Influence of Coulomb continuum wave functions in the description of high-order harmonic generation with H_2^+

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We investigate the influence of the Coulombic nature of the binding potential on high-order harmonic generation in H_2^+ molecules. We show that two-center interference effects are predicted accurately using approximated two-center Coulomb wave functions for the electron continuum state in the recombination amplitude that determines the probability for harmonic emission upon recollision.

I. INTRODUCTION

Physical phenomena in molecules are sensitive to the molecular structure and composition. In particular, the presence of two or more atomic sites leads to fundamental quantum mechanical interference effects. For example, in the electron emission from H_2 molecules by ion impact, it has been possible to observe a phenomenon that can be regarded as a Young's two-slit experiment on the atomic scale [1]. For such processes, there is a persisting effort to model the initial (bound) and final (continuum) channels. In many cases, the ground state of a molecule is well approximated using a linear combination of atomic orbitals (LCAO). On the other hand, the continuum electron in the presence of the molecular centers is difficult to model, because the exact solution of the Schrödinger equation for three or more bodies with Coulomb interaction is unknown. Nevertheless a number of approximated models have been capable of reproducing the available experimental data reasonably well. As an example, for electron impact ionization of H_2^+ and H_2 there are several approaches that take into account the multicenter nature of the initial and final molecular wave functions [2–4].

Within the area of intense laser-molecule interactions, interference patterns appear in several processes such as high-order harmonic generation (HHG) and above-threshold ionization (ATI), including both direct and rescattering ATI [5–14]. Due to the two-center interference in diatomic molecules, HHG exhibits a strong dependence on the molecular orientation so that the suppression or enhancement of certain harmonic-frequency ranges is possible [5,6,12–14].

In the semiclassical recollision model [15,16], high harmonics are generated by a three-step sequence of ionization, acceleration of the continuum electron by the laser field, and recombination with the core. The third step, i.e., the recollision of the laser-driven electron, provides the link between the two research areas of strong-field physics and collisions with external particle beams. In particular, it is expected that the molecular interference effects observed under these quite different experimental situations are closely related to each other.

A widely used semianalytical approach to describe HHG is the strong field approximation (SFA) or Lewenstein model [17], which is applicable to atoms and molecules. It can be regarded as the quantum mechanical version of the semiclassical recollision model. The Lewenstein model has the advantage of requiring less computational effort than the *ab initio* solution of the time-dependent Schrödinger equation (TDSE), which becomes very demanding at high laser intensities. Another advantage of the model is that it yields a physical interpretation of the underlying mechanisms and a certain degree of analytical description.

As the SFA model was previously used successfully to model HHG in atomic systems [17], we consider the same model for molecules. More specifically, we use it to study the two-center interference. Namely, we compare the SFA prediction of the interference-minimum position to the exact value (obtained from the *ab initio* calculations). We observe that using the two-center continuum wave functions, instead of a plane wave to describe the continuum electron, greatly improves the comparison. The usage of the continuum wave functions can be considered as an attempt to take into account Coulomb effects on the returning electron.

In [18,19] the authors propose the use of the Coulomb-eikonal Volkov states (i.e., states that at the end of the pulse become the exact free-field states, and are propagated backwards in time using the Volkov propagator, corrected for the effect of the binding potential). The agreement with *ab initio* calculations improves when compared to the standard SFA, where the electron is considered to be unaffected by the binding potential during its propagation in the continuum (i.e., it is described by a superposition of plane waves).

In HHG with molecules, the two-center interference is mostly determined by the recollision step. The simple plane-wave (PW) approximation, where the recolliding wave packet is modeled as a superposition of Volkov states, is used in most implementations of the Lewenstein model.

In the present work we investigate the influence of the Coulombic binding potential on HHG in H_2^+, namely we focus on the orientation dependence of the high harmonics and interference effects. We investigate different models for the

Coulomb continuum state based on the Coulomb-Volkov states [20] and its incorporation into the recombination amplitude of the Lewenstein model. For atoms, the influence of the Coulomb potential on HHG has been studied by several authors using various approaches: in [21] the effects of the Coulomb potential are incorporated in the three steps of the Lewenstein model, i.e., ionization, propagation of the unbound electron, and recombination (by taking into account the Stark shift of the ground state and adding the contribution of the Coulomb potential to the semiclassical action, defined in the next section); meanwhile, in [22] a Coulomb-Volkov approach has been used (the present work uses the same approach, but we focus here on the recombination process, and we apply the method specifically to H_2^+ molecules).

