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Invited Article: Refined analysis of synchrotron radiation for NIST's SURF III facility

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Abstract

We have developed a new method for the exact calculation of synchrotron radiation for the National Institute of Standards and Technology Synchrotron Ultraviolet Radiation Facility, SURF III. Instead of using the Schwinger formula, which is only an approximation, we develop formulae based on Graf's addition theorem for Bessel functions and accurate asymptotic expansions for Hankel functions and Bessel functions. By measuring the radiation intensity profile at two distances from the storage ring, we also confirm an apparent vertical emittance that is consistent with the vertical betatron oscillations that are intentionally introduced to extend beam lifetime by spreading the electron beam spatially. Finally, we determine how much diffraction by beamline apertures enhances the spectral irradiance at an integrating sphere entrance port at the end station. This should eliminate small but treatable components of the uncertainty budget that one should consider when using SURF III or similar synchrotrons as standard, calculable sources of ultraviolet and other radiation. <https://doi.org/10.1063/1.5018412>

I. INTRODUCTION

The Synchrotron Ultraviolet Radiation Facility on the Gaithersburg campus of the National Institute of Standards and Technology, referred to as SURF III since its most recent upgrade, is a calculable standard source of ultraviolet and other radiation for radiometric calibrations of instruments, and, by comparison measurements, standard lamps such as deuterium lamps.

¹ This is based on the ability to accurately calculate radiation emitted by a relativistic charged particle (to be precise, an electron) moving in a highly uniform magnetic field. Despite earlier reports on the characteristics of SURF III, we have undertaken to extend the analysis to address potential deficiencies. The analysis used here could in part be adapted for other light sources, if orbital sections in bend magnets are approximately circular arcs, whereas treatment of undulators and free-electron lasers is a field unto itself beyond the scope of this work.

The first improvement, discussed in Sec. II, is our development of an exact, efficient method to calculate the radiation fields *in lieu* of the Schwinger formula, which is approximate. Previously, since Schott's work,² Ivanenko and Sokolov³ and Schwinger⁴ developed their approximate methods that become very accurate, especially if (a) one calculates fields far

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from the tangent point of the electron's orbit, (b) the electron is highly relativistic, and (c) and fields are sought sufficiently close enough to the orbital plane. Westerveld and co-workers⁵ published tables to help readers calculate the intensity without use of the Schwinger formula.

The second improvement, discussed in Sec. III, is related to vertical betatron oscillations that are intentionally excited to spread the beam vertically, thereby reducing the rate of electron-electron collisions and increasing beam lifetime. (Moreover, SURF III has weak focusing, so that there are always horizontal betatron oscillations.) One effect of the vertical betatron oscillations is apparent fluctuations in tilt of the orbital plane as different electrons pass through a given nominal orbit tangent. Recently, improved imaging of the electron beam cross section and the temporary absence of one beamline permitted scans of the radiation profile to analyze anew how orbital tilt fluctuations affect the profile. We have developed a model that confirms the magnitude of the vertical betatron oscillations, which obviously also should be accounted for when calculating the radiometric intensity on a beamline.

The third improvement, discussed in Sec. IV, is inclusion of diffraction effects because of three apertures that were present on Beamline 2. Diffraction effects in this case, like in much of radiometry, include concentration of excess radiation on the central region of one's detector. Correcting for the bias that this causes should be included in best-practice radiometric measurements, and we report our findings on this matter as well. The results suggest that enlarging the apertures would reduce complications because of diffraction, and that understanding their effects requires good beam conditions.

II. "EXACT" CALCULATION OF SYNCHROTRON RADIATION

Consider a particle with charge q on a circular orbit with radius R_0 in a uniform magnetic field at angular frequency ω . As a function of cylindrical coordinates R , θ , and z , the time-dependent charge density is

$$\begin{aligned}\rho(R, \theta, z, t) &= \frac{q\delta(z)\delta(R - R_0)\delta(\theta - \theta_0 - \omega t)}{R_0} \\ &= \frac{q\delta(z)\delta(R - R_0)}{2\pi R_0} \sum_{n=-\infty}^{+\infty} \exp\left[in\left(\theta - \theta_0 - \omega t\right)\right].\end{aligned}\quad (1)$$

We want to know the electric and magnetic fields at a point $\mathbf{r}$, whose Cartesian coordinates are $(\rho \cos \psi, \rho \sin \psi, Z)$. By definition, at $\mathbf{r}$, $\hat{\mathbf{R}}$ and $\hat{\boldsymbol{\theta}}$ have the values, $\hat{\boldsymbol{\rho}}$ and $\hat{\boldsymbol{\Psi}}$, respectively. We denote the vector from a point on the orbit to $\mathbf{r}$ by $\mathbf{s}$. As a consequence, $\mathbf{r} - \mathbf{s}$, whose Cartesian coordinates are given by $(R_0 \cos \theta, R_0 \sin \theta, 0)$, is a point on the orbit. By the continuity equation, the time-dependent current density is

$$\begin{aligned}
 \mathbf{J}(\mathbf{r} - \mathbf{s}) &= \frac{\omega q \delta(z) \delta(R - R_0)}{2\pi} \hat{\boldsymbol{\theta}} \sum_{n=-\infty}^{+\infty} e^{in(\theta - \theta_0 - \omega t)} \\
 &= \sum_{n=-\infty}^{+\infty} \mathbf{J}_n(\mathbf{r} - \mathbf{s}) e^{-in\omega t}.
 \end{aligned} \tag{2}$$

For this, we use the fact that the current's only non-zero component is along $\hat{\boldsymbol{\theta}}$ (Fig. 1).

From Eqs. (491), (506), and (498) of Mohr,⁶ one can obtain

$$\begin{aligned}
 \mathbf{E}_n(\mathbf{r}) &= -\left(\frac{\mu_0 c k^2}{6\pi}\right) \int d^3 \mathbf{s} \mathbf{J}_n(\mathbf{r} - \mathbf{s}) h_0^{(1)}(ks) \\
 &\quad + \left(\frac{\mu_0 c k^2}{12\pi}\right) \int d^3 \mathbf{s} [s^2 \mathbf{J}_n(\mathbf{r} - \mathbf{s}) \\
 &\quad - 3\mathbf{s}(\mathbf{s} \cdot \mathbf{J}_n(\mathbf{r} - \mathbf{s}))] \left(\frac{h_2^{(1)}(ks)}{s^2}\right)
 \end{aligned} \tag{3}$$

and

$$c\mathbf{B}_n(\mathbf{r}) = -i \left(\frac{\mu_0 c k^2}{4\pi}\right) \int d^3 \mathbf{s} \left[\mathbf{s} \times \mathbf{J}_n(\mathbf{r} - \mathbf{s}) \right] \left(\frac{h_1^{(1)}(ks)}{s}\right), \tag{4}$$

all without needing to invoke the potential concept. (Throughout this work, we use a notation whereby the length of vector is indicated in non-bold italics. For instance, the length of $\mathbf{s}$ is simply s .) Also, $k = n\omega/c$ is the angular wave number of the synchrotron radiation at the n th harmonic frequency, c is the speed of light in vacuum, μ_0 is the permeability of free space, and $h_l^{(1)}$ denotes a spherical Hankel function of the first kind of order l . The same expressions for the fields can be obtained using vector and scalar potentials.

