



Theoretical and numerical approaches for Vlasov–Maxwell equations

## Case studies in space charge and plasma acceleration of charged beams



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### ABSTRACT

Plasma acceleration with electron or proton driver beams is a challenging opportunity for high-energy physics. An energy doubling experiment with electron drivers was successfully performed at SLAC and a key experiment AWAKE with proton drivers is on schedule at CERN. Simulations play an important role in choosing the best experimental conditions and in interpreting the results. The Vlasov equation is the theoretical tool to describe the interaction of a driver particle beam or a driver laser pulse with a plasma. Collective effects, such as tune shift and mismatch instabilities, appear in high intensity standard accelerators and are described by the Poisson–Vlasov equation. In the paper, we review the Vlasov equation in the electrostatic and fully electromagnetic cases. The general framework of variational principles is used to derive the equation, the local form of the balance equations and related conservation laws. In the electrostatic case, we remind the analytic Kapchinskij–Vladimirskij (K–V) model and we propose an extension of the adiabatic theory for Hamiltonian systems, which ensures stability for perturbation of size  $\epsilon$  on times of order  $1/\epsilon$ . The variational framework is used to derive the Maxwell–Vlasov equations and related conservation laws and to briefly sketch the particle-in-cell (PIC) approximation schemes. Finally, the proton-driven acceleration is examined in the linear and quasi-linear regime. A PIC simulation with the code ALADYN developed at Bologna University is presented to illustrate the longitudinal and transverse fields evolution which allow a witness electron bunch to be accelerated with a gradient of a few GeV/m. We also present some remarks on future perspectives.

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## 1. Introduction

Particle accelerators are key instruments for the research in the domain of high-energy particle physics. To explore to even further accuracy the Standard Model, higher energies are required, thus pushing the technology of particle accelerators to its limits. The challenge is being tackled in two different domains, namely the design of high-field magnets, required to control the motion of high-energy charged particles, and that of high-gradient radio-frequency (RF) systems, aimed at

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accelerating the charged particles to the energies required for probing the intimate nature of matter and forces. Collective effects, such as space charge, are relevant in the early accelerating stages and limit the intensity reachable in final ring. Their control allows one to increase the final luminosity, a key parameter for high-energy experiments. In the domain of accelerating systems, the standard approach consists in generating longitudinal electric fields using metallic RF cavities, either normal or superconducting. Technological limits arise when trying to reach accelerating gradients of the order of 100 MV/m, which would have a direct impact on the dimensions of future accelerators. In order to keep under control the size of the new instruments, gradients of the order of GV/m would be needed and a plasma could be the natural solution, as it can sustain very large accelerating fields [1–3]. It is worth recalling the efforts devoted in the last few decades to experimental verification of plasma acceleration, which reached very encouraging results [4,5]. It is also important to stress the two approaches that can be used, namely laser wakefield acceleration (LWFA) [1], whenever a laser is driving the acceleration, or plasma wakefield acceleration (PWFA) [2,3], whenever a bunch is used to drive the whole process. The fundamental principle behind both approaches is that a plasma acts as an energy transformer, i.e., transferring the energy from the driver bunch to the witness bunch. As proton bunches at the energy frontier, i.e., in the multi-TeV range, are already available, it has been proposed the use of protons, instead of electrons, as driver beams open up the possibility of generating extremely high-energy lepton beams via PWFA [6]. Furthermore, the use of protons to drive the acceleration process would be a première, never tried before.

In this paper we review the Vlasov theory and the related numerical schemes. We first examine the electrostatic case that allows one to model the space-charge effects in a beam, which are relevant at low–medium energies. Since space charge mainly affects the transverse motion, one- and two-dimensional models are adequate to describe the basic dynamical features. The analytic Kapchinskij–Vladimirskij solution [7,8], applicable to a linear lattice, and the adiabatic theory stability results, applicable to a flat beam, allow us to understand many properties of the beam dynamics such as the mismatch oscillations. However, numerical solutions for two- or three-dimensional models provided by the particle-in-cell method (PIC) are needed to define stationary solutions to the Vlasov equation and to study their stability, in particular when multipolar magnetic components are present in the accelerator lattice.

In the more general framework of laser plasma or beam plasma acceleration, the theoretical description is provided by Maxwell–Vlasov equations as long as collisional effects can be neglected. In this case, analytical results are available only for some one-dimensional models and one has essentially to rely on the numerical solutions provided by the PIC schemes. In spite of the remarkable computational power presently available, the simulation of the acceleration on long plasma channels along thousands plasma lengths is still a challenge and reduced schemes, where the fastest scales are neglected, must be adopted. The control of accuracy is important, especially for reduced schemes, and the presence of conserved variables is helpful. In this paper, we present a short review of the theoretical framework for the electromagnetic case applicable to plasma acceleration. As an example of numerical computations, we finally consider the acceleration of electrons driven by proton bunches like the AWAKE experiment on schedule at CERN.

The plan of the paper is as following: in Section 2, we introduce the Poisson Vlasov theory via the action principle, which is suitable to obtain the equations of motion and the conservation laws. In Section 3, we consider the space charge problem in a ring after recalling the Kapchinskij–Vladimirskij model and the procedure to develop numerical schemes. In Section 4, the stability problem for a flat beam is discussed using the Hamiltonian adiabatic theory and it is proved that the size of an instability does not overcome  $\epsilon \sim \|\partial f / \partial t\|$  for a time interval at least  $1/\epsilon$ . In Section 5 we consider the Maxwell–Vlasov theory starting from Low’s Lagrangian [9]. The way to obtain the local energy balance for the electromagnetic field and the charged fluid is sketched. In Section 6 we outline the procedure to obtain the PIC schemes with an interpolating basis of linear splines and sampling the distribution functions of the charged fluid with numerical particles. In Section 7 we briefly review the proposal of AWAKE experiment, discussing the acceleration of electrons driven by a proton beam in a plasma in the linear and quasi-linear regimes. The results of a simulation obtained with the code ALaDyN developed at Bologna University are presented to illustrate the accelerating longitudinal field created in the plasma. A summary and comments on future perspectives conclude the presentation.

## 2. The Poisson–Vlasov equation

We consider a system of  $N$  particles of charge  $e$  and mass  $m$  interacting via Coulomb repulsion and subject to an external electrostatic field with potential  $V^{(ex)}$ . Denoting with  $H_{\text{tot}}$  the total Hamiltonian, with  $M = Nm$  and  $Q = Ne$  the total mass and charge, we write

$$\frac{H_{\text{tot}}}{M} = \frac{1}{N} \sum_{k=1}^N H_k(\mathbf{x}_k, \mathbf{p}_k)$$

$$H_k(\mathbf{x}_k, \mathbf{p}_k) = \frac{\mathbf{p}_k^2}{2} + \frac{Qe}{m} \frac{1}{2N} \sum_{j, (j \neq k)} \frac{1}{r_{jk}} + \frac{e}{m} V^{(ex)}(\mathbf{x}_k)$$

where  $\mathbf{x}, \mathbf{p} \in \mathbb{R}^3$ . Each  $H_k$  is the Hamiltonian for a single particle, with an external potential  $V_k(\mathbf{x})$  generated by all the particles  $i \neq k$ . In the limit  $N \rightarrow \infty$ , the  $N$  body system is replaced by a continuum, whose phase space distribution  $f(\mathbf{x}, \mathbf{p}, t)$

satisfies the Liouville equation for the Hamiltonian  $H(\mathbf{x}, \mathbf{p})$  with a potential  $V$ , which satisfies the Poisson equation. The overall system is governed by

$$\frac{\partial f}{\partial t} + [f, H] = 0 \quad H = \frac{\mathbf{p}^2}{2m} + \frac{Qe}{m}V(\mathbf{x}) + \frac{e}{m}V^{(ex)}(\mathbf{x})$$

$$\Delta V = -4\pi\rho \quad \rho = e \int f(\mathbf{x}, \mathbf{p}, t) d\mathbf{p}$$

where  $[, ]$  denote the usual Poisson bracket operator.

