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SPACE-CHARGE CALCULATION FOR BUNCHED BEAMS WITH 3-D ELLIPSOIDAL SYMMETRY*

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Abstract

A method for calculating 3-D space-charge forces has been developed that is suitable for bunched beams of either ions or relativistic electrons. The method is based on the analytic relations between charge-density and electric fields for a distribution with 3-D ellipsoidal symmetry in real space. At each step we use a Fourier-series representation for the smooth particle-density function obtained from the distribution of the macroparticles being tracked through the elements of the system. The resulting smooth electric fields reduce the problem of noise from artificial collisions, associated with small numbers of interacting macroparticles. Example calculations will be shown for comparison with other methods.

I. INTRODUCTION

The repulsive space-charge forces in charged particle beams are responsible both for increased defocusing and for growth of the rms emittances. For intense, high-brightness beams from rf linacs, it is important to develop better methods for calculating these effects. The main technique used is to numerically follow the orbits of a large number of representative macroparticles in their selfconsistent fields.

In principle the space-charge forces in a numerical simulation of a charged particle beam can be calculated by summing over the coulomb interactions between point macroparticles. In practice this straightforward method fails because of the artificially large collisions that occur, because of both the enhanced charge of the macroparticles and the artificially close encounters resulting from the step-by-step numerical integration with a finite step size.

Several methods have been developed to calculate spacecharge forces in linac beams. Subroutine SCHEFF[1] uses a particle in cell (PIC) method in which a 2-D r-z mesh is superimposed on the bunch. This method results in a set of source rings from which the space-charge forces are calculated at discrete r-z mesh points. A disadvantage of this method is that it is restricted to those locations where the transverse beam cross section is round. Several versions of 3-D space-charge codes have been developed; a PIC routine, MAPRO1[2], at CERN, and a method that replaces the point-to-point interactions with interactions between finite-sized spherical clouds[3]. A disadvantage of these methods is that they are generally very time consuming on the computer.

One method for 3-D space-charge calculations, developed by CERN and called MAPRO2[2], was to represent the macroparticle distribution at each step by a continuous Gaussian charge density with ellipsoidal symmetry from which the space-charge electricfield components could be calculated by numerical integration. Although this approach leads to more rapid computation, the restriction to a Gaussian profile is in principle not compatible with realistic distributions in intense beams and could lead to inaccurate calculation of space-charge-induced emittance growth.

In this paper we have generalized the MAPRO2 method to describe 3-D ellipsoidal charge densities of otherwise arbitrary shapes. We will describe the method and then show comparisons between our routine and other existing routines.

II. ELECTRIC FIELDS FOR AN ELLIPSOIDAL BUNCH

For an ellipsoidal charge distribution, the particle density (number of particles per cubic meter) can be expressed as a function of a single generalized coordinate t_x , as

$$\mathbf{n}(\mathbf{t}_{0}) = \mathbf{n} \left(\frac{\mathbf{x}^{2}}{\mathbf{a}^{2}} + \frac{\mathbf{y}^{2}}{\mathbf{b}^{2}} + \frac{\mathbf{z}^{2}}{\mathbf{c}^{2}} \right) \quad , \tag{1}$$

where a, b, and c are the rms dimensions of the distribution, and

$$t_{o} = \frac{x^{2}}{a^{2}} + \frac{y^{2}}{b^{2}} + \frac{z^{2}}{c^{2}}$$
(2)

defines the isodensity contours of the distribution. Equation (2) defines a family of concentric ellipsoids as t_{a} varies from 0 to ∞ . The advantage of the ellipsoidal distribution is that the electric field components can be expressed as a weighted integral over the particle-density distribution. Once the rms dimensions a, b, and c have been calculated, the value of the generalized coordinate, t_{a} , can be obtained for any coordinates x, y, and z from Eq. (2).

