# Uniform onset of the long proton bunch self-modulation seeded by an electron bunch in an overdense plasma

K. Moon<sup>®</sup>,<sup>\*</sup> E. S. Yoon, and M. Chung<sup>®†</sup> UNIST, Ulsan 44919, Republic of Korea

P. Muggli<sup>‡</sup>

CERN, 1211 Geneva, Switzerland and Max Planck Institute for Physics, 80805 Munich, Germany

M. Moreira

GoLP/Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, 1049-001 Lisboa, Portugal

### M. A. Baistrukov

Novosibirsk State University, 630090 Novosibirsk, Russia and Budker Institute of Nuclear Physics, 630090 Novosibirsk, Russia

(Received 16 June 2023; accepted 25 October 2023; published 14 November 2023)

The phase, growth rate, and onset of long proton bunch self-modulation in plasma can be controlled by a preceding short charged particle bunch. In this paper, by analyzing the growth rates of the self-modulation obtained from particle-in-cell simulation results, we identify two modes of self-modulation, namely noise-seeded and externally seeded self-modulations, and investigate their onset timings. We find that a uniform onset of the self-modulation at each slice of the long proton bunch is crucial for fine-tuning its phase and amplitude. We then demonstrate that a low-energy and low-current electron seed bunch in overdense plasma generates near-axis radial wakefields similar to those observed in the blowout regime. Consequently, the resultant self-modulation is excited as a single mode simultaneously along the entire long proton bunch.

DOI: 10.1103/PhysRevAccelBeams.26.111301

#### I. INTRODUCTION

Because of much higher stored energy than that of laser pulses and electron bunches, a proton bunch could be an effective driver to create plasma wakefields for compact electron acceleration [1–5]. The optimum bunch length for generating beam-driven plasma wakefields is on the order of the plasma skin depth  $k_{pe}^{-1} = (n_{pe}e^2/\epsilon_0m_ec^2)^{-1/2}$ , where  $n_{pe}$  is the ambient plasma electron number density, *e* the elementary charge,  $\epsilon_0$  the vacuum permittivity,  $m_e$  the electron mass, and *c* the speed of light in vacuum [6]. Hence, the rms length of the proton bunch currently available in most high-intensity accelerators (e.g.,

<sup>†</sup>mchung@unist.ac.kr

approximately 6 cm in CERN SPS) is too long to effectively generate plasma wakefields. However, the envelope of the long proton bunch can be self-modulated by the transverse component of its own plasma wakefields along the beam comoving frame coordinate  $\zeta = z - ct$ . The self-modulation process forms a train of microbunches with an initially constant separation of  $2\pi/k_{pe}$ , which resonantly drives plasma wakefields, increasing the amplitude of the wakefields close to the cold, nonrelativistic plasma wavebreaking limit  $E_0 = k_{pe} m_e c^2 / e$  [1]. This amplitude can be several orders of magnitude greater than that available in conventional accelerators. The self-modulation can grow from the inherent noise of the charged particle bunch [7] or can be seeded by controlling its characteristics. It was experimentally demonstrated that the self-modulation process can be seeded by a relativistic ionization front (RIF) [8] and also by a preceding electron bunch [5]. In this paper, we mainly focus on the features of the long proton bunch self-modulation seeded by an electron bunch.

Analytical theories for the self-modulation have been developed assuming a bunch with a constant density profile in transverse and longitudinal directions [1-3,9]. The theoretical model, expressing the bunch distributions in

<sup>&</sup>lt;sup>\*</sup>Present address: Pohang Accelerator Laboratory, Gyeongbuk 37673, Republic of Korea.

<sup>&</sup>lt;sup>‡</sup>muggli@mpp.mpg.de

Published by the American Physical Society under the terms of the Creative Commons Attribution 4.0 International license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

all directions as Heaviside step functions, is advantageous in explaining the main physics while simplifying the discussion. However, it is not suitable for predicting the growth rate of the self-modulation for bunches with Gaussian or parabolic distributions. If the proton bunch self-modulation is seeded by the wakefields driven by a preceding electron bunch, the parameters of the modulated long proton bunch and the seed driver are decoupled in the analytical description. Indeed, increasing the number of degrees of freedom yields new aspects of the selfmodulation. In Ref. [9], the contribution of the seed appears with different features at the front and back of the modulated long proton bunch. However, since the analytical solution in Ref. [9] was derived using terms only up to the second order of the series-expanded seed contribution, the amplitude of the seed wakefields could not be used to precisely determine the growth rate. To analyze recent proton beam-driven wakefield experiments, therefore, it is crucial to study the seeding mechanisms of the long bunch self-modulation in more detail, considering realistic bunch distributions and higher-order terms.

In order to explore the underlying physics of the long proton bunch self-modulation seeded by a short charged particle bunch in an overdense plasma, we estimate analytically and numerically its phase and growth rate. By assuming that the self-modulation process can be analytically expressed as the linear combination of noise-seeded and externally seeded self-modulations, and by fitting the analytical expression to the results of particlein-cell (PIC) simulations, we investigate for the first time the onset timings and mode composition of two modes of the long proton bunch self-modulation. Here, fitting coefficients of the two modes indirectly suggest the onset timings of noise- and externally seeded self-modulations. In this study, we call these two fitting coefficients "onset coefficients." The mode composition which is determined by the two onset coefficients depends on  $\zeta$  for a long bunch with a nonconstant current profile, in which the long bunch self-fields are non-negligible. Furthermore, the long bunch shot noise leads to the noisy onset timing of the self-modulation. The near-axis radial wakefields driven by a preceding short, low-current, and low-energy electron bunch quickly become close to those obtained in the blowout regime of the wakefield and therefore override the self-fields and noise of the long bunch at the onset stage of the self-modulation process. In this paper, we demonstrate that the electron bunch seeding introduces the features of uniform onset of the self-modulation, such that a single mode is excited simultaneously along the entire long proton bunch. The analytical approach shows reasonable agreement with simulation results from the FBPIC code [10].

