Relativistic Lagrangian and Hamiltonian Description of a Beam with Space-Charge

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June 24, 2016

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[‡]This work has been supported by the Natural Sciences and Engineering Research Council of Canada. TRIUMF also receives federal funding via a contribution agreement through the National Research Council of Canada.

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1 Introduction

We recently became interested in a paper by H. Qin *et al.* [1] that describes a symplectic particle-in-cell (PIC) tracking algorithm. The algorithm they propose is radically different from usual PIC tracking algorithms for particle accelerators. In a usual PIC codes, the electromagnetic potential/field is recalculated 'from scratch' (from the distribution of macro particles, solving Poisson's equation) at every step; whereas in their algorithm both the potential/field and the coordinates of macro particles are pushed self-consistently over each time step using the same symplectic integrator.

In this note we describe the work we have accomplished so far toward implementing a similar algorithm to study space-charge effects in TRIUMF 500 MeV cyclotron.

2 Lagrangian

2.1 Notation

In this paper we use notation based on F.E. Low [2] and H. Cendra *et al.* [3]. All bold symbols are used to denote vectors in $\mathbb{R}^3$. Our beam/plasma is described as a continuous fluid. The position in real space of a fluid particle is written:

$$\mathbf{x}(\mathbf{x}_1, \mathbf{v}_1, t) := \mathbf{x}_1 + \boldsymbol{\Delta}\mathbf{x}(\mathbf{x}_1, \mathbf{v}_1, t - t_1), \tag{1}$$

where $\mathbf{x}_1$ and $\mathbf{v}_1$ are the position and velocity of the fluid particle at time t_1, and $\boldsymbol{\Delta}\mathbf{x}(\mathbf{x}_1, \mathbf{v}_1, 0) = \mathbf{0}$.

Φ and $\mathbf{A}$ are the electric scalar and magnetic vector potential. They are related to the electric and magnetic fields through:

$$\begin{aligned} \boldsymbol{\mathcal{E}} &= -\nabla\Phi - \frac{\partial \mathbf{A}}{\partial t}; \\ \mathbf{B} &= \nabla \times \mathbf{A}. \end{aligned} \tag{2}$$

$f(\mathbf{x}, \mathbf{v}, t) : \mathbb{R}^7 \longmapsto \mathbb{R}$ is our plasma/beam density function. The "initial" density function is defined as $f_1(\mathbf{x}, \mathbf{v}) = f(\mathbf{x}, \mathbf{v}, t_1)$.

2.2 Natural Units

We choose a system of units such that $\mathrm{e} = \mathrm{c} = \epsilon_0 = \mu_0 = 1$ (respectively: the elementary charge, speed of light, vacuum permitivity and permeability). The conversion

of electric charge, vector potential, electric field, mass, time and length to SI units follows respectively:

$$\begin{aligned} q =& \frac{\mathrm{eq}_{\mathrm{SI}}}{\sqrt{\epsilon_0}} \\ \mathbf{A} =& \frac{\mathbf{A}_{\mathrm{SI}}}{\sqrt{\mu_0}} \\ \boldsymbol{\mathcal{E}} =& \sqrt{\epsilon_0}\boldsymbol{\mathcal{E}}_{\mathrm{SI}} \\ m =& \mathrm{c}^2\mathrm{m}_{\mathrm{SI}} \\ t =& \mathrm{ct}_{\mathrm{SI}} \\ l =& l_{\mathrm{SI}}. \end{aligned} \tag{3}$$

