Analytic Space-Charge Model for Gaussian Beams with cross-plane Coupling

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Abstract

Intensities of particle beams provided by particle accelerators are raised to levels where the self-interaction of the beam particles due to electromagnetic repulsion, the so-called space-charge effect, becomes a dominant factor. It is therefore indispensable to understand the effects on the beam dynamics in the presence of strong space charge forces. As complement to existing simulation methods, we present a fully analytic space charge model valid for transverse Gaussian beams and which includes non-linear space charge forces and cross-plane coupling. We verify the validity of the model by running test simulations in a few accelerator lattice examples. Finally, we briefly explore the possibilities for future simulations regarding new insights in beam dynamics and show initial results of the development of a beam envelope (core) in a test ring, as well as the dynamics of passive spectator particles which observe the non-linear electric field generated by a beam core.

1. Introduction

One of the main challenges for high-power particle accelerators like neutron sources or neutrino factories is to avoid even the smallest particle losses. The European Spallation Source (ESS) will use a proton beam with a design power of 5 MW. With such high power, even minute beam losses will produce unwanted radiation and heat-load to the cryogenic systems of the superconducting sections. A commonly accepted beam loss limit in linear accelerators that allow hands-on maintenance without long cool-down times is below 1 W/m [1].

Space charge-driven resonances due to beam mismatch lead to the generation of a high-amplitude beam halo surrounding the beam core. These halo particles predominantly contribute to beam loss. The formation of the beam halo has been extensively studied in 2D phase space by using KV-distributions with linear space charge forces [2]. Naturally, models that study the beam halo formation can be divided into the beam core and the beam halo, called the particle-core-model. It describes the transverse dynamics of particles in the beam halo. One
of the most important discoveries was that a parametric 1:2 ratio of the single particle oscillation frequency with respect to the core oscillation frequency is a driving mechanism for particles leaving the core and to form the halo [3].

In order to model the beam core it is convenient to describe the evolution of its envelope with the so-called envelope equations. The envelope equations were first derived by Kapchinskij and Vladimirskij from the transverse equation of motion. Their model uses r.m.s beam sizes and is valid for a continuous beam with a uniform charge distribution and circular cross-sections and includes linear space charge forces [4]. Later, the envelope equations were generalized to be valid for bunched beams, four commonly encountered charge distributions and elliptical beam cross-sections by Sacherer. He found that the linear part of the space charge force mainly depends on the r.m.s beam size and not on the actual shape of the distribution. Furthermore, he noted that the time-evolution of the r.m.s emittance must be known beforehand if the envelope equations are to be applied [5]. Overall, we can infer three main limitations of the envelope equations: Linear space charge forces, no emittance growth and no cross-plane coupling. Is it possible to overcome these limitations in the modeling for a beam with a realistic particle distribution?

A closed expression for the transverse electric field of a upright, transverse Gaussian beam was found by Bassetti and Erskine [6]. Their formula was converted into a covariant form in [7]. This modification allows cross-plane coupling and makes the formula valid for Gaussian beams with any tilt angle. In our effort to overcome the aforementioned limitations, we have developed a fully analytic, transverse Gaussian beam model with non-linear space charge forces and cross-plane coupling which is based on the covariant form of Bassetti’s and Erskine’s formula. In this report, we present the full derivation of our beam model which we will use as beam core for studies related to beam halo formation, especially how the Gaussian form of the beam affects the core dynamics and the tail particle dynamics.

2. Space Charge Model

In this section we describe our treatment of non-linear space charge forces for a Gaussian beam core. Our model uses the following nomenclature for 4D phase space coordinates

\[ \vec{x} = \{x, x', y, y'\} = \{x_1, x_2, x_3, x_4\}. \quad (2.1) \]

Furthermore, we use Einstein’s sum convention for index variables appearing twice in a single expression.

In the model, a pre-defined accelerator lattice is sliced and the beam transfer matrices for all slices are stored. The lattice uses thick elements. The beam propagation of a 4D beam matrix \( \sigma_0 \) through the lattice slices is straight-forward by mapping the beam matrix \( \sigma_0 \) onto the beam matrix \( \sigma_1 \) via the transfer matrix \( R \) of the respective slice according to

\[ \sigma_1 = R\sigma_0R^T. \quad (2.2) \]
The particle distribution is given by

$$\Psi(\vec{x}) = \frac{1}{(2\pi)^2\sqrt{\det\sigma}} e^{-\frac{1}{2}\sigma^{-1}_{lm} x_l x_m}$$  \hspace{1cm} (2.3)$$

where $\sigma$ is the full 4D covariance matrix of the beam distribution. The electric field of this distribution is expressed as ([7])

$$F_0(x_1, x_3, \tilde{\sigma}) = \frac{\sqrt{\pi}}{\sqrt{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})}} \left[ w(z_1) - e^{-\frac{1}{2}\tilde{\sigma}^{-1} x_l x_m} \cdot w(z_2) \right]$$ \hspace{1cm} (2.4)$$

with

$$z_1 = \frac{x_1 + ix_3}{\sqrt{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})}} = \sum_k a_k x_k = a_1 x_1 + a_3 x_3$$

$$z_2 = \frac{(\sigma_{33} - i\sigma_{13})x_1 + i(\sigma_{11} + i\sigma_{13})x_3}{\sqrt{\sigma_{11}\sigma_{33} - \sigma_{13}^2} \sqrt{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})}} = \sum_k b_k x_k = b_1 x_1 + b_3 x_3. \hspace{1cm} (2.5)$$

where $x_1$ and $x_3$ are real space particle coordinates along the horizontal and vertical axes and $w(z)$ is the complex error function [8]. Since the field only depends on real space coordinates, the matrix $\tilde{\sigma}^{-1}$ is an inverted 4-by-4 matrix that only contains the real space elements, given by

$$\tilde{\sigma}^{-1} = \begin{bmatrix} \sigma_{33} & 0 & -\sigma_{13} & 0 \\ 0 & 0 & 0 & 0 \\ -\sigma_{31} & 0 & \sigma_{11} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \frac{1}{\sigma_{11}\sigma_{33} - \sigma_{13}^2}. \hspace{1cm} (2.6)$$

In each slice, the beam propagation is followed by a non-linear space charge kick which introduces a deflection of the particles comprising the beam. The change in angle of a single particle by the space charge kick is given by

$$\Delta x_4 + i\Delta x_2 = \tilde{K} F_0(x_1, x_3, \tilde{\sigma}) = \tilde{K} (f_3 + if_1) \hspace{1cm} (2.7)$$

and the new coordinates of a single particle that experiences the kick is described by

$$\tilde{x}_1 = x_1$$

$$\tilde{x}_2 = x_2 + \tilde{K} f_1$$

$$\tilde{x}_3 = x_3$$

$$\tilde{x}_4 = x_4 + \tilde{K} f_3. \hspace{1cm} (2.8)$$

The parameter $\tilde{K}$ reads

$$\tilde{K} = d\ell \frac{N2r_0}{\sqrt{2\pi\sigma_z^2\beta^2\gamma^3}} = d\ell K \hspace{1cm} (2.9)$$

where $N$ is the number of particles in the bunch, $\sigma_z$ is the bunch length, $r_0$ is the classical particle radius, $d\ell$ is the length over which the space charge force
is effective and $K$ the beam perveance commonly used in the literature. The derivation of $K$ is in appendix A.

From equation 2.8, we infer the new beam matrix after the kick by averaging over the beam distribution and the field distribution

\[
\bar{\sigma}_{11} = \langle \bar{x}_1 \bar{x}_1 \rangle = \langle x_1 x_1 \rangle = \sigma_{11} \\
\bar{\sigma}_{12} = \langle \bar{x}_1 \bar{x}_2 \rangle = \langle x_1 (x_2 + \bar{K} f_1) \rangle = \sigma_{12} + \bar{K} \langle x_1 f_1 \rangle \\
\bar{\sigma}_{13} = \langle \bar{x}_1 \bar{x}_3 \rangle = \langle x_1 x_3 \rangle = \sigma_{13} \\
\bar{\sigma}_{14} = \langle \bar{x}_1 \bar{x}_4 \rangle = \langle x_1 (x_4 + \bar{K} f_3) \rangle = \sigma_{14} + \bar{K} \langle x_1 f_3 \rangle \\
\bar{\sigma}_{22} = \langle \bar{x}_2 \bar{x}_2 \rangle = \langle (x_2 + \bar{K} f_1)(x_2 + \bar{K} f_1) \rangle = \sigma_{22} + \bar{K} \langle 2x_2 f_1 \rangle + \bar{K}^2 \langle f_1^2 \rangle \\
\bar{\sigma}_{23} = \langle \bar{x}_2 \bar{x}_3 \rangle = \langle x_3 (x_2 + \bar{K} f_1) \rangle = \sigma_{23} + \bar{K} \langle x_3 f_1 \rangle \\
\bar{\sigma}_{24} = \langle \bar{x}_2 \bar{x}_4 \rangle = \langle (x_2 + \bar{K} f_1)(x_4 + \bar{K} f_3) \rangle = \sigma_{24} + \bar{K} \langle x_2 f_3 \rangle + \bar{K} \langle x_4 f_1 \rangle + \bar{K}^2 \langle f_1 f_3 \rangle \\
\bar{\sigma}_{33} = \langle \bar{x}_3 \bar{x}_3 \rangle = \langle x_3 x_3 \rangle = \sigma_{33} \\
\bar{\sigma}_{34} = \langle \bar{x}_3 \bar{x}_4 \rangle = \langle x_3 (x_4 + \bar{K} f_3) \rangle = \sigma_{34} + \bar{K} \langle x_3 f_3 \rangle \\
\bar{\sigma}_{44} = \langle \bar{x}_4 \bar{x}_4 \rangle = \langle (x_4 + \bar{K} f_3)(x_4 + \bar{K} f_3) \rangle = \sigma_{44} + \bar{K} \langle 2x_4 f_3 \rangle + \bar{K}^2 \langle f_3^2 \rangle. \tag{2.10}
\]

where we assume that the beam is centered throughout the paper. We note that in each slice, the beam matrix elements are updated with inhomogeneous terms resulting from the space charge kick. The complete procedure of propagating the beam through a slice is thus given by

\[
\bar{\sigma}_1 = R \sigma_0 R^T + T \tag{2.11}
\]

where the variable $T$ collects all results of the inhomogeneous terms from eq. 2.10, representing the space charge kick.

