Reexamination of the improved strong-field approximation: Low-energy structures in the above-threshold-ionization spectra for short-range potentials

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The improved strong-field approximation (ISFA) is a version of the strong-field approximation which takes into account an additional interaction of the ionized electron with the parent ion within the first Born approximation. The ISFA describes well the middle- and high-energy parts of the electron spectra in the above-threshold ionization process. We show, using an example of a short-range potential, that the ISFA is able to describe the low-energy structure in the energy spectra if it is calculated without additional approximations. We introduce two different forms of the T-matrix element which are appropriate for application of two widely used approximations: the saddle-point approximation [i.e., its more advanced version, the uniform approximation (UA)] and the pole approximation (PA). We show that both the PA and UA are not able to describe the low-energy structure. Furthermore, the UA describes better the plateau of the spectrum than the PA. We also identify the origin of a very-low-energy structure; it is connected to the laser-free (i.e., without exchange of the laser photons) electron forward scattering.

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I. INTRODUCTION

The progress of laser technology has enabled the discovery of new nonperturbative quantum-mechanical phenomena appearing during the interaction of intense ultrashort laser pulses with atoms and molecules (see, for example, recent review articles [1–4]). One such phenomenon is above-threshold ionization (ATI) in which the ionized electron absorbs more photons than the minimum number necessary for ionization. This process was observed in 1979 [5]. Approximative theoretical approaches to ionization by strong fields had been developed much earlier. The so-called strong-field approximation (SFA) was originally formulated in 1964 [6] (see also [7]). According to this theory, once the electron has entered the continuum it only feels the laser field and not the atomic binding potential. It is described by the so-called Gordon-Volkov state [8] (the state of the free electron in the laser field which is known in analytical form). Having in mind the seminal contributions of other authors, this theory is sometimes called the Keldysh-Faisal-Reiss (KFR) approximation [6,9,10]. For a further development of the SFA-based theories see the review articles [11–15].

The process of high-order above-threshold ionization (HATI) was discovered in 1990s [16]. Semiclassically, it is described as a three-step process [17–19]. After the ATI (the first step) the ionized electron, in the second step, moves in the laser field and may return to the parent core and scatters off it (the third step). It was suggested to exploit this rescattering process as an ultrafast imaging technique, which is called laser-induced electron diffraction [20–22]. From the angle-resolved HATI spectra the differential cross section for electron-atomic ion [23] and electron-molecular ion [24] scattering was extracted. More recently, the so-called photoelectron holography was considered in Refs. [25,26].

The discovery of the HATI process has further stimulated the development of theory. The SFA theory was first generalized to approximately include the interaction with the binding potential. This has been done in a fashion of a Born series whose zeroth-order term yields the direct ATI (described by the KFR matrix element), while the term of the first order in the binding potential describes rescattering of the ionized electron off the parent core; this is the so-called improved SFA (ISFA) [27–30]. Further generalizations of the ISFA which treat more realistically (i.e., beyond the second Born approximation) the rescattering matrix element were introduced in Refs. [31–33].

Using the (I)SFA most of the strong-field processes were successfully explained [12]. However, a few years ago, in ATI experiments with long-wavelength lasers, an unexpected structure in the low-energy part of the spectrum was discovered [34,35]. It was not possible to explain this low-energy structure (LES) using the SFA and this came as a "ionization surprise" [36]. During the last four years many efforts have been made to explain this structure. The LES was reproduced by calculating the spectra using the solution of the time-dependent Schrödinger equation [34,37–40] and classical and semiclassical methods [35,41–44]. For a recent review see Sec. 4 in Ref. [2]. We will mention here some more recent publications. In Ref. [45] the very-low-energy structure (VLES) (observed in [35]) was further analyzed and related to the influence of the long-range Coulomb potential. The classical-quantum correspondence for midinfrared pulse-driven electronic dynamics was explored in Ref. [46]. Finally, in Ref. [47], in addition to the experimental results, an ISFA-based calculation in which the divergence caused by the Coulomb rescattering is removed by adding the depletion rate of the ground state in the energy denominator was presented.

A good agreement of theory and experiment, demonstrated in Ref. [47], has motivated us to further explore the ISFA. The ISFA in which laser-assisted rescattering is treated within the first Born approximation is usually calculated using additional approximations such as the saddle-point

approximation ([11,14,48–51] and references therein) and the pole approximation [52–54]. One of the aims of the present paper is to compare the results obtained using such approximations with the exact ISFA result. For this purpose two methods for exact calculation of the HATI spectra within the ISFA are developed. These methods enable us to identify those regions of the HATI spectra where the semiclassical three-step model (with backscattering) fails and also where the continuum essential state method, which is equivalent to the pole approximation, is not satisfactory anymore.

In Sec. II we introduce the transition matrix element for the HATI process, while in Sec. III we present two forms of the transition amplitude for the HATI process in the case of a linearly polarized, infinitely long, flat laser pulse. The method for calculation of this amplitude in the form of a five-dimensional integral is introduced in Appendix A, while the uniform approximation for this integral is presented in Appendix B. In Sec. IV we develop another method of exact calculation of the ISFA HATI amplitude. The obtained amplitude consists of the amplitude within the pole approximation and a correction to it expressed with the principal value integral. Numerical methods introduced in the present paper are illustrated by examples in Sec. V. Finally, conclusions and comments about the physical meaning and importance of the results obtained are presented in Sec. VI. The atomic system of units ($\hbar = |e| = m = 4\pi\varepsilon_0 = 1$) is used.

II. TRANSITION MATRIX ELEMENT

We denote the total Hamiltonian of an atom (or a negative ion) interacting with the laser field by

$$H(t) = H_0 + V_{\rm L}(t) + V(\mathbf{r}), \quad H_0 = -\nabla^2/2, \quad \boldsymbol{\nabla} \equiv \partial/\partial\mathbf{r}, \tag{1}$$

where $V_{\rm L}(t)$ is the laser-field–electron interaction, and $V(\mathbf{r}) = V_{\rm C}(r) + V_{\rm S}(r)$, with $V_{\rm C}(r) = -Z/r$ ($Z = 1$ for atoms and $Z = 0$ for negative ions, which will be considered in the present paper) the Coulomb interaction and $V_{\rm S}(r)$ a short-range interaction. The total time-evolution operator $U(t,t')$ corresponds to the Hamiltonian $H(t)$, while the evolution operator $U_{\rm L}$ and U_V correspond to the Hamiltonians $H_{\rm L} = H_0 + V_{\rm L}$ and $H_V = H_0 + V$, respectively. They satisfy the Dyson equations

$$U(t,\tau) = U_{\rm L}(t,\tau) - i\int_{\tau}^{t} d\tau' U(t,\tau')V(\mathbf{r})U_{\rm L}(\tau',\tau), \tag{2}$$

$$U(t,t') = U_V(t,t') - i\int_{t'}^{t} d\tau U(t,\tau)V_{\rm L}(\tau)U_V(\tau,t'). \tag{3}$$

