

# Proton Compression for the Muon Collider Project

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MASTER'S THESIS

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# Proton Compression for the Muon Collider Project

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# Abstract

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A muon collider is a promising future collider concept for particle physics. The International Muon Collider Collaboration (IMCC) and the Muon Collider Collaboration (MuCol) are currently conducting a design study to investigate the feasibility of such a facility. To produce muons, a high-intensity, short pulse proton beam produced in a proton complex is directed onto a target, where pions are produced, which subsequently decay into muons. This proton complex includes a compressor before final transport to the target. The collective repulsion between the protons, referred to as space-charge, is expected to be significant in the compressor, where proton bunches are to be compressed to pulse lengths below 2 ns.

Previous studies of the compressor have modeled space-charge using 2.5D Particle-in-Cell (PIC) simulations in Xsuite, whose space-charge implementation employs a static mesh, *i.e.*, the mesh does not adapt to an evolving beam size. However, 2.5D space-charge may not be sufficient to accurately describe the effects of space-charge in the compressor. In addition, a 3D model with a static mesh would be computationally inefficient due to the compression.

In this thesis, an adaptive-mesh space-charge implementation has been developed for Xsuite. Using both static- and adaptive-mesh configurations, 2.5D and 3D space-charge models have been compared for the compressor. The results indicate that 3D modeling is required to capture important aspects of the compressor dynamics. A four-fold structure has been observed in the absence of space-charge, and its cause has been investigated. Further studies have been conducted using adaptive-mesh 3D modeling, including a convergence study and a tune scan, where the latter aided in the exploration of a new working point for the compressor. No fundamental obstacle to sub-2 ns compression was identified. However, it is not fully clear whether observed microbunching phenomena are numerical or physical in nature.





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## Declaration

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I hereby affirm that this Master thesis was composed by myself and that the work herein is my own except where explicitly stated otherwise in the text. This work has not been submitted for any other degree or professional qualification except as specified. Parts of this work have been submitted to conferences HB'25 as a co-author [1] and to IPAC'26 as a primary author [2]. However, this work provides a more detailed description of the methods, assumptions, and interpretation of the results. Where other people's work has been used (either from a printed source, internet, or any other source), this has been carefully acknowledged and referenced.

AI-tools, such as Writefull, ChatGPT 4/5, and Gemini have provided assistance throughout the execution of the thesis. The usage includes clarification of conceptual questions, code assistance, and debugging as well as aid in figure generation. AI has also helped with wording, spelling, and grammar.



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## Popular Science Summary

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Want to detect dark matter? Or understand more about the Higgs boson? To accomplish these and many other goals in modern physics, we would need new particle colliders stronger than the ones we have today. One such particle collider would be the so-called Muon Collider, which would collide the particles called muons. Colliding muons would be very energy efficient, as they do not consist of several building blocks compared to protons, where their parts all use some of the useful energy. Muons would also be much more efficient compared to colliding electrons, as muons would lose much less energy when bent in a circular accelerator. However, muons come with one big drawback: a limited lifetime, which means that it is not as easy to get many of them to do meaningful collisions.

Thinking in analogy, imagine protons as colliding two round satellites together and electrons as colliding billiard balls. The satellites consist of many different parts and the energy will be spread across all of these, whereas for the billiard balls, the energy is shared only between the balls. The muons can perhaps be seen as big blocks of ice; bigger than the billiard balls yet, in a sense, still point-like. And as time progresses, the ice melts. The loss of energy at bending that is more significant for lighter objects is harder to analogize and is simply a fact to accept.

To deal with the limited lifetime of muons, several creative technical solutions are needed to make a muon collider possible. To create sufficient amounts of muons, many protons very close to each other will need to collide on a target. As equally charged particles, such as protons, repel each other, this implies significant challenges to make this possible. Before building something this expensive, we first use computer simulations to test different designs for how such a proton beam can realistically be produced. This work treats the last part of the proton complex, the compressor, where the protons are squeezed the closest together.

As some assumptions had been made in previous simulations, one goal was to see if these assumptions were realistic enough, and if not, what consequences this could have. By changing how the computer does some calculations and removing some assumptions, the results clearly differed. Following this, this work conducts

several investigations:

- To make sure that the computer is not making things up, a "convergence study" is conducted, to determine which inputs consistently give the same output.
- In some cases, the particles underwent "microbunching". Think of an accordion: when you press together the accordion to produce sound, the bellows fold on themselves. In a sense, the proton beam sometimes underwent a similar "folding", but it is not clear whether this is caused by computer calculations or by real physics.
- Through further experiments, an observed "four-fold" structure was found to have an unexpected cause. It was initially believed to be caused by a resonance. In accelerator physics, a resonance can be compared to when you push someone on a swing: if you time it a certain way, the person that you are pushing will go further and further, and may even fall off. Resonance can build up for particle beams in a similar manner and may similarly cause us to lose particles. Therefore, this work also tries to find ways to remove the resonance mentioned.
- Lastly, think of an old-school radio: you turn on the wheel to adjust frequency and connect to the channel you want. Perhaps you need to adjust the wheel slightly to make the people speaking less "noisy". This work does a similar thing to the compressor, where we try to get the best results by slightly changing the structure of the compressor multiple times. Some of the best "radio wheel" positions were then compared.

This work in many ways improves on previous simulations, attempts to better understand how to improve the compressor, and provides suggestions on what may need to be investigated further.

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## Glossary

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CERN: European Center for Nuclear Research  
CIC: Cloud-in-Cell  
DFT: Discrete Fourier Transform  
ESS: European Spallation Source  
FCC: Future Circular Collider  
FFT: Fast Fourier Transform  
FMA: Frequency Map Analysis  
FODO: Lattice cell structure (Focusing, Drift, Defocusing, Drift)  
IMCC: International Muon Collider Collaboration  
LHC: Large Hadron Collider  
MuCol: MuCol Collaboration (separate from IMCC)  
NAFF: Numerical Analysis of the Fundamental Frequencies  
NGP: Nearest-Grid-Point  
PIC: Particle-in-Cell  
PSD: Power Spectral Density  
RF: Radiofrequency  
RMS: Root-Mean-Squared  
TSC: Trilinear-Shaped-Cloud  
WP3: Work Package 3 of the MuCol collaboration



# Introduction

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In the quest to advance high-energy particle physics, future colliders with particle intensities and energies greater than those of today have been recommended [3]. One promising new concept is the muon collider, which would enable much higher effective collision energies than proton colliders while also avoiding the severe radiation losses that limit similar electron-based machines. However, a muon collider comes with its own set of constraints and requirements. As muons have a short lifetime, many muons must be produced for sufficient collision intensities [4]. To achieve this, extremely short pulses of protons must be delivered to a target where pion production will commence. These pions will thereafter decay to muons.

To produce the required proton beam, proton pulses are first accumulated to 120 ns in an accumulator ring [5, pp. 70–76]. The compressor ring is used later to compress the pulses down to 2 ns. At the required proton beam intensity and energy, the protons will exert significant electromagnetic forces on each other. These forces, collectively named space-charge, can distort the beam and adversely affect the performance of the compressor. It is therefore imperative to accurately model these effects in order to guide the design process of a compressor that would meet the requirements of the muon collider.

The focus of this thesis is to investigate both the compressor beam dynamics and the tools themselves that have been used to model the dynamics. The study will not include studies on injection or extraction. The main goal of this thesis is to determine the effects space-charge may have on the compressor's beam dynamics, as this ring is where space-charge is expected to have the strongest impact in the complex.

Previous simulation studies have used a simplified space-charge model [1]. For example, a so-called 2.5D model has been used that does not apply longitudinal energy kicks, and the simulation framework Xsuite has so far employed a static Particle-in-Cell (PIC) mesh that does not adapt to the evolving beam size. The question is therefore raised whether predictions made with this modeling would hold for 3D modeling with an adaptive mesh and, if not, what consequences this could have for an optimized design of the compressor.

A four-fold structure observed in these simulations was initially believed to be a resonance driven by space-charge, which would guide the design of upstream components of the proton complex to produce a beam of larger emittance. However, it was found that the structure was caused by sextupoles, and that it was not inherently a resonance.

The aim of this thesis is to evaluate the previous configuration and, if necessary, to improve it. This process involves understanding the Xsuite physics model as well as extending it. It evaluates a microbunching phenomenon that occurs with a new configuration. In addition, the current compressor design is evaluated. Will the current design cause resonances, space-charge driven or otherwise? Will it require a re-design? What machine tune would yield an optimal beam for the target?

In this thesis, I first give a theoretical background of beam dynamics and resonances. Further, I explain how space-charge may affect these dynamics. I then explain the simulation framework Xsuite, and how it models space-charge. The parameters chosen for the current use case are explained and then a proposed improvement is introduced to the simulation framework. Then I dive into a thorough investigation into a four-fold structure. Lastly, tune scans are performed to find an optimal working point for the current compressor design.

## Theoretical background

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This chapter introduces the muon collider concept, as well as the proton compressor. It then introduces fundamental concepts of beam physics, accelerator concepts, and theoretical framework necessary to understand resonances and space-charge effects in the compressor.

### 2.1 Current status of Accelerators for Particle Physics

#### 2.1.1 Particle colliders

Particle accelerators and particle colliders have been used since the 20th century to make a multitude of new discoveries in nuclear and particle physics [6]. Several new particles have been discovered and contributions to furthering our understanding of the standard model have been made [7] [8]. Particle colliders are widely considered one of the main tools to make new empirical discoveries in particle physics [9].

Since the discovery of the Higgs boson, many new questions have arisen in particle physics, while yet others remain unanswered. For example, the Higgs boson and its properties are still not fully understood, we do not yet understand matter-antimatter asymmetry, gravity has not been unified with the standard model (SM), and dark matter remains unexplained [8]. To gain insights that may aid in researching these and other areas in particle physics, organizations such as the European Strategy for Particle Physics (ESPP) have recommended exploring the possibilities for a 10-TeV center-of-momentum collider [10].

#### 2.1.2 The LHC and Hadron collision

The current highest-energy particle collider in the world, the Large Hadron Collider (LHC), has allowed for important discoveries in particle physics, such as the Higgs boson [11]. At the time of writing, the LHC can reach collision energies of up to 13.6 TeV [12]. However, the actual momentum/energies of the fundamental particles (the partonic Center of Momentum, or partonic Center of mass, (pCOM)) energies reached are only a fraction of these collision energies, as hadrons consist

of several partons (quarks and gluons) [3]. It is the interactions between the fundamental particles (in this case, the partons) that often are of primary interest [13, p. 236]. Furthermore, there is inherent uncertainty as to which of the constituent partons interact in the collisions [14]. In other words, the energy available for the processes of main interest is only a fraction of the collision energy in hadron colliders, and there is still uncertainty due to their composite nature, which must be considered.

### 2.1.3 Charged Lepton Colliders

In contrast to colliding hadrons, charged lepton colliders are well suited for performing "precision measurements" referring to their point-like structure [15, p. 5]. These colliders provide an alternative to hadron colliders (such as the LHC) where the accelerated particles are themselves fundamental, and these have been in use for some time in the form of electron-positron colliders; see, for example, the Large Electron-Positron Collider (LEP), which is now decommissioned [16]. For electron-positron colliders, the small mass of the electrons relative to e.g. protons provides a challenge in reaching higher collision energies [13, pp. 81–82]. Synchrotron radiation refers to the electromagnetic radiation emitted by charged particles when they are accelerated transversely, for example when they are bent along curved trajectories by magnetic fields in a circular accelerator [17, p. 52]. The amount of synchrotron radiation, and therefore lost energy, is inversely proportional to the mass of a particle [13, pp. 81–82].

### 2.1.4 The Future Circular Collider

The Future Circular Collider (FCC) is a potential new collider at CERN that would consist of two main phases. In its first stage, the aim is to collide electrons and positrons for precision measurements. The second stage is the high-energy stage, where the aim is to collide protons and heavy ions with collision energies of 100 TeV. A feasibility report was released in March 2025 [18], and a decision on whether to build the FCC will be taken in 2028. While the energy of the second stage would meet the goal of 10 TeV pCOM [3], the FCC would require a significantly bigger circumference than the LHC (the FCC circumference would be 90.7 km), and the second stage alone could cost 15 billion CHF [19] [18]. The second stage, using hadrons, would begin operation in the 2070s [18].

### 2.1.5 The case for a Muon Collider

While the FCC would achieve more precise measurements as well as reach higher energy physics, it does so by alternating the advantages and disadvantages of protons versus electrons. Muons are 200 times heavier leptons than electrons [20]. As such, they have a point-like structure, which means that their collision energies will more directly represent the energy available for fundamental interactions, comparable to the pCOM energy for hadrons [15, p. 5] [21, p. 2]. This, combined with the drastic decrease in emitted synchrotron radiation as opposed to electrons, means a muon collider could prove a compelling and cost-effective alternative for a

new collider (for example, the tunnel would be much smaller than what is proposed for the FCC) [15] [21].

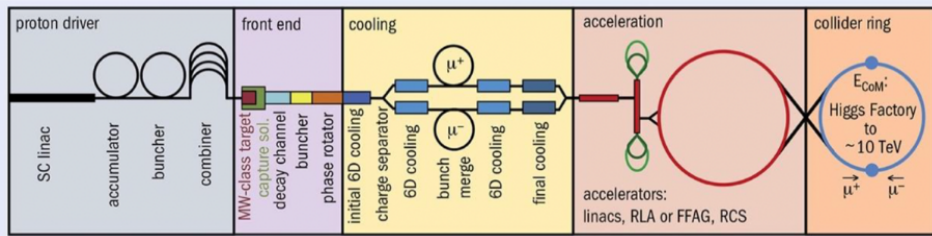
Muons do come with drawbacks of their own as they are unstable. Their limited lifetime will, among other things, result in decay products of muons in the accelerator contributing to background radiation, although neutrino products may be used for science themselves [15]. Furthermore, the short lifetime poses challenges for producing large amounts of muons with small emittance bunches [21]. For example, the muons will need to be accelerated quickly before decaying. As for the last charged lepton, the tauon, it has a lifetime roughly 8000 times shorter than that of muons [20], which makes a potential tauon collider unfeasible. To assess the feasibility of realizing a muon collider, the International Muon Collider Collaboration (IMCC) was formed in 2020. Since then, a CERN-coordinated and EU-funded design study has been initiated, called MuCol [22] [15, p. 5].

## 2.2 The MuCol project

MuCol is a design study project which was started in March 2023, and is planned to proceed until February 2027 [22]. It comprises several institutes, including the European Spallation Source (ESS). [23].

### 2.2.1 Conceptual Design

The current conceptual design of the muon collider, shown in Fig. 2.1, consists of several components: the proton driver, the front end, the cooling, the acceleration, and the collider ring [5]. Each is briefly presented below in Fig. 2.1:



**Figure 2.1:** Conceptual layout of the muon collider. Taken from [24].

- Proton complex** The proton complex is where a high-intensity short-pulse proton beam is produced [5, pp. 70–76] [15, p. 69]. This is achieved by first accelerating  $H^-$ -ions to high energies using superconducting RF-cavities and creating pulses through chopping the beam in the high-power acceleration section. Protons are produced through charge stripping and are thereafter accumulated in the accumulator. In the compressor, a  $90^\circ$  longitudinal phase space rotation is performed on the bunches to achieve the short pulse length required by the target. The compressed bunches are



lastly recombined in the transport section before hitting the target. The proton beam power will be either 2 or 4 MW, and options of either 5 or 10 GeV are being considered for the proton beam energy. A work package coordinated by ESS is dedicated to the proton complex [25].

- **Front End** The front end is where the muons are produced [15, p. 71]. When the protons hit the target, pions are produced, which decay to muons [19]. Pions and muons travel through a solenoid-focused chicane (a set of bending magnets) where high-momentum beam impurities (protons) are removed [15, p. 71]. If there are any surviving protons, these are removed in a Beryllium absorber. To allow as many remaining pions to decay as possible, the beam then enters a straight section with no additional manipulation (a drift section). Lastly, the beam is split, first into bunches, and then according to charge, before entering the cooling section.
- **Cooling** Cooling is performed to reduce the size of the beam, and is achieved through an ionization cooling system, where the beam is focused through solenoid magnets onto energy absorbers [15, p. 71]. To restore longitudinal momentum, the beam is accelerated through RF cavities, which further reduces transverse emittance. The beam is then further cooled. In the middle of the cooling section, bunches are merged before a final cooling section. At the end of this section, the bunches are re-accelerated to semi-relativistic speeds before entering the next section.
- **Acceleration** The acceleration section can be divided into two subsections; low-energy acceleration and high-energy acceleration:
  - **Low-energy section** This section consists of three superconducting linear accelerators [15, p. 75]. First, the beam is accelerated in the pre-accelerator at 352 MHz. The initial “lower” frequency is to decrease the demands on the cooling section. Thereafter, it enters into two Dogbone recirculating linacs operating at 1056 MHz. When the beam has reached an energy of 63 GeV, the beam is transferred to the high-energy subsection.
  - **High-energy section** In this subsection of the collider, the muons are accelerated to the TeV range [15, pp. 77-78]. This is achieved through a chain of rapid cycling synchrotrons, which accelerate the counter-rotating bunches (rotational direction depending on charge) in intermediate stages. They are optimized to minimize the radius, which will minimize travel time and consequently the number of decayed muons. Finally, the bunches are injected into the collider ring.
- **Collider Ring** This is the final section of the Muon Collider [15, pp. 81-82]. It has two interaction regions where muon bunches collide and where detectors are located [5, p. 95]. These straight sections will also be used for the injection of muons, extraction to the beam dump, and RF systems for acceleration. The ring also has a chromatic compensation section, as focusing will result in chromatic aberrations. The arcs are designed with negative momentum compaction to tune the momentum slip factor and keep the bunches short. As muons will decay in the ring, tungsten absorbers are

installed. A cryogenic system will handle the heat created from the decay processes.

## 2.3 A brief introduction to Beam Physics

The study of how ensembles of particles, often with roughly similar real space coordinates, called **beam**, act in electromagnetic fields is named beam physics [26, p. 4]. The field can usually be categorized into the subdivisions of **production**, **acceleration**, **transportation** and **storage**. In the following section, some important terms in beam physics are introduced.

A **beam line** is the structure that guides the beam to its intended application, and consists of components such as magnets or RF-cavities that, in one way or another, affect the bypassing beam. These components are called **elements** [27, p. 3][28, p. 15]. The arrangement of magnets along the beam line is called **lattice**. By repeating a pattern of magnets along the beam line, one may construct a **periodic lattice**. By definition, a circular accelerator lattice (also referred to as **ring**) is periodic, but segments of a lattice may themselves also be periodic, either called **superperiods** or **cells** depending on the size of the segment [29]. When a particle has traveled one complete period through a periodic lattice, this is called a **turn** [30, p. 92]. A **reference particle** is a particle that travels exactly as intended through the beam line. This path is called the **reference orbit** in a ring [26, p. 33], or more generally the **reference trajectory** [27]. The **closed orbit** is the actual orbit a particle takes in a ring, which may or may not coincide with the reference orbit [30, p. 196].

The **dynamical variables** describe the coordinates and (so-called canonical) momentum ( $p_x$  and  $p_y$ ) of the particles as functions of the distance along the beam line [30, p. 68]. **Phase space** is the space spanned by these dynamical variables [30, p. 64]. In other words, 6D phase space is spanned by  $(x, p_x, y, p_y, z, \delta)$  where  $z$  is the longitudinal coordinate relative to the reference particle, and  $\delta$  is the energy or sometimes momentum deviation. For the transverse planes, the **angle** with respect to the reference orbit is sometimes used instead of the canonical momentum, usually in connection with the use of the so-called paraxial approximation. Then the relation becomes for the x-plane with angle  $x'$ :  $\frac{p_x}{p_0} = \sin(x') \approx x'$ , where the small-angle approximation was used in the second equality, and where the momentum  $p_x$  has been scaled with the reference momentum  $p_0$ . The case is analogous for the y-plane [31, pp. 13-14]. The complete phase space is in 6D where also the longitudinal dynamical variables are included (see Section 2.7).

A **transfer map** is a map describing the evolution of the dynamical variables for a particle traveling between two points [30, p. 76]. Representing the maps as **Transfer matrices** can be advantageous as several elements in a beam line can be combined by simply multiplying the matrices together [30, p. 88]. This is mainly the case for components that can, to a good degree, be approximated as linear components (eg. dipoles, quadrupoles, drift spaces...). For higher-order elements such as sextupoles and octupoles, higher-order maps are needed to accurately represent them [30, p. 289]. It is advantageous to make use of transfer maps that

are **symplectic**, as this implies several conserved quantities during transformation. One of these quantities, assuming more than one degree of freedom and linear transformation, is the **emittance**, the phase space volume [26, pp. 1-2] [30, p. 80]. Mathematically, a transfer map with Jacobian  $J$  is symplectic if [30, pp. 76–78]:

$$J^T S J = S \quad (2.1)$$

where  $S$  is a  $2n \times 2n$  antisymmetric matrix with block diagonals given by:

$$S_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad (2.2)$$

Symplecticity may motivate the use of Hamiltonian mechanics, which is discussed in the following section.

## 2.4 Equations of motion for beam physics

While the equations of motion for a particle in an accelerator can be described using Newtonian mechanics, it may be advantageous to instead do it using the **Hamiltonian**. By inserting the Hamiltonian for a dynamical system into what is called **Hamilton's equations**, the equations of motion are produced for the system. Hamilton's equations are given by: [30, pp. 60-61]

$$\begin{cases} \frac{dx_i}{dt} = \frac{\partial H}{\partial p_i} \\ \frac{dp_i}{dt} = -\frac{\partial H}{\partial x_i} \end{cases} \quad (2.3)$$

where  $x_i$  are particle coordinates (with  $i$  corresponding to degree of freedom) and  $p_i$  are the canonical momentum components [30, pp. 61]. Any pair of variables evolving according to these equations are called **canonical variables** [30, p. 68]. For particles affected by the Lorentz force, the canonical momentum is  $\vec{p}_{\text{can}} = \vec{p}_{\text{mec}} + q\mathbf{A}$  where  $\vec{p}_{\text{mec}}$  is the more well-known mechanical momentum,  $q$  is the charge and  $\mathbf{A}$  is the magnetic vector potential [30, p. 62] [26, p. 3].

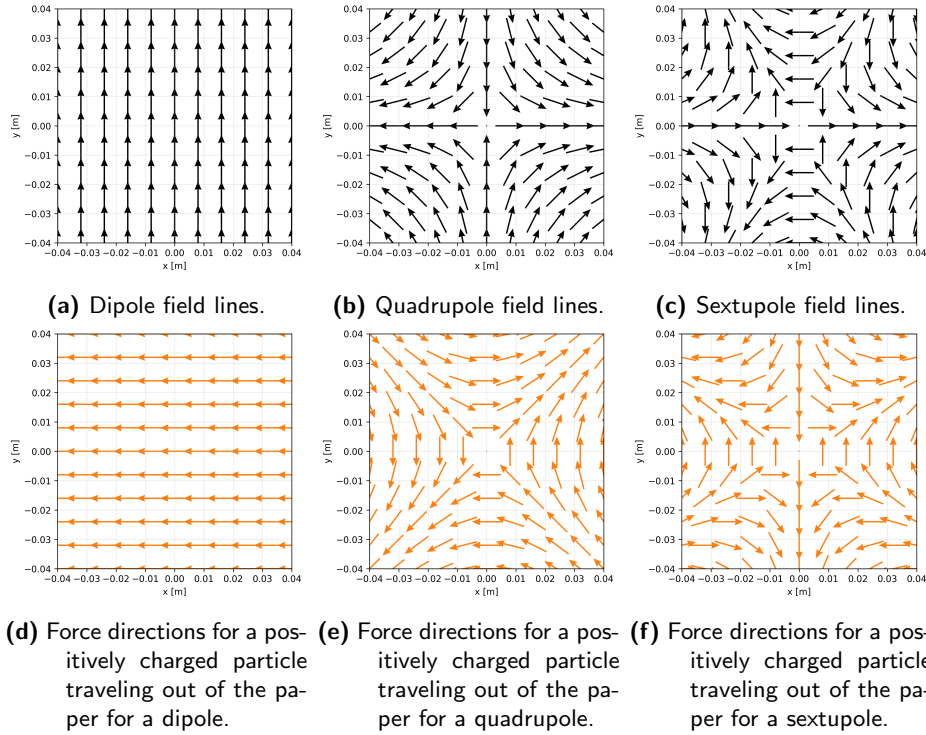
One advantage of using the Hamiltonian is that dynamical systems obeying Hamilton's equations have symplectic transfer maps [30, p. 76]. Furthermore, Hamiltonian mechanics provides a convenient way of describing the equations of motion as dependent on the location along the beamline (specifically along the reference trajectory,  $s$ ) rather than on the time, as timing the particles' flight is generally harder than simply stating that particles enter a certain element at a certain length in the beamline [30, pp. 63-64]. For Eq. (2.3), an equivalent, time-independent, form of Hamilton's equations are provided as: [32, pp. 12–14]

$$\begin{cases} \frac{dx_i}{ds} = \frac{\partial H}{\partial p_i} \\ \frac{dp_i}{ds} = -\frac{\partial H}{\partial x_i} \end{cases} \quad (2.4)$$

In Appendix A the general Hamiltonian for particles traveling in magnetic fields is described.

## 2.5 Common beam elements

The magnetic fields of the elements dipoles, quadrupoles, and sextupoles are shown in Fig. 2.2. These elements, along with the drift space, are described in the following section.



**Figure 2.2:** Field lines (black arrows) for idealized versions of a dipole, quadrupole and sextupole in subfigures a), b) and c). Force directions for positively charged particles traveling out of the paper in subfigures d), e) and f).

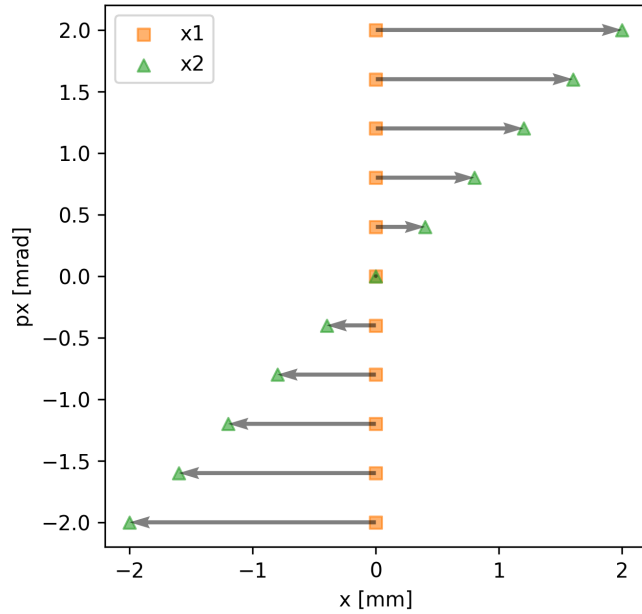
### 2.5.1 Drift space

A region of a beamline where there are no electromagnetic fields present is called a **drift space** [30, pp. 85–88]. Its Hamiltonian and the subsequent derivation of the drift linear transfer map are shown in Appendix B.0.1.

Consider a particle characterized by phase space coordinates  $\vec{x} = (x_0 \ p_{x0})^T$  where neither  $x_0$  nor  $p_{x0}$  are zero. After the drift, the particle coordinates in phase space will be:

$$\begin{pmatrix} 1 & L \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x_0 \\ p_{x0} \end{pmatrix} = \begin{pmatrix} x_0 + Lp_{x0} \\ p_{x0} \end{pmatrix} \quad (2.5)$$

In other words, while the momentum remains unchanged the coordinate changes proportionally to the length of the drift space and the momentum of the particle at the entrance. The case is equivalent for the other planes [30, pp. 87–88]. In Fig. 2.3 the phase space evolution for particles in a drift space is shown.

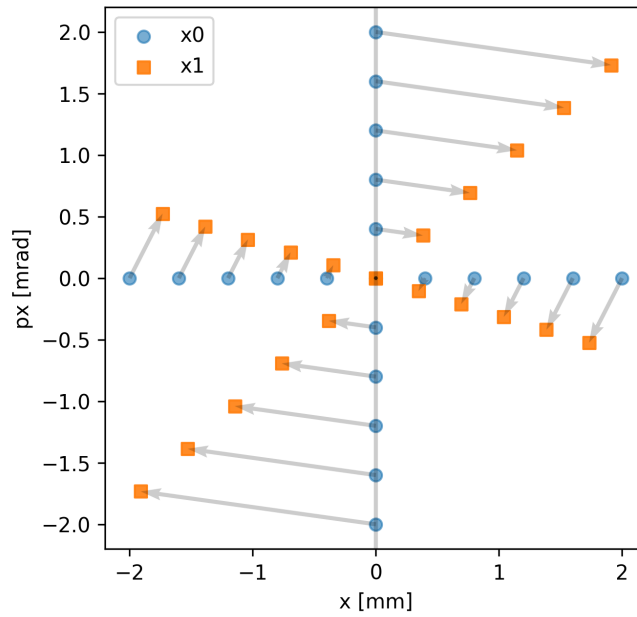


**Figure 2.3:** Phase space evolution of particles evenly distributed on a line, originally with identical  $x$  coordinates.

### 2.5.2 Dipole magnet

A **dipole magnet**, also called **bending magnet**, bends the trajectory of the particles that enter it [33]. Its transfer map and Hamiltonian are given in Appendix B.0.2. The evolution of particles travelling through a thick dipole in phase space for  $x - p_x$  and  $z - \delta$  is shown in Fig. 2.4.

If the curvature for the reference trajectory is chosen so that  $h = k_0$  in Eq. (B.8), *i.e.* it is perfectly centered, then a particle entering on the reference trajectory with no energy deviation will remain on the reference trajectory, while a particle entering on the same trajectory but with some energy deviation will deviate from the reference trajectory (and therefore have a longer/shorter path length compared to that of the reference particle). This coupling effect between the longitudinal and transverse planes is called **dispersion** [30, p. 91]. A particle entering with a transverse offset will undergo **weak focusing**, resulting in oscillations reminiscent of that of a harmonic oscillator [30, pp. 91–92]. These oscillations are treated further in Section 2.6.



**Figure 2.4:** Phase space evolution of particles in  $x - p_x$  for a horizontally bending dipole. Just like in a drift, a sloped line of the particles is created. Weak focusing causes the magnitude of  $p_x$  to increase for larger  $x$ .

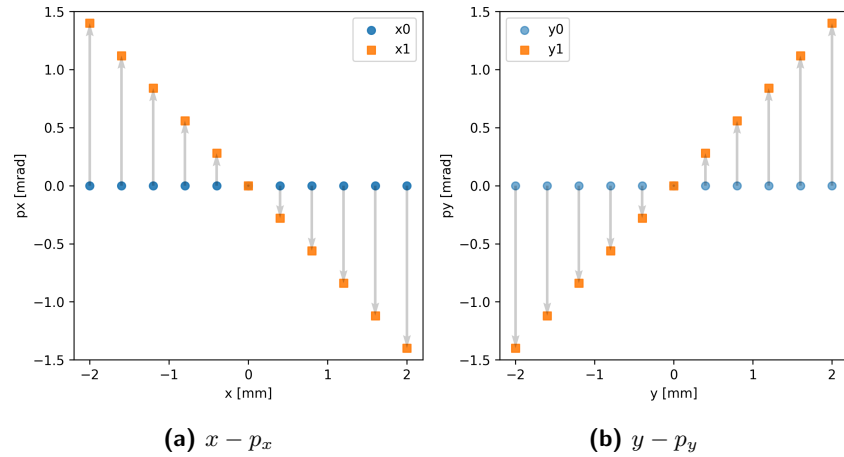
### 2.5.3 Quadrupole

Weak focusing has been mentioned as one of the effects caused by using a dipole. **Strong focusing** may instead be achieved by a **quadrupole**, simply referring to a more effective focusing with equivalent magnet strength [30, pp. 92, 94]. Its Hamiltonian and transfer map are given in Appendix B.0.3. In a quadrupole, the beam is focused (spatial spread is decreased) in one plane while defocused in the other. By effective placement relative to the betatron functions (see Section 2.6) net focusing is achieved [34, pp. 111–112]. In other terms, horizontally focusing magnets are placed where the horizontal size of the beam is expected to be big, and

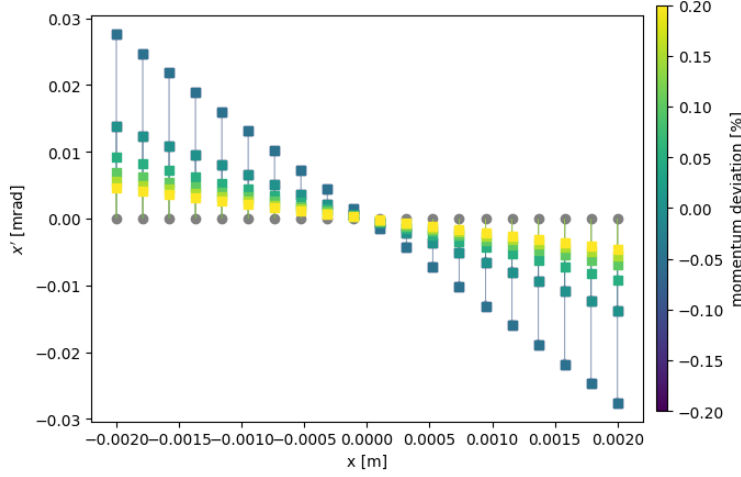
where the vertical size is expected to be small, and vice versa. When off-momentum particles enter a quadrupole, the strength of focusing will also vary [29, p. 108]. This is an effect which in periodic lattices leads to what is known as **chromaticity**. As dipoles contribute weak focusing, they also contribute to chromaticity, although generally to a lesser extent [30, p. 103][35, pp. 1–2]. Chromaticity may cause problems for accelerator operation, and its consequences are further discussed in Section 2.6.2. The quadrupole focusing strength as a function of position  $s$  around the accelerator is given as [30, pp. 102–103]:

$$k_1(s) = \frac{q}{P_0} \frac{\partial B_y}{\partial x} \quad (2.6)$$

Where  $P_0$  is the reference momentum. To model a thick quadrupole using what is known as the thin lens approximation (see Appendix B), a drift with half the quadrupole length followed by a "thin" quadrupole, followed by another drift is an example which gives a transfer map that is accurate to the second order [36, pp. 71–76]. A thin quadrupole provides a useful way of visualizing purely the quadrupole focusing effects while eliminating the "drift space" effects. The thin lens approximation is further used in simulation frameworks such as Xsuite [37]. Phase space evolution for, in the cartesian plane, initially spread out particles with the same initial momenta traveling through a thin quadrupole is shown in Fig. 2.5. Phase evolution for a thin quadrupole with different initial momenta is shown in Fig. 2.6. In the second case, the horizontal y-axis uses the angle  $x'$  as this better visualizes the immediate geometric effects of chromaticity for a thin quadrupole. In both cases the quadrupole is horizontally focusing.