The paper is organized as follows. In Sec. II we briefly describe the Lewenstein model for molecules and various approximations for the electron continuum state in the presence of the binding potential. In Sec. III, we show the resulting orientation dependence of the high harmonics and a comparison with the usual PW treatment. Finally, Sec. IV contains our conclusions and future perspectives. Atomic units are used throughout the paper.

II. THEORY

A. The strong-field approximation

We start from the dipole approximation and the length-gauge Hamiltonian for an H_2^+ molecule with fixed nuclei, irradiated by a laser pulse with electric field $E(t)$ linearly polarized along the x axis,

$$H = -\frac{\nabla^2}{2} + V(\mathbf{r},\mathbf{R}) + E(t)x, \qquad (1)$$

where V is the Coulomb interaction with the two protons and $\mathbf{R}$ is the internuclear distance, here taken as a parameter. Its orientation with respect to the laser polarization direction is arbitrary. The molecule is in the (x,y) plane and the laser propagates along the z axis.

We are interested in modeling high-order harmonic spectra from the interaction of an H_2^+ molecule with an intense and short laser pulse. Following the strong-field approximation formulated in Refs. [17,23], the time-dependent dipole moment is given by

$$\mathbf{D}(t) = -i \int_0^t dt' \int d^3p \, \mathbf{d}_{\text{rec}}^*(\mathbf{p}+\mathbf{A}(t),\mathbf{R}) d_{\text{ion}}(\mathbf{p}+\mathbf{A}(t'),\mathbf{R},t')$$
$$\times \exp[-iS(\mathbf{p},t',t)] + \text{c.c.}, \qquad (2)$$

with $S = \int_{t'}^t dt'' \{[\mathbf{p}+\mathbf{A}(t'')]^2/2 + I_p\}$ being the semiclassical action and I_p the ionization potential of the electronic ground state. Here, $\mathbf{A}(t) = -\int_{-\infty}^t \mathbf{E}(t')dt'$. The spectrum of the emitted light polarized along a certain direction $\mathbf{e}$ is obtained by modulus squaring the Fourier transform of the dipole acceleration component along that direction,

$$\mathbf{e} \cdot \mathbf{a}(\Omega) = \int_0^{T_p} dt \, \mathbf{e} \cdot \ddot{\mathbf{D}}(t)\exp(i\Omega t), \qquad (3)$$

where the integration is carried out over the duration of the laser pulse, T_p. Due to the anisotropy of the molecular system, in contrast to atoms, the emitted radiation can be polarized along other directions than the laser polarization axis. Here we consider only the harmonic radiation polarized along the direction of the laser electric field, $\hat{\mathbf{x}}$.

In Eq. (2), d_{ion} represents the ionization amplitude

$$d_{\text{ion}}(\mathbf{k},\mathbf{R},t) = \langle \psi_V(\mathbf{k})|E(t)x|\psi_0(\mathbf{R})\rangle. \qquad (4)$$

It has the simple interpretation of the electron transition amplitude from the ground state to a PW $|\psi_V(\mathbf{k})\rangle$ with momentum $\mathbf{k}$.

For the recombination step, we have

$$\mathbf{d}_{\text{rec}}(\mathbf{k},\mathbf{R}) = \langle \psi_V(\mathbf{k})| - \mathbf{r}|\psi_0(\mathbf{R})\rangle, \qquad (5)$$

describing an electron in a PW state recombining with the molecular core.

In order to calculate the dipole moment, we adopt for the molecular ground state the LCAO approximation, i.e., the ground-state wave function is taken to be

$$\psi_0(\mathbf{r},\mathbf{R}) = \frac{1}{\sqrt{2[1+s(R)]}}[\psi_h(\mathbf{r}_1) + \psi_h(\mathbf{r}_2)], \qquad (6)$$

with $\psi_h(\mathbf{r})$ being the ground state of the hydrogen atom and $\mathbf{r}_1 = \mathbf{r}+\mathbf{R}/2$ and $\mathbf{r}_2 = \mathbf{r}-\mathbf{R}/2$. Furthermore, $s(R) = \exp(-R)(3+3R+R^2)/3$ is the overlap integral between the two atomic orbitals. By using Eq. (6) in Eq. (5), the recombination amplitude reads

$$\mathbf{d}_{\text{rec}}(\mathbf{k},\mathbf{R}) = -i\sqrt{\frac{2}{1+s(R)}}\left[-\frac{\mathbf{R}}{2}\sin\left(\frac{\mathbf{k}\cdot\mathbf{R}}{2}\right)\widetilde{\psi}_h(\mathbf{k})\right.$$
$$\left. +\cos\left(\frac{\mathbf{k}\cdot\mathbf{R}}{2}\right)\frac{\partial\widetilde{\psi}_h(\mathbf{k})}{\partial\mathbf{k}}\right], \qquad (7)$$