In length gauge and dipole approximation we have

$$V_{\rm L}(t) = \mathbf{r}\cdot\mathbf{E}(t), \quad \mathbf{E}(t) = -d\mathbf{A}(t)/dt, \tag{4}$$

$$U_{\rm L}(t,t') = \int d\mathbf{k}|\chi_{\mathbf{k}}(t)\rangle\langle\chi_{\mathbf{k}}(t')|, \tag{5}$$

$$|\chi_{\mathbf{k}}(t)\rangle = |\mathbf{k} + \mathbf{A}(t)\rangle \exp[-iS_{\mathbf{k}}(t)], \tag{6}$$

where $\mathbf{E}(t)$ is the electric field vector, $U_{\rm L}(t,t')$ is the Volkov time-evolution operator, $2dS_{\mathbf{k}}(t)/dt = [\mathbf{k} + \mathbf{A}(t)]^2$, and $|\mathbf{q}\rangle$ is a plane-wave ket vector such that $\langle\mathbf{r}|\mathbf{q}\rangle = (2\pi)^{-3/2}\exp(i\mathbf{q}\cdot\mathbf{r})$.

We consider an ionization (detachment) process in which the interaction with the laser field is turned off at times t and t' so that the states $|\psi_{\mathbf{p}}(t)\rangle = |\psi_{\mathbf{p}}\rangle e^{-iE_{\mathbf{p}}t}$ and $|\psi_i(t')\rangle = |\psi_i\rangle e^{-iE_it'}$ are mutually orthogonal eigenstates of the Hamiltonian H_V with the eigenenergies $E_{\mathbf{p}} = \mathbf{p}^2/2$ and $E_i = -I_{\rm P} < 0$, respectively. E_i is the atomic or negative ion binding energy, while $I_{\rm P}$ is the atomic ionization potential or the negative ion electron affinity. The transition matrix element from the initial bound state $|\psi_i(t')\rangle$ to the final state $|\psi_{\mathbf{p}}(t)\rangle$ of the electron having the asymptotic momentum $\mathbf{p}$ we define with

$$M_{\mathbf{p}i}(t,t') = \langle\psi_{\mathbf{p}}(t)|U(t,t')|\psi_i(t')\rangle. \tag{7}$$

Introducing Eq. (3) into Eq. (7) and replacing in the resulting equation the operator $U(t,\tau)$ with Eq. (2), we obtain

$$M_{\mathbf{p}i}(t,t') = M^{\rm D}_{\mathbf{p}i}(t,t') + M^{\rm R}_{\mathbf{p}i}(t,t'), \tag{8}$$

$$M^{\rm D}_{\mathbf{p}i}(t,t') = -i\int_{t'}^{t} d\tau\langle\psi_{\mathbf{p}}(t)|U_{\rm L}(t,\tau)V_{\rm L}(\tau)|\psi_i(\tau)\rangle, \tag{9}$$

$$M^{\rm R}_{\mathbf{p}i}(t,t') = (-i)^2\int_{t'}^{t} d\tau\int_{\tau}^{t} d\tau'\langle\psi_{\mathbf{p}}(t)|U(t,\tau') \times V(\mathbf{r})U_{\rm L}(\tau',\tau)V_{\rm L}(\tau)|\psi_i(\tau)\rangle. \tag{10}$$

The upper indices D and R stand, respectively, for the direct and the rescattered part of the transition amplitude, as we will explain latter.

III. STRONG-FIELD APPROXIMATION

A. (H)ATI transition amplitude

If in Eq. (9) we approximate $\langle\psi_{\mathbf{p}}(t)|U_{\rm L}(t,\tau)$ with $\langle\chi_{\mathbf{p}}(\tau)|$, i.e., with the Volkov state that corresponds to the electron having the asymptotic momentum $\mathbf{p}$ outside the laser field, we obtain the standard SFA for the direct ATI:

$$M^{\rm SFA}_{\mathbf{p}i}(t,t') = \int_{t'}^{t} d\tau\mathcal{M}^{(0)}_{\mathbf{p}i}(\tau), \tag{11}$$

$$\mathcal{M}^{(0)}_{\mathbf{p}i}(\tau) = -i\langle\chi_{\mathbf{p}}(\tau)|V_{\rm L}(\tau)|\psi_i(\tau)\rangle. \tag{12}$$

The remaining or rest term $M^{\rm R}_{\mathbf{p}i}(t,t')$, Eq. (10), corresponds to the HATI process with the rescattering of the ionized electron off the parent ion (atom). We can approximate it using the improved strong-field approximation ([11,14,48–51] and references therein) or the low-frequency approximation [33]. In the present contribution we will consider only the ISFA. Let us elaborate this.

Using Eqs. (5) and (12), the rescattering matrix element (10) can be written in the form

$$M^{\rm R}_{\mathbf{p}i}(t,t') = \int_{t'}^{t} d\tau\int d\mathbf{k}M_{\mathbf{p}\mathbf{k}}(t,\tau)\mathcal{M}^{(0)}_{\mathbf{k}i}(\tau), \tag{13}$$

with

$$M_{\mathbf{p}\mathbf{k}}(t,\tau) = -i\int_{\tau}^{t} d\tau'\langle\psi_{\mathbf{p}}(t)|U(t,\tau')V(\mathbf{r})|\chi_{\mathbf{k}}(\tau')\rangle. \tag{14}$$

Since the amplitude $M_{\mathbf{p}\mathbf{k}}(t,\tau)$ contains the total time-evolution operator, which is difficult to treat numerically, we are forced to use some approximation. Within the ISFA, we approximate

it by the integral

$$M_{\mathbf{pk}}^{\mathrm{1BA}}(t,\tau) = -i\int_{\tau}^{t} d\tau' \langle \chi_{\mathbf{p}}(\tau')|V(\mathbf{r})|\chi_{\mathbf{k}}(\tau')\rangle, \tag{15}$$

which contains the laser-assisted scattering matrix element in the first Born approximation. Since we will use only this form of the SFA in the present paper we will omit the upper index "1BA."

B. Rescattering matrix element for long pulses and periodic field

For the case of long laser pulses we choose $t' \to -\infty$, $t \to \infty$, and denote $M_{\mathbf{p}i}^{\mathrm{R}} \equiv M_{\mathbf{p}i}^{\mathrm{R}}(\infty, -\infty)$. Then we obtain

$$M_{\mathbf{p}i}^{\mathrm{R}} = \int_{-\infty}^{\infty} dt \int d\mathbf{k}\, \mathcal{M}_{\mathbf{pk}}(t) M_{\mathbf{k}i}^{(0)}(t), \tag{16}$$

where

$$M_{\mathbf{k}i}^{(0)}(t) = -i\int_{-\infty}^{t} dt_0 \langle \chi_{\mathbf{k}}(t_0)|V_{\mathrm{L}}(t_0)|\psi_i(t_0)\rangle \tag{17}$$

and

$$\mathcal{M}_{\mathbf{pk}}(t) = -i\langle \chi_{\mathbf{p}}(t)|V|\chi_{\mathbf{k}}(t)\rangle. \tag{18}$$

