Nondipole effects in strong-field ionization

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We present a study of the relativistic nondipole effects in strong-field tunneling ionization process driven by a linearly polarized laser pulse. We consider the role of these effects in breaking the symmetry with respect to the inversion of the momentum component perpendicular to the laser-field polarization direction, which the dipole differential ionization probabilities possess. The study is based on the solution of a three-dimensional time-dependent Schrödinger equation taking into account the leading-order relativistic corrections.

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I. INTRODUCTION

Relativistic effects in the process of atomic or molecular photoionization are usually associated with either very high laser-field intensities (such as the presently achievable fields of intensity of the order of $10^{22}$ W/cm$^2$ [1]) or very high laser-field frequencies. In the former case the energy gained by the electron in the field necessitates relativistic treatment of the problem; in the latter, the nondipole effects due to the large momentum carried by a photon become important.

The relativistic nondipole effects, however, can manifest themselves even for the small frequency infrared (IR) laser fields [2,3], for the ionization in the so-called tunneling regime characterized by the values $\gamma \lesssim 1$ of the Keldysh parameter $\gamma = \omega \sqrt{2I}/E$ ($\omega$ and $E$ are the frequency and strength of the laser field, respectively, and $I$ is the ionization potential of the target system in atomic units). The reason for that is a large number of the IR photons participating in the process of the tunneling ionization [4]. Even though the momentum of an IR photon is small, the total momentum delivered to the target in the process of the tunneling ionization can be non-negligible, which offers a perspective of the experimental observation of the nondipole effects.

In the experiment [5] performed with the laser field with the typical parameters of the tunneling ionization regime (wavelengths of 800 nm) the momentum gained by the electron in the laser propagation direction was measured. Reference [6] reports breakdown of the dipole approximation in describing experimentally observed photoelectron momentum distributions, which can be considerably influenced by the formation of singularities (cusps) in the photoelectron spectra [13–16]. This fact bears a direct relation to the subject of the present work studying photoelectron momentum distributions, which can be considerably influenced by the Coulomb focusing effect.

One way of allowing us to take into account the Coulomb interaction in a relativistic calculation is a numerical solution of an appropriate relativistic generalization of the time-dependent Schrödinger equation (TDSE) describing quantum evolution of the system subjected to an external electromagnetic field. In Ref. [8] Chelkowski et al. performed a TDSE calculation taking full account of the nondipole effects for a model two-dimensional (2D) hydrogen atom. In Refs. [17,18] approaches to the solution of the time-dependent Dirac equation based on the use of the so-called split operator method were described. Nondipole effects in the angular distribution of photoelectrons were studied in [19] by solving numerically the 3D nonrelativistic Schrödinger equation including the leading-order nondipole correction.

We proposed [20] a procedure allowing us to solve a 3D Dirac equation and used it to study the problem of the tunneling time [21]. It turns out, however, that use of the Dirac equation, which takes into account all relativistic effects (excluding the quantum electrodynamic ones, of course) but is rather expensive computationally, is often quite unnecessary. In particular, the present problem of the nondipole effects in the tunneling ionization regime does not require account of the relativistic kinematic effects. The electron motion in
this case is essentially nonrelativistic; the only ingredient in the problem that requires a proper relativistic treatment is the atom–laser-field interaction. Below we describe such a procedure, providing correct account of the relativistic nondipole effects and allowing us to study their role for a realistic 3D atomic system.

The paper is organized as follows. In Sec. II we describe the numerical techniques we use to perform the TDSE calculation. Our results are presented in Sec. III. We summarize in Sec. IV. Atomic units are used throughout the paper.