We now turn to derive a fully analytic and self-consistent solutions for the calculation of the inhomogeneous terms collected in the variable $T$ in eq. 2.11. Taking a closer look at eq. 2.10, we can identify a general form of the linear inhomogeneous terms $\langle x_k F_0 \rangle$ and three quadratic inhomogeneous terms $\langle f_1^2 \rangle$, $\langle f_3^2 \rangle$ and $\langle f_1 f_3 \rangle$. We write these averages in integral form. The general form of the linear terms reads as

\[
\langle x_k F_0 \rangle = \langle x_k (f_3 + i f_1) \rangle = \int_{-\infty}^{\infty} d^4 x \, x_k \Psi(x) F_0(x_1, x_3, \bar{\sigma}). \tag{2.12}
\]

After evaluating the integral, we find a closed expression for the generalized linear term which reads

\[
\langle x_k (f_3 + i f_1) \rangle = \frac{i}{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})} \left[ \sigma_{k1} + i \sigma_{k3} - \left( \frac{\sigma_{k1}(\sigma_{33} - i\sigma_{13}) + i\sigma_{k3}(\sigma_{11} + i\sigma_{13})}{\sqrt{\sigma_{11}\sigma_{33} - \sigma_{13}^2}} \right) \right]. \tag{2.13}
\]

For the full derivation, we refer to appendix B.

Because we divide the kick function $F_0$ into its real and imaginary parts in equation 2.7, we find the following expressions for the individual quadratic terms
as
\[
\langle f_3^2 \rangle = \left( \frac{1}{2} (F_0 + \bar{F}_0) \right)^2 = \frac{1}{4} \left( F_0^2 + \bar{F}_0^2 + 2F_0 \bar{F}_0 \right)
\]
\[
\langle f_1^2 \rangle = \left( \frac{1}{2i} (F_0 - \bar{F}_0) \right)^2 = -\frac{1}{4} \left( F_0^2 + \bar{F}_0^2 - 2F_0 \bar{F}_0 \right)
\]
\[
\langle f_3 f_1 \rangle = \left( \frac{1}{4i} (F_0 - \bar{F}_0)(F_0 + \bar{F}_0) \right) = \frac{1}{4i} \left( F_0^2 - \bar{F}_0^2 \right)
\]

(2.14)

where the convolutions \( \langle F_0^2 \rangle, \langle \bar{F}_0^2 \rangle \) and \( \langle F_0 \bar{F}_0 \rangle \) are calculated in a similar way like the linear terms. In the course of the calculations we show analytically that \( \langle F_0^2 \rangle \) and \( \langle \bar{F}_0^2 \rangle \) are always zero and confirmed this with numerical tests. Consequently, the only quadratic term left to calculate is \( \langle F_0 \bar{F}_0 \rangle \) and it reads

\[
\langle F_0 \bar{F}_0 \rangle = \int_{-\infty}^{\infty} d^4 x \, \Psi(\vec{x}) F_0 \bar{F}_0.
\]

(2.15)

We also see that the terms \( \langle f_3^2 \rangle \) and \( \langle f_1^2 \rangle \) are identical under this condition. The solution for the remaining quadratic term is

\[
\langle F_0 \bar{F}_0 \rangle = \frac{-\pi}{\sqrt{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13}) \sqrt{2(\sigma_{11} - \sigma_{33} - 2i\sigma_{13})}}} \cdot P(\sigma, 1, a, \bar{a}) - P(\sigma, 2, a, \bar{b}) - P(\sigma, 2, \bar{a}, b) + P(\sigma, 3, b, \bar{b})
\]

(2.16)

where the function \( P \) is defined as

\[
P(\sigma, n, c, d) = \frac{2}{n\pi} \frac{1}{\sqrt{S_{11}S_{22} - S_{12}^2}} \left[ \frac{\pi}{2} - \arctan \left( \frac{S_{12}}{\sqrt{S_{11}S_{22} - S_{12}^2}} \right) \right]
\]

(2.17)

with

\[
S_{11} \left( \sigma, n, c, d \right) = 1 + \frac{2}{n} \left( \sigma_{11} c_1^2 + \sigma_{33} c_3^2 + 2\sigma_{13} c_1 c_3 \right)
\]
\[
S_{12} \left( \sigma, n, c, d \right) = \frac{2}{n} \left( \sigma_{11} c_1 d_1 + \sigma_{33} c_3 d_3 + \sigma_{13} c_1 d_3 + \sigma_{13} c_3 d_1 \right)
\]
\[
S_{22} \left( \sigma, n, c, d \right) = 1 + \frac{2}{n} \left( \sigma_{11} d_1^2 + \sigma_{33} d_3^2 + 2\sigma_{13} d_1 d_3 \right).
\]

(2.18)

The full derivation is given in appendix C. We also notice that there are no complex error functions left that have to be evaluated numerically which is beneficial regarding calculation speed. Further, for the case of a round beam cross-section where \( \sigma_{11} = \sigma_{33} \) and \( \sigma_{13} = 0 \), the denominator in eq. 2.4 exhibits a singularity. We show in appendix D how the singularity can be removed and how special solutions for a round beam are implemented.
3. Model Analysis

In order to verify the model, we first consider a simple beam line consisting of a single FODO cell. Therefore, we develop a simulation code in MATLAB where the complete procedure of beam propagation uses our space charge model.

We validate our model by examining the incoherent tune shift $\Delta Q_{\text{inc}}$ due to space charge in the single FODO cell. In [9], the linear incoherent tune shift is derived for a continuous KV-distribution by treating the space charge force as quadrupolar errors and integrating them over the ring. The linear incoherent tune shift is given by

$$\Delta Q_{\text{inc}} \approx \frac{1}{4\pi} \oint \Delta k \beta_r \, dl$$

where $\Delta k$ is the integrated strength of the quadrupolar error and $\beta_r$ the $\beta$-function at the location of an error. For a continuous round KV-distribution, the focusing strength of space charge is represented by

$$k_{r,\text{sc}} = -\frac{2q^2 n_q}{4\pi \epsilon_0 \beta^2 \gamma^3 a^2} = -\frac{2r_0 n_q}{\beta^2 \gamma^3 a^2}$$

(3.2)

where $a$ is the radius of the beam, $n_q$ the local particle density and $r_0$ the classical particle radius. We adapt this formula to our model, where the local charge density is given by $n_q = \frac{N}{\sqrt{2\pi} \sigma_z}$ with the total number of particles in the bunch $N$ and the bunch length $\sigma_z$. In [10], the space charge forces for uniform, round beams with radius $a$ and for Gaussian beams with beam size $\sigma$ are derived. By linearizing the force of the Gaussian beam for small $r$ (close to the beam center), we find the relation $a^2 = 2\sigma^2 = 2\epsilon r \beta r$ as conversion of the force gradient between a uniform distribution and a Gaussian distribution and write the quadrupole strength as

$$k_{r,\text{sc}} = -\frac{2Nr_0}{2\sqrt{2\pi} \sigma_z \beta^2 \gamma^3 \epsilon r \beta r}.$$ (3.3)

Putting eq. 3.3 into eq. 3.1 and integrating over the entire ring, we obtain an analytic formula of the linear incoherent tune shift for a Gaussian beam with round cross-section

$$\Delta Q_{\text{inc}} \approx \frac{1}{4\pi} \oint k_{r,\text{sc}} \beta_r(\ell) \, d\ell = -\frac{Nr_0L}{2(2\pi)^{\frac{3}{2}} \sigma_z \epsilon r \beta^2 \gamma^3}$$

(3.4)

where $L$ is the total length of the lattice and $\epsilon r$ the beam emittance.