For a $T = 2\pi/\omega$-periodic laser field we can write $M_{\mathbf{p}i}^{\mathrm{R}}$ as

$$\sum_{m=-\infty}^{\infty} \int_{0}^{T} dt' \int d\mathbf{k}\, \mathcal{M}_{\mathbf{pk}}(t'+mT) M_{\mathbf{k}i}^{(0)}(t'+mT). \tag{19}$$

In the integral over t_0 in Eq. (17) we make the substitution $t_0' = t_0 - mT$, and using the relation

$$S_{\mathbf{p}}(t+T) = S_{\mathbf{p}}(t) + (E_{\mathbf{p}} + U_{\mathrm{P}})T, \tag{20}$$

with $U_{\mathrm{P}} = \frac{1}{2}\int_0^T \mathbf{A}^2(\tau)d\tau$, and the formula

$$\sum_m e^{im(E_{\mathbf{p}}+U_{\mathrm{P}}+I_{\mathrm{P}})T} = \omega \sum_m \delta(E_{\mathbf{p}} + U_{\mathrm{P}} + I_{\mathrm{P}} - m\omega), \tag{21}$$

we obtain

$$M_{\mathbf{p}i}^{\mathrm{R}} = -2\pi i \sum_n \delta(E_{\mathbf{p}} + I_{\mathrm{P}} + U_{\mathrm{P}} - n\omega) T_{\mathbf{p}i}^{\mathrm{R}}(n), \tag{22}$$

where the T-matrix element for HATI with absorption of n photons is

$$T_{\mathbf{p}i}^{\mathrm{R}}(n) = i\int_0^T \frac{dt}{T} \int d\mathbf{k} \mathcal{M}_{\mathbf{pk}}(t) M_{\mathbf{k}i}^{(0)}(t). \tag{23}$$

The argument of the δ function in Eq. (22) displays energy conservation in terms of "absorption of laser photons." Equation (23), with Eqs. (17) and (18), contains a five-dimensional integral over the ionization time t_0, over the intermediate electron momenta $\mathbf{k}$, and over the rescattering time t. This integral can be solved using a saddle-point approximation. Various versions of this approximation were considered in our previous papers [11,12,29,48–51]. One usually applies the saddle-point method only for the integration over $d\mathbf{k}$, while the integrals over times are done by appropriate numerical quadrature. In Appendix A we will describe a numerical method for integration over $d\mathbf{k}$. In the present paper we will compare the exact results obtained solving the five-dimensional integral numerically with the results obtained solving this integral within the uniform approximation, described in Appendix B and in Ref. [50].

In the following we will present a different form of the T-matrix element. The rescattering matrix element can be written as

$$\mathcal{M}_{\mathbf{pk}}(t) = -i\sum_m T_{\mathbf{pk}}(m) e^{i(E_{\mathbf{p}}-E_{\mathbf{k}}-m\omega)t}, \tag{24}$$

where, for a linearly polarized laser field with the vector potential $\mathbf{A}(t) = \mathbf{A}_0 \cos\omega t$,

$$\begin{aligned} T_{\mathbf{pk}}(m) &= \langle \mathbf{p}|V|\mathbf{k}\rangle \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{i(m\varphi - u\sin\varphi)} \\ &= J_m(u)\langle \mathbf{p}|V|\mathbf{k}\rangle, \end{aligned} \tag{25}$$

with $J_m(u)$ the ordinary Bessel function of integer order m and argument $u = \mathbf{A}_0 \cdot (\mathbf{k} - \mathbf{p})/\omega$.

From Eqs. (23) and (24) it follows that the rescattering T-matrix element can be written as

$$T_{\mathbf{p}i}^{\mathrm{R}}(n) = \sum_m \int d\mathbf{k} T_{\mathbf{pk}}(m) \int_0^T \frac{dt}{T} M_{\mathbf{k}i}^{(0)}(t) e^{i(E_{\mathbf{p}}-E_{\mathbf{k}}-m\omega)t}, \tag{26}$$

with $E_{\mathbf{p}} = n\omega - I_{\mathrm{P}} - U_{\mathrm{P}}$. The amplitude $M_{\mathbf{k}i}^{(0)}(t)$, Eq. (17), is expressed as an integral over t_0. The integrand contains the quantity

$$\begin{aligned} \mathcal{T}_{\mathbf{k}i}^{(0)}(t_0) &= \langle \mathbf{k} + \mathbf{A}(t_0)|\mathbf{r}\cdot\mathbf{E}(t_0)|\psi_i\rangle e^{i[\mathbf{k}\cdot\boldsymbol{\alpha}(t_0)+\mathcal{U}_1(t_0)]} \\ &= \sum_{n'} T_{\mathbf{k}i}^{(0)}(n') \exp(-in'\omega t_0), \end{aligned} \tag{27}$$

which is periodic with the period $T = 2\pi/\omega$. Here $d\boldsymbol{\alpha}(t)/dt = \mathbf{A}(t)$ and $\mathcal{U}_1(t) = \int^t dt' \mathbf{A}^2(t')/2 - U_{\mathrm{P}}t$, with $\mathcal{U}_1(t+T) = \mathcal{U}_1(t)$, and

$$T_{\mathbf{k}i}^{(0)}(n) = \int_0^T \frac{dt_0}{T} \mathcal{T}_{\mathbf{k}i}^{(0)}(t_0) e^{in\omega t_0} \tag{28}$$

is the T-matrix for the direct ATI. It can be calculated using an appropriate numerical quadrature or presenting it in the form of a sum of the generalized Bessel functions. Using this and making the substitution $\tau = t - t_0$, we obtain that the integral over t in Eq. (26) gives $\delta_{m,n-n'}$, so that

$$T_{\mathbf{p}i}^{\mathrm{R}}(n) = \sum_{n'} \int d\mathbf{k} T_{\mathbf{pk}}(n-n') T_{\mathbf{k}i}^{(0)}(n') \zeta(y), \tag{29}$$

where $y = n'\omega - E_{\mathbf{k}} - I_{\mathrm{P}} - U_{\mathrm{P}}$, and [55]

$$\zeta(y) = -i\int_0^{\infty} d\tau e^{i\tau y} = \frac{1}{y+i\varepsilon} = \frac{\mathcal{P}}{y} - i\pi\delta(y). \tag{30}$$

The symbol $\mathcal{P}$ denotes the principal value of the integral over $dE_{\mathbf{k}}$. This integral appears in Eq. (29), since in spherical coordinates, $\int d\mathbf{k} = \int d\Omega_{\hat{\mathbf{k}}} \int_0^{\infty} k^2 dk = \int d\Omega_{\hat{\mathbf{k}}} \int_0^{\infty} k dE_{\mathbf{k}}$, $d\Omega_{\hat{\mathbf{k}}} = \sin\theta_{\mathbf{k}} d\theta_{\mathbf{k}} d\phi_{\mathbf{k}}$, $E_{\mathbf{k}} = \mathbf{k}^2/2$.

