

# FULLY COVARIANT TWO-PARTICLE SPACE-CHARGE DYNAMICS USING THE LIÉNARD–WIECHERT POTENTIALS

B. Folsom\*, E. Laface, European Spallation Source ERIC, Lund, Sweden

## Abstract

Space-charge models typically assume instantaneous propagation of the electromagnetic fields between particles in a bunch, describing forces in the frame of the reference particle. In this paper, we construct a space-charge tracking code from the retarded Liénard–Wiechert potentials, which are covariant by design, in a Lagrangian formulation. Such potentials are manipulated with covariant derivatives to produce the necessary equations of motion that will be solved in a test system of two-particles at various relative energies. Magnetic dipole moment dynamics are also evaluated where applicable.

## COVARIANT EQUATIONS OF MOTION

The study of retarded potential interactions between charged particles has had a renewed interest in recent years, especially for THz undulators [1, 2], electron beam interaction with high-intensity lasers [3–5], as well as being a standard tool in heavy-ion collision analysis [6–9]. We present here the framework for a fully covariant space-charge tracking routine, which easily incorporates external potentials and magnetic dipole moment dynamics.

We begin with the Liénard-Wiechert potential in covariant form [10]

$$A^\alpha(x^\alpha) = \frac{\tilde{e} V^\alpha(\tau)}{V \cdot [x - r(\tau)]} \Big|_{\tau=\tau_0}, \quad (1)$$

where  $\tilde{e}$  is source charge,  $x^\alpha$  is the observer position, and  $r^\alpha(\tau)$  is the source charge position. We use the typical arrow accent to denote the source particle, a reverse accent arrow is used for quantities pertaining to the observer, as in  $\tilde{e}^1$ . Gaussian units are used throughout the paper.

The source particle's four-position and velocity are defined in the usual way:

$$\begin{aligned} r^\alpha(\tau) &= \{c\tau, \mathbf{r}\} \\ V^\alpha(\tau) &= \{c\gamma, \mathbf{u}\}, \end{aligned} \quad (2)$$

where  $\tau$  is the *observer* proper time and where the metric  $g^{\alpha\beta} = \{1, -1, -1, -1\}$  is used going forward;  $\tau_0$  is defined by the light-cone constraint

$$[x - r(\tau_0)]^2 = 0.$$

The condition  $\tau = \tau_0$  is required for any instance of the retarded potential. This constraint can also be used to define  $R \equiv x_0 - r_0(\tau_0) = |\mathbf{x} - \mathbf{r}(\tau_0)|$  along with  $R^\rho = \{R, \hat{\mathbf{n}}R\}$ . The denominator of Eq. (1) can be reduced to

$$V \cdot [x - r] = V^\rho R_\rho = \gamma c R (1 - \boldsymbol{\beta} \cdot \hat{\mathbf{n}}), \quad (3)$$

where  $\hat{\mathbf{n}}$  is the unit vector directed from the source to the observer.

We can track a particle at the observer position using Jackson's covariant equations of motion for a charged particle in an external field [11]

$$\begin{aligned} \frac{dx^\alpha}{d\tau} &= \frac{1}{\tilde{m}} \left( \mathcal{P}^\alpha - \frac{\tilde{e}}{c} A^\alpha \right) \\ \frac{d\mathcal{P}^\alpha}{d\tau} &= \frac{\tilde{e}}{\tilde{m}c} \left( \mathcal{P}^\beta - \frac{\tilde{e} A_\beta}{c} \right) \partial^\alpha A^\beta. \end{aligned} \quad (4)$$

The canonical momentum is used here (only necessary for the observer). It is defined as

$$\mathcal{P}^\alpha = \tilde{m} V^\alpha + \frac{\tilde{e}}{c} A^\alpha. \quad (5)$$

We then turn to [12] for a workable form of  $\partial^\alpha A^\beta$ , where the velocities belong to the source particle

$$\partial^\alpha A = \left( -\frac{V^\alpha}{V^\rho R_\rho} + \frac{R^\alpha}{V^\rho R_\rho} \frac{d}{d\tau} \right) A. \quad (6)$$

