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# BEAM DYNAMICS WITH COVARIANT HAMILTONIANS

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*Abstract*

We demonstrate covariant beam-physics simulation through multipole magnets using Hamiltonians relying on canonical momentum. Space-charge interaction using the Lienard–Wiechert potentials is also discussed. This method is compared with conventional nonlinear Lie-operator tracking and the TraceWin software package.

## THEORY

Simulating particle beams in accelerators typically involves paraxial (small-angle) approximations limited to cylindrical symmetry, or Lie-operator transformations capable of modeling nonlinear effects, but still inherently relying on a series-expanded exponential about the origin in position–momentum phase space. The former is often useful in control-room software for real-time diagnostics; the latter is typically much slower and reserved for design work or other offline tasks requiring best-possible accuracy.

In either case, Hamiltonians for relativistic beams are typically renormalized in terms of longitudinal momentum [1] which can be problematic for cases such as longitudinal tracking in the ultra-relativistic limit [2].

As an alternative, we construct an integrator based on Jackson's derivations for charged particles reacting to external potentials [3], with complementary notes from Barut [4]. We begin with Jackson's covariant expression for relativistic Hamiltonians (Gaussian units, four-vectors summed over $\alpha$)

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

with the resulting equations of motion

$$\frac{dx^\alpha}{d\tau} = \frac{\partial H}{\partial P_\alpha} = \frac{1}{m}\left(P^\alpha - \frac{q}{c}A^\alpha\right), \qquad (2)$$
$$\frac{dP^\alpha}{d\tau} = -\frac{\partial H}{\partial x_\alpha} = \frac{q}{mc}\left(P^\beta - \frac{q}{c}A^\alpha\right)\partial^\alpha A^\beta,$$

where $A^\alpha$ is the external electromagnetic potential; $\tau$ is the proper time, which binds the dynamics to the rest frame of a reference particle; and $P^\alpha$ is the canonical momentum, which eliminates velocity from the Hamiltonian:

$$P^\alpha = mV^\alpha + \frac{q}{c}A^\alpha, \qquad (3)$$

wherein $V^\alpha$ is the four-velocity, constrained by $V_\alpha V^\alpha = c^2$. For multipole magnets, $A^\alpha$ only has a longitudinal component, $A_z$, which reduces Eqs. (2) to

$$\frac{dx}{d\tau} = \frac{P_x}{m} \qquad \frac{dy}{d\tau} = \frac{P_y}{m} \qquad \frac{dz}{d\tau} = \frac{1}{m}\left(P_z - \frac{q}{c}A_z\right),$$
$$\frac{P_x}{d\tau} = \frac{q}{mc}\left(P_z - \frac{q}{c}A_z\right)\frac{\partial A_z}{\partial x},$$
$$\frac{P_y}{d\tau} = \frac{q}{mc}\left(P_z - \frac{q}{c}A_z\right)\frac{\partial A_z}{\partial y} \qquad \frac{P_z}{d\tau} = 0. \qquad (4)$$

Then, using $d\tau \to \Delta t/\gamma$ (and noting that since $P_z$ is constant, these equations are position–momentum separable) we can adopt the symplectic Euler method [5]:

$$\frac{dx}{d\tau} = \frac{P_x}{m} \quad \to \quad x_{i+1} = x_i + \frac{\Delta t}{\gamma}\frac{P_x}{m},$$

and likewise for the remaining expressions in Eqs. (4). This can be evaluated iteratively with fewer operations than the Lie-operator method, whose Taylor-expanded exponential requires recursive Poisson brackets [6], typically to fourth or fifth order, for multipole-magnet tracking.

This outperforms Lie-operator tracking in terms of computational speed by at least a factor of three for fully analytic solutions – and upwards of a factor of ten when using truncated Taylor series polynomials as an optimization method. In the latter case, the Lie polynomials for $\bar{x}_{i+n}$ and $\bar{P}_{i+n}$ become fully dense, whereas the covariant trajectories remain sparse.

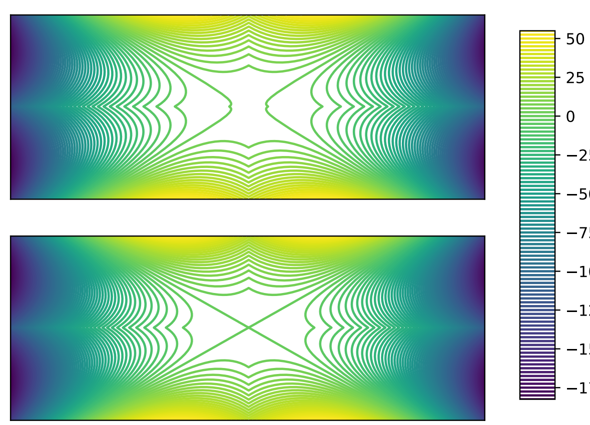


Figure 1: Lorentz forces compared in transverse space through an octupole magnet for (top) a covariant potential and (bottom) a fifth-order Lie-operator transform; the discrepancy about the origin is owing to $P_z$ dependence in the former. Both cases are consistent with an octupole's beam shaping. All units arbitrary.