The final form of the rescattering matrix element, which we will further analyze in the next section, is given by Eq. (29), with Eqs. (25), (28), and (30). It contains a sum over the number n' of (virtual) photons absorbed ($n' > 0$) or emitted ($n' < 0$) from the laser field in the ionization process which is described

by the one-dimensional integral (28) over the ionization time t_0. We also have a three-dimensional integral over the intermediate electron momenta $\mathbf{k}$. A particular problem is how to treat numerically the principal value integral.

IV. EVALUATION OF THE T-MATRIX ELEMENT (29)

Introducing the notation

$$x = E_{\mathbf{k}}, \quad x_{n'} = n'\omega - I_{\mathrm{P}} - U_{\mathrm{P}}, \tag{31}$$

the transition matrix element (29) can be rewritten as

$$T^{\mathrm{R}}_{\mathbf{p}i}(n) = \sum_{n'} F_{n'}, \quad F_{n'} = \int_0^\infty dx \frac{f_{n'}(x)}{x - x_{n'} - i\varepsilon}, \tag{32}$$

where

$$f_{n'}(x) = -k \int d\Omega_{\hat{\mathbf{k}}}\, T_{\mathbf{pk}}(n - n') T^{(0)}_{\mathbf{k}i}(n'). \tag{33}$$

We choose the z axis as the axis of quantization and as the polarization direction of the laser field. In this case, the ionization matrix element does not depend on the azimuthal angle $\phi_{\mathbf{k}}$, while the integral over this angle of the rescattering matrix element in the first Born approximation can be calculated analytically using the formula (A5). Denoting this integral by

$$I_{\mathbf{p}}(k, z_k) = \int_0^{2\pi} d\phi_{\mathbf{k}} \langle \mathbf{p}|V|\mathbf{k}\rangle, \quad z_k = \cos\theta_{\mathbf{k}}, \tag{34}$$

we have

$$f_{n'}(x) = -k \int_{-1}^{1} dz_k\, I_{\mathbf{p}}(k, z_k) J_{n-n'}(u) T^{(0)}_{\mathbf{k}i}(n'), \tag{35}$$

where $u = A_0(kz_k - p\cos\theta)/\omega$, with θ the electron emission angle with respect to the laser polarization unit vector $\mathbf{A}_0/A_0$. The integral over dz_k can be calculated using, for example, Gauss-Legendre quadrature.

A. Pole approximation

Neglecting the principal value $\mathcal{P}$ of the integral in Eq. (30), i.e., using the so-called pole approximation [52–54], we obtain that the delta function $\delta(y)$ cancels the integral over $dE_{\mathbf{k}}$ in Eq. (29), so that we have

$$T^{\mathrm{R}}_{\mathbf{p}i}(n) = i\pi \sum_{n' \geqslant n_0} f_{n'}(x_{n'}), \tag{36}$$

where $E_{\mathbf{k}} = x_{n'} = n'\omega - I_{\mathrm{P}} - U_{\mathrm{P}} \geqslant 0$. The sum in Eq. (36) is over $n' \geqslant n_0$, $n_0 = [(I_{\mathrm{P}} + U_{\mathrm{P}})/\omega] + 1$ ($[x]$ means the integer part of the number x). The final energy of the ionized electron is $E_{\mathbf{p}} = n\omega - I_{\mathrm{P}} - U_{\mathrm{P}}$, $n \geqslant n_0$.

B. Principal value of the integral

For $n' < n_0$ we have $x_{n'} < 0$, so that

$$F_{n'} = \int_0^\infty dx \frac{f_{n'}(x)}{x + |x_{n'}|}, \quad n' < n_0, \tag{37}$$

and the integral over x can be calculated using, for example, Gauss-Legendre quadrature on the interval $(0, x_{\max})$, where $x_{\max}$ is a large electron kinetic energy. For example, the well-known cutoff law [56] allows us to choose $x_{\max} > E_{\mathbf{p},\max}(\theta = 0) = 10.007U_{\mathrm{P}} + 0.538I_{\mathrm{P}}$.

The case $n' \geqslant n_0$ is more complicated since the subintegral function is ill-behaved (has a singularity) at $x = x_{n'}$. We will subtract and add to the function $f_{n'}(x)$ the function $f_{n'}(x_{n'})$ multiplied by the exponential factor $\exp[-\alpha(x - x_{n'})]$. The real parameter α is free to choose in order to achieve a convergence for large values of x (computed results should be independent of α). Therefore, we have

$$\mathcal{P}\int_0^\infty dx \frac{f_{n'}(x)}{x - x_{n'}} \approx \int_0^{x_{\max}} dx \frac{f_{n'}(x) - f_{n'}(x_{n'})e^{-\alpha(x-x_{n'})}}{x - x_{n'}} + f_{n'}(x_{n'})\mathcal{P}\int_0^{x_{\max}} dx \frac{e^{-\alpha(x-x_{n'})}}{x - x_{n'}}, \tag{38}$$

where we have omitted the principal value integral symbol $\mathcal{P}$ in front of the first integral on the right-hand side since this integral does not have the singularity at $x = x_{n'}$. The integral in the second row can be calculated analytically with the result

$$I_\alpha(x_{n'}, x_{\max}) = \mathcal{P}\int_0^{x_{\max}} dx \frac{e^{-\alpha(x-x_{n'})}}{x - x_{n'}} = \mathrm{Ei}(\alpha(x_{n'} - x_{\max})) - \mathrm{Ei}(\alpha x_{n'}), \tag{39}$$

where $\mathrm{Ei}(x)$ denotes the exponential integral. For $\alpha = 0$ this integral simplifies and we have

$$I_0(x_{n'}, x_{\max}) = \ln\left|\frac{x_{\max} - x_{n'}}{x_{n'}}\right|. \tag{40}$$

For examples considered in the present paper the parameter $x_{\max}$ is not too large and we can set $\alpha = 0$ and use the simple result (40). After an appropriate substitution, the integral in the second row in Eq. (38) can be rewritten in the form

$$\int_0^{x_{\max}} dx \frac{f_{n'}(x) - f_{n'}(x_{n'})e^{-\alpha(x-x_{n'})}}{x - x_{n'}} = \int_{-1}^{1} dt \frac{f_{n'}\left(x_{\max}\frac{t+1}{2}\right) - f_{n'}(x_{n'})e^{-\alpha(x_{\max}\frac{t+1}{2} - x_{n'})}}{t - (2x_{n'}/x_{\max} - 1)}. \tag{41}$$

This integral can be calculated using an even-point Gauss-Legendre quadrature. In conclusion, for $n' \geqslant n_0$ we will calculate the principal value integral using Eqs. (38)–(41).

V. NUMERICAL RESULTS

All numerical results in the present paper are for the above-threshold detachment of a fluorine negative ion [48,57] by a linearly polarized laser field having the wavelength 1800 nm and the intensity 1.3×10^{13} W/cm^2. The method developed is valid for arbitrary electron emission angle θ but the plateau and low-energy structures are the most pronounced for $\theta = 0^\circ$. This value will be used in all our calculations.