The underlying assumption is that in this limit the collisions can be neglected, so that statistical independence holds and the  $N$  points distribution function can be written as the product of the single particle distribution functions  $f(\mathbf{x}_k, \mathbf{p}_k, t)$  for  $k = 1, \dots, N$ . The ratio  $e/m$  as well as the total mass and charge are kept constant in this limit. The plasma frequency  $\omega_p = (4\pi\rho e/m)^{1/2}$  is constant, since  $\rho = Q/V$ , whereas the Debye length  $\lambda_D = v_{th}/(\sqrt{2}\omega_p)$  depends on the thermal velocity. Vlasov description is correct if  $\lambda_D \ll \lambda_p$  where  $\lambda_p = (2\pi c)/\omega_p$ , which is fulfilled if  $k_B T \ll mc^2$ . This collisionless model is valid since, according to the Landau model, the frequency of binary collisions is  $\nu_{coll} \approx \log(N)/N$ , which vanishes for  $N \rightarrow \infty$ .

In the Vlasov equation, the physical parameters enter as the ratios  $e/m$  and  $Q/M$ , and  $N$  has disappeared. However, it is customary to write the equation introducing the physical parameters  $e, m, N$ . Of course, these parameters can be scaled as in the PIC numerical schemes, where  $\bar{N}$  numerical particles are introduced to sample the distribution function and their charges and masses are given by  $\bar{m} = mN/\bar{N}$  and  $\bar{e} = eN/\bar{N}$ .

### 2.1. Variational formulation

We first consider the Poisson–Vlasov equations which are satisfied by a system of particles whose interaction is electrostatic. This is the case for instance of a beam in a ring once is the acceleration process is over. Low’s Lagrangian Action for the system is given by [9]:

$$A = \int_{t_a}^{t_b} \int_{\mathbb{R}^6} \ell(\mathbf{x}, \mathbf{v}, t) f_0(\mathbf{x}_0, \mathbf{v}_0) d\mathbf{x}_0 d\mathbf{v}_0 dt + \int_{t_a}^{t_b} \int_{\mathbb{R}^3} \frac{\mathbf{E}^2}{8\pi}(\mathbf{x}, t) d\mathbf{x} dt$$

where  $\ell$  and the electric field  $\mathbf{E}$  are given by

$$\ell = -\frac{m}{2}\mathbf{v}^2 - e\phi - eV^{(ex)} \quad \mathbf{E} = -\nabla\phi$$

The potential  $\phi(\mathbf{x}, t)$  and the particle trajectory  $\mathbf{x}(t)$  are kept constant at the endpoints of the time interval and  $(\mathbf{x}_0, \mathbf{v}_0)$  are the initial conditions of the trajectory. The Action is stationary for variations of  $\phi$  and  $\mathbf{x}$ , if and only if

$$m\dot{\mathbf{v}} = e\mathbf{E} + e\mathbf{E}^{(ex)} \quad \text{div}\mathbf{E} = -\Delta\phi = 4\pi\rho$$

where  $\mathbf{E}^{(ex)} = -\nabla V^{(ex)}$ . These equations must be self-consistently satisfied. The variational formulation has been used also to analyze the stability of the solutions of the Poisson–Vlasov equations [10].

We first consider the variation of the particle Action for a given potential  $\phi$  and we determine the trajectory with given endpoints  $\mathbf{x}(t_a) = \mathbf{x}_0$  and  $\mathbf{x}(t_b) = \mathbf{x}_b$ . The initial velocity  $\mathbf{v}_0$  is uniquely fixed by the boundary conditions. As a consequence, by inverting the evolution with respect to  $\mathbf{x}_0, \mathbf{v}_0$ , we obtain the distribution function in its Eulerian form  $f(\mathbf{x}, \mathbf{v}, t)$ , which satisfies the continuity or Liouville equation. In the present case the Hamiltonian is  $h = \mathbf{p}^2/2m + e\phi + eV^{(ex)}$  and

$$\frac{\partial f}{\partial t} + \mathbf{v} \frac{\partial f}{\partial \mathbf{x}} + \frac{e}{m}(\mathbf{E} + \mathbf{E}^{ex}) \frac{\partial f}{\partial \mathbf{v}} = 0$$

Imposing the variation with respect to  $\phi$  to vanish, we obtain

$$\int_{t_a}^{t_b} \int_{\mathbb{R}^3} \frac{1}{4\pi} \text{div}\mathbf{E} \delta\phi d\mathbf{x} dt - \int_{t_a}^{t_b} \int_{\mathbb{R}^6} f(\mathbf{x}_0, \mathbf{v}_0) e\delta\phi d\mathbf{x}_0 d\mathbf{v}_0 dt = 0$$

Changing the integration variable in the second integral from  $\mathbf{x}_0, \mathbf{v}_0$  to  $\mathbf{x}, \mathbf{v}$ , we can replace  $f(\mathbf{x}_0, \mathbf{v}_0)$  with its Eulerian form, since it is a canonical transformation and the Jacobian is 1. We get:

$$\int_{t_a}^{t_b} \int_{\mathbb{R}^3} \left( \frac{1}{4\pi} \text{div}\mathbf{E} - e\rho \right) \delta\phi d\mathbf{x} dt = 0 \quad \rho = e \int_{\mathbb{R}^3} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}$$

The stationary condition with respect to  $\phi$  imposes that the Poisson equation must be satisfied.

The conservation laws follow immediately in this case. Indeed, defining the current according to

$$\mathbf{j} = e \int_{\mathbb{R}^3} \mathbf{v} f \, d\mathbf{v}$$

and using the Liouville equation, we have

$$\frac{\partial \rho}{\partial t} = -e \int_{\mathbb{R}^3} \left( \mathbf{v} \frac{\partial f}{\partial \mathbf{x}} + \frac{e\mathbf{E}}{m} \frac{\partial f}{\partial \mathbf{v}} \right) d\mathbf{v} = -\operatorname{div} \mathbf{j}$$

Considering

$$\mathcal{H}^P = \int_{\mathbb{R}^3} f \frac{m}{2} |\mathbf{v}|^2 \, d\mathbf{v} \quad \mathbf{H}^P = \int_{\mathbb{R}^3} f \frac{m}{2} |\mathbf{v}|^2 \mathbf{v}_k \, d\mathbf{v} \quad S^P = \mathbf{j} \cdot (\mathbf{E} + \mathbf{E}^{(ex)})$$

where  $\mathcal{H}^P, \mathbf{H}^P, S^P$  are the energy density, flux and source for the charged fluid, and computing the second moment  $\mathcal{H}^P$  partial derivative with respect to time, we obtain the local energy balance. Setting  $\mathbf{E}^{(ex)} = 0$ , for the electric field, whose energy density is  $\mathcal{H}^F = \mathbf{E}^2/8\pi$ , a similar balance holds:

$$\frac{\partial \mathcal{H}^P}{\partial t} + \operatorname{div} \mathbf{H}^P = S^P \quad \frac{\partial \mathcal{H}^F}{\partial t} = S^F$$

where  $S^F = (4\pi)^{-1} \mathbf{E} \cdot \partial_t \mathbf{E} = -\mathbf{j} \cdot \mathbf{E}$  and is opposite to the charged fluid source if the vector  $(4\pi)^{-1} \partial_t \mathbf{E} + \mathbf{j}$  (whose divergence is zero due to the continuity equation) vanishes.

