Synchrotron Radiation

An everyday application of special relativity

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This is to all the synchrotron radiation users of the future.

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Preface

The success story of synchrotron radiation is almost unparalleled. The synchrotron provides radiation of a quality that facilitates a wide range of experiments, with applications in virtually all branches of natural sciences: from fundamental molecular and condensed matter physics, to magnetism and applied materials science, from electrochemistry to applications in solar cell, battery and environmental research, from pharmaceutics to biology, where structure determination of biological macromolecules may be the most spectacular application. Synchrotron radiation also finds users dedicated to archeology and cultural heritage, and other fields conventionally not associated with natural sciences. As the versatility is realized, new synchrotron radiation facilities are being built all around the world.

Thus, there are an increasing number of synchrotron radiation users who are specialists in scientific disciplines far from basic physics and accelerator technology. Certainly one may perform excellent experiments with the radiation with only little knowledge about the principles by which it is produced. For design of new, innovative types of experiments knowledge about fundamental opportunities and limitations is desirable, and for the personal peace-of-mind it is good to know that the brilliant radiation is not coming out of a big, magic, black box.

The radiation is produced according to the basic laws of physics, and it is fascinating that several of the most fundamental relations are needed to understand the emission process. At the heart of the process is the classical Maxwellian notion that accelerating charged particles emit electromagnetic radiation, and the properties of the radiation can be understood using classical concepts like the Doppler effect. Also, concepts from modern physics like the Heisenberg uncertainty principle are used to understand the properties of the radiation, and in particular, the principles of special relativity. The effects of special relativity are so obvious in synchrotron radiation that it may as well be used to understand special relativity as the other way around. Synchrotron radiation is by now so common that it constitutes an everyday application of special relativity.

The book is intended for the growing number of non-specialist users, and for readers who are interested in how bright x-rays can be produced. It focuses on the basic principles, which are essential for the understanding. Although the book does contain some math, the math is invariably simple and easy to follow. Synchrotron radiation is also simple in the sense that its properties often can be described by (quasi) analytical expressions. The rigorous, not-so-simple derivation of those expressions can be found in more comprehensive textbooks or research papers, to which interested readers are referred. Here, these expressions are accompanied by qualitative arguments, and statements of the ‘it-can-be-shown-that…’ form.

Acknowledgement

This book is based on lecture notes used in the ‘Synchrotron Radiation Course’ given at the master programme at Uppsala University. I am indebted to Svante Svensson who left me his lecture notes to build on when I took over the course many years ago. In my teaching I have also followed David Attwood’s comprehensive *Soft X-Rays and Extreme Ultraviolet Radiation*, and here I have borrowed from several accounts in that book. I also would like to thank my students over the years for critical remarks and discussions.

Author biography

Jan-Erik Rubensson

The author is physics professor at Uppsala University. Most of his research is based on spectroscopy using synchrotron radiation, and especially, he has been engaged in method development related to resonant inelastic soft x-ray scattering (RIXS). The new synchrotrons allow for substantial refinement of RIXS techniques, which promises progress in fields ranging from fundamental atomic and molecular physics, over electrochemistry and pharmaceutics, to magnetism and correlated-electron systems. Several advanced RIXS facilities are presently being built at the new synchrotrons, and the author is spokesperson for the VERITAS beamline at the MAX IV laboratory. In addition, the author investigates the prospects of time-resolved and non-linear inelastic x-ray scattering at free-electron lasers. His scientific focus is on ultrafast electron dynamics in free molecules, and the coupling between, spin, orbital, and nuclear degrees of freedom in general.

The author is teaching basic mechanics and optics on the bachelor level at Uppsala University, and he has the responsibility for the master-level course in synchrotron radiation.

Chapter 1

Introduction

Some perspectives on synchrotron radiation, and a short history. The use of x-rays for the study of matter.