We validate our model by a linear mapping of our space charge kick and treat it as a quadrupole which defocuses in both planes. A requirement for generating the transfer matrix of the space charge quadrupole is its effective focal lengths. By calculating the gradient of the force $\frac{\partial F_0}{\partial x_{1,3}}$ in the origin, we find the inverse focal lengths as
\[ \frac{1}{f_{x_1}} = \hat{K} \frac{\partial F_0}{\partial x_1} = \hat{K} \lim_{\alpha \to \infty} \left[ \frac{2i}{\sqrt{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})}} (a_1 - b_1) \right] \left[ \frac{2i}{\sqrt{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})}} (a_3 - b_3) \right]. \] (3.5)

We insert such a space charge quadrupole between each lattice slice, generate a new effective full-turn matrix and calculate the incoherent tune shift according to

\[ \Delta Q_{\text{inc}} = Q_{\text{inc}} - Q_{\text{bare}}. \] (3.6)

where \( Q_{\text{bare}} \) is the tune of the bare lattice and \( Q_{\text{inc}} \) the tune of the lattice including space charge quadrupoles. We obtain the tunes for the bare lattice and the linear mapping by calculating the traces of the respective full-turn matrix.

In order to compare the incoherent tune shift obtained by the linear mapping to the analytic tune shift formula in eq. 3.4, we require a beam that is as round as possible. Therefore, we use a FODO cell with 30° phase advance which produces an almost round beam along the cell. Figure 1 compares the horizontal incoherent tune shifts as a function of protons per bunch. The results show very good agreement and only differ slightly for high beam currents. The deviations arise because the beam in our model is not constantly round along the FODO cell, which we assume it to be in eq. 3.4.

Figure 1: Comparison of the linear incoherent tune shifts calculated with the analytic tune shift formula derived from ref. [9] and the linear mapping of the model for a single FODO cell with 30° phase advance.
4. Core Dynamics Simulations

In this section, we investigate the effect of the non-linear space charge force on the dynamic behavior of the beam. We expect that the space charge will lead to an overall increase in the beam size, since it is a repulsive force. The general procedure of our simulations is as follows:

First, we need to prepare a zero-current lattice. Then, we calculate the periodic solution of that lattice. In [11] Edwards and Teng presented a method to parametrize a coupled transfer matrix. In [12], this parametrization was adopted to find a corresponding representation for the beam matrix $\sigma$. The latter is given by

$$\sigma = (AT)^{-1} \begin{pmatrix} \epsilon_1 & 0 & 0 & 0 \\ 0 & \epsilon_1 & 0 & 0 \\ 0 & 0 & \epsilon_2 & 0 \\ 0 & 0 & 0 & \epsilon_2 \end{pmatrix} \left((AT)^{-1}\right)^T$$

(4.1)

where $\sigma$ is the beam matrix, $\epsilon_j$ are the eigenemittances of the transverse plane, $A$ contains the Twiss parameters and $T$ contains coupling parameters and is an identity matrix for an uncoupled lattice. Since matrix $A$ contains Twiss parameters extracted from the full-turn matrix $R$, the beam matrix is parametrized with the optical beta-functions. Consequently, the beam matrix calculated by this method is the periodic solution.

In the next step, we make the transition from the zero-current beam size to the new equilibrium beam size including space charge. For that, we propagate the beam repeatedly through the lattice in a loop. At the end of one loop iteration, we apply a damping and an excitation to the beam matrix. Damping and excitation are not related to space charge directly, but are needed to define the new beam equilibrium. They are added in the last lattice slice so that the final beam matrix after one turn through the lattice is written as

$$\tilde{\sigma} = D\sigma D^T + E$$

(4.2)

where $\tilde{\sigma}$ is the beam matrix after the iteration, $\sigma$ is the beam matrix in the final slice of the lattice, $D$ describes damping and $E$ describes excitation. Damping and excitation are calculated once before the loop is initialized. A physical example of the interplay between $D$ and $E$ is synchrotron radiation, but can also describe stochastic cooling and a beam widening due to an internal target. The radiation process is quantized and thus, a random effect. If a particle on its synchronous orbit and in a dispersive section looses energy through the emission of a photon, the synchronous orbit will be different after the emission. As a result, the particle begins betatron oscillations. The procedure in eq. 4.2 is necessary only if we have an equilibrium, because without any damping, the beam emittance would infinitely grow otherwise due to space charge. However, the additional excitation term is needed to prevent the emittance being dampened to zero in the absence of space charge forces. The initialization of $D$ and $E$ works as follows:
The damping term $D$ is simply a 4-by-4 matrix with $e^{1/N_d}$ on the diagonal

$$D = e^{1/N_d} \mathbb{1}$$  \hfill (4.3)

where $N_d$ is the damping constant in number of turns and $\mathbb{1}$ is the identity matrix.

In order to calculate the initial excitation $E$, we use a variation of a method to map Twiss parameters through a lattice, presented in [13]. They are mapped according to

$$\begin{pmatrix} \beta \\ \alpha \\ \gamma \end{pmatrix} = \begin{pmatrix} R^2_{11} & -2R_{11}R_{12} & R^2_{12} \\ -R_{11}R_{21} & R_{11}R_{22} + R_{12}R_{21} & -R_{22}R_{12} \\ R^2_{21} & -2R_{22}R_{21} & R^2_{22} \end{pmatrix} \begin{pmatrix} \beta_0 \\ \alpha_0 \\ \gamma_0 \end{pmatrix}. \hfill (4.4)$$

where $R_{nn}$ are the elements of two-dimensional transport matrix. Similarly to eq. 4.4, we find an equivalent expression to map the independent elements of the beam matrix $\sigma$ through a lattice. Eq. 4.5 shows exemplary the one-dimensional case

$$\hat{\sigma} = \begin{pmatrix} \sigma_{11} \\ \sigma_{12} \\ \sigma_{22} \end{pmatrix} = \begin{pmatrix} R^2_{11} & 2R_{11}R_{12} & R^2_{12} \\ R_{11}R_{21} & R_{11}R_{22} + R_{12}R_{21} & R_{12}R_{22} \\ R^2_{21} & 2R_{21}R_{22} & R^2_{22} \end{pmatrix} \begin{pmatrix} \sigma_{11,0} \\ \sigma_{12,0} \\ \sigma_{22,0} \end{pmatrix} = \hat{R}\hat{\sigma}_0 \hfill (4.5)$$

where the variables with a hat indicate that they are either 1-by-3 vectors or 3-by-3 matrices. Since our model uses the full transverse plane including all coupling elements, we extend eq. 4.5 to the 4D case, which then requires ten independent elements

$$\hat{\sigma} = (\sigma_{11}, \sigma_{12}, \sigma_{13}, \sigma_{14}, \sigma_{22}, \sigma_{23}, \sigma_{24}, \sigma_{33}, \sigma_{34}, \sigma_{44})^T \hfill (4.6)$$

where the vectors and matrices with a hat are now of the size 10-by-1 and 10-by-10, respectively. We use the equilibrium condition for the beam size in zero current case which is given by

$$\dot{\hat{\sigma}} = (\hat{D}\hat{R})\hat{\sigma} + \hat{E} \hfill (4.7)$$

where we calculate the fixed-point, i.e. we map the beam to itself. Rewriting eq. 4.7 leads to an expression for the excitation term

$$\hat{E} = \left[ \mathbb{1} - (\hat{D}\hat{R}) \right] \hat{\sigma}. \hfill (4.8)$$

Once the excitation is calculated, we convert the variable $\hat{E}$ to the 4-by-4 equivalent $E$ and apply eq. 4.2 at the end of each iteration.

4.1. Core Dynamics in a simple FODO Cell

In order to investigate the dynamic behavior of the beam core (envelope), we use a single FODO cell of 60° horizontal and 52° vertical phase advance. As
outlined in the simulation procedures, we first find the periodic solution for the zero-current and then the equilibrium solution with space charge by letting the beam propagate through the FODO cell in a loop. Damping and excitation are applied according to eq. 4.2. The presence of space charge renders the beam mismatched, beam oscillations start and the beam is converging toward the new equilibrium solution. This situation is comparable to injection mismatch and is illustrated in fig. 2 which shows the turn-by-turn beam sizes and eigenemittances for a damping constant of 1000 turns.

Figure 2: Turn-by-turn squared beam sizes and emittances for a single FODO cell of 60° horizontal and 52° vertical phase advance with an equivalent current of $10^9$ protons per bunch.

Figure 3 compares the zero-current periodic beta functions to the beta-functions generated by a beam with $N= 10^9$ protons per bunch at a kinetic energy of 200 MeV. The corresponding tune shift by linear approximation is $\Delta Q = -0.059$. The increase in the periodic beta-functions due to the space charge force is clearly visible.

It is of interest to examine the growth of the $\beta$-functions and the emittances as a function of particles per bunch, i.e the dependency on beam current. Figure 4 shows the horizontal periodic $\beta$-function and the horizontal turn-by-turn emittance growth as a function of particles per bunch and with constant damping time of 1000 turns.