II. THEORY

Solution of the TDSE with leading-order relativistic corrections

Our aim is to obtain the leading-order relativistic corrections to the nonrelativistic TDSE describing evolution of an atomic system

\[ \frac{i}{\hbar} \frac{\partial \Psi(r)}{\partial t} = \left( \hat{H}_\text{atom} + \hat{H}_\text{int}(t) \right) \Psi(r), \]  

(1)

where \( \hat{H}_\text{atom} \) is a Hamiltonian describing the field-free atom and \( \hat{H}_\text{int}(t) \) describes the field-atom interaction. A systematic way to do this is to consider the transition to the nonrelativistic limit of the Dirac equation [22,23]. For the case of the leading-order relativistic corrections one can use a simpler and more physically transparent procedure described below.

The leading relativistic corrections to Eq. (1) are, as we will see, of the order of \( c^{-1} \) (here \( c = 137.036 \) a.u. is the velocity of light). The field-free atomic Hamiltonian including the leading-order relativistic corrections, the so-called Breit-Pauli Hamiltonian [24], differs from the nonrelativistic Hamiltonian in the terms of the order of \( c^{-2} \). There are no relativistic corrections of the order of \( c^{-2} \) for the field-free atomic Hamiltonian, and if we are interested in the corrections of the order of \( c^{-1} \) only, we may still use the nonrelativistic expression for the field-free atomic Hamiltonian.

For the nonrelativistic atom-field interaction Hamiltonian in (1) we use the velocity gauge

\[ \hat{H}_\text{int}(t) = p \cdot A(t) + \frac{A^2(t)}{2}, \]  

(2)

where \( A(t) \) is the vector potential of the pulse, which, in the nonrelativistic dipole approximation is a function of time variable only. Relativistic corrections to this Hamiltonian arise from the fact that the vector potential of a traveling wave is in fact a function of time and space variables. We will assume that the laser pulse propagates along the \( x \) axis. The vector potential is then a function \( A(t - x/c) \) of the combination \( t - x/c \). We assume further that the pulse is linearly polarized along the \( z \) direction. The leading relativistic correction to the operator (3) can be obtained by substituting this expression for the vector potential instead of \( A(t) \) in (3), performing an expansion in powers of \( c^{-1} \) and keeping the terms linear in \( c^{-1} \). In principle, for the coordinate-dependent vector potential certain care should be exercised, since the momentum operator and vector potential may no longer commute, so one must use a symmetrized dot product of these operators in (3). For the choice of the polarization and propagation directions we made above, we need not worry about this; the first term in (3) is a product of the commuting operators \( p_z \) and \( A(t - x/c) \) [we use the notation \( A(t - x/c) \) for the \( z \) component of the vector potential]. Following this strategy, we obtain a field-atom interaction operator containing relativistic corrections linear in \( c^{-1} \):

\[ \hat{H}_\text{int}(r,t) = \hat{p}_z A(t) + \frac{\hat{p}_z x E(t)}{c} + \frac{A(t) E(t)x}{c} + \frac{A^2(t)}{2}, \]  

(3)

where we introduce the electric field of the pulse \( E(t) = -\partial A(t)/\partial t \). The last term on the right-hand side of (3) is a function of time variable only and can therefore be removed by a unitary transformation of the wave function. We therefore need not consider this term. The interaction Hamiltonian (3) can be related by a gauge transformation to the Hamiltonian uses in [19], where the laser-field–atom interaction was described using the Kramers-Henneberger gauge.

There is an additional source of relativistic corrections of the order of \( c^{-1} \) in the Hamiltonian interaction of the magnetic field of the pulse and the electron spin. These corrections cannot be obtained by simple generalization of the nonrelativistic Hamiltonian we described above, because electron spin is an essentially relativistic phenomenon following from the Dirac equation [23]. The procedure based on the systematic expansion of the Dirac equation in powers of \( c^{-1} \) gives for this term an expression [24] \( \hat{m}_m \frac{\sigma \cdot H}{c^2} \), where \( \sigma \) are the Pauli matrices and \( H \) is the magnetic field of the pulse. For the geometry we employ (the pulse propagates in the \( x \) direction and the electric field points in the \( z \) direction) the magnetic-field vector has only a \( y \) component, which for the plane wave we consider is related to the electric field as \( H_x(t) = -E_x(t) \). We arrive thus at the following expression for the field-atom interaction operator including relativistic corrections linear in \( c^{-1} \):

\[ \hat{H}_\text{int}(r,t) = \hat{p}_z A(t) + \frac{\hat{p}_z x E(t)}{c} + \frac{A(t) E(t)x}{c} - \frac{\sigma_y E(t)}{2c}. \]  