## *H* WITH *n*/2 DEPENDENCE

The Hamiltonians typically derived for multipolar magnetic potentials are linearly dependent on $A_z$. Equation (1) shows that this is not the case when using conjugate momentum. We can then assert that the quadratic dependence of $H$

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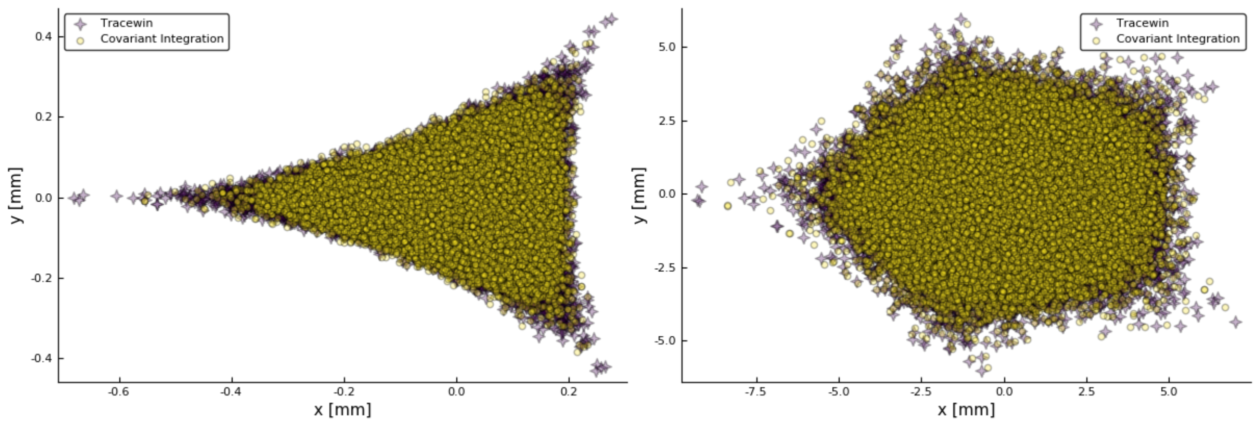


(a) (b)

Figure 2: a) 1 TeV bunch through a 1100 mm sextupole (n=3, undersized pole-tip aperture to emphasize transverse-space reshaping); $I = 20$ A, $r_0 = 1$ mm, $B_0 = 8$ T. b) 2 GeV bunch; 600 mm decapole (n=5), $I = 20$ A, $r_0 = 20$ mm, $B_0 = 5$ T.

on $A_z$ will shift the usual radial-coordinate dependence on number of dipoles $A_z \propto r^n$ to $A_z \propto r^{n/2}$.

To verify this, we use a version of Wolski's contour-integral approach [2] where the $B$-field for a single pole of a multipole magnet is only nonzero in the radial direction, and is solenoid-like:

$$B_r = C_{\frac{n}{2}} r^{\frac{n}{2}-1},$$
$$\int_{-z}^{z}\int_{0}^{r_0} B_r\,dr\,dz = \frac{\pi N I \mathcal{R}^2}{c r_0^2}, \tag{5}$$

which can be used to solve for $C_{\frac{n}{2}}$. Evaluating over all poles (i.e. introducing $\theta$-dependence) and converting to the customary Cartesian system yields

$$B_y + iB_x = \frac{n\pi N I \mathcal{R}^2 (x+iy)^{\frac{n}{2}-1}}{2 c r_0^{\frac{n}{2}+2}}, \tag{6}$$

where $N$ is number of turns per magnet coil, $\mathcal{R}$ is the effective coil radius (which we have introduced), and $r_0$ is the pole-tip aperture radius. Using $B_r = \nabla \times \bar{A} \rightarrow B_r = \frac{1}{r}\frac{\partial A_z}{\partial \theta}$, integrating, and again converting to Cartesian coordinates, we have

$$A_z = \frac{\pi^2 I N \mathcal{R}^2 (x+iy)^{\frac{n}{2}}}{c r_0^{\frac{n}{2}+2}}, \tag{7}$$

where the non-canceling units are current per $c$, which is consistent with energy in Gaussian units.