1.1 Perspectives

Synchrotrons are large-scale facilities where a radiation source with a diameter of some hundred meters is surrounded by specialized equipment which hardly looks meaningful to a first-time visitor. The equipment includes advanced instruments and detectors, with electronics and precision mechanics, the design and construction of which can take several years, but occasionally also improvised solutions to current technical problems or spontaneous setups for testing new ideas, which may include aluminum foil, clamps, paper clips and tape. The funding agency may look at synchrotrons as a place where money is delivered for the amusement of a few scientists who seem more playful than serious, and from where not much of value emanates. The inventor sees the great vision and the beautiful principle realized in the synchrotron, and the accelerator physicist sees all the wonderful optimization challenges. I assume that most readers are users or would-be users, who rather see the synchrotron as a black magic box that gives them radiation with fantastic properties for their experiment. The aim of this book is to give a glimpse inside the black box. Even though the discussion uses a mathematical language, it focuses on conceptual understanding, and not on strict derivations. It is sometimes possible to arrive at quantitative predictions from basic physical principles and rather simple algebra. I hope it can also serve as an introduction to general readers who are interested in how the brightest x-ray sources work.

There are several excellent pedagogic texts describing the principles of synchrotron radiation in more depth [1–6]. I am in debt to David Attwood's book *Soft x-rays and Extreme Ultraviolet Radiation* [1], and in several parts I follow his presentations rather closely. On his homepage [7] you can find many excellent lectures.

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Oxford University Press has published a Series on synchrotron radiation [8], and Springer has a constantly updated reference handbook entitled *Synchrotron Light Sources and Free-Electron Lasers* [9].

There are also excellent internet resources, with pedagogic introductions and analyses. An invaluable help concerning quantitative estimates of properties of radiation and its interaction with matter is the home page of Center for X-ray Optics at Lawrence Berkeley National Laboratory [10].

1.2 X-rays, structure, and dynamics

The medical use of x-rays is often emphasized, and its value can hardly be overstated. Their large penetration length has been exploited to unveil internal structure ever since their discovery by Wilhelm Conrad Röntgen in 1895. The role of x-rays in the investigation of structure and dynamics on the atomic length and time scale is not less important. The diffraction of x-rays by crystals, as observed by Max von Laue in 1912, confirmed that the wavelength of x-ray radiation is similar to atomic distances. Thus, x-ray scattering became the prime tool to investigate the structure of materials, and in 1952 the structure of DNA was determined by means of x-ray diffraction experiments, opening the door to atomic-scale biology. X-rays were also decisive for our understanding of the electronic structure of the atom, through the discovery of characteristic radiation by Charles Glover Barkla in 1909, and the systematic investigations of Henry Moseley and others. X-ray spectroscopy continues to uncover the electronic structure associated with materials properties and processes in the material world. There are several excellent books on the 20th century physics history, e.g. *Inward Bound: Of Matter and Forces in the Physical World* [11] by Abraham Pais, and a brief account of early x-ray history by Alexi Assmus can be found in [12].

Currently time-resolved experiments with short-pulse radiation are refined to reach atomic time scales: the time scale for nuclear dynamics is typically in the femtosecond range, while electron dynamics is rather in the attosecond range. For the probe radiation to have a defined frequency its period has to be substantially shorter than the pulse itself, and thus also such experiments call for x-rays.

With x-rays the properties of matter can be understood in terms of structure and dynamics on the atomic length and time scales. It is in that context that the success of synchrotron radiation can be appreciated. Synchrotrons provide brilliant x-rays with variable and well-defined energy and polarization state.

Synchrotron radiation was first observed in the General Electric synchrotron accelerator (figure 1.1) built in 1946 and announced in May 1947 in a letter [13]:

> On April 24, Langmuir and I were running the machine and as usual were trying to push the electron gun and its associated pulse transformer to the limit. Some intermittent sparking had occurred and we asked the technician to observe with a mirror around the protective concrete wall. He immediately signaled to turn off the synchrotron as ‘he saw an arc in the tube.’ The vacuum