The three components[3] of the electric field, caused by a distribution of charge q*, can be expressed in terms of the density as

$$E_{x} = \frac{q^{*} abc x}{2 e_{o}} \int_{0}^{\infty} \frac{n (t) ds}{\left(a^{2} + s\right)^{3/2} \left(b^{2} + s\right)^{1/2} \left(c^{2} + s\right)^{1/2}},$$
 (3)

where $t \equiv t(x, y, z, s) = x^2 / (a^2 + s) + y^2 / (b^2 + s) + z^2 / (c^2 + s)$, and analogous expressions are valid for E_y and E_z . For the case of a spherical bunch, it is easy to show that integration over s corresponds to an integration over all the charge within a radius x.

If the particle density is known, then E_x , E_y , and E_z can be determined by numerical integration. The integral of Eq. (3) can be made numerically tractable by changing to a new variable, u, such that

$$s = d^2 \left(\frac{1}{u}, 1\right) , \qquad (4)$$

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where $d = (abc)^{1/3}$ is chosen equal to the geometric mean of the rms beam sizes and is a scaling factor required to make the integral dimensionless and numerically well behaved. The integration limits of the field integral are then transformed into 0 and 1, giving the following new expression for the field:

÷ .

d

$$E_{x} = \frac{q^{2} \operatorname{abc} x}{2 \varepsilon_{0}} \int_{0}^{1} n(t) - u^{1/2} - x$$

$$\frac{du}{3 \left[\left(\frac{a^{2}}{d^{2}} \cdot 1 \right) u + 1 \right]^{3/2} \left[\left(\frac{b^{2}}{d^{2}} \cdot 1 \right) u + 1 \right]^{1/2} \left[\left(\frac{e^{2}}{d^{2}} \cdot 1 \right) u + 1 \right]^{1/2}$$
(5)

In our treatment, the particle-density function, n(t), will be obtained from a distribution of macroparticles determined at a given time. The macroparticle charge, q^* , will be calculated from $q^* = I/Nf$, where I is the average current in amperes, f is the bunch frequency in hertz, and N is the total number of macroparticles per bunch. The representation of the macroparticle charge density is described in the following section.

III. FOURIER DESCRIPTION OF THE MACROPARTICLE CHARGE DENSITY

Our assumption of ellipsoidal symmetry makes it necessary to describe the particle density, $n(t_0)$, only for values between $t_0 = 0$ and T, where T is the maximum t_0 – value of the distribution. However, if we artificially extend the definition of the function $n(t_0)$ for t_0 – values between -T and 0 such that $n(-t_0) = n(t_0)$, then $n(t_0)$ becomes an even function about $t_0 = 0$. The density can therefore be described as a Fourier series expansion of the form

$$\mathbf{n}(\mathbf{t}_{o}) = \frac{\mathbf{a}_{o}}{2} + \sum_{\ell=1}^{\infty} \mathbf{a}_{\ell} \cos \frac{\ell \pi \mathbf{t}_{o}}{T}, \ \mathbf{T} \leq \mathbf{t}_{o} \leq \mathbf{T} \quad . \tag{6}$$

where

$$\mathbf{a}_{\ell} = \frac{2}{T} \int_{0}^{T} \mathbf{n}(\mathbf{t}_{0}) \cos \frac{\ell \pi \mathbf{t}_{0}}{T} d\mathbf{t}_{0} \qquad (7)$$

Now we obtain a convenient expression for the integral of Eq. (7). Consider the ellipsoid defined by Eq. (2), whose squared semiaxes are $t_0 a^2$, $t_0 b^2$, and $t_0 c^2$. An element of volume inside the ellipsoid is given by

$$dV = 2\pi abct_{o}^{1/2} dt_{o} \qquad (8)$$

If the density of particles is given by $n(t_0)$, then the number of particles in a shell of thickness, dt_0 , is

$$dN = n(t_o) dV = 2\pi n(t_o) abc t_o^{1/2} dt_o$$
(9)

or rewriting,

$$\mathbf{n}(\mathbf{t}_{o}) \, \mathrm{d}\mathbf{t}_{o} = \frac{\mathrm{d}\mathbf{N}}{2\pi \mathrm{abc} \, \mathbf{t}_{o}^{1/2}} \quad . \tag{10}$$

Equation (7) can then be approximated as a summation over all N – particles by

$$a_{\ell} = \frac{1}{\pi \operatorname{abc} T} \sum_{i=1}^{N} t_{0}^{i1/2} \cos \frac{\ell \pi t_{01}}{T} \quad . \tag{11}$$

This method of describing the particle density results in a smooth distribution that can represent an arbitrary density profile (either hollow or peaked) with ellipsoidal symmetry.