2.3 Relativistic Space-Charge Lagrangian

Based on the Lagrangian proposed by F.E. Low [2] we write the Lagrangian of a given initial plasma density function f_1:

$$\begin{aligned} &L(\mathbf{x}, \dot{\mathbf{x}}, \Phi, \dot{\Phi}, \mathbf{A}, \dot{\mathbf{A}}; t) = \\ &\iint f_1(\mathbf{x}_1, \mathbf{v}_1) \left[-m\sqrt{1-\dot{\mathbf{x}}^2} + q\dot{\mathbf{x}} \cdot \mathbf{A}(\mathbf{x}, t) - q\Phi(\mathbf{x}, t) \right] \mathrm{d}\mathbf{v}_1 \, \mathrm{d}\mathbf{x}_1 \\ +&\frac{1}{2} \int \left[|\nabla\Phi(\mathbf{x}_1, t) + \dot{\mathbf{A}}(\mathbf{x}_1, t)|^2 - |\nabla \times \mathbf{A}(\mathbf{x}_1, t)|^2 \right] \mathrm{d}\mathbf{x}_1, \end{aligned} \tag{4}$$

where dots stand for partial derivatives w.r.t. time. The first term is a 6-D integral; it can be seen as a sum over the (continuous) set of fluid particle. The second term is a usual (3-D) volume integral. Note that the projection onto real-space of the 6-D volume of integration coincides with the 3-D volume of integration of the second term: this volume is the volume contained inside the vacuum chamber of our particle accelerator.

Compared to F.E. Low's Lagrangian the non-relativistic kinetic energy term has been replaced by $-m\sqrt{1-\dot{\mathbf{x}}^2}$.

We will now show how the principle of least action applied to the action associated with this Lagrangian:

$$\mathcal{S} = \int L \mathrm{d}t, \tag{5}$$

leads to well-known "equations of motion".

2.3.1 Variation of the Action in x

Variation of the action (see Appendix 5.1) in $\mathbf{x}$ leads:

$$\frac{\delta \mathcal{S}}{\delta \mathbf{x}} = f_1 \left[q\nabla(\dot{\mathbf{x}} \cdot \mathbf{A}) - q\nabla\Phi - \left. \frac{\partial \left(\gamma m \dot{\mathbf{x}} + q\mathbf{A}\right)}{\partial t} \right|_{\mathbf{x}_1, \mathbf{v}_1} \right], \tag{6}$$

where γ is the Lorentz factor: $\gamma = \dfrac{1}{\sqrt{1 - \dot{\mathbf{x}}^2}}$.
Using chain rule:

$$\begin{aligned} \left. \frac{\partial \mathbf{A}}{\partial t} \right|_{\mathbf{x}_1, \mathbf{v}_1} &= \left. \frac{\partial \mathbf{A}}{\partial t} \right|_{\mathbf{x}, \dot{\mathbf{x}}} + (\dot{\mathbf{x}} \cdot \nabla_{\mathbf{x}})\mathbf{A} + (\ddot{\mathbf{x}} \cdot \nabla_{\dot{\mathbf{x}}})\mathbf{A} \\ &= \frac{\partial \mathbf{A}}{\partial t} + (\dot{\mathbf{x}} \cdot \nabla)\mathbf{A}\,. \end{aligned} \tag{7}$$

The vector algebra identity:

$$\dot{\mathbf{x}} \times (\nabla \times \mathbf{A}) = \nabla(\dot{\mathbf{x}} \cdot \mathbf{A}) - (\dot{\mathbf{x}} \cdot \nabla)\mathbf{A}, \tag{8}$$

together with Hamilton's principle of least action:

$$\frac{\delta \mathcal{S}}{\delta \mathbf{x}} = 0, \tag{9}$$

leads to Lorentz' equation:

$$m\frac{\mathrm{d}\gamma\dot{\mathbf{x}}}{\mathrm{d}t} = q\left[-\nabla\Phi - \frac{\partial \mathbf{A}}{\partial t} + \dot{\mathbf{x}} \times (\nabla \times \mathbf{A}) \right]. \tag{10}$$

