WAVE - A COMPUTER CODE FOR THE TRACKING OF ELECTRONS THROUGH MAGNETIC FIELDS AND THE CALCULATION OF SPONTANEOUS SYNCHROTRON RADIATION

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Abstract

WAVE is developed at BESSY - now Helmholtz-Zentrum Berlin (HZB) - since 1990 to calculate spontaneous synchrotron radiation for arbitrary magnetic fields. A variety of field models for dipoles, wavelength shifters, and undulators is available. Field maps can be read and written. Many routines to handle magnetic fields are implemented, including simulations of field error e.g. due to misalignment. Coherent radiation of electrons in a bunch and energy losses due to radiation are taken into account. Phase-space distributions of the beam electrons are taken into account by various algorithms. Generating functions and linear transfer matrices for particle tracking purposes can be calculated. Subroutines to calculate the effects of insertion devices on the storage ring are included. The program runs in batch mode, controlled by input files, but a simple GUI is also provided. The results are given as ASCII data or binary formats of the programs PAW, ROOT, and HDF5. Parallel runs of WAVE on a cluster are supported. WAVE has been checked and validated with the synchrotron radiation code of the German National Bureau of Standards (PTB) based on Schwinger's formula.

INTRODUCTION

The development of WAVE started in 1990 within the framework of a study for the PTB. Subject of this study was the question, whether a superconducting wave-length shifter (WLS) can be used at the planned storage ring BESSY II for radiometry in the X-ray regime. The code was developed as a tool to calculate the synchrotron radiation of a WLS with very high precision and also to investigate the impact of the WLS on the storage ring with respect to emittance change, beam polarization and dynamical aperture. This study has become the starting point for the PhD thesis of the author [1], where more details are given. From 1994 the calculation of undulator radiation become more important and many routines to model and handle magnetic fields of undulators has been implemented. WAVE is written in FORTRAN 90 and can be compiled and used on a variety of platforms and operating systems. However, nowadays it is developed mainly for Linux.

MAGNETIC FIELDS

The periodic magnetic fields of undulators can be approximately described by analytical formulas. Although these formulas are available in WAVE, many problems, e.g. the calculations of effects of field errors or endpole configurations, require more sophisticated methods. Complex setups like helical undulators coupled by a modulator build of rotatable, cylindrical magnets [2] are treated in WAVE as an arrangement of permanent magnets. Undulator parameters as gap, shift, dimensions and magnetization of the magnets as well as taper, misalignments, and field errors can be set by the user. The magnets can be read from an external file or defined as complete devices in the input file of WAVE. The fields of the individual magnets are calculated using the current sheet method. Another very powerful method is to model the fields by a Fourier series of analytical 3D functions [1, 3]. This includes algorithms to expand the vertical field given on the longitudinal axis of an insertion device to a Maxwell conform 2D or 3D field. However, sometimes the usage of field maps is more flexible or necessary. WAVE can handle 3D field maps with different interpolation schemes. Another group of features include symmetry operations and options to make fields periodic along the longitudinal device axis. For applications not covered by WAVE, the user can also provide his own magnetic field routine.

TRACKING

The tracking algorithm of WAVE considers the magnetic field as constant for each time step. Thus, the trajectory consists of pieces of circles with orientation and bending radii according to the local field. An option allows to calculate the energy loss due to the synchrotron radiation for each tracking step and to adapt the energy of the electron accordingly. This can be done continuously or by a Monte-Carlo technique which generates discrete photons in order to take quantum fluctuations into account. For special purposes, the user may provide an own routine called for each tracking step.

SYNCHROTRON RADIATION

The spectrum calculation is mainly a numerical integration of well-known formulas given e.g. in [4]. WAVE uses a modified version:

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$$\int_0^{\Delta T} \frac{1}{R(t)} \frac{\vec{n}(t)\times[(\vec{n}(t)-\vec{\beta}(t))\times\dot{\vec{\beta}}(t)]}{(1-\vec{\beta}(t)\vec{n}(t))^2} e^{i\omega(t+R(t)/c)} dt \approx$$

$$\sum_{j=1}^{N} \frac{1}{R(t_j)} \frac{\vec{n}(t_j)\times[(\vec{n}(t_j)-\vec{\beta}(t_j))\times\dot{\vec{\beta}}(t_j)]}{(1-\vec{\beta}(t_j)\vec{n}(t_j))^2} e^{i\omega(t_j+R(t_j)/c)} \times$$

$$\frac{1-e^{i\omega(1-\vec{\beta}(t_j)\vec{n}(t_j))\Delta t_j}}{(1-\vec{\beta}(t_j)\vec{n}(t_j))\omega} \quad (1)$$

Here, $\vec{R} = R \times \vec{n}$ denotes the vector from the electron to the observer, $\vec{\beta}$ the velocity divided by c, and ω the frequency of the radiation. For the numerical integration over the time-interval ΔT, the integral of eq. 1 is approximated by a sum of N time steps. The phase is expanded up to first order, while the ω-independent factor is treated as constant within the time step. For the step the integration is then done analytically. This procedure ensures a proper integration for very rapidly varying phases with many oscillations within a step as it occurs for wigglers or dipoles. The accuracy is further increase by a recursive calculation of the phase:

$$e^{i\omega(t_{j+1}+R(t_{j+1})/c)} \approx e^{i\omega(t_j+R(t_j)/c)} \times e^{i\omega(1-\vec{\beta}(t_j)\vec{n}(t_j))\Delta t_j} \quad (2)$$

The integration yields the field amplitude for a given observation point. From this amplitude the spectral flux-density and the brilliance is calculated in terms of Stokes parameters. In addition, a similar integral for the velocity term of the field is evaluated as well. The irradiated total power and the power passing a given aperture are also determined. To calculate the flux through a rectangular or circular aperture, the calculations are carried out for each point on a rectangular or radial grid and integrated over the grid points via spline techniques. For a proper calculation of the brilliance, the size of the source is needed. It can be determined by WAVE, via a backward propagation of the field amplitudes from the grid of observation points to the device center making use of Huygens's principle.

WAVE offers two main modes for the treatment of insertion devices. In the wiggler mode all poles are treated as separate sources and added incoherently, while in the undulator mode the contributions of all steps of the trajectory are summed up coherently. Beside the normal undulator mode, a quick but less accurate mode is available, where the complex field amplitude of only one period is calculated and added up N times with the appropriate phase-shift and $1/R$-correction for N periods of the undulator. For the wiggler mode, the synchrotron radiation can also be calculated making use of Schwinger's formula [5], which is very fast and precise.

To take the emittance and energy spread of the electron beam into account two very different approaches are available. For a single electron folding procedures are applied. Alternatively, many electrons can be tracked starting from a Gaussian or user defined phase-space distribution. The radiation of all electrons of a bunch is added coherently, while the contributions of different bunches are summed up incoherently. This allows to calculate coherent radiation of bunched electrons.

If the flux through an aperture has to be calculated for a large number of electrons, a Monte-Carlo mode is available. In this mode not only the phase-space variables of the electrons are randomly generated according to their distribution, but also the coordinates of the observation point are randomly chosen within the considered aperture. Thus the flux through the aperture is calculated as fast as the flux-density for a single observation point. However, to track thousands of electrons can still be very time consuming. Therefore, WAVE can run in parallel on a cluster.

Many other features like dose rate calculations or application of filters and yield functions are available but beyond the scope of this paper.

ACCELERATOR PHYSICS

From its history WAVE was written not only for the calculation of synchrotron radiation, but also to investigate the influence of insertion devices on the storage ring. By tracking many electron through a given magnetic field, WAVE can fit the coefficients of a Taylor series of the Generating Function F_2 from the phase-space variables at the entrance and exit of the device [6, 1]. This Generating Function (GF) can be implemented in tracking codes to track a particle with a single step through a whole device. From the linear terms of the GF, the linear transfer-matrix (TM) is derived. Another method implemented to determine the TM, is to track principle trajectories and to solve a system of linear equations. As explained in details in [6], also the emittance change of the storage ring due to e.g. a superconducting wavelength-shifter as well as the degree and build-up time of the beam polarization can be estimated from the tracking through the insertion device and the parameters of the storage ring. WAVE can also calculate the beta functions of magnet configurations and determine the periodic solution, which is interesting for very long setups with many undulators and focusing elements in between.

