

Asymmetric self-injection of electrons in a laser wakefield accelerator via localized laser redshifting

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Propagation of intense laser pulses in underdense plasma always involves nonlinear evolution of the laser envelope, which leads to large deviations from the initial Gaussian intensity profile. The modulations in the intensity envelope have strong influence not only on the formation of the wakefield, but also in the process of electron injection; thus, it defines the final spectral and angular distribution of the accelerated electrons. Better understanding of the laser pulse evolution is crucial for the correct interpretation of the experimental results, especially in the highly relativistic regime. We developed a simple numerical tool, which adequately models the evolution of the laser envelope up to the point when the spectral broadening becomes significant. Our numerical modeling sheds light on the asymmetric wakefield generation and consequent off-axis injection of electrons, observed in experiments and particle-in-cell simulations.

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I. INTRODUCTION

Acceleration of high-energy electrons in underdense plasma is a result of high-amplitude plasma waves [1] having a phase velocity very close to, or even exceeding, the speed of light in vacuum [2,3]. These waves can be generated by intense laser pulses, leading to a mechanism called laser wakefield acceleration (LWFA), where electrons are accelerated behind the laser pulse, in its wake. In the nonlinear regime, when the laser's peak intensity is much larger than 10^{18} W/cm², these waves are subject to wave breaking, a process also called self-injection [4]. In this case, the velocity of the electrons, in a highly localized region, becomes larger than the phase velocity of the plasma wave; thus, high-charge and high-energy electron bunches are injected into the accelerating phase of the plasma wave. There are several methods to limit the injected charge and to control the evolution of the electron energy spectrum by shaping the gas density profile, or by employing a different injection scheme, like down-ramp injection [5,6] or ionization injection [7,8]. However, it is still important to better understand the process of self-injection in uniform density plasma, where the spectral-temporal evolution of the laser pulse plays a key role in the evolution of

the plasma wave's phase velocity. In this work, we focus on moderate energy laser pulses (on the order of 10 J), having a peak power approaching, or even surpassing, the PW (10^{15} W) level. In order to achieve wave breaking, these pulses are focused to a spot size well below 50 μ m, which also means that the diffraction length is on the order of few millimeters. In low-density plasma, the acceleration length is basically defined by the Rayleigh range, but increasing the plasma density can lead to so-called self-guiding, which is a result of the relativistic modulation of the plasma's refractive index within the laser pulse.

The self-guiding condition imposes a strong relation between the laser spot size and plasma density: $w_0 \approx \sqrt{a_0 \lambda_p} / \pi$, where $a_0 = eE_0 / (m_e c \omega_0)$ is the normalized laser field amplitude and $\lambda_p = 2\pi c / \sqrt{e^2 n_0 / m_e \epsilon_0}$ is the plasma wavelength. This means that if the laser waist radius is smaller than 30 μ m and $a_0 = 3$, then the plasma density must be larger than 4×10^{17} cm⁻³. Therefore, in experiments using a configuration with tight focusing, the plasma density is close to 10^{18} cm⁻³, which always results in significant phase modulation and redshifting of the laser pulse already after one Rayleigh length of propagation [9]. The spectral modulation is a result of the longitudinal gradients in the refractive index within the laser pulse and in some cases it causes significant electron beam-pointing instability [10] via transverse bubble oscillations. The underlying mechanism of electron injection into a wakefield driven by a combination of long and single-cycle pulse has been presented in Ref. [11]. If the electrons are injected at the right phase and acquire sufficiently large transverse momentum, this nonlinear phenomenon could be exploited to enhance betatron radiation emitted by the injected electrons [12,13].

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In this work, we thoroughly investigate the combined effects of self-focusing and self-phase modulation through numerical modeling, based on the plasma fluid equations and laser envelope model. Our theoretical model provides a deeper understanding of the nonlinear processes taking place as the laser pulse propagates and show that in certain conditions a localized single-cycle waveform evolves inside the laser pulse, which leads to the generation of asymmetric bubble [14], and to off-axis injection of relativistic electrons. Such electron beam-pointing variations are identified experimentally and in particle-in-cell simulations.

II. MODELING OF LASER WAKEFIELDS IN THE QUASISTATIC APPROXIMATION

Due to the highly nonlinear interaction between the laser pulse and the plasma, an analytical treatment is not possible; therefore, we construct a simplified model based on the cold relativistic fluid equations of quasineutral plasma. In this model, an intense laser pulse is considered moving with $v_g = c\sqrt{1 - n_e/(n_{c0}\gamma_0)}$, where $n_{c0} = \omega_0^2 m_e \epsilon_0 / e^2$ is the initial critical density, ω_0 is the laser angular frequency, and $\gamma_0 = \sqrt{1 + a_0^2/2}$ for a linearly polarized laser pulse. The laser pulse is modeled with the envelope vector potential, which is divided into longitudinal slices, and its spot radius in each slice is calculated self-consistently taking into account the local index of refraction: $\eta(\xi, r) = \sqrt{1 - n_e/(n_c \gamma)}$, where $\xi = z - ct$ is the comoving coordinate and all quantities depend on ξ and r . The critical density is defined as $n_c = n_{c0}[\omega(\xi, r)/\omega_0]^2$, where ω is calculated self-consistently using the nonuniform refractive index:

$$\frac{d\omega}{dt} = -c \frac{\omega_0}{\eta^2} \frac{\partial \eta}{\partial \xi}. \quad (1)$$

We begin with the general equation governing the plasma dynamics using a standard assumption that the generalized vorticity ($\nabla \times \nabla \times (\vec{p} - e\vec{A}_p) = 0$) is conserved and equal to zero [15]:

$$\frac{\partial \vec{p}}{\partial t} = -e\vec{E}_p - m_e c^2 \nabla \gamma, \quad (2)$$

where $\vec{E}_p = -\frac{\partial \vec{A}_p}{\partial t} - \nabla \phi$ is the plasma field and $\gamma = \sqrt{1 + |\vec{p}|^2/(m_e c)^2 + a^2/2}$, with $a = e|A_L|/m_e c$ being the normalized laser field envelope. The initial laser pulse has a Gaussian shape: $A_L = A_0(w_0/w(\xi)) \exp(-r^2/w_0^2) \exp[-2 \ln(2)(\xi - \xi_0)^2/\tau_L^2]$, where $\tau_L = ct_L$ is the FWHM of the intensity envelope. If the plasma is initially neutral, then the plasma fields are driven by the vector potential and are calculated from Ampere's law in each time step:

$$\frac{\partial \vec{E}_p}{\partial t} = -\frac{e}{\epsilon_0} n_e \vec{v} + \nabla \times \vec{B}_p, \quad (3)$$

where $\vec{v} = \vec{p}/(\gamma m_e)$ and the azimuthal magnetic field (B_p) is calculated from Faraday's law:

$$\frac{\partial \vec{B}_p}{\partial t} = -\nabla \times \vec{E}_p. \quad (4)$$

Finally, the electron density (ions are considered immobile) is updated according to the continuity equation:

$$\frac{\partial n_e}{\partial t} = -\nabla \cdot (n_e \vec{v}). \quad (5)$$

The closed set of Eqs. (2), (3), and (5) are solved numerically in cylindrical coordinate system on a spatial grid moving with the speed of light c , where the divergence operator has the form $\nabla \cdot \vec{F} = (1/r)\partial(rF_r)/\partial r + \partial F_z/\partial \xi$. For the derivatives, fourth-order centered finite difference formulas are used, where the spatial resolution is $\Delta \xi = ct_L/40$ and $\Delta r = 4\Delta \xi$, and for the time integration ($\Delta t = \Delta \xi/c$), a standard second-order predictor-corrector method is applied.

