Carrier-envelope phase effects in Laser Wakefield Acceleration with near-single-cycle pulses

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Driving laser wakefield acceleration with extremely short, near single-cycle laser pulses is crucial to the realisation of an electron source that can operate at kHz-repetition rate while relying on modest laser energy. It is also interesting from a fundamental point of view, as the ponderomotive approximation is no longer valid for such short pulses. Through particle-in-cell simulations, we show how the plasma response becomes asymmetric in the plane of laser polarization, and dependent on the carrier-envelope phase (CEP) of the laser pulse. For the case of self-injection, this in turn strongly affects the initial conditions of injected electrons, causing collective betatron oscillations of the electron beam. As a result, the beam pointing and electron energy spectrum become CEP-dependent. For injection in a density gradient these effects are reduced, as electron injection is mostly longitudinal and mainly determined by the density gradient. Our results highlight the importance of controlling the CEP in this regime for producing stable and reproducible relativistic electron beams. Mitigation of CEP effects can nevertheless be achieved using density gradient injection.

I. INTRODUCTION

Laser wakefield accelerators (LWFA) \cite{1–5} are tabletop setups that can produce relativistic electron bunches with an extremely short (fs) bunch duration \cite{6} and a small (µm) source size \cite{7}. These accelerators are based on an intense laser pulse which interacts with a plasma, exciting a plasma wave which accelerates electrons through extremely high electric fields (in excess of 100 GeV m$^{-1}$). As these setups are laser-based, the synchronisation between the electron bunch and the laser pulse is jitter free, making this source ideal for pump-probe experiments requiring high temporal resolution, with applications in solid state physics, materials science and biology \cite{8–10}.

Results obtained so far in the field of laser wakefield acceleration have mostly been on systems with a repetition rate on the order of a hertz. Part of the community is currently pushing laser plasma accelerators to a high repetition rate (kHz) \cite{11}, which is beneficial for applications requiring statistical averaging. In addition, increasing the repetition rate also improves the source stability by reducing thermal variations in the laser system. Increasing the repetition rate to a kHz-level with current Ti:Sapph laser technology means restricting the pulse energy below the 100 mJ-level. The high intensities necessary for LWFA (10\(^{18}\) – 10\(^{19}\) W cm\(^{-2}\)) can then still be achieved by compressing the pulse down to the (almost) single-cycle regime, as has recently been shown in \cite{12,13}.

In this regime, the ponderomotive approximation that is generally used in the field of laser-plasma interaction is no longer valid: the pulse envelope varies considerably over an oscillation of the electric field. The dynamics can therefore not be properly described with the pulse intensity (as is the case in the ponderomotive approximation), but the electric field itself needs to be considered instead. In this context, the carrier-envelope phase starts to become relevant, both from a theoretical point of view and as an experimental parameter that needs to be controlled in order to obtain a stable, reproducible accelerator. In addition, CEP effects can also become important in LWFA driven by longer laser pulses that reach the depletion length at the end of the interaction, where the laser pulse duration is often reduced to a few optical cycles.

The first theoretical treatment of the effect of the CEP on the LWFA process is by Nerush et al. \cite{14}, as a reaction on the plasma bubble oscillations observed in \cite{15}, initially ascribed to electron-hose instability. Developing a mathematical analysis beyond the ponderomotive model, Nerush et al. show that the higher-order terms of the plasma response contain an asymmetry that is CEP-dependent, pushing the plasma bubble off-axis. Because of plasma dispersion, the CEP changes with pulse propagation such that the plasma bubble starts to oscillate in the plane of laser polarization. As the electron self-injection region oscillates with the bubble, the electron beam is modulated in a way that depends on the CEP. One can estimate the scale on which the CEP changes by 2\(\pi\) as \cite{11,14}:

\[
L_{2\pi} \approx \frac{n_e \lambda_0}{n_e} \quad (1)
\]

where \(n_e\), \(n_c\) and \(\lambda_0\) are the electron density, critical electron density and the laser wavelength respectively.

At low intensities, where the plasma bubble does not present any asymmetry, CEP effects can still be significant, as shown by Lifschitz et al. \cite{16} for the case of ionization injection. Here, a varying CEP changes the initial conditions at which the electrons are injected, resulting in different electron energies and emission angles.

Experimentally, a first evidence of a CEP effect in a LWFA experiment is presented in \cite{11}, showing a significant change in the electron spectrum when changing the
laser CEP by $\pi/2$. It should be noted that in order to experimentally observe the CEP effect a high level of stability and control of all experimental parameters (pulse energy, pulse duration, beam profile, gas density etc.) is required.

