Analytic theory of high-order-harmonic generation by an intense few-cycle laser pulse

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We present a theoretical model for describing the interaction of an electron, weakly bound in a short-range potential, with an intense, few-cycle laser pulse. General definitions for the differential probability of above-threshold ionization and for the yield of high-order-harmonic generation (HHG) are presented. For HHG we then derive detailed analytic expressions for the spectral density of generated radiation in terms of the key laser parameters, including the number $N$ of optical cycles in the pulse and the carrier-envelope phase (CEP). In particular, in the tunneling approximation, we provide detailed derivations of the closed-form formulas presented briefly by M. V. Frolov et al. [Phys. Rev. A 83, 021405(R) (2011)], which were used to describe key features of HHG by both $\text{H}$ and $\text{Xe}$ atom targets in an intense, few-cycle laser pulse. We then provide a complete analysis of the dependence of the HHG spectrum on both $N$ and the CEP $\phi$ of an $N$-cycle laser pulse. Most importantly, we show analytically that the structure of the HHG spectrum stems from interference between electron wave packets originating from electron ionization from neighboring half-cycles near the peak of the intensity envelope of the few-cycle laser pulse. Such interference is shown to be very sensitive to the CEP. The usual HHG spectrum for a monochromatic driving laser field (comprising harmonic peaks at odd multiples of the carrier frequency and spaced by twice the carrier frequency) is shown analytically to occur only in the limit of very large $N$, and begins to form, as $N$ increases, in the energy region beyond the HHG plateau cutoff.

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I. INTRODUCTION

The high-order-harmonic generation (HHG) process is now the major means for producing ultrashort pulses in the rapidly developing field of attosecond physics (cf. recent reviews [1–5]) as well as for producing coherent radiation in the soft-x-ray regime [6]. At present it is possible experimentally to obtain HHG spectra using short (few cycle) laser pulses [2, 7–9]. The short-pulse HHG spectra are highly sensitive to the temporal behavior of the electric field of the laser pulse, i.e., to the shape of the pulse envelope, $f(t)$, and the carrier-envelope phase (CEP), $\phi$. For laser parameters in the tunneling regime, the three-step scenario [10, 11] remains applicable for understanding some basic features of HHG by atoms in a short laser pulse. However, there are at least two important differences from the monochromatic field case. First, the HHG emission becomes quasicontinuous, so that instead of analyzing HHG rates it is more appropriate to analyze the spectral density of radiation, $\rho(E_\Delta)$, where $E_\Delta = h\Omega$ is the harmonic photon energy. Second, the shape of $\rho(E_\Delta)$ as a function of $E_\Delta$ for a rapidly varying laser pulse envelope becomes sensitive to the CEP, requiring an analysis of subcycle dynamics for a proper description.

From 1998 up to the present, the key differences between short-pulse and monochromatic field HHG spectra have been delineated in numerous theoretical and experimental investigations [12–23]. The most significant differences were found in the shape and the plateau-cutoff behavior of HHG spectra for “sine” ($\phi = \pi/2$) and “cosine” ($\phi = 0$) pulses. Nearly all of the theoretical analyses of few-cycle pulse HHG spectra are based on numerical solutions of the time-dependent Schrödinger equation (TDSE) [12, 14, 15, 19, 20] or on the use of the Lewenstein et al. model [24] and its modifications. Recently, however, a closed-form formula for the spectral density of radiation, $\rho(E_\Delta)$, was presented [22], thus providing an analytic description of the short-pulse HHG spectrum similar to that for a monochromatic field [25].

A key feature of the closed-form analytic formula presented in Ref. [22] is that it confirms the validity for the case of a few-cycle pulse of the phenomenological parametrization [26–28] of the HHG yield in terms of the photorecombination cross section (PRCS) $\sigma^{(r)}$ (which describes the final step of the three-step scenario) and the “electron wave packet” (EWP) (which describes the ionization of an atomic electron and its propagation in the laser field). This parametrization is attractive since (i) it is valid for harmonics with energies in the region of the HHG plateau cutoff, which are precisely the ones used to produce attosecond pulses, and (ii) it involves a field-free atomic parameter $\sigma^{(r)}$ that describes atomic structure effects on HHG spectra [25–32]. Furthermore, the explicit form of the EWP is now known not only for monochromatic [25] and two-color [31] fields but also for the case of a few-cycle laser pulse [22]. Consequently, the closed-form
formula for the short-pulse case in Ref. [22] makes possible
the analytic exploration of many-electron atomic features in
the HHG spectrum and their modification by CEP effects. As
shown in Ref. [22], all that is required is the PRCS $\sigma^{(r)}$ for
the target atom and the solutions of some classical equations
for a given short laser pulse. Results of the analytic formula
for the HHG yield in the few-cycle laser pulse case agree well
with numerical TDSE results. Also, the dependence on the
number of cycles, $N$, in the laser pulse was shown in Ref. [22]
to reduce, for large $N$, to the analytic formula for the HHG
rate in the monochromatic field case [25].

The purpose of this paper is to present the theory upon
which the analytic predictions in Ref. [22] (for HHG by H
and Xe atom targets driven by a few-cycle laser pulse) are
based. By way of background, we note that our focus over
much of the past decade has been on developing exact (and,
when possible, closed-form analytic) results for a one-electron
model atomic system subjected to an intense laser field. The
physical insights provided by the closed-form analytic results
obtained for our model system have enabled us to generalize
those results to real, many-electron atomic systems and to
predict many-electron effects in strong-field processes for
such real systems. Thus, for example, we predicted that a
giant-dipole resonance would be seen in the HHG spectrum
of Xe [25]. (This prediction was subsequently confirmed by
experiment [33].) Also, we were able to interpret [32]
experimentally observed resonances in particular high-order
harmonics in singly ionized plasmas of Cr$^+$ and Mn$^{2+}$ [34,35]
as due to potential barrier effects that lead to a strong $3p \rightarrow 3d$
electric dipole transition, which dominates the many-electron
photoionization cross sections of the outer subshells of those
ions (as well as the corresponding PRCSs to those subshells).

The theory we have developed for our model atomic system
is the time-dependent effective range (TDER) theory [36,37].
This theory combines effective range theory (for describing a
weakly bound electron in a short-range potential of arbitrary
shape) with the Floquet or quasistationary, quasienergy state
(QQES) approach (for describing the electron’s interaction
with a monochromatic (or, more generally, periodic) laser
field). The TDER theory applies immediately to the case of
intense laser detachment of negative ions (see, e.g., its applica-
tion to laser detachment of the F$^-$ negative ion [38], which
demonstrated excellent agreement with experimental results
[39]). For the HHG process, we developed a theory applicable
in general to any system interacting with a monochromatic
laser field for which a Floquet or QQES approach is employed
[40]. We then applied this formulation for HHG specifically
to our TDER model [41]. Based on this latter application of
our new HHG formulation within TDER theory, we were able
to obtain closed-form analytic formulas for HHG rates for our
model system [42]. As noted above, the physical interpretation
of our quantum-mechanically-derived, factorized analytic
formula confirmed the well-known semiclassical three-step
scenario for HHG [10,11] and justified (for our model system)
the phenomenological factorization of the HHG rate in terms
of a PRCS and a EWP function [26–28]. Most importantly,
the clear physical interpretation of each of the three factors in
our factorized formula allowed immediate generalization for
applications to HHG spectra of real atoms [25].

In this paper we present an analytic description of HHG by
a short laser pulse based on two new theoretical developments.
First, in Sec. II we generalize the QQES approach, which is
one of the most powerful theoretical methods for accurately
describing atomic processes in a strong monochromatic laser
field, to describe the most fundamental strong-field processes
[i.e., above-threshold ionization (ATI) and HHG] in an intense,
few-cycle laser pulse. Second, in Sec. III we employ this
generalized QQES approach to extend our TDER theory for
analytic description of HHG by a monochromatic field to
the case of HHG by a periodic (nonmonochromatic) pulse
train field. In Sec. IV we derive the quasiclassical limit of the
TDER results for the HHG amplitude in the case of a periodic
(nonmonochromatic) pulse train field and, as a limiting case,
obtain closed-form analytic expressions for the HHG yield for
the case of a single short pulse. In Sec. V we generalize our
closed-form formulas to the case of real atoms. In Sec. VI we
present numerical results of our analytic formulas, including
comparisons with numerical TDSE results, illustrations of
subcycle and intercycle interferences in short-pulse HHG
spectra, and illustrations of the dependence of HHG spectra on
the CEP and number of cycles in the laser pulse. In Sec. VII we
summarize our results and present some conclusions. Finally,
in Appendices A and B we present some of the lengthier
analytic derivations of our TDER theory of HHG driven by
few-cycle laser pulses.

II. GENERALIZATION OF THE QQES APPROACH TO
THE CASE OF A SHORT LASER PULSE

A. Description of a periodic laser pulse train

We use the length gauge to describe the dipole interaction
of an active atomic electron with a short laser pulse:

$$V(r,t) = -d \cdot F(t), \quad d = e r,$$

where $F(t)$ is the electric vector of the pulse. Different ways are
used to describe a short pulse, using either the electric vector
of the pulse or its vector potential $A(t)$ [43]. In this paper, we
consider only linearly polarized pulses, so that

$$A(t) = e; A(t),$$

$$F(t) = e; F(t) = -e \frac{1}{c} \frac{\partial A(t)}{\partial t}. \quad (2)$$

Moreover, we do not specify the explicit form of $A(t)$ in our
theoretical derivations, assuming only (i) that the envelope
of $A(t)$ is different from zero in the interval $(0, \tau)$ (where $\tau$
is the pulse duration) and (ii) that the shape of $A(t)$ is such that
neither $A(t)$ nor $F(t)$ has any dc-field component. [Explicit
expressions for the fields $A(t)$ and $F(t)$ used in our numerical
examples are given in Sec. VI.]

To describe HHG and ATI in a short laser pulse of duration
$\tau$, we consider first the interaction of an atomic electron with
an infinite train of short pulses separated in time by a period
$T$ (cf. Fig. 1). Each pulse of this train is the same as for an actual
short laser pulse of duration $\tau$ described by Eqs. (1) and (2),
while $T > \tau$. The dipole interaction of such a pulse train (PT) with an atomic electron is given by

$$V_t(r,t) = \sum_{n=-\infty}^{\infty} V(r,t+nT) = -d \cdot F_t(t),$$  

where

$$F_t(t) = -\frac{1}{c} \frac{\partial A_t(t)}{\partial t} = \sum_{n=-\infty}^{\infty} F(t+nT),$$

$$A_t(t) = e_r A_t(t) = \sum_{n=-\infty}^{\infty} A(t+nT).$$

Owing to the periodicity of $V_t(r,t)$ (with period $T$), we can employ the QQES (quasienergy spectrum) approach (cf., e.g., Ref. [44]) for an ab initio treatment of nonlinear interactions of the PT with an atomic system. From the QQES expressions for the HHG and ATI amplitudes and rates for the PT, the results for a single short pulse follow by taking the limit $T \to \infty$ for fixed $\tau$. Since the QQES approach has mainly been used previously for monochromatic or two-color fields $F(t)$, in the next subsection we present the QQES results for ATI and HHG amplitudes and rates for the general case of a periodic field $F(t)$, i.e., $F(t) = F_t(t)$, as in Eq. (3).

