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Kinetic and finite ion mass effects on the transition to relativistic self-induced transparency in laser-driven ion acceleration

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Abstract

We study kinetic effects responsible for the transition to relativistic self-induced transparency in the interaction of a circularly-polarized laser-pulse with an overdense plasma and their relation to holeboring (HB) and ion acceleration. It is demonstrated using particle-in-cell simulations and an analysis of separatrices in single-electron phase-space, that ion motion can suppress fast electron escape to the vacuum, which would otherwise lead to transition to the relativistic transparency regime. A simple analytical estimate shows that for large laser pulse amplitude a_0 the time scale over which ion motion becomes important is much shorter than usually anticipated. As a result of enhanced ion mobility, the threshold density above which HB occurs decreases with the charge-to-mass ratio. Moreover, the transition threshold is seen to depend on the laser temporal profile, due to the effect that the latter has on electron heating. Finally, we report a new regime in which a transition from relativistic transparency to HB occurs dynamically during the course of the interaction. It is shown that, for a fixed laser intensity, this dynamic transition regime allows optimal ion acceleration in terms of both energy and energy spread.

1. Introduction

Modern high intensity laser technology has made the regime of relativistic optics experimentally accessible. In this regime electrons interacting with the laser-field gain relativistic velocities within an optical cycle and their motion becomes highly nonlinear. Exploiting complex laser-plasma interaction in this regime has led to a wealth of novel applications ranging from charged particle acceleration [1-3] to sources of ultra-short radiation [4, 5].

It has long been recognized that in the relativistic optics regime even the most basic properties of a plasma such as its index of refraction are profoundly affected by nonlinearities in electron motion [6, 7]. In particular, the increase of the effective electron mass due to its γ -factor dependence on the laser normalized vector potential $a_0 = eA_0/(m_ec)$ leads to an effective increase of the critical density

$$n_c^{\rm eff} = \sqrt{1 + \frac{a_0^2}{2}} n_c.$$
 (1)

Here $n_c = \epsilon_0 m_e \omega_L^2 / e^2$ is the classical critical density above which a plasma is nominally opaque to a laser pulse with angular frequency ω_L , m_e and -e are the electron mass and charge, respectively, c is the speed of light in vacuum, and ϵ_0 is the permittivity of free space.

This simple form for the relativistic critical density n_c^{eff} holds for plane waves propagating through a uniform and infinitely long plasma. By our choice of normalization of the incident laser pulse vector potential, equation (5), the laser wave amplitude a_0 relates to the wave intensity as $I_L \lambda_L^2 \simeq 1.38 a_0^2 \times 10^{18} \text{ W cm}^{-2} \mu \text{m}^{-2}$, with $\lambda_L = 2\pi c/\omega_L$ the laser wavelength. With this choice, equation (1) is valid for both circular and linear polarization, if the cycle-averaged γ -factor is used for the latter. This effective increase of the critical density is the



basis of the effect known as relativistic self-induced transparency (RSIT), in which a relativistically intense laser pulse ($a_0 \gtrsim 1$) can propagate in a nominally overdense plasma.

However, when one considers a laser pulse incident on a bounded plasma, the situation is much more complicated. In order to allow insight into the basic physical mechanisms involved and to establish connection with previous works we consider a simplified one-dimensional geometry. We consider a circularly polarized (CP) laser pulse with finite rise time τ_r and semi-infinite duration, normally incident onto a semi-infinite plasma with a constant electron density $n_0 > n_c$, and a sharp interface with vacuum, see figure 1(a). This configuration is of particular interest for ultra-high contrast laser interaction with thick targets. Since no pre-plasma is assumed, the incoming laser pulse interacts directly with a nominally overdense plasma. The ponderomotive force pushes electrons deeper into the plasma, creating a high-density peak (compressed electron layer) that may prevent the pulse from propagating further, figure 1(b). For linearly polarized pulses the strong $\mathbf{J} \times \mathbf{B}$ electron heating can lead to the destruction of the electron density peak and, to a good approximation, the threshold for RSIT is found to be in agreement with n_c^{eff} [8, 9]. By contrast, for CP pulses, the ponderomotive force is quasisteady and electron heating is reduced. As a result, the compressed electron layer forms, efficiently reflecting the incident laser pulse. An equilibrium between the ponderomotive and charge-separation forces is reached and a standing wave is formed, with the plasma boundary displaced at a new (time-independent) position x_b , figure 1(b) [10]. This situation can be described in the framework of (stationary) cold-fluid theory [11, 12], and the existence of a standing wave solution defines the opaque regime of interaction. It is found that a plasma of a given density n_0 is opaque (self-shutters) for a_0 smaller than a threshold amplitude $a_{SW}(n_0)$ such that:

$$a_{\rm SW}^2 = \bar{n}_0 (1 + a_B^2) (\sqrt{1 + a_B^2} - 1) - a_B^4/2, \tag{2}$$



Figure 2. Different transition thresholds for RSIT. The black dashed line indicates the transition boundary for infinite plane waves $n_c^{\text{eff}} = \sqrt{1 + a_0^2/2}$. The red solid line is the cold-fluid threshold for existence of a standing wave, n_{SW} , given by equation (4). The green triangles indicate the results for the transition threshold n_{th} from PIC simulations with immobile ions, see section 2. The lower end of the error bars indicates the boundary of the RSIT regime for hydrogen and helium, as determined by PIC simulations (section 2). The upper end of the error bars indicates the boundary of the B regime. The dynamic transition regime lies within the width of the error bars. For all PIC simulations in this plot a laser pulse rise time $\tau_r = 4\tau_L$ was used.

where

$$a_B^2 = \bar{n}_0 \left(\frac{9}{8} \,\bar{n}_0 - 1 + \frac{3}{2} \,\sqrt{\frac{9}{16}} \,\bar{n}_0^2 - \bar{n}_0 + 1 \right),\tag{3}$$

and $\bar{n}_0 \equiv n_0/n_c$. In the limit of high densities $n_0 \gg n_c$ we can invert these expressions to obtain [13] the density threshold for the existence of a standing wave

$$n_{\rm SW}(a_0) \simeq \frac{2}{9} (3 + \sqrt{9\sqrt{6} a_0 - 12}) n_c.$$
 (4)

Equation (4) is plotted in figure 1, and, for the range $a_0 = 5-25$ considered here, it is in excellent agreement with the exact expression equation (2). Conversely, cold-fluid theory [11, 12, 14] predicts that RSIT occurs for $n_0 < n_{\text{SW}}$. Note that equation (4) implies a different $a_0 \gg 1$ scaling for the transition to RSIT, $n_{\text{SW}} \propto a_0^{1/2}$, than equation (1) which gives $n_c^{\text{eff}} \propto a_0$.