(4)

Instead of the nonrelativistic TDSE (1) we have to solve the evolution equation with the nonrelativistic field-free Hamiltonian \( \hat{H}_\text{atom} \) and the atom-field interaction operator (4). The corresponding time-dependent wave function is of course a two-component spinor for which we will use the notation \( \Psi(r,\mu,t) \), \( r \) denoting the space and \( \mu \) the spin variables. We should note, however, that the consideration of the electron-spin effects is not necessary for the study of the nondipole effects of the order of \( c^{-1} \) that we conduct herein. The electron-spin effects were, for example, neglected in [8]. That the neglect of the spin effects is justified, as long as we are interested in the leading-order nondipole effects, can be seen by the following simple argument using classical picture of the electron motion. The effects of the electron-spin and laser-pulse–magnetic-field interaction give a correction to the energy \( U_m = -\mu \cdot H \), where \( \mu \) is the electron magnetic moment and \( H \) is the magnetic field. The corresponding correction to the total force the magnetic field exerts on the electron is then \( \Delta F = -\nabla U_m \). The spatial dependence of \( U_m \) is due to the spatial dependence of \( H \). Since the magnetic field of the propagating wave we consider is a function of the combination \( t - x/c \), the gradient of \( U_m \) acquires additional power of \( c^{-1} \), which, together with the fact that the electron magnetic moment \( \mu \) itself is proportional to \( c^{-1} \), implies that
the correction to the force due to the electron-spin–magnetic-field interaction is of the order of $c^{-2}$ and can be neglected for the nonrelativistic regime we consider. We chose, however, to include the electron-spin–magnetic-field interaction in the present study. Though, as explained above, this term in the Hamiltonian (4) does not give any significant contribution to the leading-order nondipole effects, its account provides a useful check of the accuracy of the calculation. We will discuss this issue in more detail in the next section.

As a target system we consider an argon atom described by means of the single-active-electron (SAE) approximation relying on a model potential [25]. The initial state of the system in the SAE approximation is a $p$ state. We consider below initial states with the values $M = 0$ and $M = 1$ of the orbital angular momentum projection. Electron-spin projection, as we discussed above, does not have any appreciable effect on the leading-order nondipole effects we are studying herein. We assume, therefore, that the initial electron state is a spin-up state with a $z$ component of the electron spin $\mu_0 = 1/2$.

To solve the TDSE with the interaction Hamiltonian (4) we combine the procedures we employed previously for the solution of the nonrelativistic TDSE [16,26,27] and the relativistic Dirac equation [20]. The solution of the TDSE is represented as an expansion

$$\Psi(r,\mu,t) = \sum_{l=0}^{l_{\text{max}}} \sum_{m=-l}^{l} \int d\eta r^l e^{i\mu r} Y_l^m(\eta) \psi_{l\mu}(r,\mu,t) \delta_{\mu,\mu_0},$$

where $\psi_{l\mu}(\mu) = \delta_{\mu,\mu_0}$ are the spin basis functions and $Y_l^m(\eta)$ are spherical harmonics. The vector potential in Eq. (4) was chosen as

$$A(t) = -\frac{E_0}{\omega} \sin^2 \left( \frac{\pi t}{T_1} \right) \sin \omega t$$

for $t \in (0, T_1)$ and zero otherwise. We used a base frequency $\omega = 0.057$ a.u. (with a wavelength of 790 nm) and total pulse duration $T_1 = 4T$, where $T = 2\pi/\omega$ is an optical cycle (o.c.) corresponding to the base frequency $\omega$. The electric field corresponding to the vector potential (6) is shown in Fig. 1.

