IL NUOVO CIMENTO Vol. 32 C, N. 2 Marzo-Aprile 2009
DOI 10.1393/ncc/i2009-10407-7

Colloquia: CSFI 2008

Covariant self-fields regularization in dense electron beams

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(ricevuto il 22 Giugno 2009; pubblicato online il 28 Settembre 2009)

Summary. — A critical issue in the development of coherent X-ray sources as FEL and SR facilities is the generation of high peak brilliance electron beams. Detailed simulations of such "dense" systems require self-interaction effects to be carefully accounted for in diverse dynamical conditions ranging from low energies where quasi-static space charge effects dominate, to the highly relativistic regimes of the kind encountered, *e.g.*, in magnetic compressors, where acceleration fields prevail and retarded effects cannot be neglected. In *principia prima* Monte Carlo codes the electron beam is usually modelled as a collection of mutually interacting objects, whose number is bounded because of practical computer limitations. As a consequence suitable techniques must be devised to achieve stability and suppress numerical artifacts. In this paper a covariant approach to self-fields regularization is described, in the context of TREDI simulation code, a fully 3D Monte Carlo accounting for electron beam self-interaction by means of Lienard-Wiechert retarded potentials.

PACS 52.59.Sa – Space-charge-dominated beams.
PACS 52.59.-f – Intense particle beams and radiation sources.
PACS 41.60.Ap – Synchrotron radiation.

1. – Introduction

A critical issue in the development of coherent high brilliance X-ray sources is the generation of high brilliance (high current/low emittance) electron beams. Study of such "dense" systems was the original motivation for the development of TREDI [1], a fully 3D Monte Carlo devoted to simulation of non axi-symmetric beam dynamics in RF photo-injectors by direct integration of trajectories while accounting for self-fields through Lienard-Wiechert [2] potentials. From the primal version, TREDI has now evolved to a full-fledged tool with a complete set of insertion devices that can be used, *e.g.*, for start-to-end simulations of emittance growth in magnetic beam compressors due radiative/acceleration fields (Coherent Synchrotron Radiation).

Principia prima Monte Carlo codes like TREDI usually model the beam as a collection of "macroparticles", whose number is bounded because of practical computer limitations. Therefore, in all practical cases, each macroparticle mimics a fairly large number of real electrons. As a consequence, whenever self fields cannot be neglected, suitable techniques must be devised to cancel numerical artifacts [3] like, *e.g.*, the unphysical hard collisions due to the huge electromagnetic fields that develop whenever macroparticles approach each other. While this is the typical case at low energies where short-range space charge effects dominate, other regimes exist—those occurring inside magnetic compressors, for example—where long-range radiation/acceleration fields prevail. In this respect, it is worth remarking that self-interaction must only smoothed off, not be cleared out (avove all, dominant contributions...). The variety of conditions faced by the electron beam during the acceleration, the different nature of self-interactions involved command a broader understanding of the concept itself of "proximity", and call for a unified, alternative approach to the regularization problem. The procedure adopted in TREDI to achieve regularization of velocity (Coulomb) fields to be summarized in the next section, with a some notes devoted to the work in progress on the code and concluding remarks.

2. – Smoothing of EM fields

The smoothing of EM self-fields adopted in TREDI is based on the concept of *form factor*, *i.e.* assumption that dynamical objects are extended rather than point-like charge distributions (see, *e.g.* [4]). While this approach has proven very effective in quantum electrodynamics, where examples abound, is far less common in classical electromagnetism, essentially for lack of applications, except perhaps for the rare efforts aimed at a theory free from divergencies [5]. For this reason, while in quantum electrodynamics it has been framed in a covariant fashion, it is not surprising that the solid *classical* paradigm this idea is based upon—Gauss' theorem—is invariably left aside as a concept fully compliant with special relativity.

In the classical context considered here, a covariant approach has at least two valuable properties: consistency, for the regularization procedure depends uniquely on *self-interaction*, *i.e.* smoothing turns to be *naturally* independent of the dynamical regime of the beam in the laboratory frame (which is not a covariant concept); ease of use, as the calculation can be actually carried out without transforming dynamical variables to the beam rest frame (granted for the sake of argument that it exists for a many-body system, as in numerical codes based on solution of Poisson's PDE [6]).