In this paper, we complement the work of Nerush and Lifschitz by going beyond the ponderomotive approximation and address CEP effects in laser wakefield acceleration with near-single-cycle pulses at moderately relativistic intensities (i.e. with normalized vector potential $a_0$ of 3-10). In addition, we emphasize the role of the CEP on the physics of electron injection and acceleration, and focus specifically on self-injection and density gradient (DG) injection. The paper is organized as follows: section II presents the CEP-dependent asymmetry of the accelerating structure, and its scaling with intensity. The effect of the CEP on the injection and acceleration of the electron beam is then explained in section III both for the case of self-injection and density gradient injection.

II. ASYMMETRY OF THE ACCELERATING STRUCTURE

For near single-cycle pulses, the amplitude of the electric field envelope varies considerably over the course of an optical cycle, triggering an asymmetric response of the plasma which depends on the CEP. To quantify this asymmetry, we performed particle-in-cell (PIC) simulations with parameters that correspond to what can realistically be expected in the near future from state-of-the-art near-single-cycle kHz lasers [19–20], in combination with high-density, high precision gas jets [18–20].

A. Simulation parameters

We use the spectral, quasi-cylindrical particle-in-cell code FBPIC [21]. With the laser propagating in the z-direction, the radial grid is constructed using $dz = \lambda_0/50$, $dr = \lambda_0/20$ (where $\lambda_0 = 800$ nm is the laser center wavelength), while azimuthally 5 modes are used to correctly capture all departures from cylindrical symmetry. The plasma is made of fully ionized Helium, so that ionization effects are not computed in order to save computation time. In all simulations, the laser pulse duration is 3 fs (FWHM on intensity) and the pulse is focused down to a 5 µm waist.

B. CEP dependent bubble asymmetry

We quantify the bubble asymmetry by calculating the transverse center of mass of the electron density distribution in the plane of polarization ($y = 0$), and normalizing it to the bubble radius $R \simeq w_0$:

$$\Gamma_x = \frac{1}{w_0} \frac{\int X n_e(x) x\,dx}{\int X n_e(x)\,dx},$$

where $X$ is the width of the simulation window in $x$. For $a_0 = 4$ and an electron density $n_e = 0.025n_c$ ($n_c$ being the critical electron density $1.74 \times 10^{21}$ cm$^{-3}$), figure 1 shows how the bubble asymmetry $\Gamma_x$ (blue) oscillates, driven by the CEP of the driving laser pulse (solid red), at an amplitude of 3% of $w_0$. The panel on the right shows the asymmetric bubble, with the transverse center of mass of the electron density indicated by a black dot. The gray line coincides with the $z$-axis, and indicates the length over which an average value of $\Gamma_x$ is obtained. The red and blue lines indicate the laser electric field and its envelope respectively. The CEP is calculated as the distance between the maximum of the electric field and that of the pulse envelope (each indicated by a black spot), divided by the center wavelength of the pulse. The tail of the pulse undergoes a strong redshift, causing the center wavelength to be redshifted by a factor of 2 over the course of the simulation (see Supplementary Information), an effect that was observed in [22]. Through this redshift, the effective normalized laser field strength $a_0 \propto \sqrt{\Gamma \lambda^2}$ increases considerably, peaking at 6.8 around $t = 240$ fs. As a result, the asymmetry of the plasma response increases over the course of the simulation, until depletion of the laser pulse becomes significant for times $t > 300$ fs. Interestingly, the increase in $a_0$ also increases the transverse momentum of the electrons ejected by the laser pulse, which causes the bubble top and bottom parts to flatten (see also supplementary movie). These effects cause the bubble oscillation frequency to slightly decrease, as can be seen in figure 1 in the decreasing period of $\Gamma_x$ (blue curve).

In the plane perpendicular to the laser polarization ($x = 0$) the bubble asymmetry is absent, as shown by the dotted blue line in figure 1.

C. Intensity scaling of the bubble asymmetry

The strength of the asymmetry is expected to depend on the laser intensity. We repeated the simulation for laser intensities ranging from $a_0 = 3$ to $a_0 = 10$, keeping all other parameters constant, and calculated a mean bubble asymmetry by averaging $|\Gamma|$ from the moment the bubble is formed up to the end of the plasma. Figure 2 shows this mean bubble asymmetry as a function of the laser intensity. It is interesting to compare this to the predictions from Nerush et al. [14]. According to the authors, the asymmetry becomes considerable only for $a_0 > k_0w_0$ (where $k_0 = \omega_0/c$ is the laser wave vector), i.e. for $a_0 > 12$ for our set of parameters ($\lambda_0 = 800$ nm and $w_0 = 5$ µm), but we clearly observe a strong asymmetry at lower laser intensities. This can be explained...
by the strong redshift of the laser pulse: as the center wavelength increases by a factor 2, the theoretically predicted limit drops to $a_0 > 6$, which is indeed reached by the laser field strength when normalized to the redshifted laser wavelength.