where $\widetilde{\psi}_h(\mathbf{k})$ is the Fourier transform of the hydrogen ground-state wave function, $\widetilde{\psi}_h(\mathbf{k}) = (\pi\sqrt{2})^{-1}(k^2/2+1/2)^{-2}$. The ionization amplitude has a similar form. In comparison to the atomic case, the transition amplitude (7) depends on the internuclear distance and the molecular orientation, giving rise to two-center interference effects in the harmonic spectrum [5].

In practice, the SFA model provides more accurate results when the momentum expectation value (which we refer to hereafter as the velocity form) is used to calculate the dipole acceleration [24]. According to the Ehrenfest theorem, if the exact wave function is used, this would give the same result for the harmonic spectrum as when using the length form [see Eq. (7)]. Because in the SFA model the wave function is only calculated approximately, different results are obtained from both procedures. The recombination amplitude in the dipole-velocity form reads

$$\mathbf{v}_{\text{rec}}(\mathbf{k},\mathbf{R}) = -\mathbf{k}\sqrt{\frac{2}{1+s(R)}}\cos(\mathbf{k}\cdot\mathbf{R}/2)\widetilde{\psi}_h(\mathbf{k}). \qquad (8)$$

The recombination matrix element determines the interference pattern in the harmonic generation spectrum, while the ionization matrix element mainly dictates the amplitude of the harmonic intensity. In [14] the position of the interference minimum in the harmonic spectrum obtained from the time-dependent Schrödinger equation (TDSE) has been compared with the predictions from the length form and the velocity form of the SFA recombination amplitude. While the length form overestimates by far the position of the minimum, the velocity form gives a somewhat better prediction.

While both the ionization and the recombination steps are amenable to Coulomb corrections [21,22], the purpose of this paper is to investigate whether the use of Coulomb-corrected two-center continuum wave functions in the recombination matrix element could help improve the predictive power of the SFA model for diatomic molecules. In the context of single-photon ionization (the inverse process of electron recombination), it was shown [25] that the use of two-center continuum wave functions instead of plane waves greatly improves the agreement with the *ab initio* ionization spectra. Concerning the ionization step in the HHG process, we expect that the influence of Coulomb corrections on the two-center interference is negligible. This is because in the length-gauge approach used in this work, the electrons responsible for HHG are "born" in the continuum with almost zero kinetic energy. Ionization of H_2^+ by ultrashort laser pulses based on Coulomb-Volkov solutions has recently been addressed by other authors (see [26], and references therein).

B. Two-center continuum wave functions

We will incorporate the Coulomb nature of the molecular centers in the description of the recombination step, Eq. (5). For this purpose we follow the studies carried out in single ionization of molecules by electron impact where a similar scenario takes place for the ejected electron as a consequence of the presence of the Coulombic residual nuclei [2–4].

Instead of using a plane wave $|\psi_V(\mathbf{k})\rangle$ in (5), we propose a two-center continuum (TCC) wave function for the electron moving in the combined field of the two protons,

$$\mathbf{d}_{rec}^{TCC}(\mathbf{k},\mathbf{R}) = \langle \psi_V^{TCC}(\mathbf{k},\mathbf{R})| - \mathbf{r}|\psi_0(\mathbf{R})\rangle, \tag{9}$$

where

$$\psi^{TCC}(\mathbf{k},\mathbf{r},\mathbf{R}) = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{3/2}}C(\mathbf{k},\mathbf{r}_1)C(\mathbf{k},\mathbf{r}_2) \tag{10}$$

with

$$C(\mathbf{k},\mathbf{r}) = N(\nu)\,_1F_1[i\nu,1,i(kr - \mathbf{k}\cdot\mathbf{r})], \tag{11}$$

and $\mathbf{r}_1 = \mathbf{r} + \mathbf{R}/2$ and $\mathbf{r}_2 = \mathbf{r} - \mathbf{R}/2$. Here, $N(\nu) = \exp(\pi\nu/2)\Gamma(1 - i\nu)$ is the usual Coulomb normalization factor and $\nu = 1/k$ defines the Sommerfeld parameter. Each of these wave functions corresponds to the well-known solution of the two-body Coulomb continuum problem with outgoing boundary conditions. Equation (10) is inspired from the Pluvinage approach for heliumlike systems, with one of the nuclei of H_2^+ replacing the second electron in the equation of He (see [2], and references therein). Within the framework of

