Calculation of coherent synchrotron radiation in toroidal waveguides by paraxial wave equation

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(Received 4 October 2006; published 9 May 2007)

A new technique for the simulation of coherent synchrotron radiation (CSR) and space-charge fields from a single electron bunch in straight or toroidal rectangular waveguide sections has been developed. It is based on the integration of the paraxial approximation to the wave equations, using the perturbation technique where the bending radius is large compared to the dimension of the waveguide. We have implemented an unconditionally stable integration method in the time domain with transparent boundary conditions that allows the use of a minimally sized computational domain about the bunch. This technique explicitly enforces the causality condition so that no portion of the fields can propagate faster than the speed of light, can be used with arbitrary three-dimensional charge distributions, and contains corrections for finite energy. We have also developed a method for the calculation of the transverse forces within the bunch including space-charge. This method has been developed for incorporation with a particle-in-cell code so that we may self-consistently model CSR and space-charge in combinations of bending sections with a fully dynamic electron bunch in an efficient manner. In this paper we describe the model and methods for calculation of the fields in detail and compare results to theory wherever possible.

DOI: [10.1103/PhysRevSTAB.10.054402](https://doi.org/10.1103/PhysRevSTAB.10.054402)

PACS numbers: 29.27.Bd, 41.75.Ht, 03.50.De

I. INTRODUCTION

New designs for charged particle accelerators, particularly as drivers for free electron lasers, are now in regimes of very short bunch length (picosecond or less) and very high charge per bunch (up to and exceeding 1 nC) [1–3]. These systems typically use bending sections either for energy recovery and/or bunch compression. In the bends the bunch will emit synchrotron radiation, characterized by a critical wavelength $\lambda_c = 3\pi R/\gamma^3$, where R is the bending radius and γ is the Lorentz factor [4]. At wavelengths smaller than the critical wavelength, the radiated power decreases rapidly. For the accelerator designs that we will consider, the critical wavelength will always be much smaller than the bunch length. However, the portion of the synchrotron radiation spectrum with wavelengths greater than the bunch length will be temporally coherent. In this case, the radiated coherent synchrotron radiation (CSR) power may be larger than the equivalent incoherent synchrotron radiation by up to a factor of N , the number of electrons per bunch [5]. For a Gaussian line-charge distribution, where the electrons are distributed with rms bunch length σ_z according to

$$\rho(z) = \frac{N}{\sqrt{2\pi}\sigma_z} e^{-z^2/2\sigma_z^2}, \quad (1)$$

we can easily compute the coherent enhancement for a particular wave number k as $\approx N e^{-(k\sigma_z)^2}$ which is obviously large whenever $k\sigma_z \ll 1$. In this case, the coherent portion of radiation from a bunched charge transiting a bend, which is greatly enhanced over the usual incoherent synchrotron radiation, may interact with itself in a way that will increase the transverse emittance. Simple estimates of the growth of transverse emittance from longitudinal CSR

indicate that this may be a serious problem for high brightness electron beams [6].

There are other factors that may enhance or mitigate the effect of CSR in bending systems. The presence of perfectly conducting walls as infinite parallel plates above and below the plane of motion restricts the CSR fields which can interact with the radiating bunch to wavelengths $\lambda \ll h^{3/2}R^{-1/2}$, where h is the gap size [7,8]. In the presence of conducting walls in the form of a waveguide, the modes must have phase velocity close to the speed of the bunch and therefore have a maximum wavelength which scales similarly as in the case of infinite parallel plates with gap size h , but where h is replaced by the characteristic dimension of the waveguide a , the smaller of either the height or width [9,10]. This restricts the range of CSR wavelengths to a band, limited below by the synchronous phase velocity requirement, and above by coherence, such that $\sigma_z \ll \lambda \ll a^{3/2}R^{-1/2}$.

Additionally, the effects from transverse fields can be significant and of comparable magnitude as the longitudinal forces [11,12]. However, the calculation of these transverse effects depends critically on the shape of the transverse charge distribution. Lastly, we can postulate that in the presence of the actual beam dynamics including dispersion, energy spread, betatron motion, energy chirp, and the resulting compression/decompression the actual situation may drastically vary from the ideal conditions assumed in the theoretical predictions. For these reasons, in order to obtain an accurate estimate of the potential effect of CSR and space-charge under dynamical conditions, we must develop simulation methods that include as much as possible. However, before the complications of beam dynamics are introduced, it is important to establish the capability of such a simulation to accurately calculate the

CSR fields to the extent that there is theory to compare with. So as a starting point, we remove the complexity of the beam dynamics and establish as a minimum goal to model the CSR and space-charge forces from a three-dimensional charge distribution traveling on a curved path inside a rectangular waveguide.

The simulation of the CSR force in a rectangular waveguide was first accomplished by numerical integration of a wave equation, originally derived in [13], in the *frequency domain* (i.e. Fourier transform in the longitudinal coordinate), using a three-dimensional grid [14]. Later, modifications of the basic equations were made to include space-charge [15] and the effect of resistive walls [16,17]. Starting with the same wave equation, we have developed an unconditionally stable, unitary integration method in the *time domain*, using a different set of boundary conditions in the longitudinal coordinate. As a result, we can simulate a single bunch in curved and straight sections in a manner that strictly enforces causality, and is free from any restriction of the simulation length. Additionally, we have extended and fully developed this method for an arbitrary, dynamic three-dimensional charge distribution including the effects of space-charge. In the following sections, we review the theoretical development, describe our method in detail, and compare results to theory where possible.