For the system we are considering here, the changes in bunch energy and Coulomb scattering can be assumed negligible. The main factors influencing the envelope of the long proton bunch are its transverse momentum (emittance) and the wakefields generated by both the seed and the proton bunch itself. Therefore, the root mean square (rms) radius  $r_p$  of the long proton bunch can be described by the following envelope equation [11]:

$$\frac{d^2r_p}{dz^2} - \frac{\epsilon_{n,p}^2}{\gamma_p^2 r_p^3} = \frac{e}{\gamma_p m_p c^2 r_p} [\langle rW_{\perp s} \rangle + \langle rW_{\perp m} \rangle], \quad (1)$$

where  $\epsilon_{n,p}$  is the normalized emittance of the long proton bunch,  $\gamma_p$  is the relativistic factor,  $m_p$  is the proton mass, and  $\langle rW_{\perp} \rangle$  is the average of the wakefields weighted by the particle's radial position *r*. The force term on the right-hand side of Eq. (1) incorporates both the seed wakefields  $(W_{\perp s})$ and the self-wakefields of the long proton bunch  $(W_{\perp m})$ .

## II. ENVELOPE SELF-MODULATION SEEDED BY A HIGH-ENERGY PROTON BUNCH

We consider a system in which the plasma wakefields are initially driven by a short charged particle bunch and weakly modulate the envelope of a following long proton bunch. The two relativistic bunches are colinearly propagating in a quasineutral overdense plasma  $(n_{pe} \gg n_b)$ . Here,  $n_b$  is the bunch peak number density. It is thus assumed that the bunches perturb the plasma electrons with small oscillation amplitudes and the velocities of the perturbed plasma electrons are much smaller than the speed of light. With these assumptions, the magnetic field generated by the perturbed plasma current is negligible, and other perturbed physical quantities are taken up to first order. As a result, the linearized equation for the transverse plasma wakefield driven by a charged particle bunch is [9]

$$W_{\perp} = -\left(\frac{q}{e}\right) \left(\frac{n_{b}}{n_{pe}}\right) E_{0} k_{pe}^{3} \int_{\infty}^{\zeta} d\zeta' \sin[k_{pe}(\zeta - \zeta')] f_{\parallel}(\zeta') \\ \times \left[K_{1}(k_{pe}r) \int_{0}^{r} dr' r' I_{0}(k_{pe}r') f_{\perp}(r') - I_{1}(k_{pe}r) \int_{r}^{\infty} dr' r' K_{0}(k_{pe}r') f_{\perp}(r')\right],$$
(2)

where *q* is the charge of the bunch particle and  $f_{\parallel}(f_{\perp})$  is the longitudinal (transverse) profile of the bunch. We use the approximations for Bessel functions  $I_0(k_{pe}r') \approx 1$  for  $k_{pe}r' < 1$  and  $K_1(k_{pe}r) \approx 1/k_{pe}r$  for  $k_{pe}r < 1$  for the first term and ignore the second term at the right-hand side of Eq. (2), as in Refs [3,9]. This approximation is valid when most of the bunch particles are within  $k_{pe}r < 1$ .

A preceding, short proton bunch that has the same energy and initial rms radial size as the following long proton bunch can drive linear wakefields. Although such a short proton bunch is not available in actual experiments, it can mimic the RIF seeding [8] in the theoretical analysis, providing a similar radial profile and evolution time scale as the seed wakefield driven by the sharp rising proton bunch front interacting with the plasma [1,12]. Furthermore, the analytical approach used here can be applied similarly to the electron seed bunch case. Since the rms length of the preceding seed bunch  $L_s$  is on the order of  $k_{pe}^{-1}$ , the entire bunch is within the focusing phase of its driven plasma wakefield. The transverse wakefield behind a short Gaussian proton bunch is

$$W_{\perp s,p} = -A_{s,p}^{2} E_{0} \cos(k_{pe}\zeta + \phi_{s} + \pi/2) \\ \times \frac{k_{pe}r_{s}^{2}}{r} \left[1 - \exp\left(-\frac{r^{2}}{2r_{s}^{2}}\right)\right]$$
(3)

with

$$A_{s,p} = [(n_s/n_p)\sqrt{2\pi}k_{pe}L_s \exp\left(-k_{pe}^2L_s^2/2\right)]^{1/2}, \quad (4)$$

where  $A_{s,p}$  is the normalized amplitude of the wakefields driven by the proton seed bunch. Here,  $n_s$ ,  $r_s$ , and  $\phi_s = -k_{pe}\zeta_s$  represent the peak number density, rms radius, and phase of the proton seed bunch, respectively.