**B. Basic QQES results for a periodic field**

In the QQES approach, after adiabatic turn on of the interaction (3), the wave function of a bound electron with energy $E_0$ evolves to the wave function

$$\Psi_t(r,t) = e^{-i t / \hbar} \Phi_t(r,t), \quad \Phi_t(t) = \Phi_t(t+\tau),$$

with the complex quasienergy $\epsilon = Re \epsilon - i(\hbar/2)\Gamma$, where $\Gamma$ is the total ionization rate of the initial bound state due to the field $F_t(t)$, while $Re \epsilon \to E_0$ as $F_t(t) \to 0$. Since we are describing the ionization of a bound state, the periodic-in-time QQES wave function $\Phi_t(r,t)$ satisfies the complex boundary condition in open $n$-photon ionization channels for $r \to \infty$:

$$\Phi_t(r,t) \sim \sum_{n>0} A_n(p_n) e^{i k_n r - i n \omega t} \frac{1}{R},$$

$$k_n = \sqrt{2m(\epsilon + n h \omega_t - u_p) / \hbar},$$

$$u_p = \frac{e^2}{2mc^2 \tau} \int_{-\tau / 2}^{\tau / 2} A^2(t) dt = \frac{e^2}{2mc^2 \tau} \int_{-\tau / 2}^{\tau / 2} A^2(t) dt,$$

$$R \equiv R(r,t) = r - \frac{|\epsilon|}{mc} \int_t^{t+\tau} A_r(t') dt',$$

$$\partial \epsilon / \partial \tau = \frac{1}{\partial \epsilon / \partial t} \frac{\partial \epsilon}{\partial \tau}.$$
The total ionization probability $\Gamma_{\text{tot}}$ for a period $T$ of the PT field $F_\tau(t)$:

$$\Gamma_{\text{tot}} = T \sum_{n > n_0} \int d\Omega_p \Gamma(p_n),$$  \tag{16}

where we have approximated $\epsilon$ by $E_0$ in Eq. (7), so that $n_0 = [(u_p - E_0)/(\hbar \omega)]$, $p_n = \sqrt{2m(E_0 + n\hbar \omega - u_p)}$, and $k_n = p_n/\hbar$. In the limit $\omega \tau \to 0$, the sum over $n$ in Eq. (16) can be replaced by an integral over the electron’s momentum $p$ [or energy $E_p = p^2/(2m)$], substituting

$$p_n = \sqrt{2m(n\hbar \omega + E_0 - u_p)} \to p,$$

$$\sum_{n > n_0} \to \frac{1}{m \hbar \omega} \int p \, dp = \frac{1}{\hbar \omega} \int dE_p.$$  \tag{18}

The result is

$$\Gamma_{\text{tot}} = \frac{2\pi}{\hbar \omega^2} \int \int |\Gamma(p)| dE_p d\Omega_p,$$  \tag{19}

where

$$\Gamma(p) = \frac{p}{m} |A(p)|^2. \quad A(p) \equiv A_n(p_i)|_{p_i = p}. \tag{20}$$

Thus the desired short-pulse probability $P(p)$ is given by

$$P(p) = \frac{2\pi p}{m \hbar \omega} \lim_{\omega \tau \to 0} \frac{|A(p)|^2}{\omega^2}. \tag{21}$$

To describe harmonic generation by an atom in a short laser pulse, we use the spectral density of radiation, $\rho(E_\Omega)$. Consider first the total energy radiated during a period $T$ of the PT $F_\tau(t)$:

$$E_{\text{tot}} = T \sum \hbar \Omega R_\Omega.$$  \tag{22}

As for the case of ATI, in the limit $T \to \infty$, the sum in Eq. (22) can be replaced by the integral:

$$E_{\text{tot}} = \lim_{\omega \tau \to 0} \frac{2\pi}{\omega^2} \int dE_\Omega \Omega R_\Omega \equiv \int dE_\Omega \rho(E_\Omega),$$

where the spectral density $\rho(E_\Omega)$ is

$$\rho(E_\Omega) = \frac{4\pi^2}{m \hbar |\tilde{\Omega}|^2} R_\Omega.$$  \tag{23}

We emphasize that the limit in Eq. (23) is taken at fixed $\Omega$. Generalization of the concept of a dual dipole moment to the case of a short laser pulse is obtained by substituting $\lambda_\Omega$ into Eq. (13) for $R_\Omega$ into Eq. (23) (using $A_\Omega = \tilde{\Omega}$):

$$\rho(E_\Omega) = \frac{\Omega^2}{4\pi^2} |\tilde{\Omega}|^2. \tag{24}$$

The Fourier transform, $\tilde{\Omega}$, of the dual dipole moment for a single short pulse is defined by the formal limit:

$$\tilde{\Omega}(\Omega) = \lim_{\omega \tau \to 0} \tilde{\Omega}_\Omega/\omega \tau,$$  \tag{25}

where $\tilde{\Omega}_\Omega$ [cf. Eq. (14)] is the Fourier component of the dual dipole moment for a periodic field.

The formal definitions in Eqs. (21) and (23) for $P(p)$ and $\rho(E_\Omega)$ in terms of ATI and HHG rates for a periodic field are quite general and are valid for any atomic system. However, in practice appropriate expressions for $A_n(p_i)$ and $D_\Omega$ are necessary in order that the limits in Eqs. (21) and (25) can be calculated. Such expressions are most easily obtained only for model systems, such as the one used in the TDER theory [36,37] to analyze strong-field processes in a monochromatic field. In Sec. III we describe briefly basic results of this model for the case of a periodic field, which will then be used to specify the spectral density (23) for a short pulse in the framework of TDER theory. (The TDER results for ATI by a short laser pulse will be published elsewhere.)

### III. TDER RESULTS FOR THE COMPLEX QUASIENERGY IN A PERIODIC FIELD

Within TDER theory [36,37] calculations of the complex quasienergy $\epsilon$ in Eq. (12) simplify so that most can be carried out analytically. This theory treats the electron in a short-range potential $U(r)$ of radius $r_c$ that supports only a single bound state $\psi_{\text{km}}(r)$ with energy $E_0 = (\hbar \omega \tau)^2/2m$, angular momentum $l$, and the following asymptotic behavior at large distances:

$$\psi_{\text{km}}(r) \approx C_{\text{cl}} r^{-l} e^{-\kappa r} Y_{lm}(\hat{r}),$$  \tag{26}

where $C_{\text{cl}}$ is a (dimensionless) asymptotic coefficient. In the TDER model the interaction of the active electron with the potential $U(r)$ is described by the $l$-wave scattering phase shift $\delta_l(k)$ ($k = \sqrt{2mE_0}/\hbar$). This phase is parameterized within effective range theory [49] in terms of the scattering length ($a_l$) and the effective range ($r_l$), which are the parameters of the problem.

The solution of the QQES problem within the TDER model simplifies significantly owing to the boundary condition for the QQES wave function $\Phi_{\tau}(r,t)$ in this model at small distances, $r \lesssim r_c$ (cf. Refs. [36,37] for details):

$$\int \Phi_{\tau}(r,t) Y_{lm}^* \, d\Omega \sim \frac{1}{(2l+1)!} B_l(\epsilon) (r^l + \cdots) \, g(t),$$  \tag{27}

where $\epsilon$ is the complex quasienergy in the combined field $F(t)$, which is required for calculation of the HHG amplitude according to Eq. (12):

$$F(t) = e_\tau F(t) = F_\tau(t) + F_\sigma(t).$$  \tag{28}

In Eq. (27), $g(t)$ is a periodic function with period $T$, and the parametrization of the coefficient $B_l(\epsilon)$ is very similar to that for the scattering phase $\delta_l(k)$ [49]:

$$(2l+1)!!(2l+1)!! B_l(\epsilon) = k^{2l+1} \cot \delta_l(k) = -\frac{1}{a_l} + \frac{1}{2} k^2, \quad k = \sqrt{2m\epsilon}/\hbar.$$  

Within the TDER theory, the four-dimensional (in $r$ and $t$) TDSE for $\epsilon$ and $\Phi_{\tau}(r,t)$ reduces to a homogeneous one-dimensional integro-differential equation (a key advantage), representing an eigenvalue problem for $\epsilon$ and $g(t)$. For a
bound s state, this equation is (cf. the similar results for a monochromatic field in [36,37])

\[ g(t) = \frac{\kappa r_0}{2|E_0|} \left( \Delta g(t) + i\hbar \frac{dg(t)}{dt} \right) \]

\[ = \frac{2\pi \hbar^2}{k\hbar} \int_0^\infty d\tau \left[ G(t,t+\tau) g(t+\tau) e^{i\epsilon \tau} \right] \]

\[ - G(0)(t,t-\tau) g(t) \].

(29)

Here \( \Delta \epsilon = \epsilon - E_0 \), \( G^{(0)}(t,t-\tau) \equiv G^{(0)}(r = 0, t, r' = 0, t-\tau) \) is the ordinary retarded Green’s function for a free electron, and \( G(t,t-\tau) \equiv G(r = 0, t, r' = 0, t-\tau) \) is that for an electron in the field \( \mathcal{F}(t) \). Equation (29) and the equivalent infinite system of homogeneous linear equations for \( \epsilon \) and the Fourier coefficients of the function \( g(t) \) are convenient for numerical analyses. However, for analytical analyses it is more convenient to represent Eq. (29) in terms of the quasienergy representations, \( G^{(0)}(t,t-\tau) \) and \( G_r(t,t-\tau) \), of the Green’s functions \( G^{(0)}(t,t-\tau) \) and \( G(t,t-\tau) \). An explicit form of \( G_r(t,t';t,t') \) for a monochromatic field can be found in Ref. [50]. Using the relation between \( G_r(t,t';t,t') \) and \( G_r(t,t';t,t') \) [50] (cf. also Appendix B in Ref. [41]), the integral form in Eq. (29) can be represented as

\[ \int_0^\infty [G(t,t-\tau) g(t-\tau) e^{i\epsilon \hbar \tau} - G_0(t,t-\tau) g(t)] d\tau \]

\[ = \frac{1}{T} \int_{-T/2}^{T/2} \tilde{G}_r(t,t') g(t') dt', \]

(30)

where

\[ \tilde{G}_r(t,t') \equiv \tilde{G}_r(t,t') - \tilde{G}_r^{(0)}(t,t') \]

\[ = -\frac{m}{2\pi \hbar^2} \exp \left( -\frac{i}{\hbar} \int_0^{t'} \left( \frac{e^2 \mathcal{A}^2(t'')}{2mc^2} - \tilde{u}_p \right) dt'' \right) \]

\[ \times \sum_n e^{-i\eta_n (t-t')} \frac{1}{|\mathcal{R}(t,t')|} \]

\[ \mathcal{R}(t,t') = \left| \frac{e}{mc} \right| \int_0^{t'} A''(t') dt', \]

\[ A(t) = A_r(t) - \frac{e F_h}{\Omega} \sin(\Omega t + \phi_h), \]

\[ \tilde{u}_p = \frac{e^2}{2mc^2 T} \int_{-T/2}^{T/2} A^2(t) dt, \]

\[ \hbar^2 \tilde{u}^2 = n \hbar \omega_r + \epsilon - \tilde{u}_p, \]

and \( \mathcal{A}(t) = \mathbf{e} \cdot \mathcal{A}(t) \) is the vector potential of the field \( \mathcal{F}(t) \). The result is the following alternative form of the basic TDER equation (29) for a periodic field:

\[ g(t) = \frac{\kappa r_0}{2|E_0|} \left( \Delta g(t) + i\hbar \frac{dg(t)}{dt} \right) \]

\[ = \frac{2\pi \hbar^2}{mk\hbar} \int_{-T/2}^{T/2} \tilde{G}_r(t,t') g(t') dt'. \]

(36)

IV. QUASICLASSICAL RESULTS FOR THE HHG AMPLITUDE AND SPECTRAL DENSITY \( \rho(E_\omega) \) IN TDER THEORY

We consider harmonic generation by a short pulse whose vector potential \( A(t) \) and electric field \( F(t) \) are slowly varying on the atomic time scale of order \( T_0 = \hbar/|E_0| \). For a short pulse with carrier frequency \( \omega_c \), this is equivalent to

\[ h\omega_c \ll |E_0|. \]

Moreover, we assume that

\[ \max\{|F(t)|\} \ll F_c, \quad F_c = \sqrt{8m|E_0|^2/(|e|\hbar)}, \]

(37)

where \( \max\{|F(t)|\} \) is the maximum value of \( F(t) \) in the interval \((0,T)\). When the conditions (37) and (38) are fulfilled, the TDER result for \( \rho(E_\omega) \) can be obtained in analytic form in the quasiclassical approximation. In order to carry out the limiting procedure in Eq. (25), we obtain first the quasiclassical result for the HHG amplitude \( \tilde{D}_\omega \) for small but finite \( \omega_r \), e.g., \( \omega_r \ll \omega_c \).