### 3. Space-charge effects for a 2D beam

The space-charge effects are relevant for a beam, except at extremely high energies. In a ring, the beam moves with a constant longitudinal velocity  $v_0$  close to  $c$ . If the charges are uniformly distributed over a cylinder, a test charge  $q$  experiences a radial force  $qE_r$  due to Coulomb repulsion in the beam rest frame, which in the laboratory frame becomes  $qE_r/\gamma_0^2$ ,  $\gamma_0$  being  $(1 - v_0^2/c^2)^{-1/2}$ . The coordinate along the beam axis is  $s = v_0 t$  and we define the transverse momenta as  $\mathbf{p} = \mathbf{v}/v_0 = d\mathbf{x}/ds$  so that the energy density for the transverse motion reads

$$\mathcal{E} = \mathcal{E}^F + \mathcal{E}^P = \frac{\mathbf{E}^2}{4\pi} + \int_{\mathbb{R}^2} f(\mathbf{x}, \mathbf{p}, s) h(\mathbf{x}, \mathbf{p}, s) \, d\mathbf{p}$$

where

$$h = \frac{p_x^2 + p_y^2}{2} + k_{0x}(s) \frac{x^2}{2} + k_{0y}(s) \frac{y^2}{2} + \frac{\xi}{2} \phi(x, y, s)$$

The perveance  $\xi$  is defined by

$$\xi = \frac{2eQ}{mv_0^2} \left( 1 - \frac{v_0^2}{c^2} \right) = \frac{2qQ}{mv_0^2} \left( \frac{mc^2}{E} \right)^2$$

The quadratic term in the potential is due to the quadrupoles, but higher-order polynomials, due to higher magnetic multipoles, may be present. For a brief presentation see [11], while use [8] for an exhaustive discussion.

The stationary condition implies that  $\mathbf{x}(s), \mathbf{p}(s)$  satisfy Hamilton's equations and consequently  $f$  satisfies the Liouville equation, whereas the Poisson equation holds self-consistently for  $\phi$ :

$$\frac{\partial f}{\partial s} + [f, h] = 0 \quad \Delta \phi = -4\pi \rho \quad \rho = e \int_{\mathbb{R}^2} f(\mathbf{x}, \mathbf{p}, s) \, d\mathbf{p}$$

Approximate solutions can be found using the PIC method [12–15], whose key feature is to be an efficient solver for the Poisson equation [16].

Analytic solutions are known if  $k_{0x} = k_{0y}$  and if they are  $s$  independent (constant focusing case), since the axial symmetry makes the problem one dimensional [8]. In this case, approximate analytic solutions can be found by using the Birkhoff normal forms [17].

A family of stationary solutions is given by the distributions  $f = f(H)$  with support on  $0 \leq H \leq E$ . Letting  $H = p^2/(2m) + W(r)$  where  $W = k_0 r^2/2 - \frac{1}{2} \xi V(r)$  and  $W(R) = E$  the solution reads

$$\rho = 2\pi e \int_{W(r)}^{W(R)} f(E) dE \quad \frac{1}{r} \frac{d}{dr} r \frac{d\phi}{dr} = -4\pi \rho(r)$$

with the normalization condition  $2\pi \int_0^R nr dr = 1$ . In the special case  $f(H) = \delta(H - E)f_0$ , where  $f_0 = 1/\pi R^2$ , the space density is constant  $\rho = 1/(\pi R^2)$  and the solution for the potential is  $\phi = r^2/R^2$ . The Hamiltonian becomes quadratic and the electric field is linear:

$$h = \frac{p^2}{2} + \frac{k}{2}r^2 \quad k = k_0 - \frac{\xi}{R^2} \quad \mathbf{E} = \frac{2\mathbf{x}}{R^2}$$

In the case of periodic focusing, assuming that the bunches are very elongated along the  $s$ -coordinate, an analytic solution can be found by choosing a distribution function  $f$  that depends on the invariant actions, which can be determined self-consistently assuming a priori that the potential  $\phi$  is still quadratic. This solution is due to Kapchinskij and Vladimirkij, see [7,8]. The generating function  $F = F^{(x)} + F^{(y)}$ , where  $F^{(x)} = \tan(\theta - \dot{\beta}_x/2)x^2/(2\beta_x)$  (the same for  $F_y$ ) changes  $h$  into a new Hamiltonian  $\hat{h}$  depending on the actions:

$$h = \frac{p_x^2 + p_y^2}{2} + \frac{k_x(s)}{2}x^2 + \frac{k_y(s)}{2}y^2 \quad \hat{h} = h + \frac{\partial F}{\partial s} = \frac{J_x}{\beta_x(s)} + \frac{J_y}{\beta_y(s)}$$

The function  $\beta_x$  is related to the phase of the solution for the  $x$  coordinate  $x = A(s) \cos(\Phi(s) + \gamma_x)$  by  $\beta_x = 1/\dot{\Phi}_x$ , where  $A_x(s), \beta_x(x)$  satisfy

$$\ddot{A}_x - \frac{J_{0x}^4}{A_x^3} + k_x(s)A_x = 0 \quad \frac{1}{2}\beta_x \ddot{\beta}_x + k_x(s)\beta_x^2$$

and similar equations hold for the  $y$  coordinate. The first one is the envelope equation. The distribution function is chosen according to

$$f(J_x, J_y) = \frac{1}{4\pi^2 J_{0x} J_{0y}} \delta\left(\frac{J_x}{J_{0x}} + \frac{J_y}{J_{0y}}\right)$$

and since  $[f, \hat{h}] = 0$ , it is stationary. The manifold on which  $f$  has its support is the ellipsoid  $J_x/J_{0x} + J_y/J_{0y} = 1$  foliated, by invariant tori  $\mathbb{T}^2$  defined as the product of the ellipses:

$$2\beta_x J_x = x^2 + (\beta_x p_x - \dot{\beta}_x x/2)^2 = A_x^2 \quad A_x = (2\beta_x J_{0x})^{1/2} \quad \text{and} \quad x \rightarrow y$$

The density  $\rho(x, y, s)$ , obtained from  $f$ , is constant in the ellipse with semi-axis  $A_x, A_y$ :

$$\rho = \frac{1}{\pi A_x A_y} \vartheta\left(1 - \frac{x^2}{A_x^2} - \frac{y^2}{A_y^2}\right)$$

As a consequence the electric field solution of the Poisson equation is linear within the elliptic bunch:

$$E_x = \frac{4x}{A_x(A_x + A_y)} \quad (\text{in}) \quad E_x = \frac{4x}{A'_x(A'_x + A'_y)} \quad (\text{out})$$

where  $A'_x = (A_x^2 + \chi)^{1/2}$ ,  $A'_y = (A_y^2 + \chi)^{1/2}$  are the semi-axis of the confocal ellipse; namely  $\chi$  is defined by  $x^2/A_x'^2 + y^2/A_y'^2 = 1$  and at large distance from the origin  $A'_x = A'_y \simeq \chi$ .

Since the field is linear, it is evident that the coefficients of the quadratic terms in the Hamiltonian are given by  $k_x = k_{0x} - 2\xi/(A_x(A_x + A_y))$  (and the same for  $k_y$ ) where

$$\ddot{A}_x - \frac{4J_{0x}^2}{A_x^3} + k_{0x}(s)A_x = \frac{2\xi}{(A_x + A_y)} \quad \text{and} \quad x \rightarrow y$$

This equation admits periodic solutions  $\beta(s)$  and  $A(s) = J_0 \beta^{1/2}(s)$ , which are stationary. The effect of nonlinearities in the lattice can be investigated using the normal forms in the case of constant focusing [12]. There are also quasi-periodic solutions, which are not stationary and describe the so-called mismatched beam. By linearizing the envelope equation, the frequencies of the mismatched solution can be determined [18]. In any other case, one has to rely on the PIC numerical procedure to determine the solution. The distribution function is sampled with numerical particles, the density is interpolated with linear splines and the Poisson equation is solved using a spectral or finite difference scheme. The Poisson solver is the key algorithm and an efficient spectral algorithm capable of dealing with any assigned boundary conditions has been developed by Bergamini et al. and discussed in [13].

#### 4. Adiabatic invariance for a flat 1D beam

As we have discussed in the previous section, only few explicit solutions of the Vlasov equation are known. Moreover, the stability problem of the stationary solution is still open in many cases [19].