It helps us to define dimensionless oblate spheroidal coordinates with the same azimuthal angle θ ,

$$u = \frac{k}{2} [\sqrt{(\rho + R_0)^2 + Z^2} + \sqrt{(\rho - R_0)^2 + Z^2}] \tag{5}$$

and

$$v = \frac{k}{2} [\sqrt{(\rho + R_0)^2 + Z^2} - \sqrt{(\rho - R_0)^2 + Z^2}], \quad (6)$$

implying $ks = [u^2 + v^2 - 2uv \cos(\theta - \psi)]^{1/2}$, and the parameter

$$P_n = \left(\frac{\mu_0 c k^2}{4\pi} \right) \left(\frac{\omega q R_0}{2\pi} \right) e^{-in\theta_0}. \quad (7)$$

Of the two fields, the magnetic field is easier to compute. From Eq. (4), one finds

$$\begin{aligned} c\mathbf{B}_n(\mathbf{r}) &= -iP_n \int d\theta (\hat{\mathbf{s}} \times \hat{\boldsymbol{\theta}}) h_1^{(1)}(ks) e^{in\theta} \\ &= P_n e^{in\psi} \left[(-ik\rho I_n^{(1+)} + ikR_0 I_n^{(1)}) \hat{\mathbf{z}} \right. \\ &\quad \left. + ikZI_n^{(1+)} \hat{\boldsymbol{\rho}} + kZI_n^{(1-)} \hat{\boldsymbol{\Psi}} \right]. \end{aligned} \quad (8)$$

Above and in what follows, we use the shorthand, $I_n^{(l\pm)} = (I_{n+1}^{(l)} \pm I_{n-1}^{(l)}) / 2$, with

$$I_m^{(l)} = \int_{-\pi}^{+\pi} d\phi \left(\frac{h_l^{(1)}(ks)}{(ks)^l} \right) e^{im\phi}. \quad (9)$$

For the electric field, we first note

$$\begin{aligned} \mathbf{E}_n(\mathbf{r}) &= -\frac{2P_n}{3} \int d\theta \hat{\boldsymbol{\theta}} h_0^{(1)}(ks) e^{in\theta} \\ &\quad + \frac{P_n}{3} \int d\theta [\hat{\boldsymbol{\theta}} - 3\hat{\mathbf{s}}(\hat{\mathbf{s}} \cdot \hat{\boldsymbol{\theta}})] h_2^{(1)}(ks) e^{in\theta}. \end{aligned} \quad (10)$$

Writing

$$h_2^{(1)}(ks) = \frac{3h_1^{(1)}(ks)}{ks} - h_0^{(1)}(ks), \quad (11)$$

Equation (10) can be simplified to

$$\begin{aligned} \mathbf{E}_n(\mathbf{r}) = & -P_n \int d\theta \hat{\boldsymbol{\theta}} h_0^{(1)}(ks) e^{in\theta} \\ & + P_n \int d\theta \left[\hat{\boldsymbol{\theta}} \left(\frac{h_1^{(1)}(ks)}{ks} \right) - \hat{\mathbf{s}} \left(\hat{\mathbf{s}} \cdot \hat{\boldsymbol{\theta}} \right) h_2^{(1)}(ks) \right] e^{in\theta}. \end{aligned} \quad (12)$$

By also noting

$$h_2^{(1)}(ks) = \frac{h_1^{(1)}(ks)}{ks} - \frac{1}{k} \frac{d}{ds} h_1^{(1)}(ks) \quad (13)$$

and using

$$\begin{aligned} \hat{\boldsymbol{\theta}} &= -\frac{1}{R_0} \frac{ds}{d\theta}, \\ \hat{\mathbf{s}} \cdot \hat{\boldsymbol{\theta}} &= -\frac{1}{R_0} \frac{ds}{d\theta}, \\ (\hat{\mathbf{s}} \cdot \hat{\boldsymbol{\theta}}) \frac{d}{ds} h_1^{(1)}(ks) &= -\frac{1}{R_0} \frac{ds}{d\theta} \frac{d}{ds} h_1^{(1)}(ks) = -\frac{1}{R_0} \frac{dh_1^{(1)}(ks)}{d\theta}, \end{aligned} \quad (14)$$

one can show

$$\hat{\boldsymbol{\theta}} \left(\frac{h_1^{(1)}(ks)}{ks} \right) - \hat{\mathbf{s}} \left(\hat{\mathbf{s}} \cdot \hat{\boldsymbol{\theta}} \right) h_2^{(1)}(ks) = -\frac{1}{R_0} \frac{d}{d\theta} \left[\mathbf{s} \left(\frac{h_1^{(1)}(ks)}{ks} \right) \right]. \quad (15)$$

We therefore have

$$\begin{aligned} \mathbf{E}_n(\mathbf{r}) &= -P_n \int d\theta \hat{\boldsymbol{\theta}} h_0^{(1)}(ks) e^{in\theta} + \frac{inP_n}{R_0} \int d\theta \left[\mathbf{s} \left(\frac{h_1^{(1)}(ks)}{ks} \right) \right] e^{in\theta} \\ &= P_n e^{in\psi} \left[\left(in / R_0 \right) I_n^{(1)} \mathbf{r} - i \left(n I_n^{(1+)} + I_n^{(0-)} \right) \hat{\boldsymbol{\rho}} \right. \\ &\quad \left. - \left(n I_n^{(1-)} + I_n^{(0+)} \right) \hat{\boldsymbol{\Psi}} \right]. \end{aligned} \quad (16)$$

Note that the expressions for both fields have correct transformation properties with respect to ψ .

To evaluate $I_m^{(l)}$, one can first rewrite spherical Hankel functions in terms of their cylindrical counterparts,

$$\begin{aligned}
 I_m^{(l)} &= \int_{-\pi}^{+\pi} d\phi \frac{h_l^{(1)} \left((u^2 + v^2 - 2uv \cos \phi)^{1/2} \right)}{(u^2 + v^2 - 2uv \cos \phi)^{l/2}} e^{im\phi} \\
 &= \left(\frac{\pi}{2} \right)^{1/2} \int_{-\pi}^{+\pi} d\phi \frac{H_{l+1/2}^{(1)} \left((u^2 + v^2 - 2uv \cos \phi)^{1/2} \right)}{(u^2 + v^2 - 2uv \cos \phi)^{l/2 + 1/4}} e^{im\phi},
 \end{aligned} \tag{17}$$

and apply Graf's addition theorem. This is found, e.g., in Watson,⁷ and it is also discussed in the NIST Digital Library of Mathematical Functions (DLMF),⁸ Sec. 10.23 (ii). This gives

$$\begin{aligned}
 &H_{l+1/2}^{(1)} \left((u^2 + v^2 - 2uv \cos \phi)^{1/2} \right) \\
 &= \left(\frac{u - ve^{-i\phi}}{u - ve^{+i\phi}} \right)^{l/2 + 1/4} \sum_{k=-\infty}^{+\infty} H_{l+1/2+k}^{(1)} \left(u \right) J_k \left(v \right) e^{-ik\phi}.
 \end{aligned} \tag{18}$$