Secondly, the bubble asymmetry in [14] is described to scale with $a_0^3$. Fitting a cubic function $(ax^3+b)$ yields the orange curve in the right panel of figure 2 while including the full third order polynomial (green) improves the fit only marginally. Despite the fact that the definition of the bubble asymmetry in [14] slightly differs from ours [23], the agreement with the $a_0^3$ scaling is remarkable.

In summary, our results are consistent with the predictions from [14] concerning the cubic scaling, but the bubble asymmetry appears to be considerable even at intensities lower than one may expect from the theoretical prediction, due to the strong redshift.

### III. CEP-EFFECTS ON ELECTRON INJECTION AND ACCELERATION

In a pulse so short that the ponderomotive approximation is no longer valid, the changing CEP influences not only the accelerating structure, but also the electron beam injection and acceleration. We will now show that in the case of self-injection, it is the asymmetry at the moment of injection that governs the CEP-dependent dynamics of the electron beam (rather than the oscillating bubble during acceleration).

Possibly because self-injection is easy to implement experimentally, it has been currently the most widespread injection mechanism in LWFA since its demonstration over two decades ago [24, 25]. It is based on the breaking of the plasma wave as the laser pulse reaches highly relativistic intensities. As described above, electrons at the front of the bubble collectively gain a transverse momen-
tum which is CEP-dependent. As these electrons travel towards the back of the bubble, the transverse momentum changes sign and at the moment of wave-breaking, the electrons are injected and start describing a collective betatron oscillation \cite{20}. When the injection length is small compared to \( L_{2\pi} \), the CEP at the moment of injection can thus strongly influence the electron beam produced by the accelerator. In the opposite case, the effects may be averaged out over an oscillation of the CEP.

To illustrate this effect, we study self-injection in the simulation of figure 1 (i.e. \( a_0 = 4, n_c = 0.025n_c \)) for a laser pulse with an initial CEP of \( \phi_i = 0 \) and \( \phi_i = \pi \). Figure 3 shows the moment of self-injection for these two cases. In these frames, the electron density is shown in shades of green, and the injected electrons that will constitute the accelerated electron beam are shown in a purple-yellow color scale corresponding to their final energy \( \gamma_{\text{final}} \). The asymmetric nature of the injection is evident and the color scale shows how the most energetic electrons are injected nearly on-axis, whereas the lower energy electrons are injected off-axis. As we will see below, this lower-energy tail subsequently performs large amplitude collective betatron oscillations during acceleration. Note that in the common case of longer pulses, the ponderomotive approximation still holds and the laser pulse drives a symmetric plasma bubble. Electrons injected in this symmetric structure also perform betatron oscillations, but individually, i.e. the ensemble average of the beam is symmetric in \( x \) and \( y \). What we see here is a different phenomenon, i.e. a collective betatron oscillation of the beam, which is CEP dependent. As noted in \cite{14} these CEP-dependent oscillations are also easily distinguished from beam-hose instabilities \cite{27} as such instabilities are not confined to the plane of laser polarization. To visualize this process in greater detail the reader is encouraged to explore the movies in the Supplementary Material.

We will now track the development of the electron beam throughout the acceleration. In order to get meaningful results a proper definition of “the electron beam” is crucial. We define the electron beam as: the electrons which in the final iteration (when the electron beam has left the plasma) have forward momentum \( u_z > u_{z,\text{min}} \) and lie within a 50 mrad angle of the most energetic part of the beam. Based on the electron beam’s phase space distribution, \( u_{z,\text{min}} \) is the threshold which separates the electrons in the first accelerating bucket from the background electrons, in this case corresponding to \( u_z > u_{z,\text{min}} = 26m_e c \). Following these electrons, we can track the evolution of the beam pointing and transverse normalized emittance, plotted in blue and orange in figure 4 for an initial CEP of \( \phi_i = 0 \) (the evolution of the beam charge and energy can be found in the Supplementary Information). Of these beam parameters the pointing in particular shows a clear oscillation around the symmetry axis in the plane of the laser polarization, which is the collective betatron oscillation described above. Incidentally, a similar effect was observed in \cite{28}, where collective betatron oscillations following asymmetric injection was caused by an asymmetric transverse laser profile. The reader is reminded of the characteristic frequency of betatron oscillation for an electron in a focusing wakefield, which is given by:

\[
\omega_\beta = \frac{\omega_p}{\sqrt{2\gamma}},
\]

where \( \omega_p \) is the plasma frequency. In the perpendicular plane (dotted line) no significant oscillation is observed, as expected. The evolution of the total beam charge shows that self-injection takes place from 110 to 200 fs into the simulation, which corresponds to a length of 25 \( \mu m \), or 0.8\( L_{2\pi} \). Different parts of the electron beam are thus injected at a different phase of the bubble oscillation, resulting in a superposition of multiple oscillations in the pointing of the electron beam. In addition, as the electrons gain energy from 6 to 44 MeV, their betatron oscillation period increases roughly linearly from 90 fs

FIG. 3: Simulation snapshots at \( t = 151.7 \) fs, for initial CEP values \( \phi_i = 0 \) and \( \phi_i = \pi \), showing the electron density in shades of green and the injected electrons that constitute the electron beam. The color of the injected electrons corresponds to their final energy \( \gamma_{\text{final}} \). These two frames clearly show the off-axis injection of the electron beam. High energy electrons are injected on-axis, whereas off-axis injected electrons form a lower-energy tail performing strong betatron oscillation. See Supplementary Material for the full movie.
to 225 fs. These values are consistent with the oscillations observed in figure 4. The emittance of the electron beam is significantly larger in the plane of polarization than in the perpendicular plane by a factor 3.6. Again, this is an effect that cannot be explained within the ponderomotive approximation, but is a direct consequence of the injection asymmetry. Note that although asymmetric emittances have been reported before, this mostly due to the electron beam interacting with the rear of the laser pulse [29]. In our simulation, electrons are injected through pure self-injection, and the observed effect can be attributed solely to the asymmetry of the plasma response in the plane of polarization.

We would now like to see what happens when the initial CEP of the laser pulse is varied, and how it affects the electron beam pointing, as could be observed in an experiment. We repeated the same simulation with five different initial CEP values ranging from 0 to π. The evolution of the beam pointing for these five cases (figure 5, left) clearly shows the importance of controlling the CEP to obtain a stable accelerator. As one would expect, the cases of 0 and π are symmetric with respect to the z-axis. The pointing deviation at the exit of the plasma (grey dotted line) is on the order of 10 mrad, and depends strongly on the length of the plasma. Indeed, in simulations with a shorter gas jet length of 50 µm (instead of 80, corresponding to the dephasing length) the electron beam leaves the plasma after 350 fs with a beam pointing angle of up to 20 mrad. Thus, in an experiment that aims at measuring CEP effects on the electron beam, it is crucial to keep a highly stable gas density profile.

The different phase-space trajectories followed by the electron beams for different CEP values have a significant influence on their energy spectrum, as is clear from figure 5 (right panel). The spectra for initial CEP values 0 and π overlap. Again, the importance of controlling the CEP is evident: an initial CEP of π/2 gives a quasi-monoenergetic peak of 5 % at 39 MeV, as opposed to a broad 25 % energy spectrum at a CEP of 0 or π.

B. Density gradient injection

A second injection mechanism well-adapted to LWFA with near-single-cycle pulses is injection in a density gradient (DG) [30–33]. It consists in tailoring the gas jet such that the density profile features a sharp downward gradient, causing a sudden increase of the plasma wavelength. The back of the plasma bubble thus undergoes an effective slow-down which triggers trapping of electrons. Where self-injection is triggered by the highly nonlinear response of the plasma to an ultrarelativistic laser pulse, injection in a density gradient is controlled by the relatively stable density profile. It thus allows for more controlled injection, at lower intensities. If the density gradient is over a length scale significantly smaller than $L_{2\pi}$, injection takes place at a specific CEP value and an effect on the electron beam can be expected. However, the injection geometry is to a first approximation determined by the gas density gradient, so one can expect the effect to be significantly weaker than in the case of self-injection. A similar effect, albeit with different underlying physics, is described in [34] comparing transverse and longitudinal injection in laser-plasma accelerators. In short, self-injection is typically dominated by transverse injection, i.e. electrons have are injected with an initial transverse momentum. In the case of longitudinal injection electrons remain essentially on-axis and are injected with virtually no transverse momentum, yielding an accelerator that is more robust to changes in laser profile. Similarly, in our example of DG-injection, electrons are injected with low initial transverse momentum and the resulting electron beam is more robust to changes in the CEP.

