Symplectic Integration in `elegant`

Michael Borland
ANL/APS/LS-356, Rev. 1
Original publication date February 4, 2019
Revised December 11, 2021
Argonne National Laboratory, Argonne, IL 60439, USA

1 Introduction

The program `elegant` performs symplectic integration for hard-edge dipoles and multipoles using the exact Hamiltonian. This method is not original but was cobbled together from studying several sources, e.g., [1] and [2].

We begin with a discussion of methods used for combined-function magnets for which the field expansion is defined in traditional beam-following coordinates. Following that, we describe a new method for integrating dipole magnets for which the field expansion is defined in Cartesian coordinates.

2 Hamiltonian and Definitions

The exact Hamiltonian for a combined function sector bend is[1]

$$\mathcal{H} = -\frac{eA_s(x,y)}{c} - (1+h_0x)\sqrt{\frac{E^2}{c^2} - m^2c^2 - p_x^2 - p_y^2}, \tag{1}$$

where A_s is the scalar magnetic potential, E is the energy, h_0 is the design curvature of the magnet, p_x is the transverse horizontal momentum, and p_y is the transverse vertical momentum. Defining $(1+\delta) = p/p_0$, $q_x = p_x/p_0$, and $q_y = p_y/p_0$, we have

$$H = H_f + H_d \tag{2}$$

where

$$H_f = -\frac{eA_s(x,y)}{p_0} \tag{3}$$

is the part of the Hamiltonian pertaining to fields and

$$H_d = -(1+h_0x)\sqrt{(1+\delta)^2 - q_x^2 - q_y^2}. \tag{4}$$

is the Hamiltonian for a generalized drift (possibly in curvilinear coordinates if $h_0 \neq 0$).

3 Coordinate Transformations

Because it was originally a matrix tracking code, `elegant` uses trace-space coordinates $(x, x', y, y', s, \delta)$ instead of canonical coordinates. Hence, it is necessary to transform between trace space and canonical coordinates.

To transform to canonical coordinates, we make use of the fact that $\frac{dx}{ds} = q_x/q_z$ and $\frac{dy}{ds} = q_y/q_z$, where $q_x^2 + q_y^2 + q_z^2 = (1+\delta)^2$ defines q_z. Hence,

$$\begin{aligned} q_x &= \frac{x'(1+\delta)}{\sqrt{1+x'^2+y'^2}} \\ q_y &= \frac{y'(1+\delta)}{\sqrt{1+x'^2+y'^2}}. \end{aligned} \tag{5}$$

At the exit of the element, we reverse the transformations using

$$\begin{aligned} x' &= \frac{q_x}{\sqrt{(1+\delta)^2-q_x^2-q_y^2}} \\ y' &= \frac{q_y}{\sqrt{(1+\delta)^2-q_x^2-q_y^2}}. \end{aligned} \tag{6}$$

4 Integration for a Curvilinear Dipole

The motion will be integrated using a drift-kick-drift technique (perhaps in higher order). For a drift, Hamilton's equations for the momenta are

$$\frac{dq_x}{ds} = -\frac{\partial H_d}{\partial x} = h_0\sqrt{f^2 - q_x^2}, \tag{7}$$

and

$$\frac{dq_y}{ds} = -\frac{\partial H_d}{\partial y} = 0, \tag{8}$$

where $f = \sqrt{(1+\delta)^2 - q_y^2}$ is a constant during the drift. Equation (7) is solved by

$$q_x(s) = f\sin(h_0 s + \phi), \tag{9}$$

where $\phi = \sin^{-1} q_x(0)/f$.

For the coordinates, we have

$$\frac{dx}{ds} = \frac{\partial H_d}{\partial q_x} = \frac{q_x(1+h_0x)}{\sqrt{f^2 - q_x^2}}, \tag{10}$$

and

$$\frac{dy}{ds} = \frac{\partial H_d}{\partial q_y} = \frac{q_y(1+h_0x)}{\sqrt{f^2 - q_x^2}}. \tag{11}$$

Using Equation (9) we can rewrite Equation 10 as

$$\int_{x(0)}^{x(s)} \frac{dx}{1+h_0x} = \int_0^s \tan(h_0 s + \phi), \tag{12}$$

giving

$$x(s) = \frac{1}{h_0}\left(-1 + (1+h_0x(0))\frac{\cos\phi}{\cos(h_0 s + \phi)}\right) \tag{13}$$