A. Analytic results for a periodic field

Since for a slowly varying short pulse the function \( g(t) \) in Eq. (36) also varies slowly with \( t \), we can set \( g(t) = \) constant and then average Eq. (36) in \( t \) over the period \( T \). (This procedure is similar to the adiabatic approximation used for the case of a monochromatic field [51] and its accuracy for describing HHG for this case is discussed in Ref. [41].) Thus, Eq. (36) reduces to a transcendental equation for the complex quasienergy \( \epsilon \):

\[ 1 - \frac{\kappa r_0}{2|E_0|} (\epsilon - E_0) = \mathcal{I}(\epsilon, F_h), \]

(39)

where

\[ \mathcal{I}(\epsilon, F_h) = \frac{2\pi \hbar^2}{mk\hbar T} \int_{-T/2}^{T/2} \tilde{G}_r(t,t') dt. \]

(40)

[Note that Eq. (39) at \( F_h = 0 \) gives the transcendental equation for the quasienergy \( \epsilon \) in the PT field \( \mathcal{F}_h(t) \).] Applying \( \epsilon = \epsilon + \Delta \epsilon \) (where \( \Delta \epsilon \propto F_h \)) and expanding the right side of Eq. (39) to first order in both \( F_h \) and \( \Delta \epsilon \), we obtain an expression for the linear (in \( F_h \)) correction \( \Delta \epsilon \) to the complex quasienergy \( \epsilon \) in the PT field \( \mathcal{F}_h(t) \) induced by a weak harmonic field \( \mathcal{F}_h(t) \):

\[ \Delta \epsilon = -\frac{F_h}{\kappa r_0/(2|E_0|) + \mathcal{I}_0'(\epsilon,0)}, \]

(41)

where \( \mathcal{I}_0' = \partial \mathcal{I}_0/\partial x \). In the quasiclassical approximation, the quasienergy \( \epsilon \) in Eq. (41) can be approximated by \( E_0 \). Moreover, the denominator in Eq. (41) is connected to the normalization factor for the QQES wave function [36,37] and may be approximated by its unperturbed value:

\[ \kappa r_0/(2|E_0|) = \mathcal{I}_0'(\epsilon,0) \approx -(|E_0|c_0^2)^{-1}, \]

where the asymptotic coefficient \( c_0 \) is defined by Eq. (26). Thus the result (41) for \( \Delta \epsilon \) reduces to

\[ \Delta \epsilon = F_h c_0^2 \mathcal{I}_0'(E_0,0)|E_0|. \]

(42)
As shown in Appendix A, the derivative \( \mathcal{T}_{yE} \) can be parameterized in terms of Fourier components \( \tilde{D}_{\pm \Delta} \) of the dual dipole moment [cf. Eq. (14)]:

\[
4C_{\phi 0}[E_0] \mathcal{T}_{yE} (E_0, 0) = \tilde{D}_{\pm \Delta} e^{i \phi} + \tilde{D}_{-\pm \Delta} e^{-i \phi},
\]

where the HHG amplitude \( \tilde{D}_{\pm \Delta} \) can be expressed as

\[
\tilde{D}_{\pm \Delta} = i \chi_{\pm \Delta}^{\phi} i \left( \chi_{\pm \Delta}^{\phi} \right)^*) = e^{i \phi} \left[ \tilde{C}_{\pm \Delta} e^{i \phi} + \tilde{C}_{-\pm \Delta} e^{-i \phi} \right],
\]

The labeled times \( t_n^p = \left[ t_n^p (p_n) \right] \) in Eq. (45) are roots of the saddle-point equation,

\[
P_s \left( t_n^p ; p_n \right) = \left[ C_{\pm \Delta} - \left( \sigma \right) \right] = 0,
\]

having positive imaginary part, \( \text{Im} \geq 0 \).

As in the monochromatic field case [52], Eqs. (44) and (45) for the HHG amplitude of a PT field \( F_i(t) \) have a clear physical interpretation. They express the HHG amplitude as a coherent sum of partial amplitudes corresponding to the generation of harmonics by an electron created in the continuum by \( n \)-photon ATI. For a given \( n \), these amplitudes are determined by the saddle points \( t_n^p \) of the classical action \( S(t, t_1; p_n) \) [cf. Eq. (49)], which may be interpreted as complex “ionization times.” Finally, \( \sigma = \pm 1 \) distinguishes electrons escaping in opposite directions along the polarization vector \( \mathbf{e}_z \). The number of saddle points \( n^p \) contributing to the sum over \( n^p \) in Eq. (44) depends on the phase of the vector potential \( A(t) \).

For a monochromatic field of frequency \( \omega_r \), only two saddle points (with \( \sigma = \pm 1 \)) contribute, in which case our results (44) and (45) coincide with those of Ref. [52] as well as with those obtained within the quasiclassical approximation for the TDRE model [41].

**B. Analytic results for a short pulse**

To apply the quantum results (44) and (45) for the HHG amplitude \( \tilde{D}_{\pm \Delta} \), obtained for the case of a finite \( \omega_r \), to the case of a single short pulse (i.e., in the limit \( \omega_r \rightarrow 0 \)), we use the definition of the Fourier transform \( \tilde{D} \) in Eq. (25). Replacing the sum over \( n \) in Eq. (44) by an integral over the electron’s momentum \( p \) according to Eqs. (17) and (18), the right side of Eq. (44) becomes proportional to \( 1/\mathcal{T} \) [\( \omega_r \rightarrow 0 \)], the limit \( \omega_r \rightarrow 0 \) in Eq. (25) is thus finite, giving the result

\[
\tilde{D} \left( \omega \right) = \frac{1}{\mathcal{T}} \int_{-\infty}^{\infty} \tilde{D} \left( t \right) e^{i \omega t} \, dt,
\]

where

\[
\tilde{D} \left( t \right) = \frac{1}{2\pi} \sum_{\sigma = \pm 1} \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dp \, \langle \tilde{D} \rangle \left( t, p \right),
\]

\[
\tilde{D} \left( t, p \right) = \left| E_0 \right|^2 \left( \frac{\omega_0}{\omega_0} \right)^2 e^{-i \omega_0 t} \frac{P_s \left( t^0 \right)}{\mathcal{T}} \left[ \frac{S \left( t, t^0 \right)}{2m} - E_0 \right] \left( \frac{1}{\omega} \right)^2 dt,
\]

Approximate evaluations of the integrals in Eqs. (50) and (51) (derived in Appendix B) lead to further simplifications of the HHG amplitude \( \tilde{D} \Omega \) for a single short pulse. For a short pulse with given carrier frequency \( \omega_0 \) and carrier-envelope phase (CEP) \( \phi_0 \), we parametrize the vector potential \( A(t) \) in Eq. (1) as follows:

\[
A(t) = f(t) \sin(\omega_0 t + \phi),
\]

where the pulse envelope \( f(t) \) has its maximum at \( t = 0 \).

The results in Appendix B, derived for a vector potential \( A(t) \) of arbitrary form, show that when \( A(t) \) has the form in Eq. (52), then the generation amplitude has the form presented in Ref. [22], i.e., a coherent sum of partial amplitudes \( A_j \) describing the generation of radiation with frequency \( \Omega \) by electrons ionized at each \( j \)th optical half-cycle of the pulse described by (52)

\[
\tilde{D} \left( \Omega \right) = \sqrt{-i} \left| \frac{e_0}{\omega_0} \right| \sum_{j = \pm 1} \left( A_j \right) e^{i \omega_j},
\]

\[
A_j = \chi_{j}^{(j)} \chi_{\omega}^{(j)} \chi \left( E_0 \right),
\]

\[
h \omega_j = \left( E_0 - E \right) - \frac{\mathcal{E}_{\max} \left( t_{\max} \right)}{\mathcal{T}} - E_0 \left( \mathcal{T} \right) dt,
\]

where \( E_\omega = h \omega, E_0 = \left| E_0 \right|, \) and the index \( j \) enumerates the ionization (\( t_{\max} \)) and recombination (\( t_{\min} \)) times for the \( j \)th half-cycle [where \( t_{\max} \) lies in the \( (j + 1) \)th half-cycle]. These times satisfy equations for the extreme classical trajectory (starting and ending at times \( t_{\max} \) and \( t_{\min} \)) along which an electron has zero initial velocities.

Each dimensionless partial amplitude \( A_j \) in Eq. (54) has three factors, in accord with the three-step scenario for HHG: ionization of the active electron in an atom by laser-induced tunneling, propagation along a closed trajectory driven by the laser field, and finally, recombination to the initial bound state of the parent atom accompanied by emission of a harmonic photon \( h \Omega \).

The tunneling factor (\( \chi_{\omega} \)) in Eq. (54) has the form

\[
\chi_{\omega}^{(j)} = \frac{4\pi \omega_0 e_0}{c} \int \left[ e^{-i \omega_0 t} \mathcal{T} \right] \left( \frac{\mathcal{T}}{\mathcal{T}} - \mathcal{T} \right)^2 dt,
\]

\[
\tilde{F}_{\omega} \left( \frac{\mathcal{T}}{\mathcal{T}} \right) = \frac{\mathcal{E}_{\max} \left( t_{\max} \right)}{\mathcal{T}} - E_0 \left( \mathcal{T} \right) dt,
\]

\[
\omega_j = \frac{2m \left| E_0 \right| \omega_0}{e \tilde{E}_{\omega}}, \quad \tilde{E}_{\omega} = \sqrt{m^2 \left| E_0 \right|^2 e^2},
\]

where \( \tilde{E}_{\omega} \equiv \tilde{F}_{\omega} \left( \mathcal{T} \right) \) [cf. Eq. (B17)], \( F_0 = (\omega_0)^3 |F_0|, F_\omega = \left| \right|^{2} / \left| a_0 \right|^2, a_0 = h^2 / (me^2) \) is the Bohr radius, and \( \tilde{E}_{\omega} \) is an effective
The term $w$ value of the Keldysh parameter $\chi^{(j)}$, is that it is the detachment amplitude for low-energy $[E = p^2/(2m) \rightarrow 0]$ electrons ejected by a laser pulse along its polarization axis. In the tunneling regime, the dominant term in an expansion of the short-pulse detachment amplitude, $\mathcal{A}(p, F)$, in the Keldysh parameter has a form similar to that for a monochromatic field with amplitude $F$ [54] (cf. Ref. [55]):

$$\mathcal{A}(p = 0, F) = \frac{C_{\text{v}} \sqrt{\gamma}}{2\pi} \sqrt{\frac{F}{F_0}} e^{-\frac{F}{F_0}/(3F_0)}.$$  

(59)

Comparing Eqs. (58) and (59), $\chi^{(j)}$ can be presented in terms of the detachment amplitude:

$$\chi^{(j)} = 8\pi A(\mathbf{p} = 0, \tilde{F}_j)/(k^{5/2}a_0^2).$$  

(60)

The factor $\chi^{(j)}$ in Eq. (54) describes propagation of an electron (tunnel-ionized in the $j$th half-cycle) in the laser-dressed continuum. It involves an Airy function $\text{Ai}(\xi_j)$:

$$\chi^{(j)} = \frac{\text{Ai}(\xi_j)}{\zeta_j^{1/3}(\omega_{\text{at}} \Delta t_j)^{1/2}},$$  

(61)

where $\Delta t_j = t^{(j)} - t^{(j)}$. 

$$\xi_j = -\frac{I_{\text{cut}}^{(j)}}{2I_{\text{at}}} \left( 1 - \frac{F(t^{(j)})}{F(t^{(j)}) + \tilde{F}(t^{(j)}) \Delta t_j} \right),$$  

(62)

$$\zeta_j = E - E_{\text{cut}}^{(j)},$$  

(63)

$$E_{\text{cut}}^{(j)} = E_{\text{cut}}^{(j)} + F(t^{(j)}) |E_0|,$$  

(64)

$$E_{\text{cut}}^{(j)} = \frac{e^2}{2mc^2}(A(t^{(j)}) - A(t^{(j)}))^2,$$  

(65)

and $\omega_{\text{at}} = 2.6 \times 10^{17}$ s$^{-1}$, $E_{\text{at}} = 27.21$ eV, $I_{\text{at}} = 3.51 \times 10^{16}$ W/cm$^2$.