One may next simplify the integrand using

$$\begin{aligned}
 &\frac{H_{l+1/2}^{(1)} \left((u^2 + v^2 - 2uv \cos \phi)^{1/2} \right)}{(u^2 + v^2 - 2uv \cos \phi)^{l/2 + 1/4}} \\
 &= \left(\frac{1}{u - ve^{+i\phi}} \right)^{l/2 + 1/4} \sum_{k=-\infty}^{+\infty} H_{l+1/2+k}^{(1)} \left(u \right) J_k \left(v \right) e^{-ik\phi} \\
 &= \frac{1}{u^{l+1/2}} \sum_{s=0}^{\infty} \frac{(l+1/2)_s}{s!} \left(\frac{v}{u} \right)^s \sum_{k=-\infty}^{+\infty} H_{l+1/2+k}^{(1)} \left(u \right) J_k \left(v \right) e^{i(s-k)\phi}.
 \end{aligned} \tag{19}$$

Next, trivial integration over ϕ gives

$$I_m^{(l)} = \frac{2\pi(\pi/2)^{1/2}}{u^{l+1/2}} \sum_{s=0}^{\infty} \frac{(l+1/2)_s}{s!} \left(\frac{v}{u} \right)^s H_{m+l+1/2+s}^{(1)} \left(u \right) J_{m+s} \left(v \right). \tag{20}$$

Recurrence relations for Hankel and Bessel functions imply that one can estimate the value of s for which $(v/u)^s$ renders all subsequent terms negligible, evaluate the Hankel and Bessel functions for that and the next lowest value of s , and evaluate all remaining values using the recurrence relation in order of descending s . In practice, a small value of v/u can obviate the need to evaluate the summand in order of descending s because the sum can still be found with high accuracy. Because one has $v < u$, the sum converges like a geometric series. The parameters n , u , and v are all large, v and n are similar in size, and u is larger, but not necessarily much larger, than v . Furthermore, when field strengths are computed for

increasing distance from the origin along any direction, n is constant, v approaches a finite, limiting value, and u grows indefinitely.

The Hankel function can be evaluated using Debye's asymptotic formula,⁹ also discussed in DLMF Sec. 10.19 (ii),⁸ while the Bessel function can be evaluated using Olver's uniform asymptotic expansion,¹⁰ also discussed in DLMF Sec. 10.20 (i).⁸ The latter evaluation can be problematic because of exact cancellations of divergent terms in that expansion, but we present a practical method to perform an accurate calculation (to about 12 decimal digits) in the Appendix. The leading (and dominant) behavior of a Hankel function of large argument greater than its large order is

$$H_v^{(1)}(v \sec \alpha) \sim \left(\frac{2}{\pi v \tan \alpha}\right)^{1/2} \exp\left[i\left(v \tan \alpha - v\alpha - \pi/4\right)\right] + \dots \quad (21)$$

Regarding the phase of this expression, note first that $n \cong v$. One large part of the phase, close in value to $n \tan \alpha$, accounts for phase acquired by the radiation fields because of the distance travelled from points $\mathbf{r} - \mathbf{s}$ near the tangent point to $\mathbf{r}$. Another large part, close in value to $-n\alpha$, accounts for the phase of the complex current density's n th Fourier component near the tangent point. The triangle that one can construct to relate all arguments of Bessel and Hankel functions in Eq. (18), the triangle with vertices at the origin, the tangent point and $\mathbf{r}$, and the triangle with sides $u \cong n \sec \alpha$, $n\alpha$ and $n \tan \alpha$, all become similar triangles in the relativistic limit at $Z = 0$.

To summarize the foregoing analysis, we note that it is a method to calculate synchrotron radiation exactly, without recourse to the approximations used by Schwinger and others. These approximations could be listed as follows: (1) When evaluating the $I_m^{(l)}$ integrals, the integral is approximated in terms of the Airy function or its derivative; (2) one assumes that Z/ρ is small compared to unity; (3) one assumes that ρ is arbitrarily larger than R_0 ; and (4) one assumes that the charged particle is sufficiently relativistic to justify the first three approximations.

One question worth asking is the relationship between Eqs. (8) and (16) and the more conventional Schwinger formula. By using Debye's asymptotic results for Bessel and Hankel functions of large argument and order, we have successfully derived the familiar Schwinger result. For non-negligible field strengths, the Schwinger result should render values of $\mathbf{E}$ and $c\mathbf{B}$ that are correct on the order of $n^{-1/3}$ times the in-plane electric field strength. The calculation is quite lengthy and we only summarize it here. First note that kR_0 , n , and v all have relative differences on the order of $n^{-2/3}$, as also do $k\rho$ and u , as well as v/u and $\cos \alpha$. By approximating the respective quantities just mentioned to be equal simplifies the calculation at the cost of a small error. One can introduce

$$\Psi = \frac{Z}{R_0 \tan \alpha}, \quad (22)$$

$$a = \frac{(1/\gamma^2 + \Psi^2)^{1/2}}{\pi\sqrt{3}} K_{1/3} \left(\frac{n}{3} (1/\gamma^2 + \Psi^2)^{3/2} \right), \quad (23)$$

$$b = -\frac{(1/\gamma^2 + \Psi^2)}{\pi\sqrt{3}} K_{2/3} \left(\frac{n}{3} (1/\gamma^2 + \Psi^2)^{3/2} \right), \quad (24)$$

and

$$Q = P_n e^{in\psi} \left(\frac{2\pi i^{-3/2}}{u \sin \alpha} \right) e^{i\Psi_n}, \quad (25)$$

where Ψ_n denotes the complex phase of $H_n^{(1)}(u)$, and we note that b is smaller than a by a factor on the order of $n^{-1/3}$. One can show

$$J_{n+k}(v) = (a + bk) \left[1 + O(n^{-2/3}) \right] \quad (26)$$

and

$$H_{n+\delta}^{(1)}(u) = \left(\frac{2}{\pi u \sin \alpha} \right)^{1/2} \exp(i\Psi_n - i\delta\alpha) \left[1 + O(n^{-2/3}) \right]. \quad (27)$$

Using only terms shown in Eqs. (26) and (27), one can carry out the summation in Eq. (20) and apply the result to Eqs. (8) and (16). Retaining only the leading non-zero term in each field component gives

$$E_n(\mathbf{r}) \cong Q \left[b(\hat{\rho} \cos \alpha - \hat{\Psi} \sin \alpha) + ia\Psi\hat{\mathbf{z}} \right] \quad (28)$$

and

$$c\mathbf{B}_n \cong Q \left[ia\Psi(\hat{\rho} \cos \alpha - \hat{\Psi} \sin \alpha) - b\hat{\mathbf{z}} \right]. \quad (29)$$

These approximations, which correspond to the conventional Schwinger result, differ from our exact result by a relative error on the order of $n^{-1/3}$. We also note that Ψ is at most on the order of $n^{-1/3}$ wherever field strengths are appreciable.