Plotting the equilibrium beam sizes as a function of beam current in fig. 5, we see a significant growth. We note here that increasing the current to very high values leads to a very strong decrease in tune, where at some point, linear beam transport becomes unstable. Empirically, that stability threshold is around $3 \times 10^9$ protons per bunch for the lattice and beam configurations used above.
Figure 3: Zero-current periodic beta functions for a single FODO cell with 60° horizontal and 52° vertical phase advance. The solid lines display the periodic beta-functions for the zero-current case and the dashed lines for 10^9 protons per bunch. Corresponding tune shift by linear approximation: ΔQ = −0.059

Figure 4: a) Increase in the horizontal β-function as a function of protons per bunch, b) Space charge-induced emittance growth as a function of protons per bunch. Constant damping time of 1000 turns.
Figure 5: Equilibrium beam sizes as a function of particles per bunch.
4.2. Core Dynamics in a Test Ring

In order to test our model on a realistic lattice, we set up a test ring that is used as example in [13], pages 97ff without edge focusing. The main cell of the ring consists of quadrupoles with normalized gradient $k = 1.2 \, m^{-2}$ and length $l = 0.4 \, m$, sector dipole magnets of length $1.5 \, m$ and bending angle $\theta = 22.5^\circ$, and drift spaces of length $0.55 \, m$. We close the ring by repeating the main cell 16 times. Figure 6 shows the composition of the lattice.

First, we examine the turn-by-turn data as a function of protons per bunch in shown in fig. 7. The squared beam sizes increase due to the space charge force and eventually, the beam finds its new equilibrium, similar to the FODO cell. The same happens for the eigenemittances. In both, beam size and emittance, the amount of growth is in the order of 10%. The beam size for $5 \times 10^8$ protons per bunch exhibits a strong beating, suggesting a close proximity of two
frequencies. That apparent beating can be traced to undersampling and thus is an artifact. In order to obtain the betatron tunes, we perform a FFT on the turn-by-turn squared beam sizes. Looking at the tunes as a function of beam current in fig. 8a, we see the expected linear decrease in tune shift due to space charge. The data point at $5 \times 10^8$ protons per bunch seems to be an outlier regarding the linear trend. This data point corresponds to the strong beating in the beam sizes in fig. 7a and is around the tune $Q = 0.75$. Considering the oscillation of the beam envelope with two times the betatron tune, we expect the 'beating' due to proximity of the betatron frequency to the revolution frequency to happen in intervals of 0.25. The tune regions at the border between two Nyquist zones are difficult to treat regarding a Fourier analysis. The bump in the tunes corresponding to the beating in fig. 8a is a result of an insufficient detection of the crossing point over the Nyquist frequency. Consequently, the tune is mirrored in the spectrum and appears to increase again.

![Figure 8: a) Tunes as a function of beam current. The tune is obtained by FFT of the turn-by-turn data. b) Emittance vs. tune shift.](image)

Fig. 8b shows the horizontal emittance versus the tune shift. The curve principally represents the increase in beam current, since the tune shift is proportional to it. Since emittance and tune shift are parameters that contain information about both the beam and the machine lattice encoded, the figure provides a overview over machine performance regarding beam dynamics with space charge.

5. Spectator Particle Dynamics

In this section, we examine the influence of the non-linear space charge force produced by the beam core on the dynamics of single particles. Therefore, we create a particle-core model. As core, we use the equilibrium solution obtained in the previous simulations. Additionally, we place spectator particles around the core. These particles are completely passive and observe the electric field produced by the core as well as the external fields from the lattice. The initial
spectator particles are placed in normalized phase space along the positive horizontal axis, thereby exhibiting different actions $J$. To ensure a proper placement of the particles, we choose their positions to represent multiples of the one sigma equilibrium beam size of the beam core. In normalized phase space, the action $J$ of a particle is given by

$$2J = x^2 + x'^2. \quad (5.1)$$

The beam size $\sigma_x^2$ in real space is given by

$$\sigma_x^2 = \epsilon_x \beta_x \quad (5.2)$$

which in normalized phase space becomes a circle with radius $\sqrt{2} \epsilon$ because of $\beta_x = 1$. We recall that the emittance is the average over all particle actions $J$ that comprise the beam. From here we conclude that we place a single particle on the one-sigma beam envelope if we use the rms beam emittance as particle action such as the single particle draws a circle in normalized phase space according to $2\epsilon = x^2 + x'^2$ and thus has an amplitude of $\sqrt{2}\epsilon$. Figure 9a visualizes the initial particle placement in combination with an overlay of the electric field, generated by the Gaussian beam core. Figure 9b shows the amplitude-dependent tune shift of the spectator particles with a beam current equivalent to $4 \times 10^8$ protons per bunch. As expected, particles far away from the beam core do not exhibit tune shift and thus have a tune equal to the bare tune of the lattice (dashed line). The maximum tune shift for the particles in the limit to the beam center converges to the value we obtain from the the linear approximation, where we represent space charge as defocusing quadrupoles.

![Figure 9: a) Initial placement of spectator particles around a Gaussian beam core. Overlay of the electric field, generated by the core. b) Amplitude-dependent tune shift of the spectator particles for $4 \times 10^8$ protons per bunch. The dashed line marks the bare tune of the lattice.](image)

We examine the spectator particle movement for three scenarios. Each scenario was simulated for the beam currents’ equivalent to $4 \times 10^8$ protons per
bunch and $1 \times 10^9$ protons per bunch, respectively. The results are shown as Poincaré-maps of the spectator particles in normalized phase space over 2000 turns. We recall here that the undisturbed particle draws a perfect circle in normalized phase space. The examined scenarios are:

1. Matched beam core
2. Mismatched beam core
3. Matched beam core with coupled lattice

We quantify beam mismatch with the $B_{\text{mag}}$ parameter [14]

$$B_{\text{mag}} = \frac{1}{2} \left( \frac{\beta^*}{\beta} + \frac{\beta}{\beta^*} + \left( \alpha \sqrt{\frac{\beta^*}{\beta}} - \alpha^* \sqrt{\frac{\beta}{\beta^*}} \right) \right)$$  \hspace{1cm} (5.3)

where $\alpha$ and $\beta$ are the twiss parameters before mismatch and the variables with asterisks after mismatch. The mismatch parameter quantifies the amount of non-overlapping between two ellipses in phase space, i.e. a matched beam with full overlap yields a mismatch parameter of $B_{\text{mag}} = 1$. Figure 10 shows an example of the parameter’s meaning. We note here that without further treatment, this equation is only meaningful in the absence of cross-plane coupling.

![Figure 10: Example of beam mismatch. Mismatch parameter $B_{\text{mag}}$ quantifies non-overlapping between two ellipses in phase space.](image)

5.1. Scenario 1: Matched Core

In the first scenario, the spectator particles are placed around a matched beam core. Consequently, there is no varying beam size oscillations on a turn-by-turn basis and the effect due to beam current is isolated. Figure 11 shows the Poincaré-maps of this scenario.

Comparing the maps, we observe larger amplitudes for the particles with a higher beam current. This is not a consequence of dynamical behavior, but of the initial particle placement in combination with increased equilibrium beam sizes due to a higher beam current. The beam current effect in the matched case manifests itself in blurred circles. The increase of the effect is very low, considering that the particles in the bunch were more than doubled.
Figure 11: a) Poincaré-map of spectator particles revolving around a matched beam with $4 \times 10^8$ protons per bunch and b) with $1 \times 10^9$ protons per bunch.

5.2. Scenario 2: Mismatched Core

In the second scenario, we examine the influence of beam mismatch. For that, the spectator particles are placed according to the equilibrium solution, but the core is mismatched. As a result of mismatch, the core begins beam size oscillations as it propagates through the lattice and its electric field distribution strongly varies until it is damped and reaches the equilibrium solution again. Figure 12 shows the scenario of beam mismatch. It is noticeable in both pictures that the particle which starts around the 2-σ (violet) region exhibit an increased chaotic movement over 2000 turns and migrate to orbits different than their initial ones.

Figure 12: Poincaré-map of spectator particles revolving around a mismatched beam with $B_{mag} = 1.08$ and $4 \times 10^8$ protons per bunch and b) with $B_{mag} = 1.4$ and $1 \times 10^9$ protons per bunch.
leading to a distribution density change among the spectator particles. We note here, that the underlying beam core is not subject to density change, but always stays Gaussian by construction. It is clear, that beam mismatch has a strong influence on the particles’ dynamic behavior, especially in contrast to the contribution of beam current alone. The depicted cases show an interesting difference: While the particle around the $2\sigma$ region in the left picture end up closer to the center of phase space and even below the orbit of its previously lower neighbor, the same particle ends up in a much higher orbit in the right case, where the beam current is higher and the mismatch stronger. We have not yet found criteria that predict the particles’ migration preference in such cases. In order to follow the question about this threshold, we repeated the simulations with many more particles.

Because a visualization in a Poincaré-map is not practical anymore due to the high amount of particles, we show the particles’ action displacement $\Delta J$ versus their initial action $J_{\text{init}}$ in figure 13. The ending actions are determined by the average over the last 100 turns for each particle. Further, we calculate the standard deviations of the actions and display them as error bands. The standard deviation is a measure of turbulence a particle experiences. Figure 13 provides a clearer picture about a threshold regarding particle displacement.

The particles close to the phase space origin are hardly influenced, since they observe a constant field gradient and a low field amplitude. It is noticeable that strong particle displacements and turbulences start to occur for particles that experience the non-linearity of the space charge force at least occasionally. Particles that repeatedly traverse the electric field maximum during propagation are prone to be pushed to either side. In analogy, the oscillating field maximum works like a plow, pushing the dirt out of its lane.

