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 α)

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

with the resulting equations of motion

\[
\frac{dx^\alpha}{d\tau} = \frac{\partial H}{\partial P_\alpha} = \frac{1}{m} \left( P^{\alpha} - \frac{q}{c} A^{\alpha} \right),
\]

\[
\frac{dP^{\alpha}}{d\tau} = - \frac{\partial H}{\partial x^\alpha} = \frac{q}{mc} \left( P^\beta - \frac{q}{c} A^\beta \right) \partial^{\alpha} A^\beta,
\]

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:

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

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

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

\[
\frac{P_x}{m} = \frac{q}{mc} \left( P_z - \frac{q}{c} A_z \right) \frac{\partial A_z}{\partial x},
\]

\[
\frac{P_y}{m} = \frac{q}{mc} \left( P_z - \frac{q}{c} A_z \right) \frac{\partial A_z}{\partial y},
\]

\[
\frac{P_z}{d\tau} = 0.
\]

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

\[
\frac{dx}{\Delta t} = \frac{P_x}{m} \quad \rightarrow \quad x_{i+1} = x_i + \frac{\Delta t P_x}{\gamma m},
\]

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.

**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:

\[
B_r = C_z r^{n-1},
\]

\[
\int_{-z}^{z} \int_{0}^{r_0} B_r dr dz = \frac{n \pi N I R^2}{cr^2}, \quad \text{(5)}
\]

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

\[
B_y + iB_x = \frac{n \pi N I R^2 (x + iy)^\frac{n}{2} - 1}{2cr_0^{\frac{n}{2} + 2}}, \quad \text{(6)}
\]

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 \(B_r = \nabla \times \vec{A} \rightarrow B_r = \frac{1}{r} \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\), integrating, and again converting to Cartesian coordinates, we have:

\[
A_z = \frac{n^2 \pi N I R^2 (x + iy)^\frac{n}{2}}{cr^{\frac{n}{2} + 2}}, \quad \text{(7)}
\]

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:

\[
\vec{F}_n = \left( \frac{\partial}{\partial \vec{p}} \left[ \frac{\vec{p}^2}{2m} + k \cdot \vec{A}_z \right] \right) \times \vec{B}_n
\]

\[
\propto p_z (3xy^2 - 2x^3) \hat{x} + p_x (-3yx^2 + 2y^3) \hat{y}, \quad \text{(8)}
\]

which matches the first-order Lie-operator result for \(\vec{p}/m\).

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

\[
H = \left( \vec{p}^2 - \frac{2qA_z \vec{P}}{c} + \frac{e^2 A_z^2}{c^4} \right) \frac{1}{m} - e\left[ \vec{P} - \frac{e}{c} A_z \right]. \quad \text{(9)}
\]

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

\[
F_n = \left( \frac{2\vec{P}}{m} - \frac{e\beta_z A_z}{mc} \right) \times \vec{B}_n \propto (4P_z x + 6y^2 x - 2x^3) \hat{x} + (-4P_z y + 6x^2 y + 2y^3) \hat{y}. \quad \text{(10)}
\]

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 \(R\), 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.

**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:

\[
H = mc^2 \left( \vec{p}^2 - |\vec{p}| \right) - 2e\beta y A_z + \frac{3e^2 \gamma^2 A_z^2}{mc^2}.
\]

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 $\hat{\beta}$ biased center-outward. The arrows’ horizontal components cancel when summing bins, leaving the rightmost distribution as the most $\delta$-like distribution.

$$A_z = \frac{2 \hat{\beta} m c^2}{3 \gamma q} = \frac{\hat{\beta}}{\gamma} \cdot 625.3 \text{ MV}, \quad (11)$$

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

$$|B_r| \propto \frac{n|A_z|}{r_0}, \quad (12)$$

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]

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

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

The dependence on

$$\frac{\hat{\beta}}{1 - \hat{\beta} \cdot \vec{n}} \quad (14)$$

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)).

$$A_z = |C_2| r^2 e^{\frac{3}{2} \theta} \hat{\theta},$$

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

$$F_r = -C_2^2 r^3 \cos^2(2\theta) \hat{r}. \quad (15)$$

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-$\vec{B}$, 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

$$A_r \propto -q \beta_r F_r \left(1 + \beta_r \vec{n} \right), \quad (17)$$

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

$$\vec{F}_{\text{offset}} = \frac{q^2 C_2^2 \beta_r^6 \cos^4(2\theta)}{(1 + \beta_r \vec{n})^2 R^3} \hat{\vec{z}} - \frac{4 q^2 (z - z_s) C_2^2 \beta_r^6 \sin(4\theta) \cos^2(2\theta)}{(1 + \beta_r \vec{n})^2 R} \hat{\theta}, \quad (18)$$

where the $\hat{\theta}$ component accounts for the circulatory motion, and the $\hat{\vec{z}}$ 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.
REFERENCES