The covariant smoothing is based upon the separation of the EM fields produced by a moving charge q into a "velocity" and an "acceleration" term [2]

$$\mathbf{E} = \overbrace{q\left[\frac{\mathbf{n}-\boldsymbol{\beta}}{\gamma^2\left(1-\mathbf{n}\cdot\boldsymbol{\beta}\right)^3 R^2}\right]_{\mathrm{ret}}}^{\text{velocity term}} + \overbrace{\frac{q}{c}\left[\frac{\mathbf{n}\times\left[\left(\mathbf{n}-\boldsymbol{\beta}\right)\times\dot{\boldsymbol{\beta}}\right]}{\left(1-\mathbf{n}\cdot\boldsymbol{\beta}\right)^3 R}\right]_{\mathrm{ret}}}^{\text{acceleration term}} \qquad \mathbf{B} = \mathbf{n}\times\mathbf{E} \tag{1}$$

can be cast as well in a manifestly covariant form:

$$F^{\mu\nu} = \overbrace{q\left[\frac{1}{S^3(V)}T^{\mu\nu}(V)\right]_{\mathrm{ret}}}^{\text{velocity term}} + \overbrace{q\left[\frac{1}{S^2(V)}\left\{T^{\mu\nu}(W)-\frac{S(W)}{S(V)}T^{\mu\nu}(V)\right\}\right]_{\mathrm{ret}}}^{\text{acceleration term}}. \tag{2}$$

Here $V = (\gamma, \gamma\overrightarrow{\beta})$ is the source 4-velocity (hereupon $c = 1$) and $W \equiv \mathrm{d}V/\mathrm{d}\tau$ the 4-acceleration (*i.e.* the derivative of V w.r.t. proper time τ). The subscript "ret" means fields are produced by the source at "retarded" time, *i.e.* when crossing the past light cone of the observer. In (1) R is the retarded distance, so that $(R, R\,\mathbf{n})$ ($\mathbf{n}$ is the versor from source to observer) is the space-time time separation between the emission and absorption events (note that $(R, R\,\mathbf{n})^2_{\mathrm{ret}} = 0$). The symbols S and $T^{\mu\nu}$ denote a scalar (0-form) and a tensor (2-form) function, respectively, defined as follows:

$$(3)\qquad \begin{array}{lcllcl} S(U) & = & (x-r)\cdot U & \Longrightarrow & S(V) & \equiv \gamma R(1-\mathbf{n}\cdot\boldsymbol{\beta}), \\ T^{\mu\nu}(U) & = & (x-r)^\mu U^\nu - (x-r)^\nu U^\mu & \Longrightarrow & T^{i0}(V) & \equiv \gamma R(\mathbf{n}-\boldsymbol{\beta}). \end{array}$$

It is clear that $S(V) \to 0$ for $R \to 0$ or $\boldsymbol{\beta} \approx \mathbf{n}$, or both. The Coulomb term genuinely diverges at short distances, because of its R^{-2} scaling. Acceleration field diverges as well, yet more gently because of its R^{-1} behaviour. On the other hand, even though $1 - \mathbf{n}\cdot\boldsymbol{\beta}$ cannot strictly vanish, for relativistic particles and $\boldsymbol{\beta}$ nearly parallel to $\mathbf{n}$, it can go so close to that condition to make the acceleration fields to experience a growth by many orders of magnitude. This "collinear blazing" can extend at large distances from the radiating charge because of the slow field's fall off ($\approx R^{-1}$, as compared to the $\approx R^{-2}$ behaviour of the Coulomb term). Note that $\boldsymbol{\beta} \approx \mathbf{n}$ implies $\gamma \gg 1$ as well ($\beta \approx 1$), meaning that Coulomb fields are strongly suppressed w.r.t. acceleration terms.

The previous remarks show that kinematical circumstances at which the blowing of velocity and acceleration fields occur are inherently different. This must be taken into account when devising a procedure to regularize EM fields produced by macroparticles in a Monte Carlo simulation. What seems most sensible in this respect is to put (in a covariant fashion!) in front of $F_V^{\mu\nu}$ "regularizing" terms so that $F_V^{\mu\nu}$, $F_A^{\mu\nu} \to 0$ for $R \to 0$. Regularization of $F_A^{\mu\nu}$ for $\boldsymbol{\beta} \approx \mathbf{n}$ is much more difficult, basically for lack of such a compelling physical motivation as Gauss' theorem, and will not be discussed here. In both cases preserving the tensor structure of the fields requires multiplication either by a Lorentz scalar or a 2nd-rank tensor to be partially saturated with r.h.s. of (2). For $R \to 0$ the simplest and physically cogent choice is to introduce an "effective" charge (a Lorentz scalar!) $q_{\mathrm{eff}}(\mathbf{R})$ such that

$$(4)\qquad q_{\mathrm{eff}}(\mathbf{R})/S^3(V) \to 0 \qquad \text{for} \qquad R \to 0.$$

It is easily seen from (2) that (4) implies regularization of $F_V^{\mu\nu}$ and, *a fortiori*, of $F_A^{\mu\nu}$.