electron-molecule collisions, wave functions of the type defined by Eq. (10) have been used to model the ionized electron in the presence of two Coulombic centers. The results obtained with such a scheme are in better agreement with the experimental data than other simpler ones where the electron is simply considered as a plane wave [3,27]. Furthermore, the wave function (10) possesses the correct Coulomb asymptotic conditions for one electron in a field of two nuclei,

$$\lim_{|kr - \mathbf{k}\cdot\mathbf{r}|\to\infty} [\psi_V^{TCC}(\mathbf{k},\mathbf{r},\mathbf{R})]$$
$$= (2\pi)^{-3/2}\exp[i\mathbf{k}\cdot\mathbf{r} - 2i\nu\ln(kr - \mathbf{k}\cdot\mathbf{r})]. \tag{12}$$

Using Fourier transform techniques together with the usual Nordsieck's method [28,29] it is possible to obtain suitable expressions for the integrals involved in Eq. (9) (see the Appendix).

On the other hand, we are interested in finding an analytical formula replacing Eq. (9). To this end, we approximate the Coulomb continuum wave functions $C(\mathbf{k},\mathbf{r}_1)$ and $C(\mathbf{k},\mathbf{r}_2)$ by their zeroth order around each nuclei [25] in the integral of Eq. (9), i.e., $C(\mathbf{k},\mathbf{r}_1) \approx C(\mathbf{k},\mathbf{R})$ and $C(\mathbf{k},\mathbf{r}_2) \approx C(\mathbf{k},-\mathbf{R})$, respectively. We call this model two-center approximate continuum wave functions (TCA). With this approximation an analytical expression for the recombination amplitude reads

$$\mathbf{d}_{rec}^{TCA}(\mathbf{k},\mathbf{R}) = -\frac{N^*(\nu)}{\sqrt{2[1 + s(R)]}}\Bigg\{ \exp(i\mathbf{k}\cdot\mathbf{R}/2)C^*(\mathbf{k},-\mathbf{R})$$
$$\times \left[\frac{\mathbf{R}}{2}L_0(1,\mathbf{k},\nu,\mathbf{k}) - \mathbf{K}_0(1,\mathbf{k},\nu,\mathbf{k}) \right]$$
$$+ \exp(-i\mathbf{k}\cdot\mathbf{R}/2)C^*(\mathbf{k},\mathbf{R})$$
$$\times \left[-\frac{\mathbf{R}}{2}L_0(1,\mathbf{k},\nu,\mathbf{k}) - \mathbf{K}_0(1,\mathbf{k},\nu,\mathbf{k}) \right]\Bigg\}, \tag{13}$$

where L_0 and $\mathbf{K}_0$ are defined in the Appendix.

More sophisticated wave functions to deal with an electron in a field of two nuclei have been presented recently in the study of single ionization of molecules by electron impact. The modified two-center continuum wave model (MTCC) [30] will be investigated in this work. This model emerges from the solution of the Schrödinger equation for one electron in the field of two fixed Coulombic centers, and the resulting wave functions satisfy the boundary conditions up to order $O[(kr)^{-2}]$, with k being the momentum of the electron.

In the next section we calculate the interference patterns, comparing the predictions made by the various approximations.