Nevertheless, PIC simulations have shown that even modest electron heating during the early stages of the interaction can disturb the plasma vacuum interface leading to a linear scaling for the density transition threshold, $n_{\rm th} \propto a_0$ with a coefficient that depends on the details of the interaction [13], see triangles in figure 2.

In addition, ion motion (finite ion mass) has also been found to lower n_{th} significantly in PIC simulations [15]. However, the exact mechanism responsible for this reduction has not yet been clarified. Determining the conditions and mechanisms responsible for transition from the opaque to the RSIT regime using CP light is of paramount importance as it determines the efficiency of laser energy coupling to the plasma, while it is also crucial for a wide range of applications. For example, relativistic transparency can be exploited to enhance the characteristics of laser-pulses [16], it may affect the propagation of probe pulses in plasmas with fast particles [17–19] and has led to the development of novel ion acceleration schemes [20–29].

Here we are interested in the role that RSIT may play in laser radiation pressure acceleration of ions that has recently attracted a lot of attention [16, 22, 30–32]. Indeed, when the plasma is opaque (for large enough plasma densities), and for thick enough targets, the so-called laser-driven hole-boring (HB) regime occurs [15, 30, 31, 33–36]. Ions are accelerated in the electrostatic field induced by charge separation and a double layer structure known as a *laser piston* is formed, figure 1(c). For non-relativistic ions, the resulting ion energy scales as $\mathcal{E}_{\text{HB}} \propto a_0^2 / \bar{n}_0$, where \bar{n}_0 is the normalized electron plasma density, and thus there has been considerable interest in operating HB as close to the threshold density for RSIT as possible [15, 24, 37, 38].

In this work we show that the transition from the RSIT to the HB regime is associated with a much richer dynamical behavior than previously reported, owing to the complex interplay of fast electron generation and ion motion. In order to characterize the regime of interaction we perform a parametric scan in the a_0-n_0 plane and study signatures of RSIT in section 2. In contrast to previous studies [15], which characterize the regime of interaction in the asymptotic, long time limit, we do consider the full time evolution, including transient dynamics. This is particularly important in the mobile ion case and it allows us to uncover a new *dynamic transition* regime in which the transition from RSIT to HB occurs dynamically, i.e. during the course of

interaction. In order to understand the exact mechanism we develop a dynamical systems description based on the effect of ion motion on electron phase-space separatrices in section 3. It is shown that the time scale over which ion becomes important is much shorter than usually anticipated leading to a dependence of the transition threshold on the ion charge-to-mass ratio. Moreover, the dynamic transition regime is shown to strongly depend on kinetic effects developing in the early stage of interaction and can be controlled by varying the temporal profile of the laser pulse. The importance of studying transient effects is emphasized by comparing ion spectra in the conventional near-critical HB regime and the dynamic transition regime in section 4. In the latter case much smaller energy dispersion is observed. Finally, in section 5, we discuss the differences of the dynamic transition regime with some previously explored near-critical regimes of ion acceleration [15, 23, 24], and present our conclusions.

2. Detection of the transition threshold

The transition from the HB (opaque) regime to RSIT is investigated using 1D3P PIC simulations performed with the code EPOCH [39]. The (a_0 , n_0)-parameter plane was scanned to locate the transition threshold $n_{\rm th}$ for different values of the ion charge-to-mass ratio corresponding to hydrogen, helium and immobile ions, figure 2. The simulation box extends from x = -L up to x = L, where $L = 200\lambda_L$. The plasma fills half of the box with a constant electron density n_0 and a step-like plasma-vacuum interface. The initial electron and ion temperatures are $T_i = T_e = 5 \times 10^{-4} m_e c^2$. The plasma is irradiated by a CP laser pulse with normalized vector potential

$$a_{L}(x, t) = \frac{a_{0}}{\sqrt{2}} f(t) [\hat{y} \cos \xi + \hat{z} \sin \xi],$$
(5)

where $\xi = \omega_L t - k_L x$, $k_L = \omega_L/c$ and the envelope f(t) is a flat-top profile with a sin² ramp-up of duration τ_r figure 1(a). The pulse reaches the plasma at t = 0 and the total simulation time is $t_{sim} = 2L/c$. The spatial resolution is set to $\Delta x = 0.8\lambda_D$, where $\lambda_D = \sqrt{\epsilon_0 T_e/e^2 n_0}$ is the Debye length of the unperturbed plasma, the time-step is $\Delta t = 0.95\Delta x$ and 1000 macroparticles-per-cell have been used.

In order to determine the density threshold $n_{\rm th}$ between the two regimes of interaction, we examine two different time-series which are associated to either the velocity of the pulse front or the overlap of the laser pulse with the plasma electrons.

First, the pulse front position $x_f(t)$ is identified as the largest solution of $a(x_f, t) = a_0/2$ [15], where $a(x, t) = e|\mathbf{A}(x, t)|/(m_ec)$ is the normalized amplitude of the vector potential, see figure 1(c). The pulse front position moves deeper into the plasma at a velocity v_f that strongly depends on the interaction regime. In the opaque regime, which occurs for $n_0 > n_{\text{th}}$, propagation is dominated by transfer of momentum from the laser photons to the ions and v_f equals the so-called HB (or piston) velocity [30, 40]

$$v_{\rm HB} = c\beta_0 / (1 + \beta_0),$$
 (6)

where $\beta_0 = a_0 / \sqrt{2m_i n_{i0}} / (m_e n_c)$, m_i is the ion mass and n_{i0} is the ion plasma density. As outlined in the introduction, defining the RSIT regime is not straightforward when boundaries are involved. Here, we adapt the point of view of earlier works which associated the RSIT regime in the immobile ion case with the absence of a standing wave solution [11–14]. In the RSIT regime with mobile ions no double layer (relativistic piston) is formed and transfer of momentum to ions is minimal. This operating definition of RSIT for plasmas with an interface with vacuum implies deviations from the relativistic dispersion relation applicable in plasmas of infinite extent [6, 7]. Eventhough the energy balance has been invoked in a number of works in order to determine the front propagation velocity in the RSIT regime [41–43], no generally valid, closed-form solution exists [15, 43]. Therefore, in order to determine if the laser-front velocity v_f in mobile ion simulations corresponds to propagation in the RSIT regime we compare it with v_{SIT}^{∞} , the front velocity from immobile ion simulations with otherwise identical interaction parameters. For laser amplitudes in the range $5 \le a_0 \le 25$ that we study here, it is expected that $v_{SIT}^{\infty} > v_{HB}$ [15]. We thus anticipate that at the threshold density for the transition from HB to RSIT a discontinuous change of v_f occurs.