II. SIMULATION MODEL AND METHOD

A. Theoretical model

To model the effects of CSR on an electron beam, we must be able to calculate the electromagnetic fields $\mathbf{E}$ and $\mathbf{B}$ as driven by charge density ρ and current density $\mathbf{J}$. The evolution of these fields is described by Maxwell equations in vacuum. By simple manipulation, we can form wave equations (using Gaussian units),

$$\nabla^2 \mathbf{E} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{E} = \frac{4\pi}{c^2} \frac{\partial}{\partial t} \mathbf{J} + 4\pi \nabla \rho, \quad (2)$$

$$\nabla^2 \mathbf{B} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{B} = -\frac{4\pi}{c} \nabla \times \mathbf{J}, \quad (3)$$

where $c = 2.998 \times 10^{10}$ cm/s is the speed of light in vacuum. We now define the usual accelerator coordinate system which follows a reference particle a total distance s from an arbitrary origin along the design trajectory as shown in Fig. 1. For our purposes, the reference trajectory with Lorentz factor γ_0 will only be either straight, corresponding to drift sections, or uniformly bending with constant radius R , so we use a cylindrical coordinate system and set $R \rightarrow \infty$ for drift sections. We can then specify coordinates as deviations from the reference trajectory. In the longitudinal coordinate, we define $z = s - \beta_0 \tau$, where $\beta_0 = (1 - \gamma_0^{-2})^{1/2}$ and $\tau = ct$. In the transverse directions we define $x = r - R$ as the transverse coordinate in the bending plane, and y as the vertical displacement from the

FIG. 1. Accelerator coordinate system. At any given distance s along the reference trajectory, we can assume a local radius of curvature $R(s)$. Deviations in the transverse directions are given by x (in the bending plane) and y (perpendicular to the bending plane).

bending plane. Next we write the wave equations for the transverse electric fields, denoted by the subscript $\perp$. Assuming that the transverse current density $\mathbf{J}_\perp$ is negligible,

$$\left(\nabla^2 - \frac{\partial^2}{\partial \tau^2} + 2\beta_0 \frac{\partial^2}{\partial z \partial \tau} - \beta_0^2 \frac{\partial^2}{\partial z^2} \right) \mathbf{E}_\perp = 4\pi \nabla_\perp \rho. \quad (4)$$

Next, we make the assumption that the deviation from the reference trajectory in the bending plane is small compared to the bending radius. If the width of our vacuum waveguide is a , then we state this more precisely as the restriction that $x/R < a/R \equiv \delta^2 \ll 1$, where δ is a small parameter representing the effect of curvature. Additionally, we assume the reference trajectory is such that $\gamma_0^2 \gg 1$, where $\gamma_0 = (1 - \beta_0^2)^{-1/2}$ so that we may make the expansion $\beta_0 \approx 1 - 1/2\gamma_0^2$. Lastly, we neglect solutions to Eq. (4) that are not *paraxial*, or more specifically, we ignore the second derivative $\partial^2/\partial \tau^2$ relative to other terms. We restrict ourselves to the consideration of waves with wave numbers far from the waveguide cutoff, $k \gg a^{-1}$, that propagate very nearly along the longitudinal axis. For a sustained interaction, the modes must also propagate at a similar speed (phase velocity) as the beam. As discussed in the Introduction, this restricts our description to forward wave solutions $\sim e^{i(kz - \omega t)}$ with wave numbers $ka \gg \delta^{-1}$. This leads us to a parabolic wave equation [18] for the transverse electric fields, where we only keep terms to $\sim O(\delta, \gamma^{-2})$, now given by

$$\frac{\partial^2 \mathbf{E}_\perp}{\partial z \partial \tau} = -\frac{1}{2} \left[\nabla_\perp^2 + \left(\frac{1}{\gamma^2} - \frac{2x}{R} \right) \frac{\partial^2}{\partial z^2} \right] \mathbf{E}_\perp + 2\pi \nabla_\perp \rho, \quad (5)$$

where the function $O()$ denotes order of magnitude.

The boundary conditions for $\mathbf{E}$ in a waveguide with perfectly conducting walls are

$$\hat{n} \times \mathbf{E}|_S = 0, \quad (6)$$

where $\hat{n}$ is the unit vector normal to the surface. Clearly

$E_z|_S = 0$. Additionally, we require that there are no charges in contact with the walls, so that $\rho|_S = 0$, also implying $\nabla \cdot \mathbf{E}|_S = 0$. Therefore we can derive the boundary condition for the normal component of the electric field at the rectangular waveguide walls

$$\frac{\partial}{\partial n} \hat{\mathbf{n}} \cdot \mathbf{E}|_S = 0, \quad (7)$$

keeping in mind that this too will only need be evaluated to the same order of approximation with respect to δ .

To $O(\delta, \gamma^{-2})$, we can calculate all other field quantities as a function of only the transverse electric fields and the charge density. This will be particularly important when applied to a simulation method, because it reduces the storage requirements from six fields to just two. We now describe how this can be accomplished.

To calculate the longitudinal electric force $F_z = eE_z$, we use Gauss' law $\nabla \cdot \mathbf{E} = 4\pi\rho$, where we can neglect the x -dependence, $(1 + x/R)^{-1} \partial F_z / \partial z \approx \partial F_z / \partial z$, because F_z is already $O(\delta)$, yielding

$$F_z(z) = e \int_z^\infty (\nabla_\perp \cdot \mathbf{E}_\perp - 4\pi\rho) dz', \quad (8)$$

where we have exploited the fact that $F_z(\infty) = 0$. To calculate the transverse Lorentz force $\mathbf{F}_\perp = e[\mathbf{E}_\perp + (\boldsymbol{\beta} \times \mathbf{B})_\perp]$, we first transform Faraday's law into the comoving reference frame,

$$\nabla \times \mathbf{E} = \beta_0 \frac{\partial \mathbf{B}}{\partial z} - \frac{\partial \mathbf{B}}{\partial \tau}. \quad (9)$$

Here we will assume that the energy spread is small so that $\beta \approx \beta_0$. If the energy deviation is $\Delta\gamma \equiv \gamma - \gamma_0$ then $\beta - \beta_0 \approx \Delta\gamma/\gamma_0^4$ which will always be met for $\gamma_0^2 \gg 1$. Next we note that, to the same order of approximation, $B_y = \beta E_x$. Therefore Eq. (9) can be rearranged, again neglecting all terms involving x because $F_\perp \sim O(\delta^2)$ already, and integrated to yield the following equations for the transverse Lorentz forces:

$$\mathbf{F}_\perp(z) = - \int_z^\infty \left(\nabla_\perp F_z - e\beta \frac{\partial}{\partial \tau} \mathbf{E}_\perp \right) dz'. \quad (10)$$

