Chapter 1

Introduction

In classical electromagnetism, a charged particle radiates energy in the form of electromagnetic radiation when it is subject to a force. This effect is the principle behind many useful sources of radiation across a wide range of the electromagnetic spectrum. Synchrotron radiation is one such source. In the last 60 years it has emerged as a fundamental and indispensable tool for the study of materials which encompasses a wide spectrum of sciences, technologies and applications, from life sciences to nanotechnologies, from environmental sciences and geochemistry to archeology. The main figures of merit of synchrotron radiation sources are (narrow) spectral bandwidth, photon wavelength tunability and brilliance, which defines the intensity of radiation, within a given bandwidth around the desired wavelength, that can be focused unto a sample of given area. Typical brilliance values for the highest performance “third generation” light sources are around $10^{19}$ to $10^{21}$ photons/s/mm$^2$/mrad$^2$/0.1% bandwidth.

In addition to the synchrotron radiation, a strong need has emerged over the last few years for a source of radiation with extremely high brilliance, close to full spatial and temporal coherence, a bandwidth approaching the Fourier limit and a stable and well characterized temporal structure in the femtosecond time domain. This new type of light source enables the study of not only the static structure of materials but also the dynamics of processes in complex materials and molecules. Such a source is the single-pass Free Electron Laser (FEL) that, due to a Doppler frequency up-shifting of radiation emitted by relativistic electrons, is particularly well-suited to generating short wavelength X-ray pulses with peak brilliance many orders of magnitude higher than that generated in present third generation sources and with sub-picosecond pulse lengths. There are currently no alternative sources that have such high pulse energies and short durations. The investigation domain opened by the new sources covers essen-
tially all basic science fields giving access to explorations of matter in practically unexplored regimes. The scientific opportunities will in fact impact studies of a large number of disciplines ranging from materials and biomaterials sciences, nanosciences, plasma physics, molecular and cluster femto- and nano- physics and chemistry, as well as having various connections to life, environmental, astrophysical and earth sciences.