But the possibility of describing the Vlasov dynamics as a single-particle dynamics in a self-consistent potential allows us to partially extend the averaging theorem results for Hamiltonian systems [20].

We explicitly consider when the single particle Hamiltonian reduces to a 1D integrable system with an elliptic fixed point at the origin:

$$H(x, p; f) = \frac{p^2}{2m} + V(x, t; f) \tag{1}$$

The potential  $V(x, t; f)$  has a functional dependence from the particle distribution  $f(x, p, t)$  in the phase space, that satisfies the non-linear Liouville equation:

$$\frac{\partial f}{\partial t} = -p \frac{\partial f}{\partial x} + \frac{\partial f}{\partial p} \frac{\partial}{\partial x} V(x, t; f) \tag{2}$$

Any stationary solution has to be a function of the invariants of the motion. For any given phase space distribution  $f(x, p)$ , one can introduce the action-angle variables  $(I, \theta)$  in a neighborhood of the origin:

$$I(E; f) = \frac{1}{2\pi} \oint_{H(x,p;f)=E} p(x, E) dx$$

$$\theta(x, I; f) = \left. \frac{\partial}{\partial I} F(x, I; f) \right|_x \tag{3}$$

where  $F(x, I; f)$  is the generatrix function computed from the definition

$$F(x, E; f) = \int_{H(f)=E}^x p(x, E) dx \tag{4}$$

which depends on the given distribution. Then one has to look for a self-consistent stationary distribution  $f(I)$ . We remark that, in the definition of  $F(x, I; f)$ , one can choose the origin of the angle  $\theta$  in an arbitrary way: i.e., in any section of the phase space. Letting  $H(I; f)$  the new Hamiltonian, we have the frequency of motion

$$\Omega(I; f) = \frac{dH(I; f)}{dI}$$

We assume that far from separatrix curves, the functional dependence of the Hamiltonian and the action-angle variables from the distribution  $f(x, p)$  are regular. Indeed in the Vlasov problem the potential  $V(x; f)$  is linearly dependent on the particle distribution, according to

$$V(x; f) = \int_{x' \neq x} k(|x' - x|) f(x', p') dx' dp' \tag{5}$$

where  $k(|x|)$  is the kernel that defines the electrostatic potential. Under these assumptions, if one considers a slowly varying distribution  $f(x, p, t)$

$$\left\| \frac{\partial f}{\partial t} \right\| = \epsilon \ll 1 \tag{6}$$

( $\epsilon^{-1} \gg 1$  defines the slow time scale), the single particle dynamics has the property that the action variable  $I(f)$ , computed considering the distribution  $f$  constant (frozen system), is an adiabatic invariant,

$$|I(x(t), p(t), t; f) - I_0| \leq O(\epsilon) \quad \text{for } t \leq \frac{1}{\epsilon} \tag{7}$$

where  $(x(t), p(t))$  is the solution of the Hamiltonian system (1). Eq. (7) means that, during the time evolution, the value of the initial action can be considered constant for a time  $1/\epsilon$ , which is the slow time scale. The same is true for any regular function of the action. The proof of this result is a consequence of the perturbation theory and it holds for a whole class of distribution functions  $f(x, p, t)$ , with the *adiabatic parameter*

$$\frac{\epsilon}{\Omega^2(f)} \ll 1 \tag{8}$$

as only constraint.

The condition (8) arises as we cannot apply the adiabatic theory near a separatrix curve where the unperturbed frequency  $\Omega \rightarrow 0$ . The adiabatic property of the action variable can be understood if we choose a section  $\theta = \text{const.}$  in the phase space (Poincaré section) and we denote  $\{t_n\}_{n \in \mathbb{N}}$ , the sequence of crossing times of an orbit  $(x(t), p(t))$  with the section. Since the frozen energy  $H(x, p; f)$  is conserved up to an error of order  $O(\epsilon)$ , the solution  $(x(t), p(t))$  for  $t \in [t_n, t_{n+1}]$  is close to the curve  $H(x, p; f(t_*)) = E_*$ , where  $t_* \in [t_n, t_{n+1}]$  and  $E_* \in [E_n, E_{n+1}]$ . Moreover, the dynamics of the angle variables reads:

$$\dot{\theta} = \Omega(E; f) + O(\epsilon)$$

Then we get the relation

$$dt = \frac{d\theta}{\Omega(E; f)} + O(\epsilon) \tag{9}$$

and we can use the angle  $\theta$  as a parameter for the dynamics  $(x(t), p(t))$ . According to the results of perturbation theory [21], we can write:

$$I_{n+1} - I_n = \int_0^{2\pi} \frac{1}{\Omega^2(E; f)} \left( \int_{x' \neq x} k(|x' - x|) \frac{\partial f}{\partial t} dx' dp' - \left\langle \int_{x' \neq x} k(|x' - x|) \frac{\partial f}{\partial t} dx' dp' \right\rangle \right) d\theta + O(\epsilon^2) \tag{10}$$

where  $\langle \rangle$  denotes the average with respect to the  $\theta$  variable. Since both the energy  $E$  and the distribution  $f$  can be considered constant in time during the integration up to an error of order  $O(\epsilon)$ , the integral vanishes and the previous relation implies

$$|I_{n+1} - I_n| = O(\epsilon^2) \tag{11}$$

Therefore, since the value of  $I$  varies by a quantity of order  $O(\epsilon)$  in each interval  $[t_n, t_{n+1}]$ , the adiabatic invariance holds for a time of order  $O(1/\epsilon)$ . The remark on the estimate of the adiabatic parameter (8) is needed to obtain the result (11). In the adiabatic approximation for the dynamics, the angle variable reads

$$\theta(t) = \int_0^t \Omega(I; f) dt + O(\epsilon)t$$

where  $I$  is kept constant in the integration. We will give a schematic road map to extend the previous argument to the Vlasov problem, where one has to check if a small perturbation of the stationary solution, which evolves according to the non-linear Liouville equation (2), satisfies the condition of the adiabatic approximation. Let the perturbed stationary distribution be  $f'(I, t) = f(I) + \delta f(I, \theta, t)$ , then we assume the ansatz

$$\left\| \frac{\partial f'}{\partial t} \right\| = \epsilon \ll 1 \tag{12}$$

so that the adiabatic parameter

$$\frac{1}{\Omega^2(f)} \left\| \frac{\partial f'}{\partial t} \right\| \ll 1$$

is also small. We apply the adiabatic description of motion to get an approximate solution of the non-linear Liouville equation (2)

$$f'(\theta, I, t) = f(I) + \delta f \left( \theta + \int_0^{-t} \Omega(I, s; f) ds, I \right) \tag{13}$$

with an error which remains of order  $O(\epsilon)$  for a time  $\simeq 1/O(\epsilon)$ . Then, to correctly apply the adiabatic approach, a consistency condition on the estimate of the slow time scale (6) should be satisfied. Considering the leading terms, we get

$$\left\| \frac{\partial f'}{\partial t} \right\| \leq \left\| \frac{\partial f}{\partial I} \right\| |\Delta I| + \|\delta f\| \|\Omega\| \tag{14}$$

and the adiabatic invariance for the Vlasov problem requires the consistency condition

$$\left\| \frac{\partial f}{\partial I} \right\| |\Delta I|(\epsilon) + \|\delta f\| \|\Omega\| \leq \epsilon \tag{15}$$

which can be reduced to a contraction principle if we use Eq. (10). Condition (15) can be satisfied if the derivative  $\|\partial f / \partial I\|$  is sufficiently small: i.e. the dependence of the stationary distribution from the unperturbed action variable is not too steep. In such a case, the adiabatic argument holds and the approximation (13) can be applied for a time  $\propto \|\frac{\partial f'}{\partial t}\|^{-1}$  so that we have a stable solution up to that time scale.