Neglecting the time derivative, Eq. (10) is exactly what one would have obtained using the Panofsky-Wentzel theorem [19]. We expect that the time derivative term should be small, but unfortunately cannot be neglected for an accurate calculation, because it is of the same order as $\nabla_\perp F_z$ [best seen by comparing terms in Eq. (5)]. In steady state it will be identically zero, in which case we could have derived the fields in terms of retarded potentials Φ and $\mathbf{A}$. Keeping terms to the same order, we obtain the steady-state Lorentz forces

$$F_x = -e \frac{\partial V_0}{\partial x} + \frac{eA_z}{R} \quad (11)$$

$$F_y = -e \frac{\partial V_0}{\partial y} \quad (12)$$

$$F_z = -e \frac{\partial V_0}{\partial z}, \quad (13)$$

where $V_0 = (\Phi - \boldsymbol{\beta} \cdot \mathbf{A})$. In the Appendix, we show that Eq. (10) in steady state is identical with the results from this approach. The second term in the equation for F_x is the Talman force [20] which causes some difficulty for line-charge models since it is logarithmically divergent as we take the limit of small transverse dimensions. It is shown here because we will need it to correctly derive the theoretical model for the transverse forces. The effect on the transverse dynamics is thought to be largely canceled by the change in energy from space-charge forces (also logarithmically divergent) and so can be removed for linear models [21]. The extent to which these effects cancel is a subject of debate and something our model may prove useful in resolving once we add the bunch dynamics. The problem of divergence, however, does not exist for three-dimensional models. In free space, we can solve for the retarded potentials [22]

$$\Phi(\mathbf{r}, t) = \int \frac{d^3 r_1 \rho(\mathbf{r}_1, t - \tau)}{D_{\text{ret}}}, \quad (14)$$

$$\mathbf{A}(\mathbf{r}, t) = \int \frac{d^3 r_1 \boldsymbol{\beta}_1 \rho(\mathbf{r}_1, t - \tau)}{D_{\text{ret}}}, \quad (15)$$

where $D_{\text{ret}} = |\mathbf{r} - \mathbf{r}_1|$, and $\tau = D_{\text{ret}}/c$. With a constant curvature radius of R , and in the case where we can write the charge distribution as the product of transverse and longitudinal distributions, $\rho(\mathbf{r}') = \Phi(\mathbf{x}'_\perp) \lambda(z')$ we can cast Eqs. (14) and (15) into a form suitable for numerical integration:

$$V_0(\mathbf{r}) = \int \Phi(\mathbf{x}'_\perp) [1 - \beta(x') \beta_0 \cos(\xi/R)] \times \frac{\lambda[z + \xi + \beta(x') D_{\text{ret}}(\mathbf{x}'_\perp, \xi)]}{D_{\text{ret}}(\mathbf{x}'_\perp, \xi)} d\mathbf{x}'_\perp d\xi, \quad (16)$$

$$A_z(\mathbf{r}) = \int \Phi(\mathbf{x}'_\perp) \beta(x') \cos(\xi/R) \times \frac{\lambda[z + \xi + \beta(x') D_{\text{ret}}(\mathbf{x}'_\perp, \xi)]}{D_{\text{ret}}(\mathbf{x}'_\perp, \xi)} d\mathbf{x}'_\perp d\xi, \quad (17)$$

$$D_{\text{ret}} = [(R + x)^2 + (R + x')^2 - 2(R + x)(R + x')] \times \cos\left(\frac{z' - z}{R}\right) + (y - y')^2)^{1/2}, \quad (18)$$

where $\xi = z' - z$. We have allowed for a variation in β with distance x from the reference trajectory, contrary to our previous assumption where $\beta \approx \beta_0$. This will not alter our results later in this paper, because we will always

calculate the forces along the reference trajectory where $\beta = \beta_0$ identically. The variation in β for the source, however, will be necessary for an accurate comparison with theoretical calculations of the transverse force where a rigid bunch has been assumed. To keep the bunched charge distribution fixed despite moving through a dispersive bending section, we need a linear velocity shear such that $\beta(x') = \beta_0(1 + x'/R)$.

The integrations in Eqs. (16) and (17) are over two distinct regions. When $\xi < 0$, the tail-to-head interaction regime, the radiation slowly overtakes the bunch from behind. This is the usual effect associated with CSR. The fields from the tail-to-head interaction build up slowly and only reach steady state when the overtaking length is longer than the bunch length. We also integrate over $\xi > 0$, head-to-tail interaction regime, the effect is felt almost instantaneously as the radiation and charge run towards each other. For the longitudinal force, only the tail-head interaction is significant, but for the transverse force, the head-to-tail component coming from the A_z/R is dominant.

B. Simulation method

We now describe the method we use to integrate Eq. (5). This has previously been accomplished for a rigid line charge using a Fourier transform in z , where the transverse fields can be written [14]

$$E_{\perp}(x, y, z, \tau) = \int_{-\infty}^{\infty} \tilde{E}_{\perp}(x, y, k, \tau) e^{ikz} dk. \quad (19)$$

This form is quite useful for analysis or for simulation of a line charge; however, it presents some difficulty for numerical simulation of a three-dimensional and possibly dynamic source. First, note that we will be approximating the fields on a three-dimensional grid. For a sampling window size from $-c/2$ to $+c/2$ with N grid points, the sampling locations are $z_l = -c/2 + lc/N$ with $l = 0, 1, 2, \dots$. Since the fields will be sampled on discrete intervals, we need to use a discrete Fourier transform [23]

$$E_{\perp}(z_l, \tau) = \sum_{q=0}^N E_q e^{ik_q z_l}, \quad (20)$$

where $k_q = 2\pi q/c$ for $q = 0, 1, 2, \dots$ are the discrete wave numbers. This form makes the fields periodic in z with interval c . In a waveguide section such as we are simulating, there are some frequency components which will propagate with group velocity much slower speed than the bunch. A derivation of the group and phase velocities is given later in this section. If the beam stimulates these modes as it converges/diverges, they will quickly fall behind and, if care is not taken, could reappear ahead of the bunch because of the periodic boundary conditions implicit in the discrete Fourier transform. If the computational domain is not actually periodic, this *wrap-around*

effect could contaminate the fields and furthermore violate the causality condition where signals cannot propagate faster than the speed of light.