2.3.2 Variation of the Action in Φ

The 6-D integral can be split into teo interlocked 3-D integrals, following Fubini's theorem. Variation of the action in Φ leads then to:

$$\frac{\delta \mathcal{S}}{\delta \Phi} = -\int q f_1 \mathrm{d}\mathbf{v}_1 - \nabla \cdot \left(\nabla\Phi + \dot{\mathbf{A}} \right), \tag{11}$$

where we identify:

$$\int q f_1(\mathbf{x}_1, \mathbf{v}_1)\mathrm{d}\mathbf{v}_1 = \rho(\mathbf{x}_1, t_1)\,, \tag{12}$$

as the local charge density calculated at time=t_1. Hamilton's principle of least action:

$$\frac{\delta \mathcal{S}}{\delta \Phi} = 0, \tag{13}$$

leads (at time=t_1) to Maxwell Gauss's equation:

$$\nabla \cdot \left(-\nabla\Phi - \dot{\mathbf{A}} \right) = \rho \tag{14}$$

2.3.3 Variation of the Action in A

Similarly the variation of the cation in $\mathbf{A}$ leads:

$$\frac{\delta \mathcal{S}}{\delta \mathbf{A}} = \int q\dot{\mathbf{x}} f_1 \, \mathrm{d}\mathbf{v}_1 - \frac{\partial}{\partial t}\left(\nabla\Phi + \frac{\partial \mathbf{A}}{\partial t} \right) - \nabla \times (\nabla \times \mathbf{A}) \tag{15}$$

where we recognize:

$$\int q\dot{\mathbf{x}} f_1(\mathbf{x}_1, \mathbf{v}_1) \, \mathrm{d}\mathbf{v}_1 = \mathbf{j}(\mathbf{x}_1, t_1) \tag{16}$$

as the local current density calculated at time=t_1. Hamilton's principle of least action:

$$\frac{\delta \mathcal{S}}{\delta \Phi} = 0, \tag{17}$$

leads (at time=t_1) to Maxwell Ampère's equation:

$$\nabla \times (\nabla \times \mathbf{A}) = \mathbf{j} - \frac{\partial}{\partial t}\left(\nabla\Phi + \frac{\partial \mathbf{A}}{\partial t} \right) . \tag{18}$$

3 From Lagrangian to Hamiltonian

We would like now to apply to our Lagrangian a Legendre transformation to obtain the corresponding Hamiltonian. With Lagrangians defined from a Lagrangian densities such as:

$$L = \int \mathcal{L} \, \mathrm{d}\mathbf{x} \, , \tag{19}$$

the corresponding Hamiltonian density $\mathcal{H}$ can be obtained from:

$$\mathcal{H}(\boldsymbol{\mathcal{P}}_i, q_i; t) = \sum_i (\boldsymbol{\mathcal{P}}_i \cdot \dot{q}_i) - \mathcal{L}(q_i, \dot{q}, t) \, , \tag{20}$$

where the conjugate momenta densities are defined by:

$$\boldsymbol{\mathcal{P}}_i = \frac{\partial \mathcal{L}}{\partial \dot{q}} \, . \tag{21}$$

Here again dots stand for partial derivatives w.r.t. time. The resulting Hamiltonian H then writes:

$$H = \int \mathcal{H} \mathrm{d}\mathbf{x} \,. \tag{22}$$

In our case the Lagrangian derives from two separate Lagrangian densities:

$$L = \iint \mathcal{L}_{6\mathrm{D}}(\mathbf{x}, \dot{\mathbf{x}}, \Phi, \mathbf{A}) \, \mathrm{d}\mathbf{v}_1 \, \mathrm{d}\mathbf{x}_1 + \int \mathcal{L}_{3\mathrm{D}}(\Phi, \mathbf{A}, \dot{\mathbf{A}}) \, \mathrm{d}\mathbf{x}_1 .$$

Note the variable dependencies of the Lagrangian: dotted terms that appear explicitly in one Lagrangian density do not appear explicitly in the other one. This will allow us to take the Legendre transform of each Lagrangian density independently and combine the resulting Hamiltonians.

