -i\mathcal{G}(E_0(\tau);\tau)\,\frac{\partial}{\partial\tau}\,\phi_0^{(0)}(\tau), \tag{A21}$$

where

$$\mathcal{G}(E;\tau) = [E-H(\tau)-V+i0]^{-1}. \tag{A22}$$

Equation (A21) can be also obtained by substituting Eqs. (A13) and (A15) into Eq. (A10).

In the application of this procedure to the laser-atom interaction problem, $H(\epsilon t)$ is the Hamiltonian in Eq. (1) with the potential energy term dropped, and V is the potential. In this case, Eq. (A13) reproduces the result (63) obtained in Sec. V B. The present derivation is more general. In particular, it does not rely on the explicit form of $G(t,t')$. In addition, it does not impose any restrictions on the potential V, provided that the SSs for the momentary Hamiltonian $H(\tau)+V$ exist, and hence applies also to potentials with the Coulomb tail [45]. Another advantage is that it very clearly exhibits the role of SSs in the development of the adiabatic approximation. At the same time, this derivation is only formal, because it does not specify the region of validity of the expansion (A15) which for the present problem is defined by Eq. (13).

APPENDIX B: THE KELDYSH APPROXIMATION

Substituting into Eq. (116) the unperturbed initial state [see Eq. (7)]

$$\psi_{\rm K}(\mathbf{r},t) = \phi_0(\mathbf{r})e^{-iE_0t} \tag{B1}$$

for the exact solution of Eq. (1) and integrating by parts, one obtains

$$I_{\rm K}(\mathbf{k}) = -i\int_{-\infty}^{\infty}dt\int\Phi^*(\mathbf{r},t;\mathbf{k})\mathbf{F}(t)\mathbf{r}\psi_{\rm K}(\mathbf{r},t)\,d\mathbf{r}. \tag{B2}$$

This formula is the starting point of the Keldysh theory [11]. It looks as if one had substituted the Volkov state (35) for the final state in the first-order time-dependent perturbation theory transition amplitude [52]. In contrast to Eqs. (113), (116), and (117), which are exact, Eq. (B2) is an approximation. As far as we know, the region of validity of this approximation has never been clearly defined.

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