Our goal is to efficiently simulate the CSR and space-charge fields from a three-dimensional single bunch, or as an approximation, a train of bunches that are separated by distances much greater than the bunch length while adequately resolving the forces within the bunch. This may be in individual sections or combinations of sections that are either straight or uniformly curved. Because of the difficulty associated with the wrap-around effect, we have developed a method that does not use periodic boundary conditions. Instead, we use a *time domain* method in the spatial variable z to integrate the paraxial wave equations, instead of a *frequency domain* method in the frequency variable k . We can choose the behavior at the boundaries (in z) as desired. To simulate a single bunch, at the boundary ahead of the bunch, at $z = +c/2$, we choose to set the fields to zero because it may be easily chosen to be sufficiently far enough ahead of the bunch that no radiation could ever reach it. On the other hand, for the same situation, we let any radiation passing the boundary behind the bunch, at $z = -c/2$, simply pass through as if the boundary were transparent. As long as the rear boundary is far enough away that radiation propagating to the rear boundary cannot reverse itself and come forward again, then the situation should be adequately representative of our model. We can therefore still use a relatively small (in z) window about the center of the bunch with a reasonable size, on the order of $10\text{--}20 \sigma_z$, which both models the physical situation and is computationally efficient. The transition between sections is accomplished by simply changing the value of R and continuing to advance the fields. For straight sections, $\kappa = 1/R = 0$, and for curved sections, R is set to the bending radius of the reference trajectory. The bending radius could change within a bending section but for our purposes does not.

To devise a stable integration scheme in the time domain, we found it necessary to use spectral methods in the transverse directions, where the transverse dependence is written as a series of eigenfunctions. We use either sine or cosine expansions that meet the boundary conditions in Eqs. (6) and (7) for perfectly conducting walls in a waveguide channel width a and height b . The transverse fields are written as

$$E_x = \sum_{m,n=0}^{\infty} \tilde{E}_x e_x^{m,n}, \quad (21)$$

$$E_y = \sum_{m,n=0}^{\infty} \tilde{E}_y e_y^{m,n}, \quad (22)$$

where

$$\begin{Bmatrix} e_x^{m,n} \\ e_y^{m,n} \end{Bmatrix} = \begin{Bmatrix} \cos[k_n(x - a/2)] \sin[k_m(y - b/2)] \\ \sin[k_n(x - a/2)] \cos[k_m(y - b/2)] \end{Bmatrix}, \quad (23)$$

and $k_n = n\pi/2a$, $k_m = m\pi/2b$. The exact boundary conditions at $y = \pm b/2$ are $E_x = 0$ and $\partial E_y/\partial y = 0$. At $x = \pm a/2$, $E_y = 0$, but the exact form of Eq. (7) is

$$\left. \frac{\partial E_x}{\partial x} + \frac{E_x}{R+x} \right|_{x=\pm a/2} = 0. \quad (24)$$

Since we have only retained terms to $O(\delta)$, we can also replace the boundary condition by its approximation to the same order,

$$\left. \frac{\partial E_x}{\partial x} \right|_{x=\pm a/2} \approx 0. \quad (25)$$

Therefore our eigenfunctions meet the boundary conditions individually, which in turn allows us to use an implicit method for advancing the fields because we are guaranteed to satisfy the boundary conditions area each step. By the implicit method, we mean that we can algebraically solve for the updated value at a particular time using both the previous value and current value to approximate the derivative.

The use of these eigenfunctions also allows us to easily compute the transverse spatial derivatives (from the $\nabla_\perp^2$ operator) with spectral accuracy. However this is inconsistent with terms involving x , so we need to split the transverse operator into two parts and integrate them separately and sequentially. This technique is known as *the method of fractional steps* [24]. Equation (5) then becomes two equations:

$$\frac{\partial^2 \tilde{E}_\perp}{\partial z \partial \tau} = \frac{1}{2} k_\perp^2 \tilde{E}_\perp + 2\pi k_\perp \tilde{\rho}, \quad (26)$$

$$\frac{\partial E_\perp}{\partial \tau} = \left(\frac{x}{R} - \frac{1}{2\gamma^2} \right) \frac{\partial}{\partial z} E_\perp, \quad (27)$$

where $\tilde{E}_\perp$ are the expansion coefficients. Equations (26) and (27) are integrated sequentially for each time step, using a fast Fourier transform method to change in and out of transverse eigenfunction space each step.

We now discretize the fields on a uniform mesh $x_i = a(i/N_x - 1/2)$ where $i = 0, 1, 2, \dots, N_x$ and similarly for y_j and z_l , as well as for time $\tau_n = n\Delta\tau$. For Eq. (26) we use an implicit finite difference method using only the points as illustrated in Fig. 2. Because we are only using points that are at or ahead (in z) of the point we are currently solving for, there is no mechanism for information to travel forward. As we will demonstrate later, the group velocity for all frequencies that are solutions to Eq. (26) are negative and therefore cannot propagate forward. Therefore, by using on the points as shown in Fig. 2 we are enforcing causality for this step. The discrete form of Eq. (26) is

$$\begin{aligned} \tilde{E}_{\perp,l}^{n+1} = & \frac{1-q}{1+q} (\tilde{E}_{\perp,l+1}^{n+1} + \tilde{E}_{\perp,l}^n) - \tilde{E}_{\perp,l+1}^n \\ & + \pi k_\perp \Delta\tau \Delta z (\tilde{\rho}_{l+1} + \tilde{\rho}_l), \end{aligned} \quad (28)$$

FIG. 2. Implicit integration scheme showing which points in space and time are used to solve for the point to be updated. Here the iteration runs from forward to back and requires initializing the furthest upstream point in order to solve for all others (set to zero if sufficiently upstream).

where $q = k_\perp^2 \Delta\tau \Delta z / 8$. Because the scheme needs to be initialized, we begin at the forward boundary and integrate from front to back, again consistent with causality. Note that the source term is fixed in this scheme, but could easily be advanced self-consistently under the influence of the electromagnetic fields.