It is then trivial to check that the trajectories for $dP_x/dt$ and $dP_y/dt$ by Eqs. (4) have the same leading-order dependence on $x$ and $y$ as those found by the Lie-operator method.

For a more thorough check, we compare Lorentz forces, using an octupole ($n = 4$) as a test case. Beginning with $v_i = \dot{x}_i = \partial H/\partial p_i$ in the nonrelativistic case:

$$\bar{F}_n = \left(\frac{\partial}{\partial \bar{p}}\left[\frac{\bar{p}^2}{2m} + \cancel{\kappa \cdot A_z}\right]\right) \times \bar{B}_n$$
$$\propto p_z(3xy^2 - 2x^3)\,\hat{x} + p_z(-3yx^2 + 2y^3)\,\hat{y}, \tag{8}$$

which matches the first-order Lie-operator result for $\dot{\bar{p}}/m$.

For the covariant case, Eq. (1) can be expanded

$$H = \left(\bar{P}^2 - \frac{2qA_z\bar{P}}{c} + \frac{e^2A_z^2}{c}\right)\frac{1}{m} - c|\bar{P} - \frac{e}{c}A_z|. \tag{9}$$

Then, using $\dot{x}_i = \frac{\partial H}{\partial P_i}$, the remaining non-canceling terms are

$$F_{\frac{n}{2}} = \left(\frac{2\bar{P}}{m} - \frac{e\beta_z A_z}{mc}\right) \times \bar{B}_{\frac{n}{2}} \propto (4P_z x + 6y^2 x - 2x^3)\,\hat{x}$$
$$+ (-4P_z y + -6x^2 y + 2y^3)\,\hat{y}. \tag{10}$$

Again, the $x$ and $y$ dependencies are proportional (see Fig. 1). The required $n/2$ dependence for a covariant $H$ is thus clarified a consequence of shifting to canonical momentum.

## BENCHMARKS

As a baseline, Eqs. (4) and (7) were tested against TraceWin using identical initial distributions and zero beam current. This relied on TraceWin's gradient definition—using a field-on-pole ($B_0$) approximation—to equal that of Wolski [2, 7], as well as Eq. (5). We note that neither reference includes the effective coil radius $\mathcal{R}$, and that covariant results were consistent with TraceWin for $\mathcal{R} \sim 30$ mm over a wide range of magnet types ($n$) and energies (MeV through TeV scale). Figure 2 illustrates two such cases.

## NONLINEAR BEHAVIOR

A cursory analysis in terms of relativistic velocities helps to clarify the Hamiltonian's nonlinear dependence on $A_z$. To start, Eq. (9) can be reverted to velocity dependence via Eq. (3), where we shift to the bunch frame:

$$H = mc^2\left(\bar{\beta}^2 - |\bar{\beta}|\right) - 2e\bar{\beta}\gamma A_z + \frac{3e^2\gamma^2 A_z^2}{mc^2}.$$

The quadratic $A_z$ term here is clearly dominant for low-$\beta_z$ particles; for medium- to high-$\beta_z$, a linear–quadratic threshold is now defined as

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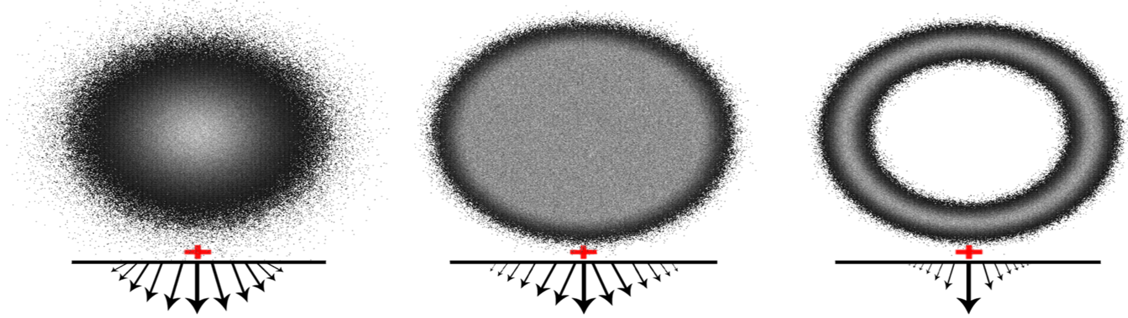

