

Anomalous effects in single-slit diffraction of light at relativistic intensities

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High-order harmonic generation via single-slit diffraction of relativistic laser pulses is investigated. Using fully kinetic two-dimensional (2D) and three-dimensional (3D) particle-in-cell simulations, we show that interesting optical phenomena emerge, including the generation of harmonic beams that are anomalously polarized orthogonal to the driver, harmonic spectrum variation depending on the incident laser polarization, and a deflection of transmitted lights that leads to a tilted harmonic intensity pattern due to total angular momentum conservation. It is shown that these anomalous effects are associated with complex peripheral electron dynamics on the plasma vacuum interface. To account for these effects, a new theoretical model is developed that can calculate harmonic fields from arbitrary 2D electron motion within the diffraction plane based on the “relativistic oscillating window” mechanism; the results agree well with the simulations. Our model indicates that the optical properties of the harmonic beams are determined by the 2D in-plane electron motion, which can be leveraged to provide immense opportunities for manipulating light-matter interaction at relativistic intensities.

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I. INTRODUCTION

With the invention of the chirped pulse amplification [1], the laser-matter interaction enters the relativistic regime, where the electron quiver motion in the laser fields approaches the speed of the light, giving rise to abundant relativistic nonlinear effects [2]. For example, the reflection of a relativistically strong laser can lead to high-harmonic generation (HHG) by the “relativistic oscillating mirror (ROM)” mechanism [3–5]. The reflected pulse is associated with a train of attosecond pulses, which promises new advances in attosecond sciences [6–9]. When the laser beam carries orbital angular momentum (OAM) [10–12], the reflection converts the OAM from the driver to the harmonics [13,14], and a deflection effect is found at oblique incidence due to the asymmetric radiation pressure of an intense vortex beam [15]. These behaviors of light not only provide fundamental insight into relativistic optics, but also promise new advances in a variety of applications, such as attosecond sciences [6–9], optical communications [16,17], and biophotonics [18].

On the other hand, another fundamental optical process, the diffraction of light, remains largely unexplored at relativistic intensities. This is probably because the prepulses tend to destroy small diffraction structures. Thanks to the progress of laser cleaning technology [19,20], the laser temporal contrast

has been steadily improving. To date, multiple diffraction effects have been reported experimentally using self-induced plasma apertures [21–23]. Thus, developing a predictive model for the relativistic light diffraction is a pressing issue that needs to be addressed in order to interpret future experiments. Recently, it is found that the diffraction of relativistic laser beams also produces high-order harmonics [24–27]. Analogous to the ROM mechanism, a “relativistic oscillating window (ROW)” model has been proposed [24], which attributes the HHG to the laser-driven peripheral electron oscillations on the rim of a diffraction window. When observed by a distant observer, this is equivalent to the oscillation of entire aperture. Consequently, relativistic Doppler effect comes into play and high-order harmonics are produced.

Despite the similarity, a unique feature of the ROW is that the electron motion that leads to HHG is intrinsically two dimensional (2D), which potentially enables vast opportunities for controlling laser-matter interaction. For instance, a circularly polarized laser drives chiral electron oscillation, and this chirality can be imprinted into the harmonics, facilitating spin-orbital interaction of light [24]. By engineering the shape of the aperture, this scheme enables independent control over the spin and orbital momentum of harmonic beams [25]. In addition, the electron acceleration associated with the relativistic diffraction can be harnessed to produce isolated subfemtosecond electron bunches [28]. However, to the best of our knowledge, previous works mainly focus on diffraction apertures with rotational symmetry [24,25], because of the potential to generate harmonic vortices. The ROW model assumes that the aperture does not change shape (“rigid window”), which is valid only for planar waves and neglecting nonlinear terms in the laser Lorentz force. As a result, it is impossible to capture the full complexity of the

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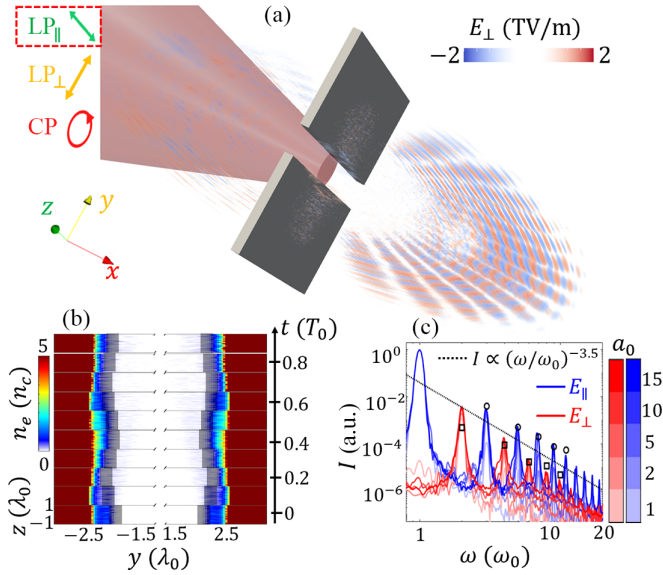