Equation (27) can be integrated a similar method, this time depending on the sign of the term $(1/\gamma^2 - 2x/R)$. If it is positive, radiation can indeed propagate ahead of the beam and vice versa if it is negative, so we use two methods:

$$E_{\perp,l+1}^{n+1} = \frac{1-p}{1+p} (E_{\perp,l+1}^n - E_{\perp,l}^{n+1}) + E_{\perp,l}^n (p > 0), \quad (29a)$$

$$E_{\perp,l-1}^{n+1} = \frac{1+p}{1-p} (E_{\perp,l-1}^n - E_{\perp,l}^{n+1}) + E_{\perp,l}^n (p < 0), \quad (29b)$$

where $p = (1/2\gamma^2 - x/R)\Delta\tau/\Delta z$.

We can estimate the error in either step by Fourier analysis (neglecting the source term), assuming $\tilde{E}_\perp \sim e^{ik_z z}$. Equations (26) and (27) separately can be integrated analytically, namely,

$$\tilde{E}_\perp(\mathbf{k}_\perp, k_z, t) = \tilde{E}_\perp(\mathbf{k}_\perp, k_z, 0) \exp\left[-i \frac{k_\perp^2}{2k_z} \tau\right], \quad (30)$$

$$E_\perp(\mathbf{x}_\perp, k_z, t) = E_\perp(\mathbf{x}_\perp, k_z, 0) \exp\left[-ik_z \left(\frac{1}{2\gamma^2} - \frac{x}{R}\right) \tau\right]. \quad (31)$$

If we write the time stepping discrete forms as $\tilde{E}_{\perp,l}^n = \lambda^n e^{il(k_z \Delta z)}$, $E_{\perp,l}^n = \mu^n e^{il(k_z \Delta z)}$, and substitute them into Eqs. (28) and (29), we obtain

$$\lambda = \frac{1 - iq \cot(k_z \Delta z/2)}{1 + iq \cot(k_z \Delta z/2)}, \quad (32)$$

$$\mu = \frac{1 - ip \tan(k_z \Delta z/2)}{1 + ip \tan(k_z \Delta z/2)}. \quad (33)$$

It is obvious that $|\lambda|, |\mu| = 1$ for all wavelengths and step sizes and therefore both steps are individually unconditionally stable.

In order evaluate the combination of steps, we use Parseval's theorem,

$$\int |\tilde{E}_{\perp,l}^n|^2 d\mathbf{k}_{\perp} = \int |E_{\perp,l}^n|^2 d\mathbf{x}_{\perp}, \quad (34)$$

to write the overall scheme in terms of the square integral of fields as a product. In our notation, the difference between n and $n+2$ will equal one complete step as $\tilde{E}_{\perp,l}^{n+1} = \lambda \tilde{E}_{\perp,l}^n$, and $E_{\perp,l}^{n+2} = \mu E_{\perp,l}^{n+1}$, therefore

$$\int |\tilde{E}_{\perp,l}^{n+2}|^2 d\mathbf{k}_{\perp} = |\lambda|^2 |\mu|^2 \int |\tilde{E}_{\perp,l}^n|^2 d\mathbf{k}_{\perp}, \quad (35)$$

$$\int |E_{\perp,l}^{n+2}|^2 d\mathbf{x}_{\perp} = |\lambda|^2 |\mu|^2 \int |E_{\perp,l}^n|^2 d\mathbf{x}_{\perp}. \quad (36)$$

Again, $|\lambda|^2 |\mu|^2 = 1$ for all longitudinal modes, regardless of step size. Since each step conserves the square integral of the fields, it is clear that it remains bounded for all time. By definition, any unstable discrete mode would grow without bound and thereby cause the square integral to grow without bound which cannot happen, therefore we conclude that all modes are stable unconditionally. The preservation of the field energy is of course consistent with our model of perfectly conducting walls which have lossless reflection. Phase accuracy, on the other hand, can only be achieved if both $4q/k_z \Delta z, pk_z \Delta z \ll 1$. The worst case scenario occurs for a maximum longitudinal wavelength of L and transverse charge distribution width of $\sigma_{\perp}$ ultimately limits that maximum time step to

$$\Delta\tau \ll \frac{\sigma_{\perp}^2}{L}. \quad (37)$$

If we look at solutions $\sim e^{i(k_z z - \omega\tau)}$ in Eqs. (26) and (27), we can obtain a separate dispersion relation for each step:

$$\omega^{(1)} = \frac{k_{\perp}^2}{2k_z}, \quad (38)$$

$$\omega^{(2)} = \left(\frac{1}{2\gamma^2} - \frac{x}{R} \right) k_z. \quad (39)$$

The phase and group velocities, $v_{\phi} \equiv \omega/k_z$, $v_g \equiv \partial\omega/\partial k_z$ are

$$v_{\phi}^{(1)} = \frac{k_{\perp}^2}{2k_z^2}, \quad (40)$$

$$v_{\phi}^{(2)} = \left(\frac{1}{2\gamma^2} - \frac{x}{R} \right), \quad (41)$$

$$v_g^{(1)} = -\frac{k_{\perp}^2}{2k_z^2}, \quad (42)$$

$$v_g^{(2)} = \left(\frac{1}{2\gamma^2} - \frac{x}{R} \right). \quad (43)$$

By considering the action of the combination of steps we can understand the scaling $k_{\min} \gtrsim R^{1/2} a^{-3/2}$ of the synchronous modes. The requirement is that the phase velocity is zero. We can approximate this by requiring that $v_{\phi}^{(1)} + v_{\phi}^{(2)} = 0$. Transverse modes will have $k_{\perp} \gtrsim a^{-1}$, and $x \lesssim a$, thus requiring $k_z \gtrsim R^{1/2} a^{-3/2}$, ignoring the small terms $O(\gamma^{-2})$.