The slicing of the laser pulse is shown in Fig. 1. The local laser spot radius (w) can be evaluated using the envelope model of Ref. [16], where w evolves according to the following equation:

$$\frac{\partial^2 w}{\partial t^2} = \frac{4}{\bar{k}^2 w^3} (1 + K), \quad (6)$$

where the wave number $\bar{k} = \langle \omega \rangle_r / c$ is averaged radially and K incorporates the plasma response assuming that the transverse laser beam profile is always Gaussian. It is evaluated numerically by performing the following integral:

$$K = k_{p0}^2 \int_0^\infty 2r(1-s)e^{-s} \frac{n_e(r)}{n_{e0}\bar{\gamma}} dr, \quad (7)$$

where $s = 2r^2/w^2$, $W = w/(w_0 a_0)$, and $\bar{\gamma} = [1 + \exp(-s)/(2W^2)]^{1/2}$. If the value of the integral is $K = -1$, then the Gaussian mode is perfectly guided as long as the energy depletion can be neglected. We note here that in reality the laser envelope does not remain Gaussian and high-order Laguerre-Gaussian modes will always appear, unless the plasma susceptibility (n_e/γ) is parabolic in radius.

In each time step, the new laser spot radii, $w(\xi)$, are calculated according to Eq. (6). Because of this, the laser field amplitude changes in each slice as $A(r=0) = A_0 w_0/w$, and the longitudinal pulse profile ($A(\xi)$) is obtained by applying a spline interpolation technique. This is needed, because the length of each slice is larger than one laser wavelength, which is larger than the mesh size in the longitudinal direction.

A spatially varying wavelength inside the laser pulse means that the local self-focusing or diffraction of the pulse is also different in each slice, which is taken into account in Eq. (6). In this simplified numerical model, the group velocity dispersion is neglected, because we consider a relatively short propagation time (t_{prop}), but one should remember that the frequency shift will cause additional change in the temporal envelope, usually referred to as self-compression.

III. REDSHIFTING IN THE LINEAR REGIME, $a_0 < 1$

After performing the derivatives in Eq. (1), the new rate equation can be written as

$$\frac{1}{\omega_0} \frac{d\omega}{dt} = -\frac{c}{2\gamma^2 \eta^2} \left(\frac{n_e}{n_{e0}} \frac{\partial \gamma}{\partial \xi} - \frac{\gamma}{n_{e0}} \frac{\partial n_e}{\partial \xi} \right) \frac{n_{e0}}{n_{c0}} \left(\frac{\omega_0}{\omega} \right)^2. \quad (8)$$

In the case of small-amplitude plasma waves ($n_e(\xi) \approx n_{e0}$) and weak pumps ($a_0 \ll 1$), it can be solved analytically

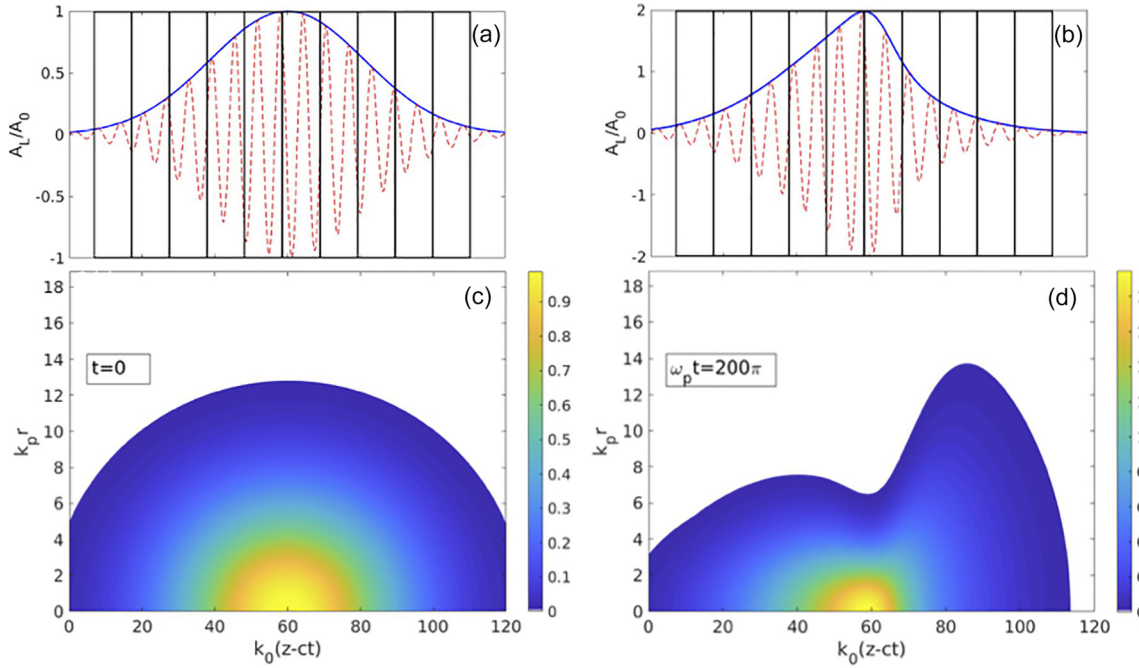


FIG. 1. Evolution of the laser pulse calculated with the slicing method. The transverse slices are shown by the black rectangles in panels (a) and (b), where the blue curve represents the envelope along the propagation axis ($r = 0$). An initially Gaussian laser pulse [panels (a) and (c)] is divided into slices along the longitudinal axis, where the evolution of the local spot radii is calculated according to the local index of refraction. The spatial distribution of the pulse envelope after $2.4z_R$ propagation is shown in panels (b) and (d). Here, the plasma density is $n_0 = 2.4 \times 10^{18} \text{ cm}^{-3}$, $w_0 = \lambda_p$, $a_0 = 2$, and $ct_L = 0.3\lambda_p$.

yielding (for $\gamma \approx 1$)

$$\frac{\omega}{\omega_0} = \left(1 - \frac{3}{2}c \frac{\partial \gamma}{\partial \xi} \frac{n_{e0}}{n_{c0}} t\right)^{1/3}. \quad (9)$$

Applying Taylor series expansion and keeping only the first-order term, the redshift can be expressed as

$$R_a = 1 - \frac{\omega}{\omega_0} \approx \frac{1}{4}c \frac{\partial a^2}{\partial \xi} \frac{n_{e0}}{n_{c0}} t_{\text{prop}}, \quad (10)$$

which predicts a linear dependence on plasma density and quadratic dependence on the laser field amplitude. It also suggests that the redshifting is stronger for shorter pulses.