FIG. 1. (a) Sketch of single-slit diffraction of relativistically strong laser pulses, with three polarization states under consideration ($LP_{\parallel}$, $LP_{\perp}$, and CP). The color-coded diffracted field in panel (a) shows the anomalously polarized harmonic fields $E_{\perp}$ driven by an $LP_{\parallel}$ driver, whereas panel (b) shows the electron density fluctuation over one laser cycle (~ 10 fs before the peak of the drive laser arrives at the target) for this case. The dark banded region represents the area over which the Kirchhoff integral is calculated to yield the harmonic fields. The HHG spectra are presented in panel (c), where the blue and red colors show the odd- and even-order harmonics that polarized parallel and perpendicular to the slit, respectively. The strength of the colors represents the $LP_{\parallel}$ driver intensity. All the harmonic spectra are normalized to the fundamental harmonic intensity in this case. The black circular and square markers in panel (c) show the saturated spectrum calculated from Eq. (2).

2D dynamics of diffraction window, which is essential for theoretical modeling of relativistic diffraction.

In this paper, we study relativistic laser beam diffraction in more general cases, with highlights on the effects of 2ω oscillating term in the laser Lorentz force and angular momenta conservation in nonrotational symmetric cases. We show that, without losing the fidelity of the HHG process, the restriction on “rigid window” can be lifted by taking into account only the contribution within a narrow band at the edge of the diffraction window. Such a quasi-one-dimensional (quasi-1D) structure can be twisted to account for arbitrary 2D electron dynamics within the diffraction plane associated with complex laser fields. Using the approach, single-slit diffraction of a relativistic laser pulse is studied and several interesting effects are identified for the first time, including the generation of harmonic beams polarized orthogonal to the driver, HHG spectral shape variation depending on incident pulse polarization, and a deflection of the harmonics due to total angular momentum conservation.

II. NUMERICAL SIMULATION SETUP

The relativistic single-slit diffraction simulation setup is sketched in Fig. 1(a): a high-power laser beam propagating along the x axis, irradiating normally on a thin foil with a single slit along the z axis. The simulations are performed with

particle-in-cell (PIC) code EPOCH [29]. The laser profile used in the simulation is

$$\begin{aligned} E_l &= E_l(\mathbf{r}) \exp(ik_0x - i\omega_0t) \\ &= \frac{\sigma_y \mathbf{e}_y + i\sigma_z \mathbf{e}_z}{\sqrt{\sigma_y^2 + \sigma_z^2}} E_0 \sin^2\left(\frac{\pi t}{\tau_0}\right) \exp\left(-\frac{y^2 + z^2}{w_0^2}\right) \\ &\quad \times \exp(ik_0x - i\omega_0t), \end{aligned} \quad (1)$$

for $0 < t < \tau_0 = 54$ fs, where $\mathbf{e}_y$ ($\mathbf{e}_z$) is the unit vector in the perpendicular (parallel) direction, E_0 is the laser amplitude, $w_0 = 5 \mu\text{m}$ is the focal spot size, $k_0 = 2\pi/\lambda_0$ the wavenumber, and $\lambda_0 = 1 \mu\text{m}$ is the wavelength.

The polarization of drive laser pulse is predominant in determining peripheral electron dynamics, which is controlled by σ_y and σ_z in the simulation. Three polarization states are considered in this work: linear polarization parallel ($LP_{\parallel}$, with $\sigma_y = 0$, $\sigma_z = 1$) and perpendicular ($LP_{\perp}$, with $\sigma_y = 1$, $\sigma_z = 0$) to the slit, as well as circular polarization (CP, with $\sigma_y = 1$, $\sigma_z = \pm 1$), as illustrated in Fig. 1(a). The default normalized laser amplitude is $a_0 = eE_0/m_e\omega_0c = 5$ for $LP_{\perp}$ and CP cases, and 10 for the $LP_{\parallel}$ case, unless otherwise specified. We adopt a higher a_0 for the $LP_{\parallel}$ driver because in this case there is no electric field component perpendicular to the plasma-vacuum interface that can drive electron oscillation directly; thus, a higher laser intensity is required for the phenomena of interest (detailed below) to appear.

The thin foil target [assumed aluminum (Al)] is modeled by a preionized plasma with a thickness of $0.2 \mu\text{m}$, and electron density $n_0 = 30n_c$, where $n_c = m_e\omega_0^2/4\pi e^2 \approx 1.1 \times 10^{21} \text{ cm}^{-3}$ is the critical density, with e , m_e , and ω_0 denoting the elementary charge, electron mass, and laser frequency, respectively. The half-width of the slit is $l_s = 2.5 \mu\text{m}$, placed at $x_0 = 2 \mu\text{m}$, with a density gradient at the boundary $n_e(y) = n_0 \exp[(|y| - l_s)/h]$ for $|y| < l_s$, where $h = 0.2 \mu\text{m}$ is the scale length.