**Figure 2.5:** Subfigures a) and b) show the phase space evolution of particles in  $x - p_x$  and  $y - p_y$  for a thin, horizontally focusing, quadrupole. In the vertical plane the particles are defocused.



**Figure 2.6:** Horizontal phase space evolution for a thin, horizontally focusing quadrupole, where particles are initially spread out in  $x$  and in  $\delta$ . The use of  $x'$  for the y-axis is to make clear the immediate geometric effects of energy deviations of the particles.

#### 2.5.4 Sextupole

**Sextupoles** provide a way to control chromaticity [35, p. 4]. They perform quadrupole-like focusing, where the effective "quadrupole strength" depends on the particle's distance from the center. This quadrupole component strength is scaled by the dispersion function and the energy deviation. When placed in regions with dispersion (typically generated by bending magnets), the sextupoles introduce a form of "controlled chromaticity" that may counter quadrupole-generated chromaticity [35, p. 5]. Its Hamiltonian and transfer map is shown in Appendix B.0.4.

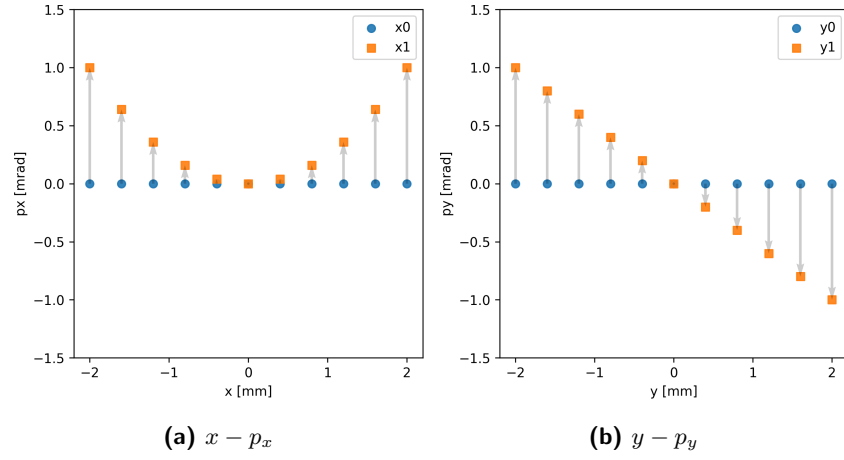
While providing a way to suppress chromaticity, sextupoles may themselves introduce unwanted higher-order effects. In Eq. (B.19), the non-linear terms introduce geometric aberration. The non-linear nature of sextupoles is shown in Fig. 2.7a. Its quadrupole-like focusing is shown in Fig. 2.7b. The fields in a sextupole are shown in Fig. 2.2c and the force directions for a positively charged particle traveling towards the paper in Fig. 2.2f.

#### 2.5.5 RF-cavity

**RF-cavities** (radiofrequency cavities) provide a way to manipulate the energies of particles at higher field strengths compared to what is feasible for conventional DC accelerators [38]. Typically, these provide sinusoidally time-varying longitudinal electric fields along the beam trajectory. An example Hamiltonian and transfer map is given in Appendix C.

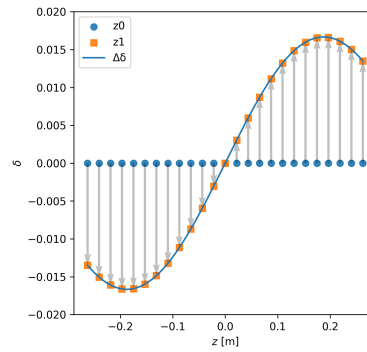
Figure 2.8 shows the energy gain as a function of relative longitudinal position a particle traveling through an RF-cavity will receive. Note that the phase of



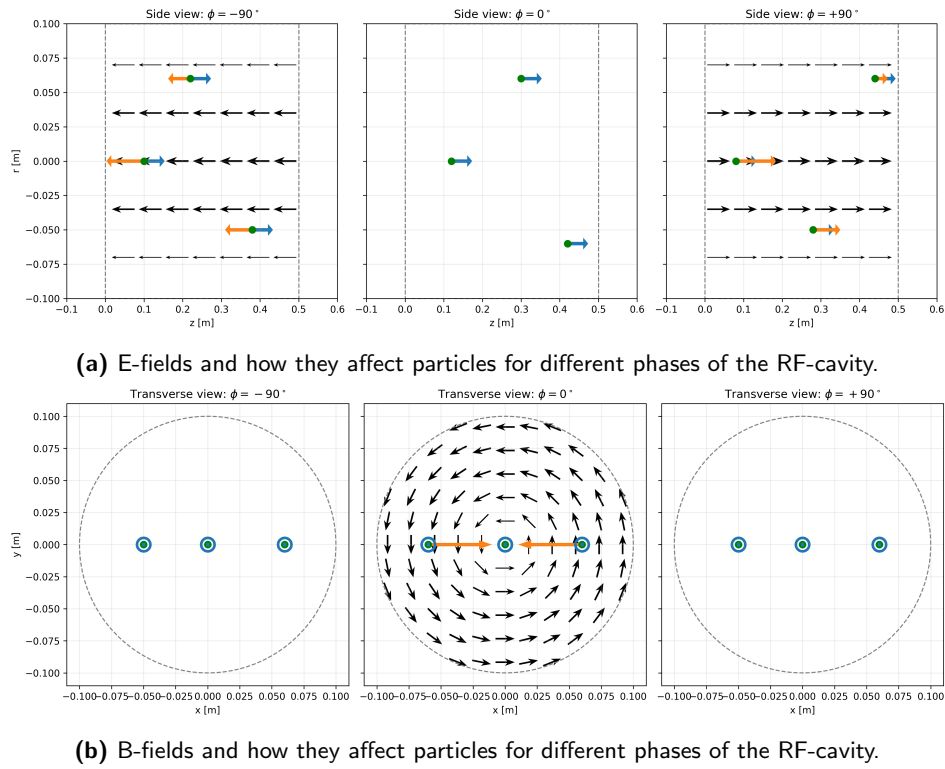


**Figure 2.7:** Subfigures a) and b) show two separate phase space evolutions of particles in  $x - p_x$  and  $y - p_y$  for a thin sextupole. In a), there is no vertical offset. In b), there is a constant horizontal offset of 1 mm in  $x$ , showing the quadrupole-like focusing in  $y$  (cf. Eq. (B.19)).

the cavity is chosen such that the synchronous particle at  $z=0$  receives no energy, meaning this RF-cavity is used for longitudinal focusing only, no net acceleration of the bunch will occur. In Fig. 2.9 The fields in an TM010 RF-pillbox cavity (see Appendix C) are shown.



**Figure 2.8:** Particles at different longitudinal positions (*i.e.* different arrival phases) in a thick RF-cavity. Bunches should ideally not be as spread out as what is shown in the picture.



**Figure 2.9:** Fields of an TM010 pillbox cavity for different phases.

Particles are shown in green, velocity in blue and forces in orange.

## 2.6 Transverse Beam dynamics

### 2.6.1 Transverse motion in a periodic lattice

If the paraxial approximation is performed directly on the Hamiltonian Eq. (A.1), the equations of motion in a periodic lattice (such as a ring) for the transverse degrees of freedom can be derived as [39, pp. 13–29]:

$$u'' + [k_u(s) + \Delta k_u(s)]u = \frac{\delta}{\rho} \quad (2.7)$$

where:

$$k_u = \begin{cases} \frac{1}{\rho^2} \mp k(s), & \text{if } u = x, \\ \pm k(s), & \text{if } u = y, \rho \rightarrow \infty \end{cases} \quad (2.8)$$

and:

$$\Delta k_u = \begin{cases} \left[ -\frac{2}{\rho^2} \pm k(s) \right] \delta, & \text{if } u = x, \\ [\mp k(s)] \delta, & \text{if } u = y \end{cases} \quad (2.9)$$

$\Delta k_u(s)$  is the chromatic perturbation term, and can be set to 0 for a linear approximation. This linear approximation is known as **Hill's equation**.

Begin by assuming no bending magnets, *i.e.*  $\rho \rightarrow \infty$  and therefore neither weak focusing nor dispersion, and focus on the case for  $x$ . Eq. (2.7) then becomes:

$$x'' + k(s)x = 0 \quad (2.10)$$

With  $k(s)$  as a non-constant restoring force, with a periodicity condition  $k(s+L) = k(s)$  ( $L$  being the **lattice period**), the general solution for a particle can be written as [40, pp. 41–43]:

$$\begin{cases} x(s) = \sqrt{\beta_x(s)J_x} \cos(\mu_x(s) + \mu_{x,0}), \\ x'(s) = -\frac{\sqrt{J_x}}{\sqrt{\beta_x(s)}} \left\{ \alpha_x(s) \cos(\mu_x(s) + \mu_{x,0}) + \sin(\mu_x(s) + \mu_{x,0}) \right\} \end{cases} \quad (2.11)$$

With the approximation that  $p_x \approx x'$  (an approximation correct for small angles relative to the reference particle, see Section 2.3). Eq. (2.10) gives [30, p. 149][40, p. 43]:

$$\begin{cases} \cos(\mu(s) + \mu_0) = \frac{x(s)}{\sqrt{J_x} \sqrt{\beta_x(s)}}, \\ \alpha_x = -\frac{1}{2} \beta'_x(s) \\ \gamma_x(s) = \frac{1 + \alpha_x(s)^2}{\beta_x(s)} \end{cases} \quad (2.12)$$

Inserting the equations in Eq. (2.12) into Eq. (2.11) gives:

$$J_x = \gamma_x x(s)^2 + 2\alpha_x(s) x(s) x'(s) + \beta_x(s) x'(s)^2 \quad (2.13)$$

The second equation in Eq. (2.12) can equivalently be expressed with  $p_x$  on the LHS. Here the approximation has simply been used for the sake of conciseness. The Courant-Snyder parameters fulfill the following condition [30, p. 146]:

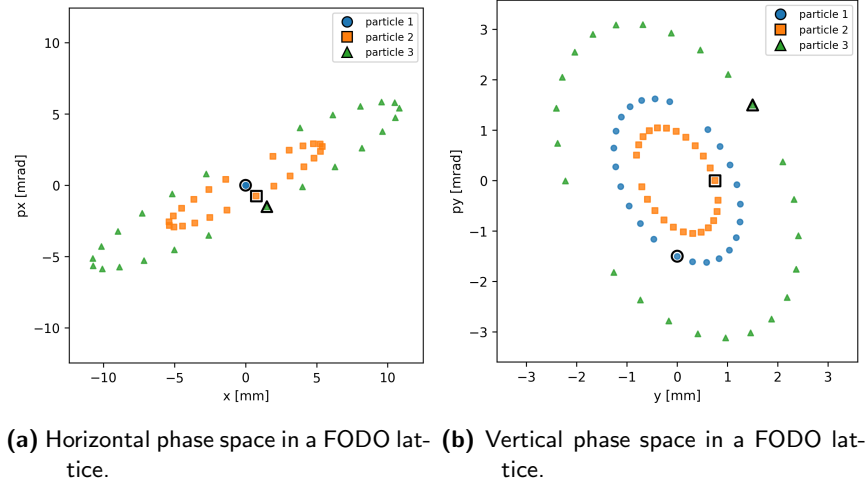
$$\beta_x \gamma_x - \alpha_x^2 = 1 \quad (2.14)$$

$J_x$  is a constant known as the **Courant-Snyder invariant** or **Action**.  $\alpha_x$ ,  $\beta_x$  and  $\gamma_x$  are together referred to as the (horizontal) **Courant-Snyder parameters** or **Twiss parameters**.  $\beta_x$  is called the **betatron function** or just **beta function** [30, pp. 133–134]. This function describes the local amplitude of the betatron oscillations, who will be periodic in a periodic lattice with a stable beam [30, pp. 137–138]. As can be seen from Eq. (2.10), a big value for beta implies bigger magnitude for  $x$  while smaller for  $x'$  and vice versa. The number of betatron oscillations performed by a particle over one turn is called the **tune**, and is defined as [40, p. 42]:

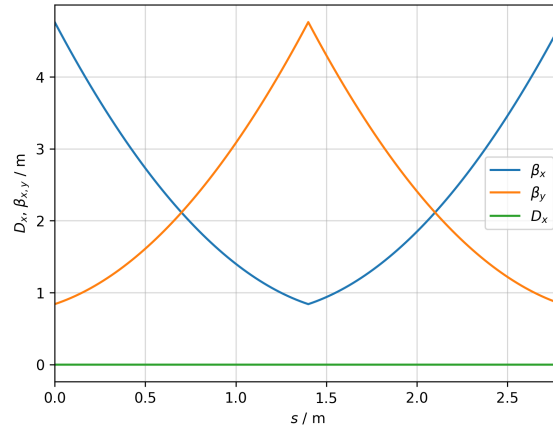
$$Q_x = \frac{1}{2\pi} \oint \frac{ds}{\beta_x(s)} \quad (2.15)$$

In a periodic beam line, a particle will move around what is called the **phase space ellipse** (see Eq. (2.13)), with an area of  $2\pi J_x$  [30, pp. 137–138]. The horizontal and vertical phase space ellipses is visualized for a single particle in a FODO lattice with no bending magnets over several turns in Fig. 2.10. The betatron and horizontal dispersion function (where the latter is 0 due to the lack of bends) for the lattice is shown in Fig. 2.11. A FODO cell consists of a focusing quadrupole (F), a drift (O), a defocusing quadrupole (D) and then another drift (O) [30, p. 128]. This is from the perspective of the horizontal transverse plane as the order of focusing and defocusing would be reversed for the vertical transverse plane.

In a realistic beam, the particles will not have exactly the same momenta and position, and therefore there is need to analyze the beam statistically. The **emittance** of a bunch may be defined as the average of the particle actions, or equivalently



**Figure 2.10:** Phase space evolution for three particles over several turns in a FODO lattice. The particles have different initial phase space coordinates (marked with black outline) to each other and depending on plane, which shows how the phase space ellipse may, for example, be small in  $x$  but big in  $y$ .



**Figure 2.11:** Betatron and horizontal dispersion function for a FODO cell with thin quadrupoles. There is no dispersion present.

as a measure of the phase-space area occupied by the bunch. The horizontal root-mean-squared (RMS) emittance is defined as, assuming no coupling between horizontal and/or longitudinal planes [30, pp. 151–152]:

$$\epsilon_x = \langle J_x \rangle = \sqrt{\langle x^2 \rangle \langle p_x^2 \rangle - \langle xp_x \rangle^2} \quad (2.16)$$

where the brackets  $\langle \cdot \rangle$  indicate the mean for all particles in a bunch. The transverse unit for emittance is expressed in length·radians, sometimes multiplied with  $\pi$  and sometimes simply expressed as a length [41, p. 13]. As the action is proportional to the area of the phase space ellipse spanned by a single particle, the emittance is proportional to the area spanned by multiple particles in phase space. The emittance in y and z is defined analogously to the x definition [30, p. 152].

Some useful relationships between phase space coordinates, the Courant-Snyder parameters and the emittance are as follows, assuming no coupling between the planes [30, p. 151]:

$$\begin{cases} \langle x^2 \rangle = \beta_x \epsilon_x \\ \langle p_x^2 \rangle = \gamma_x \epsilon_x \\ \langle xp_x \rangle = -\alpha_x \epsilon_x \end{cases} \quad (2.17)$$

In other words, the emittance and Courant-Snyder parameters are related to the mean square distribution of the particles, the mean square distribution for the momentum spread and the covariance between the spatial and the momentum spread.

## 2.6.2 Coupled periodic dynamics

### Dispersion

Eq. (2.10) is perfect in the case of no energy spread between the particles – an idealized scenario. In reality, particles will have slightly varying energies and therefore beam rigidities. For dipoles, the implication is that the particles in a bunch will be bent in varying degrees of magnitude while traversing them, which has already been mentioned in Section 2.5.2. This dependence is made clear by the  $x-z$  coupling in Eq. (B.10), is visualized for a single dipole in Fig. 2.4, and is a phenomenon known as **dispersion**. To understand the implications of dispersion, we will once again look at Eq. (2.7), but now replace the energy deviation with momentum deviation ( $\delta = \frac{p-p_0}{p_0} = \frac{\Delta p}{p_0}$ ) and focus on the case of  $u = x$  [34, p. 124]:

$$x'' + x\left(\frac{1}{\rho^2} - k(s) + \Delta k(s)\right)x = \frac{\Delta p}{p_0} \frac{1}{\rho} \quad (2.18)$$

The once homogeneous equation becomes an inhomogeneous:

$$x(s) = x_h(s) + x_i(s) \quad (2.19)$$

The **dispersion** is defined as follows:

$$D(s) := \frac{x_i(s)}{\Delta p/p_0} \quad (2.20)$$

In essence, dispersion affects the amplitude of the transverse oscillations. For a single particle, dispersion can be interpreted as an "additional orbit", which can be inferred from Eq. (2.19). For a periodic lattice we will therefore not only have a periodic, oscillating betatron function but furthermore also a periodic, oscillating dispersion function. The trajectory, with dispersion included, may be expressed as follows, for the horizontal plane [34, p. 129]:

$$\begin{pmatrix} x(s) \\ x'(s) \\ p/p_0 \end{pmatrix} = \begin{pmatrix} C(s) & S(s) & D(s) \\ C'(s) & S'(s) & D'(s) \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x(s_0) \\ x'(s_0) \\ p/p_0 \end{pmatrix} \quad (2.21)$$

Here,  $C(s)$  and  $S(s)$  are identical to the focusing horizontal elements of the dipole matrix (Eq. (B.10)) and the quadrupolar matrix (Eq. (B.14)). In Eq. (B.10), the dispersion function is divided up into  $m_{\text{dipole}}$ , a consequence of the choice of reference trajectory, and in the matrix elements  $R_{16}^{\text{dipole}}$  and  $R_{26}^{\text{dipole}}$ . As for Eq. (B.14), this needs to be modified to include dispersion, which is simply achieved by setting  $R_{16}^{\text{quad}} = D(s)$  and  $R_{26}^{\text{quad}} = D'(s)$  respectively. For a specific element, the dispersion can be calculated as follows [34, p. 125]:

$$D(s) = S(s) \cdot \int \frac{1}{\rho(\tilde{s})} C(\tilde{s}) d\tilde{s} - C(s) \cdot \int \frac{1}{\rho(\tilde{s})} S(\tilde{s}) d\tilde{s}$$

where integration is conducted over the length of the element.

While  $D(s)$  and  $D'(s)$  are general solutions, the periodic dispersion is sometimes denoted specifically as  $\eta$  and  $\eta'$  [34, p. 129]:

$$\begin{pmatrix} \eta \\ \eta' \\ 1 \end{pmatrix} = \begin{pmatrix} C & S & D \\ C' & S' & D' \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \eta \\ \eta' \\ 1 \end{pmatrix}$$

With knowledge of the emittance, the betatron function and the dispersion for a point in the lattice, the mean square beam size may be calculated as follows [30, p. 189]:

$$\langle x^2 \rangle = \beta_x \varepsilon_x + \eta_x^2 \langle \delta^2 \rangle$$

Compared to Eq. (2.17), the introduction of this transverse-longitudinal coupling leads to a direct increase in beam size. For Gaussian distributions the standard deviation is often used to express the beam size ( $\sigma_\delta$  being the rms energy spread):

$$\sigma_x = \sqrt{\beta_x \varepsilon_x + \eta_x^2 \sigma_\delta^2}$$

The change in a periodic trajectory for  $x$  and  $p_x$  as a result of dispersion can be expressed in first order, based on Eq. (2.21), as follows [30, p. 160]:

$$\begin{cases} x(\delta) = x_\beta + \eta_x \delta, \\ p_x(\delta) = p_{x,\beta} + \eta_{p_x} \delta. \end{cases} \quad (2.22)$$

where  $x_\beta$  and  $p_{x,\beta}$  represent  $x$  and  $p_x$  values with no dispersion present, while  $\eta_{p_x}$  is equivalent to  $\eta'$ . Further,  $\delta$  here represents the momentum deviation  $p/p_0$ .

### Chromaticity

The concept of **chromaticity** has already been introduced in sections 2.5.3 and 2.5.4; it describes the different degrees of focusing on particles with different energies, and is generally something we try to counteract with the use of sextupoles. The chromaticity can, in linear approximation, be expressed as follows [34, p. 140] [35, p. 1]:

$$Q' = \frac{dQ}{d\delta} \quad (2.23)$$

The **relative chromaticity** chromaticity can be expressed as follows:

$$\xi = \frac{Q'}{Q} \quad (2.24)$$

Chromaticity causes a **tune shift** for a single particle, *i.e.* a deviation from the ideal tune. For multiple particles with varying momentum deviations, chromaticity gives rise to **tune spread**, *i.e.* the particles have slightly varying tunes. This imposes challenges in the design of accelerators, further discussed in Section 2.9.

The tune shift for a single particle caused by chromaticity can be mathematically expressed as follows:

$$\Delta Q = Q' \frac{\Delta p}{p_0} \quad (2.25)$$



When momentum deviations are significant in a bunch, non-linear terms will also have to be taken into account for the chromaticity [30, p. 140]. For a lattice, the so-called **natural chromaticity** can be expressed as follows [34, p. 141]:

$$Q' = -\frac{1}{4\pi} \int k_q(s) \beta(s) ds \quad (2.26)$$

where  $k_q$  ( $= k_1$  in Eq. (2.6)) describes the quadrupole strength along the specified path. Provided net focusing, the natural chromaticity is always negative, and to compensate for this, some form of "artificial" chromaticity needs to be introduced - enter the sextupoles. With sextupoles, chromaticity in a lattice can be calculated as follows [34, p. 145]:

$$\begin{cases} Q'_x = -\frac{1}{4\pi} \oint \beta_x(s) [ +k_q(s) - m^F \cdot l_{\text{sext}} D_x(s) + m^D \cdot l_{\text{sext}} D_x(s) ] ds \\ Q'_y = -\frac{1}{4\pi} \oint \beta_y(s) [ -k_q(s) + m^F \cdot l_{\text{sext}} D_x(s) - m^D \cdot l_{\text{sext}} D_x(s) ] ds \end{cases} \quad (2.27)$$

where  $m^F$  is the focusing strength for sextupoles placed around focusing quadrupoles (for a specific plane), and  $m^D$  is the focusing strength for sextupoles placed around defocusing ones.

These equations show that without dispersion, sextupoles do not correct the chromaticity. Further, just as quadrupoles only focus in one plane each, sextupoles can similarly only "improve" the chromaticity in one plane. For both quadrupoles and sextupoles, this implies that these elements should be placed at great  $\beta_x$  ( $\beta_y$ )-values when the effect is "positive" for the horizontal (vertical) plane, and at low  $\beta_x$  ( $\beta_y$ )-values when the effect is "detrimental" for the horizontal (vertical) plane so as to have a net improvement.

The dependence on momentum deviation for sextupoles may be described as follows:

$$\Delta k_1 = \eta_x k_2 \frac{\Delta P_0}{P_0} \quad (2.28)$$

where  $k_1$  represents the equivalent "quadrupole" component strength and  $k_2$  is the sextupole strength. In other words, the effect for sextupoles will further depend on the sign of the momentum deviation of the particles.

### Transition energy

The **revolution frequency** is defined as  $f_{rev} = \frac{\beta_{\text{ref}} c}{C}$  where  $C$  is the circumference of the circular accelerator [29, p. 12]. In a ring, the revolution frequency will change with the particle energy both as a result of the speed change and as a result of the dispersion. The change in speed will dominate for lower energies but as the

particles approach the speed of light, the change in speed is closer and closer to zero. However, the length of the particles' trajectories will be increased as a result of the greater beam rigidity. The threshold energy where both effects are equal is called the **transition energy**. If a lattice operates below this energy, it is said to operate **below transition** [30, p. 166]. Otherwise it is said to operate **above transition**. Below transition, revolution frequency increases with energy as the speed increase will dominate; above transition it is the other way around. [30, p. 163] At transition, revolution frequency becomes independent of energy deviation, which is usually not desired [42]. When this happens, the ring is said to operate **isochronously**. The relative change in orbit length with respect to momentum deviation is described by the **momentum compaction factor** [42, p. 11]:

$$\alpha_p = \frac{\Delta L/L}{\Delta p/p} \quad (2.29)$$

The relative change in revolution frequency can similarly be described by the **phase slip factor**:

$$\eta_p = \frac{\Delta f_r/f_r}{\Delta p/p} \quad (2.30)$$

These two terms have the following relation [30, p. 166]:

$$\eta_p = \alpha_p - \frac{1}{\gamma_{\text{ref}}^2} \quad (2.31)$$

Indirectly, this describes the relation between the dispersion function and the particle energy in the lattice. The transition energy is defined as:

$$\gamma_T = \frac{1}{\sqrt{\alpha_p}} \quad (2.32)$$

In other words, the transition energy is defined as when the phase slip factor is 0. A negative phase slip factor implies below transition energy and vice versa.

## 2.7 Longitudinal Beam dynamics

To describe longitudinal dynamics, a 1D Hamiltonian is often used which neglects transverse components. A 1D Hamiltonian can be derived using canonical transformations from Eq. (A.2). This is provided without derivation by Wolski [30, p. 172]:

$$H(z, \delta) = \frac{qV_{\text{rf}}}{\omega_{\text{rf}}P_0c_0} \left[ \sin \phi_s \frac{\omega_{\text{rf}}z}{c} - \cos \left( \phi_s - \frac{\omega_{\text{rf}}z}{c} \right) \right] - \frac{1}{2} \eta_p \delta^2. \quad (2.33)$$

where [30, p. 169]:

- $q$  is the electric charge of the particle
- $V_{RF}$  and  $\omega_{RF}$  are the RF-voltage and RF-phase respectively. The assumption has been made that these well represent all cavities in the lattice.
- $\phi_s$  is the **synchronous phase**, *i.e.* the phase which we want the reference particle, the **synchronous particle**, to arrive on [30, p. 170] [43, p. 168]).
- $E_0$  is the reference energy

This hamiltonian is built on the assumption that the change of energy per turn can be averaged over the ring circumference [30, p. 170]. The equations of motions from this Hamiltonian are expressed as [30, p. 173]:

$$\frac{dz}{ds} = -\eta_p \delta, \quad (2.34)$$

$$\frac{d\delta}{ds} = \frac{1}{cP_0C_0} \left[ qV_{RF} \sin \left( \phi_s - \frac{\omega_{RF}z}{c} \right) - U_0 \right]. \quad (2.35)$$

Here,  $U_0$  represents energy lost e.g. due to synchrotron radiation. As discussed in Section 2.1, this is significant for electrons while less so for protons. Taking the derivative the first equation and setting  $k_z^2 = -\frac{qV_{RF}}{cP_0} \frac{\omega_{RF}}{cC_0} \eta_p \cos \phi_s$  gives [30, p. 170]:

$$\frac{d^2z}{ds^2} = -k_z^2 z \quad (2.36)$$

Here, it has been assumed that the synchrotron motion is small compared with the revolution period, and furthermore that the longitudinal oscillation amplitude is small compared with the RF-wavelength [30, p. 171]. Eq. (2.36) shows that  $k_z^2$  will need to be greater than 0 for a non-synchronous particle to perform stable oscillations [30, p. 170]. The longitudinal oscillations (similar to betatron oscillations for the transverse case) are called **synchrotron oscillations**. The number of synchrotron oscillations performed is denoted as the **synchrotron tune**:

$$\nu_s = \frac{k_z C_0}{2\pi} = \frac{1}{2\pi} \sqrt{-\frac{qV_{RF}}{cP_0} \frac{\omega_{RF}C_0}{c} \eta_p \cos \phi_s} \quad (2.37)$$

If the synchrotron tune is small, the longitudinal beta function ( $\beta_z$ ) when averaged over a bunch in a storage ring can be expressed as [30, p. 175]:

$$\beta_z = \sqrt{\frac{\langle z^2 \rangle}{\langle \delta^2 \rangle}} = \frac{\sigma_z}{\sigma_\delta} = \frac{C_0}{2\pi} \frac{|\eta_p|}{\nu_z}. \quad (2.38)$$

Values of the synchronous phase that enable stable operation will differ depending on whether the ring operates above or below transition, and further on the sign of the momentum compaction factor. Assuming a positive momentum compaction factor (*i.e.*, greater dispersion implies a lengthening of the orbit for a certain momentum deviation), the synchronous phase must satisfy:

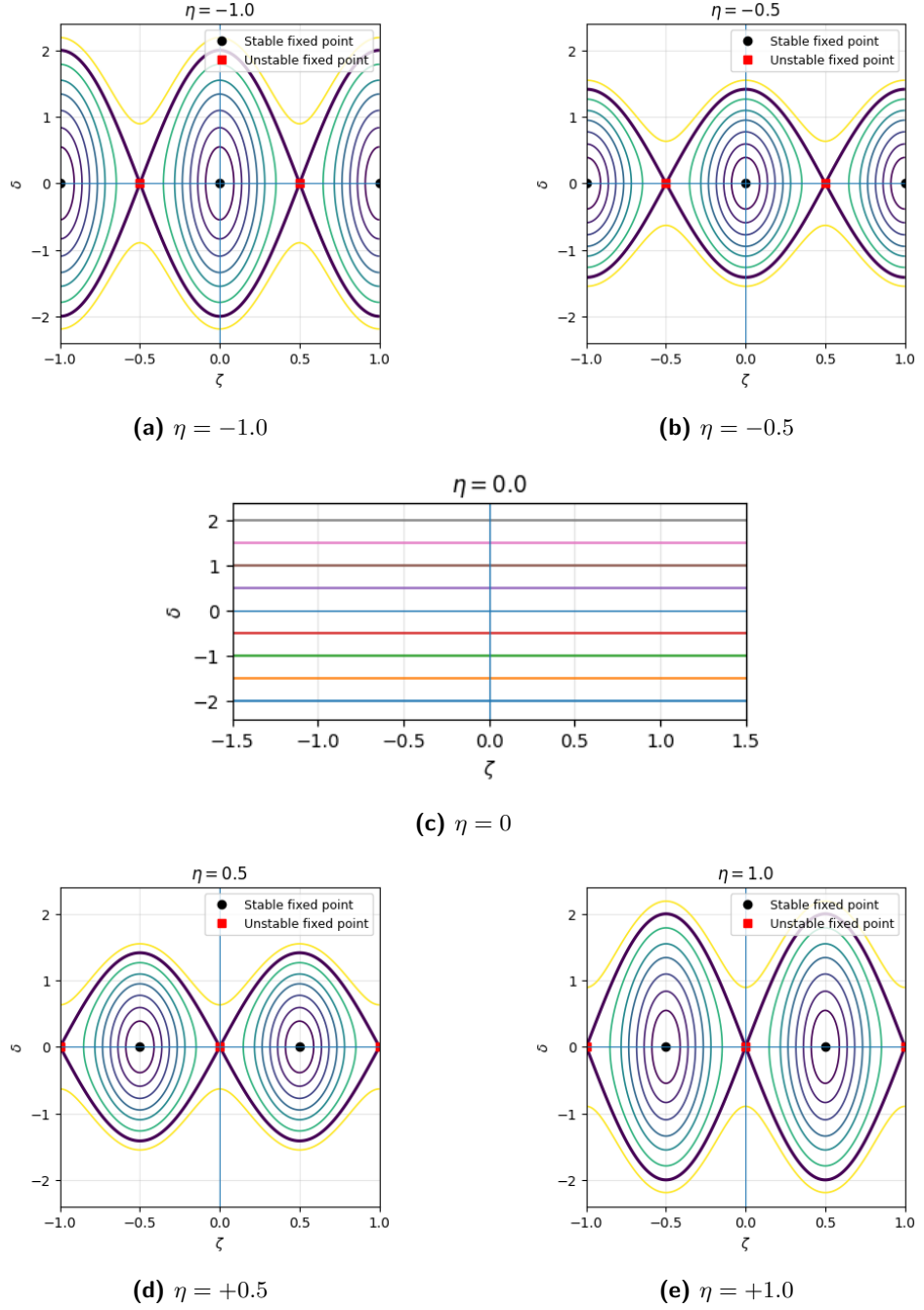
$$\begin{cases} 0 < \phi_s < \frac{\pi}{2}, & \eta_p < 0 \\ \frac{\pi}{2} < \phi_s < \pi, & \eta_p > 0 \end{cases} \quad (2.39)$$

This is known as **phase stability**: a non-synchronous particle will only oscillate around the synchronous particle if this condition is fulfilled [43, p. 210]. The previously mentioned assumption with respect to small synchrotron amplitudes cannot always be assumed [30, p. 171]. At large amplitudes, the synchrotron oscillations will become unstable. The **energy acceptance**, where the oscillations will be stable, is described by the Hamiltonian (2.33). Particles oscillating longitudinally will follow constant contours of this Hamiltonian in longitudinal phase space [30, pp. 172–173]. A **stable fixed point** is a point where the Hamiltonian contour is point like. Any particle arriving at this point will not perform longitudinal oscillations. An **unstable fixed point** is a point where contour lines cross. The contour lines that cross unstable fixed points are known as **separatrices**. The region enclosed by a separatrix where phase stability is fulfilled is known as an **RF-bucket** or simply **bucket**. Separatrices, unstable/ stable fixed points as well as buckets are shown in the case of no net acceleration in Fig. 2.12. Outside of the separatrices, a particle successively gains or loses energy each time it passes the cavity until the particle is lost from the ring. The sinusoidal RF-curve already shown in Fig. 2.8 is plotted once again in Fig. 2.13 above a corresponding separatrix plot in phase space. In this figure, it is clear that the region of phase stability shifts at transition crossing. The **RF-acceptance** is the maximum energy deviation within an RF-bucket. The **harmonic number** is the number of RF-buckets in a ring and is therefore also the maximum amount of bunches that may be present at one time. It is defined as  $h = f_{rf}/f_{rev}$ .

