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.

1. 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 \cite{1} which can be problematic for cases such as longitudinal tracking in the ultra-relativistic limit \cite{2}.

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

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

(1)

with the resulting equations of motion

\[
\begin{align*}
\frac{dx^\alpha}{d\tau} &= \frac{\partial H}{\partial P_\alpha} = \frac{1}{m} \left( P^\alpha - \frac{q}{c} A^\alpha \right) \\
\frac{dP^\alpha}{d\tau} &= -\frac{\partial H}{\partial x_\alpha} = -\frac{q}{mc} \left( P^\beta - \frac{q}{c} A^\beta \right) \partial^\beta A^\alpha ,
\end{align*}
\]

(2)

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:

\[ P^\alpha = mV^\alpha + \frac{q}{c} A^\alpha , \]

(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

$$\frac{dx}{d\tau} = \frac{P_x}{m}, \quad \frac{dy}{d\tau} = \frac{P_y}{m}, \quad \frac{dz}{d\tau} = \frac{1}{m} \left( P_z - \frac{q}{c} A_z \right)$$

(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]:

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

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.

2. $H$ 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 $H$ 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:

$$B_r = C_2 r^{\frac{n}{2} - 1} \int_{-z}^{z} \int_{0}^{r_0} B_r dr dz = \frac{\pi N I R^2}{cr_0^2},$$

(5)

which can be used to solve for $C_2$. Evaluating over all poles (i.e. introducing $\theta$-dependence) and converting to the customary Cartesian system yields

$$B_y + iB_x = \frac{n\pi N I R^2 (x + iy)^{\frac{n}{2} - 1}}{2cr_0^{\frac{n}{2} + 2}},$$

(6)

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

$$A_z = \frac{\pi^2 I N R^2 (x + iy)^{\frac{n}{2}}}{cr_0^{\frac{n}{2} + 2}},$$

(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.
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.

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:

$$\vec{F}_n = \left( \frac{\partial}{\partial \vec{p}} \left[ \frac{\vec{p}^2}{2m} + \kappa \vec{A}_z \right] \right) \times \vec{B}_n \propto p_z (3xy^2 - 2x^3) \hat{x} + p_z (-3yx^2 + 2y^3) \hat{y},$$

which matches the first-order Lie-operator result for $\dot{\vec{p}}/m$. For the covariant case, Eq. (1) can be expanded

$$H = \left( \vec{p}^2 - \frac{2qA_z \vec{P}}{c} + \frac{e^2 A_z^2}{c^2} \right) \left( \frac{1}{m} - c \frac{\vec{P}}{c} \frac{\vec{A}_z}{c} \right).$$

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

$$\vec{F}_n^2 = \left( \frac{2\vec{P}}{m} - \frac{e\beta_z A_z}{mc} \right) \times \vec{B}_n \propto (4P_zx + 6y^2x - 2x^3) \hat{x} + (4P_zy + -6x^2y + 2y^3) \hat{y}.$$ 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.

3. 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 $R$, and that covariant results were consistent with TraceWin for $R \sim 30$ mm over a wide range of magnet types ($n$) and energies (MeV through TeV scale). Figure 2 illustrates two such cases.
4. 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:

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

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

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

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

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

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

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

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

where $R = |\tilde{R}| = |\bar{x} - r(\tau_0)| = x_0 - r_0(\tau_0)$ 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.

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

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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 (a), uniform with exponential fall-off (b), and hollowed (c), respectively. All three assume a $\langle \bar{\beta} \rangle$ biased center–outward. The arrows’ horizontal components cancel when summing bins, leaving (c) as the most $\delta$-like distribution.

The dependence on

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

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]).

$$A_z = |C_n| r^2 \cos^2 \theta \hat{r},$$

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

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

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

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

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

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

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:
\[ F_{\text{offset}} = \frac{q^2 C_2^2 \beta^2 r^6 \cos^3(2\theta)}{(1 + \beta \bar{n})^2 R^3} \hat{z} - \frac{4q^2(z - z_s)C_2^2 \beta^2 r^6 \sin(4\theta) \cos^2(2\theta)}{(1 + \beta \bar{n})^2 R} \hat{\theta}, \quad (18) \]

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

6. 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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