Figure 3: Sketch of net space-charge contributions following Eq. (14) for test particles on the edges (points marked in red) of isotropic distributions: Gaussian (left), uniform with exponential fall-off (center), and hollowed (right), respectively. All three assume a $\langle\bar{\beta}\rangle$ biased center–outward. The arrows' horizontal components cancel when summing bins, leaving the rightmost distirbution as the most $\delta$-like distribution.

$$A_z = \frac{2}{3}\frac{\bar{\beta}mc^2}{\gamma q} = \frac{\bar{\beta}}{\gamma}\cdot 625.3\,\text{MV}, \tag{11}$$

where the maximum $\bar{\beta}/\gamma \approx 1/2$ occurs for 400 MeV protons. By Eqs. (5) and (7), at the magnetic pole-tip limit ($r = r_0$), we have

$$|B_r| \propto \frac{n|A_z|}{r_0}, \tag{12}$$

indicating (in Gaussian units) that this threshold falls in the multi-GV per meter regime of interest to wakefield acceleration [8, 9].

## SPACE CHARGE

Equation (2) can be populated using the Lienard–Wiechert potentials [3, 10]

$$A_0(\bar{x},t) = \left[\frac{q}{(1-\bar{\beta}\cdot\bar{n})R}\right]_{r.t.};\quad \bar{A}(\bar{x},t) = \left[\frac{q\bar{\beta}}{(1-\bar{\beta}\cdot\bar{n})R}\right]_{r.t.}, \tag{13}$$

where $R = |\bar{R}| = |\bar{x} - r(\tau_0)| = x_0 - r_0(\tau_0)$ is source to test-particle distance defined by the light-cone condition; $\bar{n}$ is the unit vector in the same direction; and all quantities are taken at the retarded time.

The dependence on

$$\frac{\bar{\beta}}{1-\bar{\beta}\cdot\bar{n}}, \tag{14}$$

cannot be overstated: velocity dependent space-charge contributions are maximized for parallel velocities, and attenuated for antiparallel velocities. Figure 3 illustrates this concept qualitatively, suggesting that a hollowed distribution represents a lowest-energy configuration for a charged-particle bunch.

We now have a toolset capable of studying more complicated cases, such as an alternating-current 4n-poles (octupoles and similar), which were shown in a previous work to effectively freeze individual particles transverse motion beyond a certain radius while inducing a circulatory trajectory with small longitudinal boost in the positive $z$ direction [11].

Starting with the full expression for $A_z$ in polar coordinates (see [2], Eq. [1.145]).

$$A_z = |C_{\frac{n}{2}}|r^{\frac{n}{2}}e^{i\frac{n}{2}\theta}\,\hat{z},$$

then, for alternating current in an octupole ($n = 4$), $\theta$ effectively fluctuates as $\pm\pi/n$. Thus, solving the force in terms of Eqs. (10) (first line) the only nonzero contribution is

$$F_r = -C^2_{\frac{n}{2}}r^3\cos^2(2\theta)\,\hat{r}. \tag{15}$$

We can expect this force to cause a shift in velocity such that

$$\beta_r \to \beta_r\left(1 + \frac{F_r\Delta t}{m}\right). \tag{16}$$

Thus despite space charge having predominantly being parallel-$\bar{\beta}$, it now has an artificial antiparallel restraint in $\hat{r}$. Using this shifted beta in Eq. (13), and assuming that $F_r\Delta t/m \ll -1$, we have for space charge

$$A_r \propto \frac{-q\beta_r F_r}{(1+\beta_r\bar{n})R}\,\hat{r}, \tag{17}$$

which, again using Eq. (10) with $R \equiv \sqrt{(r-r_s)^2 + (z-z_s)^2}$ ($s$ subscript denotes source particle) yields a force offset to the usual drift-space result:

$$\bar{F}_{offset} = \frac{q^2C^2_{\frac{n}{2}}\beta_r^2r^6\cos^4(2\theta)}{(1+\beta_r\bar{n})^2R^3}\,\hat{z} - \frac{4q^2(z-z_s)C^2_{\frac{n}{2}}\beta_r^2r^6\sin(4\theta)\cos^2(2\theta)}{(1+\beta_r\bar{n})^2R}\,\hat{\theta}, \tag{18}$$

where the $\hat{\theta}$ component accounts for the circulatory motion, and the $\hat{z}$ component is solely positive, accounting for the forward bias.

## CONCLUSION

Manifestly covariant Hamiltonians are demonstrated to be a viable alternative to conventional non-linear tracking algorithms. With multipole magnetic potentials, particle trajectories can be calculated with fewer operations, and space-charge potentials are easily incorporated. Having avoided approximations in $H$ allows for the study of longitudinal effects.

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