IV. NUMERICAL SIMULATION RESULTS

A general purpose 3-D space-charge routine (SC3DELP), based on the analytic expressions given earlier, was written and incorporated into the beam dynamics code, PARMILA. A 10-point Gaussian numerical integration was used to determine the electricfield components from Eq. (5). A five-term ($\ell = 1$ to 5) Fourier-series expansion was used to represent the macroparticle density. Figure 1 shows both the actual charge density for a 1000 macroparticle input distribution and the Fourier-series representation for comparison. T is 9.86 for this distribution.



Fig. 1 – A comparison of the charge density for a 1000 macroparticle input distribution (dotted points) and a 5-term Fourier series representation (solid line).

Two comparisons were made between the predictions of SC3DELP and other space-charge routines. First, a comparison of results on emittance growth of an expanding spherical bunch[4] was made. A Gaussian spherical input distribution, truncated after three standard deviations, was generated with the following initial parameters: $W_{in} = 2$ MeV, $\lambda = 70.5$ cm (425 MHz), input beam radius (rms) = 0.1 cm, and rms normalized input emittance, $\epsilon_{n,rms} = 0.02 \, \pi$ -cm-mrad. The bunch was then allowed to drift for varying distances. The simulation results are given in Table 1. The output emittances are given as the ratio $\epsilon_{\rm out}/\epsilon_{\rm pr}$ and are averaged over the three planes (x, y, and z). Our method agreed well with the results of both the 2-D ring code, SCHEFF, and a 3-D point-by-point (cloud-to-cloud) calculation. A space-charge calculation was made for every 1-cm step along the drift. For the 2-D calculations, a 10-interval radial mesh of 0.05-cm step size was used. The same step size, but with 20 intervals, was used longitudinally. For the 3-D point-by-point method, values of both 0.5 and 1.0 for the ratio of charge cloud diameter to Debye length were tried, achieving identical results.

As a second comparison, PARMILA simulations were run for a high-current drift-tube linac (DTL) design. The design consisted of

a 350-MHz, 3 to 35 MeV DTL incorporating a FOFODODO quadrupole-focusing scheme. Input current was varied (50-250 mA) for fixed input emittances. Figure 2 shows the transverse and longitudinal emittances using both the 2-D routine, SCHEFF, and our method, SC3DELP, for I = 125 mA. Again, we observe that the two methods give comparable results: the largest observed discrepancy is about 28%. The advantage of SC3DELP over SCHEFF is that it can also be used in situations where the transverse beam profile is not round. A space-charge calculation was made once per DTL cell. A 20 (40) interval radial (longitudinal) mesh of 0.05-cm step size was used in the 2-D calculations. SC3DELP, again, used a 5-term Fourier representation of the charge density. Increasing the number of Fourier terms (1=20) had no apparent effect.

 Table 1

 Emittance growth results for an expanding spherical bunch from simulations

Beam Current (mA)	Drift Distance (cm)	Average $\epsilon_{out}^{\prime}/\epsilon_{in}$		
		SCHEFF (2-D)	Point-by- Point (3-D)	SC3DELP (3-D)
60	100	1.13	1.14	1.13
250	50	1.44		1.47
250	100	1.59		1.66

A rough comparison of computer CPU time was also made. As expected, the required CPU time increased linearly with the number of macroparticles for a fixed number of Fourier terms used. Our 3-D method was 2-5 times slower than the 2-D calculation for an equal number of space-charge calculations. The 3-D point-bypoint calculation was approximately 15 times slower than our method.

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Fig. 2 – Transverse and longitudinal emittances as a function of cell number along a drift-tube linac from simulations using the different space-charge routines; A) SCHEFF, B) SC3DELP, C) SCHEFF, D) SC3DELP.