Looking at the evolution of action displacement from the beam center towards towards its edge, we see an interesting distinction between the two cases. Fig.

![Figure 13: Analysis of action displacement for the cases in scenario 2. a) $B_{\text{mag}} = 1.08$ and $4 \times 10^8$ protons per bunch and b) $B_{\text{mag}} = 1.4$ and $1 \times 10^9$ protons per bunch.](image)
13a exhibits a clearly visible ripple in action displacement after the chaotic region. The ripples show that the actions of the two planes are inversely phased. That is not always the case in fig. 13b, where part of the ripples appear to be in-phase. That behavior could be related to different breathing modes of the beam core and needs closer examination.

5.3. Scenario 3: Matched core, coupled lattice

In the third scenario, we use a matched beam core, but introduced a coupling between the transverse planes by adding a small skew angle to the focusing quadrupoles in our test lattice. The corresponding Poincaré-maps are shown in fig. 14. In the left picture, the particles starting at $1.5 \sigma$ and $2 \sigma$ show prominent oscillating structures without much chaos over the course of the 2000 turns. The hypothesis is that there is an action exchange between the planes due to the coupled lattice, where a part of the action leaves the horizontal phase space and enters the vertical phase space. It is the single particle equivalent to emittance exchange.

![Figure 14: Poincaré-maps of spectator particles revolving around a matched beam with cross-plane coupling for a) $4 \times 10^8$ protons per bunch and b) $1 \times 10^9$ protons per bunch. Coupling introduced by skew quadrupoles.](image)

6. Summary and Conclusion

We have developed a fully analytic space charge model valid for transverse Gaussian beams. The model includes non-linear space charge forces and cross-plane coupling. On basis of that model, a simulation code was developed in MATLAB. The model was verified at the example of a single FODO cell as a test lattice. The turn-by-turn beam core evolution in a test ring shows a $10\%$ growth in squared beam size and emittance in the investigated current range of 0 to $8 \times 10^8$ protons per bunch. Strong beating in in turn-by-turn beam sizes is attributed...
to the envelop tune being close to a resonance. The automatic calculation of the space charge tune shift by an FFT algorithm exhibits fundamental technical difficulties that are subject to further investigation. The shifted tunes are for now recovered by manual post-processing of the data.

The space charge tune shift obtained by a linear mapping shows a quadratic dependency of the chosen slice length, which was unexpected. The cause of this dependency is currently under investigation.

Passive spectator particles that observe the non-linear field produced by a previously simulated beam core show highly chaotic movement in the presence of beam mismatch. An analysis of particle action shows that the most chaotic movement seems to be locally limited to particles spending most of their time around the maximum of the self-field (between 1.5 to 2.5 $\sigma$), where also non-linearities come into effect. The pure effect of the space charge due to beam current has only little influence in the case of a matched beam. We thus conclude that the space charge effect serves as 'lever arm' for other detrimental effects like beam mismatch. In the presence of cross-plane coupling, introduced by skewed quadrupoles, an exchange of particle action between the transverse planes are observed for particles withing the 1.5 to 2.5 $\sigma$ range.

References


A. Space Charge Kick Scaling Factors

The particle deflection due to a space charge kick is given by:

\[(\tilde{x}_4 - x_4) + i(\tilde{x}_2 - x_2) = \Delta y' + i \Delta x' = \tilde{K} F_0(x_1, x_3, \sigma) = \tilde{K} (f_3 + if_1) \quad (A.1)\]

Here, we derive the scaling factor \(\tilde{K}\). We start by writing the radial Lorentz force

\[F_r = q \left( E_r - \frac{v_z}{c} B_\phi \right) = \frac{dp_r}{dt} \quad (A.2)\]

where \(\frac{dp_r}{dt}\) is the change in radial momentum, \(E_r\) the radial electric field component and \(B_\phi\) the azimuthal magnetic field component. In the relativistic case the Lorentz force and the space charge force almost compensate each other and we can replace \(\frac{v_z}{c} B_\phi = \beta^2 E_r\) since \(B_\phi\) can be expressed as \(\frac{v_c}{c} E_r\) in the relativistic limit and write

\[\frac{dp_r}{dt} = qE_r \left(1 - \beta^2\right) = \frac{qE_r}{\gamma^2} \quad (A.3)\]

where \(\gamma\) is the Lorentz factor. We have to recognize that the radial divergence of the beam is essentially the ratio between the radial momentum and the longitudinal momentum \(r' = \frac{p_r}{p_z}\). Thus, we can write the change in radial divergence as

\[dr' = \frac{dp_r}{p_z} = \frac{qE_r dt}{\gamma^2 p_z} \quad (A.4)\]

where we assume that the longitudinal momentum \(p_z\) remains constant. Now we want the kick strength to be scaled with a length \(d\ell\) instead with a time \(dt\). Therefore, we introduce the conversion \(dt = \frac{d\ell}{\beta c}\) and write

\[dr' = \frac{qE_r}{\beta c \gamma^2 p_z} d\ell. \quad (A.5)\]

Now, we can replace the longitudinal momentum \(p_z = \beta c m_0 \gamma\) insert it into eq. A.4 and obtain

\[dr' = \frac{qE_r}{\beta^2 c^2 \gamma^3 m_0} d\ell \quad (A.6)\]

where \(m_0\) is the particle rest mass. In the next step, we insert the electric field of a bi-Gaussian particle distribution with a round transverse cross-section and a constant local charge density \(\frac{dq}{dz} = \frac{N}{\sqrt{2\pi}\sigma_z}\), where \(\sqrt{2\pi}\sigma_z\) is the approximate bunch length of a longitudinal Gaussian charge distribution, and write

\[dr' = d\ell \frac{N q^2}{\sqrt{2\pi}\sigma_z 2\pi \epsilon_0 m_0 c^2 \beta^2 \gamma^3} \frac{1}{r} \left(1 - e^{-\frac{r^2}{2\sigma_z^2}}\right) = d\ell \frac{N}{\sqrt{2\pi}\sigma_z} \frac{2\sigma_z}{\beta^2 \gamma^3} \frac{1}{r} \left(1 - e^{-\frac{r^2}{2\sigma_z^2}}\right) \quad (A.7)\]
where we have used the classical particle radius 
\[ r_0 = \frac{q^2}{4\pi\varepsilon_0 m_0 c^2} \]
in the second step. In eq. A.7 we identify the beam perveance 
\[ K = \frac{N^2 r_0^2}{\sqrt{2\pi}\sigma_z\beta_0\gamma^3} \]
and conclude that 
\[ \tilde{K} = d\ell K \]
where \( d\ell \) is the length of the slice over which the space charge kick is calculated. Thus, \( \tilde{K} \) is the beam perveance, multiplied with the distance over which the space charge kick is effective.

B. Analytic Solution of the generalized linear Term

In this appendix, we show the validity of equation 2.13 and start from 2.12. The generalized linear term from equation 2.12 is given by

\[
\langle x_k (f_3 + if_1) \rangle = \frac{1}{(2\pi)^2 \sqrt{\det \sigma}} \int_{-\infty}^{\infty} d^4 x \ x_k e^{-\frac{1}{2} \sigma_{im}^{-1} x_l x_m} F_0(x_1, x_3, \tilde{\sigma}). \tag{B.1}
\]

We simplify the multiplication with \( x_k \) in the integral by completing the square and introducing a parametric differentiation \( \frac{\partial}{\partial B_k} \), writing the above equation as

\[
\langle x_k (f_3 + if_1) \rangle = \frac{1}{(2\pi)^2 \sqrt{\det \sigma} \partial B_k} \int_{-\infty}^{\infty} d^4 x \ e^{-\frac{1}{2} \sigma_{im}^{-1} x_l x_m + B_k x_k} F_0(x_1, x_3, \tilde{\sigma}) \tag{B.2}
\]

and setting \( B_k = 0 \) after the differentiation. After expanding \( F_0 \) and collecting the constant factors in the front, the linear term is written as

\[
\langle x_k (f_3 + if_1) \rangle = A_1 \int_{-\infty}^{\infty} d^4 x \ e^{-\frac{1}{2} \sigma_{im}^{-1} x_l x_m + B_k x_k} \left\{ w(z_1) - e^{-\frac{1}{2} \sigma_{im}^{-1} x_l x_m} w(z_2) \right\} \tag{B.3}
\]

with \( A_1 = \frac{\sqrt{\pi}}{(2\pi)^2 \sqrt{\det \sigma} \sqrt{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})}} \frac{\partial}{\partial B_k} \). We use the integral form of the complex error function [8]

\[
w(z) = \frac{2}{\sqrt{\pi}} \int_{0}^{\infty} d\alpha \ e^{-\alpha^2 + 2i\alpha z} \tag{B.4}
\]

to rewrite the expression and rearrange the order of integration. Changing the order of integration is allowed because Gaussian integrals always converge. The rearrangement gives the expression
\[ \langle x_k(f_3 + if_1) \rangle = A_1 \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-\alpha^2} d\alpha \left[ \int_{-\infty}^{\infty} d^4x \ e^{-\frac{1}{4}\sigma_{lm}^{-1}x_lx_m + B_k x_k + 2i\alpha z_1} \right. \\
- \left. \int_{-\infty}^{\infty} d^4x \ e^{-\frac{1}{4}\sigma_{lm}^{-1}x_lx_m - \frac{1}{4}\bar{\sigma}_{lm}^{-1}x_lx_m + B_k x_k + 2i\alpha z_2} \right] \] (B.5)

