Effect of Space Charge Forces on Particle Tracking and Generation of High Order Maps*

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Abstract

TOPKARK is a beam optics program consisting of two Fortran codes developed in parallel: a 3-D high-order mapping code and a particle tracking code; both utilize a space charge model which treats the particle bunch as a uniformly-filled 3-D ellipsoid. The map code uses the differential algebra library DA [1] to generate an arbitrary-order Taylor map describing a given lattice, then the Lie algebra library LIELIB [2] is used to obtain the Dragt-Finn factorization [3] of the corresponding Lie polynomial. The Lie polynomial generated by TOPKARK without space charge has been successfully benchmarked through third order against MARYLIE 3.0 [4] and through fifth order against TLIE [5]. With space charge on, TOPKARK generates a linear map that agrees well with TRACE 3-D [6]. The tracking code uses a symplectic integration scheme [7] when space charge is off, and it includes a more general space charge model [8] which assumes only ellipsoidal symmetry of the spatial distribution.

I. GENERAL FEATURES OF THE CODE

TOPKARK has evolved from an earlier code, which was developed during a collaboration between Grumman, LBL and BNL [9]. The mapping version is a useful design tool, while the tracking version is a useful diagnostic which resolves any ambiguities regarding *very* high order effects that might be missed by Lie algebra or mapping codes and is also required for dynamic aperture studies.

A. Mapping Version

TOPKARK employs a fourth-order, adaptive-step-size, Runge-Kutta integration scheme [10] which provides good accuracy and reasonable computational speed. The differential algebra library DA [1] is used to generate a high-order Taylor map expansion of the dynamical variables about the design trajectory (in practice up to fifth order has been used) step by numerical step along the length of the lattice. This map is used to propagate the spatial moments of the (assumed) initial particle distribution from one integration step to the next.

At each integration step, a 3-D uniformly-filled ellipsoid is constructed according to the calculated spatial moments. The exact linear electric fields associated with this ellipsoid are calculated [11] and, in combination with any magnetic fields, are used to advance to the next step. At the end of the lattice, the final Taylor map is used to calculate the emittance and Twiss parameters of the final distribution. The Lie algebra library LIELIB [2] is used to obtain the Dragt-Finn [3] factorization of the Lie polynomial corresponding to this final Taylor map.

The code includes two optimizing routines, one based on the downhill simplex method [10] and another based on Powell's method [10]. Either of these algorithms can be used by a matching routine that sets the final transverse Twiss parameters to specified values by modifying any four of the lattice parameters. This matching routine has been successfully used both with and without space charge.

Another type of matching routine, which can also use either of the optimizing algorithms, is used to zero specified terms in the Lie polynomial, sometimes while simultaneously satisfying other imposed constraints. For example, TOPKARK can determine the required strengths of three (or more) octupoles in order to eliminate third-order geometric aberrations.

B. Tracking Version

This version currently exists as a test-particle tracking code which integrates the full equations of motion, using a Hamiltonian formalism and an explicitly symplectic fourth-order integration scheme [7]. The code has been used and tested extensively; in particular, the second moments obtained at the end of example beam lines often agree well with the second moments propagated by the mapping version.

TOPKARK can generate a six-dimensional phase space ellipsoid of initial conditions, which yields the desired Twiss parameters in each of the two-dimensional phase planes. Distributions currently supported include a) uniformly-filled ellipsoid in space with gaussian distribution in momentum and b) gaussian distribution in space and momentum. The code can also read in a file of initial conditions for tracking, and it outputs the Twiss parameters and particle positions as desired.

Three distinct space charge models (described below) are being implemented in the tracking version of TOPKARK. Each imposes ellipsoidal symmetry on the spatial distribution. The Hamiltonian formalism and symplectic integration will be abandoned for space charge calculations--the equations of motion and the fourth-order adaptive-step-size Runge-Kutta [10] integrator of the mapping version will be used.

C. Features Common to both Versions

TOPKARK currently implements a number of "hard edge" or uniform-field magnet elements, including a dipole (i.e. a normal entry and exit sector bend) and quadrupole through duodecapole. Also available are "thin fringe" elements for dipole and quadrupole magnets. All of these elements, including the fringe fields, have been successfully benchmarked against MARYLIE 3.0 [4] through third order. The fringe

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field models, although calculated independently, were based on ideas developed previously by Forest [12].

TOPKARK also employs one extended-fringe magnet model. This is a line-dipole model for large-bore magnets constructed from a cylindrical array of magnetized rods, including quadrupole, octupole and duodecapole configurations [13]. TOPKARK was successfully benchmarked against TLIE [5] through fifth-order in a single test-case where these extended-fringe quadrupole and octupole models were used. New element types are easily added to the list above.