The second quantity on which we rely in order to distinguish between the opaque and transparency regimes provides a measure of the overlap of the laser pulse with plasma electrons. It is the *cross-correlation function*

$$S(t) = n_c^{-1} \lambda_L^{-1} \int_{-L/2}^{L/2} dx \ n_e(x, t) |a(x, t)|^2$$
⁽⁷⁾

introduced in [38]. In the HB regime the laser-pulse overlap with plasma electrons is limited to the electron skindepth [31, 38], see figure 1(c), and therefore S(t) is expected to remain approximately constant (and small) during the interaction. On the other hand, in the RSIT regime we expect S to increase linearly with time as the laser-pulse propagates deeper into the plasma at the constant velocity v_f .

With these two methods we can numerically determine the density threshold $n_{th}(a_0)$ that delineates the HB $(n_0 > n_{th})$ from the RSIT $(n_0 < n_{th})$ regime. We begin with the case of a hydrogen plasma and a pulse with



Figure 3. (a) Pulse front position $x_f(t)$ for $a_0 = 10$, $\tau_r = 4\tau_L$ and different densities, $n_0 = 2.6$, 2.8 and 3.3 n_c (RSIT, dynamic transition and HB regime, respectively). The upper and lower straight solid lines correspond to front propagation with $v_{\text{SIT}}^{\text{ST}}$ (with $n_0 = 2.6 n_c$) and v_{HB} (with $n_0 = 3.3n_c$), respectively. (b) Cross-correlation function S(t) for the simulations of panel (a).

 $a_0 = 10$ and ramp-up time $\tau_r = 4\tau_L$, where $\tau_L = 2\pi/\omega_L$. In figures 3(a) and (b), we plot as a function of time and for different n_0 the position of the pulse front x_f and the cross-correlation function S, respectively. For $n_0 = 3.3$, we observe that, after an initial stage of duration $\simeq \tau_r$ during which a partially standing wave [44] is formed, the front propagation velocity reaches a constant value $v_f = 0.08 c$. This matches very well the analytically predicted HB velocity $v_{\text{HB}} = 0.083 c$. Moreover, S remains approximately constant for $t > \tau_r$. This is characteristic of the HB regime, in which the overlap of the laser pulse with plasma electrons is limited to the skin depth [38].

For $n_0 = 2.6n_c$ on the other hand, the pulse front propagates with a velocity which at large times approaches the constant value $v_f = 0.24 c$, figure 3(a). This is much higher than $v_{HB} = 0.09$ and very close to $v_{SIT}^{\infty} = 0.23 c$ obtained by performing a simulation with immobile ions and identical interaction parameters. This shows that this regime of propagation is indeed dominated by electron motion effects. In addition, *S* increases approximately linearly after $t = \tau_r$. This implies that the laser overlap with plasma electrons increases with time as expected in the RSIT regime [38].

For intermediate densities, between these two clearly defined regimes of propagation, we observe a behavior that has not been identified before. As an example, we show in figure 3 the case $n_0 = 2.8n_c$ for which the pulse front propagates initially with a velocity $v_f = 0.11 c$ larger than $v_{\text{HB}} = 0.09 c$ until up to approximately $t \sim 9\tau_L$. After this time the front velocity changes abruptly and matches closely the HB velocity. The change in velocity between the initial and final stages of propagation is subtle, and thus it is essential to also examine S(t). In figure 3(b) we see that during the initial stage S grows linearly, as is typical of the RSIT regime. However, for $t > 9\tau_L$ this growth saturates and an almost constant value of S is reached, as is typical of the HB regime. This demonstrates the existence of a dynamic transition from RSIT to HB.

In order to check the applicability of these results beyond the specific case studied so far, we performed a parametric scan for the transition threshold in the (a_0-n_0) plane for immobile ions, helium and hydrogen. The results are summarized in figure 2, in which the extent of the error-bar indicates the extent of the dynamic transition regime. We observe that RSIT occurs at much lower densities for mobile than for immobile ions. Moreover, we see that the transition to RSIT occurs at lower density for ions with higher charge-to-mass ratio, as

also observed in previous numerical simulations [15]. We note that for mobile ions the transition occurs below the cold fluid theory threshold n_{SW} for existence of a standing wave with immobile ions [11, 12], shown as a red solid curve in figure 1(b). These observations suggest that we need to study the interplay of kinetic effects and ion motion in order to gain a qualitative understanding of the transition mechanism, a task that will be pursued in section 3.

3. Importance of kinetic and finite ion mass effects

3.1. Phase-space separatrices

As we will show, the transition to RSIT is in large part determined by laser energy absorption, which in nearcritical plasmas can be significant even with CP pulses [13, 41, 42, 45]. During the early stage of the interaction the ponderomotive force of the laser pulse accelerates electrons deeper into the plasma, until it is shielded by an electron density spike and wavebreaking occurs. Some of the accelerated electrons are trapped in the potential well formed by the combination of the ponderomotive and electrostatic potentials. The exact mechanism of plasma heating is highly involved and a detailed model is still lacking. Here we will show that we can gain insight into kinetic effects despite the lack of a model of electron heating by using topological information encoded in distinguished trajectories in single-electron phase-space. In the case of immobile ions the escape of electrons from single-particle separatrices at the plasma-vacuum interface was shown to be responsible for transition to RSIT [13]. In particular, it was demonstrated that the width of these separatrices decreases with decreasing density n_0 . Below a certain density n_0 , finite amplitude perturbations in longitudinal momentum p_x can then lead to electron escape to the vacuum, lowering the electrostatic field. Then the ponderomotive force prevails and pushes the electron front deeper in the target. This cycle repeats allowing laser pulse penetration in the target.