Throughout this study, we applied both 2D and three-dimensional (3D) PIC simulations, the 2D simulations are performed in a simulation domain $L_x \times L_y = 15 \mu\text{m} \times 16 \mu\text{m}$, with a high resolution $dx \times dy = 10 \text{ nm} \times 20 \text{ nm}$ to study the HHG spectra, and the numbers of macroparticles per cell are 50 for electrons and 10 for Al^{3+} ions. The 2D simulation results are presented in Figs. 1(c) and 2–4. The 3D simulations are relied on to capture the full electron dynamics on the rim of diffraction window. The simulation domain is $L_x \times L_y \times L_z = 20 \mu\text{m} \times 15 \mu\text{m} \times 15 \mu\text{m}$, and a reduced resolution $dx \times dy \times dz = 16.7 \text{ nm} \times 50 \text{ nm} \times 50 \text{ nm}$ is used for computational efficiency, with five macroparticles for electrons and three for Al^{3+} . Moreover, a larger simulation dimension in the direction perpendicular to slit ($L_y = 40 \mu\text{m}$) and a moving window are used to record the diffraction pattern shown in Fig. 5(b). In both cases, the plasma is assumed to be cold initially, open boundary conditions are applied to all the boundaries, and a high-order particle shape function is applied to suppress numerical self-heating instabilities [29].

III. GENERATION OF ANOMALOUSLY POLARIZED HARMONIC BEAMS

We first discuss the harmonic fields generated by an $LP_{\parallel}$ driver, as represented by the color-coded 3D electric field in

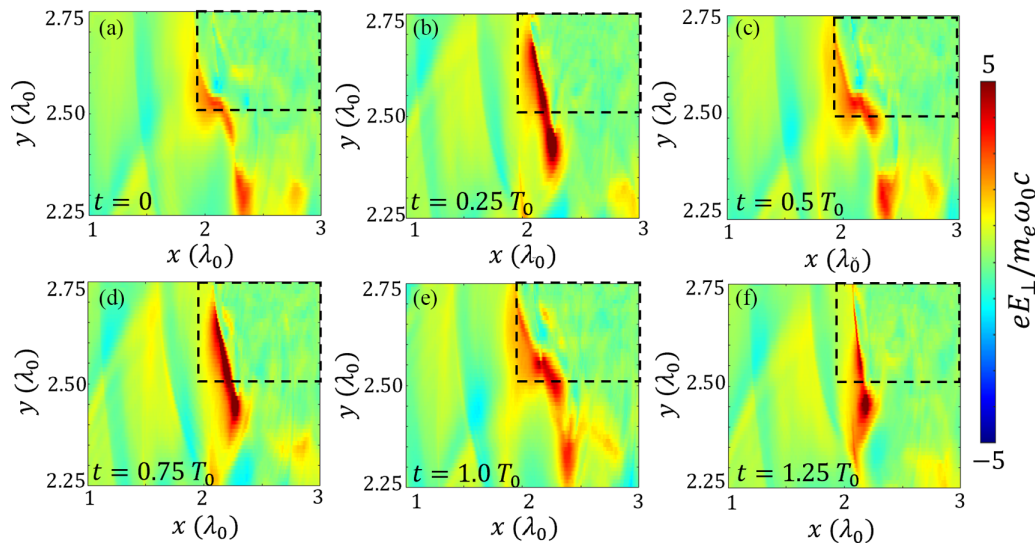


FIG. 2. The temporal evolution of the $E_{\perp}$ field at the upper boundary ($y > 0$) of the slit as the drive laser is diffracting through. The snapshots are taken successively over 1.25 laser cycles (~ 10 fs before the peak of drive laser pulse): (a) $t = 0$, (b) $t = 0.25T_0$, (c) $t = 0.5T_0$, (d) $t = 0.75T_0$, (e) $t = 1.0T_0$, and (f) $t = 1.25T_0$. The black dashed line shows the initial position of the plasma target. The thickness of the target is $1 \mu\text{m}$, which shows that this effect takes place primarily at the front surface of the target. Other parameters are the same as in Fig. 1.

Fig. 1(a), with an amplitude reaching 2 TV/m, approaching the relativistic threshold. Approximately 0.5% of the drive laser energy is converted into this field. Interestingly, this diffracting field is orthogonally polarized to the incident laser pulse and contains only even-order harmonics [Fig. 1(c)].

To understand this effect, we examine the peripheral electron motion perpendicular to the boundary, which is critical to determine the dynamics of diffraction window. For an $\text{LP}_{\parallel}$ driver, the laser field perpendicular to the slit vanishes; the electron motion is dominated by the nonlinear Lorentz force at $2\omega_0$. Consequently, the peripheral electron density oscillates at $2\omega_0$, as shown in Fig. 1(b), where $T_0 = 3.3$ fs is the laser period. Since this force has opposite signs at the $\pm y$ side, the width of the slit varies significantly. Therefore, the “rigid window” assumption in the ROW model is no longer valid in this case.