III. EFFECTS OF BETATRON OSCILLATIONS

Beam stability requires restoring forces that counter a particle's departure from an ideal circular orbit. Small departures are approximately sinusoidal oscillations about the ideal orbit in both the R - and z -direction, known as betatron oscillations. They are described, for instance, by Wiedemann,¹¹ who also cites earlier work by others. We denote departures of R by $R - R_0 = \delta R$ and departures of z from zero simply by $z = \delta z$. Either type of departure is accompanied by a velocity $\dot{R}$ or $\dot{z}$ that is 90° ahead of the departure in phase. Because the particle is always moving at a velocity near c in its forward direction, the instantaneous direction of its motion is rotated clockwise (for the case of a counterclockwise orbit) by $\theta_R = \dot{R}/c$ rad in the orbital plane and by $\theta_z = \dot{z}/c$ rad out of the orbital plane. We neglect effects that are at second or higher orders in these angles, including those $\propto \theta_R \theta_z$. The effects of both types of oscillations (horizontal and vertical) must be considered. Here we do so in the absence of beamline optics. In Sec. IV, we consider further effects when the radiation is diffracted by beamline optics such as apertures.

In either the horizontal or vertical case, we assume Gaussian distributions in the relevant degrees of freedom that we rationalize as follows (noting that this argument ignores the perturbing effects of electron-electron interaction, but is a reasonable starting point for analysis in the case of good beam conditions). First, note that any single electron's betatron oscillation of either type is generated by repeated interactions with what can be treated as a random disturbance. Let the real-space coordinate displacement be denoted by q , and its velocity divided by the betatron oscillation's angular frequency be denoted by $v = \dot{q} / \omega_q$.

Simple harmonic motion implies that q and v precess on a circular path in (q, v) phase space at angular frequency ω_q . However, they are displaced by some random amount (because of the amplitude and direction of the disturbance's force) and at a random point on an otherwise circular path in (q, v) phase space. To consider only the radius of this path, one can eliminate precession by working in a rotating frame in (q, v) phase space. Then the displacement because of each interaction would have a random magnitude and direction. After many interactions, the sum of displacements would lead to a Gaussian probability distribution in (q, v) space of the form

$$\frac{1}{2\pi[\sigma(q)]^2} \exp\left(-\frac{q^2 + v^2}{2[\sigma(q)]^2}\right). \quad (30)$$

Taken alone, interactions with the disturbance would enhance the oscillations, but oscillations are also damped for reasons such as emission of radiation, determining $\sigma(q)$.

A. Horizontal betatron oscillations

Because of the weak focusing, there are always horizontal betatron oscillations at SURF III. From Wiedemann,¹¹ we know that the radial betatron frequency is $\omega_R = (1 - n_B)^{1/2} \omega$, where

$$n_B = -\frac{R}{B} \frac{dB}{dR} \quad (31)$$

is the magnetic field index, with $n_B = 0.594$. For SURF III, this establishes a relationship between the standard deviations of radial departures and angular variations, namely, $\sigma(\theta_R) = \omega_R \sigma(\delta R)/c$. Imagery of the electron beam can be used to establish $\sigma(\delta R)$.

When considering radiation that is propagating along a beamline, it is convenient to introduce a new variable that is the distance light has travelled from the tangent to the point $\mathbf{r}$, and we denote this distance by d . Variation of θ_R can be sufficiently accurately addressed by using modified values of θ_R and d according to the replacement

$$\begin{pmatrix} \theta_R \\ \delta R \\ d \end{pmatrix} \rightarrow \begin{pmatrix} 0 \\ \delta R + R_0(1 - \cos \theta_R) \\ d - R_0 \sin \theta_R \end{pmatrix}. \quad (32)$$

This is motivated in Fig. 2 and is reasonable because an electron still maintains a path that is primarily a circular orbit with radius nearly equal to R_0 . In the case of SURF III, for $\theta_R = 1$ mrad, this would involve a change in d of 0.837 mm and be equivalent to a transverse displacement of the beamline of about 0.418 μm . Furthermore, first-order effects of θ_R do not matter because of its symmetric distribution about zero, and we find this to be the case. Effects of variation of θ_R are also small in free space because they are equivalent to an opposite transverse displacement of a beamline. Meanwhile, the radiation is emitted along every tangent of the orbit, also helping us to reduce effects of θ_R . The exception to this rule is when radiation fields are diffracted by beamline optics (discussed in Sec. IV).

B. Vertical betatron oscillations

Vertical betatron oscillations are intentionally excited for reasons already discussed. The vertical oscillations lead to variation of the orbital plane height by θ_z , which is easily incorporated into a radiometric model, but they also lead to variation of the orbital plane tilt θ_z that must be considered because the angular spread of radiation has consequences that grow with d . Again from Wiedemann,¹¹ we know that the vertical betatron frequency is given by $\omega_z = n_B^{1/2} \omega$, and we have $\sigma(\theta_z) = \omega_z \sigma(\delta z)/c$. With $\omega \cong 3.58 \times 10^8$ rad/s, we have $\omega_z \cong 2.76 \times 10^8$ rad/s. As an example, with a 0.6 mm full-width at half-maximum (FWHM) Gaussian distribution, we have a standard deviation of orbital plane height of $\sigma(\delta z) \cong 0.255$ mm. For a beam energy of 380 MeV, this implies $\sigma(\theta_z) \cong 0.235$ mrad.

Let $E_\lambda(\lambda, d, h)$ denote the spectral irradiance for wavelength λ in a vertical plane at a distance d from the tangent at height h relative to the nominal orbital plane. This is given by the pattern that one would have without betatron oscillations, i.e., $E_\lambda^{(0)}(\lambda, d, h)$, convolved with a Gaussian of fixed width because of $\sigma(\delta z)$ and a Gaussian whose width grows because of $\sigma(\theta_z)$, with $z' = \theta_z d$,

$$E_{\lambda}(\lambda, d, h) = \frac{1}{2\pi\sigma(\delta z)\sigma(z')} \int_{-\infty}^{+\infty} d(\delta z) e^{-(\delta z)^2 / [2\sigma(\delta z)^2]} \times \int_{-\infty}^{+\infty} dz' e^{-z'^2 / [2\sigma(z')^2]} E_{\lambda}^{(0)}(\lambda, d, h - h'), \quad (33)$$

where we have $h' = \theta z + z'$, with total variance $\sigma(h')^2 = \sigma(\delta z)^2 + \sigma(z')^2$. This implies

$$E_{\lambda}(\lambda, d, h) = \left(\frac{1}{2\pi\sigma(h')^2} \right)^{1/2} \times \int_{-\infty}^{+\infty} dh' e^{-h'^2 / [2\sigma(h')^2]} E_{\lambda}^{(0)}(\lambda, d, h - h') \quad (34)$$

and, in particular,

$$E_{\lambda}(\lambda, d, 0) = E_{\lambda}^{(0)}(\lambda, d, 0) + \frac{\sigma(h')^2}{2} \left(\frac{d^2 E_{\lambda}^{(0)}(\lambda, d, 0)}{d^2 h} \right) \bigg|_{h=0} + \dots \quad (35)$$

For purposes of radiometric calibrations, the pupil of an instrument undergoing calibration would be near the average orbital plane, and the irradiance at the pupil can be estimated using Eq. (35), which includes effects of vertical betatron oscillations and is an effective measurement equation for uncertainty analysis.