For the case of mobile ions the situation is more involved since the transient nature of ion motion during the early stages of the interaction implies that well-defined separatrices may not exist. In order to make progress we assume that such separatrices between escaping and confined trajectories do exist over the electron time-scale and verify this assumption *a posteriori*. In particular, we transform the single-electron Hamiltonian

$$H(x, p_x, t) = m_e c^2 \sqrt{1 + a(x, t)^2 + p_x^2 / m_e^2 c^2} - e\phi(x, t)$$
(8)

to a frame moving with the instantaneous front velocity v_f . Here, $\phi(x, t)$ is the instantaneous scalar (electrostatic) potential and p_x is the electron momentum. The Lorentz transformed Hamiltonian reads

$$H' = \gamma_f [H - \nu_f p_x], \tag{9}$$

with $\gamma_f = (1 - v_f^2/c^2)^{-1/2}$ (where a prime denotes a Lorentz-transformed coordinate). The potentials and front velocity v_f are determined from our PIC simulations. We assume that in the frame moving with velocity v_f a quasi-steady state of equilibrium between the ponderomotive and electrostatic force has been reached. In particular, we assume that the variation of the potentials due to ion motion is slow compared to the typical time-scale for electron motion and thus, H' can be treated as time-independent. Although we plot contours of H' both in and out of the plasma, we are interested in their form in the charge separation layer, where fast electron dynamics have small effect on the fields [13].

Separatrices are associated with saddle type (unstable) equilibria of the equations of motion (referred to as X-points). Taking into account Hamilton's equations, the equilibrium condition is written $\dot{x}' = \partial H'/\partial p'_x = 0$, $\dot{p}'_x = -\partial H'/\partial x' = 0$. The separatrices for electron motion are determined as iso-contours of H' associated with its local minima. Distinguishing saddle (unstable) from center (neutrally-stable) equilibria would involve examining second derivatives of H'. However, for our purposes, the distinction will be clear by inspection of phase-space plots. Examples of separatrices are plotted in figure 4, which will be discussed in detail in section 3.2. The critical momentum magnitude $|p_x^{cr}|$ is defined as the minimum momentum that an electron at the plasma boundary must have in order to escape to the vacuum. In the immobile ion case it is equal to the momentum an electron initially placed at (the vicinity of) the X-point gains by the time it crosses the plasma boundary x_b [13].

3.2. Effect of ion charge-to-mass ratio: a case study

We begin by examining the effect of ion charge-to-mass ratio on the dynamics in the total-reflection regime. In figure 4 we show the electron phase space from simulations for $n_0 = 4.5 n_c$, $a_0 = 10$, $\tau_r = 4 \tau_L$ for the cases of hydrogen, helium and immobile ions. These parameters were chosen so that all three cases correspond to the opaque regime. We show snapshots at $t = 5\tau_L > \tau_r$ so that the flat-top part of the pulse has reached the target. We choose to compare the phase space at this early stage of interaction because, as will become evident in the following, this is when the transition to RSIT is determined. We find that there are no significant differences in the width of the electron distribution close to the plasma-vacuum interface at this stage. This shows that any





differences in electron heating due to laser pulse energy being expended in ion motion are minimal and cannot explain the difference in transition threshold.

Figure 4 allows us to confirm that the electrostatic field is perturbed (compared to the immobile ion case) due to ion motion already at this early stage. The reduction in the electrostatic field in the charge separation layer (more visible for hydrogen, figure 4(c)) is larger at the position of the *X*-point x_X rather than at the position of the electron front x_f . This is due to the fact that the perturbation in ion density depends both on the magnitude of the electrostatic field and on the time over which it acts on ions. Before ion motion becomes important, the field increases approximately linearly with x,

$$E_x/E_c = \overline{n}_0 k_L x \qquad 0 < x < x_b, \tag{10}$$

with $E_c = m_e c \omega_L/e$ the so-called Compton field. Moreover, since it takes a finite time for the charge separation layer to be setup, the time over which an ion is accelerated decreases with its initial position x. As a result, ions close to the plasma boundary $x_b \simeq x_f$ did not yet have enough time to respond and the difference in the position of the front x_f between the mobile and immobile ion cases is negligible. On the other hand, the position of the X-point is determined by the balance of the ponderomotive and electrostatic force. Due to the reduction of the electrostatic field in the middle of the charge separation layer, a new equilibrium is reached at a position where the magnitude of the ponderomotive force is smaller, i.e., the X-point x_X is moved towards the left where the slope of |a| is smaller, see figure 4. At the same time the magnitute of critical momentum for escape to vacuum (the separatrix width) becomes larger as the distance of x_X and x_b increases. To understand this qualitatively, note that a test electron with small positive initial momentum placed at x_X will gain a net momentum (approximately equal to the critical momentum magnitude $|p_x^{cr}|$) while moving up to x_b , since the ponderomotive force is larger than the electrostatic force for $x_X < x < x_b$. In the mobile ion case the same electron would experience a larger average accelerating force (due to the reduction in electrostatic field) for a larger distance (due to the increase in $x_b - x_X$) therefore gaining larger net momentum.

3.3. Time-scale for ion motion

Let us now give an estimate for the time-scale over which ion motion becomes important in the sense that it can affect the electron dynamics close to the interface $x \sim x_f$. Naively, an estimate could be provided by $2\pi\omega_{pi}^{-1}$, where $\omega_{pi} = \sqrt{Z^2 e^2 n_{0i}/(\varepsilon_0 m_i)}$ is the ion plasma frequency, $n_{0i} = n_0/Z$ is the ion number density, *Z* is the atomic number of the ion species, and m_i is the ion mass. For a typical case of hydrogen with $n_{0i} = n_0 = 3$, we find $2\pi\omega_{pi}^{-1} \simeq 25\tau_L$. This appears to be too large to affect the transition dynamics according to the timeframe implied by figure 3.