Nevertheless, because the harmonic beams are generated by the nonlinear interaction between the drive laser and the oscillating peripheral electrons, HHG only takes place within a narrow area near the edge of the diffraction window, with a width approximately equal to the oscillating amplitude of electrons on the rim. The central region, where the drive pulse simply transmitted through, only affects the fundamental light, which can be safely neglected. The HHG fields in the diffracted light can then be obtained taking into account only the area relevant for harmonic generation [30],

$$\begin{aligned} \mathbf{E}_{\text{HHG}}(x, y, z, t) &= \mathbf{E}(x, y, z) \exp(-i\omega_0 t) \\ &= \frac{1}{2\pi} \nabla \times \int_B [\mathbf{e}_n \times \mathbf{E}_l(\mathbf{r}')] \frac{\exp(ik_0 R' - i\omega_0 t)}{R'} ds', \quad (2) \end{aligned}$$

where the integration is over a narrow-band area (B) near the boundary of the slit; it can be bent or twisted to account for arbitrary 2D electron motion within the diffraction plane. The unit vector $\mathbf{e}_n = \mathbf{e}_x$ is normal to the target, pointing toward

the laser propagation direction, $\mathbf{E}_l(\mathbf{r}')$ is the laser profile at the diffraction slit defined in Eq. (1), and $R' = |\mathbf{R} - d\mathbf{R}'|$ is the distance between an observer at (x, y, z) and elementary source $[ds'(x_0, y', z')]$, measured at retarded time $t' = t - R'/c$. Here, $\mathbf{R}$ is the initial distance, and $d\mathbf{R}'$ denotes the shift of ds' , which is determined by the dynamics of low-energy electrons in the plasma bulk that ds' is attached to, during the laser-plasma interaction.

In the following, we apply this method to compute the harmonic spectra produced by an $\text{LP}_{\parallel}$ drive pulse. The width of the integration band is chosen to be $\lambda_0/4$, corresponding to the maximum distance the electrons can travel in half of its oscillating period. The shift of elementary sources in the integral band is determined by the peripheral electron dynamics, which is very complicated due to collective effects in plasma. Fortunately, the harmonic beams are mostly generated in the “surface wave breaking (SWB) phase” (discussed below), where some of the oscillating surface electrons gain enough energy from the laser that they escape from the plasma [31–33]. During this period, the temporal shift of ds' can be approximated by $d\mathbf{R}'(t') = \mp \delta_2 \sin(2\omega_0 t') \mathbf{e}_y$, where δ_2 is the amplitude and the $\mp$ sign corresponds to the opposite phase at the $\pm y$ side of the slit, respectively. One can then solve for the retarded time and distance numerically to yield the harmonic fields from Eq. (2).

In the PIC simulation, the electric fields are recorded in an observational plane ($16 \mu\text{m}$ in the transverse direction) placed $10 \mu\text{m}$ behind the target, which corresponds to a half opening angle of approximately 40° . We then perform Fourier transformation for all the diffracted light within this angle; the resulting angular-dependent spectra are integrated to yield the final harmonic spectrum, which is presented by the solid curves in Fig. 1(c).

The computed HHG spectra from our model are then compared with PIC simulations for various laser normalized amplitudes. Notably two distinct groups of harmonic beams

are generated, the odd- and even-order harmonics, which are polarized orthogonal to each other. The odd-order harmonics ($E_{\parallel}$) have the same polarization direction as the driver, while the even-order (anomalous) harmonics ($E_{\perp}$) are polarized perpendicular to the incident light. In both cases, the harmonic spectra have a power-law shape $I_n \propto n^{\alpha}$, with the index α increasing with a_0 until it saturates around $\alpha \approx -3.5$. This can be interpreted as follows: The increase of peripheral electron oscillation amplitude is limited by causality; namely, δ_2 must be smaller than the maximum distance an electron can travel within half of the oscillating period. Substituting $\delta_2 = 0.25\lambda_0$ into the model, the resulting harmonic spectrum is presented by the black circles in Fig. 1(c), which agrees well with the PIC simulation.

However, since the peripheral electron oscillates with $2\omega_0$, it can only explain the odd-order (normal) harmonic beams. The generation of even-order (anomalous) harmonics requires a zero-frequency field to be present at the oscillating slit. This condition is fulfilled by the charge separation between electrons and heavy ions, which arises from the laser ponderomotive force pushing electrons into plasma. As a result, this electrostatic field is attached to a boundary that is oscillating at $2\omega_0$ and directed perpendicular to the slit.

This is illustrated in Fig. 2, which shows the $E_{\perp}$ field at the upper boundary $y > 0$ of the slit, as the drive laser is traveling through. The black dashed box represents the initial position of the plasma target. Obviously, this field is produced due to charge separation between the heavy ions (located within the blackdashed box) and the electron layer that is being pushed into the plasma. One can see that the electron layer oscillates twice in one laser cycle. We note that mobile ions are used in our PIC simulations, and replacing Al^{3+} with other ion species with higher charge-to-mass ratio does not qualitatively change our results. In general, the dynamic ion could lead to the motion of plasma bulk, but in a timescale much longer than the period of electron oscillation (T_0). Therefore, it has little influence on the harmonic generation process.