Using this, we can integrate Equation (11), obtaining

$$y(s) = y(0) + \frac{1+h_0x(0)}{fh_0} q_y \cos\phi\left(\tan(h_0 s + \phi) - \tan\phi\right). \tag{14}$$

For the kicks, we refer to the H_f part of the Hamiltonian, giving

$$\frac{dq_x}{ds} = \frac{e}{p_0}\frac{\partial A_s}{\partial x} = -\frac{eB_y}{p_0} \tag{15}$$

and

$$\frac{dq_y}{ds} = \frac{e}{p_0}\frac{\partial A_s}{\partial y} = \frac{eB_x}{p_0}. \tag{16}$$

Derivation of the expressions for B_x and B_y is beyond the scope of this note, but uses the recursion technique [3, 4]. In the case of a bending magnet, this is limited to 10^{th} order in x and y.

The kicks are imparted per

$$\Delta q_x = -\Delta s \frac{B_y}{R}(1+h_0x) \tag{17}$$

and

$$\Delta q_y = \Delta s \frac{B_x}{R}(1+h_0x), \tag{18}$$

where R is the beam rigidity and the $(1+h_0x)$ factors include the lengthening of the interval due to a beam offset. One might argue that this factor should be $\sqrt{1+x'^2+y'^2} + h_0x$, but then we'd have a kick depending on the momenta, which is not symplectic.

These equations are used to integrate motion in `elegant`'s `CSBEND` and `CSRCSBEND` elements.

5 Integration for a Non-bending Multipole

In the case where $h_0 = 0$, the expressions are considerably simplified. In particular, both q_x and q_y are constant in the drift portion. Hence,

$$x(s) = x(0) + \frac{q_x s}{\sqrt{f^2 - q_x^2}} \tag{19}$$

and

$$y(s) = y(0) + \frac{q_y s}{\sqrt{f^2 - q_x^2}}. \tag{20}$$

The expressions for the kicks are given by Equations (17) and (18) with $h_0 = 0$.

These equations are used to integrate motion in several of `elegant`'s elements:

- `KQUAD` — Quadrupole magnets, with optional fringe effects, error multipoles, and steering fields.
- `KSEXT` — Sextuple magnets, with optional weak skew and normal quadrupole, error multipoles, and steering fields.
- `KOCT` — Octupole magnets, with optional error multipoles.
- `KQUSE` — Combined quadrupole and sextupole magnets.
- `FMULT` — A general combination of many multipoles, specified from a data file.
- `MULT` — A general, single multipole

6 Integration for a Straight-pole Combined-function Dipole

A unfortunate fact of life in accelerator modeling is that codes assume that the multipole content of dipole magnets is specified in curvilinear (beam-following) coordinates, whereas magnets are often built with straight poles. This is a particular concern with combined-function magnets, since for example in curvilinear coordinates the local bending radius of a straight-pole magnet will vary along the reference trajectory, whereas in the codes it is assumed that the bending radius is constant along the reference trajectory. This is an issue even for separated-function dipoles, since the multipole errors are defined in the curvilinear coordinate system.

There are several approaches in use to address this. One is to split the dipole into segments with different bending radii and multipole content; this ignores the vertical focusing that results from the longitudinal fields that are necessarily present when the bending field varies. Another approach is to numerically integrate through simulated field maps, perhaps using such integration to construct a symplectic map; as we've found, this is easier said than done.

In this section, we present a new method of modeling dipoles that addresses this long-standing deficiency. This method was implemented in the `CCBEND` element, available since version 34.1.0 (27 February 2018).

6.1 Concept

`elegant` has several elements, such as `KQUAD` and `KSEXT`, that provide symplectic modeling of fairly general straight, hard-edge magnets. The modeling method is described in detail above. There is nothing in this method that restricts the type of fields, as long as the fields can be described as a multipole expansion in Cartesian coordinates. Other than splitting, the integrator makes no approximations to the Hamiltonian, e.g., it does not assume small angles in the motion. We realized that, for example, a `KQUAD` element with a horizontal offset is essentially a combined-function straight-pole dipole, with the exception of the fact that for a dipole we assign special meaning to certain incoming and outgoing trajectories.