In the numerical calculations, the spectral modulation within the laser pulse at $r = 0$ is quantified with the following formula:

$$R \approx \frac{\int a^2(\Delta\omega/\omega_0)d\xi}{\int a^2 d\xi}, \quad (11)$$

where $\Delta\omega = \omega_0 - \omega(\xi)$ is the frequency shift obtained from Eq. (1) at $t_{\text{prop}} \leq 2z_R/c$, where $z_R = \pi w_0^2/\lambda_0$ is the Rayleigh length.

The validity of the analytical result is confirmed in Fig. 2, where a normalized laser pulse duration of $\tau_L = ct_L/\lambda_p = 0.3$ is used. The amount of redshifting is nearly doubled when the plasma density is two times larger. Also, the dependence on laser peak intensity is the expected one, which is in agreement with Eq. (10) of Ref. [17].

IV. NUMERICAL RESULTS IN THE NONLINEAR REGIME, $a_0 > 1$

The advantage of our numerical tool is the ability to investigate the effects of various parameters, like laser spot size, pulse duration, focusing position, and others. There is a strong coupling, especially in the high-intensity regime, between the self-phase modulation and transverse focusing of the laser

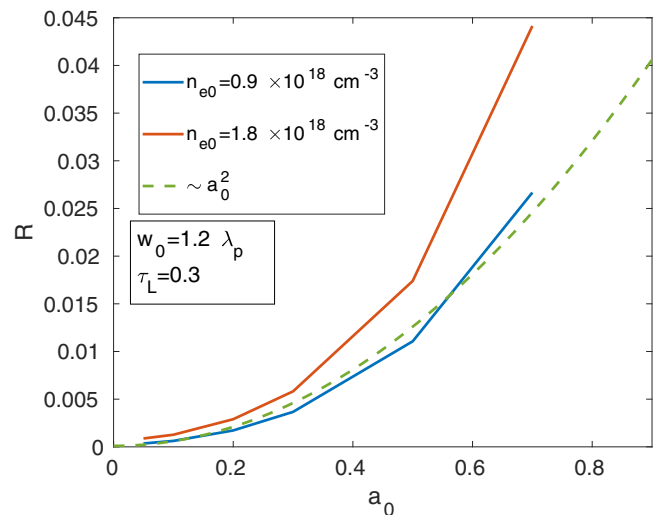


FIG. 2. The red and blue curves represent the results of our numerical modeling for two density values. The dashed green line confirms the quadratic R dependence on the laser field amplitude. Here, the propagation distance is the same in both cases.

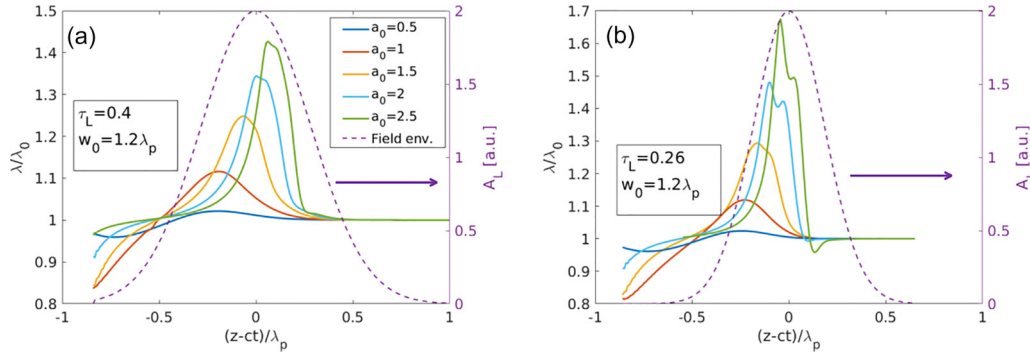


FIG. 3. Spatial variations in the laser wavelength after $t_{\text{prop}} = 1.6z_R/c$ for longer [panel (a)] and shorter [panel (b)] pulses. Here, the initial plasma density is $n_{e0} = 1.9 \times 10^{18} \text{ cm}^{-3}$.

pulse, which introduces significant deviations from the one-dimensional scaling laws.

A. Transition from linear to nonlinear case

When the laser field amplitude increases, and all other parameters are kept the same, the density profile in the wakefield changes and the role of the relativistic γ factor becomes more important in Eq. (8). Thus, the shape of the refractive index also changes, which results in a different temporal evolution of the local wavelength within the laser pulse. Due to the different self-focusing in each slice of the laser pulse, the temporal envelope can be extremely steep in a limited range, where the self-phase modulation grows very fast, leading to localized redshifting. Interestingly the position of the spectral down-shift depends on the pulse duration as well, as shown in Fig. 3. In the case of small laser field amplitudes, the frequency modulation takes place mostly in the second half of the laser, while for $a_0 \gg 1$ the radiation pressure causes a density pileup within the pulse, and the relative position of the peak density with respect to the pulse centroid depends on the pulse length. In the case of longer pulses, the spectral modulation appears in the first half of the laser pulse [Fig 3(a)], while in the case of shorter pulses it is rather in the second half [Fig. 3(b)].

The numerical results shown in Fig. 3 also show that the redshifting is stronger for shorter pulses. Obviously, there is an optimal pulse duration for maximum redshift, because using a very short laser pulse results in small wake amplitude and the self-phase modulation vanishes. It is important to note that there is a blueshifting as well, which is effective for relatively long pulses ($\tau_L \approx 0.5$ or more), and it is responsible for self-compression and self-steepening in the back of the pulse [18].

B. Effect of laser field amplitude and plasma density

Previous theoretical and experimental works [19], considering a square temporal shape of the laser pulses, predict $n_{e0}^{3/2}$ dependence on the plasma density and a_0^4 dependence in the linear, while a_0^2 in the nonlinear regimes. For a Gaussian laser pulse, these scalings are different [17]. In Fig. 2, it has been shown that the intensity and density dependence are in agreement with the findings of Ref. [17] in the linear regime

and the weak dependence on a_0 is observed in the nonlinear regime as well, when $a_0 \gg 1$.