Measurements that we carried out test the above analysis of the effects of vertical betatron oscillations. The overall intensity at and near $h = 0$ was analyzed to characterize the main effects. After summing over horizontal and vertical polarization, $E_{\lambda}^{(0)}(\lambda, d, h)$ has a local minimum in the orbital plane between maxima near the plane (symmetrically located above and below it), and the irradiance decreases rapidly far from the plane. Measurements of the effects of the betatron oscillations were performed at two distances from the tangent and for various amplitudes of vertical betatron oscillations. To isolate the effects of the oscillations, one can consider the ratio

$$X = \left(\frac{E_{\lambda}(\lambda, d, h)}{E_{\lambda}(\lambda, d, 0)} \right) \div \left(\frac{E_{\lambda}^{(0)}(\lambda, d, h)}{E_{\lambda}^{(0)}(\lambda, d, 0)} \right) \quad (36)$$

and determine the orbital tilt fluctuations that provide the best fit to measured data, whereas orbital height fluctuations can be estimated by imaging the beam. Results for three beam

energies and relatively ideal beam conditions are shown in Fig. 3. Covariance of the δz FWHM and best-fit θ_z FWHM is shown in Fig. 4 for varying beam conditions compared to the ideal case derived above. For SURF III, we estimate that the relative standard uncertainty of $\sigma(\delta z)$ is 0.02, while the relative standard uncertainty of $\sigma(\theta_z)$ is about 0.10 because of the standard deviation of the best-fit values of $\sigma(\theta_z)$ from the values expected because of the value of $\sigma(\delta z)$ and the preceding analysis. For the present uncertainty analysis, we ignore covariance of $\sigma(\delta z)$ and $\sigma(\theta_z)$ because the *measured* values of $\sigma(\delta z)$ and $\sigma(\theta_z)$ have fixed biases that are not covariant. We can use Eq. (27) to estimate the uncertainty component, related to vertical betatron oscillations (denoted below by “v.b.o.”), of the average, nominally in-plane irradiance

$$u(E_\lambda(\lambda, d, 0))_{\text{v.b.o.}} \cong \sigma\left(h'\right) u\left(\sigma\left(h'\right)\right) \left(\frac{d^2 E_\lambda^{(0)}(\lambda, d, 0)}{d^2 h} \right) \bigg|_{h=0}. \quad (37)$$

In the example that we consider in Sec. IV, the relative uncertainty in the irradiance because of imperfect knowledge of the betatron oscillations would be a few μW per W.

IV. DIFFRACTION EFFECTS OF BEAMLINE 2 APERTURES

The analysis of Secs. II and III considered irradiance because of radiation that propagated from the tangent through free space. For calibrating irradiance of deuterium lamps by a ratiometric measurement, we consider a beamline that has three non-limiting apertures and two large gate valves with glass windows upstream of an integrating-sphere entrance port that can view either a deuterium lamp undergoing calibration or the synchrotron beam. Ideally, all apertures and the sphere port are assumed to be aligned with the orbit tangent. Window transmission corrections can be deduced by having the light pass through either window or both windows while comparing measured signals.¹

Smaller sizes of the apertures compared to those in previous deuterium lamp calibrations necessitate investigating the apertures' impact on the otherwise fully understood synchrotron radiation that is incident on the sphere entrance port. The NIST Sensor Science Division and its predecessor organizations have developed computer programs that efficiently simulate the propagation of radiation through multi-staged, cylindrically symmetrical systems using the Fresnel-Kirchhoff method.¹² This is done by tracing partial waves through the optics train. Because they individually obey the Helmholtz scalar wave equation in free space, the horizontal and vertical electric field components can each be treated, at least to a good enough approximation for estimating the diffraction effects, as independent scalar wave fields, because angles of incidence and exitance at apertures are always very close to aperture and sphere port area normals, and diffraction in this case affects polarization weakly.

For what follows, many of the geometrical parameters are illustrated in Fig. 5 for the case of $\theta_R = \theta_z = 0$. Because of horizontal and vertical betatron oscillations, the actual tangent fluctuates horizontally and vertically in terms of its instantaneous location and direction. The

beamline optics are stationary, but it is convenient to consider the equivalent repositioning of the beamline entrance and direction of the beamline principal axis, which is the same as its aperture surface normals. A coordinate system whose coordinates are (x_{BL}, y_{BL}, z_{BL}) can be created for each position and direction of the beamline relative to the tangent, where z_{BL} is the distance travelled from the center of the most upstream aperture along the beamline axis, the x_{BL} direction is parallel to the (x, y) plane, and y_{BL} completes the right-handed coordinate system.

Because θ_R and θ_z are always small, in practice one can approximate their effects. Viewed from above, the angle subtended by the line segment from the orbit center to the unperturbed tangent point $\mathbf{t}$ and center of the beamline's most upstream aperture is $\phi = \cos^{-1}(R_0/\rho)$. Note that we have $\phi > 0$ even though the tangent is at $\theta = -\phi$, which is reflected in the analysis that follows. The unperturbed beamline principal axis is along the direction, $(\rho \cos \psi - R_0 \cos(\phi - \psi), \rho \sin \psi + R_0 \sin(\phi - \psi), 0)$, because we have $\mathbf{t} = R_0 \cos(\phi - \psi)\hat{\mathbf{x}} - R_0 \sin(\phi - \psi)\hat{\mathbf{y}}$.

Because of betatron oscillations, we first address effects of θ_R as described in Sec. III A, which amounts to a translation of the beamline along and transverse to the tangent direction. That is, the beamline is displaced by the difference vector,

$$R_0 \{ [(-\sin \theta_R \sin(\phi - \psi) - (1 - \cos \theta_R) \cos(\phi - \psi))\hat{\mathbf{x}} + [-\sin \theta_R \cos(\phi - \psi) + (1 - \cos \theta_R) \sin(\phi - \psi)]\hat{\mathbf{y}} \}$$

Again rotating the beamline instead of the orbital tilt to achieve the same net effect, the effective principal axis direction of the beamline can be found by first letting $\hat{\mathbf{v}}$ be a normalized vector along the unperturbed principal axis direction and including effects of θ_z by $\hat{\mathbf{z}}_{BL} = \hat{\mathbf{v}} \cos \theta_z - \hat{\mathbf{z}} \sin \theta_z$. One can next deduce $\hat{\mathbf{x}}_{BL} = (\hat{\mathbf{z}} \times \hat{\mathbf{z}}_{BL}) \sec \theta_z$ and $\hat{\mathbf{y}}_{BL} = \hat{\mathbf{z}}_{BL} \times \hat{\mathbf{x}}_{BL}$. So $\hat{\mathbf{z}}_{BL}$ is very close to parallel to the ideal tangent along the direction of the electron's travel at the tangent, $\hat{\mathbf{x}}_{BL}$ is close in value to the inwardly directed radial unit vector that would be found at the ideal tangent point, and $\hat{\mathbf{y}}_{BL}$ is close in value to $+\hat{\mathbf{z}}_{BL}$.