We can also see that the group velocity in Eq. (26) is always negative, and the group velocity in Eq. (27) may be positive or negative depending on the sign of the term $(1/2\gamma^2 - x/R)$. Therefore our choice of finite differencing in Eqs. (28) and (29) for Eqs. (26) and (27) automatically enforces causality as appropriate. We can also see that modes with large transverse wave numbers and small longitudinal wave numbers will rapidly fall behind the bunch because they have the greatest negative group velocity. Because the system is lossless, these modes could contaminate the solution if we had used periodic boundary conditions to model a nonperiodic system. The mode with the largest (negative) group velocity has $k_{\perp} \sim \sigma_{\perp}^{-1}$ and $L \sim c$, the length of the computational domain. We can estimate the maximum bend angle that can be simulated $\Delta\tau/R$ before this mode reaches the boundary,

$$\Delta\tau/R = \frac{c}{v_g R} \sim \frac{2\sigma_{\perp}^2}{cR}. \quad (44)$$

If we had used periodic boundary conditions, this would have restricted the simulation to cases where $\Delta\tau/R \ll 1$ which would be unacceptable for the range of parameters we are interested in.

III. RESULTS

We now test the simulation results to theory where possible. All examples in this section, unless specified otherwise, will use a 100 MeV, 1 nC bunch, with a three-dimensional Gaussian distribution, with longitudinal rms length, $\sigma_z = 0.23$ cm, and axisymmetric transverse rms width, $\sigma_{\perp} = 0.2$ cm,

$$\rho(\mathbf{x}) = \frac{Ne}{(2\pi)^{3/2} \sigma_{\perp}^2 \sigma_z} e^{-(x^2+y^2)/2\sigma_{\perp}^2} e^{-z^2/2\sigma_z^2}. \quad (45)$$

Note that this form remains fixed which is definitely not the correct dynamical description of the bunch dynamics in a dipole magnet. However, because the theoretical results we

will use for comparison assume a rigid bunch, we must also do so here. The bending radius where applicable is constant at $R = 120$ cm. The waveguide dimensions will vary as necessary for comparison to theory. For vacuum theory we will simply make them large enough that the results converge and shielding and reflection are negligible. For a fixed grid resolution, this means we need more grid points in the transverse directions to simulation vacuum. For the case of waveguide boundaries, our method becomes more efficient because less grid points are required. On the other hand, theories which use image charges to account for shielding become less efficient as the waveguide dimensions shrink.

We begin with space-charge. Since we have retained terms to order γ^{-2} , we should be able to recover the space-charge fields for straight line motion. To see why this should work, examine Eq. (5) with $R \rightarrow \infty$. Because we no longer have the curvature term involving x , we may find the steady-state solution by setting the time derivative to zero and Fourier transforming all the space variables:

$$\mathbf{E}(\mathbf{x}) = \int d^3x \hat{\mathbf{E}}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}}. \quad (46)$$

Then we have the steady-state straight line solution

$$\hat{\mathbf{E}}_{\perp}^{ss}(\mathbf{k}) = \frac{4\pi \nabla \hat{\rho}(\mathbf{k})}{k_{\perp}^2 + k_z^2/\gamma^2}. \quad (47)$$

First, we compute the longitudinal force using the differential form of Eq. (8):

$$\hat{F}_z^{ss}(\mathbf{k}) = \frac{-i4\pi k_z \hat{\rho}}{\gamma^2(k_{\perp}^2 + k_z^2/\gamma^2)}. \quad (48)$$

Finally we substitute this into Eq. (10) to obtain

$$\hat{\mathbf{F}}_{\perp}^{ss}(\mathbf{k}) = \frac{4\pi \nabla \hat{\rho}(\mathbf{k})}{\gamma^2(k_{\perp}^2 + k_z^2/\gamma^2)}. \quad (49)$$

The inverse Fourier transform is independent of γ , so we can explicitly demonstrate the γ^{-2} scaling as expected. Thus, we can expect that if the simulation converges to a steady-state solution it should accurately calculate the space-charge forces.

As a test, we numerically integrate Eqs. (26) and (27) with $R \rightarrow \infty$ and compute the space-charge fields which are known from theory in vacuum. The theoretical space-charge force for a three-dimensional Gaussian in free space is given by

$$F_x = \frac{2Ne^2}{\sqrt{2\pi}\sigma_z\gamma^2} \left(\frac{1 - e^{-x^2/2\sigma_x^2}}{x} \right). \quad (50)$$

The results are shown in Fig. 3 showing excellent agreement. We then calculate the coherent synchrotron radiation and space-charge longitudinal force in a curved waveguide at various times along the trajectory for a rigid charge distribution. For comparison, we take the transient theory

FIG. 3. (Color) Space-charge force x -component as a function of x in a straight 30×30 cm waveguide, taken at the center point of a three-dimensional Gaussian bunch with rms length $\sigma_z = 0.23$ cm, and rms width $\sigma_{\perp} = 0.2$ cm. Simulation results are circles, and theory is represented by a solid line. The force is normalized to $F_0 = Ne^2/\sqrt{2\pi}\sigma_z\gamma^2$.

for a Gaussian line charge [25]

$$F_z = \sqrt{\frac{2}{\pi}} \frac{Ne^2}{(3R^2\sigma_z^4)^{1/3}} G(\zeta, \eta), \quad (51)$$

where $G(\zeta, \eta)$ is a function on the order of 1 given by

$$G(\zeta, \eta) = \eta^{-1/3} [e^{-(\zeta-\eta)^2/2} - e^{-(\zeta-4\eta)^2/2}] + \int_{\zeta-\eta}^{\zeta} \frac{d\zeta'}{(\zeta-\zeta')^{1/3}} \frac{d}{d\zeta'} e^{-(\zeta')^2/2}, \quad (52)$$

where $\zeta = z/\sigma_z$ is the distance traveled in the bend and $\eta = \xi^3/(24R^2\sigma_z)$. The results are shown in Fig. 4, which also show very good agreement.