For the initial wave function of F^- we choose the Hartree-Fock-type wave function, which is given in analytical form as a series expansion in atomic Slater-type orbitals

$$\psi_i(\mathbf{r}) = \sum_a C_a \frac{(2\zeta_a)^{n_a+1/2}}{\sqrt{(2n_a)!}} r^{n_a-1} \exp(-\zeta_a r) Y_{lm}(\hat{\mathbf{r}}), \tag{42}$$

where the quantum numbers $n_a l$ and the parameters C_a and ζ_a are tabulated in Ref. [58]. There are four $2p$ orbitals ($n_a l = 21$) with (in a.u.) $C_1 = 0.4704$, $C_2 = 0.3084$, $C_3 = 0.0988$, $C_4 = 0.2470$, $\zeta_1 = 2.0754$, $\zeta_2 = 3.9334$, $\zeta_3 = 1.4660$, and $\zeta_4 = 0.9568$. The rescattering e–F potential is given by

$$V(r) = -a_1 \frac{e^{-\alpha_1 r}}{r} - a_2 \frac{e^{-\alpha_2 r}}{r}, \tag{43}$$

with the parameters (in a.u.) $a_1 = 5.137$, $a_2 = 3.863$, $\alpha_1 = 1.288$, and $\alpha_2 = 3.545$ [59]. The electron affinity of F^- is $I_P = 3.4$ eV. The potential (43) gives the correct ground-state energy, and its lowest p-orbital eigenfunction agrees well with the tabulated Hartree-Fock wave function (42), as shown in Fig. 1 in [60]. A good agreement of the ISFA spectra and the spectra obtained solving the three-dimensional time-dependent Schrödinger equation was obtained in Ref. [60]. We need the momentum space matrix element of the potential $V(r)$:

$$\langle \mathbf{p}|V|\mathbf{k}\rangle = (2\pi)^{-3} \int d\mathbf{r}\, V(\mathbf{r}) \exp[i(\mathbf{k}-\mathbf{p})\cdot\mathbf{r}], \tag{44}$$

which can be calculated analytically [see Eq. (22) in the first reference in [49]].

In Figs. 1–7 we present the results for the differential detachment rate (in a.u.) for detachment with rescattering and with absorption of n photons, which is defined by

$$w^{\mathrm{R}}_{\mathbf{p}i}(n) = 2\pi p \left| T^{\mathrm{R}}_{\mathbf{p}i}(n) \right|^2, \tag{45}$$

as a function of the detached electron kinetic energy $E_{\mathbf{p}} = n\omega - I_P - U_P$ expressed in units of ponderomotive energy U_P. All the results presented have a characteristic form of the HATI spectra: a plateau which approximately extends from $4\,U_P$ to $10\,U_P$, where an abrupt cutoff appears.

In Fig. 1 we compare the exact spectrum obtained calculating the five-dimensional integral numerically, as described in Appendix A, with the approximate spectrum obtained solving this integral within the uniform approximation (UA). We see

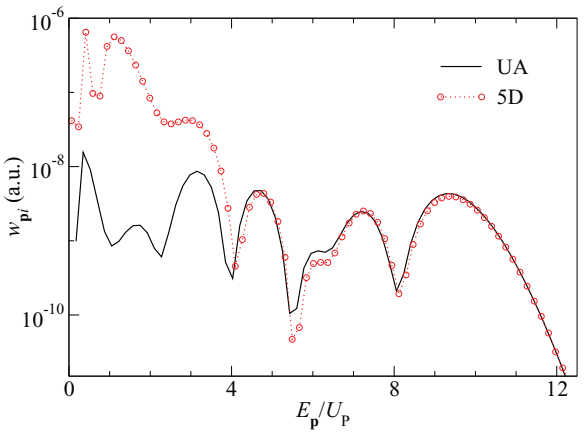

FIG. 1. (Color online) The differential detachment rates of F^- as functions of the electron energy in units of U_P. The electron emission angle is $\theta = 0^\circ$ and the wavelength and intensity of the linearly polarized laser field are 1800 nm and 1.3×10^{13} W/cm^2, respectively. Comparison of the exact result obtained calculating the five-dimensional integral (5D) with the result obtained using the uniform approximation (UA).

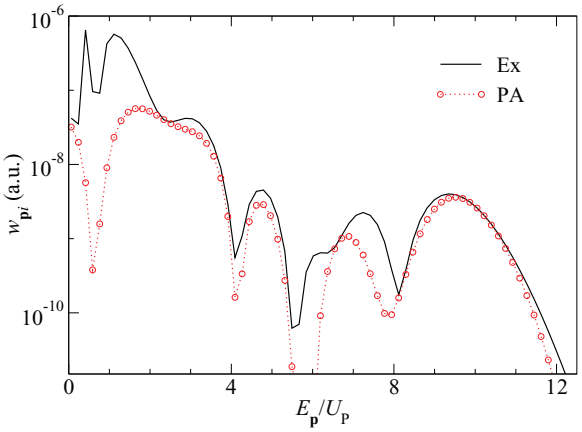

FIG. 2. (Color online) Same as in Fig. 1 but for the comparison of the result obtained using the pole approximation (PA) and the corresponding "exact" result (Ex), as described in the text.

that the plateau and the cutoff part of the spectrum ($E_{\mathbf{p}} > 4\,U_P$) are well approximated by the UA. However, the UA fails for the low-energy spectrum. The low-energy part consists of a sharp peak near $0.4\,U_P$ which resembles the VLES, followed with a broad peak near $1.1\,U_P$ which is an analog of the LES, mentioned in the Introduction. In the UA the T-matrix element is presented in the form of a sum over the solutions of the saddle-point equations [see Eq. (B4)]. These solutions include the backscattered electrons which can achieve high energy at the detector. Since the forward-scattered electrons are not included in the UA, and since such electrons are responsible for the LES [2], our finding that the LES is not reproduced by the UA is expected.

In Sec. IV we have developed another "exact" method of calculation of the T-matrix element. In Figs. 2–6 the spectrum obtained using this method is denoted by "Ex" and depicted by a black solid curve. In Figs. 2–5 this exact result is compared with the results obtained using various contributions to the exact ISFA T-matrix element. The low-energy part of the spectrum below $2\,U_P$ cannot be described well within the pole approximation, as we can see from Fig. 2. The widely used

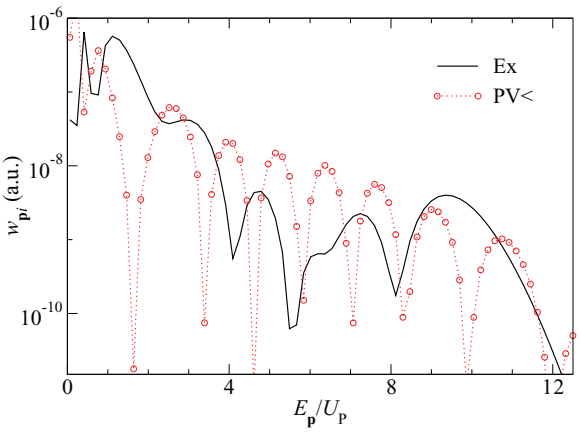

FIG. 3. (Color online) Same as in Fig. 2 but for the comparison of the result obtained solving the principal value integral for all channels with $n < n_0$ (PV<) and the "exact" result.