\[ = A_1 \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-\alpha^2} d\alpha [I_1 - I_2] \]

where two spatial integrals are nested in one parametric integral. We find the solution of the spatial integrals to be (see Appendix B.1)

\[ I_1 = (2\pi)^2 \sqrt{\text{det} \sigma} e^{\frac{1}{4}\sigma_{lm}C_lC_m} \]

\[ I_2 = \frac{(2\pi)^2 \sqrt{\text{det} \sigma}}{\sqrt{\text{det}(1 + \sigma \bar{\sigma}^{-1})}} e^{\frac{1}{2}(\sigma^{-1}(1 + \sigma \bar{\sigma}^{-1}))^{-1}_{lm}D_lD_m} \] (B.6)

with \( C_k = (B_k + 2i\alpha a_k) \) and \( D_k = (B_k + 2i\alpha b_k) \). Inserting the solutions yields a new expression for the linear term

\[ \langle x_k(f_3 + if_1) \rangle = \frac{2A_1}{\sqrt{\pi}} \int_0^\infty e^{-\alpha^2} d\alpha \left[ (2\pi)^2 \sqrt{\text{det} \sigma} e^{\frac{1}{4}\sigma_{lm}C_lC_m} \right. \\
- \left. \frac{(2\pi)^2 \sqrt{\text{det} \sigma}}{\sqrt{\text{det}(1 + \sigma \bar{\sigma}^{-1})}} e^{\frac{1}{2}(\sigma^{-1}(1 + \sigma \bar{\sigma}^{-1}))^{-1}_{lm}D_lD_m} \right] \] (B.7)

where only the parametric integral is left. Bringing the constant factors in front of the integrals, they partially cancel with the factors in the constant \( A_1 \) and we define a new constant \( A_2 = \frac{\sqrt{\pi}}{\sqrt{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})}} \frac{\partial}{\partial B_k} \). We show in Appendix B.2 that the expression \( \text{det}(1 + \sigma \bar{\sigma}^{-1}) \) is always 4 and simplify the linear term to

\[ \langle x_k(f_3 + if_1) \rangle = \frac{2A_2}{\sqrt{\pi}} \int_0^\infty d\alpha e^{-\alpha^2} \left[ e^{\frac{1}{2}\sigma_{lm}C_lC_m} - \frac{1}{2} e^{\frac{1}{2}(\sigma^{-1}(1 + \sigma \bar{\sigma}^{-1}))^{-1}_{lm}D_lD_m} \right] \] (B.8)

For a more convenient calculation, we make the substitution \( (\sigma^{-1}(1 + \sigma \bar{\sigma}^{-1}))^{-1}_{lm} = S_{lm} \), recover the parameter \( \alpha \) hidden in the expressions \( C_{lm} \) and \( D_{lm} \) and write:
\[ \langle x_k (f_3 + i f_1) \rangle = A_2 \frac{2}{\sqrt{\pi}} \left[ e^{\frac{1}{2} \sigma_{lm} B_l B_m} \int_0^\infty d\alpha \ e^{-(1+2i \sigma_{lm} a_l a_m)\alpha^2 + \frac{1}{2} \sigma_{lm} (B_l 2ia a_m + B_m 2ia a_l)} \right. \\
\left. - \frac{1}{2} e^{\frac{1}{2} S_{lm} B_l B_m} \int_0^\infty d\alpha \ e^{-(1+2S_{lm} b_l b_m)\alpha^2 + \frac{1}{2} S_{lm} (B_l 2ib a_m + B_m 2ib a_l)} \right] \\
= A_2 \frac{2}{\sqrt{\pi}} \left[ e^{\frac{1}{2} \sigma_{lm} B_l B_m} I_3 - \frac{1}{2} e^{\frac{1}{2} S_{lm} B_l B_m} I_4 \right]. \] 

(B.9)

Now we have two integrals over \( \alpha \) left to solve. We find the solution of these integrals to be (see appendix B.3)

\[ I_3 = \frac{1}{\sqrt{1 + 2 \sigma_{lm} a_l a_m}} \frac{\sqrt{\pi}}{2} \frac{\sigma_{lm} B_l a_m}{\sqrt{(1 + 2 \sigma_{lm} a_l a_m)}} \]

\[ I_4 = \frac{1}{\sqrt{1 + 2 S_{lm} b_l b_m}} \frac{\sqrt{\pi}}{2} \frac{S_{lm} B_l b_m}{\sqrt{(1 + 2 S_{lm} b_l b_m)}}. \]

(B.10)

Inserting the solutions yields

\[ \langle x_k (f_3 + i f_1) \rangle = \frac{\sqrt{\pi}}{\sqrt{2(\sigma_{11} - \sigma_{33} + 2i \sigma_{13})}} \frac{\partial}{\partial B_k} \left[ e^{\frac{1}{2} \sigma_{lm} B_l B_m} \frac{\sigma_{lm} B_l a_m}{\sqrt{(1 + 2 \sigma_{lm} a_l a_m)}} \right. \\
\left. - \frac{1}{2} e^{\frac{1}{2} S_{lm} B_l B_m} \frac{S_{lm} B_l b_m}{\sqrt{(1 + 2 S_{lm} b_l b_m)}} \right]. \]

(B.11)

At this point, we differentiate \( \frac{\partial}{\partial B_k} \) and set all \( B_k \) to zero in order to undo our transformation of \( x_k \) into the exponent in the very beginning. We show the differentiation explicitly in Appendix B.4. After the differentiation, the linear term reads as

\[ \langle x_k (f_3 + i f_1) \rangle = \frac{\sqrt{\pi}}{\sqrt{2(\sigma_{11} - \sigma_{33} + 2i \sigma_{13})}} \frac{2i}{\sqrt{2(1 + 2 \sigma_{lm} a_l a_m)}} \frac{\sigma_{km} a_m}{2} - \frac{S_{km} b_m}{2(1 + 2 S_{lm} b_l b_m)}. \] 

(B.12)

In Appendix B.5 we explicitly show that the expression \( 1 + 2 \sigma_{lm} a_l a_m = 2 \). Further, we show in appendix B.6 that \( 1 + 2 S_{lm} b_l b_m \) behaves like \( 1 + \sigma_{lm} b_l b_m = \frac{1}{2} \). We are therefore able to simplify the expression to

\[ \langle x_k (f_3 + i f_1) \rangle = \frac{2i}{\sqrt{2(\sigma_{11} - \sigma_{33} + 2i \sigma_{13})}} \left[ \frac{\sigma_{km} a_m}{2} - \frac{\sigma_{km} b_m}{2} \right]. \] 

(B.13)

After we insert the coefficients \( a \) and \( b \) from eq. 2.5, we obtain
\[ \langle x_k (f_3 + if_1) \rangle = \frac{i}{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})} \left[ \sigma_{k1} + i\sigma_{k3} - \left( \frac{\sigma_{k1}(\sigma_{33} - i\sigma_{13}) + i\sigma_{k3}(\sigma_{11} + i\sigma_{13})}{\sqrt{\sigma_{11}\sigma_{33} - \sigma_{13}^2}} \right) \right] \]

which is equation 2.13.

**B.1. Spatial Integrals**

Here, we solve explicitly the two spatial integrals from equation B.5. The first integral can be written as

\[ I_1 = \int_{-\infty}^{\infty} d^4x \ e^{-\frac{1}{2}\sigma_{lm}^{-1}x_lx_m + B_kx_k + 2i\alpha z_1} = \int_{-\infty}^{\infty} d^4x \ e^{-\frac{1}{2}\sigma_{lm}^{-1}x_lx_m + C_kx_k} \]  

(B.15)

where we use \( z_1 = a_kx_k \) and define a new variable \( C_k = (B_k + 2i\alpha a_k) \). Now we use the relation for multivariate Gaussian integrals (see in [12], Appendix A)

\[ \int_{-\infty}^{\infty} d^n x \ e^{A_{lm}x_lx_m + b_kx_k} = \frac{\pi^{n/2}}{\sqrt{\det(A)}} e^{\frac{1}{2}A^{-1}b_lb_m} \]  

(B.16)

and recognize that in our case \( A_{lm} = \frac{1}{2}\sigma^{-1} \). We solve the integral to

\[ \int_{-\infty}^{\infty} d^4x \ e^{-\frac{1}{2}\sigma_{lm}^{-1}x_lx_m + B_kx_k + 2i\alpha z_1} = \frac{\pi^2}{\sqrt{\det(A)}} e^{\frac{1}{2}\sigma_{lm}C_lC_m} = (2\pi)^2 \sqrt{\det(A)} e^{\frac{1}{2}\sigma_{lm}C_lC_m} \]  

(B.17)

leading to eq. B.6. The second spatial integral can be solved the same way with just slight differences. As before, we merge the exponent and define a new variable \( D_k = (B_k + 2i\alpha b_k) \) with \( z_2 = b_kx_k \), leading to the following equation:

\[ I_2 = \int_{-\infty}^{\infty} d^4x \ e^{-\frac{1}{2}(\sigma^{-1} + \tilde{\sigma}^{-1})_{lm}x_lx_m + D_kx_k}. \]  