We now compare our simulation with the steady-state theoretical results for shielding. By reducing the vertical gap size, keeping the horizontal dimension large, we should approximate the case of infinite parallel plates. Although there are results for parallel plate shielding for a Gaussian line charge given directly in the time domain, it is somewhat easier to calculate the results using the longitudinal coupling impedance [10]. A line charge can be approximated in our simulation by reducing the transverse dimensions so that $\sigma_{\perp} \ll \sigma_z$. An actual line charge is impossible on this simulation because it would require an infinite number of terms in the eigenfunction expansion, also reducing the maximum time step given Eq. (37) to an infinitesimal distance. So we just fix the transverse dimension of the waveguide at a large width, here 50 cm, and reduce $\sigma_{\perp}$ until the results converge. The results are shown for three different values of gap size, each obtained after the fields have reached steady state, achieved after a distance in the bend that is much longer than the characteristic

FIG. 4. (Color) Longitudinal force as a function of z (taken at $x, y = 0$) from CSR in transient states (measured in distance traveled past the entrance) from simulation (symbols) compared to vacuum theory (lines) for a three-dimensional Gaussian bunch in a 30×30 cm rectangular waveguide with a uniform bending radius of 120 cm. The longitudinal coordinate z is scaled to the rms bunch length σ_z , which is 0.23 cm, and the force is scaled to $W_0 = \sqrt{2/\pi} N e^2 (3R^2 \sigma_z^4)^{-1/3}$.

formation length $\tau \gg 2(3\sigma_z R^2)^{1/3}$, which in this case is about 42 cm. The results from the simulation were taken at $\tau = 300$ cm and, as shown in Fig. 5, once again demonstrate excellent agreement with the theory.

If we now reduce the width of the waveguide we may expect to see the effects of shielding in both transverse

FIG. 5. (Color) Longitudinal force as a function of z (taken at $x, y = 0$) from CSR in steady state with shielding from infinite parallel plates for three different gap sizes. The simulation (symbols) is compared to infinite parallel plate theory (lines) for Gaussian line charge. The bending radius is 120 cm, and the horizontal gap in the simulation is fixed at 50 cm to approximate infinite parallel plates. The longitudinal coordinate z is scaled to the rms bunch length σ_z , which is 0.23 cm, and the force is scaled to $W_0 = \sqrt{2/\pi} N e^2 (3R^2 \sigma_z^4)^{-1/3}$.

directions. For a sustained interaction with the radiation, it must propagate with a similar speed (i.e. phase velocity) as the bunch. The synchronous modes of a square toroidal waveguide must have wave numbers above $k_{\min} = 4.78R^{1/2}a^{-3/2}$ [9,10,13]. Furthermore, for these modes to be coherent with the bunch they must satisfy $k\sigma_z \lesssim 1$. In general, if $k_{\min}\sigma_z \ll 1$, there will be many synchronous modes, approaching the limiting case where the synchronous modes appear as a continuum. As a becomes very large, we approximate the vacuum (unshielded case). On the other hand, as a is made smaller, causing $k_{\min}$ to be greater, we approach the case where fewer modes will be coherent. Therefore, by carefully choosing the bunch length and a , we may be able to isolate just a single mode which is both synchronous and coherent, thereby seeing its effect clearly, appearing as a single sinusoidal signal behind the bunch. Recall that we are simulating a single bunch, and therefore no mode can be stimulated in front of it.

Using the nomenclature of [10], there are two types of modes, the “TE” mode with $E_y = 0$, and the “TM” mode with $E_x = 0$. For the square waveguide, the lowest frequency modes calculated by the method in [13] are: TE(1,0) at $k = 4.78R^{1/2}a^{-3/2}$, TM(1,0) at $k = 8.78R^{1/2}a^{-3/2}$, and TE(1,1) at $k = 12.8R^{1/2}a^{-3/2}$. For all cases using the simulation, we choose $a = b = 2.5$ cm. In order to only see the lowest mode, we pick $\sigma_z = 0.115$ cm. The resulting steady-state longitudinal force along the axis at $x = y = 0$ is shown in Fig. 6, which clearly illustrates the presence of a single sinusoidal synchronous mode stimulated behind the bunch. We can also compute the

FIG. 6. (Color) Longitudinal force as a function of z (taken at $x, y = 0$) from CSR in steady state in a square toroidal waveguide. The sinusoidal wake behind the bunch is the lowest order synchronous mode TE(1,0), and has wave number $k = 13.2$ cm. The bending radius is 120 cm, and the width and height are 2.5 cm. The longitudinal coordinate z is scaled to the rms bunch length σ_z , which is 0.115 cm, and the force is scaled to $W_0 = \sqrt{2/\pi} N e^2 (3R^2 \sigma_z^4)^{-1/3}$.

power loss of the bunch, using the results from [13], where the loss factor for a single electron with energy W is $\kappa \equiv e^{-2}dW/ds$. To calculate the average bunch power loss, we must take into account the effects of coherence as discussed in the Introduction. For the Gaussian bunch distribution, the average energy loss rate of the bunch for a single mode is

$$\frac{d\bar{W}}{ds} = \kappa r_e mc^2 N e^{-(k\sigma_z)^2}, \quad (53)$$

where $r_e = e^2/mc^2$ is the classical electron radius. Using the value from [13], with $\kappa a^2 = 4.94$ for the TE(1,0) mode, leads to a predicted average energy loss rate of 67 eV/cm when $\sigma_z = 0.115$ cm.

We can test this using the simulation with some test particles which do not move but keep track of the total energy change. Once again, the source remains fixed, as that is the assumption of the theory. After the initial transient phase in which the nonsynchronous modes fall behind, we find a steady-state energy loss rate of 66 eV/cm, which differs from the theory by 1.5%. A plot of the energy deviation from the initial average beam energy of 100 MeV vs distance s along the bend is shown in Fig. 7. The small discrepancy is attributed to differences in the assumptions of the theory and the realities of the simulation. Notably, we cannot use a line charge, but only approximate it by reducing the beam width. In the simulation the beam was a Gaussian axisymmetric distribution with $\sigma_\perp = 0.07$ cm. Additionally, the theory uses a periodic boundary at $2\pi R$, so in principle, there would be a sinusoidal wake in front of

FIG. 7. (Color) Average power loss from the TE(1,0) synchronous mode in a square toroidal waveguide as a function of distance s along the bend. The bending radius is 120 cm, and the width and height are 2.5 cm. The bunch length $\sigma_z = 0.115$ cm, and the rms beam width is $\sigma_\perp = 0.07$ cm. The symbols are the average beam energy deviation (from 100 MeV initial energy) expressed in keV, and the line is a theoretical prediction of 67 eV/cm. The simulation results reaches a steady-state loss rate of 66 eV/cm, which differs from the theoretical prediction by 1.5%.

the bunch also. The simulation, however, uses special boundary conditions where this wake will never appear in front of the bunch because all of the synchronous modes have negative group velocities. Regardless, we find a reasonable agreement between the theory and simulation in this case, as we expect the effects to be small.