To find practical equations of motion from this point, a number of identities are helpful [10, 12]

$$\begin{aligned} \frac{dV^\alpha}{d\tau} &= [c\gamma^4 \boldsymbol{\beta} \cdot \dot{\boldsymbol{\beta}}, c\gamma^2 \dot{\boldsymbol{\beta}} + c\gamma^4 \boldsymbol{\beta} (\boldsymbol{\beta} \cdot \dot{\boldsymbol{\beta}})] \equiv \dot{V} \\ \frac{d}{d\tau} [V^\rho R_\rho] &= -c^2 + R_\rho \dot{V}^\rho \\ V^\rho V_\rho &= c^2, \end{aligned} \quad (7)$$

which, using Eq. (1), yields

$$\frac{dA^\beta}{d\tau} = \tilde{e} \left[ \frac{\dot{V}^\beta}{Kc} - \frac{\dot{V}^\alpha R_\alpha V^\beta}{K^2 c^2} + \frac{V^\beta}{K^2} \right] \quad (8)$$

$$\partial^\alpha A = \tilde{e} \left[ \frac{\dot{V}^\beta R^\alpha}{K^2 c^2} - \frac{V^\alpha V^\beta}{K^2} + \frac{R^\alpha V^\beta}{K^3 c} \right], \quad (9)$$

where we have used the shorthand  $K \equiv \gamma R (1 - \boldsymbol{\beta} \cdot \hat{\mathbf{n}})$ .

Inserting Eq. (9) into Eq. (4) results in a practical equation of motion for momentum:

$$\frac{d\mathcal{P}^\alpha}{d\tau} = \tilde{e} \tilde{e} \left[ \frac{R^\alpha \dot{V}^\beta \dot{V}_\beta}{K^2 c^3} - \frac{\dot{V}^\alpha \dot{V}^\beta \dot{V}_\beta}{K^2 c} + \frac{R^\alpha \dot{V}^\beta \dot{V}_\beta}{K^3 c^2} \right]. \quad (10)$$

We can expand this equation for its zero component and  $i$ , an arbitrary position component:

$$\begin{aligned} \frac{d\mathcal{P}^0}{d\tau} &= \tilde{e} \tilde{e} \gamma \left[ \frac{\tilde{\gamma}^2 \dot{\boldsymbol{\beta}} \cdot \dot{\boldsymbol{\beta}}}{cR(1 - \dot{\boldsymbol{\beta}} \cdot \hat{\mathbf{n}})^2} - \frac{1}{R^2(1 - \dot{\boldsymbol{\beta}} \cdot \hat{\mathbf{n}})^2} \right. \\ &\quad \left. + \frac{1}{\tilde{\gamma}^2 R^2 (1 - \dot{\boldsymbol{\beta}} \cdot \hat{\mathbf{n}})^3} \right] \end{aligned} \quad (11)$$

\* ben.folsom@ess.eu

<sup>1</sup> These accents do *not* designate 3-vectors, which are set in boldface.

$$\frac{d\mathcal{P}^i}{d\tau} = \tilde{e}\tilde{e}\tilde{\gamma} \left[ \frac{\tilde{\beta}^i \tilde{\beta} \cdot \tilde{\beta}}{R^2(1 - \tilde{\beta} \cdot \hat{\mathbf{n}})^2} - \frac{n^i \tilde{\beta} \cdot \tilde{\beta}}{\tilde{\gamma}^2 R^2(1 - \tilde{\beta} \cdot \hat{\mathbf{n}})^3} - \frac{n^i \tilde{\beta} \left( \tilde{\beta} + \tilde{\beta} \left\{ \tilde{\beta} \cdot \tilde{\beta} \tilde{\gamma}^2 \right\} \right)}{cR(1 - \tilde{\beta} \cdot \hat{\mathbf{n}})^2} \right]. \quad (12)$$