(B.18)

The integral is easier to solve by using \( (\sigma^{-1} + \tilde{\sigma}^{-1}) = \sigma^{-1}(1 + \sigma\tilde{\sigma}^{-1}) \) and we obtain the solution

\[ I_2 = \frac{(2\pi)^2 \sqrt{\det(A)}}{\sqrt{\det(1 + \sigma\tilde{\sigma}^{-1})}} e^{\frac{1}{2}(1 + \sigma\tilde{\sigma}^{-1})^{-1}D_lD_m}. \]  

(B.19)

**B.2. Evaluate det(1 + \sigma\tilde{\sigma}^{-1})**

Here, we show that the expression det(1 + \sigma\tilde{\sigma}^{-1}) is always 4. First, we define the matrices \( \sigma \) and \( \tilde{\sigma} \):
We take the inverse of the integral, we write

\[ \sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} & \sigma_{14} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} & \sigma_{24} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} & \sigma_{34} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_{44} \end{bmatrix} ; \tilde{\sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{13} \\ \sigma_{31} & \sigma_{33} \end{bmatrix}. \quad (B.20) \]

We take the inverse of \( \tilde{\sigma} \)

\[ \tilde{\sigma}^{-1} = \begin{bmatrix} \sigma_{33} & 0 & -\sigma_{13} & 0 \\ 0 & 0 & 0 & 0 \\ -\sigma_{31} & 0 & \sigma_{11} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \frac{1}{\sigma_{11}\sigma_{33} - \sigma_{13}\sigma_{31}} \quad (B.21) \]

where we have filled the two missing dimensions with zeros after the inversion.

Now we take the product \( \sigma \tilde{\sigma}^{-1} \) and write

\[
\sigma \tilde{\sigma}^{-1} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} & \sigma_{14} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} & \sigma_{24} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} & \sigma_{34} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_{44} \end{bmatrix} \begin{bmatrix} \sigma_{33} & 0 & -\sigma_{13} & 0 \\ 0 & 0 & 0 & 0 \\ -\sigma_{31} & 0 & \sigma_{11} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \frac{1}{\sigma_{11}\sigma_{33} - \sigma_{13}\sigma_{31}} = \\
= \begin{bmatrix} \sigma_{11}\sigma_{33} - \sigma_{13}\sigma_{31} & 0 & -\sigma_{31}\sigma_{13} + \sigma_{33}\sigma_{11} & 0 \\ 0 & \sigma_{11}\sigma_{33} - \sigma_{13}\sigma_{31} & -\sigma_{31}\sigma_{13} + \sigma_{33}\sigma_{11} & 0 \\ 0 & 0 & \sigma_{11}\sigma_{33} - \sigma_{13}\sigma_{31} & -\sigma_{31}\sigma_{13} + \sigma_{33}\sigma_{11} \\ 0 & 0 & 0 & \sigma_{11}\sigma_{33} - \sigma_{13}\sigma_{31} \end{bmatrix} \frac{1}{\sigma_{11}\sigma_{33} - \sigma_{13}\sigma_{31}} \quad (B.22) \]

Now we add the one to the product and calculate the determinant of the whole expression

\[
\det \left( 1 + \sigma \tilde{\sigma}^{-1} \right) = \det \left( \begin{bmatrix} \frac{2}{\sigma_{11}\sigma_{33} - \sigma_{13}\sigma_{31}} & 0 & 0 & 0 \\ \frac{2}{\sigma_{11}\sigma_{33} - \sigma_{13}\sigma_{31}} & 1 & -\frac{2\sigma_{31}\sigma_{13} + \sigma_{33}\sigma_{11}}{\sigma_{11}\sigma_{33} - \sigma_{13}\sigma_{31}} & 0 \\ \frac{2}{\sigma_{11}\sigma_{33} - \sigma_{13}\sigma_{31}} & 0 & \frac{2}{\sigma_{11}\sigma_{33} - \sigma_{13}\sigma_{31}} & 0 \\ \frac{2}{\sigma_{11}\sigma_{33} - \sigma_{13}\sigma_{31}} & 0 & 0 & \frac{2}{\sigma_{11}\sigma_{33} - \sigma_{13}\sigma_{31}} \end{bmatrix} \right) = 4. \quad (B.23) \]

### B.3. Solve parametric Integrals

Here, we solve the two integrals from eq. B.10 by substitution. For the first integral, we write

\[
I_3 = \frac{1}{\sqrt{1 + 2\sigma_{1m}a_l a_m}} \int_0^\infty d\gamma \ e^{-\gamma^2 + 2i\gamma \frac{\sigma_{1m}B_{l} a_m}{\sqrt{(1 + 2\sigma_{1m}a_l a_m)}}} \quad (B.24) 
\]
were we have substituted $\gamma = \sqrt{(1 + 2\sigma_{lm}a_la_m)}\alpha$ and inferred $\frac{d\gamma}{d\alpha} = \sqrt{1 + 2\sigma_{lm}a_la_m}$.

Now we recover the integral form of the complex error function and write
\[
\frac{1}{\sqrt{1 + 2\sigma_{lm}a_la_m}} \int_0^\infty d\gamma \ e^{-\gamma^2 + 2i\gamma \frac{\sigma_{lm}B_la_m}{\sqrt{(1 + 2\sigma_{lm}a_la_m)}}} = \frac{1}{\sqrt{1 + 2\sigma_{lm}a_la_m}} \sqrt{\frac{\pi}{2}} w(m_1)
\]

where we defined a variable $m_1 = \frac{\sigma_{lm}B_la_m}{\sqrt{(1 + 2\sigma_{lm}a_la_m)}}$ for more convenient calculation.

We can apply the same method to the second integral, resulting in
\[
\frac{1}{\sqrt{1 + 2S_{lm}b_lb_m}} \int_0^\infty d\gamma \ e^{-\gamma^2 + 2i\gamma \frac{S_{lm}B_lb_m}{\sqrt{(1 + 2S_{lm}b_lb_m)}}} = \frac{1}{\sqrt{1 + 2S_{lm}b_lb_m}} \sqrt{\frac{\pi}{2}} w(m_2)
\]

where $S = (1 + \sigma\tilde{\sigma}^{-1})^{-1}\sigma$ and is $m_2 = \frac{S_{lm}B_lb_m}{\sqrt{(1 + 2S_{lm}b_lb_m)}}$ and obtain equations B.10.

**B.4. Differentiation** $\frac{d}{dB_k}$

Here, we take the derivative of the term

\[
y_1(B_k) - y_2(B_k) = \left[ e^{\frac{1}{2} \sum \sigma_{lm}B_lB_m} \left( \frac{\sigma_{lm}B_l(a_m)}{\sqrt{(1 + 2\sigma_{lm}a_la_m)}} \right) \right.
\]

\[
- \left. \frac{e^{\frac{1}{2} \sum S_{lm}B_lB_m}}{2\sqrt{(1 + 2S_{lm}b_lb_m)}} \left( \frac{S_{lm}B_l(b_m)}{\sqrt{(1 + 2S_{lm}b_lb_m)}} \right) \right]
\]

from eq. B.11 and set all $B_l$ to zero in order to reverse the parametric differentiation we introduced in eq. B.2. We consider the two parts of the difference separately. The inner and outer derivatives must be considered. Thus, we have to solve the derivative for either part as in

\[
y_k \bigg|_{B_k=0} = f'(B_k) \bigg|_{B_k=0} w(B_k) \bigg|_{B_k=0} + f(B_k) \bigg|_{B_k=0} w'(g(B_k)) \bigg|_{B_k=0} g'(B_k) \bigg|_{B_k=0}
\]

where $f$ is the factor before the complex error function and $g$ the argument of the complex error function. First, we look at the differentiation of $f(B_k)$ in the first part:

\[
f(B_k) = \frac{e^{\frac{1}{2} \sigma_{lm}B_lB_m}}{\sqrt{1 + 2\sigma_{lm}a_la_m}}
\]

The derivative of this function always contains a factor $B_l$ which is set to zero and we conclude that the function $f'(B_k) \bigg|_{B_k=0} = 0$. This reduces Eq. B.28 to the form
\[ y' \bigg|_{B_k=0} = f(B_k) \bigg|_{B_k=0} w' \bigg( g(B_k) \bigg|_{B_k=0} \bigg) g' \bigg( B_k \bigg|_{B_k=0} \bigg). \]  

(B.30)

The first remaining term is easily calculated:

\[ f(B_k) \bigg|_{B_k=0} = \frac{1}{\sqrt{1 + 2\sigma_{lm}a_l a_m}}. \]  

(B.31)

Now we look at the differentiation of the complex error function and use the relation (from [8])

\[ w'(z) = -2zw(z) + \frac{2i}{\sqrt{\pi}} \]  

(B.32)

where z is the respective argument of the function, i.e. \( g(B_i) \). Looking at

\[ g(B_k) = \frac{\sigma_{lm} B_i a_m}{\sqrt{1 + 2\sigma_{lm}a_l a_m}} \]  