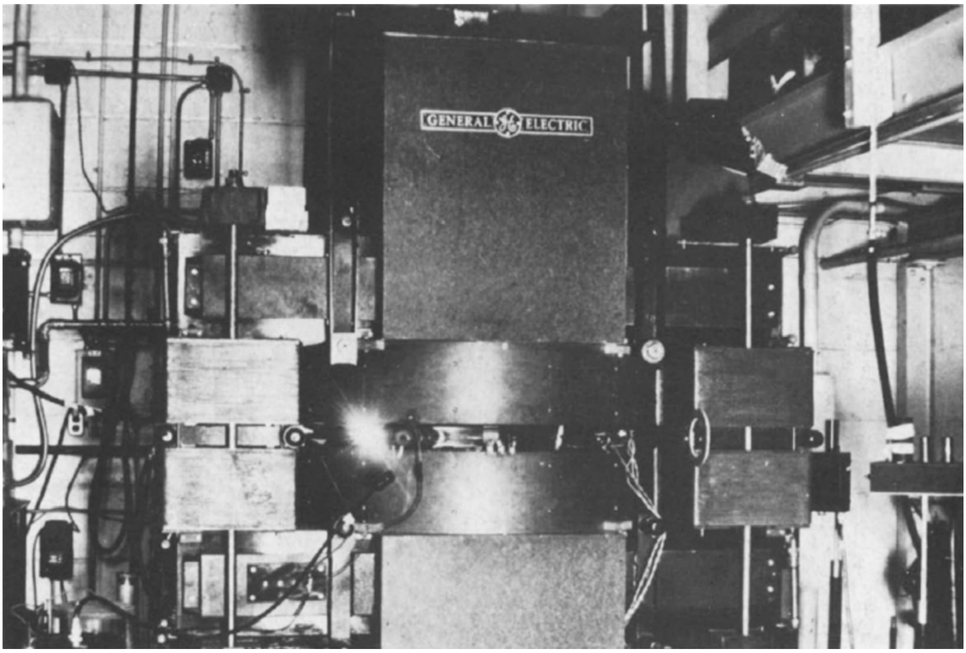

Figure 1.1. First observation of synchrotron light at the General Electric laboratory 1947 in the 70 MeV synchrotron. The image is taken from [14].

> was still excellent, so Langmuir and I came to the end of the wall and observed.

The first attempt to characterize synchrotron radiation over a large energy range was made by Hartman and Tomboulian in 1953 [15]:

> An attempt was made … to extend the region of observation to the vacuum ultraviolet. Since a grazing incidence spectrograph was available and could readily be modified for this purpose, it was decided … to proceed directly with the exploration of the soft x-ray region (50 Å to 500 Å).

The same authors followed up with thorough investigation and in their 1956 paper [16] one can find this hand-drawn figure (figure 1.2), which compares the angular distribution of the radiation from an accelerating charge at classical and relativistic speed. As a consequence of special relativity, radiation from a particle at high speed is emitted primarily in the forward direction, giving the radiation fascinating properties. In synchrotrons, electrons (or positrons) are moving very close to the speed of light. Synchrotron radiation is our most common everyday application of special relativity.

In this book I will take a heuristic approach to understanding the basic properties of synchrotron radiation, rather than attempting a formal derivation of the formulae. For those who are theoretically inclined there are several texts. A

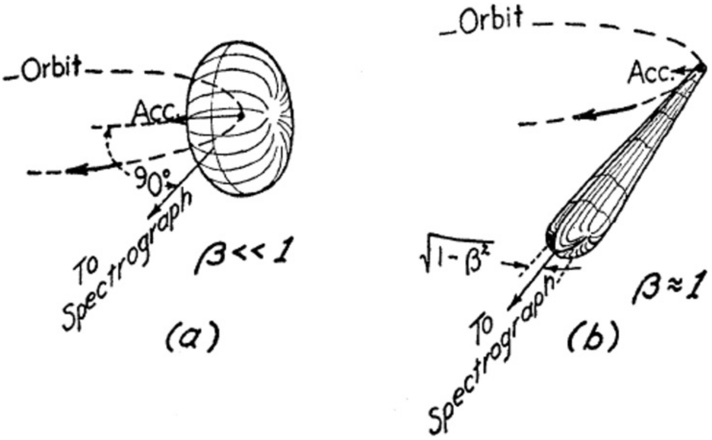

Figure 1.2. Accelerating electrically charged particles emit radiation. At slow speed the angular distribution is donut shaped with maximum intensity perpendicular to the acceleration. At relativistic speed the intensity maximum is in the forward direction. The drawing is taken from [15].