The generation of FEL radiation relies on the extraction of electromagnetic energy from kinetic energy of a relativistic electron beam by propagating it along the axis of a periodic lattice of alternating magnetic dipolar fields, known as undulator. This forces the beam to undulate transversally, thus causing the electrons to emit electromagnetic radiation. The fundamental wavelength emitted is proportional to $\lambda_u / \gamma^2$, where $\lambda_u$ is the undulator period, typically a few centimeters long, and $\gamma$ is the relativistic Lorentz factor of the electrons, which typically reaches several thousand for X-ray emission. The first theoretical works describing such undulator radiation were reported in [1] and [2] in the late 1940s to early 1950s. Experiments at Stanford in 1953 generated the first incoherent undulator radiation at visible and millimeter wavelengths [3]. A few years later, Phillips conducted research on an undulator microwave source called the ubitron. This was characterized by $\gamma \geq 1$ and minimal Doppler up-shifting of the radiation wavelength from that of one undulator period. Two main qualitative features common with a FEL interaction were already present in the Phillips’ experiment: a density modulation (bunching) of the electron beam along its direction of propagation, and radiation energy extraction from the kinetic energy of the beam. It was not until 1971 that Madey [4] published a seminal theory of the FEL that described a small gain process in a relativistic electron beam/undulator system. The first amplification and lasing from a FEL was demonstrated in a small gain infrared FEL oscillator system at Stanford a few years later. The FEL oscillator is a multi-pass electron beam/undulator system in which the undulator radiation is collected in the optical cavity of two mirrors with high reflectivity. The high FEL intensity is obtained by summing up the single-pass undulator emission over many turns of the electron beam in the optical cavity. From the late 1970s a body of work was developed that described classically what is now termed the high gain regime of FEL operation [5–9]. In this high gain regime, the radiation power increases exponentially as the electron beam and radiation co-propagate along the undulator. Thus, an initial small source, which may originate as noise, can be amplified by many orders of magnitude until the process saturates. In the X-ray FEL there is therefore no need for potentially troublesome mirrors to form an oscillator cavity. Most of the present X-ray FEL facilities and designs are based on this type of interaction, which has been made possible by many advances in electron beam generation and acceleration over the past few decades.
The remarkable step in performance of X-ray FELs – as compared with third generation light sources, ten orders of magnitude increase in peak photon brightness and two orders of magnitude reduction of pulse length – has been made possible, in part, by the advent of the photocathode RF electron gun [10] and recent progress in beam brightness preservation for linear colliders [11, 12]. Of critical importance is the normalized transverse beam emittance, \( \epsilon_n = \gamma \epsilon \), where the geometric transverse emittance \( \epsilon \) is a measure of the transverse phase space domain occupied by the beam. A limit on the geometric beam emittance for ensuring good spatial (transverse) coherence from sources of spontaneous undulator radiation was derived in [13], giving \( \epsilon \leq \lambda / (4\pi) \), where \( \lambda / (4\pi) \) is the minimum phase space area for a diffraction limited photon beam. Although this expression was derived for systems without gain, it turns out that it is also a requirement for the successful operation of a high-gain amplifier FEL. This relation gives a rough rule-of-thumb estimate of the electron energy/wavelength possibilities and shows, for example, that the minimum wavelength achievable decreases with the normalized emittance, for a given beam energy. Note that the local emittance (referred to as “slice emittance) can vary significantly along the bunch to give hot-spots where lasing can occur. In fact, in contrast to linear colliders, where particle collisions effectively integrate over the entire bunch length, the X-ray FELs usually concern only very short fractions of the electron bunch length. The integration length is given by the “FEL slippage length” that is the electron-to-photon longitudinal slippage over the length of undulator, prior to FEL power saturation. The slippage length is typically in the range 1–30 \( \mu m \), a small fraction of the total bunch length. Thus, the electron bunch slice duration can reasonably be defined of the order (or a fraction) of the FEL slippage length. The self-consistently coupled equations that describe a FEL reveal an exponential instability in both the field amplitude and the fundamental electron bunching. So, the radiation power exponentially grows until the electron/photon interaction saturates. At saturation, \( P \approx \rho P_e \) where \( P_e \) is the electron beam power and \( \rho \) [14] is seen to be a measure of the efficiency of the interaction, with typical values in the X-ray regime of \( 10^{-4} \leq \rho \leq 10^{-3} \). The relative energy spread of the electron beam at saturation is \( \sigma_\delta \approx \rho \). Hence, it becomes clear that the quality of the electron beam is of critical importance. If there is an initial electron energy spread approaching the maximum, which occurs at a FEL saturation of \( \sigma_\delta \geq \rho \), then the FEL interaction is greatly reduced. Typical electron beam parameters of the fourth generation – very high brightness – linac-based FELs (from infrared to X-rays spectral range) are: 0.2–1 nC bunch charge, 1–3 mm mrad normalized emittance, 0.5–3 kA peak current, 0.05–0.1 % relative energy spread and 1–50 GeV final electron energy.

Delivering such high machine flexibility to serve a broad range of potential applications imposes severe requirements on the quality of the electron beam.
To meet these requirements, the need of a linac design based on extensive studies of possible perturbations that may affect the electron beam dynamics, of means to correct them and of parameter optimization has emerged. The realization of a valid machine design is therefore a fundamental and critical step for the success of a FEL project. Because of the special sensitivity of the FEL generation to the electron beam emittance, relative energy spread and trajectory control [15, 16], this thesis focuses on the design strategies to control these parameters and on how the design challenges translate into modeling and simulation challenges. Some methods and results have acquired a general validity within the field of accelerator physics and have been translated into publications in refereed journals [17–21]. Some other aspects of our machine study have been developed for the specific FEL scheme known as harmonic generation. In fact, we can identify two general ways to generate X-ray FEL. The Self Amplified Spontaneous Emission (SASE) [14, 22–25] relies on the interaction of the electrons with photons that are emitted by the electron beam itself. Since the electron bunching starts to grow from the natural noise of the initial electron distribution, the SASE output radiation is relatively poor in longitudinal coherence. In the High Gain Harmonic Generation (HGHG) scheme [5–9, 26, 27], instead, the initial energy modulation is driven by an external seed laser. It is then transformed into density bunching in a dispersive section inserted in the undulator chain. In this case, the output FEL properties reflect the high longitudinal coherence of the seeding laser.