Since the following proton bunch is long  $(L_p \gg k_{pe}^{-1})$ , the radial wakefields along  $k_{pe}\zeta$  of the proton bunch alternately focus and defocus its envelope. Therefore, here, we do not treat the longitudinal and transverse integrations as separable [1–3]. The transverse wakefield from the modulated proton bunch on any slice  $\zeta$  is

$$W_{\perp m} = -\left(\frac{n_p}{n_{pe}}\right) E_0 k_{pe}^2 \int_{\zeta}^{\infty} d\zeta' \sin[k_{pe}(\zeta - \zeta')] f_{\parallel}(\zeta')$$
$$\times \frac{r_p^2}{r} \left[1 - \exp\left(-\frac{r^2}{2r_p^2}\right)\right]. \tag{5}$$

Now the envelope equation (1) can be expressed as

$$\frac{d^2 r_p}{dz^2} - \frac{\epsilon_{n,p}^2}{\gamma_p^2 r_p^3} = \frac{e}{\gamma_p m_p c^2 r_p} [\langle rW_{\perp s,p} \rangle + \langle rW_{\perp m} \rangle]$$

$$= \frac{e}{\gamma_p m_p c^2 r_p} \left[ \frac{\int_0^\infty r^2 e^{-\frac{r^2}{2r_p^2}} W_{\perp s,p} dr}{\int_0^\infty r e^{-\frac{r^2}{2r_p^2}} dr} + \frac{\int_0^\infty r^2 e^{-\frac{r^2}{2r_p^2}} W_{\perp m} dr}{\int_0^\infty r e^{-\frac{r^2}{2r_p^2}} dr} \right].$$
(6)

Hence, with the thin bunch approximation ( $k_{pe}r_{p(s)} < 1$ ), the self-modulation of the long Gaussian proton bunch seeded by a preceding short Gaussian bunch in overdense plasma is described by

$$\frac{d^2 r_p}{dz^2} - \frac{\epsilon_{n,p}^2}{\gamma_p^2 r_p^3} = -A_{s,p}^2 k_\beta^2 \cos(k_{pe}\zeta + \phi_s + \pi/2) \frac{2r_p r_s^2}{r_p^2 + r_s^2} - k_\beta^2 k_{pe} \int_{\zeta}^{\infty} d\zeta' \sin[k_{pe}(\zeta - \zeta')] f_{\parallel}(\zeta') r_p,$$
(7)

where  $k_{\beta} = (n_p e^2/2\gamma_p m_p \epsilon_0 c^2)^{1/2}$  represents the long proton bunch betatron wave number and  $n_p$  is the peak number density of the long proton bunch. At an early propagation distance in the plasma, we assume that the amplitude of the seed wakefield terms dominates over the emittance and the self-modulation growth terms. In particular, here, we consider the situation before the self-modulation becomes significant, and the Lorentz force from the magnetic field at the peak current of the long Gaussian proton bunch approximately balances the emittance, i.e.,  $\epsilon_{n,p} \sim$  $0.4\gamma_p k_{\beta} r_{p0}^2$  in our regime of interest. The factor of 0.4 has been found from FBPIC simulations.

If we consider a radially matched proton seed beam, i.e.,  $r_p \approx r_s$ , the simplified equation for the proton-bunchseeded, long proton bunch modulation amplitude, without considering the long bunch self-fields in *z*, is

$$\frac{d^2 r_p}{dz^2} \approx -A_{s,p}^2 k_\beta^2 \cos(k_{pe}\zeta + \phi_s + \pi/2) r_p.$$
(8)

At the phase where the long proton bunch is defocused [i.e.,  $\cos (k_{pe}\zeta + \phi_s + \pi/2) = -1$ ], the bunch self-modulation amplitude within the short propagation distance  $(k_{\beta}z < 1)$  is

$$r_{pD} = r_{p0} \cosh\left(A_{s,p}k_{\beta}z\right). \tag{9}$$

Once the process starts, the amplitude of envelope modulation self-consistently grows with its driven wake-fields. The contributions of the emittance and seed wakefield on the envelope quickly become negligible during the self-modulation process. Assuming  $r_p - r_{p0} = \hat{r} \exp [i(k_{pe}\zeta + \phi_s)]/2 + \text{c.c.}$  and  $|\partial_{k_{pe}\zeta}\hat{r}| \ll |\hat{r}|$ , we apply the plasma operator  $(\partial_{k_{pe}\zeta}^2 + 1)$  into Eq. (7) with Leibniz rule. We then obtain the linearized equation of the self-modulation amplitude  $\hat{r}$  [9] as

$$[\partial_{\zeta}\partial_{z}^{2} + (i/2)k_{\beta}^{2}k_{pe}f_{\parallel}(\zeta)]\hat{r} = 0, \qquad (10)$$

where the factor of 1/2 at the second term is from the estimation of the Gaussian radial profile, which can be modified for any different radial profile.

We apply the Laplace transform on Eq. (10) from z to p space and integrate the equation in  $\zeta$  space, introducing the initial conditions  $\hat{r}(z = 0, \zeta) = \delta r$  and  $\partial_z \hat{r}(z = 0, \zeta) = 0$ , where  $\delta r$  is the initial noise amplitude of the proton bunch envelope at any slice  $\zeta$ . In addition, the initial modulation