III. RESULTS AND DISCUSSION

For the study of the orientation dependence we follow Ref. [6] in order to compare directly with the numerical model developed there. As discussed above, the recombina-
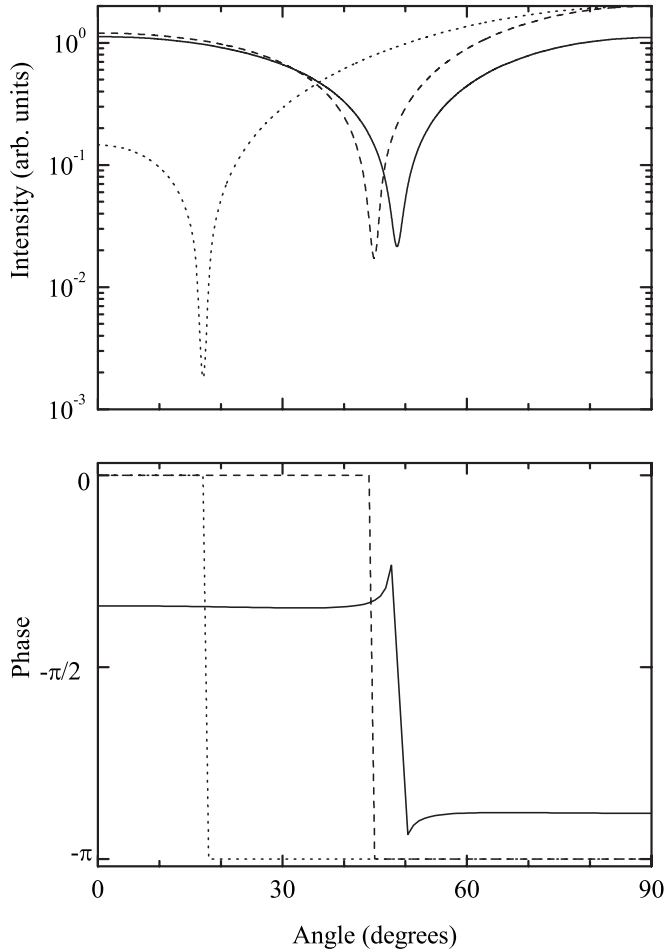
FIG. 1. Orientation dependence of the harmonic intensity and phase for the 43rd harmonic of a 780 nm laser field. Dashed line: PW velocity form ($E_k = \Omega$, see text). Dotted line: PW velocity form (with the SFA relation between electron energy and harmonic frequency). Solid line: TCA length form.
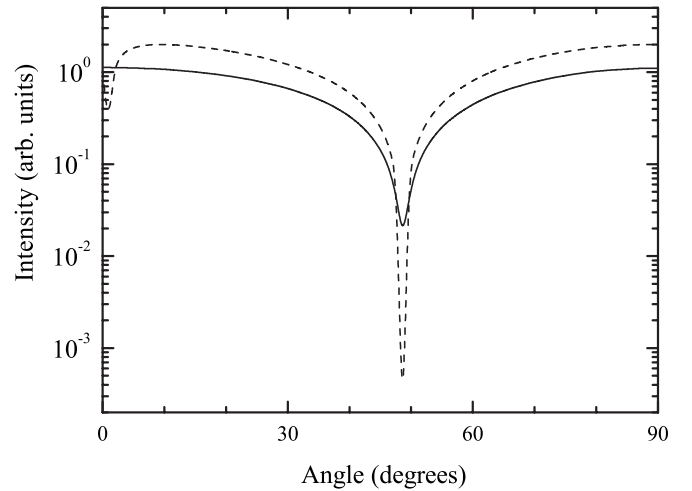

FIG. 2. Orientation dependence of the harmonic intensity for the 43rd harmonic (see Fig. 1), using the recombination matrix element in length form. Solid line: TCA approach. Dashed line: eikonal limit of the TCA approach.

tion amplitude is responsible for the interference patterns in molecules. We study the orientation dependence of the harmonics using the SFA relation $\Omega = k^2/2 + I_p$ with I_p being the ionization potential and Ω the frequency of the emitted harmonic. We begin our analysis by studying the PW approximation in the velocity form. From Eq. (8), the modulus squared of the matrix element is proportional to $\cos^2(\mathbf{k} \cdot \mathbf{R}/2)$. Consequently, destructive interference appears when $\mathbf{k} \cdot \mathbf{R} = (2n+1)\pi$, or, in terms of the projected internuclear distance $R_x = R\cos\theta$ and the electron wavelength $\lambda = 2\pi/k$,

$$R_x = (2n+1)\lambda/2, \quad n = 0, 1, \ldots . \tag{14}$$

On the other hand, constructive interference occurs when

$$R_x = n\lambda, \quad n = 0, 1, \ldots . \tag{15}$$

Note that only from the PW-velocity form, such simple interference conditions emerge.

In Fig. 1 we plot the intensity and phase of the 43rd harmonic of a 780 nm laser field versus the orientation angle θ. The prediction of the minimum using the TCA formulation

in the length form (as well as in the velocity form, not shown here) is very close to the numerical results of [6,14]. It is worth noting that the PW approach using an electron energy $E_k = \Omega$ gives surprisingly very good predictions [6], but when the SFA relation is used, i.e., $E_k = \Omega - I_p$, the results are very poor, in contrast to the very good agreement of the TCA model. Similar conclusions can be drawn for H_2 from [31]. Compared to the velocity form, the interference term is more complicated in the length form [see Eq. (7)] and the agreement is less impressive, see the results below.