The value of R saturates (becomes independent of a_0) at large a_0 values due to the shift in the position of λ_{max} , but the value of the longest wavelength increases almost linearly with a_0 . The stronger redshift with increasing laser spot size is also expected, because of the stronger self-focusing, which leads to larger laser intensity in a limited range of the plasma. The most important conclusion from Fig. 4 is that the onset of redshift-dominated regime is around a plasma density of $n_0 = 10^{18} \text{ cm}^{-3}$ for $\lambda_0 = 0.8 \mu\text{m}$, or in other words, the longitudinal pulse evolution becomes important for a normalized plasma density of $n_0/n_c > 10^{-3}$.

The bubble asymmetry is a result of a single-cycle waveform within the laser pulse [11]. Such waveform can appear if the spatial extension of the localized redshifting is comparable to the modified wavelength. This asymmetry can be quantified by calculating the accumulated transverse momentum of the electrons traversing the redshifted region of the pulse, which is a challenging task. Instead, we can model the maximum propagation distance where the redshifting is still negligible and off-axis electron injection is not expected. We denote this distance by L_m , which is obtained using the modeling as the position where the maximum wavelength within the envelope becomes 50% larger than the original carrier wavelength. After this distance, the laser propagation becomes very complicated, not only due to the dispersion effects, but also by the nontrivial self-focusing within the pulse, since it also depends on the laser wavelength. In other words, the critical density becomes spatially nonuniform.

The acceleration length limited by redshifting is presented in Fig. 5 for two scenarios: One is the matched case, when laser self-guiding is expected, and in the other case the spot size is 50% larger. The matched laser spot size in uniform plasma can be obtained from Eq. (7) requiring that $K = -1$ and assuming a small density modulation in the middle of the pulse, $n_e \approx n_{e0}$. With this simplification, evaluating the integral leads to $w_{\text{sg}} \approx \sqrt{a_0 \lambda_p} / \pi$ for $a_0 \gg 1$.

In both cases in Fig. 5, L_m is compared to the expected self-guiding distance ($L_{\text{sg}} \approx 4z_R = 4\pi w_0^2 / \lambda_0$, dashed lines) and to the energy depletion length ($L_{\text{pd}} \approx 0.5 \lambda_p n_c / n_e$, red line), and in both cases all quantities are normalized to the plasma wavelength. Our estimate for L_{sg} relies on the simulation presented in Ref. [20], where stable self-guiding of an

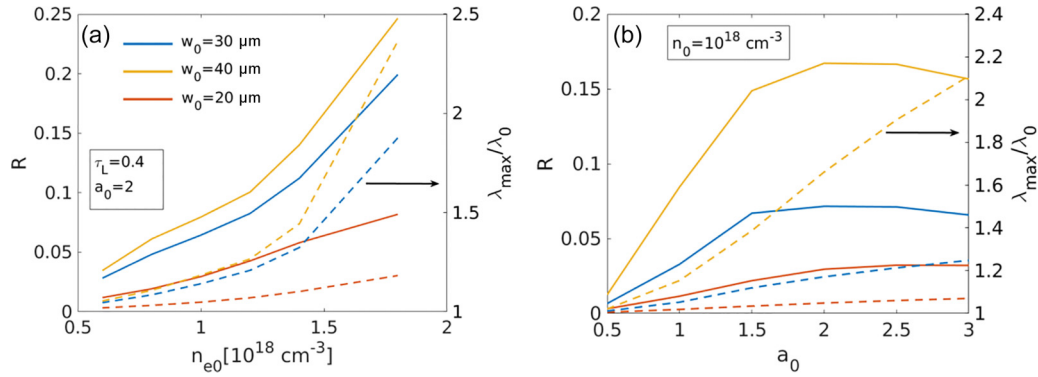


FIG. 4. Average (full lines, left axis) and maximum (dashed lines, right axis) redshifting as a function of plasma density [panel (a)] and normalized field amplitude [panel (b)]. The propagation distance is $2z_R$ in all cases, except the yellow curves in panel (a), where it was $1.6z_R$.

intense laser pulse was observed over a maximum distance of approximately $4z_R$. One can see that in the oversized case the redshifting dominates in the acceleration process, because L_m is shorter than both L_{pd} and L_{sg} . Our experiments roughly correspond to purple line in the encircled area in Fig. 5(a). With smaller laser spot L_m is a bit larger, because self-focusing is less effective and a_0 does not reach high values, but it is still smaller than L_{sg} for densities $n_e > 0.002n_c$. At lower densities, L_m can be much larger than the self-guiding distance, so external guiding is needed to extend the acceleration length, which can approach the depletion length for smaller a_0 values [see the green line in Fig. 5(b)]. This parameter scan leads to the well-known conclusion, stating that laser guiding in plasma channel is needed for $n_e/n_c < 10^{-3}$ [21], where the acceleration length can be close to the depletion (or dephasing) length if a_0 is not too large.

V. EXPERIMENTAL RESULTS AND PARTICLE-IN-CELL SIMULATIONS

A schematic of the experimental setup is presented in Fig. 6. The experiment was carried out using the HF-PW laser system at ELI ALPS, Hungary, which delivered pulses with a total energy of 4.3 J and an FWHM duration of 21 fs [22]. The laser was directed onto an $f/15$ off-axis parabolic mirror

(OAP), which focused the beam to a spot with an FWHM diameter of $18 \mu\text{m}$. In vacuum, this produced a normalized vector potential of $a_0 \approx 4$. The laser was focused on a 3-mm-wide helium gas jet, generating an LWFA, with a laser beam-pointing stability on the order of few microradians.

Electron beams emerging from the plasma were characterized using two diagnostics: an electron beam profile monitor and an electron spectrometer. The profile monitor consisted of a scintillating Lanex screen located 60 cm downstream of the gas jet and angled at 45° relative to the electron beam axis. The screen was imaged by a 16-bit charge-coupled device (CCD) camera, which provided measurements of the e-beam pointing and transverse spatial profile. After the profile screen, the electron beam entered a magnetic spectrometer. The spectrometer comprised a 1 T dipole magnet that deflected electrons according to their energies onto a pair of scintillating Lanex screens. A high-energy screen was positioned downstream of the magnet, while a low-energy screen was placed laterally to capture more strongly deflected (low-energy) electrons. The spectrometer enabled energy-resolved measurements over the range 75–400 MeV. To diagnose the plasma, a probe beam, taken as a pick-off from the main beam before reaching the OAP, was directed across the gas jet perpendicularly to the main focused beam. This probe was used to measure the plasma density using interferometry [23].