The radial variable is treated by discretizing the TDSE on a grid with the step size $\Delta r = 0.1$ a.u. in a box of the size $R_{\text{max}}$. The values of the parameters $R_{\text{max}}$ and $l_{\text{max}}$ in Eq. (5) were chosen (after the necessary convergence checks) as $R_{\text{max}} = 1000$ and $l_{\text{max}} = 60$ a.u. These relatively large values of $R_{\text{max}}$ and $l_{\text{max}}$ were dictated by the rather high values of the field strengths we consider below. We report calculations for the peak field strengths of $E_0 = 0.1, 0.15$, and 0.2 a.u. (corresponding to the intensities of $3.5 \times 10^{14}, 7.9 \times 10^{14}$, and $1.4 \times 10^{15}$ W/cm$^2$). Summation over the angular momentum projection $m$ in Eq. (5) was restricted as follows: $|m| \leq 1$ for the initial state of an Ar atom with orbital angular momentum projection $M = 0$ and $2 \geq m \geq 0$ for the initial state with $M = 1$. This choice of the ranges of $m$ values in (5) agrees with the declared accuracy of our calculation. Indeed, only the operators in the Hamiltonian (4) that contain a factor of $c^{-1}$ are nondiagonal in the basis of the states with given values of $m$. Well-known selection rules tell us that these nondiagonal operators have nonzero matrix elements between states with orbital angular momentum projections that differ by one unit. The evolution operator $\hat{U}(t,0)$ corresponding to the Hamiltonian (4), which guides the evolution of the system in time, can be found if the action of an arbitrarily high power of the Hamiltonian (4) on the initial state of the system is known (e.g., using the well-known representation of the evolution operator as a chronological exponential operator [22,23]). Applying the arguments based on the selection rules we discussed above to the powers of the Hamiltonian (4), one can see that the evolution operator can be represented as

$$\hat{U}(t,0) = \hat{U}_0(t,0) + c^{-1}\hat{U}_1(t,0) + O(c^{-2}),$$

where the zeroth-order operator $\hat{U}_0(t,0)$ is diagonal in the $m$ representation and the operator $\hat{U}_1(t,0)$ has nonzero matrix elements between the states with orbital angular momentum projections that differ by one unit. Therefore, if we are interested in the effects of the order not higher than $c^{-1}$, we can keep in the expansion (5) only the states with the orbital angular momentum projections that differ from the angular momentum projection in the initial state by not more than one unit. A system of coupled equations for the radial functions $f_{lm\mu}(r,\mu,t)$ resulting from the substitution of the expansion (5) into the TDSE was solved using the matrix iteration method [28].

For the geometry we employ (a laser pulse propagating along the $x$ direction and polarized along the $z$ direction), a convenient characteristic of the ionization process, which we will study below, is the so-called lateral or transverse electron momentum distribution (TEMD), which describes the probability distribution to detect an ionized electron with a given value $p_x$ of the momentum component along the $x$ direction. In the case of the absence of the nondipole effects, the TEMD is an even function of $p_x$ [14]. The nondipole effects break this left-right symmetry in the TEMD [8]. To actually calculate the TEMD, we project the solution of the TDSE after the end of the laser pulse on the set of the scattering states of an Ar atom with ingoing boundary conditions:

$$\psi_{p,\mu,f}^{(-)}(r) = \sum_{lm} \int \gamma_{lm}^{\ast}(p) Y_l^m(r) R_{lk}(r) \psi_{l\mu}(r,\mu,t),$$

thereby obtaining ionization amplitudes $a(p,\mu,f)$ and differential ionization probabilities $P(p,\mu,f)$, giving probability...
FIG. 2. Expectation value of the $x$ component of the electron-spin operator. The red dotted line shows $\langle \hat{S}_x \rangle$ computed as $\langle \hat{S}_x \rangle = \langle \Psi(t) | \hat{S}_x | \Psi(t) \rangle$, using the solution $\Psi(t)$ of the TDSE (1) with the Hamiltonian (4). The green solid line shows the formula $\langle \hat{S}_x \rangle = \frac{1}{2} \sin \left( \frac{\alpha}{\gamma} \right)$.