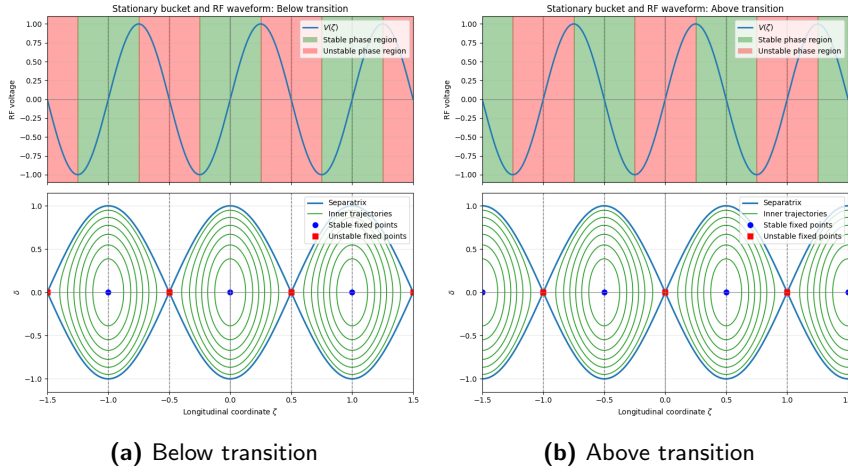
## 2.8 Compressors

In some applications, a high intensity beam is required [30, p. 265]. High intensity beams may be sensitive to collective effects, as discussed in Section 2.10.1. A common solution is therefore to generate, or accumulate, bunches with a large longitudinal spread, so that the required beam intensity and other properties of the beam may be established while keeping the peak current moderate. The required peak current may thereafter be achieved by shortening the bunch in a **compressor**.

One example of a compressor consists of an RF-cavity followed by a so-called chicane (a certain series of dipole magnets) [30, pp. 266–28]. The RF-cavity introduces a correlation between particle coordinates and momentum deviation. This



**Figure 2.12:** Example longitudinal phase space shown for several values of  $\eta$ , below, at and above transition. Stable fixed points are marked as black dots. Unstable fixed points are marked as red squares. Separatrices enclose buckets. Other contours highlight by shade their oscillation amplitude. Above transition we have kept the reference  $\zeta$  from below transition to highlight the  $\pi/2$ -difference in stable phase. These figures further show a special case of  $0$  ( $\pi$ ) synchronous phase, *i.e.* no net acceleration, implying symmetric separatrices.



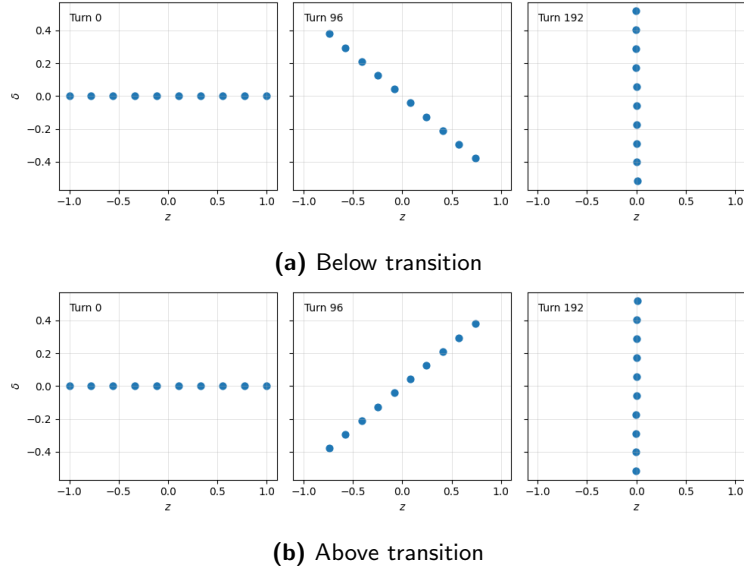
**Figure 2.13:** Comparison of the RF-voltage with the buckets, below and above transition. Longitudinally focusing areas are marked in green, while defocusing areas are marked in red. This region of stability shifts by  $\pi/2$  when crossing transition. To make this point clear, the reference position is not changed in between the two subfigures.

is then exploited by the dispersion introduced by the dipole magnets, and particles will follow different trajectories depending on momentum deviation. In this manner, longitudinal phase space may be rotated provided suitable design choices.

Another way to achieve compression is to employ a synchrotron and a suitably configured RF system [44] [45]. Essentially, no acceleration is provided to the synchronous particle while particles with larger longitudinal deviations will experience a greater accelerating gradient, something which for a single cavity is shown in Fig. 2.8. Either through the speed below transition, or through the path length above transition, the particles will focus longitudinally over several turns while simultaneously defocusing in the energy spread. An example is given in Fig. 2.14: Assuming a large spread in  $z$  and a small spread in  $\delta$ , the bunch will compress in space while increasing its energy spread.

## 2.9 Resonances

As has been seen, both the transverse and longitudinal dynamics can in a sense be described as harmonic oscillators. Periodic perturbation of a harmonic oscillator will result in resonances, and in the case of beam dynamics, resonances may lead to beam instabilities [29, p. 539]. **Linear resonances** may be caused by field errors in e.g. dipoles or quadrupoles. Higher order resonances are caused by sextupoles and higher order magnets, even if these magnets were perfect as they are nonlinear by nature [29, pp. 539–540]. For a single plane, the resonance condition is expressed



**Figure 2.14:** Idealized visualization of compression in a synchrotron over 192 turns, below and above transition. These visualizations assume a positive phase slip factor; if it were negative the cases would be reversed.

by [29, p. 543]:

$$|m| = (|l| \pm 1) \nu_0 \quad (2.40)$$

where  $|l| \leq n - 1$ , and  $m, n, l \in \mathbb{Z}$  [29, pp. 541, 543]. Here,  $|l| + 1$  is the order of the resonance [30, p. 543].  $l = 0$  implies an integer resonance which may for example be caused by dipole errors with  $n = 1$  [29, p. 541]. Quadrupole errors may cause  $n = 2$  which results in both half integer and integer resonances.  $n = 3$  is driven e.g. by sextupole fields [29, p. 542]. Eq. (2.40) can be further generalized into a ring with  $N$  superperiods:

$$|j|N = (|l| \pm 1) \nu_0 \quad (2.41)$$

where  $j \in \mathbb{Z}$ .

Expanding Eq. (2.40) into two planes gives:

$$m + k\nu_{0x} + l\nu_{0y} = \nu_x \quad (2.42)$$

with:

$$|k|+|l|+1 \leq n \quad (2.43)$$

Written in a more symmetric way, the resonance conditions may be written as, again with  $m = jN$ :

$$k\nu_{0x} + l\nu_{0y} = jN \quad (2.44)$$

The order of the resonance is then  $|k|+|l|$ . Only  $x - y$  coupling is considered in Eq. (2.42) which is in many cases sufficient [30, p. 361]. Still, synchro-betatron resonances do exist and can be expressed as:

$$k\nu_{0x} + l\nu_{0y} + m\nu_{0z} = jN \quad (2.45)$$

In choosing the working point of a lattice, resonances must be considered. In this process, low-order resonances should generally be avoided to a greater extent compared with higher-order resonances as the low-order resonances typically have larger stop bands and stronger driving terms [30, pp. 362–363] [29, pp. 555–556]. A useful tool in the choosing of a lattice working point is the so-called **resonance diagram** or **tune grid** where resonances up to a certain order are plotted [30, pp. 363–364]. An example is shown in Fig. 2.15. These diagrams only show the presence of resonances and analysis of what effects different resonances may yield will still be needed. Further, **tune shift** and **tune spread** will need to be taken into account. The tune shift is a particle's deviation from the design tune and the tune spread is the spread of tunes for an ensemble of particles. A tune shift arises from linear focusing errors, e.g. quadrupole errors. This can be expressed as [34, pp. 139–142]:

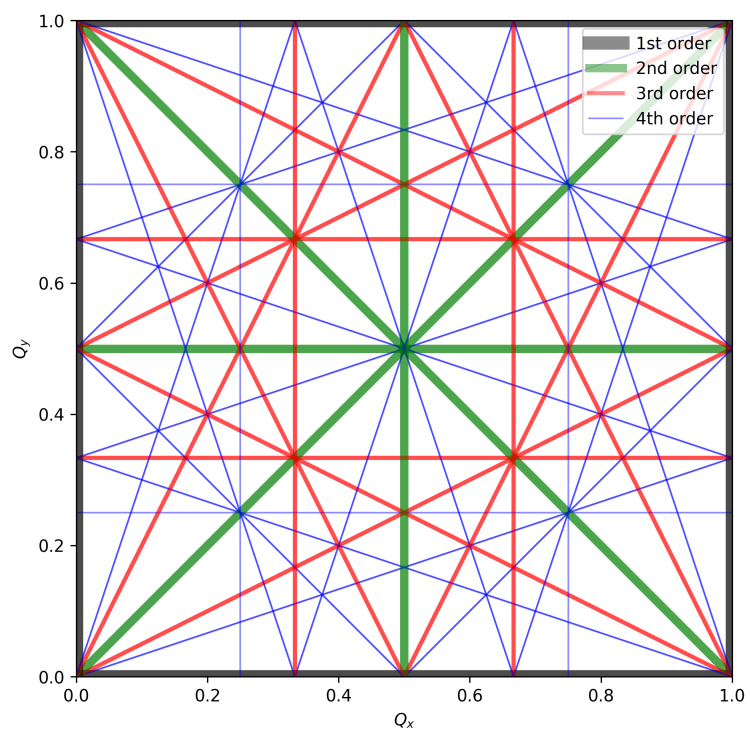
$$\Delta Q = \int_{s_0}^{s_0+l_q} \frac{\Delta k(s)\beta(s)}{4\pi} ds \quad (2.46)$$

where  $\Delta k(s)$  is the gradient error and  $l_q$  is the length of the quadrupole. As already mentioned in the section about chromaticity (section 2.6.2), variations in particle energy will lead to different degrees of focusing. This is one of many possible causes to tune spread. Non-linear elements such as sextupoles further give rise to non-linear tune spread. Tune shift and tune spread may further arise from e.g. collective effects (see sections [46][47]). In other words, even if the machine tune is chosen to avoid low-order resonance lines, particles may still be caught in these resonance stop bands due to tune shift and tune spread.

### 2.9.1 Frequency Map Analysis

In non-linear systems, it may be advantageous to analyze the tunes of the individual particles [30, pp. 384–391]. Simulation results may be used to analyze tunes as a function of particle energy or initial conditions, for example. **Frequency Map**





**Figure 2.15:** A tune diagram where resonances first to fourth order resonances are shown.

**Analysis** (FMA), describes the study where the tunes of particles are determined over a specified number of turns, and may be used to identify resonance instabilities. The tune for particles may change over time, and in this case it can be advantageous to perform FMA over specific turn intervals to see how instabilities develop. FMA is described for a discrete Fourier transform in Appendix D. There, the **Numerical Analysis of the Fundamental Frequencies** (NAFF) method is described in greater detail. This procedure can be applied not only to determine the dominant frequency, but also to identify the secondary frequency components of a particle.

## 2.10 Collective effects

The effects arising from interactions between the particles of a beam are known as **collective effects** [30, p. 395]. Collective effects are characterized by their dependence on the charge density within a bunch. Collective effects can be divided into **coherent effects** that affect a bunch as a single entity, and **incoherent effects** where the effect varies for all particles in the bunch [48]. Coherent effects generally give rise to collective tune shifts, while incoherent effects generally give rise to tune spread. As all particles will move with their own betatron amplitude, phase, and tune, incoherent effects will affect these individual attributes, rather than the bunch attributes as a whole [49, p. 313]. Space-charge effects are briefly presented below.

### 2.10.1 Space-Charge

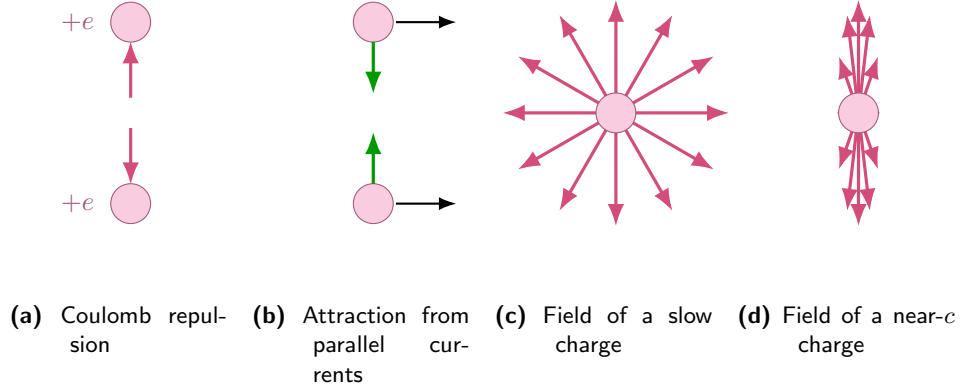
**Space-charge** comprises the effects created by self fields (**direct space-charge**) and, in the beam rest frame, electrostatic image fields induced by the surrounding vacuum chamber (**indirect space-charge**) [49, p. 311].

In beams where the transverse velocities are much smaller compared to the longitudinal velocity, the problem may be treated as electrostatic in the beam rest frame [50, p. 35]. With this assumption, the scalar potential satisfies the Poisson equation:

$$\Delta\phi = -\frac{\rho}{\varepsilon_0} \quad (2.47)$$

where  $\phi$  is the electrostatic potential,  $\rho$  the charge density and  $\varepsilon_0$  the electric permittivity in vacuum.

As bunches approach the speed of light, the field lines will approach perpendicularity with the particle, as shown in Figs. 2.16c and 2.16d, implying maximum strength for the transverse Coulomb forces. However, in the laboratory frame, the beam can be described by a current  $j = \rho\beta c$  that will generate a transverse magnetic field  $\mathbf{B}$ . These magnetic fields will result in Lorentz forces that at the speed of light negate the effects of the Coulomb forces [51, p. 338]. This is shown in Figs. 2.16a and 2.16b. Longitudinally, the contraction will cause the longitudinal



**Figure 2.16:** Illustration of electric and magnetic self-field effects for charges at different velocities.

electric field to decrease quadratically as the speed of light approaches. The fields may be described as follows:

$$\begin{cases} E_r(s=0) = \frac{q}{4\pi\epsilon_0} \frac{\gamma}{r^2} \\ B_\phi(s=0) = \frac{q\beta_{\text{ref}}}{4\pi\epsilon_0 c} \frac{\gamma}{r^2} \\ E_s(s=0) = \frac{q}{4\pi\epsilon_0} \frac{1}{\gamma^2 z^2} \end{cases} \quad (2.48)$$

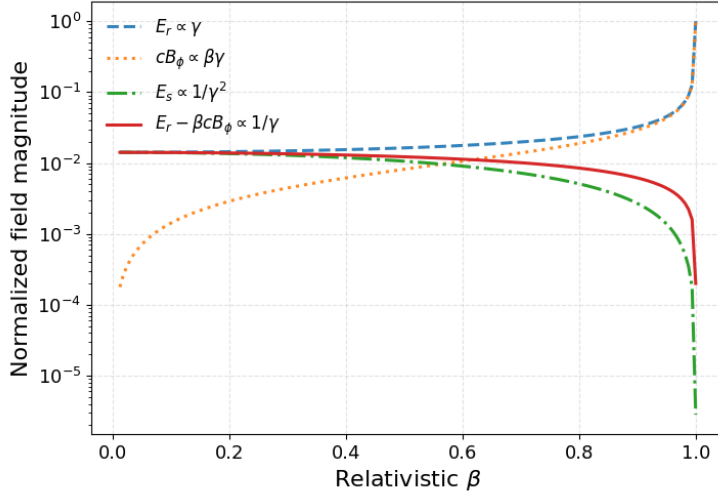
These fields, as well as the effective transverse field, are plotted in Fig. 2.17.

### Transverse space-charge

In transverse dynamics, direct space-charge acts like a defocusing quadrupole in both planes [52, p. 15]. This defocusing effect is proportional to the charge density, and will differ for particles at different transverse positions: for a test particle in the center of a uniform or Gaussian beam, the forces from the particles around it will cancel out, while the "non-symmetry" is more pronounced towards the outer edges of the beam. However, the derivative of the force with respect to transverse position is greatest at the core. By once again neglecting e.g. dispersion and looking at Hills equation, Eq. (2.10), the effect of space-charge can be introduced by adding a defocusing term:

$$x'' + (k(s) + k_x^{SC}(s))x = 0 \quad (2.49)$$

As Eq. (2.10) led to the eventual definition of the betatron function and subsequently of tune, it is perhaps not surprising that a tune shift and/or tune spread arises for the particles as a result. In fact, space-charge often causes a "tie"-like



**Figure 2.17:** The radial electric field, the azimuthal magnetic field, the longitudinal field as well as the effective electric field plotted for different relativistic beta.

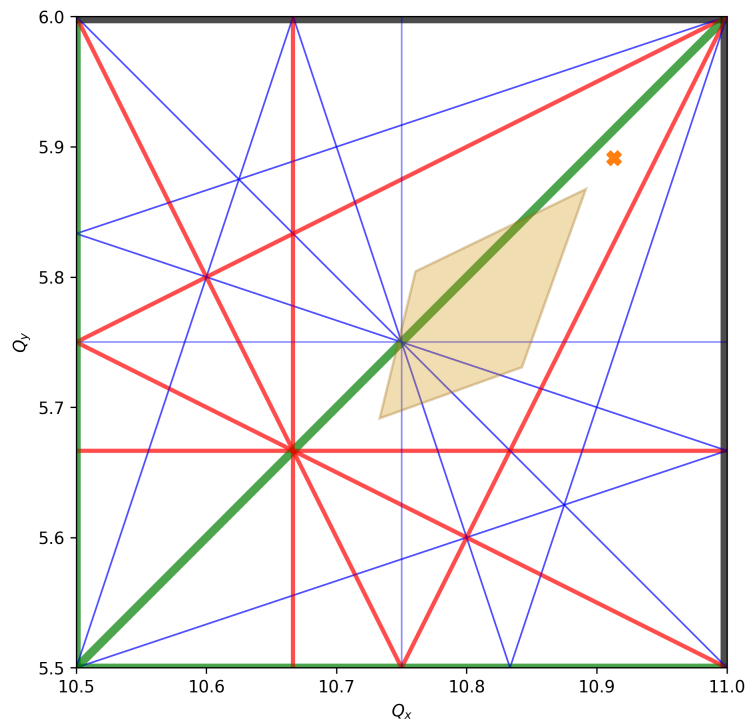
spread in tune space, where the tune spread can be loosely described as a tie shape angled below the bare tune of the machine [49, p. 18]. This is visualized in Fig. 2.18. It is important to understand that individual particles will not take a "static" place within this tune spread; they will continuously shift in tune space as a result of the space-charge, and may therefore cross the stop bands of low-order resonances multiple times. In other words, direct space-charge is often the cause of emittance blow-up and subsequently beam loss. Assuming a uniform transverse distribution, the incoherent tune shift for all particles can approximately be expressed as [51, p. 345]:

$$\Delta Q_x = -\frac{r_0 \rho_x^2 N_p}{a^2 l_0 \beta_{\text{ref}}^2 \gamma_{\text{ref}}^3 Q_x} \quad (2.50)$$

where  $r_0$  is the classical radius,  $\rho_x$  the machine radius,  $N_p$  the number of particles,  $l_0$  the bunch length,  $a$  the beam radius and  $Q_x$  the horizontal tune.

The effects of indirect space-charge will depend on the geometry and attributes of the surroundings. If a circular pipe is considered, and if the bunch studied can be approximated as a point charge at the beam center (*i.e.*, it is symmetric), then the transverse indirect space-charge forces will cancel. If a bunch is instead off-centered, the collective electric field for the bunch, as a result of the electrostatic image charges, can roughly be given for the horizontal plane as [51, p. 346]:

$$E_x^{im}(x) \approx \frac{\lambda_0}{2\pi\epsilon_0} \frac{1}{d-x} \quad (2.51)$$



**Figure 2.18:** The space-charge tune shift and tune spread visualized in a tune diagram as a shaded area below the working point of a lattice. As can be seen, several particles will have their tunes shifted towards the second order resonance.

where  $\lambda_0$  is the line charge,  $d$  is the distance from the image charge to the pipe center, and  $x$  is the distance from the real charge to the pipe center. If the approximation  $x \ll d$  holds, then the field may be approximated as:

$$E_x^{im}(x) \approx \frac{\lambda_0}{2\pi\epsilon_0} \frac{x}{b^2} \quad (2.52)$$

which will produce a linear coherent force. It should be noted that even if the beam is perfectly centered, the indirect space-charge will cause a coherent tune shift, which can be shown to be [51, p. 347]:

$$\Delta Q_x = -\frac{r_0 \rho_x^2 N_p}{b^2 l_0 \beta_{\text{ref}}^2 \gamma_{\text{ref}} Q_x} \quad (2.53)$$

Here,  $b$  is the radius of the pipe. The coherent tune shift is directly affected by the geometry of the pipe.

### Longitudinal space-charge

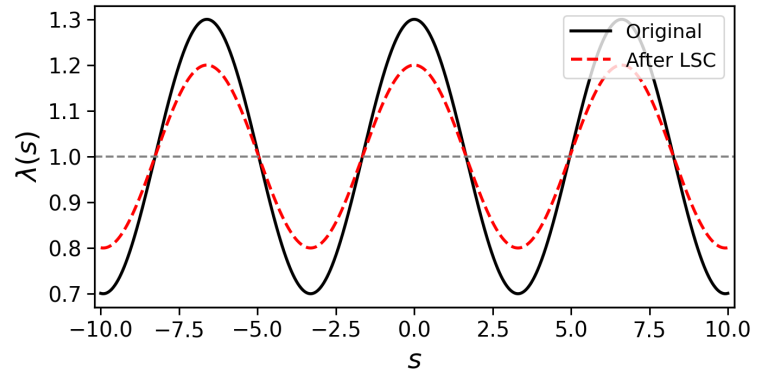
The collective electric field for longitudinal space-charge with uniform transverse density is given as [51, p. 14]:

$$E_z(r, z) = -\frac{1}{2\pi\epsilon_0\gamma^2} \left[ \int_r^a \frac{r'}{a^2} dr' + \int_a^b \frac{1}{r'} \right] \frac{\partial \lambda(z)}{\partial z} \quad (2.54)$$

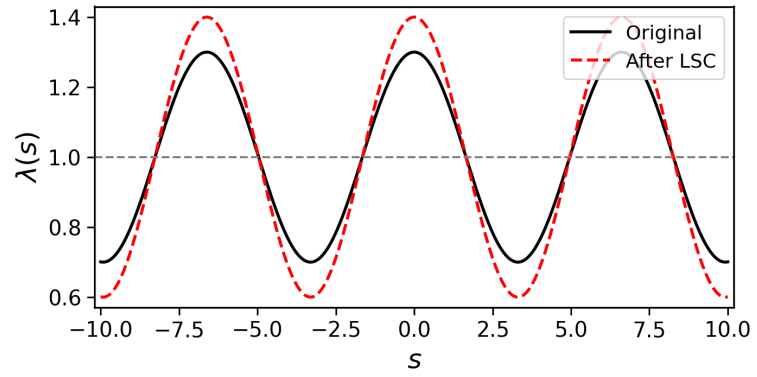
where  $a$  is the beam radius,  $b$  is the pipe radius,  $r$  is the radial position, and  $\lambda(z)$  is the longitudinal distribution. In contrast to the transverse space-charge, the longitudinal space-charge field, and therefore the force, is proportional to the derivative of the longitudinal distribution. For example, if the beam is longitudinally uniform and infinitely long, then  $\frac{\partial \lambda(z)}{\partial z} = 0$ . Longitudinal space-charge should in other words only begin affecting a bunch if it deviates from a uniform shape [53, p. 552]. For a longitudinally Gaussian bunch, the force would be negative in the tail and positive in the head. For an infinite sinusoidal bunch, the transition energy is important. Below transition, particles on positive slopes will have a longer revolution time due to their decreased energy, leading to these particles filling the "valleys" of the charge density, leading to a damping effect. Above transition, these same particles will instead have a shorter revolution time which in turn amplifies the modulation. This is known as negative mass instability [53, p. 552]. The two cases are visualized in Fig. 2.19.

### Space-charged induced resonances

The highly nonlinear nature of space-charge can give rise to higher-order resonances, and subsequently emittance growth, and can be significant in high intensity proton drivers [54]. If the phase advance of a cell or supercell reaches  $\pi/2$  (or the whole lattice having a fractional tune of  $1/2$ ), this will give rise to several fourth-order resonances (for example  $4\nu_{0x} = N$ ,  $4\nu_z = N$ ,  $2\nu_{0x} + 2\nu_{0z}$  etc).



(a) Charge density evolution below transition.



(b) Charge density evolution above transition.

**Figure 2.19:** Charge density evolution for an infinite sinusoidal bunch below and above transition.

In a similar sense, 6th-order resonances can arise from phase advances of  $\pi/3$  or fractional tune  $1/3$ , 8th-order resonances from  $\pi/4$  phase advance/fractional tune of  $1/4$  and so on. The reason for this is that space-charge for one may act as a coupling mechanism between the planes, and that space-charge may depress the betatron tunes, forcing the particles to cross dangerous resonance lines.

## 2.11 Simulating a system of interacting particles

### 2.11.1 Particle-in-Cell

The **Particle-in-Cell** (PIC) provides an efficient way of modelling space-charge. The method employs what is known as superparticles, also known as **macro-particles** [55, p. 8]. As long as the spatial wavelengths of the interparticle forces are long compared to the particle spacings, and if these spacings can be deemed as short compared to timescales for any "graininess" to appear, this description is accurate. Macro-particles represent average values, such as charge, of many particles, thereby significantly reducing the computational cost [56]. The Particle-in-Cell algorithm is given as follows [55, p. 21]:

```

1 for each time step:
2     Assign charge to mesh
3     Solve Poisson's equation on the mesh
4     Compute forces using the mesh-defined potential
5     Interpolate forces at particle positions

```

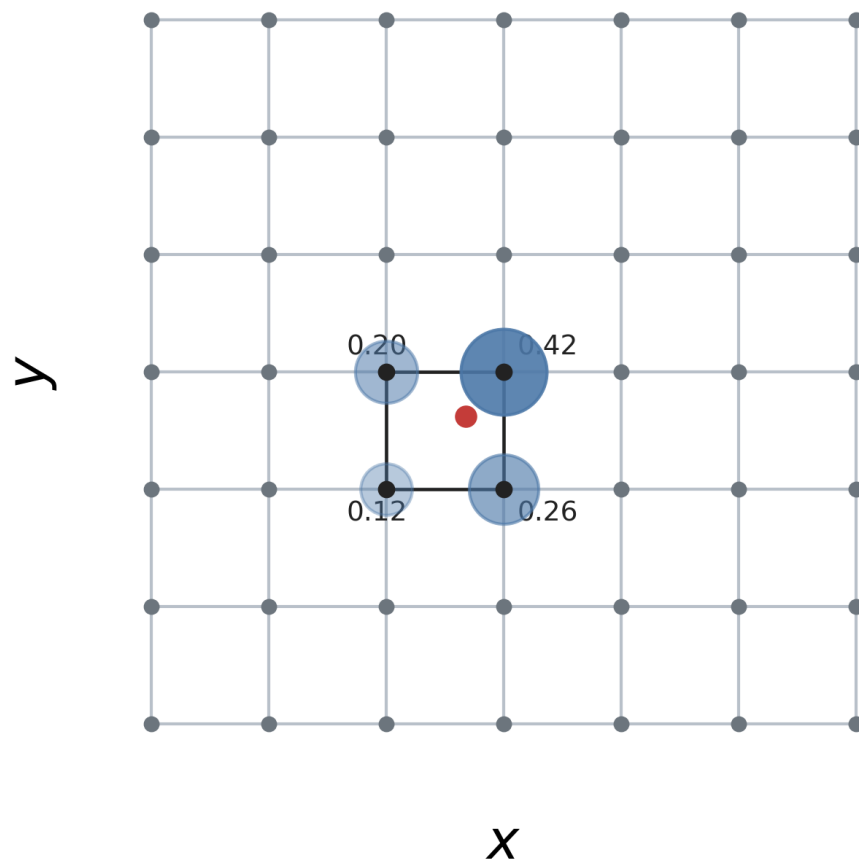
**Listing 2.1:** Pseudo code for the PIC algorithm as formalized by Hockney et al.

The **mesh** most often used in particle-in-cell codes is known as Eulerian, *i.e.* it does not move with what is modeled (in this case, the particles) [57]. The properties of a particle (*i.e.* charge) are calculated on discrete spatial points of this so-called **Eulerian grid** [56]. Henceforth, this will be simply referred to as the grid, or mesh. In one dimension of a system of length  $L$ , the grid consists of  $N$  nodes (or grid points). These nodes divide the length of the system into  $N$  cells, who are of size  $\Delta x = \frac{L}{N}$ .

Particle-in-Cell models bear the advantage of being **self driven**, *i.e.* no input assumption about the particle distribution is made [50, p. 36]. Further, Particle-in-Cell provides a computationally efficient (although in many cases still heavy) alternative to simply computing the force on every real particle as caused by all other particles [55, pp. 19–22].

Traditional Particle-in-Cell codes however comes at a disadvantage, namely that they are not symplectic [50, p. 68]. Errors arising from everything from arithmetic rounding to the finite differencing of the fields as well as the use of macro-particles give rise to a stochastic error field, which differs for each particle and causes them to undergo a random walk over each time step. This causes kinetic energy to grow for the particles, linearly over time steps, and is known as **stochastic heating** or **grid heating** [55, pp. 316–318] [50, p. 63]. **Mode coupling** is an important

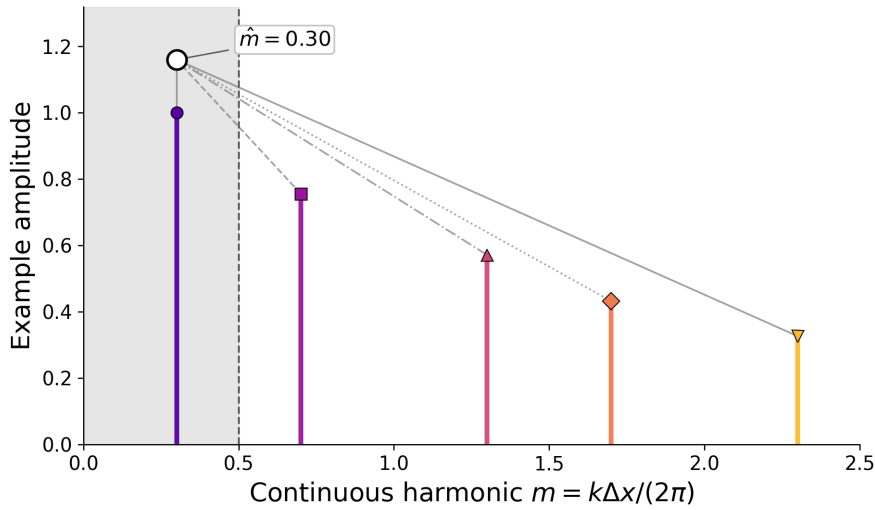




**Figure 2.20:** Visualization of a Macro particle and its charge distribution to the nearest nodes in 2D according to the CIC scheme.

example where the mesh cannot sufficiently resolve high wavenumber (high- $k$ ) physics. When forces cannot be resolved, they will alias and fold to resolvable wavelengths. An example of this is shown in Fig. 2.21. This is an effect that cannot be completely eliminated; rather, one must control the magnitude of the effect to what is considered an acceptable level. For a fixed grid size, reduction of grid heating may be accomplished through either an increase in the amount of macro-particles (*i.e.* an increase in **particle-per-cell** density) and/or use of higher order interpolation functions [55, pp. 319–320].

PIC also lacks what is known as **displacement invariance** [55, pp. 124–125]. In other words, the forces between particles will not be determined simply by their distances to each other but also by their relative distances to the mesh. For piecewise continuous interpolation, force fluctuations will occur when the particles cross cell boundaries.



**Figure 2.21:** Mode coupling example. While the physical harmonic is  $m = 0.30$ , what is sampled (open circle) will also receive contributions from higher harmonics through aliasing), yielding an increased amplitude. This gives rise to extra numerical kicks and grid heating.

## 2.12 Previous studies

Previous studies have been performed for the proton compressor with 2.5D PIC space-charge modeling [58] [1], and a detailed description of the compressor is found in Section 3.2. Previous simulations have shown significant blow-up for the 5 GeV option, especially in  $y$  with a lattice tune of (10.89, 5.77) [58]. The  $y$ -structure was especially of a four-fold nature, while the  $x$ -structure was less indicative of a certain structure. An investigation was initiated to find an optimal

tune to decrease the blow-up while still maintaining other important parameters. This scan was performed over  $\sim (10.5, 5.5)$  to  $\sim (11, 6.0)$ . It normalized equally for the lowest emittance in y (not in x, as its observed blow-up had not been as severe), the shortest bunch length, and minimal loss fraction at turn 41 (*i.e.*, the final turn). With the new chosen tune, blow-up was still observed. Higher initial emittances showed a smaller relative blow-up, but the absolute blow-up was still the same.

---

This chapter introduces the Xsuite simulation framework, the lattice parameters used, and the space-charge models employed for the compressor simulations.

### 3.1 Simulation Framework

Xsuite is an open source simulation framework for beam physics developed at CERN which combines functionalities of many previous, separate, tools [37]. It consists of several packages that work together [59, p. 6]. In this framework, functionality for simulating effects of not only single particle dynamics but also collective effects modeling is possible. Below, a brief overview will be given of how space-charge is currently implemented in Xsuite.