3.1 Temporal Gauge

The lack of explicit dependency on $\dot{\Phi}$ in our Lagrangian implies that Φ has no canonically conjugated momentum density. To overcome this degeneracy, we choose to fix $\Phi = 0$ (as in Ref. [1]). This incomplete gauge condition is referred to as temporal gauge (or Weyl gauge). Within this gauge the electric field is given by:

$$\boldsymbol{\mathcal{E}} = -\frac{\partial \mathbf{A}}{\partial t} \,. \tag{23}$$

3.2 First Hamiltonian Density

Canonically conjugated pairs associated with $\mathcal{L}_{6\mathrm{D}}$ are:

$$\mathbf{x} \text{ and } \boldsymbol{\mathcal{P}} = \frac{\partial \mathcal{L}_{6\mathrm{D}}}{\partial \dot{\mathbf{x}}} = f_1 \left(\frac{m\dot{\mathbf{x}}}{\sqrt{1 - \dot{\mathbf{x}}^2}} + q\mathbf{A} \right) . \tag{24}$$

In this case, the Legendre transformation (Eq. 20) writes:

$$\mathcal{H}_{6\mathrm{D}} = \boldsymbol{\mathcal{P}} \cdot \dot{\mathbf{x}} - \mathcal{L}_{6\mathrm{D}}. \tag{25}$$

Substituting leads:

$$\mathcal{H}_{6\mathrm{D}} = \frac{f_1 m}{\sqrt{1 - \dot{\mathbf{x}}^2}} \,. \tag{26}$$

To properly transfer into coordinate-momenta space we rearrange for $\mathbf{x}$ in terms of $\boldsymbol{\mathcal{P}}$ in Equation 24:

$$\dot{\mathbf{x}} = \frac{\boldsymbol{\mathcal{P}} - f_1 q \mathbf{A}}{\sqrt{f_1^2 m^2 + (\boldsymbol{\mathcal{P}} - f_1 q \mathbf{A})^2}} \,. \tag{27}$$

After substitution into the Hamiltonian:

$$\mathcal{H}_{6\mathrm{D}}(\mathbf{x}, \boldsymbol{\mathcal{P}}; t) = \sqrt{f_1^2 m^2 + (\boldsymbol{\mathcal{P}} - f_1 q \mathbf{A}(\mathbf{x}, t))^2} \,. \tag{28}$$

3.3 Second Hamiltonian Density

Canonically conjugated pairs associated with $\mathcal{L}_{3D}$ are:

$$\mathbf{A} \text{ and } -\boldsymbol{\mathcal{E}}\,. \tag{29}$$

The Legendre transformation gives:

$$\mathcal{H}_{3D} = -\boldsymbol{\mathcal{E}} \cdot \frac{\partial \mathbf{A}}{\partial t} - \mathcal{L}_{3D}\,. \tag{30}$$

Using Eq. 3.1 and substituting the reduced Lagrangian leads:

$$\mathcal{H}_{3D}(\mathbf{A}, \boldsymbol{\mathcal{E}}; t) = \frac{\boldsymbol{\mathcal{E}}^2}{2} + \frac{\nabla \times \mathbf{A}^2}{2}\,. \tag{31}$$

4 Resulting Hamiltonian

Combining the two Hamiltonian densities gives:

$$H(\mathbf{x}, \boldsymbol{\mathcal{P}}, \mathbf{A}, -\boldsymbol{\mathcal{E}}; t) = \iint \sqrt{\tilde{m}^2 + (\boldsymbol{\mathcal{P}} - \tilde{q}\mathbf{A}^2(\mathbf{x}, t))}\mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{x}_1 \; + \int \frac{\boldsymbol{\mathcal{E}}^2}{2} + \frac{\nabla \times \mathbf{A}^2}{2}\,\mathrm{d}\mathbf{x}_1\,, \tag{32}$$

with $\tilde{m} = f_1 m$ and $\tilde{q} = f_1 q$.

Compared to the Hamiltonian used in Ref. [1], this one is truly relativistic, and is fully expressed in terms of canonically conjugated variables; we do not need to use a modified Poisson bracket to obtain equations of motions.