**5. The Maxwell–Vlasov equations**

For simplicity, we consider the interaction of an electromagnetic field with only one species (electrons), since the extension to two or more species (electrons and ions in the plasma or in a driver bunch) is straightforward. We start again from Low’s Lagrangian Action [9] following from the system written as the sum of the Action for the field and the Action for the particle system (see [22] for a review):

$$A = \int_{t_a}^{t_b} \int_{\mathbb{R}^6} f_0(\mathbf{x}_0, \mathbf{v}_0) \ell(\mathbf{x}, \mathbf{v}, t) \, d\mathbf{x}_0 \, d\mathbf{v}_0 \, dt + \int_{t_a}^{t_b} \int_{\mathbb{R}^3} \mathcal{L}^F \, d\mathbf{x} \, dt$$

where  $\mathbf{x} = \mathbf{x}(\mathbf{x}_0, \mathbf{v}_0, t)$ ,  $\mathbf{v} = d\mathbf{x}/dt$ ,  $f_0(\mathbf{x}_0, \mathbf{v}_0)$  is the initial distribution of particles in phase space,  $\ell$  is the particle Lagrangian and  $\mathcal{L}^F$  is the field Lagrangian density, given by:

$$\ell = -\gamma^{-1}(\mathbf{v})mc^2 - e\phi + \frac{e}{c} \mathbf{v} \cdot \mathbf{A} \quad \gamma(\mathbf{v}) = \left(1 - \frac{|\mathbf{v}|^2}{c^2}\right)^{1/2}$$

$$\mathcal{L}^F = \frac{\mathbf{E}^2 - \mathbf{B}^2}{8\pi}$$

The electric and magnetic fields are expressed in terms of the scalar and vector potentials as usually

$$\mathbf{E} = -\nabla\phi - \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} \quad \mathbf{B} = \text{rot } \mathbf{A}$$

and  $\mathbf{E}, \mathbf{B}$  are invariant with respect to the gauge transformation

$$\phi \rightarrow \phi_\alpha = \phi - \frac{\alpha}{c} \frac{\partial g}{\partial t} \quad \mathbf{A} \rightarrow \mathbf{A}_\alpha = \mathbf{A} + \alpha \nabla g$$

First we impose that the variation with respect to  $\mathbf{x}$  vanishes, treating  $\phi$  and  $\mathbf{A}_k$  as assigned fields, and then we impose that the variation on the fields  $\phi, \mathbf{A}$  vanishes. As a consequence, we obtain the equations of motion and we can express the distribution function in Eulerian form  $f(\mathbf{x}, \mathbf{v}, t)$ , so that

$$m \frac{d}{dt}(\gamma \mathbf{v}) = e \mathbf{E} + \frac{e}{c} \mathbf{v} \times \mathbf{B}$$

$$\frac{\partial f}{\partial t} + \mathbf{v} \frac{\partial f}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{v}} \left[ f \left( e \mathbf{E} + \frac{e}{c} \mathbf{v} \times \mathbf{B} \right) \right] = 0$$

The equations for the fields provide the first two Maxwell’s equations

$$\text{div } \mathbf{E} = 4\pi\rho \quad \text{rot } \mathbf{B} = \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} + \frac{4\pi}{c} \mathbf{j}$$

where we have defined

$$\rho(\mathbf{x}, t) = e \int_{\mathbb{R}^3} f(\mathbf{x}, \mathbf{v}, t) \, d\mathbf{v} \quad \mathbf{j}(\mathbf{x}, t) = e \int_{\mathbb{R}^3} \mathbf{v} f(\mathbf{x}, \mathbf{v}, t) \, d\mathbf{v}$$

The remaining two Maxwell equations,  $\text{div } \mathbf{B} = 0$  and  $\text{crot } \mathbf{E} = -\partial \mathbf{B} / \partial t$ , are exactly satisfied thanks to the relation between the fields and the potentials. Formulations in a different functional setting where the distribution function  $f$  is itself a field and observables are functionals of this field have been introduced in both the Lagrangian and the Hamiltonian frameworks [23,24].

The first invariance property is obtained by imposing that the Action does not change under the gauge transformation on the fields.



The variation of the Action for the free fields and for the interaction with the charged fluid is

$$\frac{\partial A}{\partial \alpha} = \int_{\mathbb{R}^4} \left( \frac{\partial \rho}{\partial t} + \text{div} \mathbf{j} \right) \mathbf{g} \, d\mathbf{x} \, dt = 0$$

The arbitrariness of  $\mathbf{g}$  imposes that the continuity equation is satisfied.

The conservation laws in the fluid formulation have been derived using Nöther's theorem in [25].

We obtain a balance equation in the form:

$$\frac{\partial \mathcal{H}^F}{\partial t} + \text{div} \mathbf{H}^F = \mathcal{S}^F \quad \frac{\partial \mathcal{H}^P}{\partial t} + \frac{\partial \mathbf{H}^P}{\partial x_j} = \mathcal{S}^P$$

where  $\mathcal{H}^F, \mathbf{H}^F, \mathcal{S}^F$  and  $\mathcal{H}^P, \mathbf{H}^P, \mathcal{S}^P$  are the energy density, flux and source for the fields and the charged fluid.

$$\begin{aligned} \mathcal{H}^F &= \frac{\mathbf{E}^2 + \mathbf{H}^2}{8\pi} & \mathbf{H}^F &= \frac{c}{4\pi} \mathbf{E} \times \mathbf{B} & \mathcal{S}^F &= -\mathbf{j} \cdot \mathbf{E} \\ \mathcal{H}^P &= \int_{\mathbb{R}^3} \gamma(\mathbf{v}) m c^2 f \, d\mathbf{v} & \mathbf{H}^P &= \int_{\mathbb{R}^3} \gamma(\mathbf{v}) m c^2 \mathbf{v} f \, d\mathbf{v} & \mathcal{S}^P &= \mathbf{j} \cdot \mathbf{E} \end{aligned}$$

The final form of the local energy conservation law is

$$\frac{\partial}{\partial t} (\mathcal{H}^F + \mathcal{H}^P) + \text{div} (\mathbf{H}^F + \mathbf{H}^P) = 0$$

In a similar way, the local equation for the momentum balance, from which the fluid equations follow, can be obtained by considering the action of space translations on the Lagrangian density.

### 6. Particle in cell approximation schemes

In order to develop numerical schemes to solve the Poisson–Vlasov equations, one can introduce two finite bases for the potentials and for the charged fluid phase space distribution function [26,27]. Letting  $\phi_\mu$ , where  $\phi_0 = \phi$  and  $\phi_j = A_j$ , we consider the expansion

$$\phi_\mu(\mathbf{x}, t) = \sum_{\mathbf{g}} \phi_{\mu, \mathbf{g}}(t) \psi_{\mathbf{g}}(\mathbf{x}) \tag{16}$$

where  $\mathbf{g} = (i, j, k)$  and

$$\psi_{\mathbf{g}}(\mathbf{x}) = \psi_i(x) \psi_j(y) \psi_k(z) \tag{17}$$

We may choose linear interpolating spline functions. For the distribution function, the common choice is

$$f(\mathbf{x}, \mathbf{v}, t) = \frac{N}{\bar{N}} \sum_{\alpha} \zeta(\mathbf{x} - \mathbf{x}_\alpha(t)) \delta(\mathbf{v} - \mathbf{v}_\alpha(t)) \tag{18}$$

where  $\zeta(\mathbf{x} - \mathbf{x}_\alpha(t)) = \zeta(x - x_\alpha(t)) \zeta(y - y_\alpha(t)) \zeta(z - z_\alpha(t))$  and the functions have compact support.

In this case the functions are positive and normalized:  $\int \zeta(x - x_\alpha) \, dx = 1$ .