### 3.2 Lattice and Beam Model

The compressor, which is in the current Muon Collider baseline, is shown in Fig. 3.3. It has been designed by Sofia Johannesson and Natalia Milas, and is inspired by the SPL compressor design by Aiba et al [45] [58]. A large phase slip factor is desired to make the compression effective. The phase slip factor however introduces limitations through dispersion and large energy spread, as this would increase the size of the needed aperture. For this reason, negative bending magnets are introduced at points of negative dispersion to cap the maximum dispersion while still contributing positively to the slip factor (see the "outward" bends in the figure). As the chromatic tune shift would otherwise be large, sextupoles are installed and optimized to cap the chromaticity at  $\pm 0.01$ . This lattice has a length of 314 ( $100\pi$ ) m and is currently modeled with a single RF-cavity with a voltage of 4 MV, a frequency of 1.875 MHz as well as a synchronous phase of  $\pi$ . The harmonic number of the ring is 2. The ring will rotate longitudinal phase space for protons with an energy of 5 or 10 GeV. The initially used lattice tune is  $(Q_x, Q_y) \sim (10.913, 5.892)$  (see Section 2.12). The compressor operates with a positive slippage factor, meaning above transition, of  $\eta \approx 0.14$ . For compressors, this magnitude is a relatively large value. Its purpose is a quick compression over

relatively few turns. The proton energy for 5 GeV, yields  $\gamma_0 \approx 5.32$ . Parameters for both the 5 GeV and 10 GeV options are shown in Table 3.1. The initial bunch distribution is described as follows:

- **Transverse rms emittance:** Geometric:  $9.4 \text{ mm} \cdot \text{mrad}$ , Normalized:  $4.9 \text{ cm} \cdot \text{mrad}$ . The initial transverse distribution is a 4D Gaussian distribution.
- **Longitudinal distribution:** Uniformly distributed to approximate the non-Gaussian shape which will be provided by the accumulator. The initial bunch length is 120 ns (or equivalently 9 m at exactly  $\gamma_0$ ) with a uniform  $\delta$  spread of  $2.5 \cdot 10^{-2}\%$
- **Macro Particles:** Initially, 50 000 macro-particles were used (examples are found in Appendix G), which was later increased to  $1 \cdot 10^6$  macro-particles (see convergence study in Chapter 6).

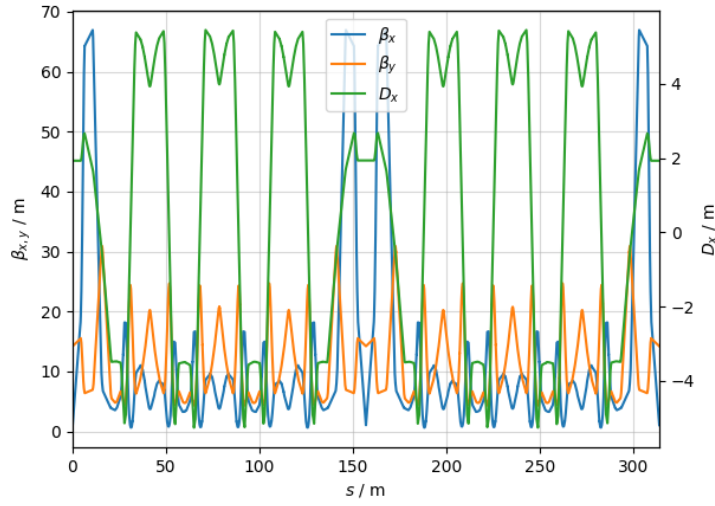
**Table 3.1:** Parameters for the two lattice options.

| Parameter                | Symbol           | Option 1  | Option 2 |
|--------------------------|------------------|-----------|----------|
| Beam Power               | $P$              | 2 MW      | 4 MW     |
| Beam Energy              | $E$              | 5 GeV     | 10 GeV   |
| Lattice Length           | $L$              | 314 m     | 628 m    |
| <i>Common parameters</i> |                  |           |          |
| Repetition Rate          | $f_{\text{rep}}$ | 5 Hz      |          |
| Initial bunch length     | $\sigma_i$       | 120 ns    |          |
| Bunch length on target   | $\sigma_f$       | 2 ns      |          |
| RF Voltage               | $V_{\text{RF}}$  | 4 MV      |          |
| RF Frequency             | $f_{\text{RF}}$  | 1.875 MHz |          |
| Synchronous Phase        | $\phi_s$         | $\pi$     |          |
| Phase slip factor        | $\eta$           | 0.14      |          |

This thesis exclusively explores the 5 GeV option. This is the baseline option; accelerating protons to 10 GeV would require the cavities in the linear accelerator to have higher voltage gradients or the addition of more cavities, the latter of which would require a larger tunnel. As is seen from Table 3.1, the compressor itself would also need a doubled lattice length to deal with the doubled beam rigidity. Min, max and average values for the beta functions, along with transverse rms bunch radii are given in Table 3.2. The second row provides initial rms bunch radii, while the third provides rms bunch radii assuming that the bunch had blown up symmetrically by a factor of 5 (this is used for calculations in section F.3). The lattice functions for the lattice is shown in Fig. 3.1. As Xsuite employs thin-element modeling, the modeled derivatives of the lattice functions are discontinuous. It should be noted that there is no position in the lattice where both the dispersion and its derivative is zero. Turn 41 was initially treated as the turn of extraction.

**Table 3.2:** Beta-function and RMS beam-size data. The amplified values are used in Section F.3.

| Quantity                              | Horizontal ( $x$ ) |         |        | Vertical ( $y$ ) |         |        |
|---------------------------------------|--------------------|---------|--------|------------------|---------|--------|
|                                       | avg                | min     | max    | avg              | min     | max    |
| $\beta$ [m]                           | 9.58               | 0.597   | 67.9   | 12.8             | 3.93    | 31.0   |
| $\sigma$ (initial) [m]                | 0.00950            | 0.00237 | 0.0253 | 0.0109           | 0.00609 | 0.0171 |
| $\sigma$ (amplified, $\times 5$ ) [m] | 0.0212             | 0.00531 | 0.0566 | 0.0245           | 0.0136  | 0.0382 |



**Figure 3.1:** Lattice functions (Twiss and dispersion) for the compressor.

### 3.3 Space-Charge modeling

Xsuite provides different alternatives on how to model space-charge, where this study has employed the PIC option. The Xsuite PIC model is largely based on the implementation developed in PyHEADTAIL-PyPIC. The following description of the Xsuite implementation is based on a source for the PyHEADTAIL implementation of PIC space-charge [50] [60] [37].

#### 3.3.1 Particle-in-Cell implementation in Xsuite

This section will discuss the 2.5D and 3D PIC implementations of PIC space-charge in Xsuite. By treating numerical calculations within the beam rest frame, the problem of determining the field gradient  $\nabla\Phi$  can be treated as an electrostatic problem provided that all particles are within a certain level of momentum deviation (i.e., the motion of the particles relative to each other can be neglected). The pseudocode for the Xsuite PIC model is given in the listing 3.1.

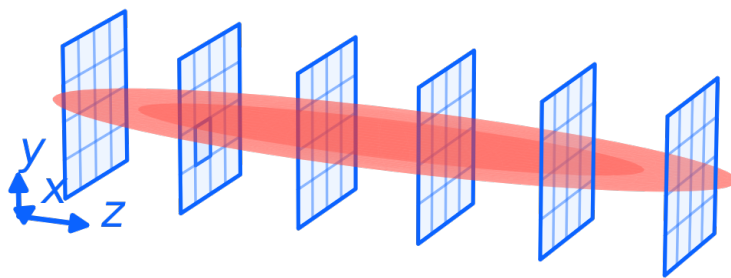
```

1 if at interaction_point:
2     deposit_charges_to_mesh()
3     Lorentz_transform() #To beam frame
4     solve_poisson_fft() # Electrostatic problem
5     compute_e_field_from_potential()
6     inverse_Lorentz_transform() #To laboratory frame
7     interpolate_fields_to_particles() #Both magnetic and
    electric fields applied
8     apply_space_charge_kicks()

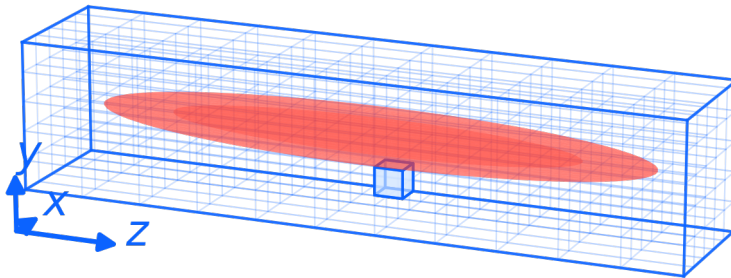
```

**Listing 3.1:** Pseudo code for the PIC algorithm in Xsuite. This is based on descriptions given in [50] but also on the author's inspection of the Xsuite source code.

In essence, it is the same scheme as described in Section 2.11, although time steps are exchanged for interaction points spread throughout the lattice. The deposition gives a discrete representation of  $\rho$ , the charge density. Multiplication with the respective integrated Green's function is done in Fourier space to save computational resources, and the result is thereafter inverse transformed to yield the field potential. The electric mesh fields are then calculated, transformed to the laboratory frame, and finally interpolated on to the macro-particles. For the 2.5D scheme, deposition is done on a 3D grid, although only transverse, 2D Poisson equations are solved using the FFT method. Essentially, the bunch is sliced longitudinally, and for each slice a 2D transverse problem is solved. For 3D space-charge, a complete 3D problem over the whole cubic grid is solved. The 2.5D and 3D schemes are shown in Fig. 3.2. It is important to know that any macro-particle outside of the mesh extents will not have any space-charge kick applied [61]. Furthermore, this method employs open boundary conditions, i.e., the bunch is modeled as if it were in free space [50].



(a) Xsuite 2.5D solver visualization.



(b) Xsuite 3D solver visualization.

**Figure 3.2:** Solver grids for 2.5D and 3D PIC space-charge in Xsuite. Red ovals represent a particle bunch. In each subfigure, one cell has been highlighted.



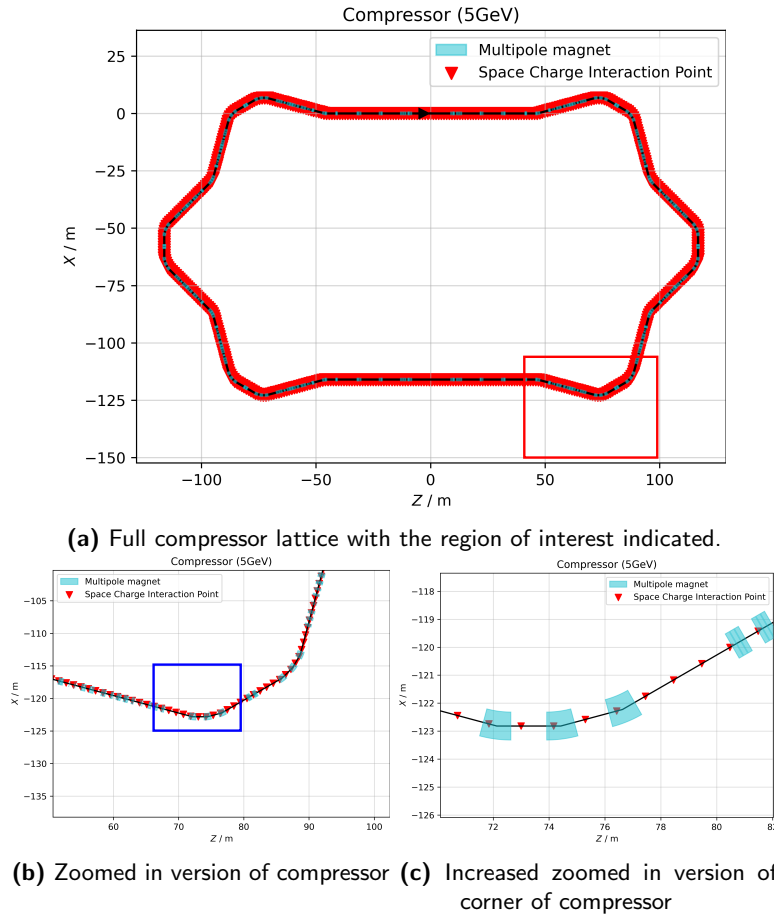
### Xsuite PIC implementation for a given lattice

The following description is based on the Xfields package (ver. 0.25.5) which is part of Xsuite [61]. Instead of using time steps as in many plasma based codes, beam physics PIC implementations usually make use of **interaction points**. In Xsuite, each interaction point is represented as a so-called "space-charge element" similar to how drifts, quadrupoles etc. are treated. At each interaction point, space-charge kicks are calculated, which are thereafter scaled by the elements' assigned length (for  $N$  interaction points with uniform distribution, this means the assigned length will be  $1/N$  for each element). In other words, the integrated space-charge effect for a single macro-particle over one turn can be expressed as a Riemann sum:

$$\sum_i F_{SC}(i) \cdot \Delta i \approx \int_0^L F_{SC}(s) ds \quad (3.1)$$

where  $F_{SC}$  is the space-charge force applied per interaction point and  $i$  is the length of each space-charge element. In Fig. 3.3, space-charge interaction points are plotted on top of the compressor, with different zoom levels. While it may look like some interaction points should act on particles as they simultaneously undergo the effects of another element, e.g. a quadrupole, this is not how Xsuite implements it. Xsuite treats all elements as thin, in the sense that effects of an element are applied at a single point, in essence several variants of the thin-lens equation is used.

Xsuite has functions which populate a given lattice with space-charge elements according to given parameters. To optimize the mesh extents per element, the 4D lattice parameters  $(x, p_x, y, p_y)$  are used to vary the transverse mesh extents along the line by applying a scaling constant. For example, given a large  $\beta_x$ , the horizontal extents of the mesh will be scaled to be greater and vice versa. The "unscaled" mesh extents are set by the user. The mesh extents are neither scaled nor changed in any way nor adapt to the evolution of the size of a bunch. As  $x$  is highly dispersive and since this is not taken into account by the aforementioned functions, the mesh extents have been chosen as 8 times the initial standard deviation of the bunch in  $x$ , as opposed to 4 times the standard deviation in  $y$ . The  $z$  mesh extents do not vary across the line. In tandem with the fact that the initial bunch is uniformly distributed in longitudinal phase space, the  $z$  mesh extents have been chosen as 2 times the standard deviation of the bunch in  $z$ .



**Figure 3.3:** Overview of compressor with 540 space-charge elements equally distributed. Red box in subfigure a) specifies zoom level in subfigure b), and blue box in subfigure b) specifies the same for subfigure c). Red triangles are interaction points, blue structures are magnets.

## 3.4 Data Analysis

### 3.4.1 Sampling

To save memory, data is only stored from  $5 \cdot 10^4$  randomly sampled macro-particles per simulation even if a larger amount has been used for the simulation itself. For simulations that use the same amount of macro-particles, the same initial particle distributions are used, and identical sampling is used for these simulations. Simulation dynamics are unchanged by the sampling, although a slight loss in resolution is to be expected for macro-particle visualizations. In addition, this is reflected in MP/bin counts which will add up to  $5 \cdot 10^4$  macro-particles regardless of the simulated amount of particles.

### 3.4.2 Dispersion correction

Unless otherwise specified, phase space figures are dispersion corrected. In this work, dispersion correction implies that the following procedure is performed in plotting scripts:

$$\begin{aligned} x &\leftarrow x - \eta_x \delta \\ p_x &\leftarrow p_x - \eta_{p_x} \delta \end{aligned}$$

Essentially, Eq. (2.22) has been solved for the values of  $x$  and  $p_x$  that would apply if no dispersion was present. This is done to better understand the pure betatron emittance of the beam.

### 3.4.3 Common configurations

Some common numerical configurations used in this work are provided in Table 3.3, and are referred to as e.g. "Configuration I" or "Configuration IV".

**Table 3.3:** Common numerical configurations used in this work. The space-charge dimensionality (2.5D or 3D) and any additional treatment such as low-pass filtering are specified separately.

| Configuration | Macro-particles | Grid size                | Mesh     |
|---------------|-----------------|--------------------------|----------|
| I             | $1 \cdot 10^6$  | $32 \times 32 \times 32$ | adaptive |
| II            | $1 \cdot 10^6$  | $32 \times 32 \times 32$ | static   |
| III           | $5 \cdot 10^4$  | $64 \times 64 \times 64$ | adaptive |
| IV            | $5 \cdot 10^4$  | $64 \times 64 \times 64$ | static   |

### 3.4.4 Tune Analysis

To perform tune analysis such as Frequency Map Analysis (FMA), see Section 2.9.1 and Appendix D, on the particles, the nafflib package has been used [62]. This is a python implementation of the NAFF algorithm where hanning filtering is

possible. As NAFF on a real signal cannot resolve  $Q$  versus  $1 - Q$ , the alternative closest to the lattice tune will be chosen. If a particle gets a tune far from the lattice tune, there is an inherent risk that this will give an incorrect, "mirrored" tune on the tune diagram, which must be accounted for. A further consideration which must be taken into account is that Xsuite elements do not, by default, have imperfections. In real life, any accelerator should expect to be more adversely affected by a working point close to resonance lines as opposed to in simulation results.



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## Improved Space Charge Model

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This chapter compares the previous with updated simulation configurations, and further discusses an observed microbunching phenomenon.

### 4.1 Previous configuration

Initial simulations of the compressor have employed 2.5D PIC space-charge. Although 2.5D PIC is a computationally efficient model compared to 3D, the evolution of longitudinal density (and therefore possibly strong longitudinal space-charge) may necessitate the use of 3D. For this reason, a simulation with 3D PIC space-charge has been made to validate the previous results. Furthermore, previous simulations have employed the static mesh mentioned above. Especially for 3D PIC modeling, a static mesh can severely decrease the resolution for later turns. In other words, one would need a very large amount of slicing along  $z$  to adequately handle the bunch length both at injection and extraction. However, as the solver step complexity scales cubically with the grid size, and due to required RAM usage, this strategy may quickly become unfeasible. A functionality to visualize the mesh in phase space has further been implemented.

### 4.2 Improved model

In this section, an adaptive mesh has been developed and tested for both 2.5D and 3D space-charge and has been employed to validate previous results. Initially, a grid resolution of 64 and macro-particle amount ( $5 \cdot 10^4$ ) was used (Configuration III and IV). However, after a new convergence study (see Chapter 6) comparisons were made again with a grid resolution of 32 and a macro-particle amount of  $1 \cdot 10^6$  (Configuration I and II).

Changes for Xfields v. 0.25.5 have been developed and can be accessed in [63]. First, a bug was fixed where no longitudinal kicks were applied for 3D space-charge. Secondly, functionality has been developed which allows the user to change the mesh extents (including solver geometry, etc) without the need to rebuild any element. This functionality has thereafter been used in a script to make the mesh

”adaptive” rather than the default ”static”, *i.e.* the mesh extent will change if the emittance in any plane changes significantly. In other words, when the mesh extents decrease, the resolution of the mesh can be increased without the need to increase the mesh size.

In Fig. 4.1, an adaptive mesh is visualized, following the development of the beam in real space. In Appendix G, further examples and figures show the development of the beam against a static versus an adaptive mesh in phase space. In it, the challenge of modeling a beam with evolving size is shown, and an adaptive mesh is motivated from a computational standpoint. In Fig. 4.2, comparisons for phase space with 2.5D vs 3D space-charge are shown, with a static mesh in Figs. 4.2a and 4.2b, as well as adaptive mesh in Fig. 4.2c. In Fig. 4.3, comparisons for phase space with static vs adaptive mesh are shown, with 2.5D in Fig. 4.3a as well as 3D in Figs. 4.3b and 4.3c.

#### 4.2.1 2.5D vs 3D

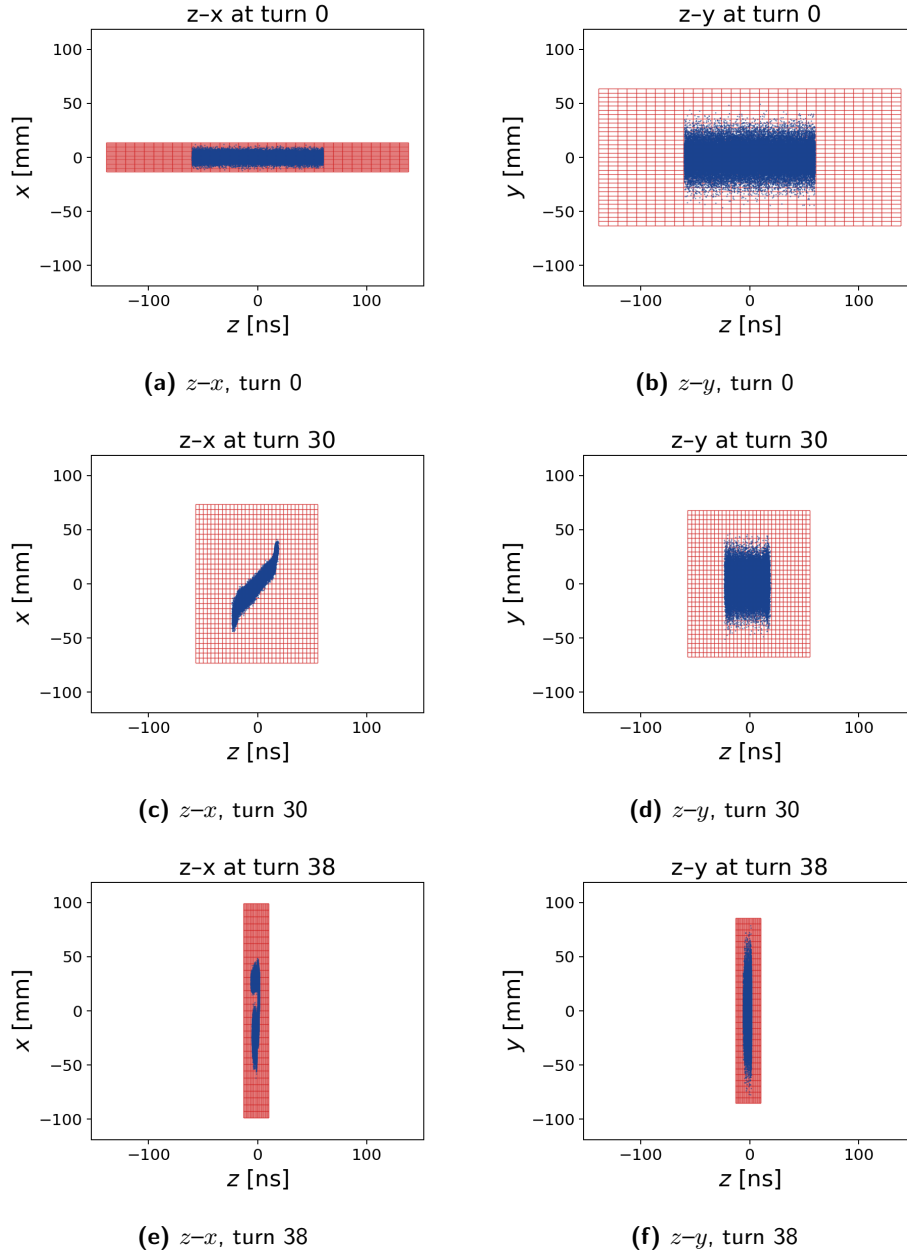
The transverse difference between 2.5D and 3D space-charge is most clear when employing an adaptive mesh (Fig. 4.2) rather than a static mesh (Fig. 4.3). Regardless, the final emittance is smaller with 3D rather than 2.5D space-charge, possibly due to increased longitudinal-transverse coupling. In the longitudinal plane, the turn where the rms bunch length ( $\sigma_z$ ) is shortest is at turn 38 instead of at turn 41 for 3D as opposed to 2.5D. This is explicitly shown in Fig. 4.4, where transverse emittances as well the bunch length are plotted against turns. As for qualitative longitudinal differences, the beam ”curls” around for 3D which is not observed for 2.5D, likely a result of the introduced longitudinal kicks. This and/or initial charge discontinuities at the edges could explain the behaviors at the tail and the head of the bunch observed, especially for a static mesh.

#### 4.2.2 Adaptive vs Static mesh

There are further differences in using an adaptive mesh over a static one, regardless of whether 2.5D or 3D space-charge has been employed. For one, the transverse emittance becomes larger with an adaptive mesh. This is seen in e.g. Fig. 4.3a, and may possibly be explained by space-charge becoming better resolved. At turn 38, the bunch is shorter with an adaptive mesh as opposed to a static mesh (see e.g. Fig. 4.3b). Perhaps this could, through better resolved space-charge and therefore stronger longitudinal-transverse coupling, explain the greater transverse emittance for an adaptive mesh as opposed to a static one. For 3D space-charge, the clearest structural differences are seen at turn 41 (Fig. 4.3c), where there is microbunching with an adaptive mesh, whereas the static mesh only show the original head/tail curling around as discussed in the previous paragraph. The microbunching is further investigated in Section 4.3.

#### 4.2.3 Chosen configuration

Motivated by the differences observed in Section 4.2.1 and Section 4.2.2, this study has proceeded with 3D adaptive space-charge. In future studies, benchmarking



**Figure 4.1:** Real-space evolution of the adaptive 3D PIC mesh for Configuration I, shown as particle scatter over projected mesh lines in the  $z-x$  and  $z-y$  planes.



should be performed in other codes to validate these choices.

#### 4.2.4 Four-fold structure

Regardless of configuration, a four-fold structure is visibly observed both in  $x$  and  $y$ . This phenomenon motivated the studies shown in chapter Chapter 5.

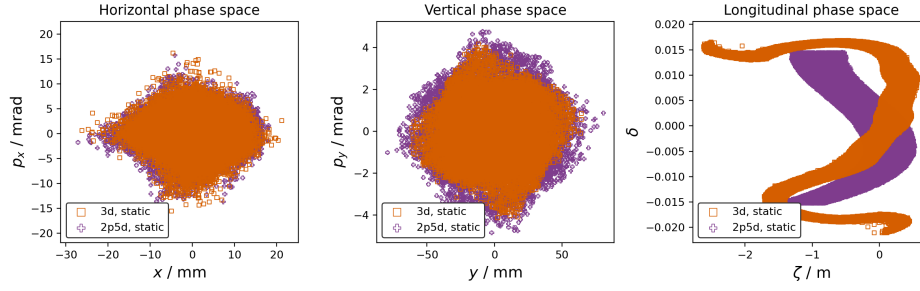
### 4.3 Microbunching

With 3D space-charge and an adaptive mesh, a longitudinal modulation in the charge density, microbunching, is observed at turn 41 (see e.g. Fig. 4.3c). Upon observation, a test was conducted in which simulations were performed with a higher-detail mesh (grid size 128 in  $z$ , while maintaining 32 for  $x$  and  $y$ ). For this case,  $8 \cdot 10^6$  macro-particles were used to maintain particle-per-cell density. The result of this test is shown in Fig. 4.5. Compared to the previous configuration, microbunching has not only increased, but is also visible for turn 38. Furthermore, the minimum bunch length has increased. In case the microbunching is completely or at least mainly numerical, a TSC inspired low-pass filter (see Appendix E) was developed and tested. A result for the baseline configuration is shown in Fig. 4.6. The filter uses a 3-point convolution with a binomial kernel on the deposited charge:

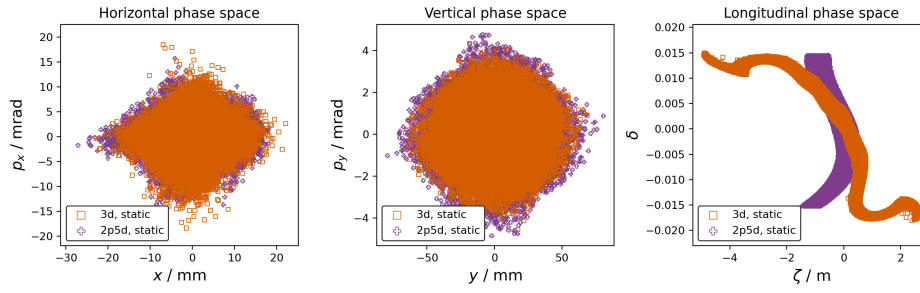
$$\rho_i \leftarrow 0.25\rho_{i-1} + 0.50\rho_i + 0.25\rho_{i+1}$$

The microbunching could either be explained by a finer mesh resolving real physics, or the adaptive mesh introducing its own numerical artifacts. The first hypothesis would be supported by the fact that the ring operates above transition. As discussed in Section 2.10.1 and as shown in Fig. 2.19, this enables natural modulation in the longitudinal density to develop. In contrast, Section 2.11.1 and Appendix E make it clear that there are many sources of numerical errors. In Section 2.11.1, it is discussed how force fluctuations appear when particles cross cell boundaries, especially if discontinuous interpolation is used. As the particle positions relative to the mesh change discontinuously at each retiling, it is possible similar force fluctuations arise. Amplified by a strong  $z - \delta$  coupling, these force fluctuations may cause microbunching. A finer mesh such as in Fig. 4.5 could possibly worsen this phenomenon by increasing retiling discontinuities, as this would imply a greater distance of relative particle positions from mesh between retiles. If this noise is not sufficiently smoothed away at the initial turns with the coarsest mesh, it will instead build and amplify through negative mass instability. As for the microbunching seen in Fig. 4.3, it could possibly be a classic example of folding (grid heating), as high spectral components in charge density resolved at turns of highest compression will fold when the mesh re-expands.

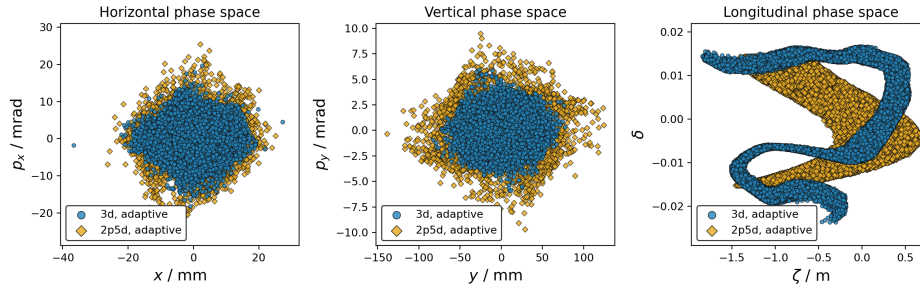
Further simulation tests should be performed. For example, a static mesh should be employed at a resolution of  $60 \cdot 32$  (given the compression factor of 60) for  $z$ , with a respective increase in macroparticles. If the microbunching persists, the source



(a) Turn 38 comparing 2p5d (purple, cross) with 3d (orange, hollow square) with a static mesh.

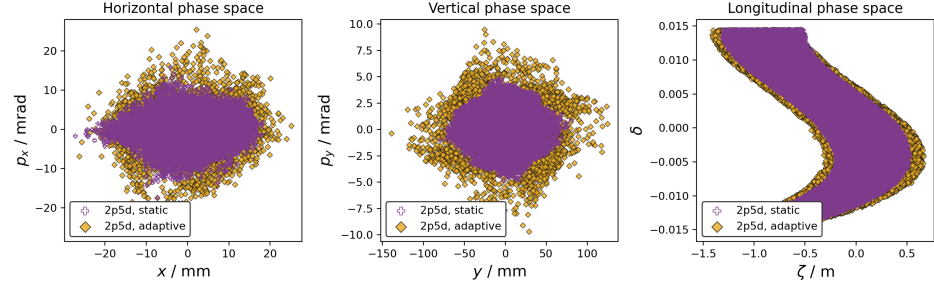


(b) Turn 41 comparing 2p5d (purple, cross) with 3d (orange, hollow square) with a static mesh.

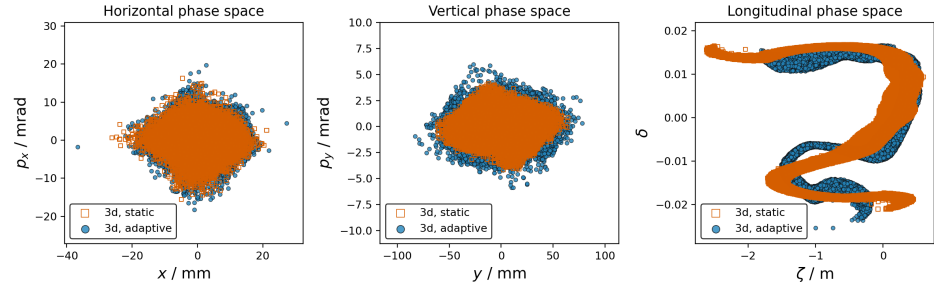


(c) Turn 38 comparing 2p5d (yellow, rhomb) with 3d (blue, circle) with an adaptive mesh.

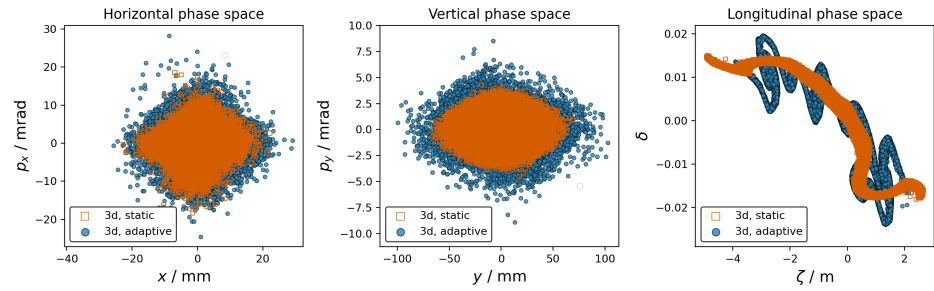
**Figure 4.2:** Simulation comparisons of 2.5D versus 3D PIC space charge. Subfigures a) and b) use Configuration II, while subfigure c) uses Configuration I.



(a) Static (purple, cross) vs adaptive (yellow, rhomb) mesh for 2.5D space-charge at turn 41.