The main problem with the above estimate is that it does not depend on the laser strength a_0 , since it does not take into account that transient ion motion can occur in the strong electrostatic field of order $\sqrt{2} a_0 E_c$ set up by the laser pulse ponderomotive force. This is particularly important here, since figure 4 shows that a relatively small change in the electrostatic field E_x can lead to change in critical momentum for escape of the order of $m_e c$. Indeed, as we are here investigating the effect of ion motion on the electron dynamics, we can anticipate that a change in electric field of the order of E_c (the typical field for relativistic electron effects), could lead to qualitative changes in dynamics despite the fact that the maximum unperturbed field is many orders of magnitude larger



Figure 5. Evolution of the local electrostatic field E_x for the PIC simulations of figure 4 ($n_0 = 4.5n_c$, $a_0 = 10$, $\tau_r = 4\tau_L$) for three different positions in the charge separation layer $x_* = 0.3$, the *X*-point x_X and the electron layer boundary x_b . Dashed horizontal lines indicate the theoretically predicted value for the maximum electrostatic field for each *x*, according to equation (10). The solution of equation (15) for $E_x(x, t)$ for each case is shown as a red, dashed curve. The initial time t_0 corresponds to the time, for each *x*, for which the electrostatic field assumes its maximum value.

than this. We will now develop a simple model for the transient ion response at the early stage of interaction in order to estimate the time required for a change in electric field of order E_c to occur.

In order to obtain an upper bound for the response time of the ions we model the interaction as a two stage process [46]. Initially the electrons are pushed by the ponderomotive force and a charge separation layer is formed. The resulting electrostatic field is a linear function of the space coordinate *x*, as described by equation (10). At a second stage, ions are accelerated in this electrostatic field. Since it takes a finite time to setup the charge separation layer, ions with smaller *x* are accelerated for a longer time (but experience a smaller electric field). Treating the ions as a cold fluid, we write the ion momentum equation as

$$m_i n_i \frac{\partial V_i}{\partial t} + m_i n_i V_i \frac{\partial V_i}{\partial x} = q_i n_i E_x(x, t), \qquad (11)$$

where $V_i(x, t)$ is the ion fluid velocity. We let $t_0 = t_0(x)$ denote the time at which the charge separation 'front' sweeps point x, and the field takes the value predicted by equation (10), i.e. the plateau in figure 5(a) is reached. The ions are assumed initially at rest, $V_i(x, t_0) = 0$, and we consider short enough evolution times that we may linearize equation (11) and drop the term $V_i \partial_x V_i$. For the same reason we also ignore relativistic ion effects. Even though the ions obtain finite momentum at early times, their density response is expected to be minimal and, since we are only interested in obtaining an upper bound on the characteristic time for ion motion to affect the electron dynamics, the effect of ion density variations in the electric field (through Poisson's equation) will not be considered. Under these assumptions, we only need the longitudinal component of Maxwell–Ampere's equation to close the model,

$$j_x = -\epsilon_0 \frac{\partial E_x}{\partial t}.$$
(12)

In the charge separation layer there are no electrons, so that $j_x = q_i n_i V_i$. Substituting equation (12) in the linearized version of equation (11) we obtain

$$\frac{\partial^2 V_i}{\partial t^2} = -\omega_{pi}^2 V_i. \tag{13}$$

This has the solution

$$V_i(x, t) = \frac{q_i}{m_i \omega_{pi}} E_x(x, t_0) \sin[\omega_{pi}(t - t_0)],$$
(14)

where for each *x*, $E(x, t_0) = \overline{n}_0 k_L E_c x$ from equation (10) is taken as initial condition and we have enforced consistency of $\partial_t V_i|_{t=t_0}$ with equation (11). Taking into account equation (14), the solution of equation (12) can be written

$$E_x(x, t) = E(x, t_0) \cos[\omega_{pi}(t - t_0)].$$
(15)

For $a_0 \gg a_b \gg 1$ we have that [13] $k_L x_b \simeq \sqrt{2} a_0 / (\overline{n}_0)$ and thus $E_x(x_b, t_0) \simeq \sqrt{2} a_0 E_c$. From equation (15) we find that an $\mathcal{O}(E_c)$ change in the electric field at x_b , $\Delta E_x \simeq -E_c$, occurs at a timescale



Figure 6. HB regime simulation ($n_0 = 3.3n_c$, $a_0 = 10$, $\tau_r = 4$, hydrogen): electron and ion density, electric field and vector potential amplitude for (a) $t = 5\tau_L$ and (b) $t = 15\tau_L$. Electron distribution fuction $f(x, p_x, t)$ and iso-contours of H' (black, solid lines), including the separatrices (red, dashed lines) in the lab frame for (c) $t = 5\tau_L$ and (d) $t = 16\tau_L$.

$$\tau_{i} = \frac{g(a_{0})}{\omega_{pi}} = g(a_{0}) \sqrt{\frac{A \ n_{c} \ m_{p}}{Z \ n_{0} \ m_{e}}} \tau_{L},$$
(16)

where

$$g(a_0) = \arccos\left(1 - \frac{1}{\sqrt{2}a_0}\right).$$

We note that equation (16) is derived under the assumption of a large initial electric field. It is valid only in the limit $a_0 \gg a_b \gg 1$, and becomes singular for $a_0 < 1/(2\sqrt{2})$. For completeness, we mention that in the large density regime, $n_0 \gg a_0^2$, the maximum electrostatic field at x_b scales as [13] $E_{x,\max}/E_c \simeq 2a_0^2/\overline{n}_0^{1/2}$ and a different limiting behavior can be derived, $g(a_0) = \arccos(1 - \overline{n}_0^{1/2}a_0^{-2}/2)$.

Figure 5 shows the evolution of the electrostatic field in the initial phase of the interaction for the three cases of figure 4 and for three different positions in the charge separation layer $x_* = 0.3$, the X-point x_X and the electron density boundary x_b . We see that the solution of equation (15) for $E_x(x, t)$ (red, dashed curve) agrees well with the simulations for smaller x, while for larger x the observed change in E_x is faster than predicted by equation (15). This is because we did not take into account the fact that ions will start to move even before the field reaches the value predicted by equation (10). Indeed, as seen in figures 5(b) and (c), the time interval during which the electric field rises is finite and increases with the position x. Although we could, in principle, account for this by solving equation (13) with initial condition $V_i(x, t_0) \neq 0$, we will not pursue this here since we are only interested in obtaining an estimate. Moreover, in the above derivation, we did not take into account the effect of ion density variation. At later times, this leads to deviation from the sinusoidal behavior predicted by equation (15). However, even in the worse case scenario of figure 5(c) this only occurs after a change of order E_c in E_x has taken place. Therefore, equation (16) constitutes a useful upper bound for the time-scale at which ion motion becomes important in our problem. For the case of helium (hydrogen) with $n_0 = 4.5n_c$ and $a_0 = 10$, equation (16) predicts a change in electric field of the order of E_c at time $\tau_i = 1.7\tau_L$ ($\tau_i = 1.2\tau_L$) after the time $t_0 = 4.1\tau_L$ at which the charge separation layer has been set up at the X-point (found from the PIC simulations, see figure 5). Although this is still a conservative upper bound, it matches much better the results of figures 4(b) and (c) than the naive scaling $2\pi\omega_{pi}^{-1} = 28 \tau_L$ and $20 \tau_L$ obtained for helium and hydrogen, respectively.