Starting from very general principles of machine design and electron beam control, the quantitative analysis reported in this thesis focuses on the FERMI@Elettra FEL case study employing the HGHG scheme. The FERMI@Elettra single-pass linac-based FEL at the Elettra Laboratory of Sincrotrone Trieste [28, 29] is one of the FEL based European projects, designed to become the international user facility in Italy for scientific investigations of ultra-fast and ultra-high resolution processes in material science and physical biosciences with ultra high brilliance X-ray pulses. With a peak brightness of about 6 orders of magnitude higher than third generation sources, full transverse coherence, (close to) transform limited bandwidth, pulse lengths of the order of a picosecond or less, variable polarization and energy tunability, the FERMI source is a powerful tool for scientific exploration in a wide spectrum of disciplines. The coherence properties will open up new perspectives for single shot imaging, allowing to study the dynamics of chemical reactions and other phenomena through single pulse coherent diffraction imaging with a spatial resolution in the nm domain and matter under extreme thermodynamic conditions (warm and dense matter phases). The high peak power will allow studying nonlinear multi-photon processes in a regime never explored before, in dilute samples that are of paramount importance in atmospheric, astrophysical and environmental physics as well as in the
characterization of nano-size materials. The short pulse duration will open the
door to visualizing ultra-fast intra-atomic and electronic dynamics. So, the ultra-
bright, ultra-short pulses will allow single photon pulse experiments to collect
images at time scales faster than radiation damage. This in turn will open the
possibility of studying the morphology and the structure of bio-systems unstable under X-ray radiation exposure. As the seed laser determines the duration,
bandwidth, and wavelength of the output radiation, all are tunable and controllable, covering a wide spectral range. The seed laser furthermore provides a reference signal throughout the FERMI facility (including the experimental beam-lines) to facilitate the femtosecond level precision timing and synchronization of all systems. The seeded FEL driven by an external laser is therefore particularly suitable for pump-probe synchronization at time scales well below 1 ps. Pump-probe experiments are usually carried out as follows. An ultra-short light pulse (pump) excites an atom, a molecule or a condensed system, while a second pulse (probe), properly delayed in time, probes the excited sample, allowing to follow the system evolution back to the non-excited state. By using fs long pulses at VUV or soft X-ray wavelengths, it will be possible to observe the atomic motion in real time. In conclusion, applications of FERMI@Elettra FEL extend from chemical reaction dynamics to biological systems, materials and surfaces, nanostructures and superconductors. The choice of design parameters allows FERMI to generate FEL radiation with a wide range of characteristics tailored to match a diversity of experimental requirements, ranging from single shot, short (≤50 fs), high brilliance, time-resolved experiments to ultra-fast pump-probe experiments, to high resolution experiments with close to transform-limited radiation on the 10’s of fs time scale.

The original contributions of this thesis are structured as follows. Chapter 2 is an introduction to the FERMI@Elettra layout based on the FERMI Technical Design Study [30]. Chapter 3 introduces for the Reader’s convenience well-established theoretical tools which are used in the following chapters to describe the electron beam dynamics and the 6-D emittance degradation. The validity of the theoretical models for the FERMI case study is discussed. Chapter 4 deals with the machine design from the point of view of the single particle dynamics, including the specification of the magnetic field tolerances and alignment, the optics design of diagnostic and production lattice and geometric collimation. Chapter 5 describes the impact of collective effects such as wake fields, space charge forces and emission of coherent synchrotron radiation on the electron beam dynamics. Chapter 6 is focused on the determination of the machine working point in terms of bunch length compression factor and final electron beam parameters. Finally, Chapter 7 reports about the FERMI@Elettra commissioning results that are relevant for a comparison with the theoretical and simulation studies carried out in the previous Chapters.