With the nominal distance along the beamline principal axis between the first optical element and the tangent being $d_0 = R_0 \tan \phi$, the effective center of the most upstream aperture is positioned at approximately

$$\mathbf{r}_{ctr} \cong \mathbf{t} + d_0 \hat{\mathbf{z}}_{BL} - \delta R \hat{\mathbf{x}}_{BL} - \delta z \hat{\mathbf{y}}_{BL}. \quad (38)$$

The aperture's area is normal to $\hat{\mathbf{z}}_{BL}$, and all effects of betatron oscillations on radiation incident on its area are sufficiently well included for purposes of estimating the diffraction effects. Here δR and δz indicate the outwardly and upwardly directed deviation of the tangent from where it would occur without betatron oscillations.

After deducing the appropriate scalar fields, which are proxies for electric field components in scalar diffraction calculations described, and are given by

$$U_x(x_{BL}, y_{BL}, z_{BL}) = \mathbf{E}(x_{BL}, y_{BL}, z_{BL}) \cdot \hat{\mathbf{x}}_{BL} \quad (39)$$

and

$$U_y(x_{BL}, y_{BL}, z_{BL}) = \mathbf{E}(x_{BL}, y_{BL}, z_{BL}) \cdot \hat{\mathbf{y}}_{BL} \quad (40)$$

everywhere on the most upstream aperture's area, diffraction calculations can proceed.

The fields on the most upstream aperture were computed on a grid in cylindrical polar coordinates to facilitate simulated propagation of partial waves further down the beamline. Because of the very large number of points required on the first optical element, the calculation was done by first tabulating the phase Φ of the leading term in $H_{n+1/2}(u)$ and the field amplitude divided by $\exp(i\Phi)$ on a two-dimensional Cartesian grid that overfilled the aperture. Fields were then obtained on the cylindrical grid using two-dimensional Lagrange interpolation of the phase and the amplitude and projected onto partial waves using fast-Fourier-transform methods. Care was taken to ensure sufficiency of all grids for accuracy of numerical quadrature and suppression of Fourier aliasing.

If we let z_N denote the value of z_{BL} on the area of the N th optical element, then the field on the subsequent element at a point $(x'_{BL}, y'_{BL}, z'_{BL})$ is given by

$$\begin{aligned} U_{x,y} \left(x'_{BL}, y'_{BL}, z_{N+1} \right) &\cong \frac{1}{i\lambda(z_{N+1} - z_N)} \int_{A_N} dx_{BL} dy_{BL} \\ &\times \exp \left\{ \frac{ik}{2(z_{N+1} - z_N)} \left[(x_{BL} - x'_{BL})^2 + (y_{BL} - y'_{BL})^2 \right] \right\} \\ &\times U_{x,y}(x_{BL}, y_{BL}, z_N). \end{aligned} \quad (41)$$

The apertures' radii and distances from the nominal tangent are given in Table I. Here A_N indicates that integration is carried out over the area of the N th aperture. This double integration becomes a single integration over radius for each partial-wave channel. One may proceed to iteratively apply Eq. (41) until finally integrating flux arriving at the sphere port. The relative diffraction effects are the ratio of flux found when apertures are included vs omitted. Many numerical tricks are used to accelerate calculations.

We have analyzed diffraction effects for the beam condition with $\sigma(\delta z) = 255 \mu\text{m}$, which implies $\sigma(\theta_z) = 235 \mu\text{rad}$, and $\sigma(\delta R) = 0.892 \mu\text{m}$, which implies $\sigma(\theta_R) = 679 \mu\text{rad}$. In principle, assessment of diffraction effects involves averaging over the distributions of δz , δR , θ_z and θ_R . In Fig. 6, we show results for 96 cubature sampling points for the spatial displacements versus several fixed values of angular displacements. The cubature was

performed by introducing $\delta R = r' \cos \eta$ and $\delta z = r' \sin \eta$. Averaging a quantity f over δR and δz can be done using

$$\begin{aligned} \langle f \rangle &= N_f \int_{-\infty}^{+\infty} d(\delta R) \int_{-\infty}^{+\infty} d(\delta z) \\ &\quad \times \exp \left[- \left(\frac{(\delta R)^2}{2[\sigma(\delta R)]^2} + \frac{(\delta z)^2}{2[\sigma(\delta z)]^2} \right) \right] f(\delta R, \delta z) \\ &= N_f \int_0^{2\pi} d\eta \int_0^{\infty} dr' r' \exp \left[- \frac{r'^2}{2} \left(\frac{\cos^2 \eta}{2[\sigma(\delta R)]^2} + \frac{\sin^2 \eta}{2[\sigma(\delta z)]^2} \right) \right] \\ &\quad \times f(r' \cos \eta, r' \sin \eta), \end{aligned} \quad (42)$$

with N_f being for normalization purposes. Introducing

$$x' = \frac{r'^2}{2} \left(\frac{\cos^2 \eta}{2[\sigma(\delta R)]^2} + \frac{\sin^2 \eta}{2[\sigma(\delta z)]^2} \right) = c(\eta) \left(\frac{r'^2}{2} \right), \quad (43)$$

we have

$$\left\langle f \right\rangle = N_f \int_0^{2\pi} \frac{d\eta}{c(\eta)} \int_0^{\infty} dx' e^{-x'} f \left(\sqrt{2x' / c(\eta)} \cos \eta, \sqrt{2x' / c(\eta)} \sin \eta \right), \quad (44)$$

allowing for cubature with regularly spaced values of η and integration over x' using the Gauss-Laguerre quadrature. Results differed very slightly whether using 12 and 8 vs 24 and 12 values of η and x' , respectively, i.e., 96 and 288 cubature points in total.

Power incident on the integrating sphere port is scaled by two factors, $F_{b.o.}$, which accounts for effects of betatron oscillations (shown in red, see Fig. 6), and F_{diff} , which accounts for diffraction effects (shown in green). It is clear that F_{diff} only depends weakly on angular displacements (the effects shown in blue) so that such a mixed effect can be neglected, with an associated relative uncertainty component for the power $\sim 100 \mu W/W$. These results are for a wavelength of 400 nm, and this latter dependence should be smaller at shorter wavelengths. We show the theoretical F_{diff} versus wavelength for two sets of cubature points (points) in Fig. 7, as well as a best-fit parabolic curve (solid line). The diffraction effects mimic those for the case of a point source near the tangent.

V. UNCERTAINTY ANALYSIS

From Shaw *et al.*,¹ one uncertainty component expresses the level of confidence in knowledge of the spectral irradiance because of synchrotron radiation at an integrating sphere entrance port. We would append to this several additional components that became

evident in this work. These include uncertainty in the diffraction effects, uncertainty in the effects of vertical betatron oscillations, and uncertainty in the overall numerical finesse of the diffraction calculations, which may result in part from the use of the Fresnel approximation, because of a 0.06% difference between the apparent value of $\lim_{\lambda \rightarrow 0} F_{\text{diff}}$ and unity. We therefore combine these uncertainty components with the uncertainty in the irradiance because of the SURF radiation to suggest a new value for that component in the case of calibration of deuterium lamps. This is detailed in Table II.