As a result, even-order harmonics emerge, whose polarization is naturally orthogonal to the driving pulse. By adding an electrostatic field in Eq. (2), namely, we replace $\mathbf{E}_l(\mathbf{r}') \exp(ik_0 R' - i\omega_0 t)$ with a constant static field $E_s \mathbf{e}_y$ ($E_s > 0$ for $y > 0$ and $E_s < 0$ for $y < 0$), the even-order harmonics can be reproduced from our model, as shown by the black squares in Fig. 1(c). Notably, they follow the same power-law spectral slope as the odd-order harmonics, but with weaker strength; this is mainly because the nonlinear term in the numerator of Eq. (2) is missing for an electrostatic field. The intensity of the second-order harmonic is significantly stronger than our prediction. This is probably because of high-energy electrons generated from laser-plasma interaction. Since two electron bunches are produced per laser cycle, their near field and coherent transition radiation due to such spatial modulation are added to the $2\omega_0$ harmonic in the PIC simulation [34–36]. We note that in this study we are only interested in the power-law scaling of the HHG spectral shape; a quantitative comparison is beyond the scope of the current work.

It is worth noting that a similar phenomenon was reported in the reflection of s -polarized intense laser pulses [3,4]. Although the single-slit diffraction of an $\text{LP}_{\parallel}$ driver can be

regarded as the reflection of two s -polarized laser beams on a plasma target at grazing incidence, it is not obvious to compare qualitatively our model with the one presented in Ref. [4], because the source term in Eq. (19a) of Ref. [4] becomes infinite at grazing incidence. Nevertheless, we would like to point out that according to Eq. (19a) of Ref. [4], a zero-frequency term must exist for the production of even-order harmonics.

IV. THE HARMONIC SPECTRAL SHAPE

In general, spectral intensity decreases slower with frequency at higher a_0 , until it saturates at some point, after which the relative intensities between the harmonics stay the same when a_0 further increases [as shown in Fig. 1(c)]. We thus call power-law scaling (index α) “saturated.” With the nonlinear $2\omega_0$ oscillating term in the Lorentz force of the drive laser pulse been correctly addressed by the model, we can then discuss the saturated power-law HHG spectral shape $I_n \propto n^{-3.5}$ (the “SWB limited spectrum” hereafter). Such a spectral profile is observed for the $\text{LP}_{\parallel}$ driver when $a_0 = 15$, as shown in Fig. 1(c), and also seen in the CP case when $a_0 = 8$ [Fig. 3(a)]. Moreover, it also emerges in the pinhole diffraction case, as discussed in Ref. [24]. However, the harmonic spectra presented in Fig. 3(b) for an $\text{LP}_{\perp}$ follow a different trend. One can see that the spectrum reaches saturation at smaller a_0 with the CP case, and the saturated HHG power-law index is slightly higher $\alpha \approx -8/3$, similar to the ROM mechanism.

The numerical model suggests that the SWB limited spectrum arises when (1) the peripheral electron oscillation can be estimated by a *harmonic oscillation* during SWB phase and (2) its amplitude is limited by causality. The HHG spectra shown in Figs. 1(c) and 3 imply that these criteria are satisfied in the $\text{LP}_{\parallel}$ and CP cases, but not for the $\text{LP}_{\perp}$ driver.

To see this, the peripheral electron dynamics are compared in detail for the CP and $\text{LP}_{\perp}$ drivers in Fig. 4, where upper panels depict electron density evolution at lower boundary of the slit ($y < 0$) and the lower panels show the harmonic energy increasing over the same period of time. In these plots, the energetic electrons ($\gamma > 3$) that escaped the plasma have been

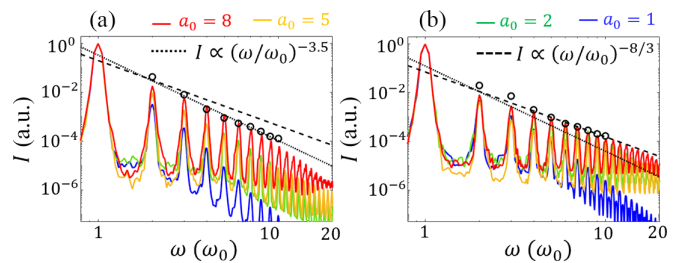


FIG. 3. The HHG spectra from (a) the CP and (b) $\text{LP}_{\perp}$ drivers, where the solid lines show the results from PIC simulations with color representing the normalized laser amplitude and the black circular makers show the saturated spectrum calculated from Eq. (2). In both plots, the harmonic spectra are normalized to the fundamental harmonic intensity. The black dashed line and dotted lines represent the previously known power-law scaling of $I \propto (\omega/\omega_0)^{-8/3}$ [5] and $I \propto (\omega/\omega_0)^{-3.5}$ [24], respectively.