Lindberg [5] has described the coordinate transformations necessary between the angled input trajectory needed for a symmetric dipole and the natural coordinate system of a straight magnet. Such transformations are used in the `BRAT` element, for example, which integrates (non-symplectically) through 3D field maps. Hence, our basic concept is to use the existing straight-element integrator together with appropriate coordinate transformations at the entrance and exit. Some details must be considered, such as fringe fields and trajectory errors.

6.2 Fringe fields

Fringe fields provide vertical focusing and are handled using a simple kick approximation at the ends. The field expansion is

$$B_y(z) = B_0(z) + xB_1(z) + \frac{B_2(z)}{2}(x^2 - y^2). \tag{21}$$

The longitudinal field is related to B_y by

$$\frac{\partial B_z}{\partial y} = \frac{\partial B_y}{\partial z}, \tag{22}$$

giving

$$B_z \approx y\left(\frac{\partial B_0(z)}{\partial z} + x\frac{\partial B_1(z)}{\partial z} + \frac{1}{2}\frac{\partial B_2(z)}{\partial z}(x^2 - y^2)\right). \tag{23}$$

We define a new coordinate system (q, p) rotated at an angle $\alpha = \theta/2$ relative to the (x, z) system, where θ is the bending angle. The reference particle enters along p with $q = 0$, with velocity βc. B_z has a component along the q axis, given by $B_q = B_z \sin\alpha$. The integrated vertical kick from this component is

$$\Delta y' = -\frac{y}{H}\left(B_0(c) + xB_1(c) + \frac{1}{2}B_2(c)(x^2 - y^2)\right)\sin\alpha, \tag{24}$$

where $z = c$ is a point well inside the magnet where the fields reach their final values and H is the rigidity. A more convenient form is

$$\Delta y' = -\frac{y}{1+\delta}\left(\frac{1}{\rho_0} + xK_1 + \frac{1}{2}K_2(x^2 - y^2)\right)\sin\alpha, \tag{25}$$

We see that the explicit magnet gradient (K_1) produces a normal-sextupole term in the vertical plane, with no comparable effect on the horizontal plane. Hence, this is a pseudo-sextupole. Similarly, the explicit magnet sextupole term (K_2) provides an pseudo-octupole term.

6.3 Trajectory issues

Trajectory errors can result in combined-function, straight-pole magnets because, as noted earlier, the bending radius varies with distance along the reference trajectory. This can be resolved by making the magnet stronger or weaker overall, or by displacing it in the horizontal plane. In addition, we want to center the reference trajectory in the magnet, i.e., center it about $x = 0$, so that we make best use of the good field region. Hence, we adjust both the field strength and the horizontal position to simultaneously center the trajectory and obtain the desired deflection angle. This is done by tracking the reference trajectory from the entrance (plane P0) to the exit plane (plane P2). A Simplex optimization of the fractional strength error (FSE) and horizontal offset is performed targeting $X(P2) = X(P0)$ and $p_X(P2) = -p_X(P0)$, where X and p_X are the position and momentum in the Cartesian coordinate system. We also target $X(P0) = -X(P1)$, where plane P1 is the longitudinal midplane; this ensures that the central trajectory is centered in the magnet.

6.4 Symplecticity tests

To test whether it is symplectic, we computed the change in the Hamiltonian for each particle at the end of each integration step. The Hamiltonian is given by

$$H = -\sqrt{(1+\delta)^2 - q_x^2 - q_y^2} + K_0 x + \frac{1}{2}K_1(x^2 - y^2) + \frac{1}{6}K_2(x^3 - 3xy^2). \tag{26}$$

Using a 0.5-m-long bending magnet with an angle of 0.2 rad, we found that the changes in H were less than 10^{-15}, which demonstrates that the model is symplectic. We also used a combined-function magnet with quadrupole and sextupole terms, getting the same result.