For the non-PW approaches, nonanalytical formulas result and it is necessary to study the interference minima and maxima numerically. However, if we proceed using the asymptotic limit, i.e., taking $|kR - \mathbf{k} \cdot \mathbf{R}| \to \infty$, in the approximated Coulomb continuum wave functions $C(\mathbf{k}, \mathbf{R})$ and $C(\mathbf{k}, -\mathbf{R})$ (this limit is known in collision physics as the *eikonal limit*), we can obtain an analytical formula for the interference patterns.

To explore the TCA behavior in the eikonal limit we do a similar analysis as in [23] to *isolate* the interference behavior. Consequently we rewrite (13) as

$$d_{\text{rec},x}^{\text{TCA}}(\mathbf{k}, \mathbf{R}) = r_+^{\text{TCA}} \exp[i\mathbf{k} \cdot \mathbf{R}/2 + i\nu \ln(kR + \mathbf{k} \cdot \mathbf{R})]$$
$$+ r_-^{\text{TCA}} \exp[-i\mathbf{k} \cdot \mathbf{R}/2 + i\nu \ln(kR - \mathbf{k} \cdot \mathbf{R})]. \tag{16}$$

From this length form of the recombination amplitude [see Eq. (16)], it is still not possible to obtain a simple analytical form of the interference term. However, in the velocity form, the interference term appearing in the modulus squared $|v_{\text{rec},x}^{\text{TCA}}|^2$, is proportional to $\cos^2\left(\mathbf{k} \cdot \mathbf{R} + \nu \ln\frac{kR+\mathbf{k} \cdot \mathbf{R}}{kR-\mathbf{k} \cdot \mathbf{R}}\right)$. For $\nu = 0$, i.e., for the high-velocity electrons, one recovers the PW form of the interference factor in the velocity formulation, see Eq. (8). The interference minima appear thus when
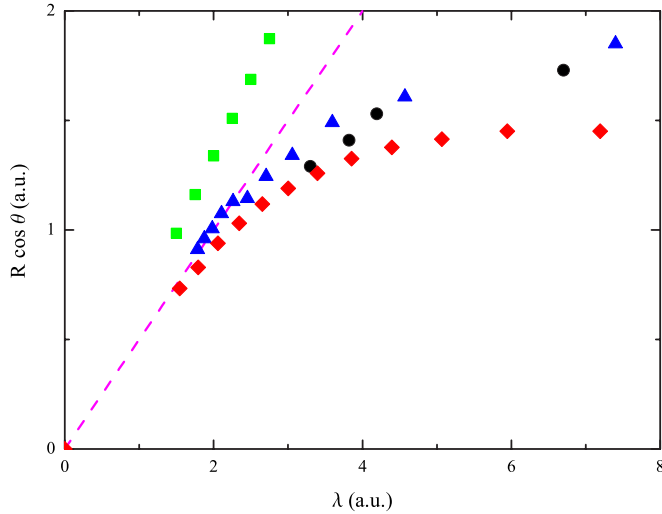
FIG. 3. (Color online) Projected internuclear separation for interference minima vs electron wavelength. Dashed line: plane wave in the velocity form. ($\blacksquare$) Plane wave in the length form, ($\blacklozenge$) TCA model in the length formulation, ($\blacktriangle$) 2D model from Lein *et al.* [6] for $I=1\times10^{15}$ W/cm^2, ($\bullet$) exact from Kamta *et al.* [14].

$$\mathbf{k}\cdot\mathbf{R} + \nu\ln\left(\frac{kR+\mathbf{k}\cdot\mathbf{R}}{kR-\mathbf{k}\cdot\mathbf{R}}\right) = (2n+1)\pi, \quad n=0,1,\dots\ ,$$

$$(17)$$

or in terms of R_x and λ,

$$R_x + (\lambda/2\pi)^2\ln\frac{1+\cos\theta}{1-\cos\theta} = (2n+1)\lambda/2, \quad n=0,1,\dots\ .$$

$$(18)$$

The logarithmic shift in the above formula depends on the molecular structure only through the geometrical factor $\cos\theta=\mathbf{k}\cdot\mathbf{R}/kR$, not through the value of kR. Similar results were obtained for molecular photoionization [25].

Figure 2 shows the behavior of the eikonal limit and its comparison with the TCA formulation in the length gauge. The eikonal limit predicts exactly the same value of the orientation angle minimum. Only a slight difference in the amplitude appears. Furthermore, the phases predicted by this model are identical to those that emerge from the TCA formulation and for this reason we omit the phase plot.