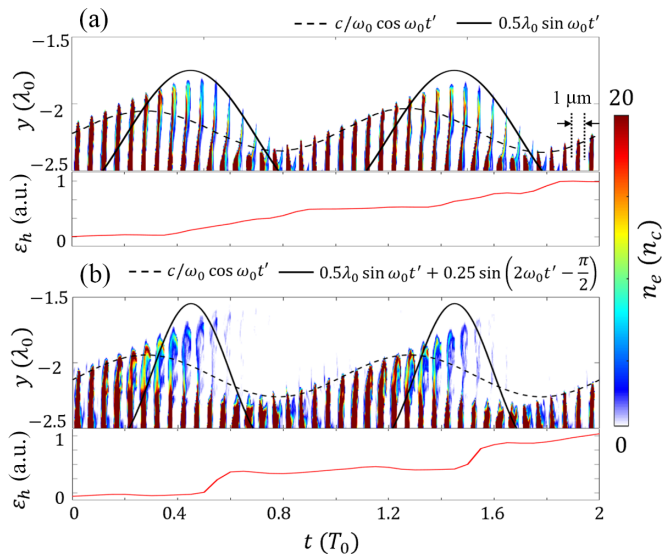


FIG. 4. Upper panel: The low-energy ($\gamma < 3$) electron density oscillation at the lower boundary of slit for (a) the CP and (b) LP $_{\perp}$ drivers, where each column represents a snapshot of n_e within $x = x_0 \pm 0.5 \mu\text{m}$ temporally spaced by $0.05T_0$. The black solid and dashed curves show the boundary electron layer trajectories $d\mathbf{R}'(t')$ (specified in the corresponding plot) we used for calculating the harmonic fields. Lower panel: The harmonic energy (with $\omega \geq 2\omega_0$) evolution over the same period of time. The normalized laser amplitude employed in this plot is $a_0 = 5$ for both CP and LP $_{\perp}$ cases.

excluded from n_e , as they just copropagate with the light along x axis and do not contribute to the dynamics of diffraction window. Apparently, when the electrons oscillate toward the plasma bulk, the temporal trajectory of slit boundary roughly follows $d\mathbf{R}'(t') = c/\omega_0 \cos(\omega_0 t') \mathbf{e}_y$ (dashed lines) for both cases, and the HHG during this phase is negligible. Notably, the dashed lines in Fig. 4 also indicate the phase of $E_{\perp}$, because when the electrons are oscillating into the plasma bulk, their collective motion is in phase with the driving electric field. On the other hand, when the electrons oscillate towards vacuum, periodic outbursts of SWB are observed. This is when the harmonic fields are predominantly generated.

Importantly, the peripheral electron dynamics in two cases deviate during this phase. For the CP drivers, our simulation suggests that during the SWB phase, the dynamics of low-energy electrons can still be estimated by a harmonic motion $d\mathbf{R}'(t') = 0.5\lambda_0 \sin(\omega_0 t') \mathbf{e}_y$ [black solid line in Fig. 4(a)]. By substituting this relation into Eq. (2), our model yields the SWB limited spectrum as expected, which agrees with PIC simulations [Fig. 3(a)].

This simple harmonic behavior of low-energy electrons can be understood as the drive force is a harmonic one (electric force of the laser field). One may think that the electron motion would still be nonlinear when they become relativistic. However, it is the dynamics of nonrelativistic (and weakly relativistic) electrons during the SWB phase that matters, because these are the majority of electrons in the oscillating plasma layer, which practically determine the motion of diffraction window. Note that a similar argument can apply to the LP $_{\parallel}$ case.

When both the laser electric field and the $2\omega_0$ term in the Lorentz force play a role, this assumption is no longer valid. In this case, as illustrated in Fig. 4(b), the electron dynamics is characterized by a sharp rising ramp and an abrupt falling in each cycle. It cannot be modeled by a harmonic motion due to the $2\omega_0$ oscillating term in the Lorentz force. Therefore, the resulting HHG could potentially surpass the SWB limit because of additional nonlinearity in the system.

Nevertheless, our model can be easily modified to account for such nonlinear oscillations. By adding a second harmonic term, namely, $d\mathbf{R}'(t') = [0.5\lambda_0 \sin(\omega_0 t') \mp 0.25\lambda_0 \sin(2\omega_0 t' - \pi/2)] \mathbf{e}_y$ [black solid curve in Fig. 4(b)], where the $\mp$ sign corresponds to the $\pm y$ side of the slit, our model is able to reproduce the saturated HHG spectrum for the LP $_{\perp}$ case, as shown by the black circles in Fig. 3(b). Here, the nonlinear ($2\omega_0$) term is shifted by $\pi/2$ with respect to the first term our model, which leads to sharp peaks of electron oscillation, consistent with the PIC simulation results. Physically, this can be attributed to the locked phase of the SWB effect [31,37].