The last factor, $\chi_{\sigma}(E)$, in Eq. (54) describes the recombination step of the three-step scenario:

$$\chi_{\sigma}(E) = C_{\text{v}} \frac{q}{(q^2 + 1)^2},$$  

(66)

where $q = \sqrt{E/|E_0|} = p/(\hbar v$).

Substituting the amplitude (33) into Eq. (24), the spectral density $\rho(E_{\text{th}})$ acquires the factorized form [26–28]

$$\rho(E_{\text{th}}) = w(E, F) e^{\sigma^{(j)}(E)}.$$  

(67)

Here $\sigma^{(j)}(E)$ is the TDER result for the differential PRCS of an electron with momentum $p$ ($p = \sqrt{2mE}$) parallel to the polarization direction $\mathbf{e}_0$ of the harmonic (recombination) photon of energy $E_{\text{th}}$ (cf. Ref. [42]):

$$\sigma^{(j)}(E) = a^2 \chi_{\sigma}^{(j)}(E)(\frac{q^2 + 1}{q})^{2} a_0^2, \quad a = e^2/(\hbar c).$$  

(68)

The term $w(E, F)$ in Eq. (67) is the EWP, which can be presented as follows:

$$w(E, F) = \sum_{j,k} s_{jk} \sqrt{\frac{w_j}{w_k}} \cos(\phi_j - \phi_k).$$  

(69)

where $s_{jk} \equiv (-1)^{i+j} \text{sign}(\chi_{\sigma}^{(j)} u_{\text{th}}^{(j)})$. As for the case of a monochromatic field [25], the partial EWP $w_j$ for the $j$th half-cycle can be presented as a product of tunneling ($I_j$) and propagation ($\nu_j$) factors:

$$w_j = \frac{\pi \Omega}{2a_0} I_j \nu_j,$$  

(70)

$$I_j = \frac{1}{16\pi} (\chi^{(j)}(\kappa a_0))^6 \frac{\nu_j}{\pi \kappa v_{\text{at}}},$$  

(71)

$$\nu_j = \frac{p}{m a_0^2} (\chi_{\sigma}^{(j)})^2 = \frac{p}{m} (v_{\text{at}} \Delta t_j)^2 \zeta_j^{-2/3},$$  

(72)

where $\Gamma_{\sigma}(\tilde{F}_j)$ is the decay rate for a weakly bound $s$-state electron in a static electric field $F$ [56]:

$$\Gamma_{\sigma}(F) = C_{\text{v}} \sqrt{\frac{F}{F_0}} e^{-2F_0/(3F_0)} |E_0| / \hbar.$$  

(73)

As Eqs. (70)–(72) show, the magnitude of the $j$th EWP $w_j$ is governed by the dc ionization rate $\Gamma_{\sigma}(\tilde{F}_j)$, where $\tilde{F}_j$ is close to the maximum value of the field $F(t)$ during the $j$th half-cycle. Since the magnitude of $\Gamma_{\sigma}(\tilde{F}_j)$ decreases exponentially with decreasing $\tilde{F}_j$, only a few optical half-cycles near the peak intensity of a short pulse contribute significantly to the sum in Eq. (69). For each half-cycle, the propagation factor $\nu_j$ describes plateau structures in the spectrum of harmonics generated by electrons created during this half-cycle. In particular, the position of the $j$th plateau cutoff, $E_{\text{cut}}^{(j)}$, is given by an equation similar to that for a monochromatic field [42]:

$$E_{\text{cut}}^{(j)} = |E_0| + \varepsilon_{\text{cut}}^{(j)} (I_j - I_j^{(j)}),$$  

(74)

\[ \frac{F(t^{(j)})}{F(t^{(j)})} |E_0| - 1.019 \xi_j^{1/3} E_{\text{at}}. \]

V. GENERALIZATION TO THE ATOMIC CASE

The TDER results for $\rho(\Omega)$ presented in Sec. IV are valid for a weakly bound electron in an $s$ state. However, we have confirmed that the derivations described in Appendix B can be generalized for the case of a weakly bound state with nonzero angular momentum $l$ in a way similar to that used to obtain our TDER HHG results for a bound $p$ state in a monochromatic field [41]. As in the latter case, since the centrifugal barrier suppresses the return of a continuum electron with $l > 0$ to the atomic core, the harmonic yield for substates with nonzero angular momentum projection $m$ (in which case $l \geq |m|$) is suppressed by a factor $|E_0| \Delta t_j / \hbar^{2|m|} \sim |E_0| / \hbar \omega^{2|m|}$ compared to the case $m = 0$. Nevertheless, our analysis (not presented) shows that the spectral density $\rho(\Omega)$ for $m = 0$ has the factorized form (67) with the same partial propagation factors (72) as for $l = 0$. Thus $\nu_j$ is essentially independent of the spatial symmetry of the bound state, while both $I_j$ and $\sigma(E)$ are sensitive to $l$. Moreover, we note that the TDER PRCS (68) coincides with that in the Born approximation since, as a consequence of dipole selection rules, it is determined by the $p$-wave scattering phase, which is zero in the TDER model for a single bound $s$ state. However, our recent analysis in Ref. [57] for the TDER model with two ($s$ and $p$) bound states
shows that, indeed, the TDER HHG results involve the exact (non-Born) result for the PRCS \( \sigma(E) \).

The analytic results (67)–(72) describing HHG by a short laser pulse thus involve only two constituents, \( \mathcal{I}_j \) and \( \sigma(E) \), that depend on the atomic model employed. Since both of these constituents have a transparent physical meaning, it is reasonable to expect that the generalization of the TDER results for \( \rho(\Omega) \) to the case of neutral atoms (as well as their positive and negative ions) requires only the replacement of \( \mathcal{I}_j \) and \( \sigma(E) \) by their corresponding atomic counterparts. The result (71) for \( \mathcal{I}_j \) should thus be replaced by

\[
\mathcal{I}_j = \frac{4\pi^2 \Gamma_{\text{at}}(\tilde{F}_j)}{(2l + 1)\pi \kappa_{\text{at}}},
\]

\[
\Gamma_{\text{at}}(\tilde{F}_j) = \left( \frac{E_0}{\hbar} \right)^2 \left( \frac{2F_{\text{at}}}{\tilde{F}_j} \right)^{2l+1} e^{-2F_{\text{at}}/(3\tilde{F}_j)},
\]

where \( \Gamma_{\text{at}}(F) \) is the tunneling rate for a bound atomic electron [in the state \( \psi_{\text{clm}}(r) \) with energy \( E_0 \), angular momentum \( l \), and projection \( m = 0 \) in a static electric field \( e\tilde{F}_j \) [56], and \( C_j \) is determined by the asymptotic form of \( \psi_{\text{clm}}(r) \) [cf. Eq. (26)]:

\[
\psi_{\text{clm}}(r)_{kr>1} = C_j \sqrt{\tilde{r}} e^{-r} Y_{lm}(\hat{r}),
\]

where \( r = Z/(\kappa a_0) \) and \( Z \) is the charge of the atomic core. Also, the TDER PRCS (68) should be replaced by the corresponding cross section \( \sigma^{(2)}(E) \) for the specific atom considered. For the ground-state H atom, \( \sigma^{(2)}(E) \) is known analytically [58],

\[
\sigma^{(2)}(E) = 32\pi^2 \alpha^4 \frac{e^{-4\pi \sqrt{q}} \text{arc}(q)}{q^2(1 + q^2)^2(1 - e^{\pi q/q})^2}, \quad q = \frac{pa_0}{\hbar},
\]

while for other atoms experimental or theoretical data for \( \sigma^{(2)}(E) \) should be used.

We present the resulting generalized expression for the spectral density \( \rho(E_\Omega) \) in a way that separates terms with \( j = k \) and \( j \neq k \) in the sum in Eq. (69):

\[
\rho(E_\Omega) = w(E) \sigma^{(2)}(E),
\]

where the EWP \( w(E) \) is given by

\[
w(E) = w_{\text{dir}} + w_{\text{int}}.
\]

The “direct” term \( w_{\text{dir}} \) includes only terms with \( j = k \) and is given by the sum of half-cycle EWPs \( w_j(E) \):

\[
w_{\text{dir}} = \sum_j w_j(E),
\]

\[
w_j(E) = \frac{\pi \Omega}{2\Omega^2} \mathcal{I}_j W_j,
\]

where \( \mathcal{I}_j \) and \( W_j \) are given by Eqs. (72) and (75). The “interference” term \( w_{\text{int}} \) originates from the interference between the half-cycle amplitudes \( A_j \) and \( A_k \) (\( j \neq k \)) and thus involves their phase difference:

\[
w_{\text{int}} = \sum_{j \neq k} s_{kj} \sqrt{w_j(E)w_k(E)} \cos(\varphi_j - \varphi_k),
\]

where the phase \( \varphi_j \) is given by Eq. (55).

VI. NUMERICAL RESULTS

A. Comparison with TDSE results

In order to check the accuracy of our analytical results, we present comparisons with results of direct numerical solutions of the three-dimensional (3D) TDSE. The TDSE was solved by two different methods, both of which used the dipole length gauge:

(i) in spherical coordinates using a spherical harmonic expansion of the wave function (cf. Refs. [59,60]), and

(ii) in cylindrical coordinates using a split-step method with a fast Fourier transform with respect to \( z \) and a discrete Fourier-Bessel transform with respect to \( \rho \) (cf. Refs. [31,61,62]).

In the first method, \( f(t) \) in Eq. (52) has a sin² shape:

\[
f(t) = -\frac{cF}{\omega} \left\{ \begin{array}{cl}
\sin^2 \left( \frac{\tau}{\tau_g} \right), & t \in [0, \tau], \\
0, & \text{otherwise},
\end{array} \right.
\]

where \( F \) is the peak value of the electric field \( F(t) \), \( \tau = 2\pi N/\omega \), and \( N \) is the number of optical cycles in the laser pulse. In Fig. 2 we present numerical results for a peak intensity \( I = cF^2/(8\pi) = 10^{14} \text{ W/cm}^2 \) and a wavelength \( \lambda = 3.1 \mu\text{m} \) (\( \hbar \omega = 0.4 \text{ eV} \)). For these parameters, the convergence of the numerical results is achieved by solving the TDSE within the sphere defined by \( 0 \leq r \leq 5000 a_0 \), with a uniform radial grid step \( \Delta r = 0.022 a_0 \), a uniform temporal step \( \Delta t = 0.022 T_{\text{at}}(E_\text{at} = \hbar/\epsilon_{\text{at}} \approx 2.42 \times 10^{-17} \text{s} \), and including orbital angular momenta \( L \) up to \( L_{\text{max}} = 500 \).

In the second method, a Gaussian-like parametrization of the laser pulse is used:

\[
\mathcal{A}(t) = \frac{\partial \mathcal{A}(t)}{\partial t}, \quad \mathcal{F}(t) = -\frac{1}{c} \frac{\partial^2 \mathcal{A}(t)}{\partial t^2},
\]

\[
\mathcal{A}(t) = e^{-\frac{t^2}{a^2}} \tilde{f}(t) \cos(\omega t + \phi),
\]

\[
\tilde{f}(t) = \exp \left[ -2\ln(2) \left( \frac{t^2}{\tau_g^2} \right)^{-1} \right],
\]

where \( \tau_g = 2\pi N/\omega \), and \( N \) is the number of optical cycles in the full width at half maximum (FWHM). (Note that the FWHM for a sin²-shaped pulse is about three times smaller than for a Gaussian pulse with the same \( N \).) Numerical results are presented for \( \lambda = 1.6 \mu\text{m} \) (\( \hbar \omega = 0.775 \text{ eV} \)) and \( I = 2 \times 10^{14} \text{ W/cm}^2 \). Calculations for this case (cf. Fig. 3) were performed within the cylinder bounded by \( -z_{\text{max}} \leq z \leq z_{\text{max}} \), \( 0 \leq \rho \leq \rho_{\text{max}} \), with \( z_{\text{max}} = 614 a_0 \), \( \rho_{\text{max}} = 59 a_0 \). To avoid reflection from the boundary of the cylinder, the imaginary potential method [63] was used to absorb the wave function at the boundary. A uniform grid was used for both the integrations over time (with grid step size \( \Delta t = 0.025 T_{\text{at}} \)) and over \( z \) (with \( \Delta z = 0.3 a_0 \)), whereas the grid nodes in \( \rho \) were placed nonuniformly: The grid was more dense near \( \rho = 0 \), and the total number of nodes, \( N_{\rho} \), was 420.