Both codes use MKS units, with all momenta normalized to the longitudinal design momentum p_0. We define the longitudinal variables $\delta\tau \equiv c(t-t_0)$ and $\delta p_\tau \equiv (E_0-E)/p_0c$, and the magnetic rigidity $B\rho \equiv p_0/e$. For straight elements, the equations of motion are:

$$\frac{dx}{dz} = \frac{\beta_x}{\beta_z}; \quad \frac{dy}{dz} = \frac{\beta_y}{\beta_z}; \quad \frac{d\delta\tau}{dz} = \frac{1}{\beta_z} - \frac{1}{\beta_0}; \tag{1a}$$

$$\frac{dp_x}{dz} = \frac{1}{B\rho}\left(\frac{\beta_y}{\beta_z} B_z - B_y + \frac{1}{\beta_z c} E_{x\ eff}\right); \tag{1b}$$

$$\frac{dp_y}{dz} = \frac{1}{B\rho}\left(-\frac{\beta_x}{\beta_z} B_z + B_x + \frac{1}{\beta_z c} E_{y\ eff}\right); \tag{1c}$$

$$\frac{d\delta p_\tau}{dz} = -\frac{1}{B\rho c}\left(\frac{\beta_x}{\beta_z} E_{x\ eff} + \frac{\beta_y}{\beta_z} E_{y\ eff} + E_{z\ eff}\right). \tag{1d}$$

The electric field components $E_{x\ eff}$, etc. include the self-magnetic field of the particles and relativistic effects (see below). The corresponding equations of motion for bending elements have been given elsewhere [14].

II. SPACE CHARGE MODELS

We consider only models with ellipsoidal symmetry, meaning that the spatial density distribution has the form

$$\rho(x, y, \delta z) = \rho_0 f(u) , \tag{2a}$$

where the function $u(x,y,\delta z)$ is defined by the equation

$$u^2(x,y,\delta z) \equiv \frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{\delta z^2}{c^2} , \tag{2b}$$

with $a^2 = \langle x^2 \rangle$, etc. Thus the one-parameter family of 3-D ellipsoids defined by Eq. (2b) are isodensity contours.

Such models yield electric fields of the following form (for all points *within* the distribution) [15], [8]:

$$E_{xB} = \frac{q\rho_0}{2\varepsilon_0} abc\, x \int_0^\infty ds\, \frac{f[u(x,y,\delta z)]}{(a^2+s)^{3/2}\,(b^2+s)^{1/2}\,(c^2+s)^{1/2}} , \tag{3}$$

with analogous results for E_{yB} and E_{zB}. These electric fields are calculated in the *bunch* frame, then relativistically transformed to the laboratory frame.

The length of the bunch as observed in the lab frame is shortened due to relativistic length contraction, so the lab frame distribution is first stretched out in the z-direction before calculating the fields: $\delta z_B = \gamma_0 \delta z_L$. This reduces the particle density: $n_B = n_L/\gamma_0$, so E_{xB}, E_{yB}, E_{zB} are all reduced by a factor γ_0 from what one would naively calculate in the lab. However, the fact that the distribution is stretched out in z effectively increases the value of E_{zB} by γ_0 at the position of each particle, thus negating the decrease in E_{zB} noted above. This stretching of the bunch also alters the geometry of the distribution, which affects the values of all three components of $\mathbf{E}_B$ accordingly.

Particle velocities are neglected in the bunch frame, so the Lorentz transformations yield:

$$\mathbf{E}_L{}^{\parallel} = \mathbf{E}_B{}^{\parallel}; \quad \mathbf{E}_L{}^{\perp} = \mathbf{E}_B{}^{\perp}; \tag{4a}$$

$$\mathbf{B}_L{}^{\parallel} = \mathbf{B}_B{}^{\parallel} = 0; \quad \mathbf{B}_L{}^{\perp} = \gamma_0\, \mathbf{B}_B \times \mathbf{E}_B/c . \tag{4b}$$

The Lorentz force equation is:

$$\frac{1}{q}\mathbf{F}_L = \mathbf{E}_L + \mathbf{v} \times \mathbf{B}_L . \tag{4c}$$

Combining these results yields an *effective* electric field:

$$\mathbf{E}_{L\ eff} = \mathbf{E}_B{}^{\parallel} + \mathbf{E}_B{}^{\perp}/\gamma_0 . \tag{4d}$$

This is the quantity used to advance the particles. The longitudinal field is altered by geometric effects only, while the transverse fields are *also* reduced by a factor of γ_0^2.

A. Mapping Version

TOPKARK works with a Taylor-series expansion about the design trajectory, so the obvious question arises: How then does one propagate a particle distribution down the beamline? This has been explained in detail elsewhere [14], but essentially one calculates the second moments at a given point in the lattice by using second and higher moments of the initial distribution.

