Space Charge Tracking in Accelerators

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Introduction

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- The Liénard–Wiechert potentials: a fundamental definition of space charge.
- Two-particle force
- Multiparticle picture
- Simplifying pairwise distance calculation

The Liénard–Wiechert Potentials

$$\Phi = \left[\frac{q}{\left(1 - \vec{\beta}_{s(t)} \cdot \hat{n}\right) R} \right]_{t=t_r} \quad ; \quad \vec{A} = \left[\frac{q\, \vec{\beta}_{s(t)}}{\left(1 - \vec{\beta}_{s(t)} \cdot \hat{n}\right) R} \right]_{t=t_r}$$

[1] Jackson, *Classical Electrodynamics*, pp661–663.

[2] Feynman, Leighton, and Sands, *The Feynman Lectures on Physics, Vol. 2: Mainly Electromagnetism and Matter*, pp14-4,25-5.

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These are derived solely from an assumption of EM fields propagating at c. The unit vector $\hat{n}$ points from the source to the test particle. The quantity R is the distance between the two.[1,2]

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The dependence on $\frac{\vec{\beta}}{1-\vec{\beta}\cdot\hat{n}}$ implies an attractive limit of $\vec{\beta} \to -1$ but a divergence as $\vec{\beta} \to 1$ for $\vec{\beta} \cdot \hat{n} \approx 1$.

[1] Jackson, *Classical Electrodynamics*, pp661–663.

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The Liénard–Wiechert Potentials

The $\vec{E}$ and $\vec{B}$ field definitions resulting from these potentials are more complicated.

$$\vec{E} = q\left[\frac{\hat{n} - \vec{\beta}}{\gamma^2(1 - \vec{\beta}\cdot\hat{n})^3 R^2}\right]_{t=t_r} + \frac{q}{c}\left[\frac{\hat{n}\times\left\{(\hat{n} - \vec{\beta})\times\dot{\vec{\beta}}\right\}}{(1 - \vec{\beta}\cdot\hat{n})^3 R}\right]_{t=t_r}$$

$$\vec{B} = [\hat{n}\times\vec{E}]$$

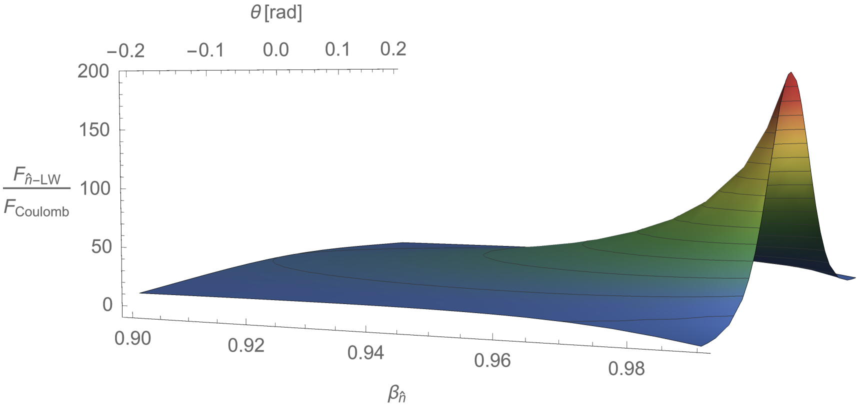
Two-particle Force

Ignoring radiation, the Lorentz-forces in the $\hat{n}$ direction are then

$$F_{\vec{B}} = \frac{-q^2\beta^2(1-\beta^2)(1-cos^2(\theta))}{(1-\beta cos(\theta))^3\,R}\hat{n}$$

$$F_{\vec{E}} = \frac{q^2(1-\beta^2)\,(1-cos(\theta))}{(1-\beta cos(\theta))^3\,R}\hat{n}$$