FIG. 3. The TEMD for different field strengths and different initial states of an Ar atom for the pulse with the shape shown in Fig. 1.
FIG. 4. Ionization from the initial $M = 0$ state. Shown are differential distributions $W(p_x, p_z)$ (left column) for the initial $M = 0$ state and antisymmetrized distributions $W_a(p_x, p_z)$ (right column) defined in Eq. (12) for field strengths of 0.1 a.u. (top row), 0.15 a.u. (middle row), and 0.2 a.u. (bottom row).

equations:

$$v\left(-\frac{1}{2}, t\right) = \sin \frac{A(t)}{2c},$$

$$v\left(\frac{1}{2}, t\right) = \cos \frac{A(t)}{2c},$$

(10)

where $A(t)$ is the vector potential given by Eq. (6). Since the vector potential vanishes at the end of the pulse, $v(-1/2)$ should vanish too, implying that the state initially polarized along the $z$ direction becomes polarized again after the end of the pulse. This is of course a consequence of our choice to consider only effects not higher in $c^{-1}$ than the linear term. To obtain a nonzero probability of a spin-flip process, we should include spin-orbit interactions in the Hamiltonian (terms of order $c^{-2}$ [24]). For this reason we could, as we mentioned above, dispense with the spin part of the wave function altogether in our calculation. We kept it, however, retaining the spin-magnetic-field interaction term in the Hamiltonian (4) and using the two-component spinor wave functions for
two reasons. First, it provides us with a basis for future generalizations, including the spin-orbit effects. Second, it provides a convenient additional accuracy check of the present calculation. In particular, it is easy to see that for the evolution of the components of the spin wave function given by exact analytic equations (10), expectation values of the spin operator as functions of time are \( \langle S_x \rangle = \frac{1}{2} \sin \frac{4\pi t}{c} \) and \( \langle S_y \rangle = 0 \). We used these equations as an additional check of the accuracy of our solution of the TDSE. An illustration is shown in Fig. 2, where we compare results for the expectation values \( \langle S_x \rangle \) computed analytically and computed as \( \langle \Psi(t)|S_x|\Psi(t) \rangle \), where \( \Psi(t) \) is the solution of the TDSE (1) with the Hamiltonian (4), obtained using the procedure described above.

### III. RESULTS

In Fig. 3 we present results for the TEMD obtained for different field strengths and different \( M = 0 \) and \( M = 1 \) initial states of an Ar atom for the pulse with the shape shown in Fig. 1. Results are compared to the results of the dipole (completely nonrelativistic) calculation obtained by dropping all relativistic corrections from the Hamiltonian (3).

One can see that for both \( M = 0 \) and \( M = 1 \) the initial states of the TEMD begin deviating appreciably from the dipole results for the field strength of 0.15 a.u., the difference of the nondipole and dipole results becoming quite apparent for the field strength of 0.2 a.u. The overall behavior of the nondipole TEMD is quite consistent with that found in the 2D TDSE calculation reported in [8]. Nondipole effects increase, in general, the number of electrons with momenta parallel to the beam propagation direction for which \( p_x \gtrsim 0.1 \) a.u., compared to the dipole case. At the same time, the nondipole effects generally decrease the number of electrons with momenta antiparallel to the beam propagation direction for which \( |p_x| \) is not too large. More detailed information can be obtained from the analysis of the differential distributions in \( (p_x, p_z) \) plane defined as

\[
W(p_x, p_z) = \int_{-\infty}^{\infty} P(p_x)dp_z.
\]  

In the dipole case the distribution \( W(p_x, p_z) \) (11) clearly possesses a symmetry with respect to the transformation \( (p_x, p_z) \rightarrow (-p_x, p_z) \). To better reveal the role of the nondipole effects breaking this symmetry, we will also consider an antisymmetrized function

\[
W^a(p_x, p_z) = W(p_x, p_z) - W(-p_x, p_z). \tag{12}
\]

We will consider below these distributions separately for the cases of \( M = 0 \) and \( M = 1 \) initial states.