In Fig. 3 we plot the projected internuclear separation versus electron wavelength using various approximations and we compare them with numerical calculations made in [6,14]. We can observe that in the small- to intermediate-wavelength region, 1 a.u.$\leqslant\lambda\leqslant4$ a.u. (corresponding to high-energy electrons), the TCA model gives very good predictions. On the other hand, when the electron wavelength increases, the TCA model is not able to reproduce adequately the predictions of the numerical calculations. An explanation of this lies in the fact that the low-energy electrons are sensitive to the quality of the two-center continuum wave functions, and the TCA model is not accurate in the so-called condensation region, i.e., when all the particles are close. In
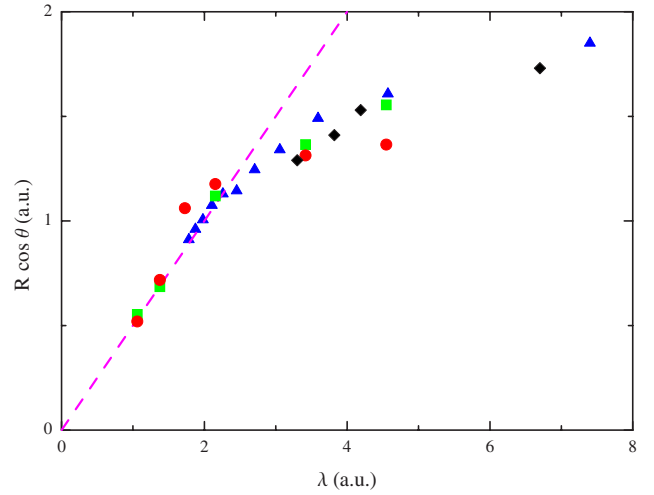

FIG. 4. (Color online) Same as Fig. 3 but using other two-center Coulomb models. Dashed line: plane wave in the velocity form. ($\bullet$) TCC in the length form, ($\blacksquare$) MTCC model in the length form, with $z_3=0.25$ and $z_4=0$ (see text), ($\blacktriangle$) 2D model from Lein *et al.* [6] for $I=1\times10^{15}$ W/cm^2, ($\blacklozenge$) exact from Kamta *et al.* [14].

these cases more elaborate wave functions or numerical wave functions are needed.

To complete our analysis we calculate the internuclear separation versus electron wavelength using the TCC and more sophisticated models (MTCC) (Fig. 4). Here we observe that the more sophisticated two-center models allow us to predict interference minima in a larger range of wavelengths. The MTCC shows the best global performance, since it reaches the region of low electron energy and the results are comparable with fully numerical models, but with less computer requirements. The parameters z_3 and z_4 (see Fig. 4) are *free variational* parameters [30], and we choose their values such as to obtain overall good agreement with the exact position of the interference minima. For a complete prediction of the molecular interference features, including the full range of the ionized electron energy, a better description of the electron in the continuum of the two atomic centers is needed, e.g., using functions that result from the numerical solution of the Schrödinger equation.

IV. CONCLUSIONS

We have investigated how the incorporation of the Coulomb binding potential of the atomic centers modifies the prediction of two-center interference in HHG with H_2^+ molecules. Using instead of plane waves various types of Coulomb corrections for the electron continuum state, we have demonstrated that the prediction of two-center interference is improved, in particular in the region of small electron wavelengths. In previous work [6], a simple formula for the interference minimum had been derived from the plane-wave approximation, but good agreement with the exact interference minimum was obtained only when using a heuristic relation between electron momentum and harmonic frequency. Here, we have derived an interference formula in a systematic way from an approximated Coulomb correction (velocity-form

TCA) in the eikonal limit. Unfortunately, this approach gives only modest improvement with respect to the PW approach. On the other hand, one of the more involved Coulomb corrections is very close to the exact results in the entire investigated energy range, but is not amenable to deriving a simplified analytical formula. Future work will address the calculation of harmonic spectra using the SFA with Coulomb corrections.

APPENDIX

The integrals involved in the calculation of Eq. (9) can be of two types: a *scalar* one

$$I = e^{\pm i\mathbf{k}\cdot\mathbf{R}/2} \int d^3 r_1 e^{-i\mathbf{k}\cdot\mathbf{r}_1} e^{-ar_1} {}_1F_1[-i\nu,1,-i(kr_1-\mathbf{k}\cdot\mathbf{r}_1)]$$

$$\times {}_1F_1[-i\nu,1,-i(kr_2-\mathbf{k}\cdot\mathbf{r}_2)] \qquad (A1)$$

and a *vectorial* one

$$\mathbf{J} = e^{\pm i\mathbf{k}\cdot\mathbf{R}/2} \int d^3 r_1 e^{-i\mathbf{k}\cdot\mathbf{r}_1} e^{-ar_1} \mathbf{r}_1 {}_1F_1[-i\nu,1,-i(kr_1-\mathbf{k}\cdot\mathbf{r}_1)]$$