A covariant expression for the effective charge fulfilling the (4) can be devised assuming the macroparticle in its rest frame to be described by the static charge density:

$$(5)\qquad \rho(\mathbf{R}) = \frac{q}{\sqrt{\det\widehat{\sigma}}}\cdot\mathcal{F}\left[\mathbf{R}^T\cdot\widehat{\boldsymbol{\sigma}}^{-1}\cdot\mathbf{R}\right],$$

where $\mathbf{R}$ is the 3-distance between emitter and observer, $\widehat{\boldsymbol{\sigma}}$ is a symmetric, definite positive, 3×3 matrix so that the argument of the scalar form factor $\mathcal{F}$ (usually chosen to be concave) is a quadratic form of $\overrightarrow{R}$'s components. Now, charge density is the time component of the charge density 4-vector J which depends, in general, both on space and time coordinates. Moreover, signals propagate at the speed of light, and retard condition must be fulfilled also for a still charge distribution, even though in this case only the geometry (*i.e.* space location) of the observer matters and time delays are irrelevant. These prerequisites and covariance of (5) can be consistently fulfilled

postulating heuristically that the argument of $\mathcal{F}$ to be the completely saturated product (*i.e.* a Lorentz scalar) $R^T \cdot \widehat{\Sigma}^{-1} \cdot R$ where R is the full 4-distance connecting field emitter and observer, while $\widehat{\Sigma}^{-1}$ is a symmetric 4-D tensor with space components equal to $\widehat{\boldsymbol{\sigma}}^{-1}$ and vanishing (in macroparticle's rest frame) time components ($\widehat{\Sigma}^{-1}_{0i} = \widehat{\Sigma}^{-1}_{0i} = 0$ i, j $= 1 \ldots 3$). It is easily shown [7] that in the lab frame the following relation holds:

(6)
$$\widehat{\Sigma}'^{-1} = \begin{pmatrix} \boldsymbol{\beta}^T \widehat{\boldsymbol{\sigma}}'^{-1} & -\boldsymbol{\beta}^T \widehat{\boldsymbol{\sigma}}'^{-1} \\ -\widehat{\boldsymbol{\sigma}}'^{-1}\boldsymbol{\beta} & \widehat{\boldsymbol{\sigma}}'^{-1} \end{pmatrix}, \qquad \text{with} \qquad \begin{cases} \widehat{\boldsymbol{\sigma}}'^{-1} &= \widehat{A} \cdot \widehat{\boldsymbol{\sigma}}^{-1} \cdot \widehat{A}, \\ \widehat{A} &= \widehat{1} + \dfrac{\gamma^2}{1+\gamma} \boldsymbol{\beta} \otimes \boldsymbol{\beta}^T. \end{cases}$$

As a final consistency check, observe that $\det \widehat{\boldsymbol{\sigma}}' = \gamma^{-2} \det \widehat{\boldsymbol{\sigma}}$, implying that casting (5) in the lab frame correctly reproduces the transformation properties of charge density:

$$\rho'(R) = \frac{q}{\sqrt{\det \widehat{\sigma}'}} \cdot \mathcal{F}\left[R'^T \cdot \widehat{\Sigma}'^{-1} \cdot R'\right] = \gamma \cdot \frac{q}{\sqrt{\det \widehat{\sigma}}} \mathcal{F}\left[R^T \cdot \widehat{\Sigma}^{-1} \cdot R\right] = \gamma \rho(x). \tag{7}$$

A functional effective charge based on previous concepts is practically implemented in TREDI via the choice $\mathcal{F}(z) = (2\pi)^{-3} \exp[-z/2]$ (other options are possible, though) as

$$q_{\text{eff}} = \int_{\mathcal{R}^2(\mathbf{x}) \le \mathcal{R}^2_{\mathcal{O}}} \rho(\mathbf{x}) \mathrm{d}\mathbf{x} = q \left[\operatorname{erf}\left(\frac{\mathcal{R}_O}{\sqrt{2}}\right) - \sqrt{\frac{2}{\pi}} \cdot \mathcal{R}_O \cdot \exp\left[-\frac{\mathcal{R}^2_O}{2}\right] \right] \tag{8}$$

(see App. A in ref. [7] for details) where $\mathcal{R}^2(\mathbf{x})$ is the Lorentz scalar $\mathbf{x}^T \cdot \widehat{\boldsymbol{\sigma}}^{-1} \cdot \mathbf{x}$, while $\mathcal{R}^2_{\mathcal{O}}$ is the same quantity evaluated for the observer. It is easily seen that $q_{\text{eff}} \propto \mathcal{R}^3_{\mathcal{O}}$ for $\mathcal{R}_{\mathcal{O}} \ll 1$, thus fulfilling short-range regularization requirements.

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The authors warmly acknowledge P. LONDRILLO for addressing his attention to a few papers that proved relevant to further development of TREDI, and helpful suggestions.

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