#### A. The \( M = 0 \) initial state

Differential distributions \( W^a(p_x, p_z) \) for the \( M = 0 \) initial state are shown in Fig. 4. A considerable asymmetry of the spectra with respect to \( p_z \) is noticeable, i.e., in the pulse polarization direction. This is a well-known phenomenon due to the carrier-envelope-phase effects, which manifests itself for driving pulses of short duration, and we will not dwell upon this issue. Antisymmetrized distributions \( W^a(p_x, p_z) \) for the \( M = 0 \) case are shown in the right column in Fig. 4.

From the plots showing the distributions \( W^a(p_x, p_z) \), one can see that major contributions to the effect of the antiparallel nondipole shift (we recall that in our calculation the pulse propagates in the positive \( x \) direction) are due to the local maxima of \( W^a(p_x, p_z) \) in the half plane \( p_x < 0 \) corresponding to the low-momentum electrons. For a field strength of 0.1 a.u., the region in the \( (p_x, p_z) \) plane where these electrons are concentrated is approximately defined by the inequalities \( |p_x| < 0.1 \) a.u. and \( |p_z| < 0.3 \) a.u. For larger fields the local maximum of \( W^a(p_x, p_z) \) corresponding to these low-energy electrons becomes less pronounced but still remains visible. As one can surmise from the plots in Fig. 4, for a field strength of 0.2 a.u., momenta of the low-energy electrons exhibiting the antiparallel shift satisfy approximately \( |p_x| \lesssim 0.2 \) a.u. and \( |p_z| \lesssim 1 \) a.u. These approximate bounds agree well with the bounds given in [8], where Chelkowski et al. performed a calculation including the nondipole effects for a model 2D hydrogen atom and found that electrons with the momenta antiparallel to the pulse propagation direction are the electrons with \( p_x \lesssim 0.1 \) a.u., and \( p_z^2 < U_p/3 \) (here \( U_p = E^2_0/4\omega^2 \) is the ponderomotive energy). For the field parameters we use these bounds imply that electrons with the momenta shifted in the direction antiparallel to the pulse propagation...
FIG. 6. Ionization from the initial $M = 1$ state. Shown are differential distributions $W(p_x, p_z)$ (left column) for the initial $M = 0$ state and antisymmetrized distributions $W_{as}(p_x, p_z)$ (right column) for field strengths of 0.1 a.u. (top row), 0.15 a.u. (middle row), and 0.2 a.u. (bottom row).

On the other hand, the electrons with the momenta shifted in the direction parallel to the pulse pulse propagation direction are the electrons with larger momenta. These electrons are more evenly distributed in the $(p_x, p_z)$ plane, with the distribution $W_{as}(p_x, p_z)$ showing in the half plane $p_x > 0$ not sharp maxima, but rather broad elevated plateaus. These plateaus occupy a considerable area in the $(p_x, p_z)$ plane, which results in the overall predominance of the ionization in the pulse propagation direction (we will discuss this issue in more detail below). As can be inferred from the approximate location of these elevations of $W_{as}(p_x, p_z)$ in the half plane $p_x > 0$, typical values of the momentum component $p_x$ for the fast electrons, exhibiting parallel shift, belong to the interval $|p_z| \approx 1.5–2$ a.u. Typical values of the momentum component $p_z$ parallel to the pulse propagation direction for these electrons are $p_z = 0.2–0.3$ a.u.
B. The $M = 1$ initial state

For the ionization from the $M = 1$ initial state the TEMD in Fig. 3 exhibits structures near $p_x = 0$ that are absent in the $M = 0$ case. The origin of these structures is purely geometrical and can be easily elucidated. In Fig. 5 we show the photoelectron momentum distribution $P(p_x, p_y, p_z)$ (note that this is a full 3D electron momentum distribution, without integration over the $p_z$ component of the electron momentum) for two fixed values of the $p_x$ component, $p_z = 0$ and 0.1 a.u.