As shown in Figs. 2 and 3, the results of the analytic formula in Eq. (78) are in excellent agreement with the numerical TDSE results, reproducing even the most minor details of the HHG spectra at the high-energy end of the plateaus. Small deviations of the analytic results from the TDSE results shown
in Fig. 3 at the lower energy end of the HHG spectrum originate from the depletion (∼20%) of the ground state in an intense field, whereas this depletion is negligible (<2%) for the longer wavelength results shown in Fig. 2. It is well established by many theoretical and experimental groups that the shape of $\rho(E_\text{cut})$ depends crucially on the CEP [12–16,18–21] (see also reviews [2,7–9]); i.e., for $\phi = 0$ [cf. Figs. 2(a)–2(c) and 3(a)], two-plateau structures in HHG spectra are observed, while for $\phi = \pi/2$ there is sometimes only a single plateau in each HHG spectrum [cf. Figs. 3(d)–3(f)]. We note that the shapes of the high-energy plateaus in Figs. 2 and 3 are sensitive to the partial ($j$th half-cycle) Keldysh parameters $\tilde{\gamma}_j$ [cf. Eq. (58) and Table I]. In particular, for the low-frequency case: (i) two-plateau structures are observed even for the sine-like ($\phi = \pi/2$) pulse [cf. Figs. 2(e)–2(f)]; and (ii) additional bump-like structures can appear beyond the second plateau cutoff [cf. Figs. 2(d)–2(e)]. Such crucial dependence of the shapes of HHG spectra on the laser parameters (e.g., CEP, wavelength, and pulse envelope) can be clearly explained in the framework of the present analytic theory, as we show in the following three subsections.

### TABLE I. Numerical values of $I_j$ (75), $E^{ij}_\text{cut}$ (74), and $\tilde{\gamma}_j$ (58) for three half-cycles in Figs. 2(b) and 2(e). $|E_\text{cut}| = 13.605$ eV.

<table>
<thead>
<tr>
<th>$\phi = 0$</th>
<th>$\phi = \pi/2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$j$</td>
<td>$I_j$</td>
</tr>
<tr>
<td>2</td>
<td>5.76(−9)</td>
</tr>
<tr>
<td>3</td>
<td>5.40(−6)</td>
</tr>
<tr>
<td>4</td>
<td>1.18(−5)</td>
</tr>
</tbody>
</table>

FIG. 2. (Color online) HHG spectra of the H atom for a sin²-shaped pulse [cf. Eq. (83)] with peak intensity $I = 10^{14}$ W/cm² and $\lambda = 3.1$ μm. Gray area: Spherical coordinate TDSE results (see text); solid (blue) lines: analytic results using Eq. (78). Results are given for three values of $N$, the number of cycles per pulse, and two values of the CEP, $\phi$, as shown in each panel. Arrows mark the positions of $E^{ij}_\text{cut}$ [cf. Eq. (74)] given in Table I for three half-cycles $j$.

FIG. 3. (Color online) The same as in Fig. 2, but for a Gaussian pulse [cf. Eq. (84)] with $I = 2 \times 10^{14}$ W/cm² and $\lambda = 1.6$ μm. Gray area: Cylindrical coordinate TDSE results (see text).
B. Subcycle and intercycle interferences in short-pulse HHG spectra

To understand the interference features of the short-pulse HHG spectra, it is necessary to examine the role of the various contributions to the spectra. The contribution of a partial wave packet $w_j$ to the total HHG amplitude is governed by both the ionization [cf. Eq. (75)] and the propagation [cf. Eq. (72)] factors. However, the ionization factor determines only the magnitude of $w_j$ and does not depend on the harmonic energy $E_\Omega$. Its value depends only on the ionization potential $|I_j|$ and the electric field $\tilde{F}_j$ at the moment of ionization [in fact, this field is close to the maximum value of $F(t)$ during the $j$th half-cycle]. In the contrast, the propagation factor depends essentially on $E_\Omega$. This factor oscillates for $E_\Omega < E_{\text{cut}}^{(j)}$ and decreases exponentially in the region beyond the cutoff, $E_\Omega > E_{\text{cut}}^{(j)}$, where the cutoff energy for the $j$th half-cycle is given by Eq. (74). If for a given laser pulse there are only a few half-cycles with large values of $E_{\text{cut}}^{(j)}$, but for which $E_{\text{cut}}^{(j)}$ is considerably larger than $E_{\text{cut}}^{(j)}$, while $\tilde{F}_j < \tilde{F}_j$, and $E_{\text{cut}}^{(j)} > E_{\text{cut}}^{(j)}$ but $\tilde{F}_j < \tilde{F}_j$, and so on, then a multiplateau structure is formed in the high-energy part of the HHG spectrum owing to the absence of overlapping partial HHG amplitudes, $A_j$. In Table I we present the three largest values of $E_{\text{cut}}^{(j)}$ together with the ionization factors $I_j$ and the effective Keldysh parameters $\tilde{\gamma}_j$ for the laser parameters applicable to the results in Figs. 2(b) and 2(e). For the cosine-pulse ($\phi = 0$) results in Fig. 2(b), the partial amplitude for $j = 2$ is suppressed relative to the partial amplitudes with $j = 3$ and $j = 4$ owing to the smallness of the ionization factor $\tilde{\gamma}_2$, while for the sine-pulse ($\phi = \pi/2$) results in Fig. 2(e) the contributions from all three half-cycles (with $j = 2, 3, 4$) are clearly visible.

The difference in HHG spectra for cosine-like ($\phi = 0$) and sine-like ($\phi = \pi/2$) pulses is clearly seen in Figs. 2 and 3: For $\phi = 0$, high-energy plateaus exhibit large-scale oscillations [cf. Figs. 2(a), 3(a)], while for $\phi = \pi/2$ these oscillations are modulated by fine-scale oscillations [cf. Figs. 2(f) and 3(d)]. The origin of the large-scale oscillations is the same as for a monochromatic field [25]; i.e., these oscillations originate from the interference of long and short electron trajectories for a given $j$th half-cycle and are described by the Airy function in Eq. (72). The fine-scale modulations originate from interference between different amplitudes $A_j$; they are described by the term $\tilde{w}_{\text{int}}$ in Eq. (82) [22]. This term simplifies when the interference of only two neighboring amplitudes in $\tilde{w}_{\text{int}}$ is significant:

$$\tilde{w}_{\text{int}} \approx 2 s_{j_1, j_2} \sqrt{w_{j_1} w_{j_2}} \cos (\varphi_{j_1} - \varphi_{j_2}).$$

(85)

Equations (85) and (55) allow one to estimate the distance $\Delta E_\Omega$ between two adjacent fine-scale peaks as the distance over which the phase difference in Eq. (85) changes by $2\pi$:

$$\Delta E_\Omega = \frac{2\pi \hbar}{\Delta t_0^{(j)}},$$

(86)

where $\Delta t_0^{(j)}$ is the difference between recombination times for two $(j+1)$th and $j$th neighboring half-cycles: $\Delta t_0^{(j)} = t_0^{(j+1)} - t_0^{(j)}$. (Since $t_0^{(j)} \sim \omega^{-1}, \Delta E_\Omega$ is of order $\hbar \omega$.) For a single-cycle ($N = 1$) cosine-like pulse, the fine-scale interference pattern appears in the region of the first plateau [cf.

FIG. 4. (Color online) Dependence of ionization factors $I_j$ (75) and cutoff energies $E_{\text{cut}}$ (74) on the half-cycle number $j$ for laser parameters as in Fig. 3. Panels (a), (b): $\phi = 0$; panels (c), (d): $\phi = \pi/2$. Red lines with circles: $N = 1$; black lines with squares: $N = 2$; blue lines with triangles: $N = 3$.

Fig. 3(a) since it originates from the interference of amplitudes $A_j$ with $j = 2$ and $j = 3$ as is clear from Figs. 4(a) and 4(b)]. For $E_\Omega > E_{\text{cut}}^{(j=3)}$, the interference term $\tilde{w}_{\text{int}}$ is negligible since the partial EWP $w_{j=3}$ decreases exponentially with increasing $E_\Omega$ and thus fine-scale oscillations disappear. The fine-scale interferences are pronounced for the sine-like pulse for $N = 1$ [cf. Fig. 3(d)] because there are two neighboring half-cycles with close values of both $E_{\text{cut}}^{(j)}$ and $I_j$, as shown in Figs. 4(c) and 4(d) (i.e., for $N = 1$, half-cycles with $j = 2$ and $3$ contribute to $\tilde{w}_{\text{int}}$). With increasing $N$, the results for both cosine and sine-like pulses exhibit fine-scale modulation patterns in the cutoff region.

C. Dependence of quasiharmonic structures in short-pulse HHG spectra on the CEP

The most prominent feature visible in Figs. 3(c)–3(f) is the formation of quasiharmonic patterns in the dependence of $\rho(E_\Omega)$ on $E_\Omega$ in the cutoff region and beyond. In previous studies [12,13,16,18,21] (see also Ref. [64]) these structures have been attributed to the real (but shifted) HHG peaks. However, our analytic results show that these structures have no relation whatsoever to the usual $2\hbar \omega$-spaced HHG peaks typical of a monochromatic driving laser field. Rather, these structures originate from the interference of two neighboring
D. Evolution of HHG spectra with increasing pulse duration

With increasing pulse duration, the number of half-cycles that contribute to the interference term $w_{\text{int}}$ (82) for a given harmonic energy $E_{\Omega}$ increases gradually and leads to some unexpected interference patterns. For instance, for a Gaussian pulse with $N = 10$ the interference of many half-cycle amplitudes $A_j$ leads to the appearance of an $\hbar \omega$-spaced HHG spectrum (cf. Fig. 6 for $\phi = 0.25$). As discussed above, the energy positions of such quasiharmonics may be tuned by varying $\phi$. For example, in Fig. 6 the green (light gray) curves with $\phi = 0.25$ have peaks at integer values of $E_{\Omega}/\hbar \omega$ while the orange (dark gray) curves with $\phi = 0.11$ have peaks at half-integer values. The customary HHG peaks (i.e., $2\hbar \omega$-spaced peaks located at odd integer values of $\hbar \omega$, independent of $\phi$) begin to form in the beyond-cutoff region for large $N$, as shown by the black curve for $N = 50$ in Fig. 6.

The case of a monochromatic laser field (whose entire HHG spectrum is composed of a sequence of $2\hbar \omega$-spaced, CEP-independent peaks located at odd integer values of $\hbar \omega$) is obtained by taking the limit $\tau \to \infty$ (or $N \to \infty$) in our analytic results. In this limit, the vector potential $A(t)$ can be approximated by that of a monochromatic field and Eqs. (56) and (57) have the solution

$$\alpha \Omega_{1,\phi} \approx \alpha E_{\Omega} + \beta \phi + \gamma,$$

where $\alpha$, $\beta$, and $\gamma$ are constants independent of $E_{\Omega}$ and $\phi$. Considering $\rho(E_{\Omega}, \phi)$ along the line $\alpha E_{\Omega} + \beta \phi + \gamma = 2n\pi$ for a fixed integer $n$, we maximize the interference term and, as a result, the spectral density has maximal values along these lines. In the contrast, moving in the direction perpendicular to the stripes, the argument of the cosine in Eq. (87) changes continuously, so that the interference term $w_{\text{int}}$ varies between its maximum and minimum values, leading to corresponding maxima and minima (i.e., quasiharmonic patterns) in $\rho(E_{\Omega}, \phi)$.
where \( \tau_r \approx -2.83 \) and \( \tau_r \approx 1.26 \). Since each half-cycle is the same [except for the sign of \( A(t) \) and \( F(t) \)], \( \chi^{(i)}(k) = \chi^{(k)}(k) \), \( \chi^{(i)} \), \( \chi^{(k)}(k) \), and \( \phi_j - \phi_k = \pi(j - k)E_\Omega/h\omega \) [cf. Eq. (55)].