$$\times {}_1F_1[-i\nu,1,-i(kr_2-\mathbf{k}\cdot\mathbf{r}_2)]. \qquad (A2)$$

We begin by defining the function

$$\Gamma(\mathbf{r}_2) = e^{-\epsilon r_2} {}_1F_1[-i\nu,1,-i(kr_2-\mathbf{k}\cdot\mathbf{r}_2)]$$

$$= \frac{1}{(2\pi)^{3/2}} \int d^3\tau \Psi(\boldsymbol{\tau}) e^{i\boldsymbol{\tau}\cdot\mathbf{r}_2}, \qquad (A3)$$

with

$$\Psi(\boldsymbol{\tau}) = \frac{1}{(2\pi)^{3/2}} \int d^3 r_2 \Gamma(\mathbf{r}_2) e^{-i\boldsymbol{\tau}\cdot\mathbf{r}_2}, \qquad (A4)$$

where we include a parameter $\epsilon \to 0$ to avoid numerical instabilities. Using Eq. (A4) in Eqs. (A1) and (A2), one obtains

$$I = \frac{e^{\pm i\mathbf{k}\cdot\mathbf{R}/2}}{(2\pi)^{3/2}} \int d^3\tau \Psi(\boldsymbol{\tau}) e^{-i\boldsymbol{\tau}\cdot\mathbf{R}}$$

$$\times \int d^3 r_1 e^{i(\boldsymbol{\tau}-\mathbf{k})\cdot\mathbf{r}_1} e^{-ar_1} {}_1F_1[-i\nu,1,-i(kr_1-\mathbf{k}\cdot\mathbf{r}_1)]$$

$$(A5)$$

and

$$\mathbf{J} = \frac{e^{\pm i\mathbf{k}\cdot\mathbf{R}/2}}{(2\pi)^{3/2}} \int d^3\tau \Psi(\boldsymbol{\tau}) e^{-i\boldsymbol{\tau}\cdot\mathbf{R}}$$

$$\times \int d^3 r_1 e^{i(\boldsymbol{\tau}-\mathbf{k})\cdot\mathbf{r}_1} e^{-ar_1} \mathbf{r}_1 {}_1F_1[-i\nu,1,-i(kr_1-\mathbf{k}\cdot\mathbf{r}_1)],$$

$$(A6)$$

using that $\mathbf{r}_2 = \mathbf{r}_1 - \mathbf{R}$.

Now using the definitions

$$L_0(a,\mathbf{q},\alpha,\mathbf{p})$$

$$= \frac{1}{\pi^2}(a/2)^{3/2} \int d^3 r e^{-i\mathbf{q}\cdot\mathbf{r}} e^{-ar} {}_1F_1[-i\alpha,1,-i(pr-\mathbf{p}\cdot\mathbf{r})]$$

$$(A7)$$

and

$$\mathbf{K}_0(a,\mathbf{q},\alpha,\mathbf{p})$$

$$= \frac{1}{\pi^2}(a/2)^{3/2} \int d^3 r e^{-i\mathbf{q}\cdot\mathbf{r}} e^{-ar} \mathbf{r} {}_1F_1[-i\alpha,1,-i(pr-\mathbf{p}\cdot\mathbf{r})],$$

$$(A8)$$

it is possible to write (A5) and (A6) as

$$I = (\pi/a^3)^{1/2} e^{\pm i\mathbf{k}\cdot\mathbf{R}/2} \int d^3\tau \Psi(\boldsymbol{\tau}) e^{-i\boldsymbol{\tau}\cdot\mathbf{R}} L_0(a,\mathbf{k}-\boldsymbol{\tau},\nu,\mathbf{k})$$

$$(A9)$$

and

$$\mathbf{J} = (\pi/a^3)^{1/2} e^{\pm i\mathbf{k}\cdot\mathbf{R}/2} \int d^3\tau \Psi(\boldsymbol{\tau}) e^{-i\boldsymbol{\tau}\cdot\mathbf{R}} \mathbf{K}_0(a,\mathbf{k}-\boldsymbol{\tau},\nu,\mathbf{k}).$$

$$(A10)$$

The remaining three-dimensional integral in the $\boldsymbol{\tau}$ variable can be evaluated numerically using quadratures. The integrals (A7), (A8), and $\Psi(\boldsymbol{\tau})$ are usual in collision physics and can be calculated analytically using the Norsdieck method as described in [29].

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