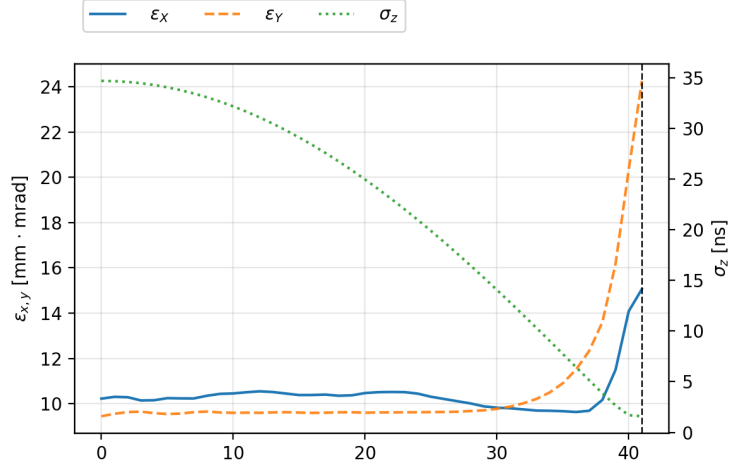


(b) Static (orange, hollow square) vs adaptive (blue, circle) mesh for 3D space-charge at turn 38.

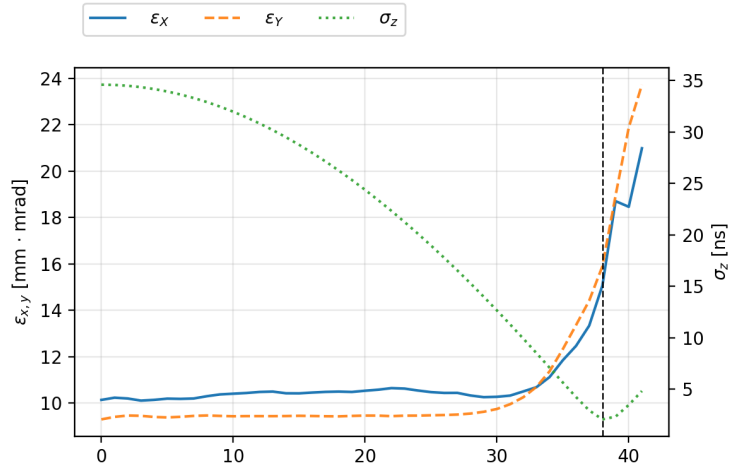


(c) Static (orange, hollow square) vs adaptive (blue, circle) mesh for 3D space-charge at turn 41.

**Figure 4.3:** Simulation comparisons of static versus adaptive mesh for 2.5D and 3D PIC space charge using Configurations I and II.



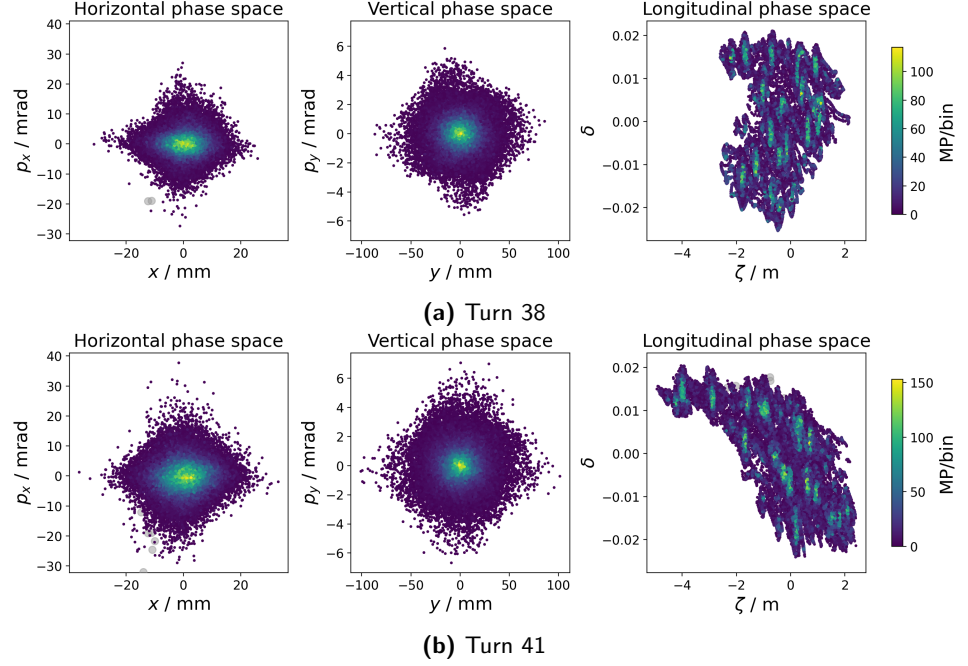
(a) Evolution of emittance and bunch length for 2.5D PIC space charge with Configuration I.



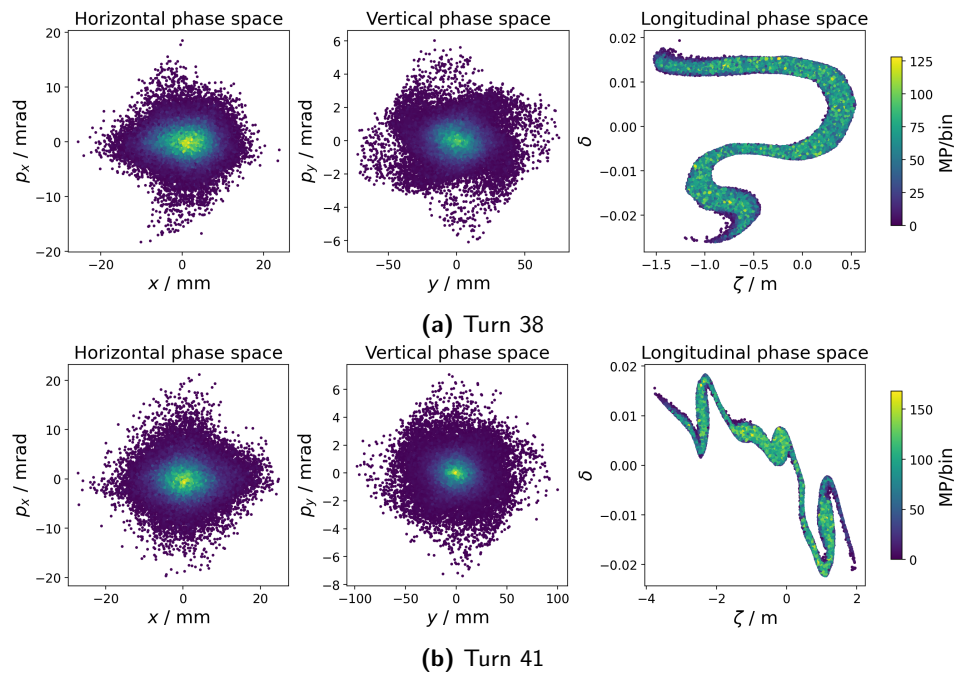
(b) Evolution of emittance and bunch length for 3D PIC space charge with Configuration I.

**Figure 4.4:** Evolution of emittance and bunch length for 2.5D and 3D PIC space charge with Configuration I. A black line marks the turn of shortest bunch length.

problem is not driven by the retiling mechanic, and in that case is more likely to be caused by physical negative mass instability, or yet some other phenomena. If the microbunching is numerical, higher-order interpolation could possibly be motivated by the smoothing seen in Fig. 4.6. However, the smoothing would need to be greater than what is currently achieved.



**Figure 4.5:** Phase space for turn 38 (smallest  $\sigma_z$ ) and for turn 41 for  $z-x$  and  $z-y$  with transverse grid sizes of 32, longitudinal grid size of 128 and macro-particle count of  $8 \cdot 10^6$ .



**Figure 4.6:** Phase space for Configuration I at turn 38 (smallest  $\sigma_z$ ) and for turn 41 with low pass filter active in all dimensions. The filter dampens microbunching, although it is still present at turn 41.



## Four-fold effect investigation

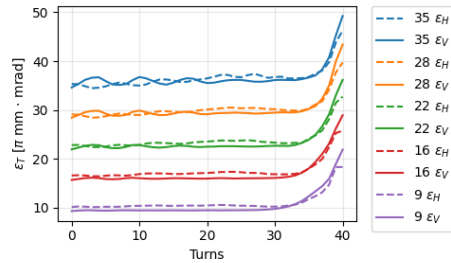
Several hypotheses have been established as to the cause of the four-fold structure observed for both  $x$  and  $y$  in the previous chapter. This chapter covers a number of tests conducted to determine the cause of the structure.

### 5.1 Hypothesis: Space-charge driven resonance

As discussed in Section 2.10.1, space-charge can induce resonances. If this is the case, an increased initial emittance, and therefore a lower particle density, should imply a lower charge density, and in turn should dampen the effects of space charge. The transverse emittances for these tests are plotted over turns in Fig. 5.1. The phase space at turn 41 for the different initial emittances is plotted in Fig. 5.2.

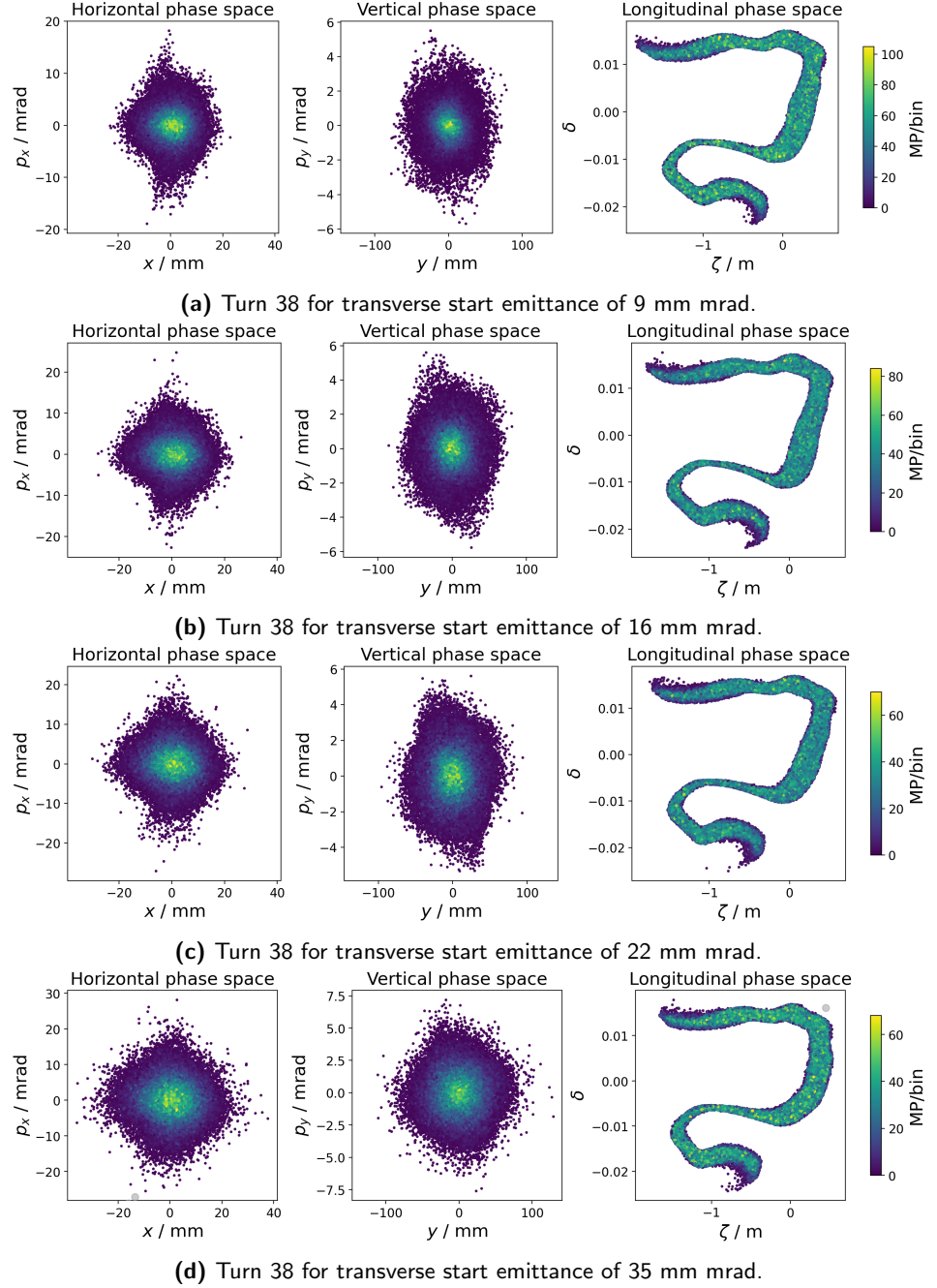
While the relative emittance blow-up decreases, this can simply be attributed to the increased initial emittance. The fact that the absolute emittance blow-up in both transverse planes do not decrease with increasing emittance may indicate that there is a baseline mechanism causing the structure. Space-charge may in turn excite a resonance.

For this reason, the following chapter will investigate the cause of the structure

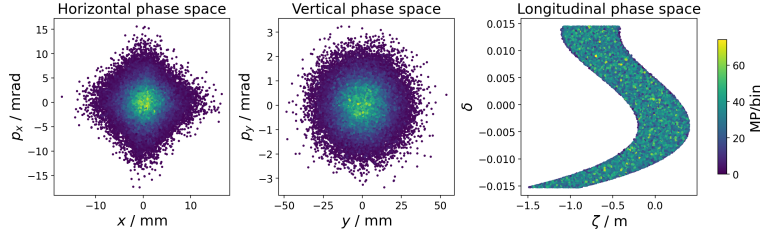


**Figure 5.1:** Emittance / turn for different initial emittances.





**Figure 5.2:** Turn 38 for different start emittances. The four-fold structure appears in all cases.



**Figure 5.3:** Simulation with no space-charge at turn 41. As can be seen, a four-fold structure is present in  $x$ .

with space-charge turned off in simulations. As the particles will therefore not interact, these simulations have employed  $5 \cdot 10^4$  macro-particles for the sake of computational efficiency. An initial simulation is shown in Fig. 5.3, which confirms the presence of the structure in  $x$  even with no space-charge active. Still, it confirms that the space-charge induces a significant  $x - y$  coupling, creating a structure in  $y$ .

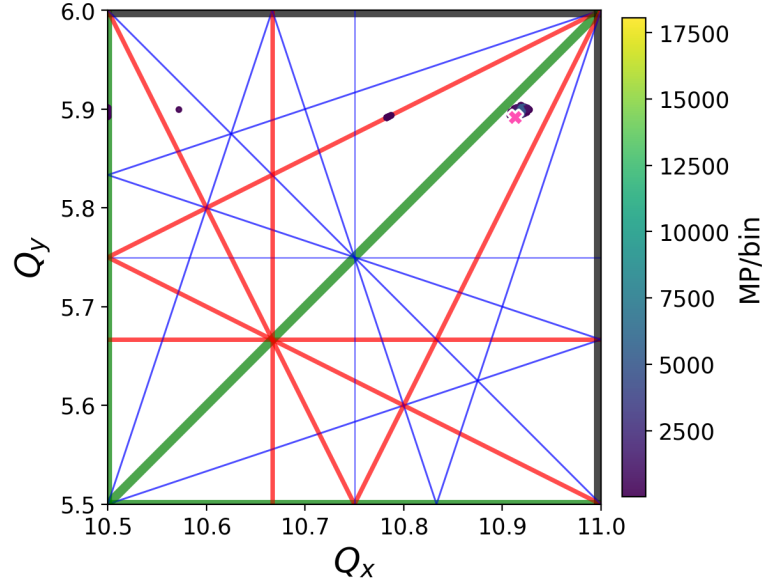
## 5.2 Hypothesis: Crossing of resonance line

FMA (see Section 2.9.1) was used in a simulation of  $5 \cdot 10^4$  macro-particles without space-charge. The intention was first to confirm that the particles did not cross a clear resonance line. The results of this is shown in Fig. 5.4. FMA was thereafter employed only on the particles at the "petals" of the structure, both with and without space charge, to determine whether this would clarify any specific resonance. This was done through "masking", where particles consistently close to the center over turns 34-37 were removed so as to only keep the "petal"-particles. On these particles, FMA was thereafter performed over turns 35-48, where the four-fold structure becomes most clear. Masking is shown with no space-charge in Fig. 5.5 and with space-charge in Fig. 5.6. The respective tune scatters using FMA is shown in Fig. 5.7. In it, some resonance lines are overlapped by a few particles, although there is no clear dominance of a single resonance.

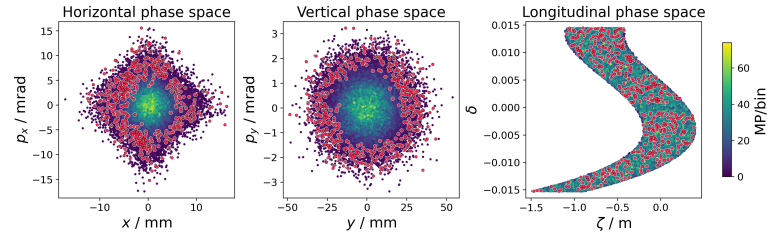
From the mask in Figs. 5.6 and 5.7, it can be seen that particles that have at least some level of energy deviation correspond to the outer transverse particles, including the ones caught in the four-fold structure. As is almost explicit in Fig. 5.6, particles with no energy deviation are not caught in the four-fold structure. This indicates that the cause of the structure is in some way dependent on the longitudinal phase space.

## 5.3 Hypothesis: Sextupole overcompensation

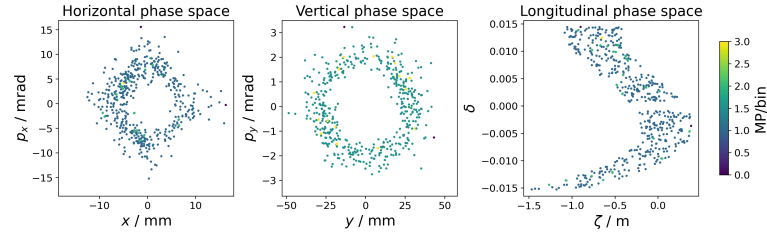
An initial hypothesis was that the structure was caused by synchro-betatron coupling. Tests conducted to explore this theory may be found in Appendix H. Another theory was that the current lattice matching for a relative chromaticity of  $\xi = 0$ , while suppressing chromaticity, could cause the structure. Sextupoles may,



**Figure 5.4:** Tune scatter over turns 0 to 41 with no space charge active. The cross marks the bare tune. While a few particles cross a third order resonance line and some others a second order resonance line (at  $Q = 10.5$ ), there is no clear dominant resonance.

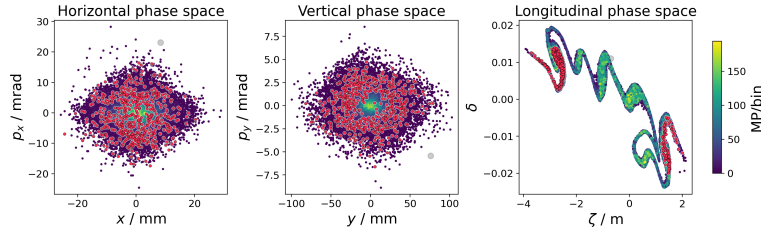


**(a)** Highlighted particles (kept) overlaid on all particles from no space-charge simulation.

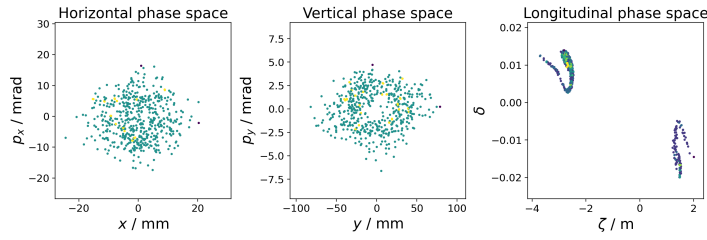


**(b)** Only kept particles from no space-charge simulation.

**Figure 5.5:** Masking shown in two pictures for no space-charge.

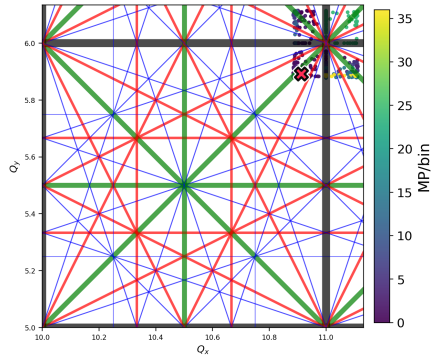


(a) Highlighted particles (kept) overlaid on all particles from space-charge simulation.

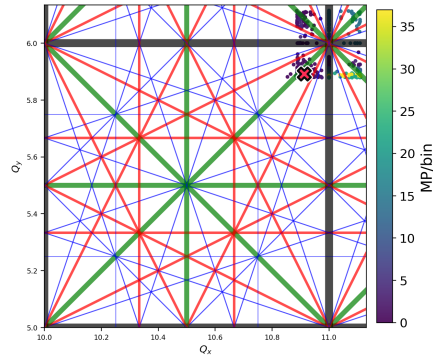


(b) Only kept particles from space-charge simulation.

**Figure 5.6:** Masking shown in two pictures for space-charge.



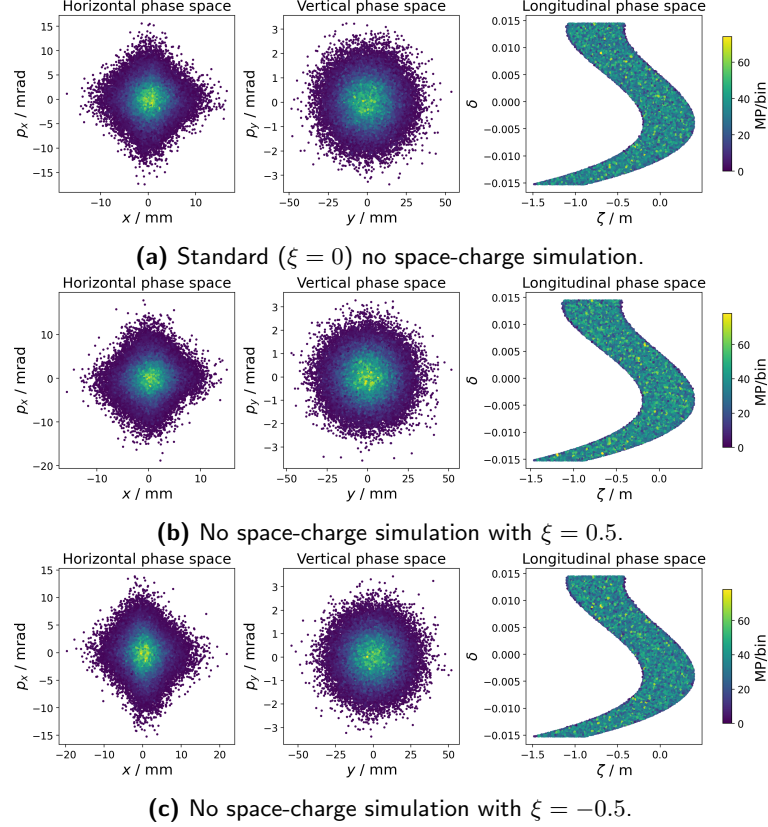
(a) Tune scatter for the masked no space-charge particles over turns 35–48.



(b) Tune scatter for the masked space-charge particles over turns 35–48.

**Figure 5.7:** Tune scatters over turns 35-48 for the no space-charge and the space-charge case.

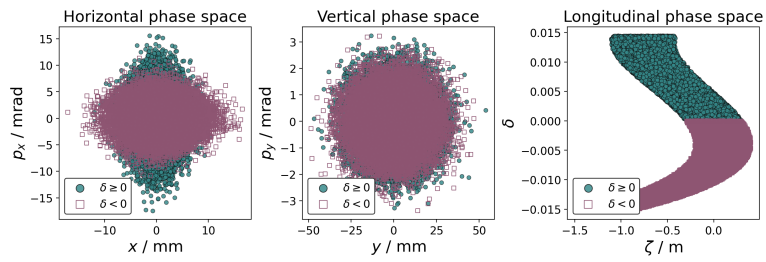
in second-order, excite four-order resonances [64]. For this reason, tests were conducted where the chromaticity was adjusted to be non-zero. The results for two examples,  $\xi = -0.5$  and  $\xi = 0.5$ , compared with  $\xi = 0$ , are shown in Fig. 5.8.



**Figure 5.8:** Comparison of no space-charge simulations with  $\xi = 0$ ,  $\xi = 0.5$  and  $\xi = -0.5$  respectively.

## 5.4 Chromatic beta-beating

Shinji Machida (Science and Technology Facilities Council) has confirmed through additional experiments that the structure, while caused by sextupoles, is not inherently a resonance [65]. Rather, non-linear chromaticity-like effects (chromatic beta-beating) for high momentum deviation particles in the sextupoles will, for these particles, adjust their phase space ellipses (see Section 2.6 and especially Fig. 2.10). As the horizontal beta functions are dependent on sign (see Eq. (2.28)), this effect will either increase the ellipse amplitude in  $x$  (negative momentum deviation) or  $p_x$  (positive momentum deviation). Together, these particles superpose in phase space to form the four-fold structure, which may thereafter be excited as a real resonance by space-charge. This superposition is shown in Fig. 5.9.



**Figure 5.9:** Simulation with no space-charge at turn 41. Positive momentum deviation particles (circles, light green) versus negative momentum deviation particles (squares, purple) are highlighted to make the non-linear chromatic effects clear.

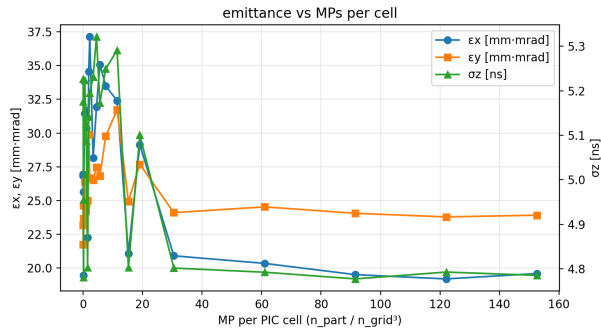


## Convergence study

Inspired by studies in [66], a particle-per-cell convergence study was conducted. The goal of this convergence study has been to determine what macro-particle per PIC cell density is needed to remove the numerical uncertainty to a sufficient degree.

For the convergence study, macro-particle counts of  $[5 \cdot 10^3, 5 \cdot 10^4, 5 \cdot 10^5, 1 \cdot 10^6, 2 \cdot 10^6, 3 \cdot 10^6, 4 \cdot 10^6, 5 \cdot 10^6]$  have been used, and grid sizes have been  $[32, 64, 96, 128, 160]$ . The transverse emittance and the bunch rms length has thereafter been compared at turn 41. The result is shown in Fig. 6.1.

After a density of  $\frac{1 \cdot 10^6}{31250}$  macro-particles/cell is achieved, the oscillations flatten out and stay within 1 mm mrad and 0.03 ns. For the purposes of this study, this is considered numerically convergent. The cheapest convergent configuration (1 million MP:s, grid size of 32, Configuration I) was chosen as the new baseline.



**Figure 6.1:** Transverse emittances and the rms bunch length against different MP/cell densities.





## Parametric study

This chapter presents the results of tune scans which were performed to determine optimal working points, and further to investigate whether the beam blow-up could be mitigated.

### 7.1 No space-charge

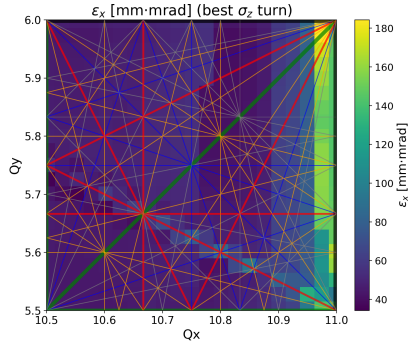
A tune scan was first performed with no space-charge, in order to see if the structure discussed in Chapter 5 could be minimized (and further to confirm that the structure was an inherent phenomenon to the lattice and not simply dependent on working point). For these simulations,  $5 \cdot 10^4$  macro-particles were employed. In  $Q_x$  and  $Q_y$ , 21 values equally spaced in the ranges  $[10.50, 10.99]$ ,  $[5.50, 5.99]$  were tested. Higher-order decimals (e.g. 0.0235642) were added to avoid testing tunes that were too close to the stop bands of resonances. For each run, the following was measured at the turn of best (shortest)  $\sigma_z$ : Transverse emittance, longitudinal rms bunch length, and loss percentage. The beam size should be minimized in order to decrease the demands on the aperture, as well as meet the conditions set by the target [15]. The loss percentage should be minimized to maximize the number of produced pions. Further, a high loss percentage and/or high emittance may indicate e.g. the presence of a resonance. Then a composite value with the same weights from these metrics was calculated. The results are shown in Fig. 7.1. The composite heat maps represent all the results normalized, weighted equally, and added together.

Some observations include what appears to be excitation of a third-order resonance visible in Fig. 7.1c, Fig. 7.1b and to a lesser extent in Fig. 7.1a. Fig. 7.1a generally has a larger resulting emittance compared to Fig. 7.1b likely due to dispersion. In Fig. 7.1d, the shortest bunch length achieved seems to vary in an almost periodic way with  $Q_x$ . In Fig. 7.2, a lower  $Q_x$  indicates that the turn where  $\sigma_z$  is the shortest for a simulation is earlier. Possibly, this could be explained by the longitudinal-horizontal coupling through dispersion present in the compressor. As  $Q_x$  changes, so does the horizontal oscillation pattern, which in turn should affect the evolution of the synchrotron phase. As the sextupoles, which in Chapter 5 were stated to

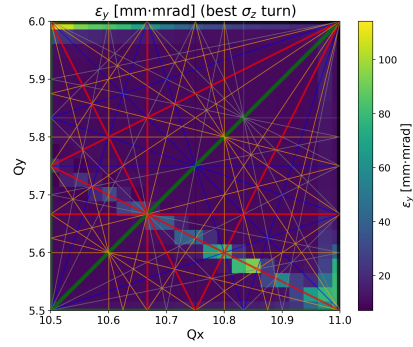
significantly affect the dynamics of the lattice, are also dependent on the position and momentum deviation of particles (cf. Appendix B.0.4), this may further be a source of affected longitudinal particle dynamics.

## 7.2 With space-charge

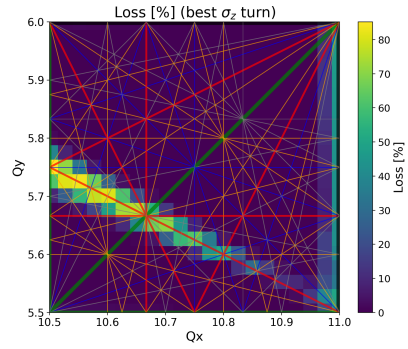
A second tune scan with space-charge active was performed using 3D PIC space charge with Configuration I. The goal was to see whether results from previous, 2.5D and static, tune scans would differ significantly and in that case if a better working point than the previous ( $[10.913, 5.891]$ ) could be found. The results are found in Fig. 7.3.



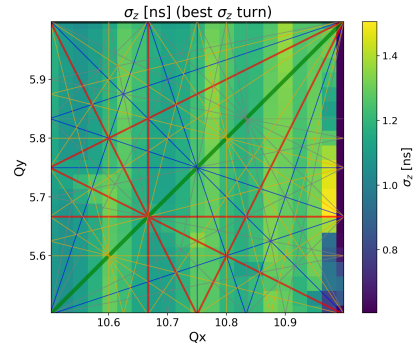
(a) Heat map for horizontal emittances.



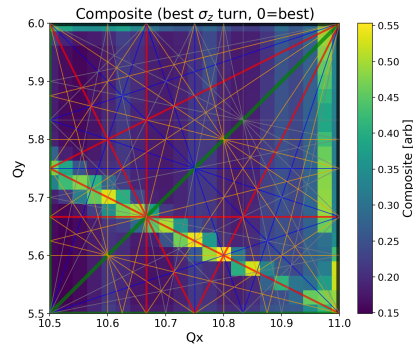
(b) Heat map for vertical emittances.



(c) Heat map for loss percentage.

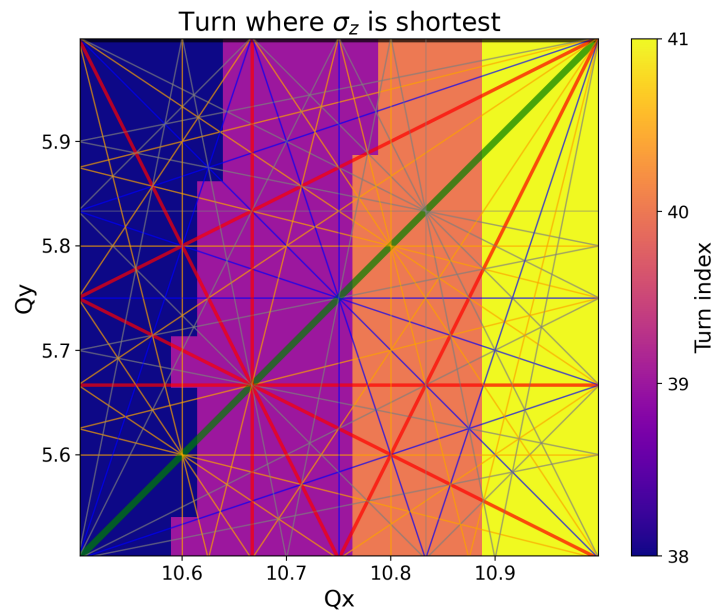


(d) Heat map for rms bunch length.

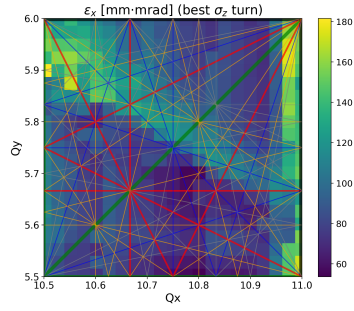


(e) Composite results.

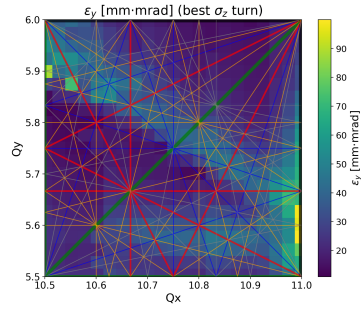
**Figure 7.1:** No space-charge tune scan results for  $21 \times 21$  runs at their turns of best  $\sigma_z$  with tunes varying between  $[10.50, 10.99]$ ,  $[5.50, 5.99]$ .