description of synchrotron radiation was worked out early on in the classical paper by Schwinger [17]. A more recent comprehensive theoretical description is given by Kim [18], and the basics are treated in several textbooks on electromagnetic field theory.

The development of synchrotron radiation techniques since the early days is a success story. The first generation synchrotrons were built for collision experiments, with synchrotron radiation as an unwanted by-product. The usage of the radiation was termed ‘parasitic’. The second generation storage rings were dedicated to and optimized for producing synchrotron radiation, and the third generation sources feature so-called insertion devices, magnetic structures with which the radiation can be tailored for specific purposes. For the next generation the *ultimate* storage ring is envisioned, for which the performance is limited by fundamental principles only. Closely related is the recent development of x-ray free-electon lasers, which I will describe briefly here.

Taking the brilliance of the radiation as a figure of merit, the improvement since the discovery emulates Moore’s law for microelectronics integration: whereas computer speed is only doubled in 18 months, synchrotron radiation brilliance is tripled (figure 1.3). The concept of brilliance will be discussed in more detail later, but briefly it reflects the number of photons of a certain wavelength that can be concentrated in a small area (as compared to the number of microelectronic functions in a small area). This development creates overwhelming new opportunities for experiments which rely on x-rays.

There are a large number (>50) of dedicated synchrotron laboratories around the globe, and they are easy to find via their homepages [19]. Many of them have a lot of information and nice animations which describe synchrotron radiation.

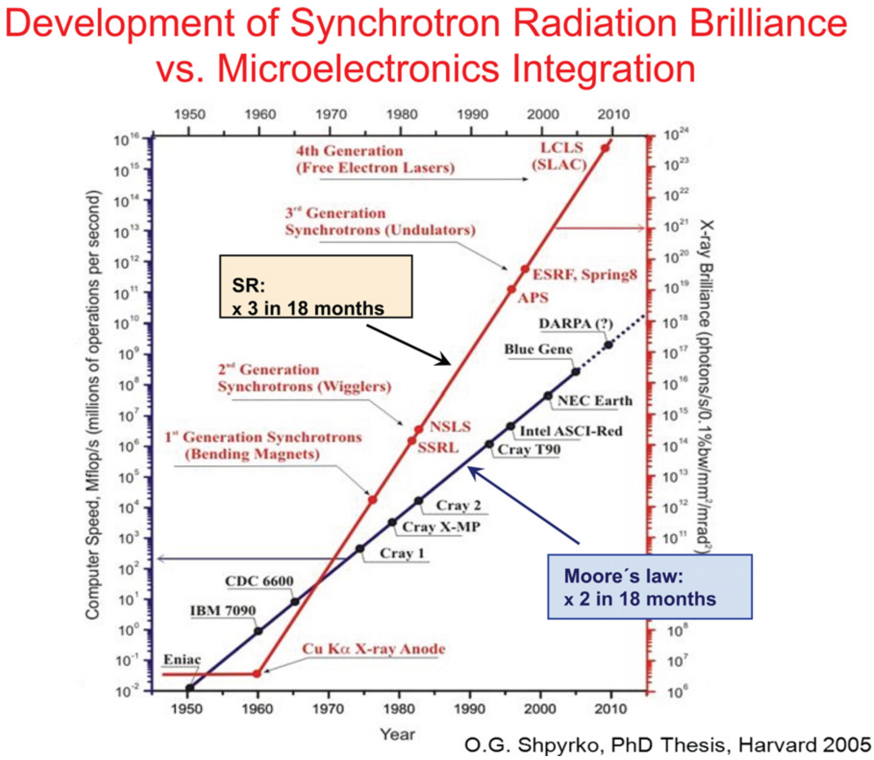

Figure 1.3. Until around 1960 the best x-ray sources were x-ray tubes, based on the same principle as used by Röntgen. With synchrotron radiation brilliance is increasing rapidly. Courtesy of O G Shpyrko [20].