3.4. Transition to relativistic self-induced transparency

In order to establish the connection of the separatrix width to the transition to RSIT, we now concentrate in the case of a hydrogen plasma and reduce the density, compared to figure 4(c), to the lowest possible density $n_0 = 3.3 n_c$ for which dynamics is still in the HB regime. In figure 6 we show, for two different times $t = 5\tau_L$ and $t = 15\tau_L$, the results of a simulation with $a_0 = 10$, $n_0 = 3.3 n_c$. For these parameters cold fluid theory with immobile ions predicts that no standing wave solution exists and electrons from the dense electron layer would be able to escape to the vacuum leading to RSIT according to the scenario in [13, 14]. However, we see in figure 6(c) that due to ion motion a separatrix merely wide enough that no electrons escape to the vacuum during the initial stage of the interaction exists. The separatrix width is smaller than in the case $n_0 = 4.5n_c$ of



Figure 7. RSIT regime simulation ($n_0 = 2.6n_c$, $a_0 = 10$, $\tau_r = 4$, hydrogen): electron and ion density, electric field and vector potential amplitude for (a) $t = 5\tau_L$ and (b) $t = 15\tau_L$. Electron distribution function $f(x, p_x, t)$ and, when applicable, iso-contours of H' (black, solid lines), including the separatrices (red, dashed lines) in the lab frame for (c) $t = 5\tau_L$ and (d) $t = 16\tau_L$.

figure 4 because it takes longer for ion effects to become important in this case of lower density (according to equation (16), $\tau_i = 1.4\tau_L$). With time, a double layer is formed and propagates deeper into the plasma as a laser piston (figures 6(b) and (d)). At this stage the separatrix becomes wider in p_x as ions catch up with the electrons, reducing the charge separation induced electrostatic field. This contributes to the stability of the HB process as electrons cannot escape at this point.

We next examine typical dynamics in the RSIT regime, i.e., at lower density ($a_0 = 10$, $n_0 = 2.6 n_c$, figure 7). Lowering the density further decreases the effect of ion motion, $\tau_i \simeq 1.6$, preventing the plasma to reach a quasistatic state which could trap electrons. As electrons escape, the space-charge is largely reduced and the ions remain essentially immobile during the course of the simulation. Therefore, the immobile ion results apply: the interaction is in the RSIT regime since $n_0 < n_{SW}$ [11–14]. Since the quasi-static approximation does not hold in this case, we do not plot separatrices in figure 7. However, we note that the fact that electron escape in the PIC simulations occurs for all values below $n_0 = 3.3$ for which the separatrix (figure 6(c)) was marginally wide enough to prevent electron escape justifies using the Lorentz-transformed Hamiltonian in order to define separatrices of confined and escaping electrons. We note that laser propagation in this RSIT regime is not associated to the destruction of the electron density peak; the latter remains higher than the threshold n_c^{eff} predicted by equation (1), see figure 7(b). Rather, while some electrons are pushed into the plasma, other electrons continuously escape in the region where they interact with the laser-pulse through a mechanism akin to beatwave heating [45]. We thus conclude that, as in the case of immobile ions [13], electron escape drives transition to RSIT.

For intermediate densities $2.7 < n_0/n_c < 3.3$ between the hole boring and RSIT regimes we find the dynamic transition regime. As an example we see in figure 8 that for $a_0 = 10$, $n_0 = 2.8n_c$ electrons are initially escaping (panels (a) and (c)). The estimate for the ion response time, $\tau_i \simeq 1.5$, is slightly smaller than in the RSIT case, while at the same time the RSIT velocity v_{SIT}^{∞} decreases with the density [13, 15]. Therefore ions in the charge separation layer gain enough momentum to catch up with the electron front. This leads to the eventual formation of a piston and of a potential well in which electrons are trapped (panels (b) and (d)). Electron escape then saturates and the subsequent dynamics are of the HB type.

For completeness, we note that for even larger laser field amplitudes ($a_0 \ge 20$), interaction in the dynamic transition regime can be even more complex and a transition may also occur in the reverse direction, from HB to RSIT, since electrons accelerated by the beatwave heating mechanism [45] can re-enter the plasma and destabilize the relativistic piston.

4. Effect of laser envelope on the transition threshold and ion energy distribution

4.1. Effect on the transition threshold

Since kinetic effects in the early phase of interaction play an important role in the transition between the different regimes, we can, to some extent, control the transition by varying the shape of the laser pulse. The ponderomotive force associated to a pulse with a shorter rise-time is larger than for one with a longer rise-time and this is expected to lead to stronger electron heating in the former case [42]. In order to illustrate this, we



Figure 8. Dynamic transition regime simulation ($n_0 = 2.8n_c$, $a_0 = 10$, $\tau_r = 4$, hydrogen): electron and ion density, electric field and vector potential amplitude for (a) $t = 5\tau_L$ and (b) $t = 15\tau_L$. Electron distribution fuction $f(x, p_x, t)$ and iso-contours of H' (black, solid lines), including the separatrices (red, dashed lines) in the lab frame for (c) $t = 5\tau_L$ and (d) $t = 16\tau_L$.

choose fixed values of $a_0 = 10$ and $n_0 = 2.7n_c$ and perform simulations with different pulse rise-times, $\tau_r = 4$, 7 and $12\tau_L$.

In figure 9 we show that for the shortest value $\tau_r = 4\tau_L$ the pulse propagates in the RSIT regime, while as τ_r increases to $\tau_r = 7\tau_L$ and $\tau_r = 12\tau_L$, the dynamic transition and HB regimes are reached, respectively. The relation of this effect to electron heating is illustrated in figure 10(a), where the electron spectra are compared at an early interaction time, $t = 4.4 \tau_L$, before electrons escape in any of these cases. We find that electron spectra in the case of shorter rise-time are broader than for longer rise-times, showing that electron heating indeed occurs at a higher rate for the pulse with shorter rise time τ_r . Moreover, it was verified by plotting the electron separatrices (not shown) that the transition mechanism is identical to the one described above. In the case of $\tau_r = 4\tau_L$ the stronger electron heating leads to electron escape and triggers RSIT. For $\tau_r = 12\tau_L$ no electrons gain enough momentum to escape to the vacuum and we have HB. Finally, for $\tau_r = 7\tau_L$ some electrons escape but eventually ion response leads to a dynamic transition to HB.