Because DG-injection is well adapted for applications with limited laser pulse energy, and in order to avoid self-injection, we performed the DG simulations at a (vacuum) laser field strength of $a_0 = 3$. The peak electron density at the start of the gas jet is $0.015n_e$, which drops to $0.01n_e$ over a length of 10 µm (see Supplementary Information for the gas density profile).

As in figure 3 for the case of self-injection, figure 6 shows the two frames corresponding to the moment of electron beam injection (t=156.9 fs) in the density gradient, for initial CEP values of 0 and π. Indeed, the injection is highly axisymmetric and, to a first approximation, independent of the CEP, in line with the above-mentioned reasoning that the injection is determined by the geometry of the gas density profile (i.e. longitudinal). It should be noted however that due the lower electron density, the tail of the laser is not as redshifted as in the example on self-injection, which reduces the asymmetry of the plasma response (the bubble asymmetry is...
FIG. 5: (a) Pointing of the electron beam as a function of time, for initial CEP values from 0 to $\pi$. Note the exact symmetry between the trajectories 0 and $\pi$. The gray dotted line indicates the plasma-vacuum interface. (b) The final electron beam energy spectra for the different CEP values. The spectra for 0 and $\pi$ overlap.

CEP which changes with propagation through plasma dispersion. As the laser redshifts during propagation, $a_0$ increases up to 6.8 (compared to 4.0 in vacuum), causing an increasingly asymmetric plasma response. For the case of self-injection, the transverse momentum gained by the electrons causes them to be injected off-axis and subsequently launches large amplitude collective betatron oscillations. While such large oscillations may be beneficial to the generation of betatron X-ray radiation, they also cause a degradation of the transverse emittance as well as oscillations of the beam pointing along propagation. This collective betatron oscillation depends on the betatron frequency and on the extent to which the injection is localized in time (if the injection time is more than a fraction of the CEP period, a superposition of several oscillations is observed). The angle at which the electron beam leaves the accelerator is thus influenced by the initial CEP of the laser. The energy spectrum of the electron beam is also shown to be strongly CEP-dependent. These effects are strongly reduced in the case of injection in a density gradient, where injection is axisymmetric to a first approximation.

IV. CONCLUSION

Through PIC simulations we explored the effect of the CEP on injection and acceleration in a laser-plasma accelerator, in particular the cases of self-injection and density gradient injection with near-single cycle laser pulses at moderately relativistic laser intensities. For such short pulses, the ponderomotive approximation is no longer valid and the plasma response becomes asymmetric in the plane of laser polarization. In contrast to what one may expect from theoretical predictions [14], bubble asymmetry is found to be significant even at these moderate intensities due to significant redshifting of the laser pulse. The observed oscillation of the bubble is locked to the CEP which changes with propagation through plasma dispersion. As the laser redshifts during propagation, $a_0$ increases up to 6.8 (compared to 4.0 in vacuum), causing an increasingly asymmetric plasma response. For the case of self-injection, the transverse momentum gained by the electrons causes them to be injected off-axis and subsequently launches large amplitude collective betatron oscillations. While such large oscillations may be beneficial to the generation of betatron X-ray radiation, they also cause a degradation of the transverse emittance as well as oscillations of the beam pointing along propagation. This collective betatron oscillation depends on the betatron frequency and on the extent to which the injection is localized in time (if the injection time is more than a fraction of the CEP period, a superposition of several oscillations is observed). The angle at which the electron beam leaves the accelerator is thus influenced by the initial CEP of the laser. The energy spectrum of the electron beam is also shown to be strongly CEP-dependent. These effects are strongly reduced in the case of injection in a density gradient, where injection is axisymmetric to a first approximation.

These findings show to which extent CEP control, especially in the case of self-injection, is crucial in establishing a laser wakefield accelerator capable of producing relativistic electron bunches using near single-cycle pulses, with a stable and reproducible beam pointing and energy spectrum. Alternatively, using a density gradient injection scheme loosens the requirements on the CEP stability of the laser, which is relevant for systems where CEP-stabilization is challenging or absent. These findings are an important step in the maturation of these unique sources.

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FIG. 6: Simulation snapshots at $t = 156.9$ fs, for initial CEP values 0 and $\pi$, showing the electron density in shades of green and the injected electrons that constitute the electron beam. The color of the injected electrons corresponds to their final energy $\gamma_{\text{final}}$. These two frames clearly show how the injection is axisymmetric to a first approximation.

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FIG. 7: Injection in a density gradient. (a) Pointing of the electron beam as a function of time, for initial CEP values from 0 to $\pi$. Again, the trajectories for 0 and $\pi$ are symmetric with respect to the z-axis. The gray dotted line indicates the plasma-vacuum interface. (b) The final electron beam energy spectra for the different CEP values.

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