We also note that during the SWB phase, the simple harmonic motion indicated by the black solid curve in Fig. 4(a) is shifted by $\pi/2$ with respect to the laser electric field $E_{\perp}$ (black dashed line). This is expected as the electron momentum P_y reaches maximum at the nodes of $E_{\perp}$; thus, electrons are more likely to escape from the plasma [37]. We note that this is not the same as in Ref. [24], where the motion of the electron layer is assumed to be antiparallel with respect to the laser electric field for simplicity. Nevertheless, this assumption is justified as the exact phase of the electron oscillation does not change the key results of the HHG spectrum and OAM of the harmonic beams. In the case of Fig. 4(b), when both the laser electric field and the ponderomotive effects play a role, our results suggest that they are approximately in phase with each other. This is obtained by fixing the phase of drive laser pulse and the ω_0 term in $d\mathbf{R}'(t')$, and adjusting the phase of the ponderomotive ($2\omega_0$) term to fit the electron density evolution and the HHG spectra.

Notably, the HHG spectrum produced by a relativistic LP $_{\perp}$ drive pulse diffracting through a single slit becomes almost the same as the ROM scenario [5]. This is because when a high-power laser is obliquely incident on a reflective plasma foil, the oscillating electron layer follows a similar nonlinear motion as discussed in Ref. [4]. However, there is a small difference; unlike the ROM being a quasi-1D model [4], the diffracted lights are spatially inhomogeneous. The HHG spectra reported in this work are obtained by integrating over all diffracting angles; this might be responsible for the discrepancy with the results reported in Ref. [38].

V. DEFLECTION OF THE HARMONIC BEAMS

Finally, we discuss another anomalous effect in the relativistic single-slit diffraction. It stems from the total angular momentum conservation in the HHG process driven by a CP pulse. When N laser photons are converted into one N th harmonic photon during the diffraction, their (spin) angular momenta $N\sigma_z \hbar$ must be transferred to the harmonic photon generated, where $\sigma_z = 1$ and -1 corresponding to right-handed and left-handed circular polarization, respectively.

Previous study [24] shows that this effect converts the spin angular momentum of the drive CP pulse into the intrinsic OAM of the harmonics in relativistic pinhole diffraction. However, this process requires rotational symmetry, thus cannot occur in single-slit diffraction. It is therefore not clear whether and how the angular momentum is conserved for single-slit diffraction HHG driven by a CP laser. Regarding the breaking of rotational symmetry, we note that our work is different from Ref. [25] as the single-slit setup has spatial translational symmetry, which prevents any singularity from emerging; therefore, the harmonic lights cannot obtain intrinsic OAM.

The answer to this dilemma lies in the extrinsic OAM gained by the harmonics due to the tangential electron motion with respect to the boundary of the slit. When the peripheral electrons move towards vacuum during the SWB phase, the conservation of transverse canonical momentum leads to $\mathbf{P}_\perp = -(\mathbf{e}_y + i\sigma_z \mathbf{e}_z)a_0 \exp(-i\phi_{\text{swb}})$, where ϕ_{swb} is the optical phase where SWB effect occurs.

This indicates a tangential shift of the peripheral electrons as they oscillate, which is controlled by the polarization of drive pulse. Although it is challenging to determine the exact value of ϕ_{swb} , due to symmetry of the system, it should differ by a phase of π between the $+y$ and the $-y$ side of the slit. Therefore, the direction of the tangential shift is also opposite, which could potentially change the diffraction pattern of the harmonic beams.

To study this effect, we perform 3D PIC simulation of single-slit diffraction of a right-handed CP laser and calculate the total angular momentum of each harmonic beam that aligned with the beam axis by $L_x = [\mathbf{r} \times \mathbf{P}_n]_x$, for the harmonic numbers $n = 1, 2, 3, 4$ ($n = 1$ being the fundamental laser), where $\mathbf{P}_n = \varepsilon_0 \int \mathbf{E}_n \times \mathbf{B}_n dV$ is the linear momentum of the n th harmonic. The high-order harmonics with $n \geq 5$ are omitted because their energies are too low. In addition, we calculate the angular momentum carried by each species (electrons + ions) in the plasma. One can see that the fundamental laser loses around 10% of its (spin) angular momentum, which is transferred to the plasma and harmonic beams.

The inset shows that for a right-hand drive CP pulse, the peripheral electrons simultaneously stream toward $+z$ ($-z$) when they oscillate inward at the $-y$ ($+y$) side of the slit, as expected. Notably, as indicated by the phase-space diagram shown in the inset, it is expected that the plasma picks up a negative angular momentum antiparallel to the drive pulse because of the tangential shift; this is observed during the early stage of the diffraction process for $6T_0 < t < 10T_0$. However, only the electron on the rim of diffraction window behaves in this way. Therefore, this trend is reversed soon as the positive (spin) angular momenta carried by the right-handed CP driver is gradually transferred to the bulk of hot electrons during laser-plasma interaction, and eventually to ions as well.