Substituting these results in Eqs. (24), (53), and (54), we obtain

\[
\rho(E_\Omega) = \frac{\pi\hbar^2}{2\omega^2 N} W(E)\sigma^{(\ell)}(E)D(n, \Omega),
\]

where \( W(E) \) is the EWP for a monochromatic field [25], \( n \) is the number of half-cycles \( (n = 2N) \), and

\[
D(n, \Omega) = \sum_{j=1}^{n} (-1)^{j} \left( \frac{1}{\sin \frac{\Omega}{\omega} j} \right)^2 \left( \frac{\sin \frac{\Omega}{\omega} j x}{\sin \frac{\Omega}{\omega} x} \right)^2, \quad (90)
\]

where

\[
x = \pi \left( \frac{\Omega}{\omega} - 1 \right).
\]

For \( N \to \infty \), \( D(n, \Omega) \) becomes a sum of \( \delta \) functions [66]:

\[
D(n, \Omega)|_{\ell \to 0} \to \frac{2\omega^2}{\pi} T_N \sum_{k=0}^{N} \delta[\Omega - (2k + 1)\omega], \quad (91)
\]

where \( T_N \) is the pulse duration, \( T_N = 2\pi N/\omega \). For a long pulse, it is useful to introduce the power of emitted radiation, \( W_{\text{tot}} \), i.e., the ratio of total energy radiated during the pulse, \( E_{\text{tot}} \), to pulse duration:

\[
W_{\text{tot}} = \lim_{N \to \infty} E_{\text{tot}}/T_N. \quad (92)
\]

Substituting Eq. (91) into Eq. (89) and integrating the latter over \( E_\Omega \), we obtain the total power \( W_{\text{tot}} \) as

\[
W_{\text{tot}} = \sum_{k} W_{2k+1}, \quad W_{2k+1} = (2k + 1)\hbar\omega \mathcal{R}_{2k+1}, \quad (93)
\]

where the partial power of the \((2k + 1)\)th harmonic \((W_{2k+1})\) is expressed in terms of the HHG rate \( \mathcal{R}_{2k+1} \) for the \((2k + 1)\)th harmonic [25,42].

The above analysis shows that our analytical results for short pulses uniformly approach those for a monochromatic laser field in the limit that the pulse duration becomes infinitely long. We emphasize that it is the interference term \( W_{\text{int}} \) that is responsible for the formation of \( 2\hbar\omega \)-spaced HHG peaks (located at odd-integer multiples of the carrier frequency) as the number of optical cycles, \( N \), in the pulse becomes large. For a given pulse shape, the monochromatic field limit is reached when (i) the magnitudes of the half-cycle amplitudes \( A_j \) are close in value to each other, and (ii) the phase differences between the half-cycle amplitudes are essentially independent of the peak intensity. These two conditions can only be satisfied simultaneously for quasimonochromatic pulses. However, the critical number of optical cycles, \( N_r \), at which a stable shape (i.e., independent of the CEP \( \phi \)) of the HHG spectrum begins to form in the cutoff energy region, depends crucially on both the shape of the laser pulse and its peak intensity \( I \). For instance, for a trapezoidal pulse, \( N_r \approx 3 \) and the shape of the HHG spectrum is only slightly sensitive to the intensity \( I \). For this reason, a trapezoidal pulse shape is the most appropriate one for analyzing the monochromatic field limit. In contrast, for Gaussian pulses, \( N_r \) depends significantly on the intensity; e.g., \( N_r \approx 40 \) for \( I = 4 \times 10^{14} \text{ W/cm}^2 \), \( \approx 15 \) for \( I = 2 \times 10^{14} \text{ W/cm}^2 \) (cf. Fig. 7), and \( \approx 10 \) for \( I = 10^{14} \text{ W/cm}^2 \).

Finally, we remark that our analytical description provides a remarkably clear illustration of how the regular \((2\hbar\omega)-\text{spaced}\) feature of HHG spectra begins to form (with increasing number \( N \) of optical cycles) from the often complicated spectral structure of short-pulse HHG radiation. Since for small \( N \) the intercycle interferences are highly sensitive to the CEP, as shown in Fig. 6, the evolution of these interferences with increasing \( N \) can best be seen by considering spectra that are averaged over the CEP. In Fig. 7 we present such CEP-averaged spectral densities \( \rho(E_\Omega) \) for the same Gaussian pulse as in Fig. 6 for four values of \( N \), from 10 to 40. Such averaging smooths out the fine-scale oscillations for \( N = 10 \) (seen in Fig. 6 for two values of the CEP). Such averaging, however, is less significant for \( N = 15 \) or 20, and beginning from \( N = 40 \), the results do not depend on \( \phi \). As shown in Fig. 7, a stable harmonic structure gradually appears with increasing \( N \) beginning for energies \( E_\Omega \) well beyond the plateau-cutoff energy, with the first signature of this structure appearing for \( N = 10 \) as horizontal steps centered close to the positions of odd harmonics, \( E_\Omega = (2k + 1)\hbar\omega \). For larger \( N \), the regular structure becomes more distinct and extends toward the plateau cutoff position (corresponding to the \( 213\text{th harmonic} \) with gradually increasing peak heights and narrowing peak widths centered at the odd-harmonic energies. Such evolution of the short-pulse HHG spectrum is not surprising. Indeed, with increasing \( N \), the half-cycle ionization factors \( \bar{l}_j \) (which do not depend on the harmonic energy \( E_\Omega \) and which determine the absolute values of both the partial EWP's \( w_j \) and the amplitudes \( A_j \) become independent of the half-cycle number \( j \)). However, condition (ii) (cf. prior paragraph) for the phase difference, \( \Delta_{jk} = \phi_j - \phi_k \), between half-cycle amplitudes \( A_j \) and \( A_k \) is fulfilled for energies \( E_\Omega \) primarily beyond the plateau cutoff. This is because in this region the first (linear in \( E_\Omega \)) term in Eq. (55) for \( \phi_j \) exceeds the second (intensity- and CEP-dependent) term, allowing the realization of the condition \( \Delta_{jk} = (t^{(j)} - t^{(k)})E_\Omega/h\omega \approx \pi(j - k)E_\Omega/h\omega \) that is necessary for "constructive" interference of half-cycle HHG amplitudes at odd integers of the ratio \( E_\Omega/h\omega \) [cf. Eq. (90)]. The results in Fig. 7, which employ a Gaussian approximation for the pulse envelope, are useful
VII. SUMMARY AND CONCLUSIONS

In this work we have derived quantum-mechanically closed-form analytical formulas for the spectral density \( \rho(E_\Omega, \phi) \) of coherent radiation emitted by an atomic system subjected to an intense, short laser pulse with CEP \( \phi \). Our main results consist, first, in generalizing our TDER theory [36,37] (for describing a weakly bound electron in a short-range potential subjected to an intense, monochromatic laser field) to the case of an intense, few-cycle laser pulse. The key idea is to treat the case of an infinitely long pulse train of short laser pulses and then to take the limit that the time between pulses becomes infinite. We then derive closed-form analytic expressions for the spectral density \( \rho(E_\Omega, \phi) \) of generated radiation by a few-cycle laser pulse that includes the dependence on the number of cycles \( N \) in the pulse and on the CEP \( \phi \) of the pulse. The resulting formulas factorize into factors corresponding to the three steps of the well-known three-step scenario [10,11]. These formulas also confirm the phenomenological parametrization [26–28] of the HHG yield in terms of the PRCS \( \sigma^{(3)} \) (which describes the final step of the three-step scenario) and the EWP (which describes the ionization of an atomic electron and its propagation in the laser field). Most importantly, we provide a closed-form expression for the EWP factor for the case of a few-cycle laser pulse. Moreover, we generalize the analytic formulas derived for our TDER model system to treat HHG by real atoms in a few-cycle laser pulse.

Our analytic formulas show that the spectral density \( \rho(E_\Omega, \phi) \) is highly sensitive to both the CEP, \( \phi \), and the number of optical cycles, \( N \), in the pulse. The fine-scale oscillation pattern of the HHG plateau near the high-energy cutoff is shown to originate from interference between EWP ionsized from a few neighboring half-cycles in the vicinity of the peak of the laser pulse intensity envelope. Moreover, the CEP \( \phi \) can be used to tune the energy locations of peaks in the plateau spectrum of \( \rho(E_\Omega, \phi) \). Only in the limit that \( N \to \infty \) does the interference pattern become the one expected for a monochromatic laser field: harmonics separated in energy by \( 2\hbar\omega \) and located at odd integer values of the carrier frequency \( \omega \). The closed-form analytic formula derived for our TDER model system was easily generalized to describe HHG by real atoms owing to the transparent physical meaning of each of the three factors of which it is composed. This formula is thus applicable for describing HHG by atoms in a few-cycle laser pulse provided only that the intensity and carrier frequency of the pulse lie in the tunneling regime.

We conclude by emphasizing the valuable insight into strong-field processes provided by closed-form analytic formulas. Although such formulas can be derived only for model systems and/or within limited ranges of the laser parameters, they allow one to obtain a detailed understanding of the underlying physics applicable to real systems. We note, finally, that ours is not the only theory capable of providing closed-form analytic formulas for strong-field processes. Recently, O. I. Tolstikhin, T. Morishita, and S. Watanabe presented a general adiabatic theory of ATI and applied this theory to the case of a one-dimensional zero-range-potential model [67]. This work obtained a factorized analytic formula describing ATI for that model that is consistent with the suggested factorization proposed in Ref. [26] and is applicable in the limit that the driving laser period is long compared to electronic time scales in atoms. Various details of the simple model system treated in Ref. [67] differ from those of our three-dimensional TDER model system that was applied in Ref. [55] for analytic description of ATI in a monochromatic laser field. However, the advantage of such analytical approaches is that (in addition to the physical insight they provide) the closed-form formulas provide experimentalists with the means both to plan experiments and to probe any differences between results of different theoretical models.

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APPENDIX A: DERIVATION OF EQUATIONS (43) AND (44)

To evaluate \( I_{E_\Omega}(E_0,0) \) in Eq. (42), we express the integral (40) in an alternative form. Using the definition (31) for \( \tilde{g}_\nu(t,t') \) and proceeding as in Ref. [68], the integrand of Eq. (40) can be written as a sum of two terms,

\[
\frac{e^{i\tilde{k}_n |R(t,t')|}}{|R(t,t')|} = \frac{\cos \tilde{k}_n |R(t,t')|}{|R(t,t')|} - \frac{\sin \tilde{k}_n |R(t,t')|}{|R(t,t')|},
\]

(A1)

where the first term on the right is an even function of \( \tilde{k}_n \), while the second term is odd. Expanding the even term in a series in \( \tilde{k}_n \) [cf. Eq. (35)] and substituting this expansion into the integral (40), the contribution of the \( \tilde{k}_n \)-even term becomes

\[
I_{E} = \int_{-T/2}^{T/2} \sum_{n=-\infty}^{\infty} \sum_{s=1}^{\infty} \frac{(-1)^s \tilde{k}_n^2 g_s(t,t') e^{-i\text{int}(t-t')}}{(2\nu)!} dt dt',
\]

\[
g_s(t,t') = |R(t,t')|^{2s-1} \exp \left\{ -i \int_{t'}^{t} \left[ \frac{e^2 A^2(\tau)}{2mc^2} - \tilde{u}_p \right] d\tau \right\},
\]

where \( g_s(t,t') \sim |t-t'|^{2s-1} \) at \( t \to t' \). Using the definition of \( \tilde{k}_n \) in Eq. (35), the integral \( I_{E} \) becomes

\[
I_{E} = T \sum_{n=1}^{\infty} \sum_{s=0}^{\infty} \int_{-T/2}^{T/2} \frac{(1)^{-s} C_{2s}(\varepsilon - \tilde{u}_p)^{2s}}{(2\nu)!} \times (i\hbar)^{s} \delta(t-t') g_s(t,t') dt dt',
\]

(A2)
where $C_{2n}$ is a binomial coefficient and $\delta^{(t)}(t' - t)$ is the s-fold derivative of the $\delta$ function in the space of periodic functions:

$$\delta^{(t)}(t' - t) = \sum_{n} (-i \omega_n t')^n e^{-i \omega_n (t' - t)}. \quad (A3)$$

Using Eq. (A3), the integrations in Eq. (A2) can be performed straightforwardly and show that $I_n = 0$.