With this basis, the Lagrangian for the particles and their interaction with the fields becomes:

$$L^P = \sum_{\alpha=1}^{\bar{N}} \frac{\bar{m}}{2} \mathbf{v}_\alpha^2 + \sum_{\mathbf{g}} \left( -\rho_{\mathbf{g}} \phi_{\mathbf{g}} + \frac{1}{c} \mathbf{j}_{\mathbf{g}} \cdot \mathbf{A}_{\mathbf{g}} \right)$$

where we have defined the current and the density components

$$\rho_{\mathbf{g}} = \bar{e} \sum_{\alpha=1}^{\bar{N}} S_{\mathbf{g}}(\mathbf{x}_\alpha(t)) \quad \mathbf{j}_{\mathbf{g}} = \bar{e} \sum_{\alpha=1}^{\bar{N}} \mathbf{v}_\alpha S_{\mathbf{g}}(\mathbf{x}_\alpha(t))$$

In the equations above,  $\bar{e} = Ne/\bar{N}$  and  $\bar{m} = Nm/\bar{N}$  denote the charge and the mass of the so called numerical particles.  $S_{\mathbf{g}}(\mathbf{x}_\alpha(t))$  are new basis functions defined by

$$S_{\mathbf{g}}(\mathbf{x}_\alpha(t)) = \int \psi_{\mathbf{g}}(\mathbf{x}) \zeta(\mathbf{x} - \mathbf{x}_\alpha(t)) \tag{19}$$

In a similar way one may compute the field Lagrangian that becomes a quadratic form in the field components  $\phi_{\mathbf{g}}$  and  $\mathbf{A}_{\mathbf{g}}$ .

By taking the variations of the Action  $A = \int (L^P + L^F) dt$  with respect to the macro-particles coordinates  $\mathbf{x}_\alpha$  and the potential components  $\phi_{\mathbf{g}}, \mathbf{A}_{\mathbf{g}}$ , one can obtain a set of ordinary differential equations for these variables. An explicit integration scheme in time, like the fourth-order Runge–Kutta one, allows us to obtain an approximate solution, where the conservation laws are preserved up to the error due to the integration numerical scheme.

### 6.1. Standard particle in cell formulation

The more traditional scheme consists in solving the exact Maxwell equations for the fields  $\mathbf{E}, \mathbf{B}$  after expanding them on the basis  $\phi_{\mathbf{g}}(\mathbf{x})$ , according to [28,29].

$$\mathbf{E}(\mathbf{x}, t) = \sum_{\mathbf{g}} \mathbf{E}_{\mathbf{g}}(t) \psi_{\mathbf{g}}(\mathbf{x}) \quad \mathbf{B}(\mathbf{x}, t) = \sum_{\mathbf{g}} \mathbf{B}_{\mathbf{g}}(t) \psi_{\mathbf{g}}(\mathbf{x}) \quad (20)$$

By choosing for instance linear splines, one can obtain the discrete Maxwell equations projected on a staggered mesh (Yee's lattice) according to

$$\frac{d\mathbf{B}_{\mathbf{g}}}{dt} = -\mathbf{D} \times \mathbf{E}_{\mathbf{g}} \quad \frac{d\mathbf{E}_{\mathbf{g}}}{dt} = \mathbf{D} \times \mathbf{B}_{\mathbf{g}} - \frac{4\pi}{c} \langle \mathbf{J} \rangle_{\mathbf{g}}$$

where  $\mathbf{D}$  is the 2-point finite-difference operator. The condition  $\mathbf{D} \cdot \mathbf{B} = 4\pi \langle \rho \rangle_{\mathbf{g}}$ , true at  $t = 0$ , is satisfied for  $t > 0$  by centered time differences. The condition  $\mathbf{D} \cdot \mathbf{E}_{\mathbf{g}} = 4\pi \rho_{\mathbf{g}}$ , if true at initial time, is satisfied for  $t > 0$  if the continuity equation holds. It can be forced to hold following Esirkepov's procedure. However, in this case, energy conservation is lost.

A parallel PIC code `ALaDyn`, based on second- and fourth-order schemes, has been developed by the group of the University of Bologna [30,31]; a code based essentially on the same algorithms has been implemented on the GPU architectures [32]. Other approximations, based on a truncated moments expansion of the distribution function, suitable also to describe the beam plasma interaction, have been proposed [33,34].

## 7. Beam plasma acceleration

In recent years, the AWAKE collaboration [35] has been created, with the aim of exploring the beam-driven Plasma WakeField Acceleration (PWFA) based on protons as driver beam. Special emphasis was put on the analysis of the several key processes that are needed to achieve successfully the goal of PWFA.

The first step in this process has been the proposal of using high-energy protons for performing PWFA of electrons [6]. Numerical simulations [36] showed that a 1-TeV proton bunch, composed of  $10^{11}$  particles and with an rms length of 100  $\mu\text{m}$ , can generate a large enough plasma wave. The key point is the generation of such a short proton bunch, which is a true challenge. However, a milestone was achieved when numerical simulations showed [37,38] that even much longer bunches, comparable with those that can be generated in existing facilities, can excite a plasma wave, as long as the intensity of the proton bunch is modulated along its length. This opened the possibility of experimental verifications of the proposal, and hence the AWAKE collaboration has been set up to [35]:

- study the detail of the process of self-modulation of the long proton bunches;
- probe the acceleration process properly, by studying the properties of the generated wakefield;
- study the injection mechanism of multi-GeV electron bunches;
- develop plasma cells and mechanisms to generate short proton bunches.

The issue of generating short bunches is certainly a crucial one and it has been considered in detail, e.g. in Ref. [39], where several options have been considered, based on the performance of existing CERN accelerators and even including new techniques. In a first stage, the use of proton bunches extracted from the CERN Proton Synchrotron (PS) at 24 GeV was considered and numerical simulations [38] confirmed the validity of this option. Nevertheless, additional considerations, based both on physical arguments and on available infrastructure, suggested that the best choice would be to use a 400-GeV proton beam extracted from the CERN Super Proton Synchrotron (SPS) and this option (see Refs. [40–42] for more detail) was retained in the official proposal [35]. In the following, the key points of the AWAKE Design Report are addressed. In the case of LWFA, the driver is a laser pulse of length  $\sigma_z$ , comparable to the plasma wavelength  $\lambda_{pe}$ :

$$\sigma_z = \lambda_e \quad \text{with } \lambda_e = \frac{2\pi c}{\omega_e} \quad \text{and } \omega_e = \left( \frac{4\pi e \rho_e}{m_e} \right)^{1/2}$$

Under these conditions, a longitudinal accelerating field can be generated proportional to the breaking field EWB [43], which in turn is proportional to  $\rho_e^{1/2}$ . All this favors short length for the laser pulse and high density for the plasma. Whenever the typical bunch length  $\sigma_z$  is of the order of  $100\lambda_{pe}$ , then one has to operate in the so-called self-modulated PWFA regime [37]. In this regime, the transverse bunch size  $\sigma_r$  has to satisfy  $k_{pe}\sigma_r < 1$ , with  $k_{pe} = \omega_{pe}/c$ . Hence, the condition on a short bunch length can be translated into one on a small transverse bunch size, much easier to achieve even with conventional focusing devices available in a beam transfer line.

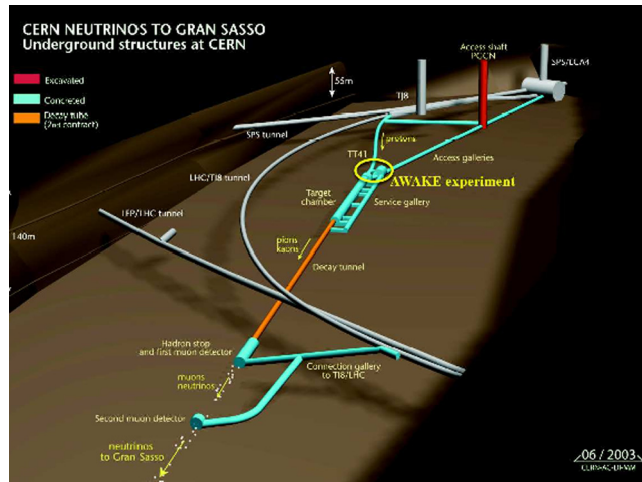


Fig. 1. (Color online.) Layout of the CNCS transfer line including the region where the AWAKE experiment should be installed (from Ref. [49]).