Two-particle Force



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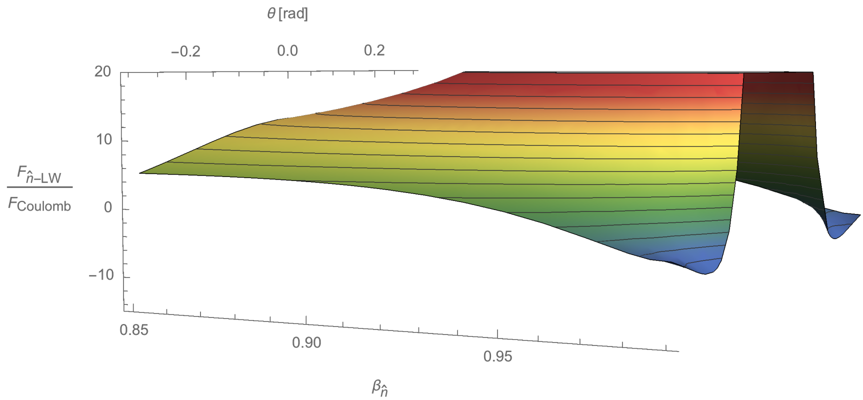
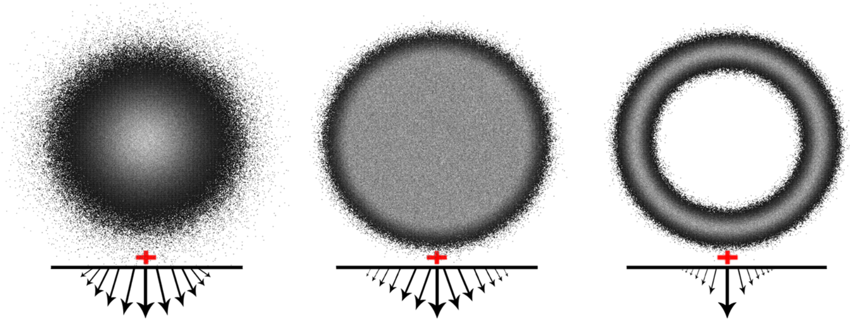


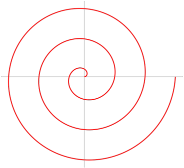
Multiparticle Picture

For an ensemble, the $\vec{A}$ contributions at an exterior point are then distinct:



Folsom and Laface, "Beam Dynamics with Covariant Hamiltonians". (With thanks to V. Vislavicious)

Simplifying Pointwise Distance Calculation



A typical bunch in an accelerator beamline contains a population N of roughly 10^{10} to 10^{13} particles. We can reduce the number of operations required for each Cartesian distance calculations can be reduced by using Archimedian spiral coordinates.[3]

[3] Parker, "Dynamics of the interplanetary gas and magnetic fields."

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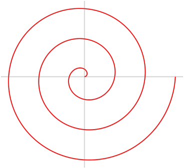

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Simplifying Pointwise Distance Calculation

Here $r = \pm b\theta^{\frac{1}{n}}$. Then using $n = 1$, and taking an arbitrary spacing of $b = 1$ and projecting into spherical coordinates:

$$x = \theta \sin(\theta) \cos(\phi)$$
$$y = \theta \sin(\theta) \sin(\phi)$$
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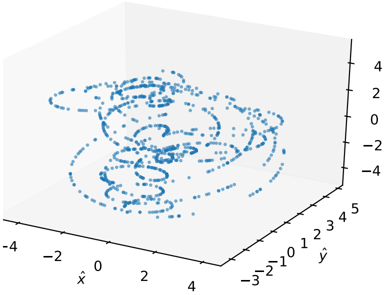
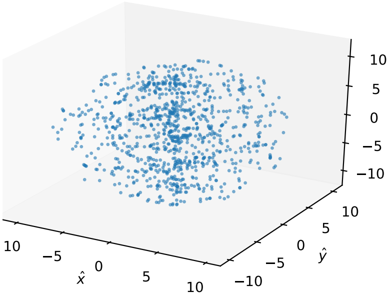
Then defining $\phi = \theta\epsilon$, where ϵ is irrational, one can populate 3D space with a single dynamical variable θ.

Simplifying Pairwise Distance Calculation





Random uniform spiral-coordinate distributions in θ (8π and 40π for left and right plots, respectively).

Simplifying Pairwise Distance Calculation

Here, the 3D distance formula goes as

$$d = \sqrt{(x_1 - x_0)^2 + (y_1 - y_0)^2 + (z_1 - z_0)^2}$$

$$\downarrow$$

$$d = \sqrt{\theta_1^2 + \theta_0^2 - 2\theta_1\theta_0\left[\sin(\theta_1)\sin(\theta_0)\cos(\epsilon\{\theta_1 - \theta_0\}) - \cos(\theta_1)\cos(\theta_0)\right]}$$

[4] An even simpler formula arises for $r = (\theta_1 + \theta_0)$, but introduces the constraints $y_1 = y_0$ and $r_1 = r_0$.