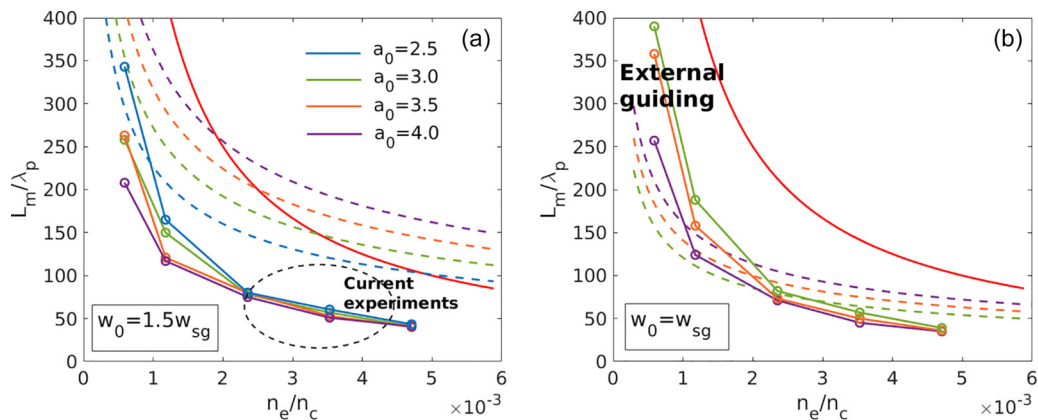


FIG. 5. Maximum acceleration distance (L_m) defined by the redshifting in the case of oversized [panel (a)] and matched for self-guiding [panel (b)] laser waist radii. The full lines with circle marks are obtained with our numerical modeling tool, the dashed lines represent the self-guiding distance, which is roughly $4z_R$, and the red line shows the pump-depletion length. In all cases, $\tau_L = 0.3$.

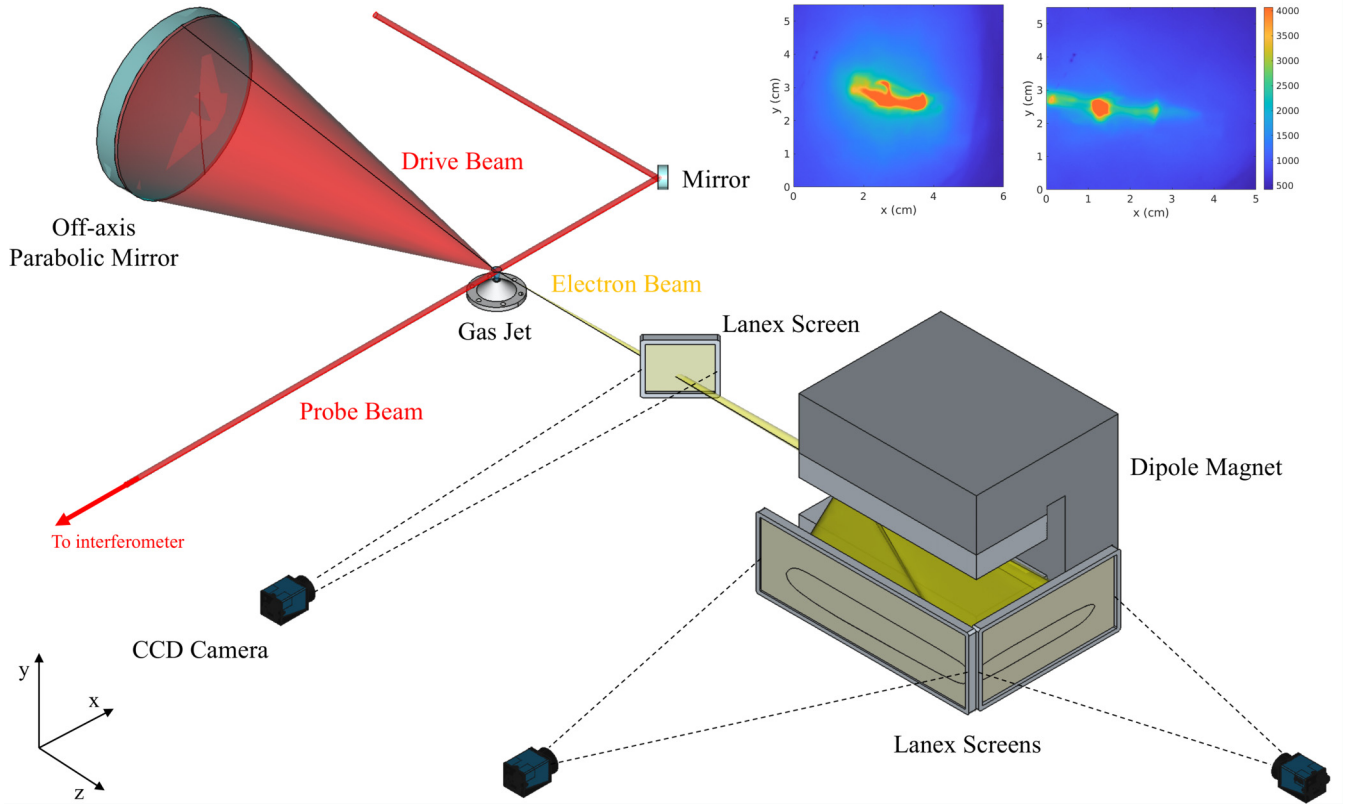


FIG. 6. Laser beams, target, and diagnostics used in experiment. The transverse e-beam profiles (in the top right) are detected by the first lanex screen after the gas jet.

The experimental results were compared with three dimensional (3D) particle-in-cell simulations, presented in Fig. 7. The electron beam profile in Fig. 7(a) is calculated from the electron's momentum obtained in the simulation at the end of the gas jet. The simulated beam profile is very similar to the measured ones, shown in the inset of Fig. 6. The simulation suggests that the e-beam divergence is not symmetric in the plane of polarization of the laser pulse [see Fig. 7(b)], which is the topic of this work. The reason is the self-phase modulation of the laser field, which in turn generates an asymmetric bubble, where the electrons are injected with large transverse momentum. The physics of electron injection into an undulating bubble is presented in Ref. [11]. It is very important that in the orthogonal plane the electron spectra is fully symmetric in angle [see Fig. 7(c)], as it should be in the case

of a perfectly rotation symmetric laser envelope. However, in experiments the angular distribution of electrons is not symmetric in this plane, which can be attributed to the imperfect intensity distribution in the focal plane. Another reason is the vertical nonuniformity in the gas density, which generates a small gradient in the refractive index and bends the laser's propagation direction along the y axis. The larger divergence and nonzero pointing angle of the low-energy (<200 MeV) electrons in the orthogonal plane were measured consistently in all data shots, as shown in Fig. 8. Here, the presented quantities are calculated after excluding the high-energy electrons. We assumed that the direction of the most energetic electrons is at the center of the saturated region and deleted the data values lying inside a small circle corresponding to 5 mrad half angle. Although the electron's angular-energy