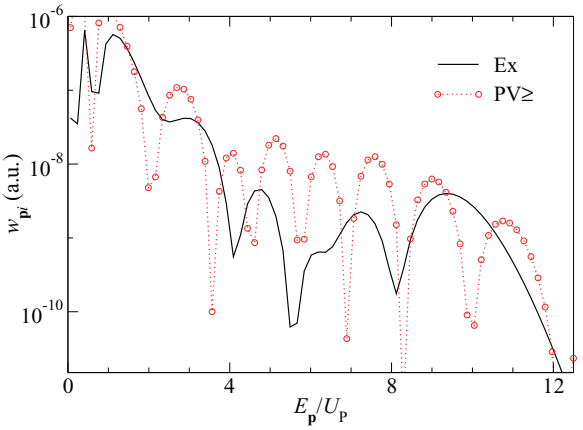

FIG. 4. (Color online) Same as in Fig. 2 but for the comparison of the result obtained solving the principal value integral for all channels with $n \geqslant n_0$ (PV$\geqslant$) and the "exact" result.

pole approximation [52–54] does not reproduce either the LES or the exact shape of the high-energy spectrum at $6\,U_\mathrm{P}$–$8\,U_\mathrm{P}$.

In Figs. 3–5 we have compared the "exact" result with the results obtained taking into account only the principal value integral part of the transition amplitude. In Fig. 3, with a dotted curve with circles, denoted by PV$<$, we have presented the result obtained using Eq. (37), which corresponds to the channels with $n' < n_0$ that are closed in the pole approximation. The principal-value-integral result for $n' \geqslant n_0$, obtained using Eqs. (38)–(41), is shown in Fig. 4 (the curve denoted by PV$\geqslant$). Both the PV$<$ and PV$\geqslant$ spectra exhibit a high plateau with large oscillations, but the interference of the corresponding amplitudes leads to the spectrum shown in Fig. 5 (PV curve) in which the exact low-energy structure is perfectly reproduced. Furthermore, the PV amplitude in combination with the amplitude obtained using the pole approximation exactly reproduces the plateau and the cutoff of the spectrum.

The low-energy structure in ATI spectra was observed in the experiments [34,35] as a big surprise, as we have discussed in the introduction. Various mechanisms of this process were proposed and the scientists mainly agree that the

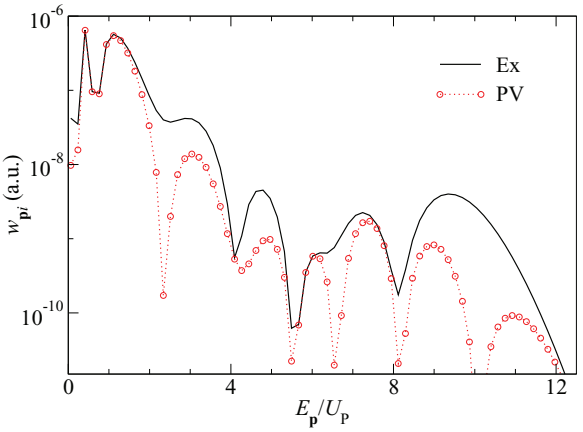

FIG. 5. (Color online) Same as in Fig. 2 but for the comparison of the result obtained solving the principal value integral for all channels (PV) and the "exact" result.

LES is a consequence of an interplay of laser-assisted forward scattering of the ionized electron wave packet on the parent ion and the Coulomb effect. For Coulomb potential the rescattering matrix element is proportional to $\langle \mathbf{p}|V_\mathrm{C}|\mathbf{k}\rangle \propto 1/(\mathbf{p}-\mathbf{k})^2$ and is singular for forward scattering for which $\mathbf{p} = \mathbf{k}$. In fact, in Ref. [47] it was shown that for $n' = n$ (in our notation) the partial contribution $F_{n'}$ [see Eq. (32)] to the matrix element $T^\mathrm{R}_{\mathbf{p}_f}(n)$ is logarithmically divergent, similarly to that in the case of field-free Coulomb scattering. In Ref. [47] this divergence was avoided by adding a decay factor into the phase of the T-matrix element. Using this method a relatively successful simulation of the experimentally observed LES has been done, but the VLES was not explained. In our case of short-range potential we do not have the Coulomb singularity, but, nevertheless, we observed a peak at very low energy as well as a broader LES. Since $\langle \mathbf{p}|V_\mathrm{S}|\mathbf{k}\rangle \propto 1/[(\mathbf{p}-\mathbf{k})^2 + \lambda^2]$ for a short-range potential of the Yukawa type $V_\mathrm{S}(r) \propto e^{-\lambda r}/r$, the rescattering matrix element is maximal for forward scattering $\mathbf{p} = \mathbf{k}$. We expect that from all terms in the sum over n' the term $n' = n$ is responsible for the VLES peak observed in the "exact" calculation. Physically, this case corresponds to rescattering of the ionized electron with no exchange of photons since $E_\mathbf{k} = n\omega - I_\mathrm{P} - U_\mathrm{P} = E_\mathbf{p}$. In Fig. 6 we presented the contribution of the amplitude F_n [see Eq. (45) with Eq. (32)] to the low-energy spectrum. Its contribution to the high-energy spectrum is negligible. As expected, the term F_n is responsible for the VLES at $E_\mathbf{p} \approx 0.4\,U_\mathrm{P}$. This term together with the terms which correspond to the laser-assisted scattering with absorption (emission) of more laser photons, is responsible for the remaining part of the LES. In addition, in Fig. 6 we compared the spectra obtained calculating the ISFA amplitude with two different "exact" methods and found an excellent agreement.

Finally, let us compare the contribution to the detachment rate from the direct SFA, Eqs. (11) and (12), and the exact

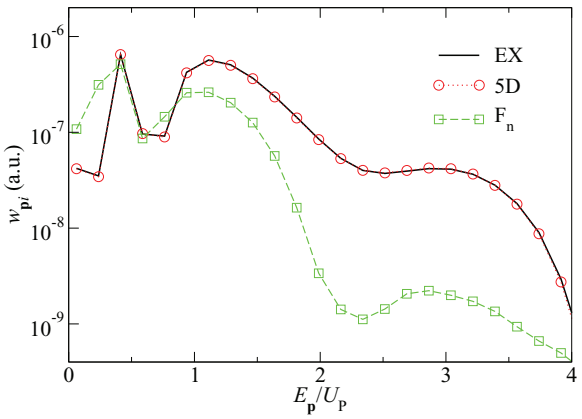

FIG. 6. (Color online) Same as in Fig. 1 but for the comparison of the results obtained using two different "exact" methods of calculations: EX, summation over all intermediate photon channels and integration over all ionization times and the intermediate electron momenta; 5D, five-dimensional integral over the ionization and travel times and over the intermediate electron momenta. The low-energy part of the spectrum ($E_\mathbf{p} \leqslant 4\,U_\mathrm{P}$) is presented in order to better show the contribution of the $n' = n$ term of the T-matrix element, which is described by the amplitude F_n (dashed green line with squares). See the text for explanation.