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Or in terms of the cosine law we can use more compact form

$$d = \sqrt{\theta_0^2 + \theta_0^2 - \theta_1\theta_0\left[2\cos(\gamma)_{LUT}\right]}$$

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The use of lookup tables here leads to one fewer operation with spiral coordinates than Cartesian.[4]

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Simplifying Pairwise Distance Calculation

Euclidean case:

$$\sqrt{\underbrace{(x_1 - x_0)}_{=A}^2 + \underbrace{(y_1 - y_0)}_{=B}^2 + \underbrace{(z_1 - z_0)}_{=C}^2} \quad \text{3 parallel subtraction}$$

$$\sqrt{\underbrace{A^2}_{=D} + \underbrace{B^2}_{=E} + \underbrace{C^2}_{=F}} \quad \text{3 parallel powerings}$$

$$\sqrt{\underbrace{D + E}_{=G} + F} \quad \text{1 serial addition}$$

$$\sqrt{\underbrace{G + F}_{=H}} \quad \text{1 serial addition}$$

$$\sqrt{H} \quad \text{1 square root}$$

Simplifying Pairwise Distance Calculation

Spiral case:

$$\sqrt{\underbrace{\theta_1^2}_{=A} + \underbrace{\theta_0^2}_{=B} - \underbrace{\theta_1\theta_0}_{=C}\underbrace{[2cos(\gamma)]}_{=D}}$$ 4 parallel (2 power, 1 mult., 1 lookup)

$$\sqrt{\underbrace{A + B}_{=E} - \underbrace{C \cdot D}_{=F}}$$ 2 parallel (1 addition, 1 mult.)

$$\sqrt{\underbrace{E - F}_{=G}}$$ 1 serial addition

$$\sqrt{G}$$ 1 square root

Conclusion

- Machines are typically designed “around” space charge, with the weighty assumption that since average transverse β values are low, the Coulomb potential is a sufficient approximation for particle–particle effects. This may be inadequate for simulating ultrarelativistic or unusually shaped beams/bunches.

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- Machines are typically designed “around” space charge, with the weighty assumption that since average transverse β values are low, the Coulomb potential is a sufficient approximation for particle–particle effects. This may be inadequate for simulating ultrarelativistic or unusually shaped beams/bunches.
- As new accelerator designs demand high-brightness and high-precision, relativistic accuracy via the Liénard–Wiechert potentials may become critical.

Supplement: An Explicit, Covariant, Symplectic Integrator for Simulating Space Charge

Symplecticity is inherent to any system obeying Hamilton's equations of motion and leads to preservation of phase-space for each spatial axis. It is a facet of beam physics–a symplectic tracking code can predict beam stability over millions of cycles in a ring, where a simpler energy-conservation tracking code might gradually drift.

Explicitness, in this context, refers to an integrator which does not require an implicit solver to determine the equations of motion for a particle's trajectory at each timestep.

Covariance then ensures that a simulation's results are frame-independent, with the additional benefit of "adaptive" proper-time rescaling.[5]

[5] Wang, Liu, and Qin, "Lorentz Covariant Canonical Symplectic Algorithms for Dynamics of Charged Particles".

Beginning with Jackson's covariant Hamiltonian[6]

$$H = \frac{1}{m}\left(P_\alpha - \frac{q}{c}A_\alpha\right)\left(P^\alpha - \frac{q}{c}A^\alpha\right) - c\sqrt{\left(P_\alpha - \frac{q}{c}A_\alpha\right)\left(P^\alpha - \frac{q}{c}A^\alpha\right)} \quad (1)$$

where the conjugate momentum is

$$P^\alpha = mV^\alpha + \frac{q}{c}A^\alpha \quad (2)$$

where A^α is a function of four-position $r_\alpha = (t, -x, -y, -z)$, $P^\alpha = (\gamma + \Phi, -\vec{P})$, $A_\alpha = (\Phi, -\vec{A})$, and V^α is constrained by the light-cone condition:

$$V_\alpha V^\alpha = c^2 \quad (3)$$

this yields the following equations of motion in proper time ($d\tau = \frac{dt}{\gamma}$)

$$\frac{dr^\alpha}{d\tau} = \frac{\partial H}{\partial P_\alpha} = \frac{1}{m}\left(P^\alpha - \frac{q}{c}A^\alpha\right)$$
$$\frac{dP^\alpha}{d\tau} = -\frac{\partial H}{\partial r_\alpha} = \frac{q}{mc}\left(P_\beta - \frac{q}{c}A_\beta\right)\partial^\alpha A^\beta \tag{4}$$

where m is particle mass, and the ordering of indices α and β merits careful consideration.