1.3 Outline

I will start by introducing concepts which are often used to describe electromagnetic radiation and radiation sources in chapter 2. In chapter 3 we will see how the properties of synchrotron radiation emerge, by considering the emission from particles traveling close to the speed of light. The analysis is simplified when the acceleration and the velocity directions of the emitting particles are perpendicular, and we shall see that a simple understanding only requires acceptance of the most basic assumptions of special relativity. In chapter 4 I will discuss so-called ‘insertion devices’, and especially the undulator, which today is the most common radiation source at synchrotron radiation facilities. In chapter 5 I will briefly describe the basic ideas behind x-ray free-electron lasers. Although this is different from synchrotron radiation facilities, it is closely related. Finally, in chapter 6 I will describe x-ray optical properties and the implications for the optical elements and beamline design.

Basic understanding of the phenomena is at the forefront throughout the book. The large number of equations may be discouraging to many would-be synchrotron-radiation users and generally interested readers with little mathematical background. Mathematics is unavoidable to appreciate the importance of the various parameters for the properties of the radiation. However, the mathematical reasoning in this book is simple, and rarely advances beyond the level of Pythagoras' theorem. In cases where a rigorous analysis and quantitative predictions require more advanced algebra, I will refer to other texts.

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Chapter 2

Properties of radiation

Before describing the properties of synchrotron radiation we introduce some key concepts, by which electromagnetic radiation in general is described.

2.1 Intensity

The energy density associated with electric, $\overrightarrow{E}$, and magnetic, $\overrightarrow{B}$, fields in vacuum is

$$u = \frac{1}{2}\varepsilon_0 E^2 + \frac{1}{2\mu_0}B^2 \tag{2.1}$$

where in SI units the vacuum permittivity is $\varepsilon_0 = 8.8541878 \cdot 10^{-12}$ AsVm^{-1}, and the vacuum permeability is $\mu_0 = 4\pi \cdot 10^{-7}$ Vm^{-1}. In an electromagnetic plane wave

$$B = \frac{E}{c} = \sqrt{\varepsilon_0\mu_0}\,E \tag{2.2}$$

so that

$$u = \frac{1}{2}\varepsilon_0 E^2 + \frac{\varepsilon_0\mu_0}{2\mu_0}E^2 = \varepsilon_0 E^2. \tag{2.3}$$

Intensity is defined as the average energy, u_{average}, per unit time, Δt, traveling through cross section with area, A (see figure 2.1). The corresponding volume is $V = Ac\Delta t$. For a harmonic wave in vacuum with amplitude E_0 we have $E^2_{\text{average}} = \frac{1}{2}E_0^2$, and the intensity is

$$I = \frac{u_{\text{average}}V}{A\Delta t} = \frac{\varepsilon_0 E^2_{\text{average}}Ac\Delta t}{A\Delta t} = \frac{1}{2}\varepsilon_0 c E_0^2 \tag{2.4}$$

The speed of light in vacuum is $c = 2.99792458 \cdot 10^8$ ms^{-1}, and E_0 is the amplitude of the wave in [Vm^{-1}]. Intensity has the unit [Wm^{-2}] as expected. If

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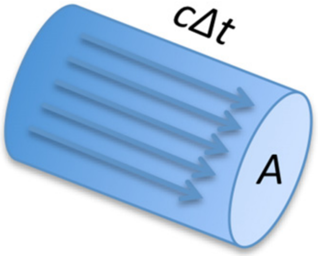

Figure 2.1. Intensity is the average energy per unit time flowing through the cross section area A. The intensity of a plane harmonic wave is given by the average energy contained in a cylinder with area A and length $c\Delta t$.

you don’t feel comfortable with these considerations you may consult electricity and optics text books. This discussion is covered e.g., in [1].