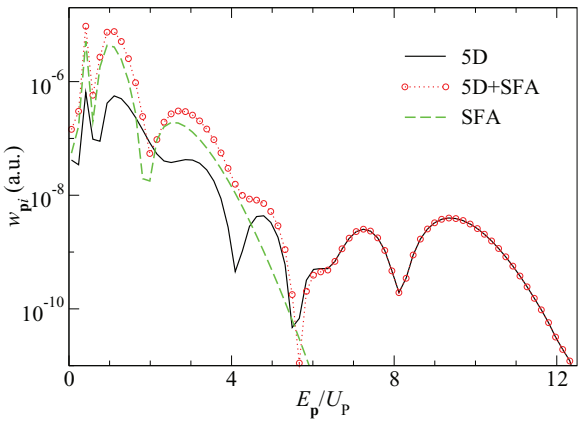

FIG. 7. (Color online) Comparison of the results obtained using the ISFA calculated using the five-dimensional integral (5D, black solid curve) with the results obtained with the direct SFA alone (green dashed curve) and the coherent sum of the SFA and ISFA (5D + ISFA, red dotted curve with circles). The negative ion and laser parameters are as in Fig. 1.

ISFA calculated using five-dimensional integration described in Appendix A. It is expected from the results of Ref. [48] that the direct SFA rate is dominant in the low-energy part of the spectrum. The results presented in Fig. 7 show that the direct SFA rate is really larger than the rescattering ISFA rate for energies $E_{\mathbf{p}} < 4.5U_{\mathrm{P}}$. However, the coherent sum of both the SFA and ISFA results is larger than the direct SFA alone, so that the ISFA cannot be neglected even in this low-energy region. Furthermore, it was shown in [48] that for the heavier halogen ions the rescattering plateau becomes higher. For example, for iodine I^-, which has a large number of scattering centers, the rescattering plateau is lower than the direct part of the spectrum by a factor only 40. Since the (V)LES part of a rescattering spectrum is more than two orders of magnitude higher than the high-energy plateau, we expect that (V)LES can be observed in the experiments with heavier negative-halogen ions. In fact, one of the motivations of our work was to develop code for more precise calculation of the low-energy spectra in order to be able to better simulate the experimental spectra for Br^- [57], for which the rescattering plateau was observed for the first time for negative ions. Since the laser intensity in this experiment is far above saturation value, in addition to the averaging over the spatiotemporal distribution of the intensity in the laser focus, the depletion of the negative ion during interaction with the laser pulse needs to be taken into account.

In this paper we have considered the case of negative ions and short-range potentials. For H(ATI) of neutral atoms one should take into account both the long-range Coulomb potential $V_{\mathrm{C}}(r)$ and the short-range potential $V_{\mathrm{S}}(r)$. The forward-scattering cross section for the Coulomb potential is much larger than that of short-range potentials. Therefore, for neutral atoms the (V)LES should be much more pronounced than in the negative ion case. The problem with long-range Coulomb potential is the well-known Coulomb-related divergence. This divergence can be eliminated in different ways. For example, one can cut off the Coulomb potential at a safe distance away from the atom [29,33]. Another method for eliminating the Coulomb divergence was used in Ref. [47], where the depletion of the atomic ground state due to an applied laser field was taken into account. Also, one can consider various methods of regularization of the S matrix and use the Coulomb asymptotic states [61], but this is a difficult task, which we leave for future investigations.

VI. CONCLUSIONS

We have presented two equivalent forms of the T-matrix element of the HATI process within the ISFA in which an additional interaction of the (virtually) ionized electron with the parent core is taken into account within the first Born approximation. Numerical methods for exact calculation of these two forms are introduced. This has enabled us to check some approximations which were used previously for calculation of the HATI spectra.

In particular, we have shown that the saddle-point approximation for five-dimensional integral, or even the corresponding more precise method, the so-called uniform approximation, describes well the middle- and high-energy parts of the spectrum (plateau and cutoff) but fails to describe the LES. Since the LES is absent in the uniform approximation which takes into account only the quantum orbits of backscattered electrons, our result indicates that the LES is related to the interference of forward-scattered-electron amplitudes.

The second derived form of the ISFA matrix element is used to introduce the pole approximation in which the δ function cancels the integral over the intermediate electron energy so that only the intermediate resonance continuum states (the so-called continuum essential states [53]) having the energy $E_{\mathbf{k}} = x_{n'} = n'\omega - I_{\mathrm{P}} - U_{\mathrm{P}} \geqslant 0$ contribute. By calculating the correction to this approximate result, i.e., by calculating the principal value part of the integral, we have shown that the pole approximation fails both for low energies and for the electrons in the plateau region at $6\,U_{\mathrm{P}}$–$8\,U_{\mathrm{P}}$. The exact result is recovered if we take into account the intermediate states with the electron energy $x_{n'} < 0$ as well as those with $x_{n'} \geqslant 0$. The interference of the amplitudes of all these contributions gives the exact ISFA result. We have also shown that the amplitude with fixed $n' = n$, which corresponds to the rescattering without exchange of the laser photons, is responsible for the very-low-energy structure (VLES).

All numerical results presented are for short-range potential. For long-range Coulomb potential we expect that the VLES and LES structures are more pronounced due to the Coulomb singularity. This is exactly what has been observed in experiments. The investigation of LES in ATI spectrum is presently a very active area of research in strong-field physics and we hope that our results shed some light on this phenomenon.

ACKNOWLEDGMENTS

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APPENDIX A: INTEGRATION OVER THE INTERMEDIATE ELECTRON MOMENTA

After an appropriate change of the time-integration variables, $\tau = t - t_0$, Eq. (16) can be rewritten as

$$M^{\mathrm{R}}_{\mathbf{p}i} = -\int_{-\infty}^{\infty} dt\, e^{iS_{\mathbf{p}}(t)} \int_0^{\infty} d\tau\, e^{iI_{\mathrm{P}}(t-\tau)} \times \exp\left[-\frac{i}{2}\int_{t-\tau}^{t} dt' \mathbf{A}(t')^2\right] J_{\mathbf{p}i}(t,\tau), \quad \text{(A1)}$$

where

$$J_{\mathbf{p}i}(t,\tau) = \int d\mathbf{k}\, e^{-ik^2\tau/2 + i\mathbf{k}\cdot\mathbf{k}_{\mathrm{s}}\tau} h_{\mathbf{p}i}(\mathbf{k}), \quad \text{(A2)}$$

with $\mathbf{k}_{\mathrm{s}}$ the stationary electron momentum in the intermediate state

$$\mathbf{k}_{\mathrm{s}} \equiv -\int_{t-\tau}^{t} dt'' \mathbf{A}(t'')/\tau, \quad \text{(A3)}$$

and

$$h_{\mathbf{p}i}(\mathbf{k}) = \langle \mathbf{p}|V|\mathbf{k}\rangle \langle \mathbf{k} + \mathbf{A}(t-\tau)|\mathbf{r}\cdot\mathbf{E}(t-\tau)|\psi_i\rangle. \quad \text{(A4)}$$

The integrals over the ionization and rescattering times are done using appropriate numerical quadrature.