(often considered as bunch noise [7]) and the external seed are set as  $\hat{r}(z, \zeta = 0) = \Theta[\delta r + r_{p0} \sum_{\ell=1} (A_{s,p} k_{\beta} z)^{2\ell} / (2\ell)!]$ , where  $\Theta(z)$  is the Heaviside step function and  $r_{p0} \sum_{\ell=1} (A_{s,p} k_{\beta} z)^{2\ell} / (2\ell)! = r_{pD} - r_{p0}$  is the series expanded amplitude of the externally seeded modulation at the early propagation distance. Here, for the sake of simplifying the analysis, we have neglected any unknown coupling mechanisms and have modeled the self-modulation process as a linear combination of noise- and externally seeded modulations. The equation arranged for the Laplace transformed self-modulation amplitude is

$$\mathcal{L}_{z}[\hat{r}(z,\zeta)] = \left[\frac{\delta r}{p} + r_{p0} \sum_{\ell=1}^{\infty} \frac{A_{s,p}^{2\ell} k_{\beta}^{2\ell}}{p^{2\ell+1}}\right] \exp\left(\frac{i}{2} \frac{k_{\beta}^{2} k_{pe} \Phi}{p^{2}}\right),$$
(11)

where  $\Phi = \int f_{\parallel}(\zeta) d\zeta$  is the integration along the long bunch current profile.

In order to obtain the phase locked asymptotic solution, we use the method of steepest descent while inversetransforming Eq. (11) using the Bromwhich integral. Assuming that the effects of initial modulation and external seed are small when compared to the selfmodulation growth, the resultant self-modulation amplitude in  $(k_{pe}\zeta, k_{\beta}z)$  space is

$$\hat{r} \approx \left[\delta r + r_{p0} \sum_{\ell=1} \left\{ \exp\left(-i\frac{\pi}{6}\right) R_{c,p} \right\}^{2\ell} \right] \\ \times \left(\frac{\sqrt{3}}{8\pi}\right)^{1/2} \exp\left(N + i\frac{N}{\sqrt{3}} + i\frac{5\pi}{12}\right) N^{-1/2}, \quad (12)$$

where  $r_{p0}$  is the initial rms radius of the long proton bunch,  $R_{c,p} = A_{s,p} (k_{\beta}z/k_{pe}\Phi)^{1/3}$  the radius of convergence with the Gaussian proton seed bunch in the series expansion, and  $N = (3^{3/2}/4) (k_{\beta}^2 z^2 k_{pe} \Phi)^{1/3}$  the e-folding number for the exponentially growing self-modulation without the seed wakefield contribution. We note that by selecting a specific order of seed ( $\ell$ ), this series solution is partly reduced to the ones in Refs [3,9].

By taking the real part from Eq. (12), we obtain the asymptotic solution of the envelope self-modulation for a long Gaussian proton bunch seeded by a short, radially matched, and high-energy Gaussian proton bunch in  $(k_{pe}\zeta, k_{\beta}z)$  space as below.

$$r_{p} - r_{p0} \approx \left(\frac{\sqrt{3}}{8\pi}\right)^{1/2} r_{p0} \frac{e^{N}}{\sqrt{N}} \times \left[\frac{\delta r}{r_{p0}} \cos(\psi) + \sum_{\ell=1} R_{c,p}^{2\ell} \cos\left(\psi + \frac{\pi\ell}{3}\right)\right],$$
(13)

where  $\psi = -5\pi/12 - k_{pe}\zeta + \phi_s - N/\sqrt{3}$  is the phase of the self-modulation without the contribution of the external seed wakefields. In Eq. (13),  $R_{c,p}$  shows the dominance of the seed wakefield over the long bunch self-field in  $(k_{pe}\zeta, k_{\beta}z)$  space. Meanwhile,  $\pi \ell/3$  in each term of the externally seeded series solution shifts its phase against the phase slippage from the self-modulation process [2,3], which is determined by  $-N/\sqrt{3}$ . When the self-modulation is dominated by the seed wakefield (i.e.,  $R_{c,p} \sim 1$ ), the phase slippage from the self-modulation process is negligible. Therefore, the effect of  $\pi \ell/3$  inside the phase argument of the externally seeded solution is physical only when the resultant phase does not surpass the phase of the seed wakefield. Since  $R_{c,p} < 1$  in the regime of interest, the series converges.

For the PIC simulations, the physical and numerical parameters are set as follows: The ambient plasma electron number density is  $n_{pe} = 1.0 \times 10^{14} \text{ cm}^{-3}$ . For the initial parameters of the short Gaussian proton seed bunch, the peak number density  $n_s = 1.8 \times 10^{12} \text{ cm}^{-3}$  $(Q_s \approx 150 \text{ pC})$ , the mean relativistic gamma  $\gamma_s = 426$ , the rms length  $L_s = 1.4/k_{pe} \approx 744 \ \mu\text{m}$ , the rms radius  $r_{s0} = 0.4/k_{pe} \approx 213 \ \mu\text{m}$ , and the normalized transverse emittance  $\epsilon_{n,s} = 1 \mu m$ . For the initial parameters of the long Gaussian proton bunch, the peak number density  $n_p =$  $2.4 \times 10^{12} \text{ cm}^{-3}$  ( $Q_p \approx 16 \text{ nC}$ ), the mean relativistic gamma  $\gamma_p = 426$ , the rms length  $L_p = 113/k_{pe} \approx 6$  cm, the rms radius  $r_{p0} = 0.4/k_{pe} \approx 213 \ \mu\text{m}$ , and the normalized transverse emittance  $\epsilon_{n,p} = 0.4 \gamma_p k_\beta r_{p0}^2 \approx 1.8 \ \mu\text{m}.$ The simulation geometry is 2D axisymmetric, and the resolution is set to  $\Delta z = 0.02/k_{pe}$ ,  $\Delta r = 0.005/k_{pe}$ , and  $\Delta t = \Delta z/c$  in the laboratory frame. In order to avoid the situation in which the long proton bunch front is cut by the front of the simulation window, and therefore the sharp rising bunch front generates undesired wakefield, the length of the simulation window is set to  $L_w = 4L_p$ . Only the front half of the long Gaussian proton bunch is simulated. The radius of the simulation window is set to  $R_w = 1.88/k_{pe} \approx 1.1$  mm, which is large enough for observing the early stage of the long proton bunch self-modulation. Each simulation particle of the seed and the long proton bunches represents 1000 physical particles.