4.2. Effect on the ion energy distribution

In either the case of $\tau_r = 7 \tau_L$ (dynamic transition) or $\tau_r = 12 \tau_L$ (HB) the long time dynamics corresponds to HB. It is therefore worth asking whether there are any differences in ion spectra in these cases. The ion spectra at $t = 200 \tau_L$ are shown in figure 10(c). We observe that in the HB regime ($\tau_r = 12\tau_L$) the spectrum has a multipeak structure around the HB energy $\mathcal{E}_{HB} = 15.8$ MeV. By contrast, for a typical simulation in the dynamic transition regime ($\tau_r = 7 \tau_L$ and all other parameters kept unchanged), we see in figure 10(c) that the spectrum has a much lower energy spread. The peak energy $\mathcal{E} \simeq 15.6$ MeV is very close to the analytical prediction for HB, $\mathcal{E}_{HB} = 15.8$ MeV, and the energy spread (1 MeV or 6% FWHM) is much smaller than in the pure HB regime for $\tau_r = 12\tau_L$ (correspondingly, $\mathcal{E} \simeq 16.3$ MeV, and energy spread of $\simeq 5$ MeV or 30% FWHM).

To explain the differences in the ion spectra, one has to examine into more detail the dynamics of the double layer structure. Indeed, the broadening of the spectrum in the conventional HB regime is usually attributed to large amplitude periodic oscillations of the double layer, known as piston oscillations [31, 32, 40]. These oscillations are illustrated in figure 12(a) (for the conventional HB case ($\tau_r = 12\tau_L$)), where large scale ($\Delta E_{x,\max}/E_{x,\max} \simeq 0.3$) periodic fluctuations are observed in the temporal evolution of the maximum value electrostatic field. These oscillations result in ions being reflected at different phases of the oscillating piston and therefore accelerated to different energies as described in [40], thus leading to ion bunching and modulation of the ion beam in x - p, phase space, sometimes referred to as 'rib-cage' structure, and illustrated in figure 11(b).

Although the exact mechanism behind these oscillations is still largely not understood, e.g. no model yet describes the time at which they set in nor why they appear, one can still get a deeper understanding of how they proceed by examining more closely the time evolution of the maximum values of the electrostatic field and electron/ion densities, as shown in figures 12(a)–(c).

The following discussion focuses on non-relativistic HB velocities, and builds on the previous analysis of piston oscillations as a three-step process presented in [31], where the piston structure was also described within the framework of stationary cold fluid theory.





In a first stage (region I in figures 12(a)-(c)), an ion bunch is formed in the charge separation layer close to the laser front, associated with an increase of the maximum ion density as shown in figure 12(b). This can be seen more clearly in the supplemental movie 1 available online at stacks.iop.org/NJP/19/123042/mmedia.

In a second stage (region II in figures 12(a)–(c)), this ion bunch crosses the charge separation layer and is launched into the plasma. This results in the abrupt decrease of the electrostatic field evidenced in figure 12(a). Note that stage I and II are characterized by the maxima of ion and electron density as well as electric field being in a very close vicinity (supplemental movie 1). Furthermore, ion bunches launched into the target during the second stage have a velocity $\sim 2\nu_{\text{HB}}$. This can be seen in figure 12(c) where the velocity computed from the position of the maximum ion density is about twice that computed from the maximum electron density moving at ν_{HB} (note that the discontinuity in the position of the maximum ion density occurs when the ion bunch launched into the target becomes more dense than the the ion density peak in the charge separation layer and vice versa).

The characteristic time for these two first stages is related to the thickness Δ_e of the compressed electron layer. As shown in [31], $\Delta_e \simeq c/\omega_{pe}$, and the duration of these first two stages is negligible with respect to the characteristic time of the piston oscillations.

Of particular importance is the third stage (region III in figures 12(a)–(c)), during which not yet reflected ions move deeper into the charge separation layer, thus increasing the charge imbalance and enhancing the electrostric field as observed in figure 12(a). The rate of increase of the electrostatic field can be estimated from Ampère's equation as $dE_x/dt \sim Zen_{i0}v_{\rm HB}/\epsilon_0$, and the characteristic duration of this stage is $\tau_3 \simeq 2\Delta_i/v_{\rm HB}$, where Δ_i is the width of the charge separation layer. The latter can be estimated from the piston model proposed in [31] as $\Delta_i \simeq v_{\rm HB}/(3\omega_{pi})$, for $v_{\rm HB} \ll c$. This leads $\tau_3 \sim 2/(3\omega_{pi})$, much larger than the characteristic duration of the first two stages ($\infty \omega_{pe}^{-1}$) so that the characteristic duration of an oscillation is $\tau_{\rm osc} \sim \tau_3 \simeq \omega_{pi}^{-1}$. The total increase of the electrostatic field during this stage can then be computed as $\Delta E_x \sim 2 Zen_{i0}v_{\rm HB}/(3 \epsilon_0 \omega_{pi})$ $\simeq \frac{\sqrt{2}}{3} a_0 m_e c\omega_0/e$. Recalling that the (normalized) maximum electrostatic field is $eE_{x,\max}/(m_e c\omega_0) \simeq \sqrt{2} a_0$, one then finds that the relative amplitude of the electrostatic field oscillations are of the order $\Delta E_x/E_{x,\max} \simeq 1/3$.



Figure 10. Energy spectra for $a_0 = 10$, $n_0 = 2.7 n_c$ and different rise-times $\tau_r = 4 \tau_L$ (RSIT), $\tau_r = 7 \tau_L$ (dynamic transition regime) and $\tau_r = 12\tau_L$ (HB). (a) Electron spectra for electrons with $x > x_f$ obtained at $t = 4.4 \tau_L$, (b) same as above but for at $t = 200 \tau_L$ and (c) spectra for ions with $p_x > 0$ obtained at $t = 200 \tau_L$.