Of course, we must assume a *convenient* initial distribution function, and one that is consistent with our assumption of a uniformly-filled 3-D ellipsoid in space. Such a distribution has been found and implemented [14]. The projection of this distribution in the x-p_x plane has the form:

$$g(x,p_x) = \frac{3}{4\sqrt{10\pi}\ \varepsilon_x}\left(1 - \frac{x^2}{5\varepsilon_x\beta_x}\right) \exp\left[-\frac{\beta_x}{2\varepsilon_x}\left(p_x + \frac{\alpha_x}{\beta_x}x\right)^2\right] , \tag{5}$$

for $x^2 \le 5\varepsilon_x\beta_x$ (otherwise, g=0). We are using RMS Twiss parameters, which means that $\langle x^2 \rangle \equiv \varepsilon_x\beta_x$, $\langle xp_x \rangle \equiv -\varepsilon_x\alpha_x$, and $\langle p_x{}^2 \rangle \equiv \varepsilon_x\gamma_x$. The linear bunch frame electric fields can be found analytically in terms of complete elliptic integrals [11].

B. Tracking Version

Three distinct space charge models are being implemented in the tracking code. One assumes a uniformly-filled ellipsoid in space, for which f(u)=1. Another assumes a gaussian ellipsoid in space, for which $f(u)=\exp(-u^2/2)$. The third is a more general scheme developed by Garnett and Wangler [8] in which f(u) is Fourier expanded.

The uniform model will start with the same distribution function as is assumed by the mapping code. This general form will continue to be imposed on the actual particle distribution, with only the second moments being determined directly from the particles. The extent to which this imposed form is actually preserved by the particles will provide a direct check on the validity of the mapping code.

For particles within the bounds of the assumed 3-D ellipsoid, the purely linear space charge forces can be found analytically in terms of complete elliptic integrals [11]. For those few particles outside these bounds, the now-nonlinear fields can be calculated analytically in terms of *in*complete elliptic integrals [11], requiring the phase-like quantity λ, which is the real positive root of the following equation:

$$\frac{x^2}{5a^2+\lambda} + \frac{y^2}{5b^2+\lambda} + \frac{\delta z^2}{5c^2+\lambda} = 1 \ . \qquad (6)$$

The gaussian model has been used previously [15], although not in a beam optics code like TOPKARK. Here, the integrals cannot be evaluated in closed form. The favored numerical method [8], [15] is to use ten-point gaussian quadrature [10]. In this model, the space charge forces will have strong nonlinear components. The extent to which an initial gaussian distribution is preserved and the extent to which the results of this model differ from those of the uniform model will help to clarify the relative importance of how one models the beam distribution for high-brightness high-order beam optics applications.

For the more general scheme of Garnett and Wangler [8], f(u) is left arbitrary. One Fourier expands f(u), obtaining the expansion coefficients directly from the particle positions. It was shown [8] that keeping the first six terms of the expansion is probably adequate. Again, ten-point gaussian quadrature will be used to evaluate the electric fields.

III. DISCUSSION

The mapping code has already demonstrated [14] that three-dimensional space charge forces cause a new class of geometric aberrations to appear. These aberrations result from the introduction by space charge of an asymmetry in the longitudinal variable $\delta\tau$. This result is contrary to the physical intuition developed from the use of linear codes with 3-D space charge models and high-order optics codes with 2-D models. This result was partially confirmed [14] in a given example by comparison with the PARMILA code, and the results are consistent [14] with analytic considerations based on a Green's function approach to estimating nonlinear effects [16].

Our approach is faster and simpler than a particle-in-cell (PIC) or point-to-point particle code, and it is free of the strong numerical noise associated with such codes. On the other hand, because we impose a *smooth* form on the distribution, we must be in a regime where the combined field of the particles is predominantly smooth and individual collisions are a secondary effect. This condition is generally satisfied [17] if there are many particles within a Debye sphere.

The algorithms used by TOPKARK cannot follow the development of any structure within a bunch (unless, in the case of the Garnett and Wangler scheme, such structures preserve ellipsoidal symmetry), such as might arise due to plasma waves or instabilities. Thus the transit time through a lattice should not be much longer than a plasma period [17].

IV. CONCLUSIONS

The mapping version of TOPKARK is a tested and reliable high-order optics code in which a TRACE3D-like space charge model has been successfully implemented. Implementation of three distinct space charge models--uniform, gaussian and more general--into the tracking version is currently under way.

Used in a complementary fashion, the mapping and tracking versions of TOPKARK will provide a unique tool for investigating basic physics issues associated with space charge. These codes will also serve as powerful design and diagnostic tools for high-brightness beam optics applications.

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