Since the rms radial size of the long proton bunch averaged in  $\zeta$  slowly diverges or focuses by the choice of  $\epsilon_{n,p}$  along the Gaussian current profile, we estimate, based on the PIC simulation results, the normalized amplitude of the self-modulation  $(r_{p,\text{max}} - r_{p,\text{min}})/2r_{p0}$ , which is plotted in Figs. 1(a) and 1(b). Plots are made at two longitudinal positions of the long proton bunch [indicated by red dotted vertical lines in Figs. 1(c)–(e)]. Here, the maximum and minimum rms radial sizes  $r_{p,\text{max}}$  and  $r_{p,\text{min}}$  are sampled with the slice length  $0.1\pi/k_{pe}$  within the range  $2\pi/k_{pe}$ .



FIG. 1. Amplitudes of the long proton bunch envelope self-modulation, seeded by the radially matched proton bunch for  $n_s/n_p = 0.75$ , as a function of  $k_{\beta z}$  at (a) the longitudinal center of the long bunch and (b)  $2L_p$  ahead from the center. Equation (13) (solid curves) is fitted to the PIC simulation result (dotted curves) by introducing the onset coefficients:  $\alpha$  for noise-seeded modulation and  $\beta$  for externally seeded modulation. Dashed curve in (b) represents the amplitude of the seeded modulation without the long bunch self-fields. (c) Current profiles of the proton seed bunch (orange curve) and long proton bunch (blue curve) in  $k_{pe}\zeta$  space. (d) Colormap of  $R_{c,p} = A_{s,p} (k_{\beta z}/k_{pe} \Phi)^{1/3}$  (radius of convergence with the Gaussian proton seed bunch) in  $(k_{pe}\zeta, k_{\beta}z)$  space. (e) Onset coefficients  $\alpha$  (blue circles with error bars) and  $\beta$  (orange circles with error bars) along  $k_{pe}\zeta$ . Circles and error bars indicate the average values and standard deviations, respectively, calculated over five simulations. The blue and orange shaded areas represent the data intervals of  $\alpha$  and  $\beta$ , respectively. In (c) and (d), two red, dotted vertical lines represent the positions of the longitudinal center of the long bunch and  $2L_p$  ahead from the center, respectively. (f) Phase shifts of the modulation at the long bunch center: (solid curve)  $-\Delta \arg(0.8\hat{r}_0 + 0.12\hat{r}_{s,p})$  from the shifted phase argument of Eq. (13), (dashed curve)  $-N/\sqrt{3}$  from the self-modulation growth without seed and onset coefficients, and (dotted curve) from the PIC simulation.

Figure 1(a) is for the longitudinal center of the long proton bunch,  $k_{pe}\zeta = k_{pe}\zeta_0 \sim -452$ , and Fig. 1(b) is the case at  $2L_p$  ahead from the center,  $k_{pe}\zeta = k_{pe}(\zeta_0 + 2L_p) \sim -226$ , where  $\zeta_0$  represents the position of the longitudinal center of the long proton bunch. We note that for  $k_{\beta}z \leq 0.1$ , the noise associated with the finite number of simulation particles is responsible for the initial modulation amplitudes [i.e.,  $\delta r$  in Eq. (13)] in Figs. 1(a) and 1(b).

In order to fit the prediction of Eq. (13) to the PIC simulation results, we set the normalized amplitude of the self-modulation for Eq. (13) as

$$(r_p - r_{p0})/r_{p0} \equiv \alpha \hat{r}_0 + \beta \hat{r}_{s,p}.$$
 (14)

Here,  $\hat{r}_0$  and  $\hat{r}_{s,p}$  are the first and the second terms normalized by  $r_{p0}$  in the right-hand side of Eq. (13), respectively. The coefficients  $\alpha$  and  $\beta$  are relevant for the onset timings of the two modes and are determined when the simulation data are fitted with Eq. (13) [see black solid curves in Figs. 1(a) and 1(b)]. The onset coefficients  $\alpha$  and  $\beta$  indicate the dominance of the long proton bunch self-field and the seed wakefield, respectively, in the early stage growth rate of the self-modulation. Here, we define the growth rate as  $\partial_{k_{\beta z}} \{ (r_p - r_{p0})/r_{p0} \}$ . At the longitudinal center of the long bunch [Fig. 1(a)], since  $n_s/n_p = 0.75$ , the amplitude of the self-magnetic focusing field of the long proton bunch is comparable to the radial seed wakefield [13]. The resultant growth rate is estimated as a mixture of two modes ( $\hat{r}_0$  and  $\hat{r}_{s,p}$ ). At  $2L_p$  ahead from the center [Fig. 1(b)], the self-fields of the long bunch are negligible compared to the seed wakefields, and only the externally seeded mode ( $\hat{r}_{s,p}$ ) survives. We note that right behind the seed bunch,  $R_{c,p} > 1$  [see Figs. 1(c) and 1(d)], and the asymptotic solution of the seeded self-modulation does not converge. In Fig. 1(e), the fitting coefficient  $\alpha$  is averaged over five simulations for a given  $\zeta$ . The variation of  $\alpha$  with respect to  $\zeta$  resembles the current profile of the long bunch. The bunch shot noise is the main contributor to the large error bars and the wide intervals between the minimum and maximum values.