VI. CONCLUSIONS

We have shown that it is straightforward to calculate *exact* field strengths for synchrotron radiation, which is largely aided by the use of Graf's addition theorem for Bessel functions as well as Debye's and Olver's asymptotic expansions for Bessel functions of large argument and order. We have also confirmed that betatron oscillation amplitudes can be estimated based on beam imagery for the oscillations' effects on practical radiometry. We have also shown that diffraction effects of beamline optics on the spectral power received at a receiving port of an integrating sphere can be treated with sufficient confidence. Analysis of uncertainties in regards to the above issues suggests an additional component to include in the uncertainty budget of Shaw *et al.*¹ for the case of Beamline 2 being used for calibration of deuterium lamp irradiance scales. This component is modest in size so that use of Beamline 2 in its present state is feasible for such calibration if good beam conditions are maintained.

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APPENDIX:: USE OF OLVER'S RESULT

We seek to evaluate $J_n(nz)$ for large, positive n and z both positive and near 1. From Olver,¹⁰ one has

$$J_n(nz) \sim \left(\frac{4\zeta}{1-z^2} \right)^{1/4} \times \left[\frac{\text{Ai}(n^{2/3}\zeta)}{n^{1/3}} \sum_{k=0}^{\infty} \frac{a_k(\zeta)}{n^{2k}} + \frac{\text{Ai}'(n^{2/3}\zeta)}{n^{5/3}} \sum_{k=0}^{\infty} \frac{b_k(\zeta)}{n^{2k}} \right]. \quad (\text{A1})$$

Functions $a_k(\zeta)$ and $b_k(\zeta)$ are defined below. For $z < 1$, ζ is positive and given by

$$\frac{2}{3}\zeta^{3/2} = \ln \left(\frac{1 + \sqrt{1-z^2}}{z} \right) - \sqrt{1-z^2}. \quad (\text{A2})$$

Using

$$(1 - \sqrt{1 - z^2})(1 + \sqrt{1 - z^2}) = z^2, \quad (\text{A3})$$

we have

$$\begin{aligned} \frac{2}{3}\zeta^{3/2} &= \frac{1}{2} \ln \left(\frac{1 + \sqrt{1 - z^2}}{1 - \sqrt{1 - z^2}} \right) - \sqrt{1 - z^2} \\ &= \sum_{s=0}^{\infty} \frac{(1 - z^2)^{(2s+1)/2}}{2s+1} - \sqrt{1 - z^2} \\ &= (1 - z^2)^{1/2} \left[\frac{1}{3}(1 - z^2) + \frac{1}{5}(1 - z^2)^2 + \frac{1}{7}(1 - z^2)^3 + \dots \right], \end{aligned} \quad (\text{A4})$$

from which follows

$$\begin{aligned} \zeta &= (1 - z^2) \left\{ \frac{1}{2} \left[1 + \frac{3}{5}(1 - z^2) + \frac{3}{7}(1 - z^2)^2 + \dots \right] \right\}^{2/3} \\ &= (1 - z^2) \left[{}_2F_1(1, 3/2; 5/2; 1 - z^2) / 2 \right]^{2/3} \\ &= (1 - z^2) (F/2)^{2/3}. \end{aligned} \quad (\text{A5})$$

Therefore ζ can be written as a series expansion in $1 - z^2$. In the case of synchrotron radiation, field strengths are negligible unless we have $\zeta \lesssim n^{-2/3}$ because of the highly damped behavior of the Airy function and its derivative. This ensures that $1 - z^2$ is small compared to unity. In the last step of Eq. (A5), we abbreviate the hypergeometric function as F . Analogous logic and a different definition of ζ applies for $z > 1$, with the same result as Eq. (A5). Analyticity near $z = 1$ also allows for complex z .

We have

$$\left. \begin{aligned} a_k(\zeta) &= \sum_{s=0}^{2k} \mu_s \zeta^{-3s/2} u_{2k-s} \left((1 - z^2)^{-1/2} \right) \\ b_k(\zeta) &= -\zeta^{-1/2} \sum_{s=0}^{2k+1} \lambda_s \zeta^{-3s/2} u_{2k-s+1} \left((1 - z^2)^{-1/2} \right) \end{aligned} \right\}. \quad (\text{A6})$$

Here we have

$$\left. \begin{aligned} \lambda_s &= \frac{(2s+1)(2s+3)\cdots(6s-1)}{s!(144)^s} \\ \mu_s &= -\frac{6s+1}{6s-1}\lambda_s \end{aligned} \right\}, \quad (\text{A7})$$

while the u functions are from Debye,⁹ with $u_0(t) = 1$ and

$$u_{l+1}\left(t\right) = \frac{1}{2}t^2\left(1-t^2\right)\frac{du_l(t)}{dt} + \frac{1}{8}\int_0^t d\tau\left(1-5\tau^2\right)u_l\left(\tau\right). \quad (\text{A8})$$

From this, one can automatically determine all required u_l^m to deduce

$$u_l(t) = t^l \sum_{m=0}^l u_l^m t^{2m}. \quad (\text{A9})$$

With arguments of u functions always being $(1-z^2)^{-1/2}$, negative powers of ζ appearing in Eq. (A6), and F having a series expansion in non-negative powers of $(1-z^2)$, $a_k(\zeta)$ and $b_k(\zeta)$ also have series expansions in $(1-z^2)$. Different terms in Eq. (A6) diverge as $z \rightarrow 1$ because their expansion begins with negative powers of $(1-z^2)$, but the behavior of Bessel functions in the transition region ensures that such terms must cancel.

It is therefore desirable to partition problematic terms from the rest, at which time it is also convenient to demonstrate, if desired, that leading negative-power terms do indeed cancel. To this end, we make the series expansion of F^P explicit,

$$F^P = \sum_{q=0}^{\infty} f_q^P (1-z^2)^q, \quad (\text{A10})$$

and denote partial summations of terms in F^P with powers shifted as follows:

$$r_Q^P = \sum_{q=0}^{\infty} f_{Q+q}^P (1-z^2)^q. \quad (\text{A11})$$

We then have

$$\begin{aligned}
a_k(\zeta) &= \sum_{s=0}^{2k} \mu_s (1-z^2)^{-3s/2} 2^s F^{-s} u_{2k-s} \left((1-z^2)^{-1/2} \right) \\
&= F^{-2k} \sum_{s=0}^{2k} 2^s \mu_s F^{2k-s} \sum_{m=0}^{2k-s} u_{2k-s}^m (1-z^2)^{-k-m-s} \\
&= F^{-2k} \sum_{s=0}^{2k} 2^s \mu_s \sum_{m=0}^{2k-s} u_{2k-s}^m \\
&\quad \times \left[\sum_{q=0}^{k+m+s-1} f_q^{2k-s} (1-z^2)^{q-k-m-s} + r_{k+m+s}^{2k-s} \right]
\end{aligned} \tag{A12}$$