For $p_z = 0$ the photoelectron momentum distribution $P(p_x, p_y, p_z)$ exhibits a sharp drop in intensity along the line $p_z = 0$. This is a consequence of the structure of the evolution operator (and hence of the TDSE wave function), summarized in Eq. (7). For $p_z = 0$ and $p_y = 0$ the expansion (8) for the ingoing scattering state contains only the terms with $m = 0$. Consequently, the projection of the TDSE wave function developing from the initial $M = 1$ state on such a scattering state can have a nonzero value only due to the relativistic nondipole effects [represented by the term proportional to $c^{-1}$ on the right-hand side of Eq. (7)]. If we consider a purely nonrelativistic case, keeping only the first term on the right-hand side in the expansion for the propagator (7), the momentum distribution $P(p_x, 0, p_y)$ will have a nodal line $p_z = 0$ in the $(p_x, p_y)$ plane. The TEMD for the $M = 1$ case in Fig. 3 exhibits a tendency to drop (or at least not to grow as fast as in the $M = 0$ case) when $p_z$ approaches zero. It does not, however, drop considerably at $p_z = 0$. This is because the TEMD is obtained by integrating differential probabilities over all momentum components perpendicular to $p_z$, in particular the $y$ component of the electron momentum. If the $y$ component of the momentum vector is not zero, the above symmetry reasoning, which forced the momentum distribution $P(p)$ to vanish if $p_z = 0$ and $p_y = 0$, does not apply. In fact, as Fig. 5 shows, for fixed $p_y ≠ 0$ the distribution $P(p)$ has local maxima lying on the line $p_z = 0$. The maxima of differential momentum distributions present for $p_y ≠ 0$ compensate partially for the sharp drop of $P(p)$ at $p_z = 0$ when $p_y = 0$ and lead to the structures observed in the TEMD in the vicinity of $p_z = 0$ for the $M = 1$ case.

Apart from this difference between the $M = 0$ and $M = 1$ cases, which, as we saw, has a purely geometrical origin, the $p_z$-integrated differential distribution $W(p_x, p_y)$ and its antisymmetrized counterpart $W^a(p_x, p_y)$ provide essentially the same information as in the $M = 0$ case; $W(p_x, p_y)$ and $W^a(p_x, p_y)$ for the ionization from the initial $M = 1$ state are shown in Fig. 6.

One can see that, as in the $M = 0$ case, the distribution $W^a(p_x, p_y)$ has local maxima for small momenta in the half plane $p_x < 0$, corresponding to the electrons for which nondipole effects lead to the antiparallel shift. Local maxima of $W^a(p_x, p_y)$ in the half plane $p_x > 0$, corresponding to the electrons experiencing the momentum shift parallel to the propagation direction, on the other hand, are concentrated mainly in the regions of larger momenta, approximately satisfying the bounds on the momentum components obtained in [8], which we quoted above.

As in the $M = 1$ case, the electrons experiencing the positive shift are more broadly distributed in the $(p_x, p_y)$ plane, which leads to the overall dominance of the ionization in the $p_x > 0$ hemisphere. This can be conveniently illustrated using an asymmetry parameter defined as $β = (P_+ - P_-)/(P_+ + P_-)$, where $P_+$ and $P_-$ are the total probabilities to detect an electron in the $p_x > 0$ and $p_x < 0$ hemispheres, respectively. The asymmetry parameter as a function of the laser-field strength is shown in Fig. 7.