4.1 Equations of Motions from Hamiltonian

Hamilton's equations for continuous systems writes:

$$\frac{\partial q_i}{\partial t} = +\frac{\delta H}{\delta \boldsymbol{\mathcal{P}}_i}, \quad \frac{\partial \boldsymbol{\mathcal{P}}_i}{\partial t} = -\frac{\delta H}{\delta q_i}; \tag{33}$$

where $\frac{\delta}{\delta}$ stand for functional derivatives(see Appendix 5.1). From the Hamiltonian given in Eq. 32 we derive the following equations of motions:

$$\begin{aligned} \dot{\mathbf{x}} &= \frac{(\boldsymbol{\mathcal{P}} - \tilde{q}\mathbf{A})}{\sqrt{\tilde{m}^2 + (\boldsymbol{\mathcal{P}} - \tilde{q}\mathbf{A})^2}} \\ \dot{\boldsymbol{\mathcal{P}}} &= -\tilde{q}\nabla(\dot{\mathbf{x}} \cdot \mathbf{A}) \\ \dot{\mathbf{A}} &= -\boldsymbol{\mathcal{E}} \\ -\dot{\boldsymbol{\mathcal{E}}}(\mathbf{x}_1, t_1) &= -\nabla \times (\nabla \times \mathbf{A}(\mathbf{x}_1, t_1)) + \mathbf{j}(\mathbf{x}_1, t_1) \end{aligned} \tag{34}$$

where dots are partial time derivatives.

Note that the last equation of motion is only valid at time=t_1, since the current density $\mathbf{j}$ is calculated at t_1. To obtain this equation of motion at a time=t_2, one has to start from a different Hamiltonian H_{f_2} expressed using t_2 as "initial" time. This approach is perfectly compatible with a step-wise integration of the equation of motion, and implies that $\mathbf{j}$ has to be re-calculated at every step.

5 Appendix

5.1 Functional Derivative

Let $\mathcal{C}$ be the configuration space of derivable functions from $\mathbb{R}^n$ to $\mathbb{R}$. Let $\mathcal{S}$ be a mappings from $\mathcal{C}$ to $\mathbb{R}$ (called a functional) such that:

$$\mathcal{S}(g) = \int \mathcal{L}(g, \frac{\partial g}{\partial x_1}, \frac{\partial g}{\partial x_2}, .., \frac{\partial g}{\partial x_n}) \mathrm{d}x_1 \mathrm{d}x_2 .. \mathrm{d}x_x, \tag{35}$$

where g is an element of $\mathcal{C}$. The functional derivative of $\mathcal{S}$ with respect to g is defined as:

$$\frac{\delta \mathcal{S}}{\delta g} = \frac{\partial \mathcal{L}}{\partial g} - \frac{\partial}{\partial x_1} \frac{\partial \mathcal{L}}{\partial \frac{\partial g}{\partial x_1}} - \frac{\partial}{\partial x_2} \frac{\partial \mathcal{L}}{\partial \frac{\partial g}{\partial x_2}} .. - \frac{\partial}{\partial x_n} \frac{\partial \mathcal{L}}{\partial \frac{\partial g}{\partial x_n}}, \tag{36}$$

see for instance Ref. [4].

For the purpose of this paper it is useful to generalize this definition to a configuration space $\mathcal{C}^3$ of functions from $\mathbb{R}^n$ to $\mathbb{R}^3$; in this case $\mathcal{S}$ becomes a mappings from $\mathcal{C}^3$ to $\mathbb{R}$. Let now $g \in \mathcal{C}^3$ such as:

$$g(x_1, x_2, .., x_n) = \begin{pmatrix} g_1(x_1, x_2, .., x_n) \\ g_2(x_1, x_2, .., x_n) \\ g_3(x_1, x_2, .., x_n) \end{pmatrix}, \tag{37}$$

then:

$$\frac{\delta \mathcal{S}}{\delta g} = \begin{pmatrix} \frac{\delta \mathcal{S}}{\delta g_1} \\ \frac{\delta \mathcal{S}}{\delta g_2} \\ \frac{\delta \mathcal{S}}{\delta g_3} \end{pmatrix}. \tag{38}$$

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