The integral (40) thus simplifies upon substituting,

$$\frac{e^{i \bar{k}_n R(t,t')}}{|R(t,t')|} \rightarrow \frac{e^{i \bar{k}_n R(t,t')} - e^{-i \bar{k}_n R(t,t')}}{2 |R(t,t')|}, \quad (A4)$$

and representing the integral $\mathcal{I}(\epsilon, F_h)$ as a summation over simpler integrals $I_n$:

$$\mathcal{I}(\epsilon, F_h) = \frac{1}{2 \kappa T^2} \sum_{n=0}^{\infty} I_n, \quad (A5)$$

$$I_n = \int_{T/2}^{T/2} \frac{e^{-i S_n^+(t,t')}}{R(t,t')} dt \bar{d}t', \quad (A6)$$

where $S_n^+(t,t')$ is the classical action:

$$S_n^+(t,t') = \int_{t'}^{t} \left[ \frac{P_n^+(t')}{2m} - \epsilon \right] dt'', \quad (A7)$$

$$P_n^+(t) = \bar{p}_n \pm \frac{e |A(t)|}{c} \bar{A}(t), \quad (A8)$$

To extract explicitly the linear in $F_h$ result in the expansion of $\mathcal{I}(\epsilon, F_h)$ in the limit $F_h \to 0$, we transform first the expression (A6) for $I_n$ (presenting it as $I_n = I_n \to I^+_n$) as follows:

$$I^+_n \equiv \int_{T/2}^{T/2} \frac{e^{-i S_n^+(t,t')}}{R(t,t')} dt \bar{d}t'$$

$$= \int_{T/2}^{T/2} \frac{e^{-i S_n^+(t,t')}}{R(t,t')} \left( \alpha \frac{S_n^+}{\alpha S_n^+} + \beta \frac{S_n^+}{\beta S_n^+} \right) dt \bar{d}t'$$

$$= \frac{i \hbar \alpha}{2} \left. \int_{T/2}^{T/2} d\bar{d}t \left[ e^{-i S_n^+(t,t')} \bar{R}(t,t') \left( \alpha \frac{S_n^+}{\alpha S_n^+} + \beta \frac{S_n^+}{\beta S_n^+} \right) \right] \right|_{t=t'}$$

$$= \frac{i \hbar \beta}{2} \left. \int_{T/2}^{T/2} d\bar{d}t \left[ e^{-i S_n^+(t,t')} \bar{R}(t,t') \left( \alpha \frac{S_n^+}{\alpha S_n^+} + \beta \frac{S_n^+}{\beta S_n^+} \right) \right] \right|_{t=t'} \quad (A9)$$

where $\alpha$ and $\beta$ are free parameters. [Note that the derivatives, $\partial S_n^+/\partial t$ or $\partial S_n^+/\partial t'$, of the function $S_n^+(t,t')$ depend only on the single variable, $t$ or $t'$, respectively.] Next, we integrate by parts in Eq. (A9), keeping only terms of the lowest order in $1/R$, to obtain

$$I^+_n \approx \frac{i \hbar \alpha}{2} \int_{T/2}^{T/2} e^{-i S_n^+(t,t')} \frac{S_n^+}{R(t,t')} dt \bar{d}t'$$

$$+ \frac{i \hbar \beta}{2} \int_{T/2}^{T/2} e^{-i S_n^+(t,t')} \frac{S_n^+}{R(t,t')} dt \bar{d}t', \quad (A10)$$

Finally, we use the saddle-point method to estimate the integral over $t'$ in the first term in Eq. (A10) and that over $t$ in the second term. The derivative $\partial S_n^+/\partial t$ or $\partial S_n^+/\partial t'$ in the denominator of the first (second) integral in Eq. (A10) becomes zero since it determines the corresponding saddle-point equation. Thus the free parameters $\alpha$ and $\beta$ do not enter the final result for $I_n$:

$$I_n \approx i \hbar \sum_{v} \frac{2 \pi i h}{S_n^+(t_v)} \int_{-T/2}^{T/2} \frac{2 \pi h}{S_n^+(t_v)} dt \bar{d}t'$$

$$+ \frac{2 \pi h}{S_n^+(t_v)} \int_{-T/2}^{T/2} \left[ \frac{P_n(t)}{2m} - E_0 \right]^{2} dt \bar{d}t', \quad (A11)$$

where $S_n^+(t) = \frac{[P_n^+(t)]^2}{2m} - \epsilon$, $S_n^{--}(t) = \frac{[P_n(t)]^2}{2m} - E_0$. The saddle-point equations for $t^+_n$ are

$$\frac{[P_n^+(t^+_n)]^2}{2m} = E_0, \quad (A12)$$

where $\epsilon$ is approximated by $E_0$ and $t^+_n$ are the roots of Eq. (A14) for which the imaginary parts of $S_n^{--}(t^+_n)$ are positive.

Consider first the imaginary part of $\mathcal{I}$ for real $\epsilon < 0$ [to which only open $n$-photon ATI channels contribute, as follows from (A6)]. Its expression in terms of $I_n$ is

$$\tilde{\mathcal{I}} = \text{Im} \mathcal{I}(\epsilon, F_h) = \frac{\mathcal{I} - \mathcal{I}^*}{2} = \frac{1}{2 \kappa T^2} \sum_{n=0}^{\infty} I_n, \quad (A15)$$

where $n_0 = \lfloor (\mu - \epsilon)/\hbar \omega \rfloor$ (where $\lfloor x \rfloor$ is the integer part of $x$) and $\mu_0$ is defined by Eq. (34). Assuming $\hbar \Omega \gg |E_0|$, we can neglect in Eq. (A11) for $I_n$ any dependence of $P_n^+$, $S_n^+$, $S_n^{++}$, $\bar{R}$, and the saddle points $t^+_n$ on $F_h$ in the limit $F_h \to 0$, other than that stemming from the terms $F(t)$ and $\bar{F}(t)$ in the derivatives $S_n^{--}(t)$ and $S_n^{++}(t')$ [cf. Eq. (A13)] in the numerators of the integrals in Eq. (A11). Thus the linear in $F_h$ term in the expansion of $I_n$ in $F_h$ follows only from the linear dependence of $F(t)$ on $F_h$ [cf. Eq. (28)] in Eq. (A13) for these derivatives. Hence, the derivative (in $F_h$) of $\tilde{\mathcal{I}}$ is obtained as

$$\tilde{T}_{F_h}^+ \equiv \frac{\partial \tilde{\mathcal{I}}}{\partial F_h} \bigg|_{F_h=0} = e^{i \phi} \Phi_{\Omega} + e^{-i \phi} \Phi_{-\Omega}, \quad (A16)$$

where

$$\Phi_{\pm \Omega} = \frac{i \hbar |e|}{4 m \kappa T^2} \sum_{n=0}^{\infty} \sum_{v} \int_{-T/2}^{T/2} e^{-i S_n^{xx}(t_v)} \frac{P_n^{-}(t)}{2m - E_0} dt \bar{d}t'$$

$$+ \frac{2 \pi i h}{S_n^{xx}(t_v)} \int_{-T/2}^{T/2} \left[ \frac{P_n(t)}{2m} - E_0 \right]^{2} dt \bar{d}t', \quad (A17)$$

Finally, we use the saddle-point method to estimate the integral over $t'$ in the first term in Eq. (A10) and that over $t$ in the second term. The derivative $\partial S_n^+/\partial t$ or $\partial S_n^+/\partial t'$ in the denominator of the first (second) integral in Eq. (A10) becomes zero since it
and definitions of \( S_{ji}^\pm(t, t') \), \( P_{ji}^\pm(t) \), and \( R(t, t') \) are given by Eqs. (A7) (with \( \varepsilon = E_0 \)), (A8), and (32) with \( F_0 = 0 \), while \( t_{ji}^\pm \) are given by Eq. (A14) with \( P_n^0 \rightarrow P_n^\pm \). Moreover, since Eq. (A17) involves only integrals over the period \( T \), the vector potential \( A_j(t) \) can be replaced by \( A(t) \) in these integrals [cf. Eq. (4)].

Since \( \tilde{I} \) determines only the imaginary part of \( I \) [cf. Eq. (A15)], to find an explicit form for \( \tilde{I}_F (E_0, 0) \) in Eq. (42), it is necessary to express Eq. (A16) for \( \tilde{I}_F \) as a difference of two terms similar to that of \( I - I' \) in Eq. (A15). For this purpose, we separate the saddle points \( t_{ji}^\pm \) in the integrals for \( \Phi_\Omega \) in Eq. (A17) into two groups:

(i) Saddle points from the first group satisfy the equation

\[
    p_n \pm A(t_{ji, \pm}^\pm) = -i \hbar \kappa, \tag{A18}
\]

where we label those as \( t_{ji, \pm}^\pm \), and

(ii) saddle points from the second group (labeled as \( t_{ji, 0}^\pm \)) satisfy the equation

\[
    p_n \pm A(t_{ji, 0}^\pm) = +i \hbar \kappa. \tag{A19}
\]

The solutions of (A18) and (A19) are related as follows:

\[
    t_{ji, \pm}^\pm = [t_{ji, 0}^\pm]^*. \tag{A20}
\]

To separate the contributions of these two groups of saddle points to \( \Phi_\Omega \) in Eq. (A17), we rewrite \( \Phi_\Omega \) as

\[
    \Phi_\Omega = \Phi_\Omega^{(1)} + \Phi_\Omega^{(-1)}, \tag{A21}
\]

where \( \Phi_\Omega^{(j)} \) corresponds to the \( j = \pm 1 \) saddle-point group:

\[
    \Phi_\Omega^{(j)} = \frac{i \hbar |e|}{4 \pi m T^2} \sum_{\sigma = \pm 1} \sum_{n = 0} \sum_{t_{ji, 0}^\pm} \left[ \frac{2 \pi m \sigma j}{\mu_{ji, \sigma}^\pm} \right] F(t_{ji, \sigma}^\pm) \kappa \int_{-T/2}^{T/2} e^{-i S_{ji}^\pm(t, t_{ji, 0}^\pm)/\hbar} P_{ji}^\pm(t) \left[ \frac{P_{ji}^\pm(t)}{2m} - E_0 \right] dt, \tag{A22}
\]

where \( \mu_{ji, \sigma}^\pm = \pm 1 \) is the sign of the imaginary part of the saddle point \( t_{ji, 0}^\pm \). [Eq. (A22) follows from Eq. (A17), taking into account Eqs. (A13) and (A18)-(A20).] Though saddle points with both positive and negative parts contribute to Eq. (A22), the contributions of those with \( \text{Im} \ t_{ji, 0}^\pm < 0 \) are negligible for \( \Omega > |E_0| \). Indeed, the saddle points of the integrand in Eq. (A22) satisfy

\[
    \mu_{ji, \sigma}^\pm \left( \frac{P_{ji}^\pm(t)^2}{2m} - E_0 \right) = \hbar \Omega. \tag{A23}
\]

For \( \mu_{ji, \sigma}^\pm = -1 \) and \( \Omega > |E_0| \), the saddle points are complex, so that the corresponding integrals are small, whereas for \( \mu_{ji, \sigma}^\pm = 1 \) the saddle points are real and the integrals are not small. Thus we substitute \( \mu_{ji, \sigma}^\pm = +1 \) and neglect contributions of saddle points with \( \text{Im} \ t_{ji, 0}^\sigma < 0 \).

From the symmetry relation (A20) and the explicit form (A22) for \( \Phi_\Omega^{(j)} \), it follows that

\[
    \Phi_\Omega^{(1)} = -\Phi_\Omega^{(-1)}. \tag{A24}
\]

This symmetry relation allows us to write \( \tilde{I}_F \) as

\[
    \tilde{I}_F = \frac{I_{\tilde{F}_F} - I_{\tilde{F}_F^*}}{2}, \tag{A25}
\]

where

\[
    I_{\tilde{F}_F} = 2 \Phi_\Omega^{(1)} \Theta(t_0^\pm - t_0^\pm), \tag{A26}
\]

Finally, from Eqs. (A15), (A25), and (A26), we obtain

\[
    4C_{\varepsilon_0}^2 |E_0| I_{\tilde{F}_F} (E_0, 0) = \tilde{D}_0 \Theta(t_0^\pm - t_0^\pm), \tag{A27}
\]

where the HHG amplitude, \( \tilde{D}_0 = 8C_{\varepsilon_0}^2 |E_0| \Phi_\Omega^{(1)} \), is given by Eqs. (44)-(48).