Figure 7 also shows the shifts of the central cusp of the TEMD in Fig. 3 as a function of laser-field intensity for the ionization from the $M = 0$ state (as can be seen from Fig. 3, the cusp shift has a meaning only for the ionization from the $M = 0$ state; therefore, we do not consider the $M = 1$ case). One can see that, despite the overall dominance of the ionization in the laser-beam propagation direction, the cusps of the TEMD are shifted in the opposite direction. This picture agrees qualitatively with the one described in [8]. The value of the cusp shift of the TEMD reported in [8] was approximately $−0.01$ a.u. for a field intensity of $10^{15}$ W/cm$^2$. In the present case the shifts are much smaller, which can be attributed to the difference of the wavelengths used in the two calculations. The cusp shifts reported in [8] were found to be of the order of $−⟨E_{el}/c⟩$, where $⟨E_{el}⟩$ is the expectation value of the electron energy. An order of magnitude estimate for this quantity is the ponderomotive energy, which for the wavelength of 800 nm used herein is considerably smaller than for the wavelength of 3400 nm employed in [8].

IV. CONCLUSION

We have presented the results of a full 3D calculation of the nondipole effects in strong-field tunneling ionization. The overall picture we presented above agrees qualitatively with the picture presented in [8], where a 2D TDSE calculation and a classical analysis of the nondipole effects were performed. The separation of the electrons in the groups of slow electrons, exhibiting a negative momentum shift, and the faster electrons, exhibiting the positive momentum shift, apparently survives, adding one more spatial dimension. Given the vastly different field parameters used in [8] and in the present work (a wavelength of 3.4 μm used in [8] against 790 nm used in the present work), we may conclude that this separation is indeed an important part of the mechanism of the nondipole effects in strong-field ionization.
In [8] Chelkowski et al. presented the results of a classical simulation of the ionization processes, with the conclusion that slow electrons are mainly the rescattered electrons following the long quantum orbits. We did not perform an analogous classical study in the present 3D case. The traces of the rescattering process in the present quantum calculation can, however, be discerned. The most prominent local maxima of the \( W_{\text{SHA}}(p_x, p_z) \) in the half plane \( p_z < 0 \), representing electrons experiencing antiparallel momentum shift, are generally very sharp and are located at the points with very small \( p_z \), for example, \( p_z \approx -0.05 \) a.u. for a field strength of 0.1 a.u. in Fig. 4. The lateral momentum distribution predicted by the Keldysh theory of strong-field ionization is given by the well-known formula [31] \( W_{\text{SHA}}(p_z) = P \exp \left(-\frac{\gamma^2 p_z^2}{2} \right) \), where \( \gamma \) is the Keldysh parameter and the prefactor \( P \) is a slowly varying function of the momentum components, which can be neglected [32] for the purposes of the qualitative analysis. For the field strength of 0.1 a.u. and the wavelength of 790 nm we have used in the present paper, this formula would imply that the distribution of the momentum component perpendicular to the polarization direction (e.g., the distribution of the \( p_z \) component) should be a smooth Gaussian function with a width of approximately 0.25 a.u. This formula for the lateral momentum distribution has been derived for the so-called direct electrons, which never return to the core after ionization has taken place. Deviation of the momentum distribution from the strong-field approximation, which we observed in Figs. 4 and 6, is well understood. In particular, the narrowing of the electron velocity distribution in the directions perpendicular to the laser-field polarization vector is due to the presence of the Coulomb field [13], which rescattered electrons experience upon returning to the ionic core. The electrons with small negative \( p_z \) in our calculation, responsible for the antiparallel shift, are therefore the rescattered electrons, which agrees with the conclusions made in [8].

Finally, we may say that the framework we used in this calculation (a semirelativistic approach taking into account the leading-order effects in \( c^{-1} \)) can be easily extended to include spin-orbit and kinematic effects by including the next-order terms in \( c^{-1} \) in the Hamiltonian, which can be done using the Breit-Pauli Hamiltonian [24]. This aim is left for future work.

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