We can uncover more modes by decreasing the bunch length. We now take $\sigma_z = 0.028$ cm and again run the simulation to a steady-state situation. In this case, we should see the three lowest frequency modes as described above. To confirm the presence of these modes, we can identify them more clearly in a spectral analysis which is shown in Fig. 8. Here, we now see the TE(1,0), TM(1,0), and TE(1,1) modes. The modes above these frequencies do not appear with any significant power because there are not coherent at this bunch length.

Last, we compute the steady-state transverse coherent synchrotron force and space-charge force (in the plane of motion) as shown in Fig. 9. For comparison, we numerically integrated Eqs. (16) and (17). The nonsymmetric shape is an effect of the finite transverse dimensions of the bunch. It should be noted that the theoretical result can only be obtained under artificial constraints, specifically here we must assume a linear velocity shear in order to make a rigid charge distribution fixed in the local coordinate system. Of course, this is unphysical because, if the reference trajectory is close to the speed of light, the outer particles will exceed it. In an actual uniformly bending section, the bunch would be continuously deforming in a combination of betatron motion in the horizontal plane coupled with longitudinal bunching/debunching all with period $2\pi R$. In this case, the forces would never reach a

FIG. 8. (Color) Power spectrum of E_z (taken at $x, y = 0$) from CSR in steady state in a square toroidal waveguide, showing the three lowest frequency synchronous modes. The bending radius is 120 cm, and the width and height are 2.5 cm. The three modes have predicted wave numbers of 13.2, 24.3, and 35.5 cm^{-1} , respectively. The beam is a fixed three-dimensional Gaussian with $\sigma_z = 0.028$ cm and $\sigma_\perp = 0.07$ cm.

FIG. 9. (Color) Transverse coherent synchrotron radiation force in steady state as a function of z , taken along the center $x, y = 0$ of a three-dimensional Gaussian bunch given by simulation (shown in circles). The theoretical value (line) was calculated by numerical integration of Eqs. (16) and (17). The longitudinal coordinate z is scaled to the rms bunch length σ_z and the force is scaled by $F_{x0} = 2Ne^2/R$.

steady state and we would be left without anything to compare to. Despite these violations of our assumptions it is interesting to note that simulation implicitly took care of this while the theory had to be modified.

IV. CONCLUSIONS

We have shown that the integration of the paraxial wave equation in the time domain can be accomplished and can accurately reproduce results from theory for vacuum, infinite parallel plates, and a rectangular waveguide for rigid charge distributions. Additionally, we have devised a method to calculate the transverse self-fields as well. However, this method has far more capability than the current state of theory can deal with. The most obvious case is in a waveguide where shielding is significant, most theoretical solutions only apply to a steady-state condition. Even for a rigid distribution in sector dipole magnet, steady state is rarely achieved before exiting each sector magnet because the formation length is long. If we included the actual beam dynamics for a bunch, we would never reach a steady-state condition. Furthermore, we would like to have the bunch respond in a self-consistent way to the CSR and space-charge fields. This simulation can naturally handle all of these situations in a fully three-dimensional way. The extent to which these effects are canceled by space-charge fields is the subject of further investigation. The simulation we have developed encompasses all the major aspects of the real physical situation such as three dimensionality, time dependence, boundary conditions and space-charge forces. What is most encouraging is that method may easily be coupled with a particle-in-cell code with all the

relevant dynamics, therefore creating a truly self-consistent model.

ACKNOWLEDGMENTS

This work was supported by the Joint Technology Office and the Office of Naval Research.

APPENDIX: DERIVATION OF THE RELATIONSHIP BETWEEN TRANSVERSE AND LONGITUDINAL FORCES IN STEADY STATE

In this Appendix, we will show the details of the derivation leading to Eq. (10).

We start by expressing the electric and magnetic fields in terms of potentials ϕ and A ,

$$\mathbf{E} = -\nabla\phi - \frac{1}{c}\frac{\partial}{\partial t}\mathbf{A} \quad (\text{A1})$$

$$\mathbf{B} = \nabla \times \mathbf{A}. \quad (\text{A2})$$

The force felt by a test particle moving at speed βc along an arc of a circle with radius r is given by the Lorentz force law,

$$\mathbf{F} = e[\mathbf{E} + \boldsymbol{\beta} \times \mathbf{B}]. \quad (\text{A3})$$

In a cylindrical coordinate system $\{r, \theta, z\}$ if we take the particle's motion to be in the θ -direction, we have the two following components:

$$F_r = e\left(-\frac{\partial\phi}{\partial r} - \frac{1}{c}\frac{dA_r}{dt} + \frac{\beta}{r}\frac{\partial}{\partial r}rA_\theta\right), \quad (\text{A4})$$

$$F_\theta = e\left(-\frac{1}{r}\frac{\partial\phi}{\partial\theta} + \frac{\beta}{r}\frac{\partial A_\theta}{\partial\theta} - \frac{1}{c}\frac{dA_\theta}{dt}\right), \quad (\text{A5})$$

where we have substituted the total time derivative defined by

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \frac{\beta c}{r}\frac{\partial}{\partial\theta}. \quad (\text{A6})$$

Subsequently, we neglect the total time derivative, consistent with our approach of using the paraxial wave equation where the fields evolve slowly in the comoving reference frame.

Lastly, we compute the difference in the derivatives as follows:

$$\frac{1}{r}\frac{\partial F_r}{\partial\theta} - \frac{\partial F_\theta}{\partial r} = \frac{e}{r}\left(-\frac{1}{r}\frac{\partial\phi}{\partial\theta} + \frac{\beta}{r}\frac{\partial A_\theta}{\partial\theta}\right), \quad (\text{A7})$$

noting that the right-hand side F_θ/r if we neglect the total derivative. Rearranging terms, we have

$$\frac{1}{r}\frac{\partial F_r}{\partial\theta} = \frac{\partial F_\theta}{\partial r} + \frac{F_\theta}{r}. \quad (\text{A8})$$

This is essentially Eq. (10) if we change variables to $x = r - R$ and $z = R\theta$ and neglect small terms in $x/R \ll 1$.

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