The self-modulated instability (SMI) generates a modulation of the bunch intensity along its length, and hence it can drive resonantly the plasma so that wakefields are generated. Unfortunately, the instability destroys the micro-bunching structure soon after the peak field is reached [44–46]. A mitigation measure was found in generating a plasma density gradient. It is worth mentioning that seeding the SMI is also an important point that will be probed with AWAKE. Indeed, the natural noise in the plasma should be enough to trigger the rise of the SMI [36]. Nonetheless, the SMI can be more efficiently induced by means of a short bunch preceding the long driver bunch or by a short laser pulse. The SMI can arise together with another instability, the hose instability (HI) [47] and in this respect seeding helps SMI to overcome HI [45,46]. The witness electron bunch will be side-injected into the plasma cell [48] at a longitudinal position where the amplitude of the wakefield generated by the long proton bunch has already reached saturation. The long,  $\sigma_z \gg \lambda_{pe}$ , low-energy electron bunch should be injected with an angle of few milli-radians with respect to the proton beam axis. The electrons will approach the seeding bunch and will be trapped into the wakefield, and later will be accelerated by the resulting buckets from the wakefield. In principle, a fraction of the electrons in the witness bunch corresponding to 5–40% should be trapped and accelerated to higher energies with a rather small relative energy spread, at the level of a percent. The scientific goals of the AWAKE collaboration rely heavily on the state-of-the-art in the field of instrumentation. The various devices are based on transition radiation (TR), which is emitted when charged particles traverse media with different refraction indexes. This type of radiation allows for fast diagnostic device, at the level of picoseconds. Two flavors of TR, namely optical transition radiation (OTR) and coherent transition radiation (CTR), will be used for a complete characterization of the bunch density distribution. An integral part of the beam instrumentation will be the electron spectrometer aimed at an accurate measurement of the electron bunch energy at the end of the process. The final choice for the location of the AWAKE experiment has been made: it will be located in the CERN Neutrino to Gran Sasso (CNCS) area (see Fig. 1).

The beam line to transfer the SPS-extracted proton beams towards the CNCS target will be re-used. However, the AWAKE experiment will be housed just upstream of the target station (see Fig. 2 for a layout of the experimental area). This will entail the modification of the last section of the existing proton beam line, in order to provide the required transverse focusing of the driver bunch at the location of the plasma cell. Moreover, an additional beam line to transport the electron beam to the plasma cell will be built.

The study and installation of the AWAKE experimental facility will be staged between the proton beam line, the proper experimental area, and the electron source and related beam line [35]. These activities will span a time period of about four years. The experimental activities with protons will be starting by the end of 2016, while those with electrons one year later. Overall the data taking should take place over a period of three to four years.

### 7.1. PIC simulations

As an example of applications of the Vlasov equations, we consider the case of a driver beam of electrons or protons exciting plasma waves by which a witness electron beam is accelerated. In a background plasma with electron density  $\rho_e$ , an electron or proton bunch with density  $\rho_b \ll \rho_e$  excites linear plasma waves whose longitudinal accelerating field is a few GV/m. In linear regimes, reached for higher densities  $\rho_b \gg \rho_e$ , the wave breaks and a bubble is formed in the plasma just like when the driver is a laser pulse. An energy doubling experiment in a nonlinear regime was carried out with a driver beam of 42 GeV in a plasma wakefield accelerator of 85 cm at SLAC [5] and the accelerating field was of 52 GV/m. In the bubble (blow out) regime, first proposed in [50], the radial confining field is linear  $E_r \approx 2\pi\rho_e r$  so that the electrons of the witness beam are accelerated just as in a conventional RF cavity. The drawbacks of the bubble regime are the instabilities

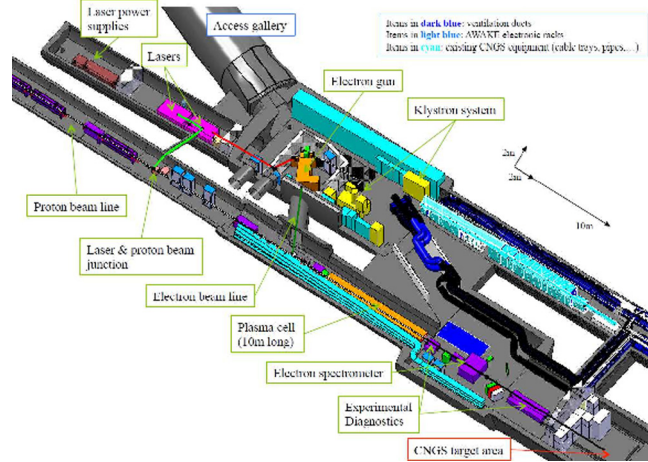


Fig. 2. (Color online.) Layout of the CNGS transfer line including the region where the AWAKE experiment should be installed (from Ref. [22]).

(wave-breaking spike on the first oscillation behind the beam driver), which do not allow a stable resonant response over large distances.

To overcome these limitations, a quasi-nonlinear regime (QNL) has been proposed [51] to preserve some aspects of the linear regime such as a constant plasma wavelength and maintain the resonance conditions.

The key parameter has then identified by the dimensionless charge quantity  $\hat{Q} = N_b (k_p)^3 e / \rho_e$ , which is the beam charge normalized to the electron charge located in a cubic plasma length  $k_p^{-1} = c / \omega_p$ . As usual,  $\omega_p = \sqrt{4\pi e \rho_e / m_e}$  is the electron plasma frequency.  $N_b$  is the number of protons in the bunch.

For a bi-Gaussian beam charge distribution with  $(\sigma_z, \sigma_r)$  sizes, the normalized charge reads:

$$\hat{Q} = (2\pi)^{3/2} \frac{\rho_b}{\rho_e} k_p^3 \sigma_z \sigma_r^2$$

where  $k_p = 2\pi / \lambda_p = \omega_p / c$ . A linear regime is characterized by  $\hat{Q} \ll 1$ . A QNL regime needs the peculiar condition that  $\rho_b / \rho_e > 1$  for bubble formation, but it has  $\hat{Q} < 1$  to preserve some linear features of the wakefield.

The linear response requires  $k_p \sigma_z \simeq \sqrt{2}$ , so that the QNL regime thus requires very thin beams  $\sigma_r \ll \sigma_z$ . In this parameter range, linear relations for the wakefield longitudinal field  $E_z$  can be extended, up to a limiting value of the  $\rho_b / \rho_e$  ratio, where wave breaking occurs:

$$E_z \simeq \frac{mc\omega_p}{e}, \quad \sim 100 \sqrt{\rho_e / e} [\text{cm}^{-3}] \text{ V m}^{-1}$$

Numerical simulations using 3D OSIRIS PIC code [52] or 2D cylindrical [53,54] have already documented some aspects of QNL regimes, relevant for experimental applications. For a proton bunch in the linear regime the maximum available longitudinal field [6] is:

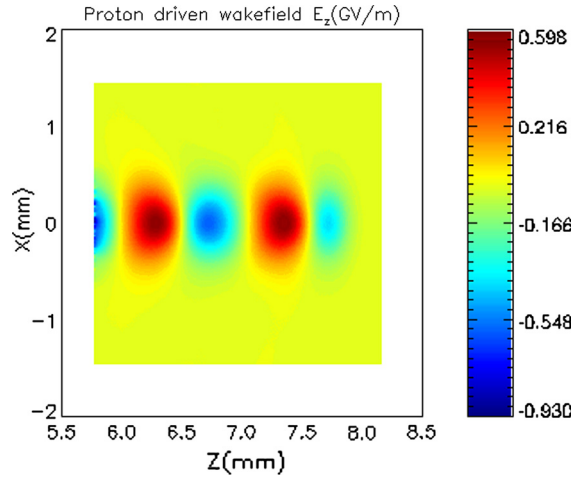
$$E_z = 240 \left( \frac{N_b}{4 \times 10^{11}} \right) \left( \frac{0.6}{\sigma_z (\text{mm})} \right)^2$$

A specific implementation of the standard PIC schemes has been achieved in the code ALaDyn [55] to include the beam-driven PWFA conditions, in order to ensure accuracy and efficiency. As a first application, some examples of QNL regime formation on short time scale, in configurations with one-driver or three-driver beams, have been provided. A similar approach holds when the driver is a proton beam; the condition for linearity  $\hat{Q} \ll 1$  is the same.