For a qualitative look, we can take the following case:  $\tilde{\beta}$  and  $\hat{\mathbf{n}}$  are parallel (perfectly head-on approach) such that  $\tilde{\beta} \cdot \hat{\mathbf{n}} = \tilde{\beta}$ . For further simplification, we take the source velocity as constant, and the observer velocity is negligible. This leaves

$$\left| \frac{d\mathcal{P}^\alpha}{d\tau} \right|^2 = \left\{ \frac{e^2}{R^2} \left[ -\frac{1}{(1 - \tilde{\beta})^2} + \frac{1}{\tilde{\gamma}^2(1 - \tilde{\beta})^3} \right] \right\}^2, \quad (13)$$

where the high and low energy limits can be found by expanding the  $\tilde{\gamma}$  in the denominator of the second term.

$$\left| \frac{d\mathcal{P}^\alpha}{d\tau} \right| \Big|_{\tilde{\beta} \rightarrow 1} \approx \frac{e^2 \tilde{\gamma}^2}{R^2} \Big|_{\tilde{\beta} \rightarrow 0} \approx \frac{e^2}{R^2}. \quad (14)$$

The  $\gamma^2$  dependence as  $\tilde{\beta} \rightarrow 1$  indicates that such velocity-dependent interactions can be substantial beyond the femtometer scale where they are typically studied [6]<sup>2</sup>. This approximation is non-radiative, since we have taken  $\dot{\tilde{\beta}} = 0$ ; typically, such velocity-dependent forces are considered near-field. However, it is clear that for  $\gamma \gg 1$ , the relevant distance scale may be greater. One should keep in mind, however, that this is a peak value, only for perfectly aligned particles.

## SPIN DYNAMICS

Here we follow [13], which derives spin as a consequence of symmetries in Minkowski space, thus requiring no magnetic monopoles or current loops. Ignoring the anomalous magnetic moment, we use

$$\frac{ds^\alpha}{d\tau} = \frac{\tilde{e}}{m} F^{\alpha\beta} s_\beta - \frac{d_m}{m} s \cdot \partial (F^{*\alpha\beta}) s_\beta, \quad (15)$$

where  $\frac{\tilde{e}}{m} F^{\alpha\beta}$  is the standard Lorentz force applied to the classical spin four-vector  $s$ , defined in the lab frame as

$$s_{(\text{LF})}^\mu = \{\tilde{\beta} \cdot \mathbf{s}, \mathbf{s}\}, \quad (16)$$

which is chosen to satisfy  $V \cdot s = 0$ ; this requires defining the variable  $d_m$  as a magnetic dipole constant analogous to charge:

$$d_m \equiv \frac{|\mu|}{c^2 |\mathbf{s}|},$$

where  $\mu$  is the observer particle's magnetic dipole moment.

For the Liénard–Wiechert potentials, the electromagnetic tensor  $F^{\alpha\beta}$  is

$$\begin{aligned} F^{\alpha\beta} &= \partial^\alpha A - \partial^\beta A \\ &= \tilde{e} \left[ \frac{\dot{V}^\beta R^\alpha - \dot{V}^\alpha R^\beta}{c^2 K^2} + \frac{R^\alpha V^\beta - R^\beta V^\alpha}{c K^3} \right] \end{aligned} \quad (17)$$

<sup>2</sup> Although this pertains to the magnitude of the canonical momentum  $|\mathcal{P}^\alpha|$ , one can use Eqs. (5), (8), and (14) to show that  $m \left| \frac{dV}{d\tau} \right| \propto \frac{e^2}{R^2} \left[ \gamma^2 + \frac{1}{\gamma^2} \right]$ .

and  $F^{*\alpha\beta} = \epsilon^{\alpha\beta\gamma\delta} F_{\gamma\delta}$  is its Hodge dual.

With equations of motion for the spin itself, we now have all the necessary components to reconstruct the momentum equation from Eq. (4) to account for the Stern–Gerlach force using the Gilbert model [14]:

$$\begin{aligned} \frac{d\mathcal{P}^\alpha}{d\tau} &= \frac{\tilde{e}}{\tilde{m}c} \left( \mathcal{P}_\beta - \frac{\tilde{e}A_\beta}{c} \right) \partial^\alpha A^\beta - d_m s \cdot \partial (F^{*\alpha\beta}) V_\beta \\ &= \frac{\tilde{e}}{c} \tilde{V}_\beta \partial^\alpha A^\beta - \frac{|\mu|}{c^2} \hat{s} \cdot \partial (F^{*\alpha\beta}) \tilde{V}_\beta \\ &= \frac{\tilde{e}}{c} \tilde{V}_\beta \partial^\alpha A^\beta - \frac{|g\tilde{e}|}{2mc^3} s \cdot \partial (F^{*\alpha\beta}) \tilde{V}_\beta, \end{aligned} \quad (18)$$