We can immediately test how these equations of motion will discretize, thanks to Heirer's explicit symplectic form[7]

$$P^{k+1,\alpha} = P^{\alpha,k} - \Delta\tau \frac{\partial H}{\partial r}\left(P^{k+1,\alpha}, r^{\alpha,k}\right) =$$
$$\underset{+1}{P} = P^{\alpha} - \Delta\tau \frac{\partial H}{\partial r}\left(\underset{+1}{P}^{\alpha}, r^{\alpha}\right) = P^{\alpha} + \frac{\Delta\tau q}{mc}\left(\underset{+1}{P}_{\beta} - \frac{q}{c}A_{\beta}\right)\partial^{\alpha}A^{\beta} \tag{5}$$

and for position:

$$r^{k+1,\alpha} = r^{\alpha,k} + \Delta\tau \frac{\partial H}{\partial r}\left(P^{k+1,\alpha}, r^{\alpha,k}\right) =$$
$$\underset{+1}{r} = r^{\alpha} + \Delta\tau \frac{\partial H}{\partial r}\left(\underset{+1}{P}^{\alpha}, r^{\alpha}\right) = r^{\alpha} + \frac{\Delta\tau}{m}\left(\underset{+1}{P}^{\alpha} - \frac{q}{c}A^{\alpha}\right) \tag{6}$$

where we have condensed the notation for updated coordinates with an underset $+1$, and leaving the originating coordinates unmarked, that is

$$P^{k+1} \rightarrow \underset{+1}{P} \quad ; \quad P^{k,\alpha} \rightarrow P^{\alpha} \tag{7}$$

This clarifies the upcoming linear algebra needed to decouple P_β from the right-hand side terms.
We can then attempt to isolate $\underset{+1}{P}$ terms for a fully explicit algorithm. Such a potential reduces to

$$\underset{+1}{P}^{x} = P_x + \frac{\Delta\tau}{mc}\left(-\underset{+1}{P}^{z} + \frac{q}{c}A^z\right)\frac{\partial A^z}{\partial x} \tag{8}$$

where here and moving forward we use the notation

$$\partial^\alpha \equiv \frac{\partial}{\partial x_\alpha} = \left(\frac{\partial}{\partial x^0}, -\vec{\nabla}\right)$$
$$\partial_\alpha \equiv \frac{\partial}{\partial x^\alpha} = \left(\frac{\partial}{\partial x_0}, \vec{\nabla}\right)$$
$$A^\alpha = (A^0, A^\alpha) \quad ; \quad A_\alpha = (A_0, -\vec{A})$$
$$\therefore \partial^\alpha A_\alpha = \partial_\alpha A^\alpha = \frac{\partial A^0}{\partial x^0} + \vec{\nabla}\cdot\vec{A} = 0 \text{ (in the Lorenz gauge)}$$
$$\partial^\alpha A^\alpha = \partial_\alpha A_\alpha = \frac{\partial A^0}{\partial x^0} - \vec{\nabla}\cdot\vec{A} \tag{9}$$

along with the Minkowski metric

$$
\begin{aligned}
g_{00} = 1 \quad &; \quad g_{11} = g_{22} = g_{33} = -1 \\
g^{\alpha\beta} = g_{\alpha\beta} \quad ; \quad g_{\alpha\gamma} g^{\gamma\beta} &= \delta^{\beta}_{\alpha} \quad ; \quad \delta^{\beta}_{\alpha}\delta^{\alpha}_{\beta} = \delta^{\alpha}_{\alpha} = 4 \\
x^{\alpha} = g_{\alpha\beta} x^{\beta} \quad ; \quad x^{\alpha} &= g^{\alpha\beta} x_{\beta} \quad ; \quad x^{\alpha} = x^{\beta}\delta^{\alpha}_{\beta}
\end{aligned}
\tag{10}
$$

Since the $\underset{+1}{r}^{\alpha}$ expression is explicit as-is, we can focus solely on the momentum, first rearranging terms and extracting $g_{\alpha\beta}$'s

$$
\begin{aligned}
\underset{+1}{P}^{\alpha} - \left(\frac{\Delta\tau q}{mc}\right) \underset{+1}{P_{\beta}} \partial^{\alpha} A^{\beta} &= P^{\alpha} - \left(\frac{\Delta\tau q^2}{mc^2}\right) A_{\beta}\, \partial^{\alpha} A^{\beta} \\
g^{\beta\alpha} \underset{+1}{P_{\beta}} - \left(\frac{\Delta\tau q}{mc}\right) \underset{+1}{P_{\beta}} \partial^{\alpha} A^{\beta} &= g^{\beta\alpha} P_{\beta} - \left(\frac{\Delta\tau q^2}{mc^2}\right) A_{\beta}\, \partial^{\alpha} A^{\beta}
\end{aligned}
\tag{11}
$$