and

$$\begin{aligned}
b_k(\zeta) &= -(F/2)^{-1/3} (1-z^2)^{-1/2} \sum_{s=0}^{2k+1} \lambda_s (1-z^2)^{-3s/2} 2^s F^{-s} u_{2k+1-s} \left((1-z^2)^{-1/2} \right) \\
&= -F^{-2k-4/3} \sum_{s=0}^{2k+1} 2^{s+1/3} \lambda_s F^{2k+1-s} \sum_{m=0}^{2k+1-s} u_{2k+1-s}^m (1-z^2)^{-k-m-s-1} \\
&= -F^{-2k-4/3} \sum_{s=0}^{2k+1} 2^{s+1/3} \lambda_s \sum_{m=0}^{2k+1-s} u_{2k+1-s}^m \left[\sum_{q=0}^{k+m+s} f_q^{2k+1-s} (1-z^2)^{q-k-m-s-1} + r_{k+m+s+1}^{2k+1-s} \right],
\end{aligned} \tag{A13}$$

with contributions because of the first terms in brackets summing to zero, and those because of the second terms giving $a_k(\zeta)$ and $b_k(\zeta)$. One can also introduce coefficients that are independent of z ,

$$\left. \begin{aligned}
A_k^q &= \sum_{s=0}^{2k} 2^s \mu_s \sum_{m=0}^{2k-s} u_{2k-s}^m f_{k+m+s+q}^{2k-s} \\
B_k^q &= \sum_{s=0}^{2k+1} 2^s \lambda_s \sum_{m=0}^{2k+1-s} u_{2k+1-s}^m f_{k+m+s+1+q}^{2k+1-s}
\end{aligned} \right\}, \tag{A14}$$

which gives

$$\left. \begin{aligned}
a_k(\zeta) &= F^{-2k} \sum_{q=0}^{\infty} A_k^q (1-z^2)^q \\
b_k(\zeta) &= -2^{1/3} F^{-2k-4/3} \sum_{q=0}^{\infty} B_k^q (1-z^2)^q
\end{aligned} \right\}. \tag{A15}$$

To this end, readers are referred to a similar, more fully developed expansion by Temme.¹³ Because of their utility, we present nonzero values of the A_k^q and B_k^q coefficients related to all terms up to and including contributions that are $O(\pi^{-7})$ in Table III. This is based on setting $1 - \mathcal{Z}^2 < C\pi^{-2/3}$ and bounding C so that the argument of the Airy function and its derivative are not very large. If such a bounding condition is not met, the Bessel function is very small and so not of interest. The coefficients are all rational numbers, but many have numerators and denominators that are too large for standard 64-bit arithmetic. To prevent transcription error, we provide values output by a computer program.

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FIG. 1.

Coordinate system and related parameters. Cartesian axes are shown in black, the orbit and sense of orbit are shown in red, the vector $\mathbf{s}$ is shown in green, points $\mathbf{r}$ and $\mathbf{r} - \mathbf{s}$ are indicated, orbit radius and lengths of several line segments (R_0 , ρ , and Z) are shown in blue, and measures of angles θ and ψ are indicated using dashed lines and arcs.

FIG. 2.
Geometrical construction for assessing effects of θ_R .

FIG. 3. Measurements (points) and best-fits (curves) of ratio X at three beam energies. The beam vertical FWHM was 2 mm.

FIG. 4.
Best-fit FWHM for θ_z given the δz distribution FWHM (points) vs their theoretical ratio (line).

FIG. 5. Schematic with various quantities and coordinates. The electron orbit direction is indicated.

FIG. 6. Factors $F_{\text{b.o.}}$, F_{diff} , and dependence of F_{diff} on angular displacements for 400 nm radiation.

FIG. 7. Enhancement of flux expressed by the scaling factor, F_{diff} , including effects of betatron oscillations for several wavelengths.

TABLE I.
Radius (mm) and distance from tangent (m) of beamline apertures and integrating-sphere port.

Element	Radius (mm)	Distance from tangent (m)
Aperture #1	13.855	0.414
Aperture #2	11.43	2.11
Aperture #3	11.43	4.82
Integrating sphere port	4.75	11.6

TABLE II.
Modification of relative standard uncertainty component in irradiance because of the
SURF radiation's uncertainty.

Uncertainty reported in Ref. 1	0.003 60
Diffraction effect uncertainty	0.001 00
Betatron oscillation effect uncertainty	0.00050
Numerical finesse uncertainty	0.000 60
Root sum of squares	0.003 82
Expanded uncertainty ($k = 2$)	0.007 63

TABLE III.
Coefficients defined by Eq. (A14) formatted for inputting into numerical calculations.

k	q	A_k^q
0	0	1.000 000 000 000 000
1	0	$-4.444\,444\,444\,444\,493 \times 10^{-3}$
1	1	$-6.255\,411\,255\,411\,250 \times 10^{-3}$
1	2	$-6.604\,506\,604\,506\,618 \times 10^{-3}$
1	3	$-6.311\,237\,263\,618\,194 \times 10^{-3}$
1	4	$-5.769\,176\,357\,411\,631 \times 10^{-3}$
1	5	$-5.157\,331\,488\,600\,777 \times 10^{-3}$
1	6	$-4.554\,816\,814\,878\,820 \times 10^{-3}$
1	7	$-3.994\,400\,819\,072\,884 \times 10^{-3}$
2	0	$6.937\,355\,413\,353\,593 \times 10^{-4}$
2	1	$1.897\,207\,044\,416\,996 \times 10^{-3}$
2	2	$3.230\,911\,258\,443\,270 \times 10^{-3}$
2	3	$4.414\,287\,138\,261\,381 \times 10^{-3}$
2	4	$5.302\,265\,784\,506\,415 \times 10^{-3}$
3	0	$-3.542\,119\,697\,628\,188 \times 10^{-4}$
3	1	$-1.431\,324\,374\,334\,131 \times 10^{-3}$
k	q	B_k^q
0	0	$-1.428\,571\,428\,571\,429 \times 10^{-2}$
0	1	$-1.587\,301\,587\,301\,588 \times 10^{-2}$
0	2	$-1.515\,151\,515\,151\,515 \times 10^{-2}$
0	3	$-1.398\,601\,398\,601\,399 \times 10^{-2}$
0	4	$-1.282\,051\,282\,051\,282 \times 10^{-2}$
0	5	$-1.176\,470\,588\,235\,294 \times 10^{-2}$
0	6	$-1.083\,591\,331\,269\,349 \times 10^{-2}$
0	7	$-1.002\,506\,265\,664\,160 \times 10^{-2}$
0	8	$-9.316\,770\,186\,335\,404 \times 10^{-3}$
1	0	$1.184\,859\,584\,858\,651 \times 10^{-3}$
1	1	$3.066\,750\,709\,608\,478 \times 10^{-3}$
1	2	$5.144\,688\,178\,301\,632 \times 10^{-3}$
1	3	$7.132\,511\,642\,705\,032 \times 10^{-3}$
1	4	$8.901\,694\,906\,684\,041 \times 10^{-3}$
1	5	$1.041\,196\,757\,573\,656 \times 10^{-2}$
2	0	$-4.382\,918\,093\,603\,083 \times 10^{-4}$
2	1	$-1.758\,058\,116\,017\,036 \times 10^{-3}$
2	2	$-4.184\,637\,309\,616\,559 \times 10^{-3}$