where the simplification in the second line contains a unit vector  $\hat{s}^\alpha = s^\alpha/|s|$ , and the third line is shown for reference, using  $|s| = \hbar/2$  for a spin 1/2 particle and  $|\mu| = (g\tilde{e}\hbar)/(2mc)$  where  $g$  is the spin  $g$ -factor and  $\hbar$  is Planck's constant.

An elementary analysis of Eq. (18) gives the following thresholds for spin terms becoming dominant in  $\frac{d\mathcal{P}^\alpha}{d\tau}$ ; first for  $\dot{\tilde{\beta}} = 0$  considering the  $R^\alpha V^\beta$  term for the diagonal components in a head-on interaction (i.e.  $1 - \tilde{\beta} \cdot \hat{\mathbf{n}} = 1 - \tilde{\beta}$ ):

$$\frac{R}{2\tilde{\gamma}} \approx \frac{|\mu|}{|e|} = 193.2 \text{ fm} = \frac{\lambda_e}{4\pi}, \quad (19)$$

where  $\lambda_e$  is the Compton wavelength. Then for  $\dot{\tilde{\beta}}$  dependence in the high  $\tilde{\beta}$  limit

$$\dot{\tilde{\beta}} \tilde{\gamma}^3 \Big|_{\tilde{\beta} \rightarrow 1} \approx \frac{|e|c}{|\mu|} = 1.5 \cdot 10^{21} \text{ Hz} \approx 4\pi \omega_e, \quad (20)$$

where  $\omega_e$  is the Compton frequency. We again observe that a high- $\gamma$  source particle may bring typically negligible interactions (in the context of accelerator tracking) to a more appreciable scale.

Note that we have not used the canonical momentum formalism for spin in Eq. (15) and, in turn, Eq. (18). Such formalism stems from the least-action principle and produces symplectic equations of motion. However, in the case of the Stern–Gerlach force, the addition of spin-dependent terms to the action requires a solution with recursive  $ds/d\tau$  terms [13].

This formalism for spin is only truly symplectic, then, in cases where the forces dependent on  $ds/d\tau$  can be ignored. Such forces can be incorporated *ad hoc* by using, for example, the full Gilbert model of the Stern–Gerlach force, but we presume their effects to be negligible for most Liénard–Wiechert tracking in the context of accelerator simulation, including spin-polarized beam tracking. Exceptions may be the incorporation of ultra high-frequency external fields, or tracking classical spin trajectories to the picometer scale for a smooth transition regime as a precursor to investigating quantum-scale interactions.

## INTEGRATION ALGORITHM

We first consider the discrete form of Eq. (4). For example, to construct a first-order, symplectic Euler integrator one

can choose from

$$\begin{aligned}\mathcal{P}_{+1}^\alpha &= \mathcal{P}^\alpha - \Delta\tau \frac{\partial H}{\partial x} \left( \mathcal{P}^\alpha, x_{+1}^\alpha \right) \\ x_{+1}^\alpha &= x^\alpha + \Delta\tau \frac{\partial H}{\partial \mathcal{P}} \left( \mathcal{P}^\alpha, x_{+1}^\alpha \right)\end{aligned}\quad (21)$$

or

$$\begin{aligned}\mathcal{P}_{+1}^\alpha &= \mathcal{P}^\alpha - \Delta\tau \frac{\partial H}{\partial x} \left( \mathcal{P}_{+1}^\alpha, x^\alpha \right) \\ x_{+1}^\alpha &= x^\alpha + \Delta\tau \frac{\partial H}{\partial \mathcal{P}} \left( \mathcal{P}_{+1}^\alpha, x^\alpha \right),\end{aligned}\quad (22)$$

where the +1 notation indicates a component value at a new timestep<sup>3</sup>. In our case, the only position dependence in the derivative terms arises from  $A^\alpha(R[x, r], \vec{\beta}, \dot{\vec{\beta}})$ . Composition of these sets of equations using the implicit midpoint rule of equations leads to conventional second and higher-order symplectic integrators [16].