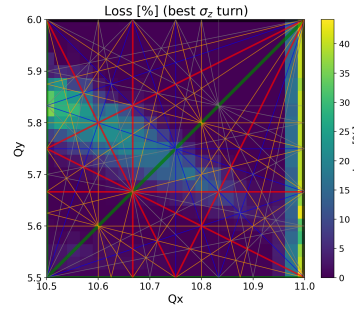
**Figure 7.2:** Turns where  $\sigma_z$  is shortest depending on the lattice tune.



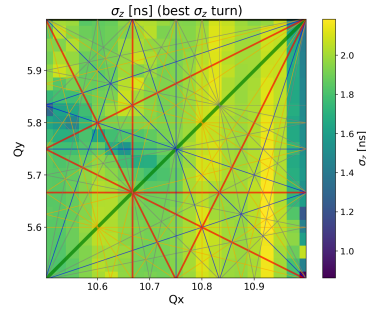
(a) Heat map, horizontal emittances.



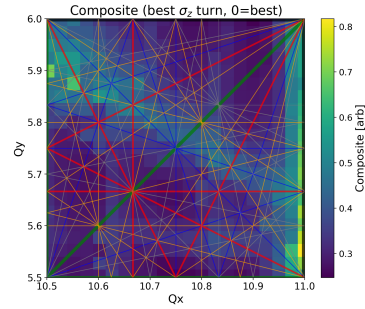
(b) Heat map, vertical emittances.



(c) Heat map for loss percentage.

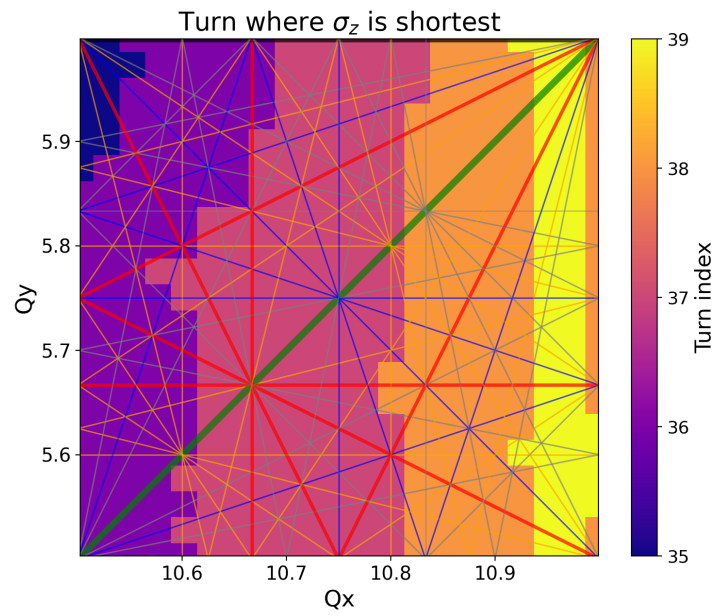


(d) Heat map for rms bunch length.



(e) Composite results.

**Figure 7.3:** Space-charge tune scan results for  $21 \times 21$  runs using 3D PIC space charge with Configuration I, evaluated at their turns of best  $\sigma_z$  with tunes varying between  $[10.50, 10.99]$  and  $[5.50, 5.99]$ .



**Figure 7.4:** Turns where  $\sigma_z$  is shortest depending on the lattice tune.

### 7.3 Comparison of candidates

To evaluate how the parameters of the beam may vary for different lattice tunes, and if the four-fold structure could be minimized for simulations with and/or without space-charge, some sample candidates have been compared. In choosing these candidates one low-ranking candidate of each case has been chosen for the sake of comparison. For high-ranking candidates, only ones some distance away from integer- and half-integer resonance lines have been chosen to account for potential systematic resonances. The selected candidates are summarized in Table 7.1.

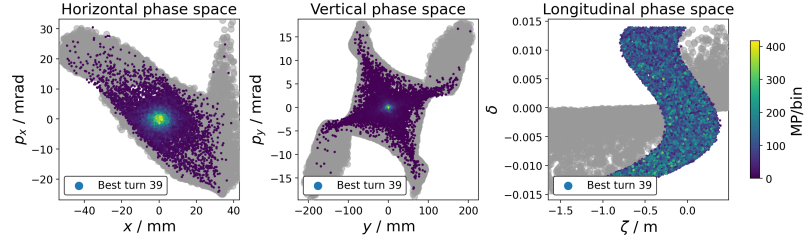
**Table 7.1:** Candidate selected for comparison.

| Candidate | Case            | $Q_x$  | $Q_y$ | Ranking               |
|-----------|-----------------|--------|-------|-----------------------|
| A         | No space-charge | 10.701 | 5.651 | low-ranked (rank 434) |
| B         | No space-charge | 10.552 | 5.948 | well-ranked (rank 9)  |
| C         | Space-charge    | 10.999 | 5.701 | low-ranked (rank 437) |
| D         | Space-charge    | 10.775 | 5.973 | well-ranked (rank 17) |

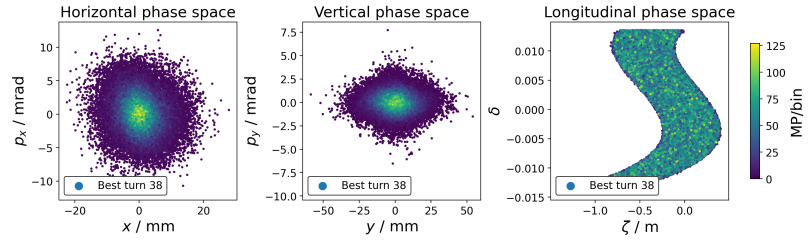
#### 7.3.1 No space-charge candidates

In Fig. 7.5, chosen no space-charge candidates are shown in phase space. Candidate A (Fig. 7.5a) shows a four-fold structure in  $y$ , as well as lost particles. Fig. 7.5b shows a four-fold structure in  $y$ , more reminiscent of the one observed in  $x$  for Fig. 5.3. However, the beam is not completely centered. In Fig. 7.6, their longitudinal macro-particle distributions are plotted together with the transverse beam size variation. In Fig. 7.5a, the surviving particles are mainly in  $z - \langle z \rangle = 1$  ns, with a smaller beam size than for the other surviving particles. In Fig. 7.7, tune scatters for the candidates are shown. In Fig. 7.7a, the beam is seen to cross several resonance lines at once. Likely at least one of these drives the loss of particles for the candidate. In Fig. 7.7b, some particles are crossing the integer line. This possibly explains the offset beam in Fig. 7.5b. Despite its high ranking, the candidate would likely not be suitable for a real accelerator where imperfections would lead to amplified orbit distortions. In other words, more factors than the ranking itself must be taken into account when choosing a suitable working point.

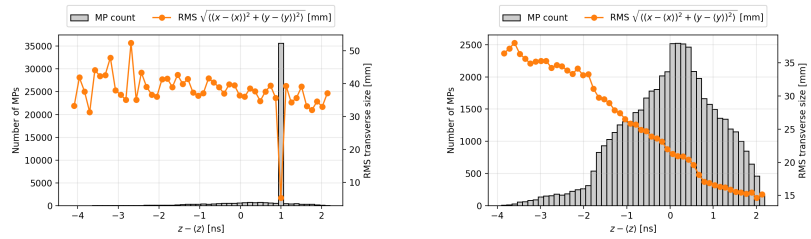




(a) Phase space for Candidate A.



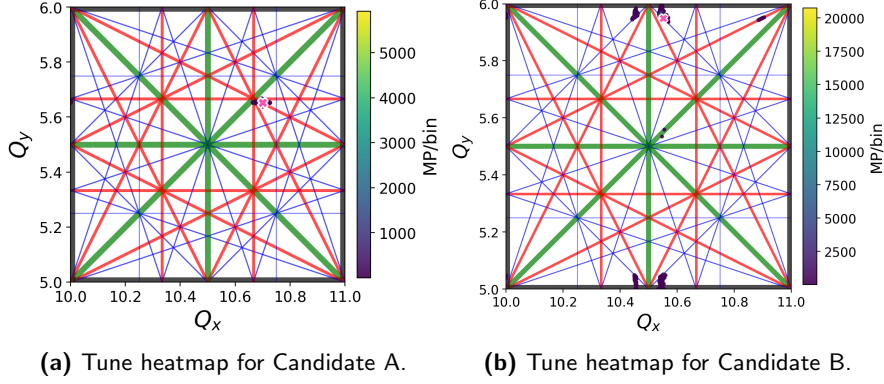
(b) Phase space for Candidate B.

**Figure 7.5:** No space-charge: phase-space comparison at the best sigma-z turn.

(a) Longitudinal macro-particle distribution vs transverse emittance for Candidate A.

(b) Longitudinal macro-particle distribution vs transverse emittance for Candidate B.

**Figure 7.6:** No space-charge: longitudinal macro-particle distribution vs transverse emittance.



**Figure 7.7:** No space-charge: tune heatmaps.

### 7.3.2 Space-charge candidates

All space-charge candidate figures in this subsection use 3D PIC space charge with Configuration I. In Fig. 7.8, the phase spaces of the space-charge candidates are shown. Fig. 7.8a shows visible particle loss, a pronounced four-fold structure in  $y$  and an almost triangular structure in  $x$ . In  $z$ , it can be seen that particle loss mainly has occurred for negative momentum deviation. For Candidate D in Fig. 7.8b, the four-fold structure in  $y$  is, while present, less pronounced than in Fig. 7.8a. In  $x$ , the four-fold structure is also present. For both candidates, the longitudinal phase space "curls" upon itself, similar to previous observations in Chapter 4.

In Fig. 7.11, longitudinal macro-particle distribution is compared against transverse beam size. There is some similarity in high-ranking versus low-ranking candidates as seen for no space-charge in Fig. 7.6: For the low-ranking candidate, surviving candidates are concentrated almost at a single point longitudinally, with a smaller beam size at this point. Fig. 7.11b has two peaks rather than one as seen in Fig. 7.6b, perhaps caused by space-charge interacting with the non-linear dynamics.

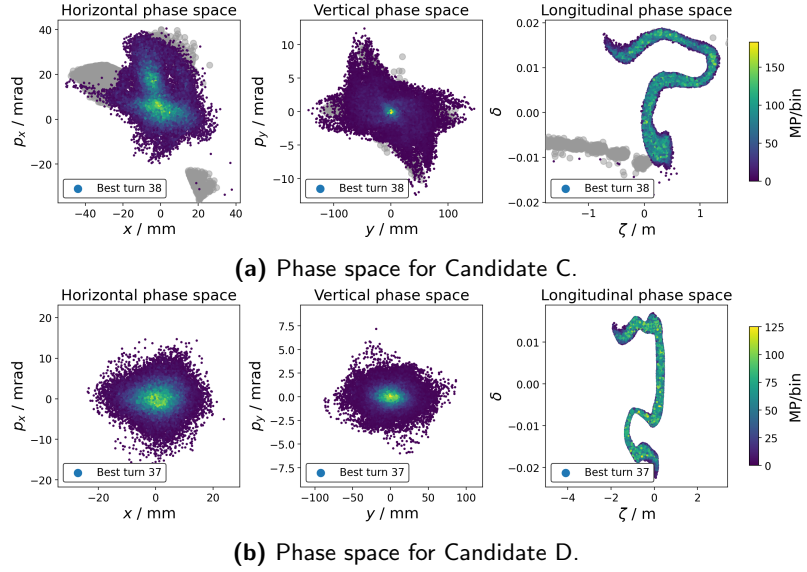
In Fig. 7.9 and Fig. 7.10, real space  $z - x$  and  $z - y$  scatters are shown, both for the best  $\sigma_z$  turn and for turn 41. Similarly to what was observed in Chapter 4, the longitudinal modulation of the bunch increases after the optimal turn. This eliminates the possibility that the microbunching would be working-point dependent.

In Fig. 7.12, emittance and bunch length per turn is plotted for the two candidates. For the low-ranking candidate in Fig. 7.12a, the horizontal emittance has blown up already by turn 20, and a further jump is seen up to turn 38 when momentum spread is high. For the high-ranking candidate, Fig. 7.12b, both transverse emittances blow up close to turn 37. In Fig. 7.13, transmission per turn is plotted for the two candidates. From Fig. 7.13a, loss of particles begins already at turn 10, and more than 20% of the particles have been lost by turn 20, further reach-

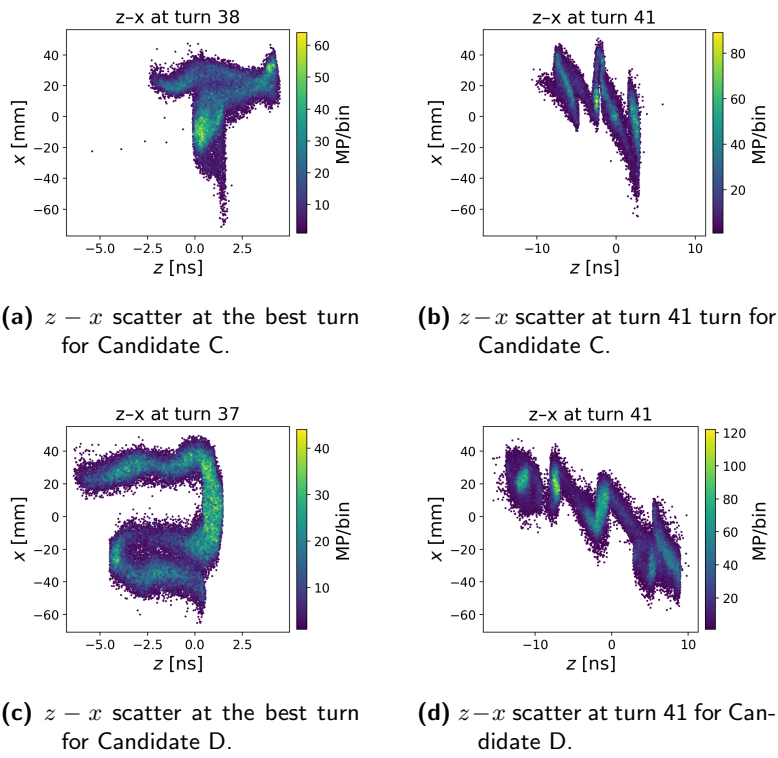
ing almost 60% by turn 38. In contrast, no transmission loss is observed for the high-ranking candidate in Fig. 7.13b. While the horizontal blow-up at turn 20 for the low-ranking candidate is likely caused by some form of resonance, the blow-ups observed close to the final turns possibly have the same reason as observed and discussed in Chapter 5: it is likely a sextupolar-driven effect for particles of high-momentum deviation.

In Fig. 7.14, tune heatmaps for the candidates are shown. For the low-ranking candidate in Fig. 7.11a, a high concentration of particles are seen on the integer line, as well as on the half-integer line, aligning with the discussion in the previous paragraph. In Fig. 7.14b, a tune spread more akin to what is discussed in Section 2.10.1 is seen. It avoids crossing any half-integer line, and avoids the vertical integer line thanks to the space-charge tune shift.

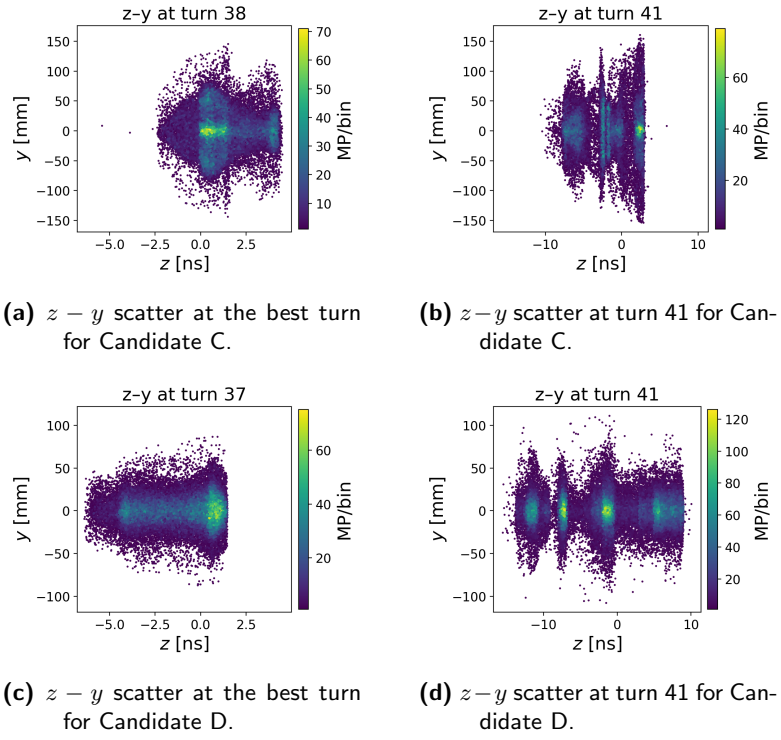
While Candidate D may need to be further evaluated, for example through modeled imperfections to confirm that the integer line would not be crossed, it may provide a promising example. As it reaches a final bunch length of 1.95 ns, it fulfills the constraints set for the 5 GeV option.



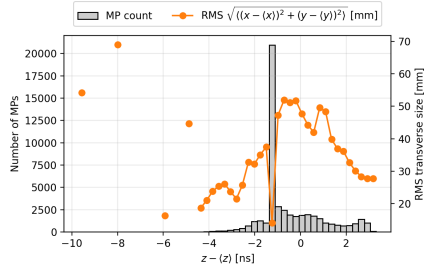
**Figure 7.8:** Space-charge: phase-space comparison at the best sigma-z turn.



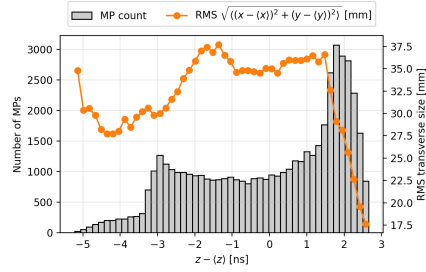
**Figure 7.9:** Space-charge:  $z-x$  scatter comparison at the best  $\sigma_z$  turn and at turn 41 for candidates C and D.



**Figure 7.10:** Space-charge:  $z - y$  scatter comparison at the best  $\sigma_z$  turn and at turn 41 for candidates C and D.

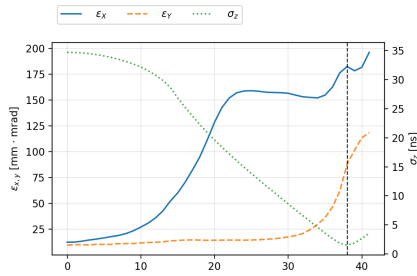


(a) Longitudinal macro-particle distribution vs transverse emittance for Candidate C.

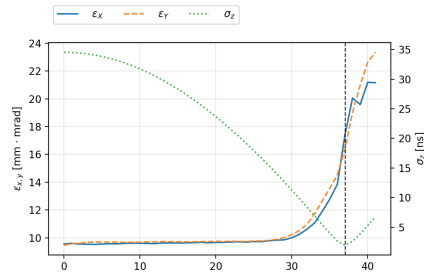


(b) Longitudinal macro-particle distribution vs transverse emittance for Candidate D.

**Figure 7.11:** Space-charge: longitudinal macro-particle distribution vs transverse emittance.

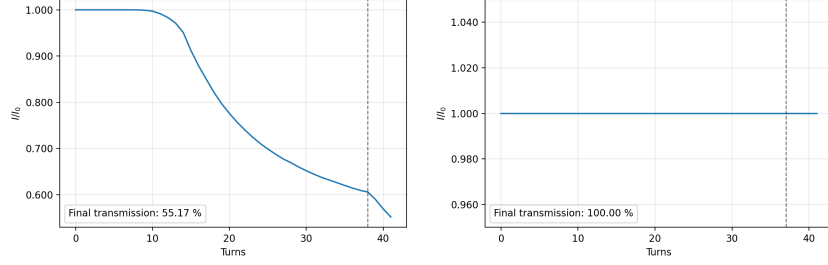


(a) Emittance vs turns for Candidate C.



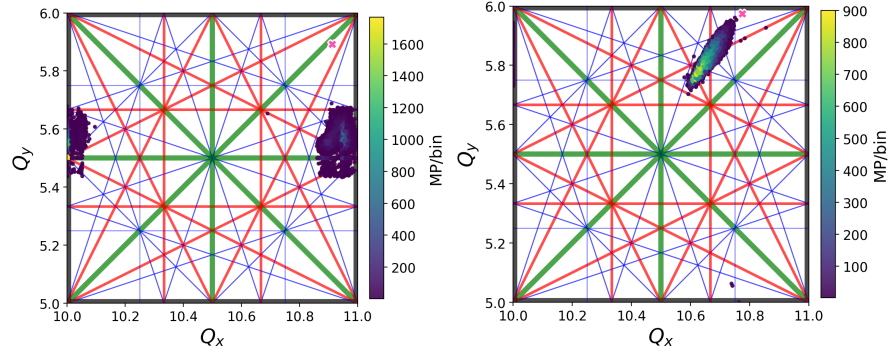
(b) Emittance vs turns for Candidate D.

**Figure 7.12:** Space-charge: emittance vs turns.



(a) Transmission for Candidate C.

(b) Transmission for Candidate D.

**Figure 7.13:** Transmission for space-charge candidates.

(a) Tune heatmap for Candidate C.

(b) Tune heatmap for Candidate D.

**Figure 7.14:** Space-charge candidates: tune heatmaps between turn 0 and respective best  $\sigma_z$  turns.

## 7.4 Discussion

While Candidate D fulfills target constraints, this work will need to be iterated upon before drawing any final conclusions. As shown in Appendix F, the lack of boundary conditions likely implies a degree of loss of meaningful physics. As observed in Appendix G, discontinuities at the longitudinal edges of the beam possibly distort the results. The microbunching discussed in Chapter 4 is not fully understood. To remove the four-fold structure discussed in Chapter 5, additional sextupole families may be needed. If adjustments are performed, to address any of these concerns, it is possible the optimal working point will yet again need to be evaluated. Still, Candidate D will be a suitable starting point for any further investigations.

## Conclusion

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This study has evaluated the current design for the IMCC Muon Collider proton compressor. Further, it has evaluated the limits of previous and new simulations performed with Xsuite with the goal to determine if it is sufficient to model the dynamics of the system. It has further aimed to improve upon previous simulations through additions to the Xsuite source code, such as developing an adaptive mesh as well as adding a low-pass filter. A convergence study for the improved space-charge configuration has been conducted. A four-fold structure has been investigated, and different design alterations to the current lattice have been explored. Tune scans have further been conducted, both without space charge, and with an altered Xsuite space-charge model.

It has been found that employing 3D space-charge with an adaptive mesh gives a result that significantly differs compared to previous 2.5D simulations which further employed a static mesh. This is expressed most clearly in the longitudinal phase space, which is significantly altered. In addition, the likely turn of extraction is changed with the new configuration. The new configuration introduces longitudinal microbunching when the mesh re-expands and when grid resolution is increased. This may be partially suppressed if a low-pass filter is applied. However, it is not known whether the microbunching is fully numerical or physical in nature. Experiments have determined that the four-fold structure is likely caused by the sextupoles, and external research has confirmed that this is thereafter excited as a true resonance by space-charge. A new tune scan has provided a new working point for the compressor that performs sub-2 ns compression. However, the four-fold structure is not eliminated. For this reason, alternate designs of the lattice should be explored, for example, through the addition of more sextupole families.

As it is not yet clear to which degree the observed microbunching is physical or numerical, further investigations are needed. It would be advisable to test a high-resolution mesh with a sufficient amount of macro-particles to determine whether the adaptive mesh causes, or at least amplifies, the microbunching. Further, as the space-charge should be significantly affected by boundary conditions, Xsuite will, in its current form, not capture the complete dynamics of the proton compressor.



Validative studies, using other codes and/or empirical measurements, are therefore needed to confirm any findings in this study that have employed 3D space charge.

This study has shown that the dynamics of space-charge is changed by using 3D space-charge rather than 2.5D space-charge, and similarly for using an adaptive mesh versus a static one. It has been found that a 3D model as well as using an adaptive mesh greatly changes the dynamics of the compression. Most likely, a 3D model together with the higher resolution offered by the adaptive mesh is needed to evaluate the compressor design. The current compressor design can compress to 2 ns; however, the investigated four-fold structure could not be completely suppressed, and further design iterations would be needed to fully eliminate it. In conclusion, the current design is limited not only by space-charge but also by a four-fold structure driven by sextupoles, further excited as a resonance by space-charge. These simulations do not indicate this to be a major showstopper, but more studies, especially empirical ones, are needed to make any conclusive statements.

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## General Hamiltonian

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The Hamiltonian for a particle traveling in a magnetic field, for which derivation can be found in [30, p.59-80], is:

$$H = -(1+hx) \left( \frac{\delta}{\beta_{\text{ref}}} \sqrt{\left( \delta + \frac{1}{\beta_{\text{ref}}} - \frac{q\phi}{cP_0} \right)^2 - (p_x - a_x)^2 - (p_y - a_y)^2 - \frac{1}{\beta_{\text{ref}}^2 \gamma_{\text{ref}}^2}} + a_s \right) \quad (\text{A.1})$$

Here,  $H$  is directly or indirectly dependent on the following:

- $x$  (horizontal coordinate) and  $y$  (vertical coordinate) are the coordinates for a plane perpendicular to the reference trajectory, while  $s$  is the length along the reference trajectory [30, p. 75].  $z$  is the longitudinal offset and  $\delta$  the energy deviation from the reference particle (both make up the longitudinal coordinates) [30, p. 71]
- $h$  is the curvature of the reference trajectory with  $h = \frac{1}{\rho}$  where  $\rho$  is the radius of the curvature [30, pp. 73, 75]
- $\beta_{\text{ref}}$  is the speed of the reference particle scaled by the speed of light and  $\gamma_{\text{ref}} = \frac{1}{\sqrt{1-\beta_{\text{ref}}^2}}$  [30, p. 70]
- $P_0$  is the reference momentum [30, p. 68]
- $\phi$  is the scalar potential [30, p. 16]
- $c$  is the speed of light [30, p. 20]
- $a_x$ ,  $a_y$  and  $a_s$  are components of the scaled vector potential in the direction of increasing  $x$ ,  $y$  and  $s$  respectively. [30, p. 75]
- $p_x$  and  $p_y$  are canonical momenta who depend on  $x$ ,  $y$  as well as their time derivatives, vector potentials and indirectly on  $z$  as well as  $\delta$ . [30, pp. 74, 75]

Eq. (A.1) is not a description of the energy of a system, but rather describes the evolution of the system along  $s$ . This Hamiltonian can represent a straight beamline by setting  $\rho$  to be infinite ( $\Rightarrow h = 0$ ), giving the following equation [30, p. 75]:

$$H = \frac{\delta}{\beta_{\text{ref}}} - \sqrt{\left(\delta + \frac{1}{\beta_{\text{ref}}} - \frac{q\phi}{cP_0}\right)^2 - (p_x - a_x)^2 - (p_y - a_y)^2 - \frac{1}{\beta_{\text{ref}}^2 \gamma_{\text{ref}}^2}} - a_s \quad (\text{A.2})$$

This Hamiltonian may then be used to derive element-specific transfer maps, which is done in following appendices.

## Hamiltonian derivations for magnets

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### B.0.1 Drift space

Since the ideal drift space is a region with no applied fields or forces, the scalar and vector potential can be set to zero with an appropriate gauge [30, p. 85]. With a bending radius of zero, this gives the following Hamiltonian:

$$H = \frac{\delta}{\beta_{\text{ref}}} - \sqrt{\left(\delta + \frac{1}{\beta_{\text{ref}}}\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_{\text{ref}}^2 \gamma_{\text{ref}}^2}} \quad (\text{B.1})$$

Instead of deriving the equations of motion from this Hamiltonian and then linearizing the solutions, the Hamiltonian is first linearized to ensure the transfer map remains symplectic (as described in Section 2.3, symplecticity is conserved under linear transformation). Expanding the Hamiltonian (B.1) to second order in the dynamical variables gives, omitting constant, third order and higher order terms: [30, p. 87]

$$H_2 = \frac{p_x^2}{2} + \frac{p_y^2}{2} + \frac{\delta^2}{2\beta_{\text{ref}}^2 \gamma_{\text{ref}}^2} \quad (\text{B.2})$$

Inserting this into Hamilton's equations finally gives the linear transfer map ( $L$  being the length of the element): [30, pp. 86-87]

$$\begin{cases} x_1 = x_0 + Lp_{x0} \\ p_{x1} = p_{x0} \\ y_1 = y_0 + Lp_{y0} \\ p_{y1} = p_{y0} \\ z_1 = z_0 + \frac{L}{\beta_{\text{ref}}^2 \gamma_{\text{ref}}^2} \delta_0 \\ \delta_1 = \delta_0 \end{cases} \quad (\text{B.3})$$

where second order terms have been omitted. The subscript 0 indicates the state just before entering the drift space, and the subscript 1 indicates just after [30, p. 86]. While this transfer map was derived using the Hamiltonian, it can also be realized by reflecting on the physical system; if a particle enters a system with constant momentum and is not accelerated, its transverse coordinates will change proportionally to the momentum and the length it is traveling. The true non-linear map also accounts for non-ideal particles, as these will have a different path length in the drift depending on their longitudinal momentum. Usually, this difference between ideal and non-ideal particles can be neglected, and (B.3) is sufficient [30, p. 86].

The linear transfer map (B.3) may be described in a more concise way using matrices:

$$\vec{x}_1 = R_{\text{drift}} \vec{x}_0 \quad (\text{B.4})$$

where  $\vec{x} = (x \quad p_x \quad y \quad p_y \quad z \quad \delta)^T$  and the transfer matrix of the system is:

$$R_{\text{drift}} = \begin{pmatrix} 1 & L & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & L & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & \frac{L}{\beta_{\text{ref}}^2 \gamma_{\text{ref}}^2} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{B.5})$$

This matrix is block diagonal, and if one wishes to work only with a certain plane, one may simply pick out the relevant block (and relevant components from  $\vec{x}$ ). All block matrices can be seen to be 2x2 identity matrices with the addition of a positive constant at (1,2).

### B.0.2 Dipole magnet

Due to the bent trajectory, the Hamiltonian (A.1) is needed as the particle path will be curved [30, p. 88]. Compared to a drift space, there is now also a magnetic field applied to particles passing through the dipole. Assuming the dipole has a constant strength  $\mathbf{B} = (0, B_0, 0)$ , the scaled vector potential is chosen to be [30, pp. 89–90]:

$$\mathbf{a} = \frac{q}{B_0} \mathbf{A} = \left( 0, 0, -k_0 x + \frac{k_0 h x^2}{2(1 + hx)} \right) \quad (\text{B.6})$$

where  $k_0$  is defined as the normalized field strength:

$$k_0 = \frac{q}{F_0} B_0 \quad (\text{B.7})$$

Inserting (B.6) into (A.1) and once again performing the paraxial approximation gives:

$$H_2 = \frac{p_x^2}{2} + \frac{p_y^2}{2} + \frac{\delta^2}{2\beta_0^2\gamma_0^2} + \left(k_0 - h \left(1 + \frac{\delta}{\beta_0}\right)\right)x + \frac{k_0 h x^2}{2} \quad (\text{B.8})$$

The transfer map is expressed as follows:

$$\vec{x}_1 = R_{\text{dipole}} \vec{x}_0 + \vec{m}_{\text{dipole}} \quad (\text{B.9})$$

Below, the transfer matrix for a horizontal bending magnet with a uniform field and edges orthogonal to the reference trajectory is presented, where  $L$  is the element length [30, p. 95]:

$$R_{\text{dipole}} = \begin{pmatrix} c_x & s_x & 0 & 0 & 0 & \frac{\bar{h}(1-c_x)}{\omega_x^2} \\ -\omega_x^2 s_x & c_x & 0 & 0 & 0 & \bar{h} s_x \\ 0 & 0 & 1 & L & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ -\bar{h} s_x & -\frac{\bar{h}(1-c_x)}{\omega_x^2} & 0 & 0 & 1 & \frac{L}{\beta_{\text{ref}}^2 \gamma_{\text{ref}}^2} - \frac{\bar{h}^2(L-s_x)}{\omega_x^2} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{B.10})$$

where

$$\vec{m}_{\text{dipole}} = \begin{pmatrix} (h - k_0) \frac{1-c_x}{\omega_x^2} \\ (h - k_0) s_x \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

and

$$s_x = \frac{\sin(\omega_x L)}{\omega_x}, \quad c_x = \cos(\omega_x L), \quad \bar{h} = \frac{h}{\beta_{\text{ref}}}, \quad \omega_x = \sqrt{\bar{h} k_0} \xrightarrow{k_0=h} \sqrt{\bar{h} h}.$$

The vertical phase space is completely uncoupled (elements for row 2 and 3 are 0 at columns not 2 and 3 and vice versa), while this is not the case for the horizontal and longitudinal phase space.