Moreover, we estimate the spin angular momentum by $L_s \approx W_n/(n\omega_0)$ for each harmonic order n , where $W_n = \int_{(n-0.5)\omega_0}^{(n+0.5)\omega_0} [\int (\varepsilon_0 E_n^2 + B_n^2/\mu_0) dV] d\omega$ is the electromagnetic energy of the harmonic beams. It is found that their sum (blue dashed line) is much smaller than their total angular momenta. This indicates that the harmonic beams are carrying significant (extrinsic) OAM.

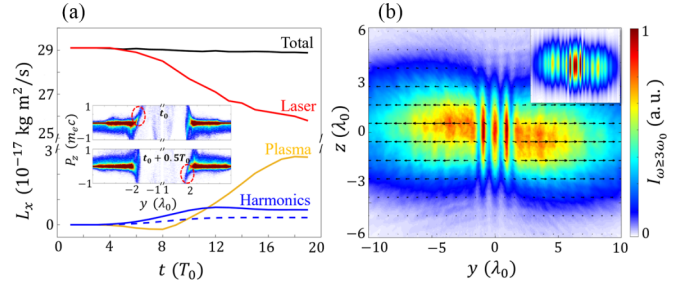


FIG. 5. (a) The temporal evolution of total angular momentum aligned with beam axis carried by each component in the 3D PIC simulations is presented by the solid curves, and the blue dashed line shows the spin angular momentum of the harmonic beams estimated by their total energy. The inset of (a) shows phase space diagram ($y - p_z$) for peripheral electrons at two times separated by $0.5T_0$, where the red dashed circles highlight the electrons undergoing the SWB process. (b) The tilted near-field intensity pattern of harmonic fields ($\omega \geq 3\omega_0$), where the black arrows represent the transverse momentum of the harmonics, and the inset shows the prediction from our model.

Figure 5(b) depicts the near-field harmonic intensity pattern ($n > 3$), which is recorded at $30 \mu\text{m}$ behind the target. The transverse components of the electromagnetic momenta $\mathbf{P}_n$ are represented by the black arrows superposed on the plot, where the fundamental and the second harmonic fields are filtered out. Obviously, an extrinsic OAM aligned with $+x$ arises due to the tilted harmonic intensity pattern. This ensures total angular momentum conservation for the HHG process. In order to explain this effect, one needs to consider a drive pulse with finite focal spot. Thus, the tangential shift of peripheral electrons leads to the deformation of the (effective) diffraction window. Fortunately, this effect can now be investigated with the present model. By submitting $d\mathbf{R}(t') = -0.5\lambda_0(\mathbf{e}_y + i\sigma_z \mathbf{e}_z) \exp(-i\omega_0 t')$ into Eq. (2), the calculated harmonic intensity pattern [inset of Fig. 5(b)] is in reasonable agreement with the 3D PIC simulations. We noted that the tangential motion of electrons does not change the harmonic spectrum; it only modifies the intensity pattern due to conservation of total angular momenta.

VI. CONCLUSION AND OUTLOOK

In conclusion, we have developed a theory that allows for calculating HHG fields from arbitrary 2D electron motion on the rim of a diffraction window. This work removes a critical restriction (“rigid window” assumption) on the theoretical modeling, such that it can capture the full complexity of the 2D electron dynamics, which paves the way toward full-degree-of-freedom control over high-power laser-matter interaction.

Using this model, we identify and study a few interesting effects in the single-slit diffraction of a relativistically strong light.

(1) The generation of anomalously polarized harmonic beams for $\text{LP}_{\parallel}$ drivers, where the even-order harmonics are polarized orthogonal to the incident laser pulse. This is because a charge separation (electrostatic) field is generated perpendicular to the plasma-vacuum interface as the

ponderomotive force pushes the electrons into the plasma. In the meantime, the oscillating term in the laser Lorentz force drives the electron layer to oscillate at $2\omega_0$, thus producing the even-order harmonics polarized perpendicular to the slit.

(2) The saturated harmonic spectral profile is dependent on polarization. By examining the electron dynamics, we conclude that only when the motion of low-energy electrons in the plasma layer during the SWB phase can be estimated by a simple harmonic oscillation, the saturated HHG spectral profile is $I_n \propto n^{-3.5}$. This applies to the CP and $LP_{\parallel}$ drivers. While in the $LP_{\perp}$ case, since both laser electric field and the $2\omega_0$ term in the Lorentz force play a role, such limit can be surpassed as additional nonlinearity is introduced into the system, the saturated HHG spectrum is similar to the ROM mechanism $I_n \propto n^{-8/3}$.

(3) A deflection of the harmonic beams is observed for single-slit diffraction of a high-power CP laser pulse. This effect is attributed to extrinsic OAM that arises due to tangential peripheral electron motion.

Notably, these effects involve deformation of the diffraction window, thus can only be studied by the presented model. Our work thus creates a new paradigm for

theoretical modeling of light diffraction at relativistic intensities. With this model, a general solution to any nonplanar wave diffraction problem can be obtained, which is critical for interpreting complex electromagnetic wave diffraction, such as Laguerre Gaussian beams [10,11], vector light fields [39,40], and spatial-temporal optical vortices [41]. These are discussed in other works [42,43].

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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