Analytical estimation of the phase shift, with two modes interfering with each other [solid curve in Fig. 1(f)], is smaller in magnitude than the case without the external seed [dashed curve in Fig. 1(f)]. The PIC simulation result of the phase shift [dotted curve in Fig. 1(f)], representing the phase trace of the zeros of the longitudinal wakefield, exhibits an anomalous behavior, which is distinguished from the established analytical expectations [2,3]. This occurs because the  $\beta$ -mode wakefield experiences delayed growth and interferes with the  $\alpha$ -mode wakefield that has already grown earlier at the center of the long bunch. We note that since the analytical estimation of the phase shift does not take into account the self-modulation onset delay when the mode composition of the self-modulation is polarized along  $\zeta$  as shown in Fig. 1(e) (i.e., the  $\alpha$  mode is dominant near the long bunch longitudinal center and the  $\beta$  mode is dominant right behind the seed bunch), the phase shift cannot be explained by Eq. (13). The coefficients  $\alpha$ and  $\beta$  may depend on the profiles and amplitudes of the long bunch's self-fields and the seed wakefields, as well as the magnitude of the long bunch noise. Therefore,  $\alpha$  and  $\beta$ are, in general, functions of  $\zeta$ .

Section II with Fig. 1 illustrates that when the radial profile and the amplitude of the seed wakefields are comparable to those of the self-fields from the following long proton bunch, the composition of the two modes and their onset timings are significantly affected by the shot noise and the current profile of the long bunch.

# III. ENVELOPE SELF-MODULATION SEEDED BY A LOW-ENERGY ELECTRON BUNCH

The radial equilibrium of the charged particle beam in an overdense plasma is found as a collective behavior of the beam particles that have different oscillation frequencies [14]. Since the ratio of the betatron frequency of the low-energy (~18 MeV) electron seed bunch to that of the modulated high-energy (400 GeV) proton bunch is approximately 150, the seed bunch is focused to its radial equilibrium at the very early stage of the self-modulation process. In the regime of interest, the electron bunch peak number density after the focusing surpasses  $n_{pe}$ , and the

perturbed plasma number density reaches  $n_{pe}$  on the bunch propagation axis. A radial profile of the perturbed plasma density behind the low-current (~25 A) electron driver at its radial equilibrium is found as  $f_e(r) \propto \exp(-2r/r_B)$ from the PIC simulations. Here,  $r_B$  is known as the blowout radius of the plasma electrons defined by  $r_B = 2(n_s/n_{pe})^{1/2}r_{s0}$  [15]. Replacing the driver bunch density with this perturbed plasma electron number density in the linearized plasma wakefield equation [9], the radial wakefield behind the short, low-energy, and low-current electron bunch at its radial equilibrium is obtained as

$$W_{\perp s,e} \approx E_0 k_{pe} r_B^2 [\{1 - \exp(-2r/r_B)(1 + 2r/r_B)\}/4r] \\ \times [\sqrt{2\pi} k_{pe} L_s \exp(-k_{pe}^2 L_s^2/2)] \\ \times \cos(k_{pe}\zeta + \phi_s + \pi/2).$$
(15)

Within  $r < r_B$ , this radial wakefield is close to that obtained from the blowout regime.

For an analytical simplicity, as the electron bunch energy loss is negligible at the early stage of the self-modulation process, we assume that the electron seed bunch profile remains the same, which is valid while  $\gamma_s m_e c^2 \gg eW_{\text{Dec}} z$ , where the decelerating wakefield  $W_{\text{Dec}} \approx E_0 k_{pe} r_B \{1 - 3 \exp(-2)\} \{\sqrt{2\pi} k_{pe} L_s \exp(-k_{pe}^2 L_s^2/2)\}/16$ . Since  $\langle rW_{\perp s,e} \rangle$  is not integrable in the integration limit  $0 \le r < \infty$  with the proton bunch Gaussian radial profile, we set the integration upper limit as  $\sqrt{3} r_p$  and expand the long bunch Gaussian radial profile near the axis up to  $r^6$ order. Then, considering the low current seed bunch, i.e.,  $r_B \ll r_p$ , the equation for the electron-bunch-seeded, long proton bunch modulation amplitude, without considering the long proton bunch self-fields in z, is

$$\frac{d^2 r_p}{dz^2} \approx \frac{93}{256} \frac{n_{pe}}{n_p} \frac{k_\beta^2 r_B^2}{r_p} \left[ \sqrt{2\pi} k_{pe} L_s \exp\left(-k_{pe}^2 L_s^2/2\right) \right] \\ \times \cos(k_{pe} \zeta + \phi_s + \pi/2).$$
(16)