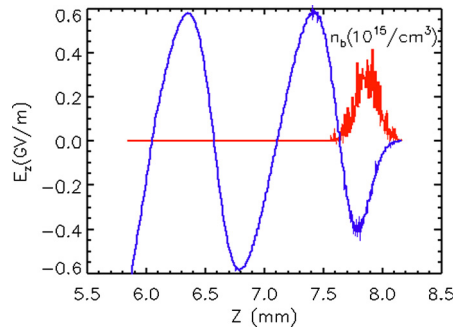
Labeling with  $(\mathbf{x}_e, \mathbf{p}_e)$  and  $(\mathbf{x}_b, \mathbf{p}_b)$  the positions and momenta for electrons (macroparticles) of the background plasma and of the bunch, we can say that both species have the same equations of motion. Charge densities and currents are split according to  $\rho = \rho_b + \rho_e$ ,  $\mathbf{J} = \mathbf{J}_b + \mathbf{J}_e$ . Each species satisfies the corresponding set of Maxwell equations with its proper charge density and current. For initial conditions, represented by a beam freely moving in space at speed  $\mathbf{v}_0$  along the  $z$  axis with a density  $\rho_0(\mathbf{x})$  in the comoving frame, the initial current distribution is  $\mathbf{J}_{0b} = \mathbf{v}_0 \rho_{0b}$  in the rest frame. The potentials fields in rest frame satisfy the equations

$$\left[ \frac{1}{\gamma_0^2} \frac{\partial^2}{\partial z^2} + \nabla_{\perp}^2 \right] \phi_b = -\omega_p^2 \rho_{0b}, \quad A_z^{(b)} = \beta_0 \phi_b \mathbf{A}_{b\perp} = 0$$

The corresponding electric and magnetic fields immediately follow, and it is clear that the components of the fields orthogonal to the propagation direction are dominant and provide the leading contribution to the Lorentz force. The sources



**Fig. 3.** (Color online.) Two-dimensional plot of the  $E_z$  wakefield on the  $(z, x)$ ,  $y = 0$  plane. The position for optimal acceleration of an electron witness bunch is at  $z \simeq 6.8$  mm.



**Fig. 4.** (Color online.) Lineout of the  $E_z(z)$  field with superposed density of the proton driver, to document the forward shifted wake structure compared to the case of electron driven wakefield.

and the fields evolve by pure advection on a short time-scale and on a long time-scale they are modified by the plasma wakefield.

On the computational side, this scale separation entails stiffness and errors on numerical integration. The transverse fields decay as  $1/r$  and involve problems with the boundary condition. This problem was solved by separating fields and sources for the beam into the advected part and a remainder [54].

$$\begin{aligned} \rho_b &= \rho_{0b}(z - v_0t, x, y) + \delta\rho_b & \mathbf{J}_b &= \mathbf{J}_{0b}(z - v_0t, x, y) + \delta\mathbf{J}_b \\ \mathbf{E}_b &= \mathbf{E}_{0b}(z - v_0t, x, y) + \delta\mathbf{E}_b & \mathbf{B}_b &= \mathbf{B}_{0b}(z - v_0t, x, y) + \delta\mathbf{B}_b \end{aligned}$$

the residual parts can be evolved separately or can be reabsorbed in the plasma field components. Symbols with the zero subscript denote initial values.

The application of this strategy to the case when the proton beam acts as a driver does not imply any significant change. In the specific case of AWAKE, where the plasma wavelength is 1.35 mm and the longitudinal bunch length is 0.1 mm, choosing a grid spacing  $\Delta z = 10 \mu\text{m}$  should allow one to simulate the beam propagation for about 1 m using a moderate size parallel architecture.

Here we shortly report on a preliminary numerical investigation of a proton-driven wakefield, following the computational design introduced previously (see Figs. 3–5).

We have considered a Gaussian proton beam with size  $\sigma_z = 0.1$  mm,  $\sigma_x = \sigma_y = 2\sigma_z$ , and density parameter  $\rho_b/\rho_e = 0.3$ , where  $(\rho_e/e) = 1.0 \times 10^{15} \text{ cm}^{-3}$  is the electron density of the background plasma. The driven wakefield is in the linear regime, allowing us to check the resulting maximum values of the longitudinal  $E_z$  accelerating field against the available analytical formulas [56].

## 8. Conclusions

The space-charge effects in high intensity accelerators and plasma acceleration, driven by a charged beam or a laser pulse, have a common theoretical framework: the Vlasov equation coupled self-consistently with the Poisson or the Maxwell

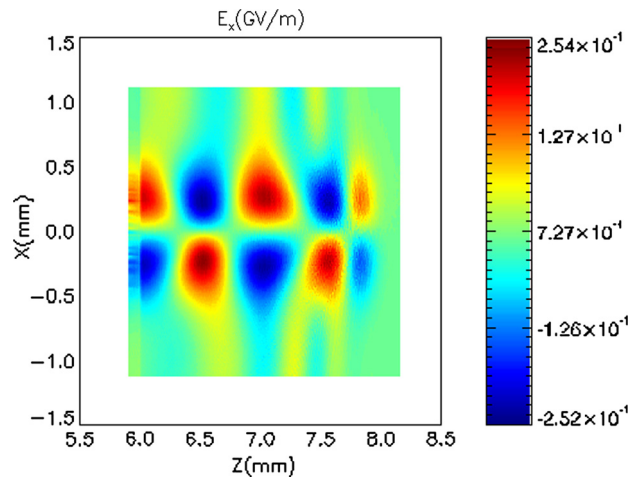


Fig. 5. (Color online.) The  $E_x$  wake field, documenting the focusing–defocusing action of the transverse electric field.

equation. We have presented a brief review of this theory starting from the variational principles, which are the natural framework to discuss the conservation laws and develop approximation schemes, like the particle-in-cell (PIC) method. For the space charge, the analytic KV theory applicable to a 2D beam and the general adiabatic theory applicable to a flat 1D beam have been summarized. For these problems, the core PIC approximations are an efficient Poisson solver. In the electromagnetic case, the Maxwell–Vlasov equations have been presented in the same variational framework. We have sketched how to obtain the conservation laws and how to formulate the PIC approximation schemes. The result is based on the introduction of a finite basis for the potentials and on sampling the distribution function with shaped numerical particles. The exact formulation of the balance equations and conservation laws for PIC schemes is still an open problem, but the variational framework is appropriate to provide the right answers. Finally, the problem of electron accelerators in the wake field of plasma waves excited by a charged driver has been considered and illustrated with a simulation, based on the code ALaDyn, in conditions similar to the AWAKE experiment, where the driver is a proton beam. The possibility of achieving fields of some GV/m in the linear regime is confirmed starting from short bunches (below 1 mm). Their generation via modulation instabilities, even though it has been suggested by simulations, is waiting to be experimentally confirmed. In spite of the challenges which include the stability on several meters of the driver and the control of longitudinal and transverse growth, the AWAKE project opens a new route for electron acceleration up to the TeV threshold. On the computational side, the search for more efficient and reliable PIC approximation is continuing. It was shown that high-order schemes may have an advantage in the description of a laser pulse, since they improve the dispersion relation and reduce the noise. A better control on the numerical heating and on the conservation laws for charge, energy and momentum might be achieved, within the theoretical framework we have presented. Improvement of the PIC algorithms and of the underlying hardware might allow us to gain one order of magnitude in performances within the next few years, as required for planning and interpreting new challenging experiments like AWAKE.

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