We will now show how the integral over the intermediate electron momenta can be calculated numerically. This form of the integral appears in many problems in strong-field physics. We will present a general solution and omit the problem-dependent indices $\mathbf{p}i$. In the spherical coordinates we have $\int d\mathbf{k} \equiv \int_0^{\infty} k^2 dk \int_0^{\pi} \sin\theta_{\mathbf{k}}\, d\theta_{\mathbf{k}} \int_0^{2\pi} d\phi_{\mathbf{k}}$. We choose the z axis as the axis of quantization and as the polarization direction of the laser field. In this case, the ionization matrix element does not depend on the azimuthal angle $\phi_{\mathbf{k}}$, while the integral over this angle of the rescattering matrix element in the first Born approximation can be calculated analytically using the formula

$$\int_0^{2\pi} d\phi_{\mathbf{k}}/(1 + a\cos\phi_{\mathbf{k}}) = 2\pi/\sqrt{1-a^2}. \quad \text{(A5)}$$

The remaining two-dimensional integral we will calculate using an appropriate method of numerical integration.

Denoting $a = k_{\mathrm{s}}\cos\theta_{\mathbf{k}}$ and $g(k,\theta_{\mathbf{k}}) = k^2 \int_0^{2\pi} d\phi_{\mathbf{k}} h(\mathbf{k})$, we can rewrite the integral (A2) as

$$J(t,\tau) = \int_0^{\pi} \sin\theta_{\mathbf{k}} d\theta_{\mathbf{k}} e^{ia^2\tau/2} I(\theta_{\mathbf{k}}),$$
$$I(\theta_{\mathbf{k}}) = \int_0^{\infty} dk g(k,\theta_{\mathbf{k}}) \exp[-i\tau(k-a)^2/2]. \quad \text{(A6)}$$

Using the substitution $(k-a)^2 = x$, for $a \leqslant 0$ we obtain

$$I(\theta_{\mathbf{k}}) = \int_{a^2}^{\infty} \frac{dx}{2\sqrt{x}} g(a+\sqrt{x},\theta_{\mathbf{k}}) e^{-i\tau x/2}, \quad \text{(A7)}$$

while for $a > 0$ we have

$$I(\theta_{\mathbf{k}}) = \int_0^{a^2} \frac{dx}{2\sqrt{x}} g(a-\sqrt{x},\theta_{\mathbf{k}}) e^{-i\tau x/2} + \int_0^{\infty} \frac{dx}{2\sqrt{x}} g(a+\sqrt{x},\theta_{\mathbf{k}}) e^{-i\tau x/2}. \quad \text{(A8)}$$

For numerical calculation of the integrals of this type we use a powerful numerical quadrature, based on the double exponential formula for Fourier-type integrals, adapted to slowly decaying analytic functions [62].

APPENDIX B: UNIFORM APPROXIMATION

The uniform approximation for HATI and high-order harmonic generation processes was introduced in Refs. [63] and [64], respectively. We will present it briefly following Ref. [50].

The matrix element in the integrand of Eq. (16) can be represented in the form $A_{\mathbf{p}i}\exp(iS_{\mathbf{p}i})$ where the action $S_{\mathbf{p}i}$ consists of three parts,

$$S_{\mathbf{p}i}(t,t_0,\mathbf{k}) = -\int_t^{\infty} dt' [\mathbf{p} + \mathbf{A}(t')]^2/2 - \int_{t_0}^{t} dt' [\mathbf{k} + \mathbf{A}(t')]^2/2 + I_{\mathrm{P}} t_0, \quad \text{(B1)}$$

in accordance with the three-step model. The integral over the intermediate electron momentum $\mathbf{k}$ can be solved using the saddle-point method: The action is stationary, i.e., $\nabla_{\mathbf{k}} S_{\mathbf{p}i}(t,t_0,\mathbf{k}) = \mathbf{0}$, for the momentum $\mathbf{k} = \mathbf{k}_{\mathrm{s}} = -\int_{t_0}^{t} dt' \mathbf{A}(t')/(t-t_0)$ [see Eq. (A3)]. This condition corresponds to the requirement that the electron returns to its parent ion. The stationarity conditions with respect to the remaining two integration variables t_0 and t lead to the relations

$$\tfrac{1}{2}[\mathbf{k}_{\mathrm{s}} + \mathbf{A}(t_0)]^2 = -I_{\mathrm{P}}, \quad \text{(B2)}$$

$$\tfrac{1}{2}[\mathbf{k}_{\mathrm{s}} + \mathbf{A}(t)]^2 = \tfrac{1}{2}[\mathbf{p} + \mathbf{A}(t)]^2. \quad \text{(B3)}$$

Physically, these two conditions correspond to energy conservation at time t_0 of ionization and at time t of rescattering. Application of the saddle-point method to the double integral over the times t_0 and t leads to a sum over solutions $\{t_{0s}, t_s\}$ of the system of Eqs. (B2) and (B3). The corresponding T-matrix element has the form $\sum_s A_s e^{iS_s}$, where $S_s \equiv S(t_{0s},t_s)$, with $S(t_0,t) = E_{\mathbf{p}}t + \mathbf{p}\cdot\boldsymbol{\alpha}(t) + E_{\mathbf{k}_{\mathrm{s}}}(t-t_0) + (U_{\mathrm{P}} + I_{\mathrm{P}})t_0 + \mathcal{U}_1(t_0)$. For a linearly polarized monochromatic laser field, the solutions $\{t_{0s}, t_s\}$ are characterized by a multi-index consisting of the three numbers $s \equiv \alpha\beta m$ [50]. With this notation the T-matrix element in the uniform approximation takes the form

$$T^{\mathrm{R,UA}}_{\mathbf{p}i}(n) = \sum_{\beta m} (6\pi S_-)^{1/2} \exp(iS_+ + i\pi/4) \times \left[\frac{A_-}{\sqrt{z}}\mathrm{Ai}(-z) + \frac{iA_+}{z}\mathrm{Ai}'(-z)\right], \quad \text{(B4)}$$

where Ai and Ai′ are the Airy function and its first derivative, respectively, and $z = (3S_-/2)^{2/3}$. The quantities $A_{\pm}$ and $S_{\pm}$ are related to the weights and the actions of the saddle points: $A_{\pm} = (A_{1\beta m} \pm iA_{-1\beta m})/2$ (in Ref. [50] was a misprint in this formula: the imaginary unit in front of $A_{-1\beta m}$ was omitted), $S_{\pm} = (S_{1\beta m} \pm S_{-1\beta m})/2$. In Eq. (B4), beyond the cutoff the argument z must be replaced by $z\exp(i2\beta\pi/3)$, in order to select the proper branch of the Airy functions, and $A_{\alpha\beta m}$ should change its sign.

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