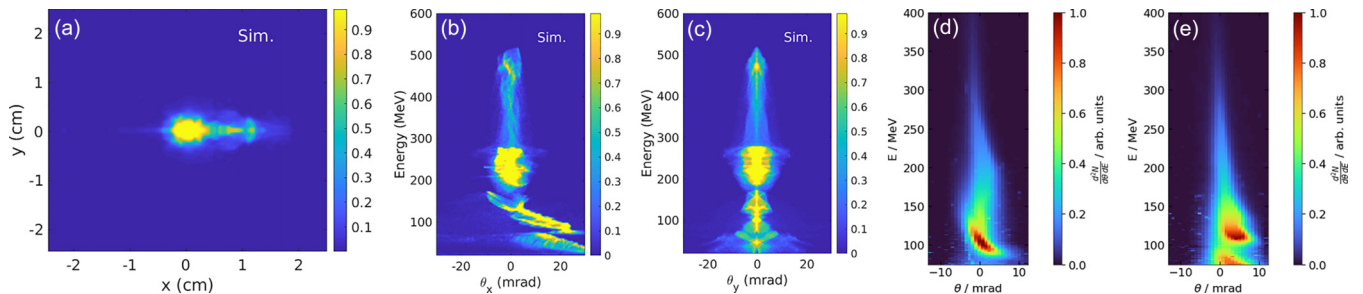


FIG. 7. (a) Simulated beam profile at 0.5 m distance from the gas jet. (b), (c) The angle-resolved energy spectrum of the accelerated electrons in both planes. (d), (e) Example spectra from experiments in the plane perpendicular to the laser's polarization plane.

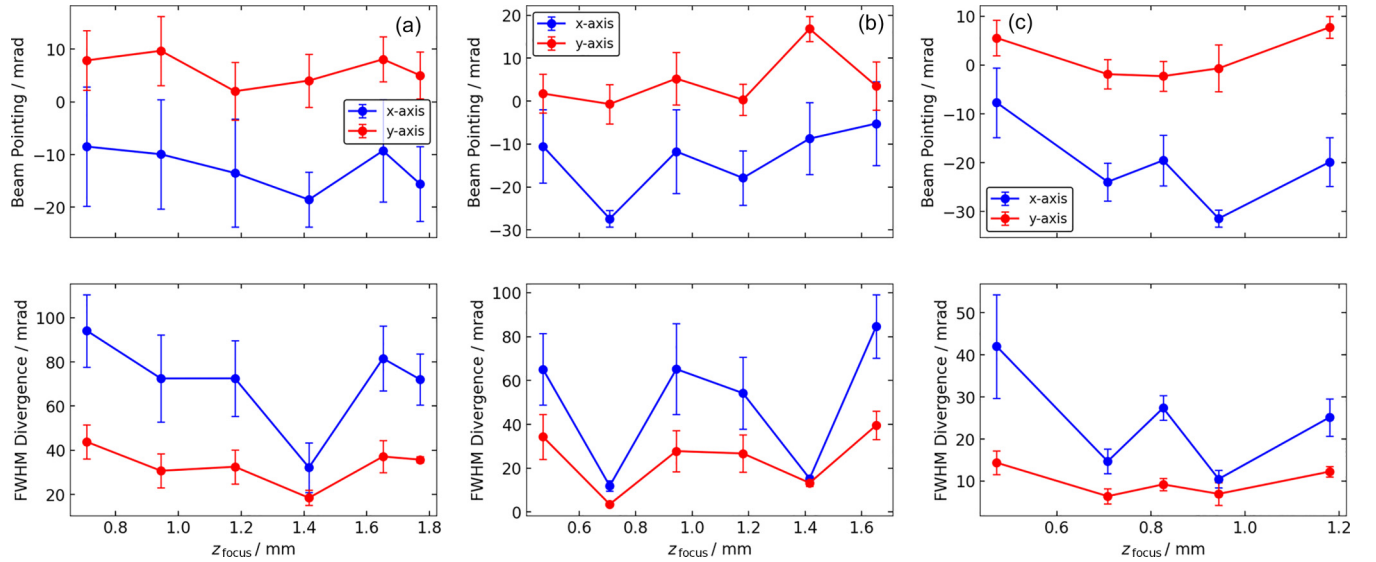


FIG. 8. Electron beam pointing (top) and divergence (bottom panels) measured in experiments. Both quantities are larger along the x axis. The gas pressures were 17 bar ($n_e \approx 4 \times 10^{18} \text{ cm}^{-3}$) [panel (a)], 20 bar ($n_e \approx 5.5 \times 10^{18} \text{ cm}^{-3}$) [panel (b)], and 22 bar ($n_e \approx 7 \times 10^{18} \text{ cm}^{-3}$) [panel (c)].

distribution in the orthogonal plane was not measured, the transverse beam profiles provide clear evidence of nonsymmetric self-injection. This phenomenon is explained and analyzed in the following sections.

In order to investigate the physics behind the angular asymmetry, a Particle-in-Cell (PIC) simulation was performed with the quasi-3D code, FBPIC [24], using the following parameters: FWHM of the laser-intensity envelope is $15 \mu\text{m}$ ($w_0 = 12.7 \mu\text{m}$) in the radial direction and the FWHM pulse duration is 21 fs ($t_L = 18 \text{ fs}$). The normalized peak laser field amplitude is $a_0 = 4$ and the laser wavelength is $\lambda = 0.8 \mu\text{m}$. The laser is polarized in the x direction, like in the experiment. The plasma density up-ramp is represented by a semi-Gaussian function $n_e = n_0 \exp(-z^2/\sigma^2)$, where $n_0 = 7 \times 10^{18} \text{ cm}^{-3}$ and $\sigma = 250 \mu\text{m}$, which is followed by a 1-mm-long uniform region (plateau), then the plasma ends with the same density (down-)ramp. The cell size of the simulation grid is 35 nm in the z direction, while it is 160 nm in the radial direction, and four azimuthal modes are used. In each grid cell, 64 electrons (quasiparticles) are placed zero temperature and the ions are immobile. The size of the simulation box is $70 \mu\text{m} \times 80 \mu\text{m}$; thus, the total number of grid points is $N_z \times N_r = 2000 \times 500$.