These forms are implicit, meaning they must use iterative methods to solve for the +1 dependent components on the right-hand sides of Eqs. (21) and (22). For Hamiltonians separable into kinetic and potential terms (i.e.  $H = U(mV^\alpha) + K(x^\alpha)$ ) such integrators are explicit, meaning they can be solved for all unknown +1 components exactly at each timestep. Otherwise, if  $\frac{\partial H}{\partial x^\alpha}$  has a component that does not depend on  $x$  — or if  $\frac{\partial H}{\partial \mathcal{P}^\alpha}$  has one which does not depend on  $\mathcal{P}$  — routes to explicitness are possible.

Although our choice of Hamiltonian and canonical momentum is suitable for tracking a lab-frame timestep as well as incorporating external potentials, the dependence of our equations of motion on both  $\mathcal{P}^\alpha$  and  $A^\alpha$  in every component does not provide such a shortcut to explicitness.

A simple method for making Eq. (21) explicit can be constructed by enforcing a condition that  $|\Delta\vec{x}| \ll |R|$  at every integration step, such that  $|R_{+1}| \approx R$ . Combining this with an explicit version of Eq. (22) would yield a Störmer–Verlet type second-order integrator. On inspection, finding similar  $\mathcal{P}$ -independent partial derivatives for Eq. (22) seems impossible with our choice of Hamiltonian. However, a renormalization derived in a previous work is suitable here [17]

$$\mathcal{P}_{+1}^\alpha = \frac{\mathcal{P}^\alpha + \frac{\Delta\tau q}{mc} \left( \mathcal{P}_\beta - \frac{q}{c} A_\beta \right) \partial^\alpha A^\beta - \frac{\Delta\tau^2 q^3}{m^2 c^3} A^\alpha \left( \frac{\partial \Phi}{\partial \tau} \right)^2}{1 - \frac{\Delta\tau^2 q^2}{m^2 c^2} \left( \frac{\partial \Phi}{\partial \tau} \right)^2}, \quad (25)$$

<sup>3</sup> It is worth considering the  $x^0$  component in discrete form, following Eq. (22) and [15]:

$$t_{+1} = t + \frac{\Delta\tau}{m} \left( p_{+1}^0 - \frac{\tilde{e}}{c} A^0 \right) = t + \frac{\Delta\tau}{m} \left( \dot{\gamma} + \frac{\tilde{e}}{c} [\Phi - \Phi] \right), \quad (23)$$

where  $\Phi$  is the scalar potential. For head-on interactions, one can take  $R_{+1} = R(1 + \beta)$ . This yields an upper limit on the ratio of tracked lab time and observer's proper time:

$$\frac{\Delta t}{\Delta \tau} \leq \dot{\gamma}_{+1} + \frac{\tilde{e}\tilde{e}}{cR} (\dot{\gamma}^2 - \dot{\gamma} [1 + \vec{\beta}]), \quad (24)$$

which reduces to the familiar  $\Delta t/\Delta \tau = \dot{\gamma}_{+1}$  for low source velocity.

where  $\frac{\partial \Phi}{\partial \tau} = \partial^0 A^0$  is the time derivative of the scalar potential<sup>4,5</sup>. Although the resulting common prefactor of  $q^4/(m^2 c^4)$  for these two terms is approximately  $10^{-29} [\text{m}^{-2}]$  we again have a countervailing  $\gamma$  dependence:  $(\partial \Phi / \partial \tau)^2 \propto \dot{\gamma}^8 \vec{\beta} / R^2$ .