we then introduce a dummy index λ and left-hand multiply both sides by $g^{\lambda\alpha}/g_{\lambda\alpha}$, which are identical and which can commute past β-only factors. This yields

$$\delta_\lambda^\beta \underset{+1}{P_\beta} - \left(\frac{\Delta\tau q}{mc}\right)\partial_\lambda A^\beta = \delta_\lambda^\beta P_\beta - \left(\frac{\Delta\tau q^2}{mc^2}\right) A_\beta \, \partial_\gamma A^\beta \tag{12}$$

where δ_λ^β is analogous to the identity matrix here, and thus $\delta_\lambda^\beta P_\beta$. We then have

$$\underset{+1}{P_\beta}\left(\delta_\lambda^\beta - \frac{\Delta\tau q}{mc}\partial\lambda A^\beta\right) = P_\beta \delta_\lambda^\beta - \left(\frac{\Delta\tau q^2}{mc^2}\right) A_\beta \, \partial_\lambda A^\beta \tag{13}$$

which, for $P_{\beta}\delta_{\lambda}^{\beta}$, and $\lambda = x$ still reduces to Eqn. 8. We then multiply both sides bu $(\delta_{\lambda}^{\beta} + \frac{\Delta\tau q}{mc}\partial^{\lambda}A_{\beta})$, leaving

$$\underset{+1}{P_{\beta}}\left(4 - \frac{\Delta\tau^2 q^2}{m^2c^2}\partial_{\lambda}A^{\beta}\cdot\partial^{\lambda}A_{\beta}\right) = \left(P_{\beta}\delta_{\lambda}^{\beta} - \frac{\Delta\tau q^2}{mc^2}A_{\beta}\,\partial_{\lambda}A^{\beta}\right)\left(\delta_{\beta}^{\lambda} + \frac{\Delta\tau q}{mc}\partial \tag{14}$$

where $\partial_{\lambda}A^{\beta}\cdot\partial^{\lambda}A_{\beta}$ contracts to a scalar. We can now isolate $\underset{+1}{P_{\beta}}$ by division, and expand the right-hand side terms:

$$\underset{+1}{P_{\beta}} = \frac{4P_{\beta} + \frac{\Delta\tau q}{mc}P_{\beta}\delta_{\lambda}^{\beta}\,\partial^{\lambda}A_{\beta} - \frac{\Delta\tau q^2}{mc^2}A_{\beta}\,\partial_{\lambda}A^{\beta}\delta_{\beta}^{\lambda} - \frac{\Delta\tau^2 q^3}{m^2c^2}A_{\beta}\,(\partial_{\lambda}A^{\beta})^2}{4 - \frac{\Delta\tau^2 q^2}{m^2c^2}(\partial_{\lambda}A^{\beta})^2} \tag{15}$$

we can now resolve the Kronecker deltas and finally left-hand multiply by $g^{\lambda\beta}$ to return $\underset{+1}{P}$ to contrariant form

$$\underset{+1}{P}^{\lambda} = \frac{4P^{\lambda} + \frac{\Delta\tau q}{mc} P^{\beta}\,\partial^{\lambda} A_{\beta} - \frac{\Delta\tau q^2}{mc^2} A^{\lambda}\,\partial_{\lambda} A^{\lambda} - \frac{\Delta\tau^2 q^3}{m^2 c^2} A^{\lambda}\,(\partial_{\lambda} A^{\beta})^2}{4 - \frac{\Delta\tau^2 q^2}{m^2 c^2}(\partial_{\lambda} A^{\beta})^2} \tag{16}$$

For $A^{\alpha} = A^{z}(x, y)$ (i.e. the ideal form of multipole magnet's potential) the x- and z-components of momentum are

$$\underset{+1}{P}^{x} = \frac{4P^{x} - \frac{\Delta\tau q}{mc} P^{z} \frac{\partial A^{z}}{\partial x}}{4 - \frac{\Delta\tau^2 q^2}{m^2 c^2}\left(-\frac{\partial A^{z}}{\partial x} - \frac{\partial A^{z}}{\partial y}\right)^2} \quad ; \quad \underset{+1}{P}^{z} = P^{z} \tag{17}$$

[6] Jackson, *Classical Electrodynamics*, p585.

[7] Hairer, Lubich, and Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations; 2nd ed.* p3.

Equation (15) and the already explicit $\underset{+1}{r}^{\alpha}$ four-position from Eq. (5) now fulfill the ideal criteria: long-term stability (symplecticity by Hairer's method), frame independence (Lorentz invariance via covariant formalism), and efficiency/precision (via an explicit integrator).