At the phase where the proton bunch is focused [i.e.,  $\cos (k_{pe}\zeta + \phi_s + \pi/2) = -1$ ], by selecting a monotonically decreasing solution of Eq. (16) and using  $\exp \left[-\text{erf}^{-1}(z)^2\right] = 2 - \cosh \left[(\pi/2)^{1/2}z\right] + \mathcal{O}(z^6)$  for z < 1, we obtain the bunch modulation amplitude without considering the long bunch self-fields in the form of hyperbolic cosine function as we did with the radially matched high-energy proton seed, i.e.,

$$r_{pF} \approx r_{p0} [2 - \cosh\{1.2A_{s,e}k_{\beta}z\}],$$
 (17)

where  $A_{s,e} = [(I_s/I_p)\sqrt{2\pi}k_{pe}L_s \exp(-k_{pe}^2L_s^2/2)]^{1/2}$  with  $I_s$  and  $I_p$  the seed and proton bunch peak currents, respectively. Now the resultant contribution of seed wake-fields depends on the currents of the electron seed and long



FIG. 2. Amplitudes of the long proton bunch envelope self-modulation, seeded by the tightly focused electron bunch for  $I_s/I_p = 0.75$ , as a function of  $k_\beta z$  at (a) the longitudinal center of the long bunch and (b)  $2L_p$  ahead from the center. Equation (18) (solid curves) is fitted to the PIC simulation result (dotted curves) by introducing the onset coefficients:  $\alpha$  for noise-seeded self-modulation and  $\beta$  for externally seeded self-modulation. (d) Colormap of  $R_{c,e} = 1.2A_{s,e}(k_\beta z/k_{pe}\Phi)^{1/3}$  (radius of convergence with the tightly focused electron seed bunch) in  $(k_{pe}\zeta, k_{\beta}z)$  space. (f) Phase shifts of the self-modulation at the long bunch center: (solid curve)  $-\Delta \arg(0.3\hat{r}_{s,e})$  from the shifted phase argument of Eq. (18), (dashed curve)  $-N/\sqrt{3}$  from the self-modulation growth without seed and onset coefficients, and (dotted curve) from the PIC simulation.

proton bunches. This analytical result is obtained by adopting the concept of the blowout radius, which depends on the seed bunch current, and by estimating the average of the seed wakefields across the radial profile of the proton bunch.

Since now the mathematical form of  $r_{pF} - r_{p0}$  is the same as  $r_{pD} - r_{p0}$ , we simply replace  $R_{c,p}$  in Eq. (13) with  $R_{c,e} \equiv 1.2A_{s,e}(k_{\beta}z/k_{pe}\Phi)^{1/3}$  the radius of convergence with the tightly focused electron seed bunch. Therefore, the modified equation is

$$r_{p} - r_{p0} \approx \left(\frac{\sqrt{3}}{8\pi}\right)^{1/2} r_{p0} \frac{e^{N}}{\sqrt{N}} \times \left[\frac{\delta r}{r_{p0}} \cos(\psi) + \sum_{\ell=1} R_{c,e}^{2\ell} \cos\left(\psi + \frac{\pi\ell}{3}\right)\right].$$
(18)

The dominance of the electron bunch driven seed wakefield over the long proton bunch self-field depends on their bunch currents, not on their densities. Since the peak value of the radial seed wakefield is limited by its narrow blowout radius, the wakefields amplified from the self-modulation growth are dominant over the seed wakefield. Therefore, the long proton bunch betatron frequency appears  $\zeta$ dependent, which is known to suppress the hosing of long charged particle bunches in overdense plasmas [16].

As for the PIC simulations, from the previous simulation parameter set, we replace the mass  $m_s = m_p$ , the mean relativistic gamma  $\gamma_s = 426$ , and the (+) sign for the seed bunch charge with  $m_s = m_e$ ,  $\gamma_s = 35.2$ , and the (-) sign, respectively.

In order to estimate the fitting coefficients of two modes with the tightly focused low-current electron seed bunch, we set  $(r_p - r_{p0})/r_{p0} \equiv \alpha \hat{r}_0 + \beta \hat{r}_{s,e}$ , where  $r_{s,e}$  represents the second term normalized by  $r_{p0}$  in the right-hand side of Eq. (18). Figures 2(a) and 2(e) show that at the longitudinal

center of the long proton bunch, the fitting coefficient  $\beta$ , which accounts for the externally seeded self-modulation, dominates in determining the growth rate. The self-modulation term, represented by the fitting coefficient  $\alpha$ , is estimated to be negligible compared to the externally seeded self-modulation. Therefore, for simplicity,  $\alpha$  is set to zero. At  $2L_p$  ahead from the center, the PIC simulation result in Fig. 2(b) of the self-modulation amplitude (dotted curve) shows a mismatch with the analytical expectation (solid curve) at  $k_{\beta z} \sim 1$ . The mismatch is due to the energy loss of the seed bunch, which was not considered in our analytical approach. Comparison of Figs. 2(c) and 2(d) with Figs. 1(c) and 1(d) indicates that the electron seed bunch at its radial equilibrium leads to a larger growth rate than the high-energy proton seed bunch case. Whereas both cases have the same seed bunch current, the radius of convergence  $R_c$  is larger for the electron seed bunch for the same  $\zeta$  and z, which leads to a larger  $\partial_{k_{\beta}z}\{(r_p - r_{p0})/r_{p0}\}$ .