7 Synchrotron Radiation

Synchrotron radiation is implemented in a less rigorous fashion. In particular, radiation kicks are imparted after the magnetic field kicks are imparted. Both the classical and quantum nature of the radiation must be modeled. In `elegant`'s `CSBEND`, `CCBEND`, `KQUAD`, and `KSEXT` elements these can be independently turned on and off. The classical radiation is simple to simulate. Since these elements are already simulated using numerical integration, we just insert additional kicks for the change in energy due to classical synchrotron radiation. To do this, we use the fact that the synchrotron radiation power is[6]

$$P_\gamma = \frac{1}{6\pi\epsilon_0}\frac{e^2 c}{\rho^2}p^4 \tag{27}$$

where we use MKS units, ρ instantaneous bending radius, and $p = \beta\gamma$ is the momentum. We can now find the rate of change of the average of $\delta = (p - p_0)/p_0$

$$\frac{\partial\delta}{\partial s} = \frac{1}{6\pi\epsilon_0}\frac{e^2}{m_e c^2 \rho_0^2}(1+\delta)^2 p_0^3, \tag{28}$$

where ρ_0 is the instantaneous bending radius for an on-momentum particle, i.e., it contains any strength error (`FSE` in `elegant`) and also any variation in field with particle position. Of course, when integrating this we must take into account the variation in path-length due to x, x', and y':

$$\Delta s = \Delta s_0 \sqrt{(1 + x/\rho_d) + x'^2 + y'^2}, \tag{29}$$

where ρ_d is the radius of the design orbit.

The quantum effects are trickier to simulate. For `CSBEND` elements, `elegant` allows simulating the actual photon distribution with angle-spread effects. We've found this makes very little difference in practical applications. Hence, for the present, we describe the simpler simulation in which we simulate the quantum emission using gaussian-distributed random numbers. At each kick location, a random variation in the energy change is included. Of course, in reality the quanta are not necessarily emitted at the particular locations we've chosen for kicks. For one thing, the number of quanta emitted in single pass around the APS is about 900. This means that about 11 photons are emitted in each dipole on each turn. However, if we split a dipole into 20 parts and use a 4th-order integrator, we are imparting noise to the beam at 60 locations per dipole. If the noise is equivalent in an rms sense this error should average out over many turns. Comparison with a more fundamental approach, described above, confirms this expectation.

The growth rate of the mean square deviation of the energy due to quantum excitation is [6]

$$N\langle u^2\rangle = \frac{55}{24\sqrt{3}}\frac{r_e \hbar m_e c^4 \gamma^7}{\rho^3}. \tag{30}$$

We can express this more conveniently as

$$\frac{\partial\delta^2}{\partial s} = \frac{55}{24\sqrt{3}}\frac{r_e\hbar}{m_e c}\frac{p_0^5}{\rho_0^3}(1+\delta)^4 \tag{31}$$

The expected change in δ^2 in a section of length Δs is simply

$$\Delta\delta^2 = \Delta s \frac{\partial \delta^2}{\partial s}, \tag{32}$$

which we can model by adding gaussian random deviates of magnitude

$$\Delta\delta = \sqrt{\Delta s \frac{\partial \delta^2}{\partial s}}. \tag{33}$$

8 Discussion and Conclusion

We have exhibited expressions showing how `elegant` performs symplectic integration of hard-edge dipoles and multipoles. The expressions involve no approximations to the Hamiltonian or equations of motion, beyond the drift-kick-drift factorization. Hence, they are good for arbitrary momentum offset and coordinate deviations. This describes the implementation underlying the `CSBEND`, `KQUAD`, `KSEXT`, `KQUSE`, `KOCT`, `FMULT`, and `MULT` elements.

We have also described a new method of symplectically integrating through dipoles that are defined in Cartesian coordinates, implemented as the `CCBEND` element.

This document is a compilation of several internal technical notes written to document methods used by the program `elegant` [7] for sympletic integration of dipoles and multipoles. These technical notes span the period from 2005 to 2018.

9 Acknowledgements

Thanks to Y. Roblin (JLab) and L. Emery (ANL) for comments on an earlier version of this document. Thanks to R. Lindberg (ANL) for providing the coordinate transformations needed by the `CCBEND` element.

10 Revision Notes

- December 11, 2021, Revision 1: The original version of this note stated in Section 3 that $q_x^2 + q_y^2 + q_z^2 = (1-\delta)^2$, which is incorrect. This has been replaced by the correct expression, $q_x^2 + q_y^2 + q_z^2 = (1+\delta)^2$.

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