INTERFACES

Two different kinds of interfaces are available: User defined subroutines and output data for external codes. The interface routines are provided by the user to be compiled and linked to WAVE. These interfaces exist for the magnetic field routine, the input routine and the output routine for WAVE as well as for the tracking routine on step level. Output interfaces exist for the ray-tracing and field propagation codes RAY [7] and PHASE [8] to make use of sources calculated by WAVE.

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EXAMPLE

WAVE has become a standard tool for the calculation of synchrotron radiation at BESSY (now HZB), and the results are confirmed by a variety of measurements. However, with the FEL, new challenges came up with the need of new features to calculate the spontaneous synchrotron radiation of very long sections of undulators including focusing elements. These includes energy-loss of the electrons, quantum fluctuations, and tracking of many electrons with a realistic phase-space distribution. As an example, the following figure shows spectra of a 215.25 meter long straight section build of 35 cells. Each cell consists of an undulator with a period-length of 4 cm and 125 periods, phase-shifters, and quadruples. WAVE offers an option to find the periodic beta-functions for the cells. It is used here to tune the quadrupoles such that the maxima and minima of the horizontal and vertical beta-functions are 23 and 9.5 meter.

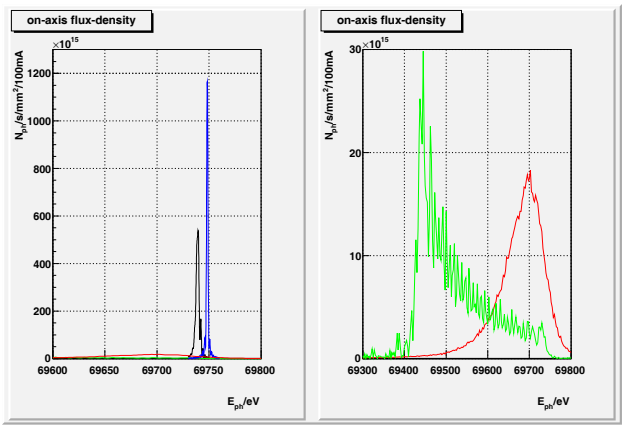

Figure 1: Spectra of the 9th harmonic of 35 undulator sections: Blue: Pencil beam, no energy loss, no taper. Green: Pencil beam, continuous energy loss, no taper. Black: Pencil beam, continuous energy loss, with compensating taper. Red: Broad beam including all effects, i.e. energy loss with quantum fluctuations, beam emittance, energy spread, and taper.

The main problem is, that the harmonics of so many coupled undulators are so narrow, that a minor change of the parameters of the considered particle changes the harmonics dramatically. As a consequence, folding procedures to take the beam emittance and energy spread into account are not applicably. Thus, a representative sample of many electrons has to be tracked. About one million integration steps per electron are require making the calculations very time consuming. An analysis of the performance of WAVE has shown that the calculation of the magnetic field is a crucial point, depending on the field model used. To speed up calculations, the complex magnetic field of the undulators (current sheet method), of the quadrupoles, and of the phase-shifters is written to a 3D field map in a first WAVE run. This takes some minutes, and the size of the map file for this examples is 235 MBytes. In the following runs, the spectra are calculated using this field map. This is much faster, and allows to calculate the spectrum of 1000 electrons for 201 photon energies within 5 hours on a conventional PC with a single processor.

Figure 1 shows the importance of the new features of WAVE, especially the treatment of the energy loss during the passage of the electrons through the undulators and the capability of tracking many electrons. The blue curve shows the pure on-axis spectrum of an electron without energy loss. The green curve shows the same situation, but with a continuous energy loss. Due to this effect, the 9th harmonic is completely spoiled. The black curve shows the effect with a continuous energy loss but compensated by a taper. The tapering is done such that the field of each undulator is scaled to keep the position of the harmonic. This restores the harmonic to about half of the original peak value. However, when all effects are included, the harmonic goes down by a factor of about 60 (red curve) compared to the pencil beam case without energy loss. This examples illustrates that WAVE is ready (although not yet cross-checked) for the calculation of spontaneous synchrotron radiation of FEL beamlines.

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