This simple estimate turns out to be in very good agreement with our numerical simulations, for example for figure 12(a) we find $\Delta E_{x,\max}/E_{x,\max} \simeq 0.3$. It is also confirmed by all our simulations performed in the pure HB (near critical) regime where piston oscillations have been observed, all of them exhibiting oscillations $\Delta E_x/E_{x,\max} \sim 0.3$, independently of the initial plasma density n_0 and laser field amplitude a_0 .

This three-step process suggests that, to set in, piston oscillations require a clear separation between the ion and electron layers, so that the third stage lasts long enough for the electrostatic field perturbation to build up. While this is the case in most of our pure HB simulations, this clear separation does not hold when considering the dynamic transition regime (for $\tau_r = 12\tau_L$). In that case indeed, some of the electrons that escape into the



vacuum during the initial stage interact with the standing wave and form energetic bunches through beatwave heating [45]; they then return to the plasma leading to enhanced electron heating by beam-plasma instabilities, see figure 10(b), where electron spectra are plotted at late interaction time $t = 200\tau_L$, figure 11 and supplemental movie 2. This electron heating actually prevents the formation of the double layer with clearly separated ion and electron layers, as can be seen in figure 11(b) for the dynamic transition regime, in contrast with figure 11(a) for the pure HB regime. This henceforth prevents piston oscillations to set in, as is confirmed in figures 12(b), (d) and (f) where none of the three stages discussed for the pure HB case are observed. In that case indeed some residual oscillations in the maximum electrostatic field, albeit with a decreased amplitude $\Delta E_{x,max}/E_{x,max} \simeq 0.15$, can be observed. Their irregular nature prevents a strong imprint on the ion energy spectrum as they cannot not coherently contribute to acceleration or deceleration of the fast ions around their mean velocity, see figure 11, and explains the smaller energy spread in the fast ion spectrum observed in figure 10(c).

As a result, operating in the dynamic transition regime may allow to produce ion beams via HB with a low energy spread. In contrast to operating in the pure HB regime at lower intensity (or conversely larger density), a situation which has been shown not to be prone to piston oscillation [31], small energy dispersion is here obtained without sacrificing mean energy.

Let us finally note that the effect of electron heating to prevent piston oscillations was also discussed in a previous work [47]. In that case however, the authors relied on the use of elliptically polarized light to allow for electron heating to set in.

5. Discussion and conclusions

Before concluding on this work, we wish to briefly stress that various ion acceleration mechanisms have been identified in near-critical plasmas, which are clearly different from the ion acceleration process in the dynamic transition regime discussed here. At the boundary of the RSIT regime $n_0 \simeq n_{\text{th}}$ an energetic ion bunch can be formed and accelerated to energies much higher than expected from a pure HB scenario, as discussed in [24]. In [15] an incomplete HB regime has been reported, which occurs for much larger intensities ($a_0 \simeq 100$) when



Figure 12. Difference in piston oscillations for simulations with hydrogen and $a_0 = 10$, $n_0 = 2.7 n_c$ for the two values of the rise time $\tau_r = 12\tau_L$ (HB, left column) and $\tau_r = 7\tau_L$ (dynamic transition regime, right column). (a), (d) Maximum longitudinal electric field $E_{x,\text{max}}$ normalized to the Compton field $E_c = m_e c \omega_L/e$ versus time. (b), (e) Maximum density $n_{s,\text{max}}$ for electrons (solid lines) and ions (dots). (c), (f) Position of the maximum of the density spike x_s for electrons (solid lines) and ions (dots).

 $v_{\text{SIT}}^{\infty} \simeq v_{\text{HB}}$. Finally, in the presence of a long enough pre-plasma, trace light ions can be accelerated by the charge separation field in the pre-plasma [23, 48]. In all these regimes ion spectra scale differently than those obtained in the dynamic transition regime, which follows the usual HB scaling.

To conclude, we have studied the transition from the opaque (HB) to a transparent (RSIT) regime in the interaction of relativistic laser pulses with plasmas using a combination of PIC simulations and Hamiltonian dynamics. The transition to RSIT is found to be linked to an instability of the plasma-vacuum interface triggered by fast electron generation during the early stages of the interaction, as revealed by studying single-electron separatrices. Remarkably, this instability can be saturated by an ion-motion-induced deepening of the trapping potential at the plasma boundary. We therefore find that ion motion is involved in a transition which is commonly thought of as a purely electron effect. As shown in section 3, this occurs because the strong electrostatic field $E_{x,\max} \propto a_0$ at the charge separation layer causes ion response on a time-scale shorter than the naive $2\pi\omega_{pi}^{-1}$ estimate. An upper bound for this time-scale which depends on both ω_{pi} and, importantly, on a_0 has been derived.

We showed that transient effects are important and identified a new dynamic transition regime from RSIT to HB. Surprisingly, the short, transient RSIT phase in this regime has a long-lasting impact on the properties of the accelerated ions. HB spectra in near critical plasmas suffer from broadening due to periodic piston oscillations. We analyzed these oscillations for non-relativistic HB as a three-step process and estimated the electric field oscillation amplitude to be approximately 30%, independently of a_0 and n_0 , in very good agreement with PIC simulations. Enhanced electron heating in the dynamic transition regime prevents this three-step process from setting in, therefore ameliorating the effect of the oscillations on the ion spectrum. As a result an optimal ion spectrum is obtained both in terms of mean energy and energy spread.

The transition between the transparent and opaque regimes of interaction, and the dynamic transition regime in particular, are characterized by complex dynamics which have been here studied in a reduced 1D geometry. In realistic (3D) geometries, further complicating factors may play an interesting role. Transverse, instabilities developing at the laser-plasma interaction surface [30, 34, 49–51] can trigger additional electron heating [52, 53] thus modifying the threshold density in a complex way. It is therefore important that these 3D effects are taken into account in future works and that mitigation strategies for transverse instabilities relying, for

example, on tuning the laser polarization [54] or intensity profile [55] be employed. Recently developed optimization strategies drawing on the field of complexity science, such as those that rely on genetic algorithms to control adaptive optics [56], suggest that there is a potential to operate laser-driven ion acceleration in the dynamic transition regime despite the inherently complex dynamics at play.

These results are of fundamental importance for our understanding of relativistic laser-plasma interaction and for a wide-range of applications, from particle acceleration to fast ignition, as they open new paths, for example for the optimization of laser-driven ion beams.

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