In Fig. 9, the evolution of the laser pulse is shown and compared with the simplified model presented above. This comparison clearly shows that the modulation in the waveform occurs exactly at the same place where the localized redshifting is predicted by the model: near the positions $z = 1.152 \text{ mm}$ in Figs. 9(b1) and 9(b2), and $z = 1.432 \text{ mm}$ in Figs. 9(c1) and 9(c2). Furthermore, the shapes of the envelope agree fairly well in the upper and lower pictures. After $\approx 1 \text{ mm}$ of propagation, the laser pulse loses only 15% of its initial energy; therefore, the laser envelope evolution has a stronger effect on the self-phase modulation compared to the pulse-front depletion. The longitudinal envelopes would be different at later stages of the propagation, not shown here, because group velocity dispersion (GVD) and energy depletion is neglected in our fluid-envelope model. However, this simplified

approach serves as a quick numerical tool for the investigation of pulse evolution, at least over a distance corresponding to 1–2 Rayleigh lengths, and can provide a reliable description of the redshifting, which is not uniform, but strongly localized in the nonlinear regime. According to Ref. [11], this off-axis injection leads to the formation of microbunches, but it could be possible to achieve nanometer-scale bunch lengths after careful tuning and optimization of the pulse evolution. Our modeling provides a platform for such optimization, which could ultimately lead to the emission of coherent betatron radiation in the XUV range.

We can get deeper insight into the bubble evolution as well by showing the density and velocity distribution of electrons in Fig. 10. The symmetric wakefield structure can be easily recognized from the bubble shape in the initial stage of LWFA, as shown in Fig. 10(c). This symmetry originates from the axis-symmetric repulsion of the electrons by the Gaussian laser pulse, which results in antisymmetric velocity distribution, meaning that the radial velocities below and above the axis ($x = 0$) have opposite signs, but the absolute values are identical. With the notations $v_x^+ = v_x(x > 0)$ and $v_x^- = v_x(x < 0)$, we can express the asymmetric part of the electrons distribution as $v_a = |v^- + v^+|/2c$ and the symmetric part as $v_s = |v^- - v^+|/2c$. Here, the velocity map is calculate as the ratio of the current density and charge density: $v_x = j_x/(en_e)$. In Fig. 10(a), one can see that v_a is completely zero behind the laser pulse in the first bubble, which means complete rotation symmetry. In the second bubble, this symmetry already breaks because of the finite number of azimuthal modes and probably due to the insufficient number of particles in the simulation. Later, in Fig. 10(b), when the single-cycle waveform appears in the laser pulse v_a is not zero anymore, which results in the off-axis injection and coherent transverse oscillation in the tail of the electron beam, seen in Fig. 10(d). This asymmetry is a signature of transverse wobbling of the bubble, as it is depicted in Ref. [11].

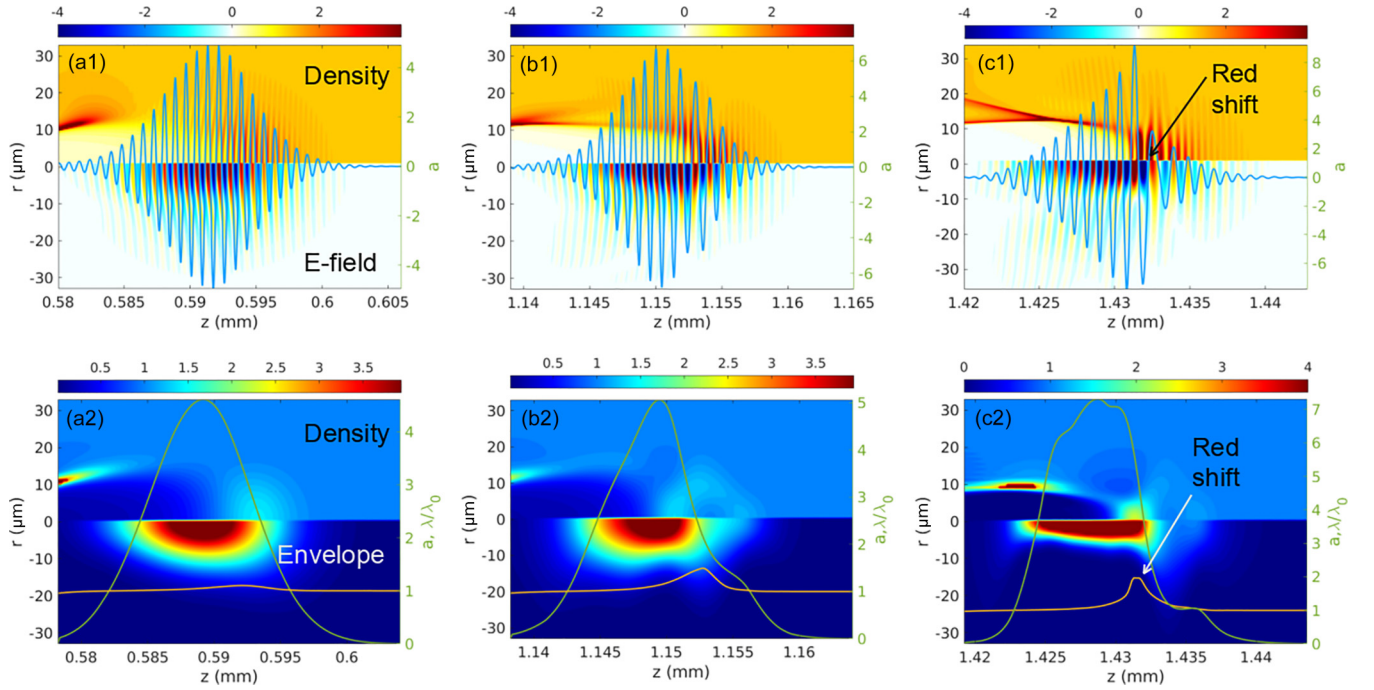


FIG. 9. Comparison between a PIC simulation [panels (a1), (b1), and (c1)] and our fluid-envelope model [panels (a2), (b2), and (c2)]. The upper part of each picture shows the electron density distribution and in the lower part the laser field (or envelope) is shown. The blue (and green) curves show the lineout of the laser field (and envelope) along the propagation axis and the orange curve in the lower pictures shows the normalized laser wavelength (or redshifting). The density is normalized to $5 \times 10^{18} \text{ cm}^{-3}$ in all cases.