### B.0.3 Quadrupole

As the reference trajectory through a quadrupole is straight, (A.2) may once again be used as Hamiltonian [30, pp. 92, 94]. Using Eq. (2.6), the vector potential for a quadrupole can be expressed as the following [30, p. 129]:

$$\mathbf{a} = \left( 0, 0, -\frac{k_1}{2}(x^2 - y^2) \right) \quad (\text{B.11})$$

Inserting into (A.2) gives:

$$H = \frac{\delta}{\beta_{\text{ref}}} - \sqrt{\left(\delta + \frac{1}{\beta_{\text{ref}}}\right)^2 - p_x^2 - p_y^2} - \frac{1}{\beta_{\text{ref}}^2 \gamma_{\text{ref}}^2} - \frac{k_1}{2}(x^2 - y^2) \quad (\text{B.12})$$

Once again performing the paraxial approximation and dropping zero-order/third-order-and-higher terms gives:

$$H_2 = p_x^2 + p_y^2 + \frac{\delta^2}{2\beta_{\text{ref}}^2 \gamma_{\text{ref}}^2} + \frac{k_1}{2}(x^2 - y^2) \quad (\text{B.13})$$

The transfer matrix then becomes, where  $L$  is the quadrupole length and  $\omega = \sqrt{k_1}$ :

$$R_{\text{quadrupole}} = \begin{pmatrix} \cos(\omega L) & \frac{\sin(\omega L)}{\omega} & 0 & 0 & 0 & 0 \\ -\omega \sin(\omega L) & \cos(\omega L) & 0 & 0 & 0 & 0 \\ 0 & 0 & \cosh(\omega L) & \frac{\sinh(\omega L)}{\omega} & 0 & 0 \\ 0 & 0 & \omega \sinh(\omega L) & \cosh(\omega L) & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & \frac{L}{\beta_{\text{ref}}^2 \gamma_{\text{ref}}^2} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{B.14})$$

The nature of the horizontal and vertical block will depend on if  $k_1$  is positive or negative. If  $k_1$  is positive, then  $\omega$  is real, implying that particles will be focused in the horizontal plane while defocused in the vertical plane. If  $k_1$  were instead negative, we would have hyperbolic functions in the horizontal block while the vertical would now have sin- and cosine elements. In other words, the case would be reversed. For the focusing plane, particles will have the movement of a harmonic oscillator. These transverse oscillations are called **betatron oscillations** [30, p. 92]. Usually, the length of components that cause betatron oscillations are only a fraction of the oscillations' wavelength [30, pp. 102–103]. While this matrix shows no coupling between the longitudinal plane and the horizontal/vertical, the momentum will in reality affect the strength of the focusing in the form of chromaticity [29, p. 108].

The matrix (B.14) may be further simplified using the so-called **thin lens approximation**. In this approximation, the length of the quadrupole is set to 0 while  $k_1 L \rightarrow \frac{1}{f}$  where  $f$ , the **focal length**, is constant. A vertically focusing matrix is obtained simply by switching  $f$  with  $-f$  [30, pp. 129–130]. The horizontally focusing quadrupole then has the transfer matrix:

$$R_{\text{quad\_thin\_x}} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{f} & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{f} & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{B.15})$$

The thin lens approximation thus leaves the coordinates unchanged while applying opposing focusing kicks in the transverse planes.

#### B.0.4 Sextupole

The vector potential for a sextupole is, with  $k_2 = \frac{q}{P_0} \frac{\partial^2 B_y}{\partial x^2}$  [30, p. 282]:

$$\mathbf{a} = (0, 0, -\frac{1}{6}k_2(x^3 - 3xy^2)) \quad (\text{B.16})$$

With a straight reference trajectory through the sextupole, (A.2) is used with the vector potential which gives [30, p. 283]:

$$H = \frac{\delta}{\beta_{\text{ref}}} - \sqrt{(\delta + \frac{1}{\beta_{\text{ref}}})^2 - p_x^2 - p_y^2} - \frac{1}{\beta_{\text{ref}}^2 \gamma_{\text{ref}}^2} + \frac{1}{6}k_2(x^3 - 3xy^2) \quad (\text{B.17})$$

As the sextupole is a non-linear element, their fields cannot be linearized. Nevertheless, a simpler form of the Hamiltonian is given by assuming a thin sextupole [30, p. 284]:

$$H = \frac{1}{6}k_2(x^3 - 3xy^2) \quad (\text{B.18})$$

A matrix representation is not possible due to the sextupoles' non-linear nature. Inserting (B.18) into Hamilton's equations gives the following transfer map, where  $k_2 L_{\text{sext}}$  is the integrated sextupole strength:

$$\begin{cases} \Delta p_x = -\frac{1}{2}k_2 L_{\text{sext}}(x^2 - y^2) \\ \Delta p_y = k_2 L_{\text{sext}}xy \end{cases} \quad (\text{B.19})$$

Unlike the quadrupole case, the quadratic dependence on the transverse coordinates makes the sextupole intrinsically non-linear.





## RF-cavities

---

The transfer map for the RF-cavity will depend on the shape of the cavity itself and its operating mode [38]. The following section will derive the transfer map for a  $TM_{010}$  pillbox cavity [30, pp. 109–110]. The geometry of a pillbox cavity allows us to derive analytical solutions, and is approximately similar to "real" elliptical cavities where edges are rounded rather than hard [38]. The pillbox and elliptical cavities are examples of standing wave cavities, *i.e.* the electric fields are standing waves as opposed to traveling along the structure.

The electric and magnetic fields in the cavity can be written using cylindrical polar coordinates as:

$$\begin{cases} \mathbf{E} = (0, 0, E_0 J_0(kr) \sin(\omega t + \phi_0)) \\ \mathbf{B} = (0, \frac{E_0}{c} J_1(kr) \cos(\omega t + \phi_0), 0) \end{cases} \quad (\text{C.1})$$

where  $r = \sqrt{x^2 + y^2}$ ,  $E_0$  is the field amplitude, while  $J_0$  and  $J_1$  are the zeroth- and first order Bessel functions respectively [30, p. 56]. The frequency  $\omega$  is given by  $\omega = \frac{k}{c}$  with  $k = \frac{p_{01}}{a}$  where  $p_{01}$  is the first zero of  $J_0$  and  $a$  is the cavity radius. [30, p. 110] For the purpose of maximum acceleration of the particles, the cavity length should ideally be  $\frac{L}{\beta_{\text{ref}} c} = \frac{\pi}{\omega}$ . As the electric field will oscillate with time, having a longer length would eventually result in the particles experiencing deceleration as the field changes sign [30, p. 111]. A shorter length will on the other hand provide less time for the particles to be accelerated.

The potential for these fields, with a suitable gage choice, is given by [30, p. 111]:

$$\mathbf{A} = (0, 0, \frac{E_0}{\omega} J_0(kr) \cos(\omega t + \phi_0)) = (0, 0, \frac{E_0}{\omega} J_0(kr) \cos(\frac{ks}{\beta_{\text{ref}}} - kz + \phi_0)) \quad (\text{C.2})$$

where the time dependence is replaced with a dependence on the independent variable  $s$  in the second equality.  $\phi_0$  is a phase offset. Finally, since the reference

trajectory is straight, the Hamiltonian (A.2) may once again be used which gives [30, p. 111]:

$$H = \frac{\delta}{\beta_{\text{ref}}} - \sqrt{\left(\delta + \frac{1}{\beta_{\text{ref}}}\right)^2 - (p_x - a_x)^2 - (p_y - a_y)^2 - \frac{1}{\beta_{\text{ref}}^2 \gamma_{\text{ref}}^2}} - \frac{qE_0}{P_0 \omega} J_0(kr) \cos\left(\frac{ks}{\beta_{\text{ref}}} - kz + \phi_0\right) \quad (\text{C.3})$$

As the field in an RF-cavity varies with time, which implies that (C.3) is explicitly dependent on  $s$ , solving the equations of motion is comparatively harder than for the previous elements. A practical simplification is simply taking the average of the Hamiltonian over the cavity (*i.e.* integrating it for the cavity length and divide by  $L$ ) and then performing the paraxial approximation once again. This gives [30, p. 112]:

$$H_2 = \frac{p_x^2}{2} + \frac{p_y^2}{2} + \frac{\delta^2}{2\beta_{\text{ref}}^2 \gamma_{\text{ref}}^2} + \frac{\alpha}{4\pi} \cos(\phi_0) k^2 (x^2 + y^2) - \frac{\alpha}{\pi} \sin(\phi_0) kz + \frac{\alpha}{2\pi} \cos(\phi_0) k^2 z^2 \quad (\text{C.4})$$

with:

$$\begin{cases} \alpha = \frac{qV_0}{P_0 c} \\ \frac{V_0}{L} = E_0 T \\ T = \frac{2\pi\beta_{\text{ref}}}{k^2 L^2} \sin\left(\frac{kL}{2\beta_{\text{ref}}}\right) \end{cases} \quad (\text{C.5})$$

where  $V_0$  is the **cavity voltage**, and  $T$  is the **transit-time factor**. The transit-time factor is the ratio between the average accelerating potential and the maximum accelerating potential (*i.e.* a ratio for particles who require time in passing the cavity and thus experiencing a time variation of the accelerating potential, versus conceptual particles instantly passing the cavity at maximum potential) [43, p. 185]. The fourth term in (C.4) implies simultaneous focusing in  $x$  and  $y$ . The fifth term gives a change in energy that depends on the phase  $\phi_0$  and is proportional to  $V_0$ . The sixth term is also dependent on these, but also introduces a dependence on the particle coordinates, providing longitudinal focusing. Now, using (C.4) to finally solve the equations of motion gives the linear transfer map [30, p. 113]:

$$\vec{x}_1 = R_{rf} + m_{rf} \vec{r}_f \quad (\text{C.6})$$

with:

$$R_{\text{rf}} = \begin{pmatrix} c_{\perp} & s_{\perp} & 0 & 0 & 0 & 0 \\ -\omega_{\perp}^2 s_{\perp} & c_{\perp} & 0 & 0 & 0 & 0 \\ 0 & 0 & c_{\perp} & s_{\perp} & 0 & 0 \\ 0 & 0 & -\omega_{\perp}^2 s_{\perp} & c_{\perp} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{\parallel} & \frac{1}{\beta_{\text{ref}}^2 \gamma_{\text{ref}}^2} s_{\parallel} \\ 0 & 0 & 0 & 0 & -\beta_{\text{ref}}^2 \gamma_{\text{ref}}^2 \omega_{\parallel}^2 s_{\parallel} & c_{\parallel} \end{pmatrix}, \quad (\text{C.7})$$

$$\vec{m}_{\text{rf}} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ (1 - \cos(\omega_{\parallel} L)) \frac{\tan \phi_0}{k} \\ \beta_{\text{ref}}^2 \gamma_{\text{ref}}^2 \omega_{\parallel} \sin(\omega_{\parallel} L) \frac{\tan \phi_0}{k} \end{pmatrix}. \quad (\text{C.8})$$

The transverse components are given by:

$$\begin{cases} c_{\perp} = \cos(\omega_{\perp} L) \\ s_{\perp} = \frac{\sin(\omega_{\perp} L)}{\omega_{\perp}} \\ \omega_{\perp} = k \sqrt{\frac{\alpha \cos \phi_0}{2\pi}} \end{cases} \quad (\text{C.9})$$

and the longitudinal by:

$$\begin{cases} c_{\parallel} = \cos(\omega_{\parallel} L) \\ s_{\parallel} = \frac{\sin(\omega_{\parallel} L)}{\omega_{\parallel}} \\ \omega_{\parallel} = \frac{k}{\beta_{\text{ref}} \gamma_{\text{ref}}} \sqrt{\frac{\alpha \cos \phi_0}{\pi}} \end{cases} \quad (\text{C.10})$$

The focusing-like effects described above are present in (C.7). Meanwhile, the vector (C.8) provides the following acceleration for a particle with originally  $z = 0$  [30, p. 114]:

$$\Delta\delta = \beta_{\text{ref}}^2 \gamma_{\text{ref}}^2 \omega_{\parallel} \sin(\omega_{\parallel} L) \frac{\tan \phi_0}{k} = [\omega_{\parallel} L \ll 1] = \frac{qV_0}{P_0 c} \frac{kL}{\pi} \sin \phi_0 \quad (\text{C.11})$$

For maximum acceleration, the cavity length should be  $kL \approx \pi$  giving:

$$\Delta\delta \approx \frac{qV_0}{P_0 c} \sin \phi_0 \quad (\text{C.12})$$

A higher-order map of the RF-cavity would introduce a dependence on the energy deviation of particles. In the provided transfer map, acceleration is described by  $\delta$  while the reference momentum is unchanged. For large changes in energy and therefore in  $\delta$ , one may wish to change the reference momentum. However, this comes at the cost of losing symplecticity [30, pp. 114–115].

It is also possible to make a thin approximation of an RF-cavity. By taking  $L \rightarrow 0$ , with  $\frac{1}{f_{\parallel}} = \frac{qV}{P_0 c} k \cos \phi_0$  [67, pp. 29–30]:

$$R_{\text{rf}} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{f_{\parallel}} & 1 \end{pmatrix}, \quad (\text{C.13})$$

and:

$$\vec{m}_{\text{rf}} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \frac{qV}{P_0 c} \sin \phi_0 \end{pmatrix}. \quad (\text{C.14})$$

In other words, the thin-lens RF cavity does not affect the transverse planes, and provides purely a phase-dependent longitudinal kick.

## Frequency Map Analysis

---

In one dimension, provided normalized coordinates, a complex quantity  $w$  is given as:

$$w = x_n - ip_{x,n} = \sqrt{2J_x} e^{i\phi_x} \quad (\text{D.1})$$

Furthermore, given the initial phase  $\phi_{x0}$  and the tune  $Q_x$ , this quantity becomes on the  $n$ :th turn:

$$w_n = \sqrt{2J_x} e^{i\phi_{x0}} e^{2\pi i n Q_x} \quad (\text{D.2})$$

The DFT of  $w$  is given as:

$$\hat{w}_m = \frac{1}{N} \sum_{n=0}^{N-1} e^{-2\pi i m n / N} w_n \quad (\text{D.3})$$

where  $m \in [0, N - 1]$ . Inserting Eq. (D.2) into Eq. (D.3) gives:

$$\hat{w}_m = \sqrt{2J_x} e^{i\phi_{x0}} \frac{1 - e^{2\pi i \Delta}}{1 - e^{2\pi i \Delta / N}} \quad (\text{D.4})$$

where  $\Delta = N\{\nu_x\} - m$ . If  $m$  is allowed to take any real value, one can numerically search the fractional part of the tune as follows:

$$\{Q_x\} = \frac{\tilde{m}}{N} \quad (\text{D.5})$$

where  $\tilde{m}$  is the value of  $m$  which maximizes  $\hat{w}$ . The process in which determining which  $m$  gives the maximum  $\hat{w}$  is the basis for what is known as **Numerical Analysis of the Fundamental Frequencies** (NAFF). This process can be done not only to find the dominant frequency, but also the secondary frequency and so

on by simply repeating the process. In non-linear systems, the tunes of particles may have several spectral components. Additional frequencies in the spectrum of a particle may appear from e.g. betatron coupling (the vertical tune appearing in the horizontal spectrum and vice versa), or simply from numerical errors. The presence of multiple frequencies affect the accuracy of identifying the correct main frequency. By simply employing the DFT, the accuracy scales as  $1/N$ . By employing NAFF (searching for  $m$  maximizing  $\hat{w}$ ) gives an improved accuracy of  $1/N^2$ . The use of a Hanning filter:

$$\chi_p(n) = \frac{2^p(p!)^2}{(2p)!} \left(1 + \cos \frac{2\pi n}{N}\right)^p \quad (\text{D.6})$$

where  $\hat{w}$  is calculated as follows:

$$\hat{w}_m^{(p)} = \frac{1}{N} \sum_{n=0}^{N-1} e^{-2\pi i m n / N_t} w_n \chi_p(n) \quad (\text{D.7})$$

will further improve the accuracy according to  $1/N^{2p+2}$ .

## Particle-in-Cell Theory

---

The way in which the charge of macro-particles is deposited onto the mesh depends on the interpolation technique. One of the simplest methods is the so-called Nearest Grid Point (NGP) scheme [55, pp. 123–124]. In this scheme, the complete charge of a macro-particle is assigned to the closest grid-point in the mesh. Although computationally efficient, the crudeness of this technique can lead to significant numerical errors. This motivates the use of higher-order interpolation, such as the **Cloud-in-Cell** (CIC) model, which is piecewise continuous, or even the **Triangular-Shaped-Cloud** (TSC) model, which is piecewise quadratic [55, pp. 125–127, 135–136]. The three schemes are compared in Fig. E.1. In Fig. E.1a, the 1D shape functions of each scheme is shown for the central grid point. Depending on where the actual charge is located, this represents how much of the charge will be distributed to the grid point. In Fig. E.1b, it is visualized how a charge at the red dotted line deposits its charge to nearby grid points. In Fig. E.1c, aliasing is visualized for the three schemes; it shows a trade-off of locality versus smoothness and reduced aliasing. A 2D CIC scheme is shown in Fig. 2.20.

For CIC, an ensemble of  $N$  particles in a one dimensional system, the mesh-deposited charge function can be described as follows: [55, pp. 123–127]

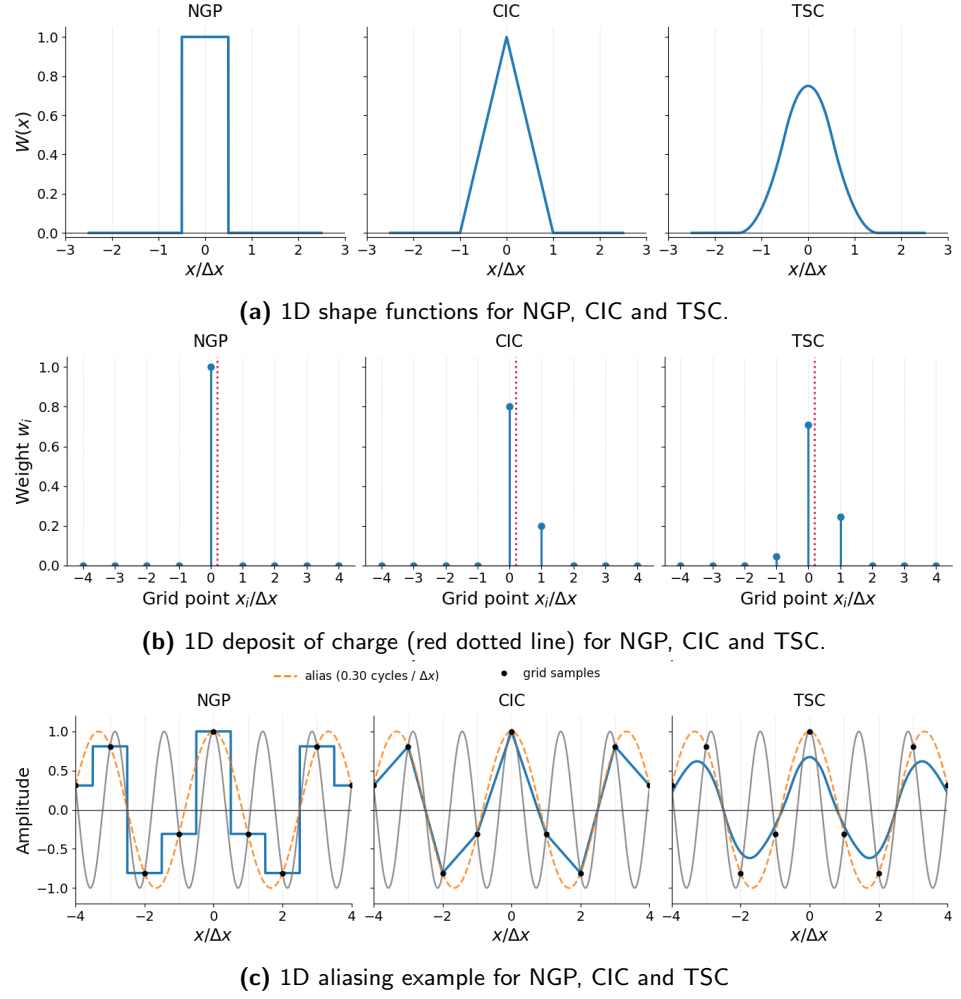
$$\rho(x_p) = \frac{1}{L} \sum_{i=1}^N q_i W(x_i - x_p) \quad (\text{E.1})$$

where  $x_p$  is the position of the mesh point  $p$ , while  $x_i$  and  $q_i$  are the position and charge of particle  $i$ .  $W$ , the shape function, is given as:

$$W(x - x_p) = \begin{cases} 1 - \frac{|x - x_p|}{H}, & \text{if } |x - x_p| \leq H \\ 0, & \text{otherwise} \end{cases} \quad (\text{E.2})$$

where  $H$  is the cell size. The force interpolation function is also used for the force calculation:





**Figure E.1:** 1D comparison of NGP, CIC and TSC. Subfigure a) shows the shape function, b) charge deposit and c) an example of how the three schemes treat a signal above the Nyquist limit.

$$F(x) = \sum_p W(x - x_p) E(x_p) \quad (\text{E.3})$$

where  $E$  is the mesh-deposited electric field. In 2D and 3D, the force interpolation function becomes  $W(x, y) = W(x)W(y)$  and  $W(x, y, z) = W(x)W(y)W(z)$  respectively [55, p. 140]. Eq. (E.1) becomes valid either by exchanging  $L$  with the total area  $A$  or the total volume  $V$  for these two cases. For CIC, the number of grid points on which charge is deposited is  $2^d$  [55, p. 144]. In other words, this implies two grid points for one dimension, four grid points for 2D and 8 for 3D.

As Particle-in-Cell employs a discrete mesh, the particle distribution will to some degree be undersampled (see Fig. E.1c) [55, p. 225]. Intuitively, think what happens between two particles if one of them crosses a cell border into another: for NGP, the interparticle force will go from zero to its max, and the same is the case for the first derivative in CIC [55, pp. 124–125, 136]. High wavenumber (high- $k$ ) harmonics (meaning short wavelength in real space) will therefore alias into lower harmonics in the so-called **principal zone** (also known as the first Nyquist zone):

$$|k| < \frac{\pi}{\Delta} \quad (\text{E.4})$$

where  $k$  is the wavenumber and  $\Delta$  the mesh spacing. Harmonics beyond this wavenumber, and therefore of wavelength  $2\Delta$ , will contribute to harmonics in the principal zone with wavenumber  $k' = k \bmod k_g$ . These aliases are the source of unphysical mode coupling, introducing errors in the forces [55, pp. 236–241]. If large enough, these errors will contribute to non-physical instabilities as well as to the previously mentioned grid heating.

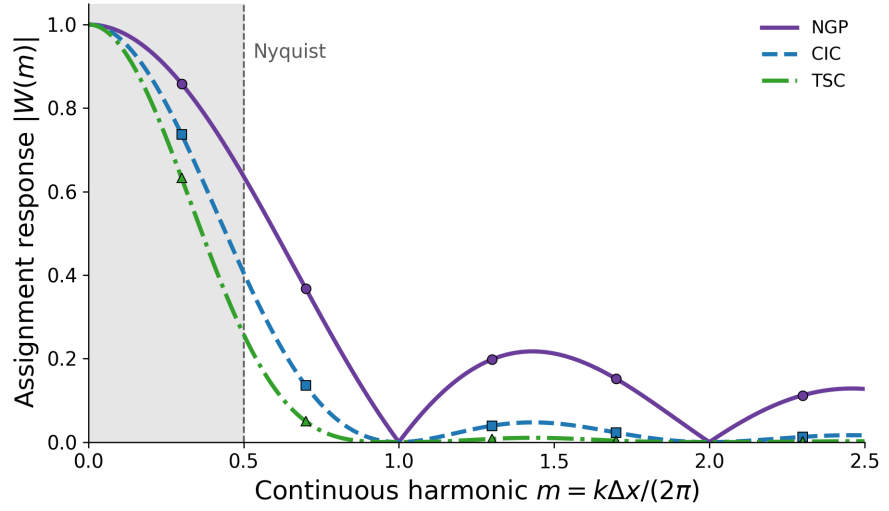
One solution to these sources of errors is sometimes to increase the mesh size (and thereby decreasing the mesh spacing), which would also require an increase in the number of macro-particles used to maintain particle-per-cell density. Examples of this is given in [66] and [55, p. 424]. However, if the physical system of interest is sufficiently modeled at a decreased mesh size, it may, from a computational perspective, be of interest to choose an assignment function acting as a low pass filter where Hockney et al suggests for this purpose to use higher-order interpolation functions [55, p. 272]. This is a balancing act, as while higher-order interpolation may reduce e.g. required number of macro-particles, it introduces extra algorithmic steps [55, pp. 258–259]. To understand the smoothing effect according to interpolation order better, interpolation function in three dimension can be written as:

$$W(\mathbf{x}) = \frac{1}{V_c} w\left(\frac{x}{\Delta_1}\right) w\left(\frac{y}{\Delta_2}\right) w\left(\frac{z}{\Delta_3}\right) \quad (\text{E.5})$$

where

$$w(x) \xrightarrow{\mathcal{F}} \hat{w}(k) = \left( \frac{\sin(k/2)}{k/2} \right)^{p+1} \quad (\text{E.6})$$

Where  $p$  denotes the interpolation order. As can be seen, Eq. (E.6) is a sinc-function in  $k$ -space, where higher orders will result in stronger smoothing. It is important to note that smoothing schemes should only be considered provided the high- $k$  harmonics have little importance for the collective behaviour of a particle ensemble, as smoothing applies not only to high- $k$  errors, but also to high- $k$  physics [55, pp. 272, 320]. The Fourier response of NGP, CIC and TSC is shown in Fig. E.2 and an example of mode coupling is shown in Fig. 2.21.



**Figure E.2:** Fourier response of the particle-shape/deposition scheme. Higher order interpolation suppresses high- $m$  (and therefore high- $k$ ) content more strongly than lower order interpolation.

## Direct versus indirect space-charge

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### F.1 Transverse Space Charge

By dividing equation (2.50) with (2.53), an approximate measure of the relative effect of indirect vs direct transverse space charge may be calculated:

$$\frac{\Delta Q_x^{indir}}{\Delta Q_x^{dir}} \approx \frac{\gamma^2 a^2}{b^2} \quad (\text{F.1})$$

This may thus be used as a simple order-of-magnitude estimate for the relative importance of indirect versus direct space-charge.

### F.2 Longitudinal Space Charge

To determine the relative direct vs indirect contribution to the tune shift, Zhao et al provides a way in [68]. There, Eqs. 4 and 5 give formulas for the direct and indirect longitudinal focusing. This focusing may be treated as proportional to the tune shift, and therefore provides a way to calculate the ratio [30, p. 417]. Zhao et al's equations 4 and 5 are as follows:

$$\Delta k_{\text{direct}} = \frac{2N\eta r_c}{\beta^2 \sqrt{\pi}} \int_0^\infty dq \frac{1}{\sqrt{(2\sigma_x^2 + q)(2\sigma_y^2 + q)(2\bar{\sigma}_z^2 + q)^3}} \quad (\text{F.2})$$

$$\Delta k_{\text{indirect}} \simeq \frac{4N\eta r_c}{\beta^2 \sqrt{\pi}} \sum_{n=1}^{\infty} (-1)^n \int_0^\infty dq \frac{\exp\left[-\frac{(2nb)^2}{q}\right]}{q(2\bar{\sigma}_z^2 + q)^{3/2}} \quad (\text{F.3})$$

where  $N$  is the number of particles,  $\eta$  the phase slip factor,  $r_c$  the classical particle radius,  $b$  the half-gap of the vacuum chamber,  $\bar{\sigma}_z = \gamma_{\text{ref}} \sigma_z$  and where  $q$  is a geometric parameter derived from convolution with Green's function. Let us now

make use of these equations. For the sake of simplicity, let us assume that  $\sigma_x \sim \sigma_y \sim \sigma_r$  while  $\bar{\sigma}_z \gg \sigma_x, \sigma_y$ .

### F.2.1 Direct contribution

First, let us look at eq. (F.2):

**Case A:**  $q < 2\bar{\sigma}_z$ :

$$(2\bar{\sigma}_z^2 + q)^{3/2} \sim (2\bar{\sigma}_z^2)^{3/2} \sim \bar{\sigma}_z^3 \quad (\text{F.4})$$

This gives:

$$\Delta k_{direct}^A \sim \frac{1}{\bar{\sigma}_z^3} \int_0^{\bar{\sigma}_z^2} \frac{dq}{2\sigma_r^2 + q} \sim \frac{1}{\bar{\sigma}_z^3} \ln \frac{\bar{\sigma}_z^2}{\sigma_r^2} \quad (\text{F.5})$$

The upper limit for the integral was chosen as the breakpoint for the validity of case 1.

**Case B:**  $q > 2\bar{\sigma}_z$ : Here the integrand becomes  $\frac{1}{q^{5/2}}$ . This gives:

$$\Delta k_{direct}^B \sim \int_{\bar{\sigma}_z^2}^{\infty} dq q^{-5/2} = \left[ -\frac{2}{3} q^{-3/2} \right]_{\bar{\sigma}_z^2}^{\infty} = 0 + \frac{2}{3} (\bar{\sigma}_z^2)^{-3/2} = \frac{2}{3} \frac{1}{\bar{\sigma}_z^3} \quad (\text{F.6})$$

Finally:

$$\Delta k_{direct} \sim \Delta k_{direct}^A + \Delta k_{direct}^B = \frac{1}{\bar{\sigma}_z^3} \ln \frac{\bar{\sigma}_z^2}{\sigma_r^2} + \frac{2}{3} \frac{1}{\bar{\sigma}_z^3} \quad (\text{F.7})$$

Thus the direct longitudinal focusing may be calculated.

### F.2.2 Indirect contribution

Let us now turn to the indirect contribution and look at equation (F.3). Assume only one image charge,  $n = 1$ , as higher order image terms enter logarithmically with alternate signs and should not change the order of magnitude. Then,  $q = (2b)^2$  is treated as a lower cutoff motivated by the exponential term. Divide up in two cases as previously:

**Case A:**  $q < 2\bar{\sigma}_z$ :

$$(2\bar{\sigma}_z^2 + q)^{3/2} \sim (2\bar{\sigma}_z^2)^{3/2} \sim \bar{\sigma}_z^3 \quad (\text{F.8})$$

This gives:

$$\Delta k_{indirect}^A \sim \frac{1}{\bar{\sigma}_z^3} \int_{(2b)^2}^{2\bar{\sigma}_z^2} \frac{dq}{q} \sim \frac{1}{\bar{\sigma}_z^3} \ln \frac{\bar{\sigma}_z^2}{b^2} \quad (\text{F.9})$$

**Case B:**  $q > 2\bar{\sigma}_z^2$ : For this case, the exponential term should approach 1. This gives the following integral:

$$\Delta k_{indirect}^B = \int_{\bar{\sigma}_z^2}^{\infty} dq q^{-5/2} \sim \bar{\sigma}_z^{-3} \quad (\text{F.10})$$

Assuming  $\bar{\sigma}_z \gg \bar{\sigma}_r$ , this contribution will be negligible. Therefore:

$$\Delta k_{indirect} \sim \frac{1}{\bar{\sigma}_z^3} \ln \frac{\bar{\sigma}_z^2}{b^2} \quad (\text{F.11})$$

Thus the indirect longitudinal focusing may be calculated.

### F.2.3 Direct vs indirect contribution

The contribution to the tune shift of the indirect space charge relative to the direct will then be of the following order of magnitude:

$$\frac{\Delta Q_{indirect}}{\Delta Q_{direct}} = \frac{\Delta k_{indirect}}{\Delta k_{direct}} \sim \frac{\ln(\bar{\sigma}_z^2/b^2)}{\ln(\bar{\sigma}_z^2/\sigma_r^2) + 2/3} \quad (\text{F.12})$$

This may thus be used to determine the relative effect of indirect longitudinal space-charge versus direct longitudinal space-charge.

## F.3 Analysis: Transverse indirect space-charge

The relative tune spread between indirect and direct transverse space-charge can be calculated using Eq. (F.1) with  $\gamma_0 = 5.32$ ,  $b = 0.15$  and assuming a rms beam radius of  $a = 0.02$  m:

$$\frac{5.32^2 \cdot 0.02^2}{0.15^2} \approx 0.6 = 60\% \quad (\text{F.13})$$

With an rms beam radius of 5 cm, this value increases to 300%. Only if the beam radius would be close to its original value could the indirect contribution be considered minor.

## F.4 Analysis: Longitudinal indirect space charge

As for the longitudinal case, (F.12) may be used to get a rough estimate. In Tables F.1 (initial transverse bunch) and F.2 (blown-up transverse bunch), estimates are given based on initial and final predicted bunch lengths, and an average assuming the bunch length changes linearly from start to end. The average beta functions as given in Table 3.2 have been used.

**Table F.1:** Ratio  $\Delta k_{\text{indirect}}/\Delta k_{\text{direct}}$  for different bunch lengths using initial emittance.

| Case            | $\sigma_z$ [m] | $\bar{\sigma}_z = \gamma\sigma_z$ [m] | ratio ( $\langle\beta_x\rangle$ ) | ratio ( $\langle\beta_y\rangle$ ) |
|-----------------|----------------|---------------------------------------|-----------------------------------|-----------------------------------|
| Initial, 120 ns | 8.99           | 47.9                                  | 0.651                             | 0.662                             |
| Final, 2 ns     | 0.150          | 0.799                                 | 0.351                             | 0.362                             |
| Average in $z$  | 4.57           | 24.4                                  | 0.622                             | 0.633                             |

**Table F.2:** Ratio  $\Delta k_{\text{indirect}}/\Delta k_{\text{direct}}$  assuming blown-up transverse size  $\sigma_r$  by a factor 5.

| Case            | $\sigma_z$ [m] | $\bar{\sigma}_z = \gamma\sigma_z$ [m] | ratio ( $\langle\beta_x\rangle$ ) | ratio ( $\langle\beta_y\rangle$ ) |
|-----------------|----------------|---------------------------------------|-----------------------------------|-----------------------------------|
| Initial, 120 ns | 8.99           | 47.9                                  | 0.716                             | 0.729                             |
| Final, 2 ns     | 0.150          | 0.799                                 | 0.422                             | 0.438                             |
| Average in $z$  | 4.57           | 24.4                                  | 0.690                             | 0.704                             |

As can be seen, the lack of image charges will understate the contribution from longitudinal space charge.

## Adaptive vs Static mesh visualizations

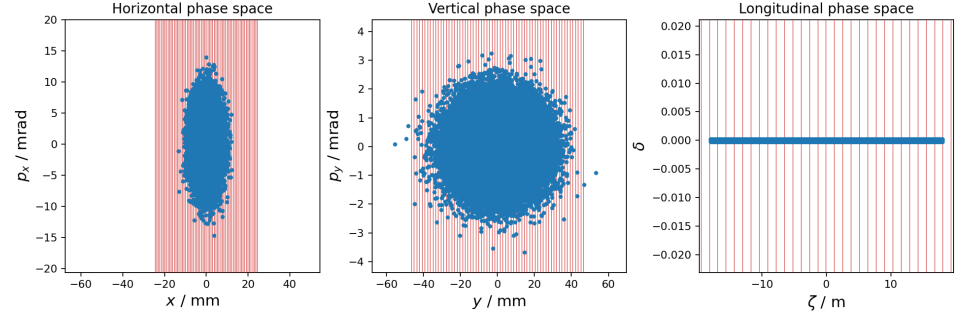
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The initial and final turn for static 3D space-charge is shown, for low macro-particle/cell density in Fig. G.1 and for high density in Fig. G.2. The evolution of phase space with 3D space-charge and an adaptive mesh is shown for several turns with low macro-particle/cell density in Fig. G.3 and with high macro-particle/cell density in Fig. G.4.