An alternative approach improves on the  $|\Delta x| \ll |R|$  approximation by presuming information is available for the source particle's trajectory in the upcoming timestep (i.e. the lapse between present and retarded time is greater than the chosen timestep by at least a factor of two:  $|\tau - \tau_0| = |R|/c \geq 2|\Delta\tau|$ ). We can now form a composite of Eqs. (21) and (22) analogous to the Störmer–Verlet method with the ordering as follows, beginning with Eq. (25) with  $\Delta\tau \rightarrow \Delta\tau/2$ .

$$\begin{aligned}\tilde{\mathcal{P}}_{+1/2}^\alpha &\left\{ \text{following Eq. (25), with } A \left( x^\alpha, r^\alpha, \vec{\beta}, \dot{\vec{\beta}} \right) \right\} \\ x_{+1/2}^\alpha &= x^\alpha + \frac{\Delta\tau}{2m} \left[ \tilde{\mathcal{P}}_{+1/2}^\alpha + \frac{\tilde{e}}{c} A \left( x^\alpha, r^\alpha, \vec{\beta}, \dot{\vec{\beta}} \right) \right] \\ \tilde{\mathcal{P}}_{+1}^\alpha &= \tilde{\mathcal{P}}_{+1/2}^\alpha + \frac{\Delta\tau \tilde{e}}{2mc} \left[ \tilde{\mathcal{P}}_{+1/2}^\alpha + \frac{\tilde{e}}{c} A^\alpha \left( x_{+1/2}^\alpha, r_{+1/2}^\alpha, \vec{\beta}_{+1/2} \right) \right] \partial^\alpha A^\beta \\ x_{+1}^\alpha &= x_{+1/2}^\alpha + \frac{\Delta\tau}{2m} \left[ \tilde{\mathcal{P}}_{+1}^\alpha + \frac{\tilde{e}}{c} A \left( x_{+1/2}^\alpha, r_{+1/2}^\alpha, \vec{\beta}_{+1/2} \right) \right],\end{aligned}\quad (27)$$

where the  $\partial^\alpha A^\beta$  derivatives have equivalent timestep dependencies as the  $A^\alpha$  terms in the same expression. In this way, inter-particle dependent terms are evaluated on coherent timesteps. From here, extension to higher-order symplectic integration would employ Lie transformations [18, 19], where the necessary Poisson brackets can be constructed using Eq. (10) or a derivative form of Eq. (25), along with the position components from Eq. (4).

## CONCLUSION

We formulated fully covariant equations of motion with the Liénard-Wiechert potential between two particles including the contribution of the spin in terms of magnetic momentum. We then wrote two explicit algorithms to evaluate such equations for each step of integration. This model provides an *ab initio* means to treat ultra-relativistic effects between charged particles with classical electromagnetic fields.

<sup>4</sup> For cases where this derivative is negligible, Eq. (25) reduces to an explicit form of Eq. (21) for time-independent  $\phi$ . In other words, if  $\Phi_{+1} - \Phi \rightarrow 0$  in Eq. (23), then we have a  $\frac{dx^\alpha}{d\tau} = \frac{\partial H}{\partial \mathcal{P}}$  component which does not depend on other  $x^\alpha$  components, which allows for a first-order explicit integrator [15, 16].

However, in the case of the Liénard–Wiechert potentials  $\frac{\partial \Phi}{\partial \tau} \neq 0$  unless  $R \gg \Delta x$  and  $\vec{\beta} \cdot \hat{\mathbf{n}} = 0$ .

<sup>5</sup> We have ignored spin here, but note instead that one may use a modified canonical momentum to have composite potential:

$$P^\alpha = \tilde{m}V^\alpha + \frac{\tilde{e}}{c} A^\alpha + \frac{\tilde{e}}{c} \tilde{B}^\alpha = \tilde{m}V^\alpha + \frac{\tilde{e}}{c} \tilde{A}^\alpha, \quad (26)$$

where  $\tilde{B}^\alpha = \left[ \frac{|g| \text{sgn}(\tilde{e})}{2mc} F^{*\alpha\beta} s_\beta \right]$ , and one can then substitute  $\tilde{A}^\alpha$  into Eq. (25). This implies by Eq. (18) that  $\partial^\alpha \tilde{B}^\beta = \frac{|g\tilde{e}|}{2mc^3} s \cdot \partial (F^{*\alpha\beta})$ , which agrees with the definition in [13] of  $B^\alpha = \frac{\tilde{e}}{c} \text{sgn}(\tilde{e}) \tilde{B}^\alpha \equiv F^{*\alpha\beta} s_\beta d$ .

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