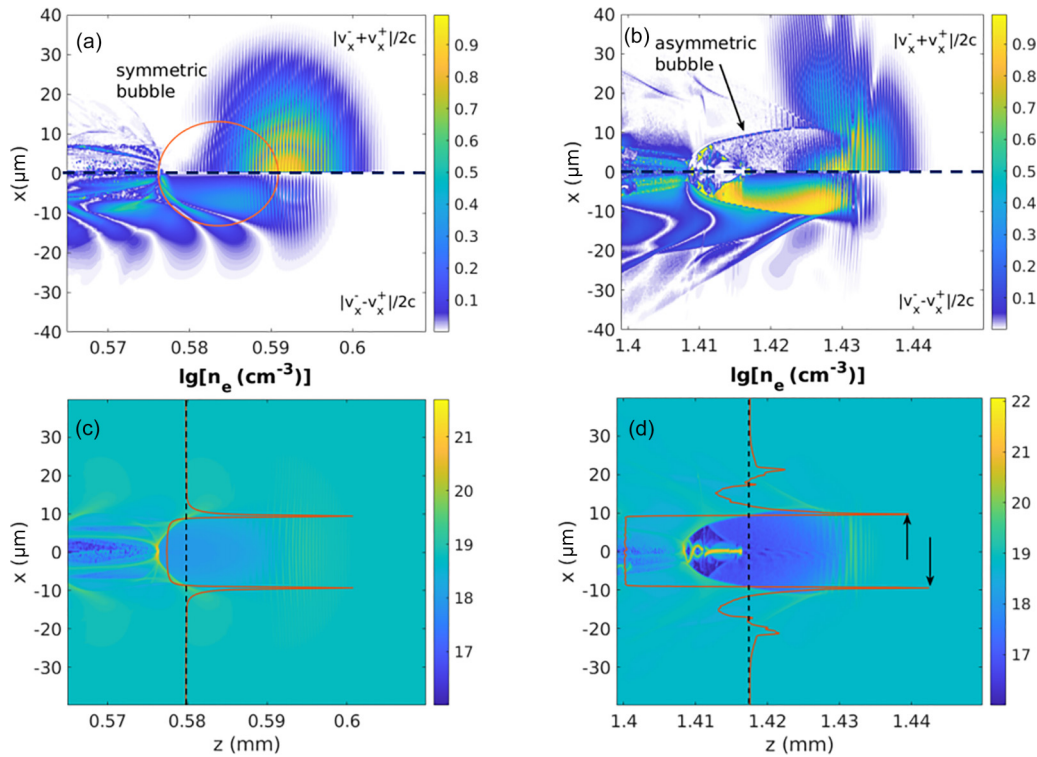


FIG. 10. Velocity maps [panels (a) and (b)] and electron density distributions [panels (c) and (d)] at an early time of the interaction [panels (a) and (c)] and later [panels (b) and (d)], when the redshifting becomes significant. The red lines show the density lineouts (linear scale, arbitrary units) across the bubble.

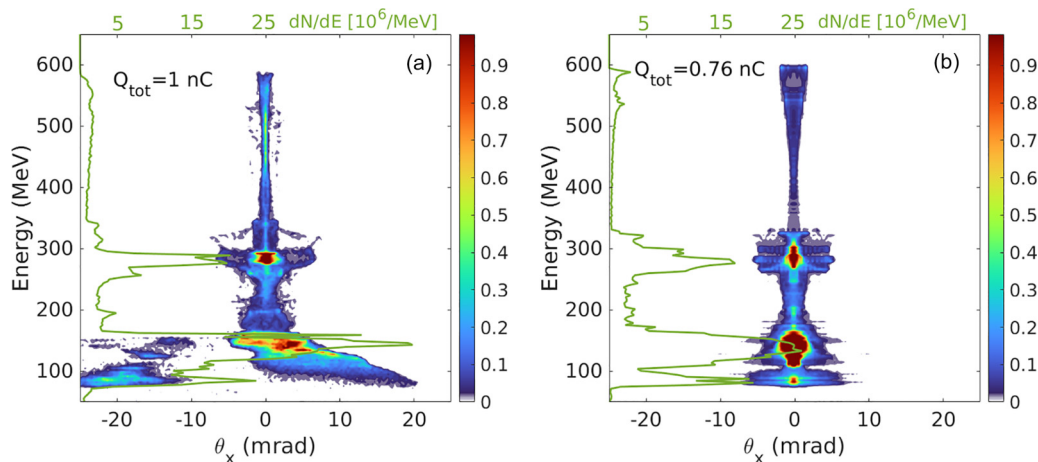


FIG. 11. Angular-energy distribution of injected electrons using a standard PIC field solver [panel (a)] and the envelope solver [panel (b)]. The spectra integrated in angle are also shown with the green lines.

In order to show the impact of subcycle dynamics of the plasma electrons on the self-injection (and acceleration), we compare the results of simulations performed with full electromagnetic solver (the laser pulse propagates as a wave) and with the envelope solver (the electrons do not have a quiver motion). For this, we use our recently developed PIC code [25], based on an exponential field propagator, which has an accuracy similar to the spectral solvers. The results are presented in Fig. 11, which shows almost identical distribution in the case high-energy electrons, but there is an asymmetry below 200 MeV when the full laser field is modeled. Interestingly, the off-axis injected charge is larger in this portion of the spectrum. The larger injected charge can be explained with the Hamiltonian analysis performed for expanding [26] and undulating [11] bubbles. In both cases, the change in the Hamiltonian increases the probability of electron trapping; therefore, when both modulations are present, as in Fig. 11(a), more charge is expected.

VI. CONCLUSIONS

A quick numerical method is presented, which is suitable to model the longitudinal phase evolution of the laser pulse by taking into account the local variations in the refractive index given by the fluid density and momentum inside the wakefield. The model has a limited validity, because the envelope equation in the longitudinal direction is not solved; therefore, group velocity dispersion is neglected in the calculations. However, our numerical tool reproduces the self-phase modulation of a high-intensity laser pulse observed in particle-in-cell simulations; therefore, it can provide reliable pulse evolution if the local laser frequency shift is below 100%. Our findings are in good agreement with self-consistent one-dimensional theory [17], which gives us the confidence that our approach is valid up to the point when the self-compression or energy depletion of the pulse becomes significant.

In general, we can conclude that the self-phase modulation becomes significant after a few Rayleigh lengths of

propagation if the density is larger than $n_{e0} > 10^{18} \text{ cm}^{-3}$ for a laser wavelength of $\lambda_0 = 800 \text{ nm}$, or $n_{e0} > 5 \times 10^{-4} n_{c0}$. This is an important remark for all PW-class lasers used for LWFA, because the local wavelength variation has to be taken into account to correctly describe the guiding or self-focusing processes in a constant density plasma. In plasma channels, the density is typically smaller and the transverse laser beam dynamics are more important than the longitudinal phase modulation, which allows the guiding nearly up to the pump depletion length.

The most important consequence of the redshifting is the asymmetric electron injection, which results in large e-beam divergence in the plane of laser polarization. These electrons will have a larger betatron oscillation amplitude in the bubble, which potentially can lead to higher x-ray yield via betatron radiation emission. Controllability of the waveform evolution still remains the main question for future studies aiming to exploit the transverse asymmetry in nonlinear wakefields.

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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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