In a quantum mechanical description the intensity is related to number of photons per time and area. The energy density is related to the number of photons, n_{ph}, and their frequency, υ:

$$u = \frac{n_{\mathrm{ph}} h\upsilon}{V} \tag{2.5}$$

where $h = 6.626076 \cdot 10^{-34}\ \mathrm{Js}^{-1}$ is Planck’s constant. Assuming a constant flux of photons, the intensity (average energy per unit time traveling through the area A) is then

$$I = \frac{u_{\mathrm{average}} V}{A\Delta t} = \frac{n_{\mathrm{ph}} h\upsilon}{A\Delta t}. \tag{2.6}$$

The classical equation (2.4) and the quantum mechanical equation (2.6) appear very different. As long as we are doing experiments in the ‘linear regime’, where excitations are made with one-photon-at-a-time, it is convenient to count the number of photons, as opposed to considering the E-field amplitude. Thus, equation (2.6) is a more convenient starting point. For typically 10^{12} photons per second with an energy of 1 keV, the power is 0.16 mW, and focused in a 1 mm^2 spot the intensity is around 160 Wm^{-2}, corresponding to a classical E_0 field amplitude in a harmonic wave of around 350 Vm^{-1}.

Intensity is a property of the radiation, and not of the source.

2.2 Flux

Many experiments require monochromatic radiation. Therefore, the spectral purity of the source is an important parameter. One has introduced a number of concepts which are relevant for experiments. On most of these concepts there is no consensus on the terminology, so one has to be careful and look at the definition in each specific case. The flux of a source is normally defined:

$$\Phi = \frac{n_{\mathrm{ph}}}{\Delta t \frac{\Delta\omega}{\omega}} \tag{2.7}$$

with the unit

$$\frac{\text{number of photons}}{\text{s} \cdot 0.1\%\ \text{BW}}.$$

The notation may be confusing; the intention is that only photons within the 0.1% frequency bandwidth (BW) are to be counted (figure 2.2). In this way 'flux' does take the spectral purity into account, e.g. at a nominal photon energy of 1000 eV, only photons/second within the 999.5–1000.5 eV band contributes to Φ.

2.3 Emittance and Liouville's theorem

The usefulness of a source is also critically dependent on its *size and the angular divergence* of the emitted radiation. The spatial extensions are often given as the standard deviation of a distribution, σ_x and σ_y, in the horizontal and vertical direction, respectively. Similarly, the angular distribution of the flux is characterized by the standard deviation of the intensity around a nominal direction, σ_x' and σ_y', with respect to the horizontal and vertical plane, respectively. These measures contain an implicit assumption of a statistical distribution of the intensity. In addition, since the two dimensions are separated, the solid angle defined by $\sigma_x'\sigma_y'$ gets the unit rad^2 rather than sterad. This is convenient as long as small angles are considered.

The *emittance* in the horizontal and vertical directions is defined (figure 2.3):

$$\varepsilon_x = \sigma_x\sigma_x' \tag{2.8}$$

$$\varepsilon_y = \sigma_y\sigma_y'. \tag{2.9}$$

It is immediately realized that small emittance is desirable for a radiation source. As intensity is inversely proportional to the cross section area, decreasing spatial extension implies increasing intensity. Also, one can realize that a source is more useful if all the photons go in the same direction, than if they are isotropically distributed. No focusing optics is needed to increase intensity if we have a hypothetical point source, which radiates in one direction only. This would imply zero emittance, which is unphysical: for any number of photons per second the intensity

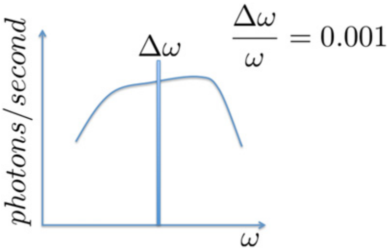

Figure 2.2. Only photons in 0.1% bandwidth contribute to the flux at a certain photon energy.