Figure 2(e) shows that the onset coefficient  $\alpha$  for the noise-seeded self-modulation is negligible, whereas the onset coefficient  $\beta$  for the externally seeded self-modulation is approximately constant along  $\zeta$  with negligible deviation. This implies that long proton bunch self-modulation is simultaneously seeded as a single mode along  $\zeta$ , effectively overriding the  $\zeta$  dependence of the self-fields of the long proton bunch and the initial noise on the envelope. We define this characteristic as the "uniform onset." The phase behavior of the long proton bunch self-modulation now can be explained by the shifted phase argument of Eq. (18) with a single mode, i.e., in terms of  $\Delta \arg[\beta \hat{r}_{se}]$ , without any mode interference. Moreover, the PIC simulation result of the self-modulation phase shift [dotted curve in Fig. 2(f) does not exhibit the anomalous behavior that was observed in Fig. 1(f).

#### **IV. CONCLUSION**

This work indirectly demonstrates that the onset timing of the long proton bunch self-modulation seeded by the RIF can be significantly affected by the shot noise and current profile. In particular, when the mode composition of the self-modulation is polarized along the current profile of the long proton bunch, the mode interference causes an anomalous phase shift during the self-modulation process.

On the other hand, the tightly focused, low-current electron bunch uniformly seeds bunch self-modulation along  $\zeta$ , even for the long proton bunch with a nonconstant current profile, while suppressing mode polarization and the noisy onset timing. This feature is critical when introducing the plasma density step or the density gradient [2,17] at the early stage of the self-modulation process.

The analytical and numerical tools developed in this work will be useful for the design and analysis of proton beam-driven wakefield experiments, such as the Advanced Wakefield Experiment (AWAKE) at CERN.

#### ACKNOWLEDGMENTS

This work was supported by the National Research Foundation of Korea (Grants No. NRF-2016R1A5A1013277, No. NRF-2020R1A2C1010835, and No. RS-2022-00154676).

- N. Kumar, A. Pukhov, and K. Lotov, Self-modulation instability of a long proton bunch in plasmas, Phys. Rev. Lett. **104**, 255003 (2010).
- [2] A. Pukhov, N. Kumar, T. Tückmantel, A. Upadhyay, K. Lotov, P. Muggli, V. Khudik, C. Siemon, and G. Shvets, Phase velocity and particle injection in a self-modulated proton-driven plasma wakefield accelerator, Phys. Rev. Lett. 107, 145003 (2011).
- [3] C. B. Schroeder, C. Benedetti, E. Esarey, F. J. Grüner, and W. P. Leemans, Growth and phase velocity of self-modulated beam-driven plasma waves, Phys. Rev. Lett. 107, 145002 (2011).
- [4] AWAKE Collaboration, Acceleration of electrons in the plasma wakefield of a proton bunch, Nature (London) 561, 363 (2018).
- [5] L. Verra *et al.* (AWAKE Collaboration), Controlled growth of the self-modulation of a relativistic proton bunch in plasma, Phys. Rev. Lett. **129**, 024802 (2022).
- [6] W. Lu, C. Huang, M. Zhou, W. B. Mori, and T. Katsouleas, Limits of linear plasma wakefield theory for electron or positron beams, Phys. Plasmas 12, 063101 (2005).
- [7] K. V. Lotov, G. Z. Lotova, V. I. Lotov, A. Upadhyay, T. Tückmantel, A. Pukhov, and A. Caldwell, Natural noise and external wakefield seeding in a proton-driven plasma accelerator, Phys. Rev. ST Accel. Beams 16, 041301 (2013).
- [8] F. Batsch, P. Muggli *et al.* (AWAKE Collaboration), Transition between instability and seeded self-modulation of a relativistic particle bunch in plasma, Phys. Rev. Lett. **126**, 164802 (2021).
- [9] C. B. Schroeder, C. Benedetti, E. Esarey, F. J. Grüner, and W. P. Leemans, Coherent seeding of self-modulated plasma wakefield accelerators, Phys. Plasmas 20, 056704 (2013).
- [10] R. Lehe, M. Kirchen, I. A. Andriyash, B. B. Godfrey, and J. L. Vay, A spectral, quasi-cylindrical and dispersion-free particle-in-cell algorithm, Comput. Phys. Commun. 203, 66 (2016).
- [11] E. P. Lee and R. K. Cooper, General envelope equation for cylindrically symmetric charged-particle beams, Part. Accel. 7, 83 (1976).
- [12] Y. Fang, V. E. Yakimenko, M. Babzien, M. Fedurin, K. P. Kusche, R. Malone, J. Vieira, W. B. Mori, and P. Muggli, Seeding of self-modulation instability of a long electron bunch in a plasma, Phys. Rev. Lett. **112**, 045001 (2014).
- [13] J. Krall and G. Joyce, Transverse equilibrium and stability of the primary beam in the plasma wake-field accelerator, Phys. Plasmas **2**, 1326 (1995).
- [14] K. V. Lotov, Radial equilibrium of relativistic particle bunches in plasma wakefield accelerators, Phys. Plasmas 24, 023119 (2017).
- [15] W. Lu, C. Huang, M. Zhou, M. Tzoufras, F.S. Tsung, W. B. Mori, and T. Katsouleas, A nonlinear theory for

multidimensional relativistic plasma wave wakefields, Phys. Plasmas **13**, 056709 (2006).

- [16] J. Vieira, W. B. Mori, and P. Muggli, Hosing instability suppression in self-modulated plasma wakefields, Phys. Rev. Lett. **112**, 205001 (2014).
- [17] P. I. Morales Guzmán, P. Muggli *et al.* (AWAKE Collaboration), Simulation and experimental study of proton bunch self-modulation in plasma with linear density gradients, Phys. Rev. Accel. Beams **24**, 101301 (2021).