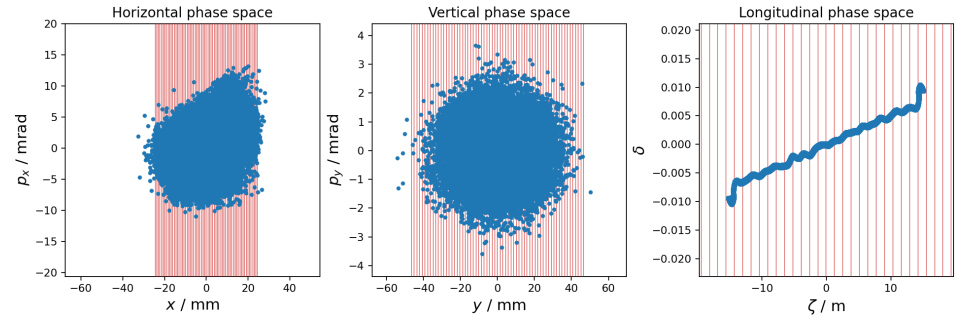
As seen in Figs. G.1 and G.2, it is clear that while a static mesh may be initially suitable, only adapting the mesh extents to the original beam size quickly becomes problematic. At later turns, a significant amount of macro-particles are outside the mesh extents in horizontally, and will therefore not experience space-charge kicks. In  $z$ , the resolution of the mesh is severely decreased for progressing turns, which could cause effects such as grid heating. A suitable static mesh should instead be adapted to the most extreme beam sizes, both in terms of mesh extents and in grid size. For the cases seen in Figs. G.1 and G.2, this would require the mesh extents to be almost tripled in  $x$  (which would therefore also require a tripling of the grid size to maintain resolution). As the bunch is to compress longitudinally 60 times in size, this would further require an mesh increase by 60 times. Further, macro-particle amount would accordingly need to be significantly increased in order to maintain macro-particle/cell density. If any of these changes would further imply a larger emittance in  $y$ , this would also need to be accounted for. With the computational resources available, this was not feasible.

A visualization of the static mesh vs the adaptive mesh for a few initial turns with 3D PIC space-charge,  $5 \cdot 10^4$  macro-particles and a grid size of 64 is shown for the longitudinal phase space in Fig. G.5. It is clear that the interpolation causes discontinuities between the cell borders for a static mesh (grid heating), while the distribution is much smoother for the adaptive mesh. One possible explanation is that continuously evolving positions of the grid points contributes to an indirect low-pass filter which combats the effects of grid heating. Something that is present in both configurations, although more clear for the static mesh, is a deviation in the momentum spread for the edges of the bunch compared with the inner bunch. This is possibly the result of outer mesh cells having a cut-off in macro-particle distribution due to the uniform distribution. In turn, this

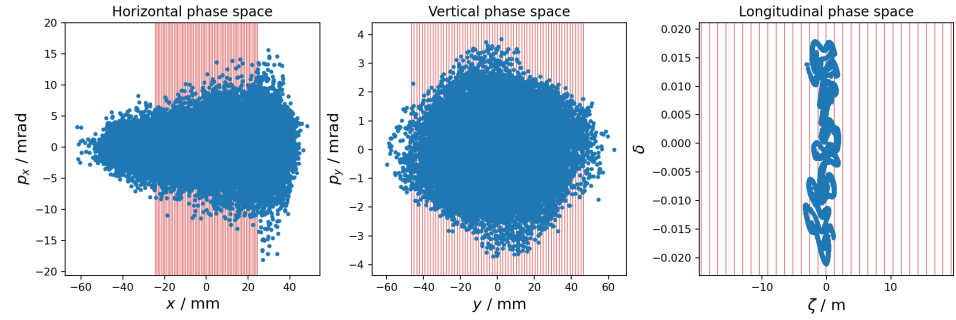




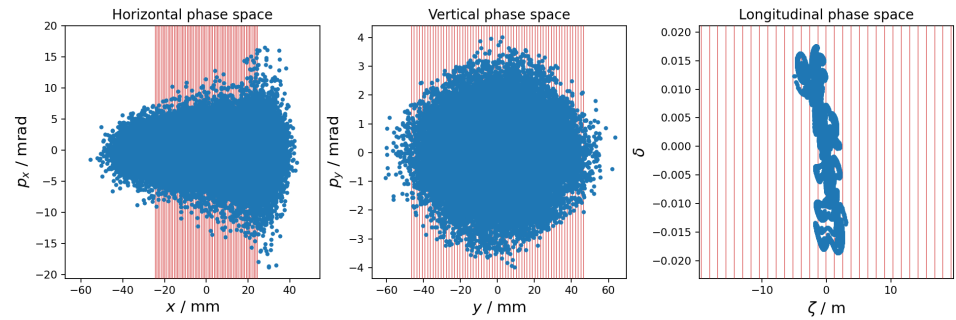
(a) Turn 0 with 3D, static mesh.



(b) Turn 14 with 3D, static mesh.

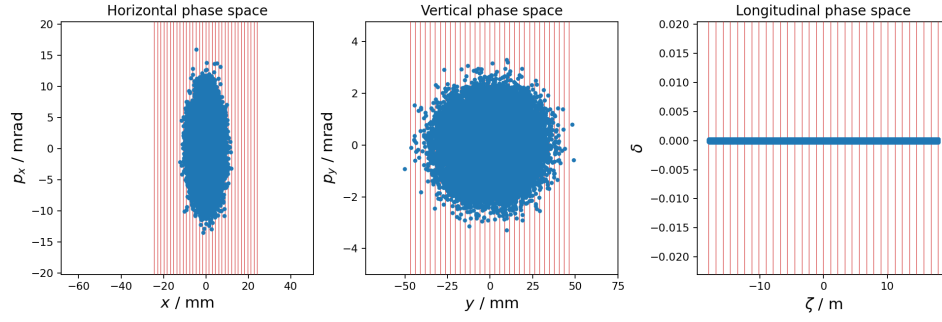


(c) Turn 38 with 3D, static mesh.

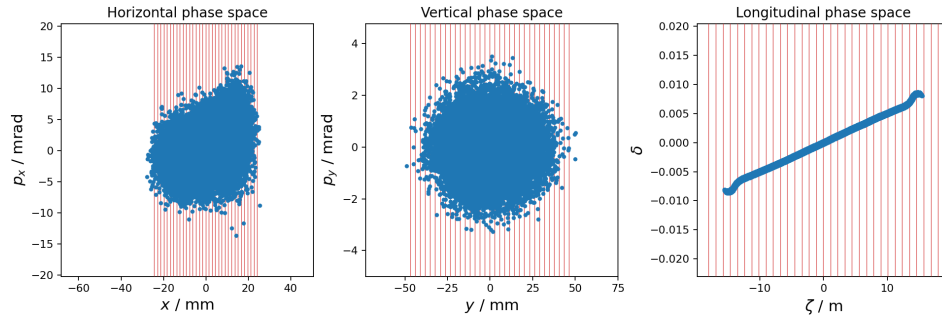


(d) Turn 41 with 3D, static mesh

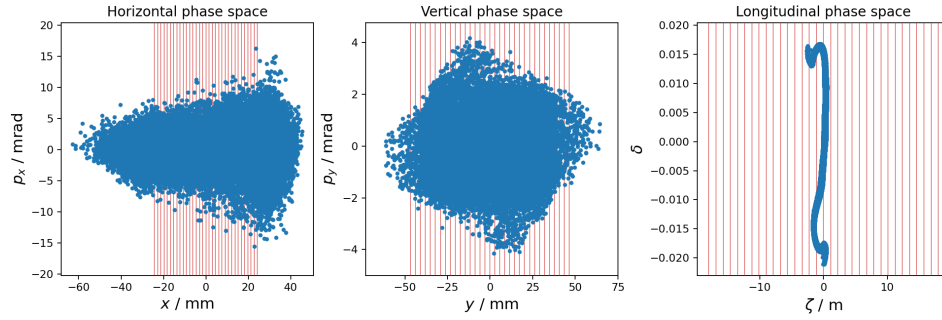
**Figure G.1:** Phase space for turns 0, 14, 38 and 41 with 3D PIC space charge and static mesh (Configuration IV). No dispersion correction has been performed to better illustrate how the bunch develops relative to the mesh.



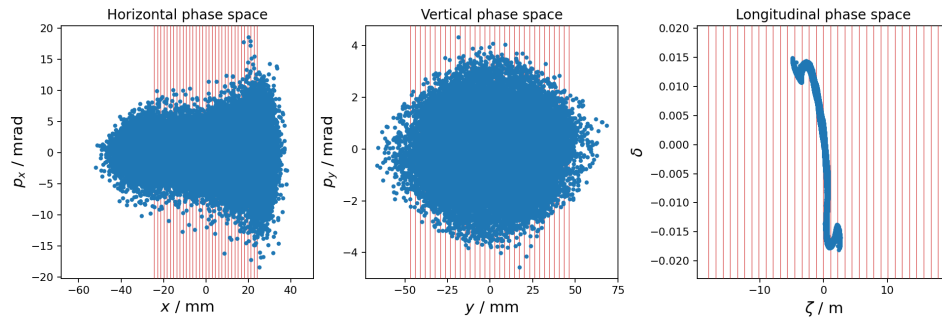
(a) Turn 0 with 3D, static mesh.



(b) Turn 14 with 3D, static mesh.

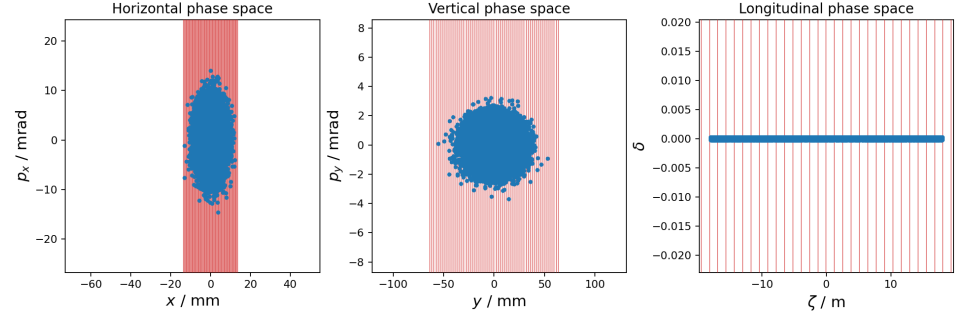


(c) Turn 38 with 3D, static mesh.

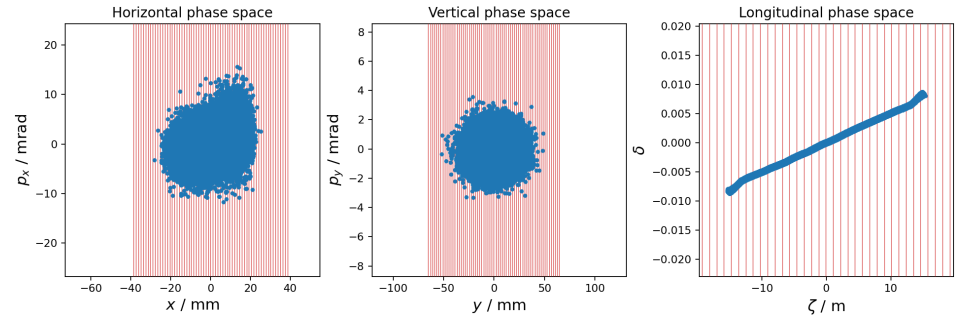


(d) Turn 41 with 3D, static mesh

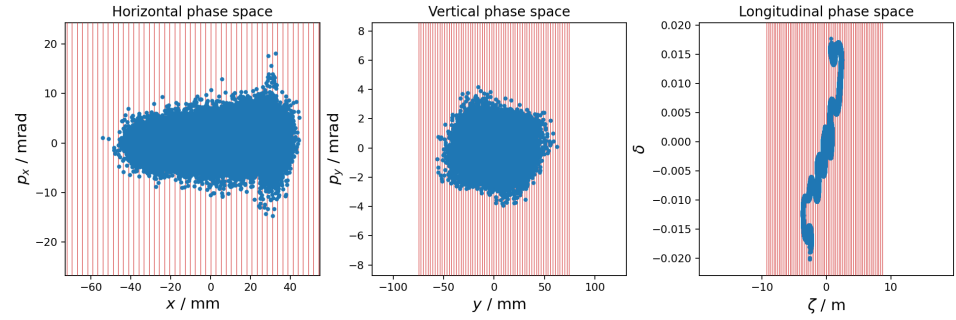
**Figure G.2:** Phase space for turns 0, 14, 38 and 41 with 3D PIC space charge and static mesh (Configuration II). No dispersion correction has been performed to better illustrate how the bunch develops relative to the mesh.



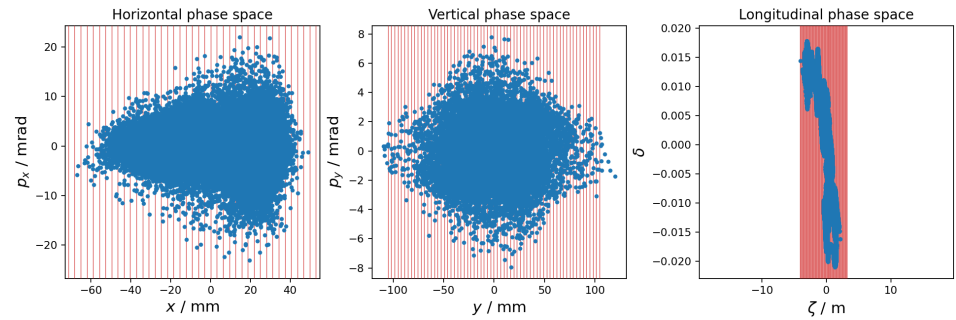
(a) Turn 0 with 3D, adaptive mesh.



(b) Turn 14 with 3D, adaptive mesh.

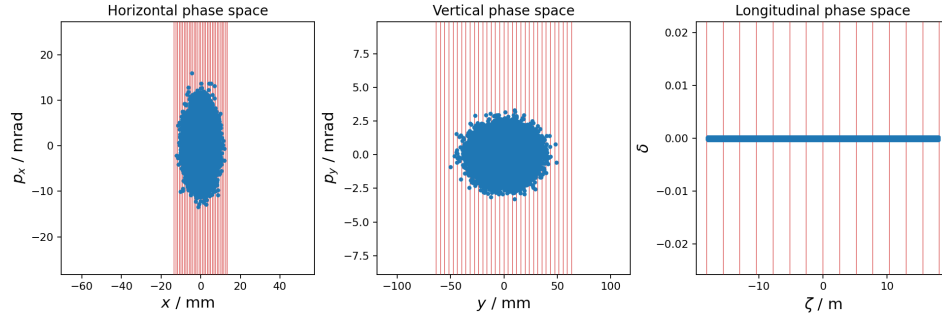


(c) Turn 35 with 3D, adaptive mesh.

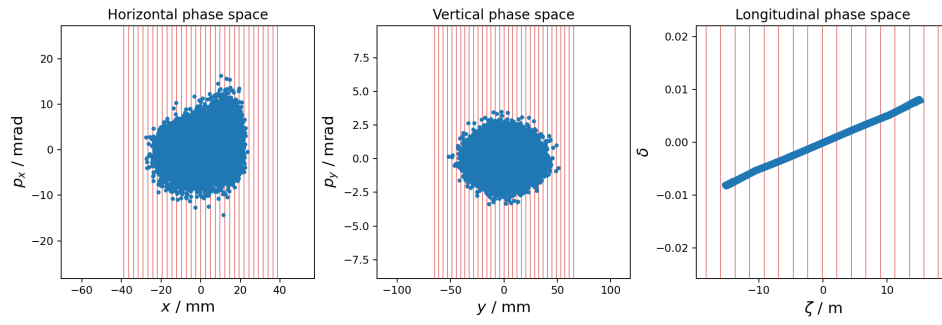


(d) Turn 41 with 3D, adaptive mesh

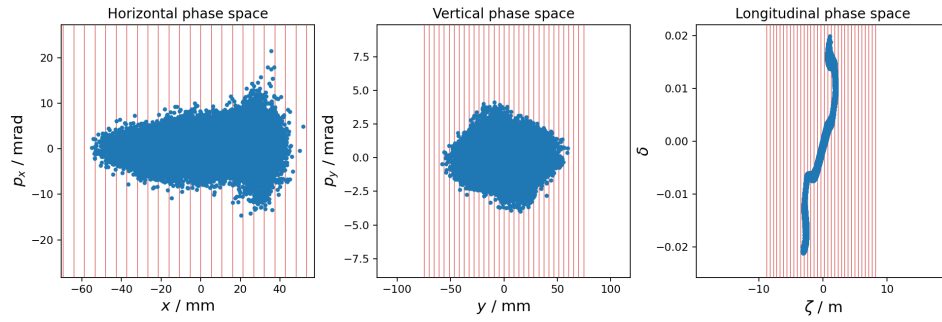
**Figure G.3:** Phase space for turns 0, 14, 35 and 41 with 3D PIC space charge and adaptive mesh (Configuration III). No dispersion correction has been performed to better illustrate how the mesh adapts to the bunch.



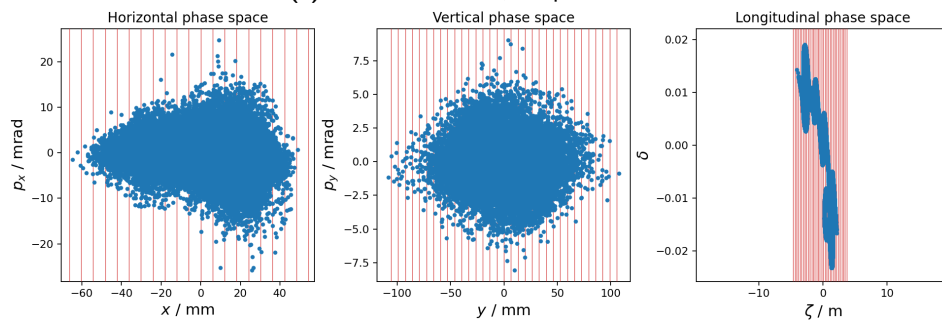
(a) Turn 0 with 3D, adaptive mesh.



(b) Turn 14 with 3D, adaptive mesh.



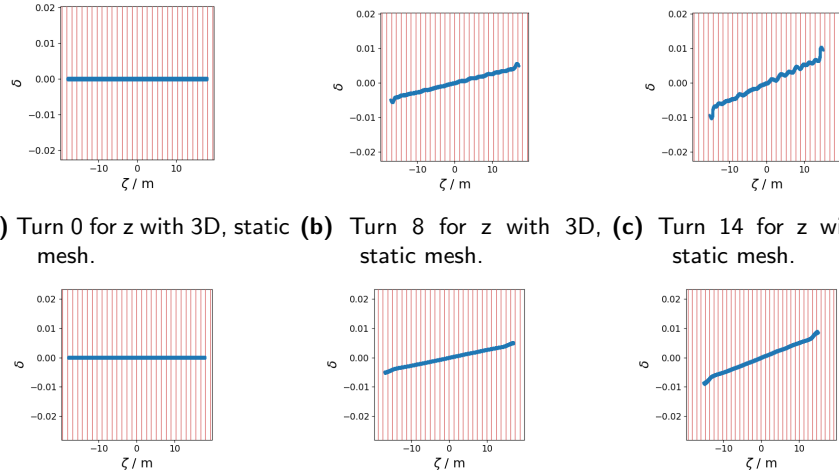
(c) Turn 35 with 3D, adaptive mesh.



(d) Turn 41 with 3D, adaptive mesh

**Figure G.4:** Phase space for turns 0, 14, 35 and 41 with 3D PIC space charge and adaptive mesh (Configuration I). No dispersion correction has been performed to better illustrate how the mesh adapts to the bunch.

likely results in drastically differing charge density in the outer cells, implying large gradients and therefore a large space-charge force applied on these particles. While it is clear that the adaptive mesh suppresses the momentum deviation for the outer edges, it is still present. This effect is even further suppressed, although not completely gone, when using the configurations with  $1 \cdot 10^6$  macro-particles and 32 grid resolution. Instead of using a uniformly distributed bunch in  $z$ , using a bunch from accumulator simulations could possibly alleviate the problem somewhat, as we should expect some degree of tapering in the longitudinal edges of the bunch and therefore less extreme derivatives.



(a) Turn 0 for  $z$  with 3D, static mesh. (b) Turn 8 for  $z$  with 3D, static mesh. (c) Turn 14 for  $z$  with 3D, static mesh.  
 (d) Turn 0 for  $z$  with 3D, adaptive mesh. (e) Turn 8 for  $z$  with 3D, adaptive mesh. (f) Turn 14 for  $z$  with 3D, adaptive mesh.

**Figure G.5:** Longitudinal phase space at turns 0, 8 and 14 for 3D PIC space charge. Subfigures a)–c) use Configuration IV, while subfigures d)–f) use Configuration III.

## Further four-fold identification tests

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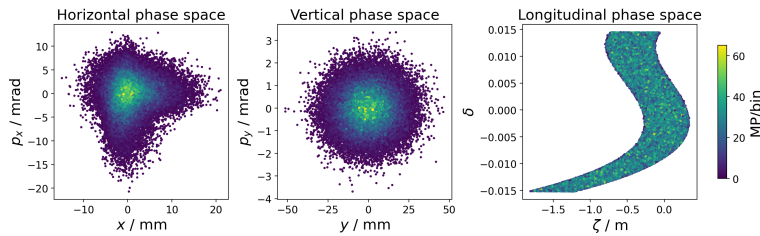
### H.1 Hypothesis: Synchro-Betatron coupling

Several tests were conducted to determine if the four-fold structure visible in Fig. 5.3 was driven by synchro-betatron coupling.

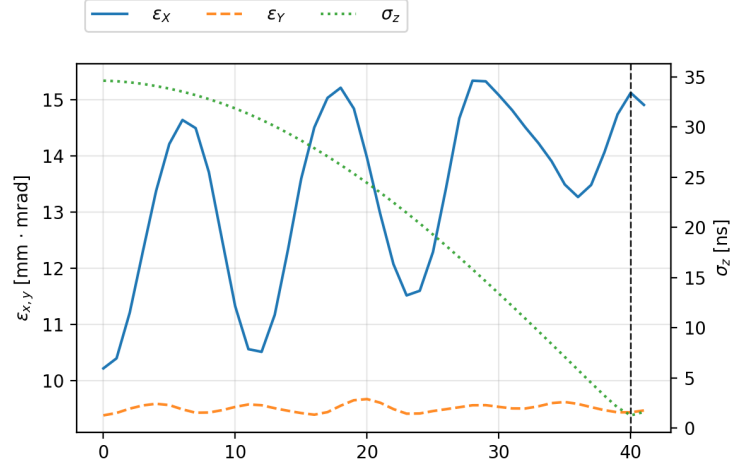
#### H.1.1 Test: Movement of RF-cavity

As the structure was deemed to be longitudinal-transverse in nature, an initial test was conducted to see if the structure could be suppressed by moving the RF-cavity, initially at a position with periodic dispersion with  $\eta = 1.89 \text{ m}$  and  $\eta' = 0$  ( $s = 0 \text{ m}$ ) to a position of  $\eta = 0 \text{ m}$  and  $\eta' = -0.457$  ( $s = 14.69 \text{ m}$ ). The resulting phase space is shown in Fig. H.1 while the transverse emittances and the longitudinal bunch length are plotted against turns in Fig. H.2.

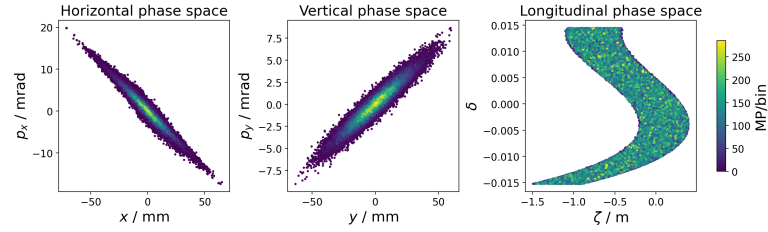
In Fig. H.1, the structure is still present. Compared to previously, it is further off-centered. Investigating Fig. H.2 explains the off-centered nature: This could be interpreted as a first order resonance further being hit, causing orbit distortions. Even if this were not the case, the four-fold structure remaining would either indicate that the longitudinal-transverse coupling is still significant due to periodic dispersion derivative  $\eta' \neq 0$ , or it could indicate that the structure is in fact not



**Figure H.1:** Phase space at shortest  $\sigma_z$  (turn 40) with cavity moved to position with periodic dispersion  $\eta = 0 \text{ m}$  and  $\eta' = -0.457$ .



**Figure H.2:** Transverse emittance and longitudinal bunch length vs turns with cavity moved to position with periodic dispersion  $\eta = 0$  m and  $\eta' = -0.457$ .



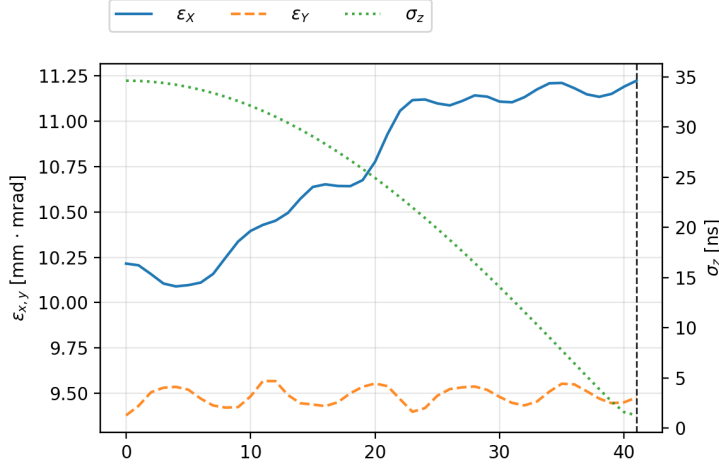
**Figure H.3:** Phase space at shortest  $\sigma_z$  (turn 41) with data observation point moved to position with periodic dispersion  $\eta = 0$  m and  $\eta' = -0.457$ .

caused by transverse-longitudinal coupling. For subsequent tests the RF-cavity and the observation point are at their default locations.

### H.1.2 Test: Movement of observation point

Another test was conducted where the data observation point in the lattice was moved to the same point as in Appendix H.1.1 ( $s = 14.69$  m) with  $\eta = 0$  m and  $\eta' = -0.457$ . This was motivated by the fact that injection regions for lattices are generally dispersion free, and simulations for conventional lattices usually collect data at these dispersion free points. Possibly, the structure would not be as amplified at a point of no dispersion. The results are shown in Figs. H.3 and H.4.

Notwithstanding that the beam is horizontally focused and vertically defocused at  $s = 14.69$  m, the four-fold structure is still visible in x.



**Figure H.4:** Transverse emittance and longitudinal bunch length vs turns with cavity moved to position with periodic dispersion  $\eta = 0$  m and  $\eta' = -0.457$ .

### H.1.3 Test: Removal of RF-cavity

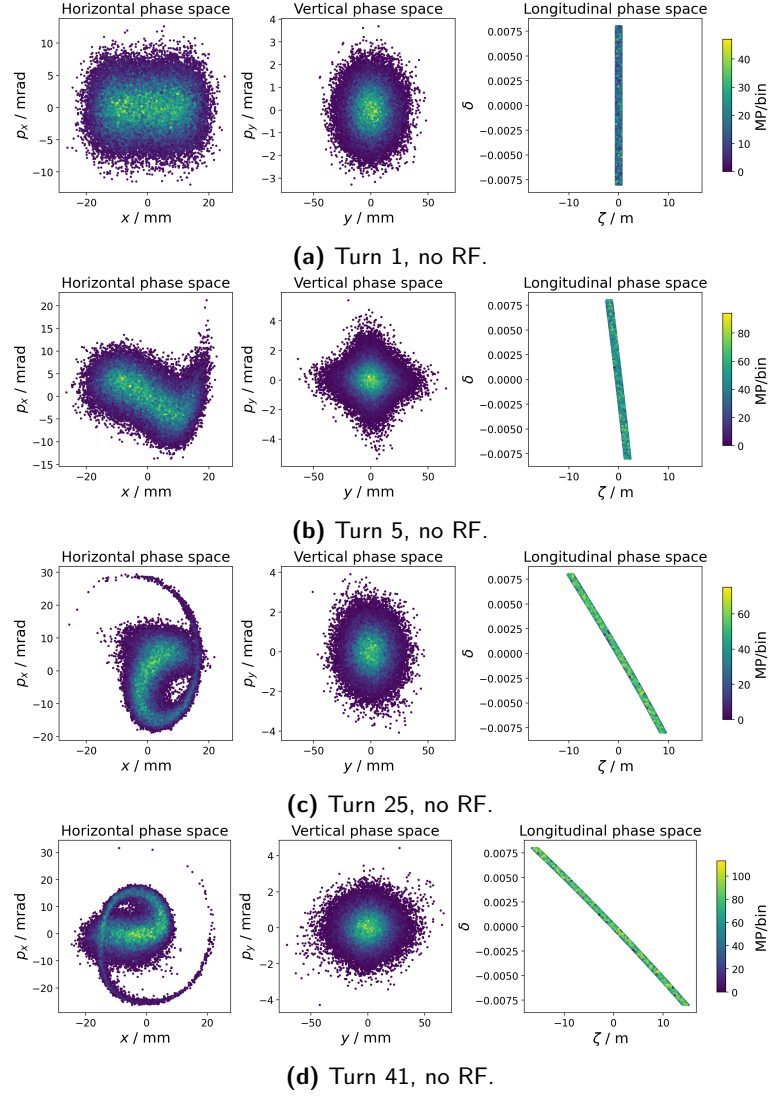
As the experiments in subsections H.1.1 and H.1.2 did not produce any conclusive results, a new test was conducted where the RF-cavity was completely removed and the simulation was started as if the bunch had already been compressed. The purpose of this test was to see if the four-fold structure would still develop; if it would remain, this would disprove the hypothesis of synchro-betatron coupling as the structure would still develop despite no synchrotron oscillations. The result is shown in Fig. H.5.

As can be seen, the structure first develops in  $y$ , before disappearing as a four-lobed oscillation starts in  $x$ . This confirms that while synchro-betatron coupling is not the cause of the structure, it is caused by longitudinal-transverse coupling.

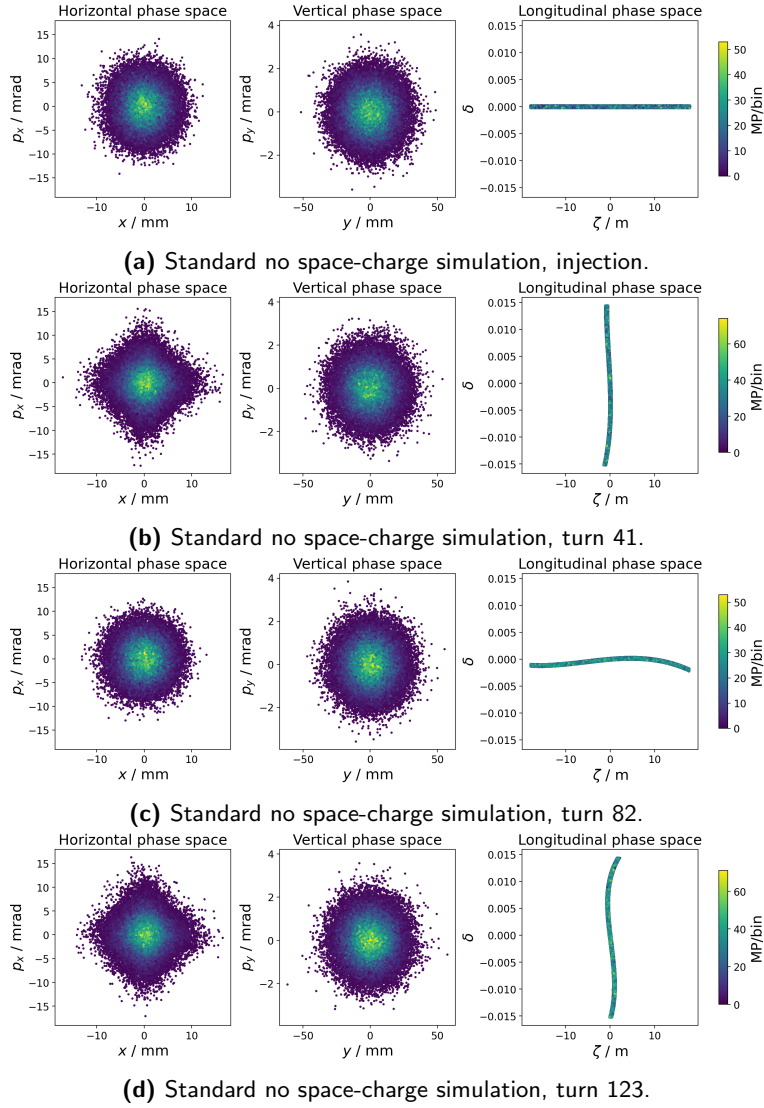
### H.1.4 Test: Simulation over 123 turns

To confirm if high energy deviation could be the driver of the structure in itself, a simulation was further conducted over 123 turns, with the results shown in Fig. H.6. As can be seen, the four-fold structure only appears at high energy deviations, further strengthening the hypothesis that the structure is indeed dependent on longitudinal phase space.





**Figure H.5:** Simulation with no space charge, longitudinal phase space already rotated and no RF-cavity.



**Figure H.6:** Standard no space charge simulation from injection to turn 123. The four-fold shape is only seen at high energy deviation.



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