**APPENDIX B: ANALYTIC ESTIMATES OF THE HHG AMPLITUDE FOR A SHORT LASER PULSE**

To simplify the result (51) for the HHG amplitude in the low-frequency limit (\( \hbar \omega_0 \ll |E_0| \)), we estimate the integral over \( p \) by the saddle-point method. The saddle point \( \tilde{p} = \tilde{p} \) and the second derivative of the classical action \( S(t, t_\nu^\pm; p) \) in Eq. (47) at \( p = \tilde{p} \) are given by

\[
    \tilde{p} = \sigma q, \quad q = -\frac{|e|}{c} \int_{t_\nu^\pm}^t A(\tau) d\tau, \tag{B1}
\]

\[
    \left\| \frac{\partial^2 S}{\partial p^2} \right\|_{p=\tilde{p}} \approx \frac{m}{\hbar k} \frac{\partial^2 S}{\partial p^2} \approx \frac{t - t_\nu^\pm}{m}, \tag{B2}
\]

so that the saddle-point result for \( \tilde{D}(t) \) is

\[
    \tilde{D}(t) = |e| \int_{\sigma = \pm 1} \tilde{a}_\sigma(t), \tag{B3}
\]

where

\[
    \tilde{a}_\sigma(t) = \int_{t_\nu^\sigma} f_{\sigma, \sigma}(t) \left[ \frac{|e| |e| F(t_\nu^\sigma) - E_0} \right] dt, \tag{B4}
\]

and the equation for the saddle points \( t_\nu^\sigma \) follows from Eq. (49) upon substituting there \( p_n \rightarrow \tilde{p} \):

\[
    |e| \int_{t_\nu^\sigma} f_{\sigma, \sigma}(t) \left[ \frac{1}{|e| |e| F(t_\nu^\sigma) - E_0} \right] dt, \tag{B5}
\]

To estimate the integral over \( t \) for \( \tilde{D}(\Omega) \), we use the techniques suggested in Ref. [69] for evaluating integrals involving functions with two close (nearly equal) saddle points, as used recently in Refs. [31,42] (cf. also Ref. [70]). Briefly, for the integral in Eq. (50), one expands \( \tilde{S}(t, t_\nu^\sigma) \) in (B3) in powers...
of $t$ (up to the cubic term) about the point $\tilde{t}_v$, at which the second derivative of $\tilde{S}$ is zero, and then evaluates the integral in terms of Airy functions, $\text{Ai}(x)$.

Double differentiation of $\tilde{S}(t, t_v')$ in Eq. (B4) yields the equation for $\tilde{T}_v'$:

$$\frac{F(t_v') \tilde{P}(t)}{|e|F(t_v') - i\sigma \hbar \kappa} - F(t) = 0,$$  \hspace{1cm} (B6)

where $\tau = \tilde{t}_v$. To evaluate $\tilde{D}(\Omega)$, we substitute (B2) and (B3) in Eq. (50) and, taking into account the equation for the saddle points of the function $\exp[-i\tilde{S}(t, t_v')/\hbar - \Omega \tau]$, remove the pre-exponent from the integrand in the integral over $t$ upon substituting there $\tilde{P}(t) \to \sqrt{2mE}$, $(t - t_v') \to (\tilde{t}_v - t_v')$. Then, after approximating $\tilde{S}$ in (B3) by the cubic polynomial in $t$, we obtain $\tilde{D}(\Omega)$:

$$\tilde{D}(\Omega) \approx \frac{e^{-1}}{\pi} \frac{2\sqrt{2mE}}{(E - E_0)^2} \sum_{\sigma, \nu} f_{\sigma, \nu} \int_{-\infty}^{\infty} e^{-i\tilde{S}(t, t_v')/(\hbar + \Omega t)} dt \approx \frac{e^{-1}}{\pi} \frac{2\sqrt{2mE}}{(E - E_0)^2} \sum_{\sigma, \nu} f_{\sigma, \nu} e^{-i\tilde{S}(t, t_v')/(\hbar + \Omega t)} \int_{-\infty}^{\infty} e^{-i(E-\nu\omega(t-t_v'))/\hbar} dt$$

$$= 2e^{-1} \frac{2\sqrt{2mE}\hbar}{(E - E_0)^2} \sum_{\sigma, \nu} f_{\sigma, \nu} e^{-i\tilde{S}(t, t_v')/(\hbar + \Omega t)} \text{Ai}(\xi_{\sigma, \nu}),$$  \hspace{1cm} (B8)

where we have introduced the notations $\tilde{S}_{\sigma, \nu} \equiv \tilde{S}(\tilde{t}_v, t_v')$, $f_{\sigma, \nu} \equiv f_{\sigma, \nu} (\tilde{t}_v)$, and

$$\xi_{\sigma, \nu} = \frac{E - \xi_{\sigma, \nu}}{\xi_{\sigma, \nu}},$$  \hspace{1cm} (B9)

$$\xi_{\sigma, \nu} = \frac{e^{2}}{2me^{2}} \left[ A(t_v') - \frac{f_{t_v'}}{F(t_v')} \right]^{2},$$  \hspace{1cm} (B10)

$$\xi_{\sigma, \nu} = \frac{e^{2}}{2me^{2}} \left[ A(t_v') - \frac{f_{t_v'}}{F(t_v')} \right]^{2} \left[ 1 - \mathcal{L}^{(-1)} \right]$$

$$\xi_{\sigma, \nu} = \frac{e^{2}}{2me^{2}} \left[ A(t_v') - \frac{f_{t_v'}}{F(t_v')} \right]^{2} \left[ 1 - \mathcal{L}^{(-1)} \right]$$

Further simplification of the complicated general result (B8) that allows for a better physical interpretation follows by using an approximate solution of the basic Eqs. (B5) and (B6) for the times $t_v'$ and $\tilde{t}_v$. Both $t_v'$ and $\tilde{t}_v'$ are complex owing to the terms $\sim \hbar \kappa$, which have a quantum origin (cf. Ref. [42]).

As for the case of a monochromatic field [42], for an intense, low-frequency pulse field $F(t)$ with vector potential (52), the quantum term $i\sigma \hbar \kappa$ in Eqs. (B5) and (B6) can be treated iteratively. In our case, this means that the “effective Keldysh parameter,” $\tilde{\gamma} = \hbar\kappa/(|e| \tilde{F}^{-1})$ [where $F$ is a characteristic value of the field $F(t)$], is small: $\tilde{\gamma} \ll 1$. In the tunnel limit ($\tilde{\gamma} \to 0$), (B5) and (B6) reduce to the classical equations,

$$A(t_v^{(0)}) - \frac{1}{t_v^{(0)} - t_v^{(0)}} \int_{t_v^{(0)}}^{t_v^{(0)}} A(\tau) d\tau = 0,$$  \hspace{1cm} (B13)

$$A(t_v^{(0)}) - \frac{1}{t_v^{(0)} - t_v^{(0)}} \int_{t_v^{(0)}}^{t_v^{(0)}} A(\tau) d\tau + F(t_v^{(0)}) = 0,$$  \hspace{1cm} (B14)

for closed classical trajectories of an electron in the field $F(t)$, along which an electron with zero velocity at the initial (ionization) time $t_i \equiv t_v^{(0)}$ gains the maximum kinetic energy from the field $F(t)$ at the final (recombination) time $t_r \equiv t_v^{(0)}$. We consider only classically allowed closed trajectories, for which $t_i$ and $t_r$ are real and the return time is smaller than the optical period of the pulse, i.e., $(t_r - t_i) < 2\pi/\omega$. For a short pulse (52) involving $N$ optical cycles of frequency $\omega$, the index $v$ enumerates the ionization ($t_v^{(0)}$) and recombination ($t_v^{(0)}$) times for the $v$th half-cycle [where $t_v^{(0)}$ lies in the $(v + 1)$th half-cycle].

The solution of Eqs. (B5) and (B6), taking account of the quantum terms $\sim \hbar \kappa$, perturbatively, has the form

$$t_v' \approx t_i - i \frac{\hbar \kappa}{|e| \tilde{F}(t_i)} + \delta t_i,$$  \hspace{1cm} (B15)

$$t_r' \approx t_r + \delta t_r,$$  \hspace{1cm} (B16)

where

$$\tilde{F}(t_i) = \sigma F(t_i) > 0,$$  \hspace{1cm} (B17)

$$\delta t_i = \frac{\hbar^2 \kappa^2}{2e^2 F(t_i)^2 \Delta t} \left[ 1 + \frac{\tilde{F}(t_i)}{F(t_i)} \Delta t + \frac{F(t_i)}{F(t_i)} \alpha \right],$$  \hspace{1cm} (B18)

$$\delta t_r = \frac{\hbar^2 \kappa^2 \alpha}{2e^2 F(t_i)^2 \Delta t},$$  \hspace{1cm} (B19)

$$\alpha = \frac{1 - \frac{F(t_i)}{F(t_i)}}{1 - \frac{F(t_i)}{F(t_i)} + \frac{F(t_i)}{F(t_i)} \Delta t \Delta t},$$  \hspace{1cm} (B20)

$$\Delta t = t_r - t_i.$$  \hspace{1cm} (B21)

With the use of expansions (B15) and (B16), all parameters in the expression (B8) for $\tilde{D}(\Omega)$ can be presented in terms of the classical times $t_i$ and $t_r$. Numerically, the quantum corrections in Eq. (B11) for $\xi_{\sigma, \nu}$ are found to be negligible, so that we can make the approximations

$$\xi_{\sigma, \nu} \approx -\tilde{E}_{\text{eff}} \xi_{\sigma, \nu}.$$  \hspace{1cm} (B22)

$$\xi_{\sigma, \nu} \approx \frac{E_{\text{max}}}{(t_i) - (t_r)} |eF(t_i)^2|/\hbar^2.$$  \hspace{1cm} (B23)

where

$$\tilde{E}_{\text{eff}} = \frac{\hbar^2 \kappa^2}{2e^2 F(t_i)^2 \Delta t} \left[ 1 + \frac{\tilde{F}(t_i)}{F(t_i)} \Delta t + \frac{F(t_i)}{F(t_i)} \alpha \right].$$  \hspace{1cm} (B24)
Taking into account the results (B22) and (B23), we obtain for the argument $\xi_{\sigma,\nu}$ of the Airy function in Eq. (B8):

$$\xi_{\sigma,\nu} \approx \xi = \frac{E - E_{\text{max}}}{\xi_{\nu}^{1/3}E_{\text{int}}}.$$  \hspace{1cm} \text{(B25)}

The expansion of the classical action $S_{\nu}^c$ in Eq. (B8) involves an imaginary term stemming from $\text{Im} \tau_{\nu}$ [cf. Eq. (B15)]:

$$S_{\nu}^c \approx S_0 = \int_{t_i}^{t_f} \left[ \frac{\epsilon_{\text{cl}}(t_i,t_f)}{E_{\text{int}}} - E_0 \right] dt + \frac{2 \hbar |E_0|}{3 |e| F(t_i)}.$$  \hspace{1cm} \text{(B26)}

Since the last term in Eq. (B26) involves $\hbar |E_0| \sim (\hbar \kappa)^3$, it would seem that the term involving $\Delta t$ should also be expanded up to terms of order $(\hbar \kappa)^3$. However, we find that these latter corrections give such a small contribution that they may be neglected.

Substituting Eqs. (B8), (B22), (B25), and (B26) into Eq. (50), we obtain the HHG amplitude in the form (53), in which we use the summation index $j$ (instead of $\nu$) for enumerating the solutions ($t_{j0}^{(t)}, t_{j1}^{(r)}$) of the classical equations (B13) and (B14).