(B.33)

we see that the only part left from the differentiation of the complex error function after setting \( B_i \) to zero is

\[ w'(B_k) \bigg|_{B_k=0} = \frac{2i}{\sqrt{\pi}} \]  

(B.34)

which gives us the second factor of the chain differentiation. Last, we look at the differentiation of the function \( g(B_i) \). We see that for every differentiation step, one \( B \) becomes unity due to the differentiation and another \( B \) that is constant with respect to the \( B \) which was differentiated after. That constant \( B \), however, becomes zero and thus, these terms vanish. The remaining term and the last missing in the differentiation chain thus is:

\[ g'(B_k) \bigg|_{B_k=0} = \frac{\sigma_{lm} a_m}{\sqrt{1 + 2\sigma_{lm}a_l a_m}} = \frac{\sigma_{km} a_m}{\sqrt{1 + 2\sigma_{lm}a_l a_m}}. \]  

(B.35)

Note that due to the differentiation, the term above is non-zero only for the \( B \) that was differentiated after. Thus, the index \( i \) can be replaced by \( k \) in the final expression. The solution to the differentiation of the first part is

\[ y_1'(B_k) \bigg|_{B_k=0} = \frac{1}{\sqrt{1 + 2\sigma_{lm}a_l a_m}} \frac{\sigma_{km} a_m}{\sqrt{1 + 2\sigma_{lm}a_l a_m}} \frac{2i}{\sqrt{\pi}} = \frac{\sigma_{km} a_m}{1 + 2\sigma_{lm}a_l a_m} \frac{2i}{\sqrt{\pi}}. \]  

(B.36)

Performing the same calculations for the second part of the derivation, we obtain its solution

\[ y_2'(B_k) \bigg|_{B_k=0} = \frac{1}{2\sqrt{1 + 2S_{lm}b_l b_m}} \frac{S_{km} b_m}{\sqrt{1 + 2S_{lm}b_l b_m}} \frac{2i}{\sqrt{\pi}} = \frac{S_{km} b_m}{2(1 + 2S_{lm}b_l b_m)} \frac{2i}{\sqrt{\pi}}. \]  

(B.37)
B.5. Evaluate \((1 + 2\sigma_{lm}a_l a_m)\)

Here, we evaluate the term \((1 + 2\sigma_{lm}a_l a_m)\) from equation B.12 by inserting the respective elements from the \(\sigma\)-matrix and the variable \(a_{l,m}\):

\[
(1 + 2\sigma_{lm}a_l a_m) = 1 + 2 \left( \sigma_{11}a_1^2 + 2\sigma_{13}a_1 a_3 + \sigma_{33}a_3^2 \right) \\
= 1 + 2 \left( \sigma_{11}a_1^2 + 2i\sigma_{13}a_1^2 - \sigma_{33}a_3^2 \right) \\
= 1 + 2a_1^2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13}) \\
= 1 + \frac{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})}{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})} = 2.
\]  

(B.38)

B.6. Show that \((1 + 2S_{lm}b_l b_m) = \frac{1}{2}\)

Here we show that the term \((1 + 2S_{lm}b_l b_m)\) from eq. B.12 is \(\frac{1}{2}\). The variable \(S\) is defined by

\[
S = (\sigma^{-1} (1 + \sigma\tilde{\sigma}^{-1}))^{-1} = (1 + \sigma\tilde{\sigma}^{-1})^{-1}\sigma.
\]  

(B.39)

In eq. B.23, we already calculated the term \((1 + \sigma\tilde{\sigma}^{-1})\) and it reads

\[
(1 + \sigma\tilde{\sigma}^{-1}) = \begin{bmatrix}
\frac{2}{\sigma_{11} - \sigma_{33} - 2i\sigma_{13}} & 0 & 0 & 0 \\
0 & \frac{1}{\sigma_{11} - \sigma_{33} - 2i\sigma_{13}} & 0 & 0 \\
0 & 0 & \frac{2}{\sigma_{11} - \sigma_{33} - 2i\sigma_{13}} & 0 \\
0 & 0 & 0 & \frac{1}{\sigma_{11} - \sigma_{33} - 2i\sigma_{13}}
\end{bmatrix}
\]  

(B.40)

Now, we invert the matrix and write

\[
(1 + \sigma\tilde{\sigma}^{-1})^{-1} = \begin{bmatrix}
\frac{1}{2} & 0 & 0 & 0 \\
-\frac{1}{2}a & 1 & -\frac{1}{2}b & 0 \\
0 & 0 & 1/2 & 0 \\
-\frac{1}{2}c & 0 & -\frac{1}{2}d & 1
\end{bmatrix}.
\]  

(B.41)

The multiplication of that matrix with the matrix \(\sigma\) yields the matrix \(S\) and it reads

\[
S = \begin{bmatrix}
\frac{1}{2} & 0 & 0 & 0 \\
-\frac{1}{2}a & 1 & -\frac{1}{2}b & 0 \\
0 & 0 & 1/2 & 0 \\
-\frac{1}{2}c & 0 & -\frac{1}{2}d & 1
\end{bmatrix} \sigma = \begin{bmatrix}
\sigma_{11} & \sigma_{12} & \sigma_{13} & \sigma_{14} \\
\sigma_{21} & \sigma_{22} & \sigma_{23} & \sigma_{24} \\
\sigma_{31} & \sigma_{32} & \sigma_{33} & \sigma_{34} \\
\sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_{44}
\end{bmatrix}
\]  

(B.42)

where \(w, x, y\) and \(z\) are terms which are different from one half of their respective matrix element and they have the indices 22, 24, 42 and 44. Since the next step contains a multiplication with \(b_l b_m\) and \(b_2 = b_4 = 0\), these elements will disappear in the sum and we treat \(S\) like \(\frac{1}{2}\sigma\) with respect to the remaining elements. Consequently, we show in the next step that \((1 + \sigma_{lm}b_l b_m)\) is always \(\frac{1}{2}\) by inserting the respective elements from the \(\sigma\)-matrix and the variables \(b_{l,m}\):
\[(1 + \sigma_{lm} b_l b_m) = 1 + \left[ \sigma_{11} b_1^2 + 2\sigma_{12} b_1 b_2 + \sigma_{33} b_3^2 \right] \]

\[= 1 + \frac{\sigma_{11}(\sigma_{33} - i\sigma_{13})^2 + 2\sigma_{13} [(\sigma_{33} - i\sigma_{13})(i\sigma_{11} - \sigma_{13})] + \sigma_{33}(i\sigma_{11} - \sigma_{13})^2}{\sqrt{\sigma_{11}\sigma_{33} - \sigma_{13}^2 \sqrt{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})}}} \]

\[= 1 + \frac{\sigma_{11}\sigma_{33}^2 - 2i\sigma_{11}\sigma_{13}\sigma_{33} - \sigma_{13}^2\sigma_{33} + 4\sigma_{11}\sigma_{13}\sigma_{33} - 2\sigma_{11}\sigma_{13}^2 + 2\sigma_{13}^2\sigma_{33} - 4i\sigma_{13}}{2\sigma_{11}\sigma_{33} - 2\sigma_{11}\sigma_{33}^2 + 4i\sigma_{11}\sigma_{13}\sigma_{33} - 2\sigma_{11}\sigma_{13}^2 + 2\sigma_{13}^2\sigma_{33} - 4i\sigma_{13}} \]

\[= 1 - \frac{1}{2} = \frac{1}{2}. \quad \text{(B.43)} \]

\[\text{C. Analytic Solution of the quadratic Term}\]

In this appendix, we evaluate the quadratic terms of the space charge kick from eq. 2.14. We start by evaluating the term \(\langle F_0^2 \rangle\) constructed from eq. 2.4 and write its explicit expression

\[\langle F_0^2 \rangle = \frac{\pi}{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})} \frac{1}{2\pi \sqrt{\det \sigma}} \int_{-\infty}^{\infty} d^2x \quad e^{-g} \left[ w(z_1) - e^{-g}w(z_2) \right]^2 \]

\[= A \int_{-\infty}^{\infty} d^2x \quad e^{-g} \left[ w(z_1)w(z_1) - 2e^{-g}w(z_1)w(z_2) + e^{-2g}w(z_2)w(z_2) \right] \quad \text{(C.1)}\]

with \(A = \frac{\pi}{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})} \frac{1}{2\pi \sqrt{\det \sigma}}\) and \(g = \frac{1}{2} \sum \sigma_{lm}^{-1} x_l x_m\).

In the integral, we distinguish between three terms

1. \(e^{-g} w(c_1 x_1 + c_3 x_3)w(d_1 x_1 + d_3 x_3)\)
2. \(e^{-2g} w(c_1 x_1 + c_3 x_3)w(d_1 x_1 + d_3 x_3)\)
3. \(e^{-3g} w(c_1 x_1 + c_3 x_3)w(d_1 x_1 + d_3 x_3)\)

Where variables \(c \) and \(d \) are coefficients appearing in the arguments of the complex error functions. With these terms we create a function \(P(\sigma, n, c, d)\) and write the above integral in the generalized form

\[P(\sigma, n, c, d) = \frac{1}{2\pi \sqrt{\det \sigma}} \int_{-\infty}^{\infty} d^2x \quad e^{-ng} w(c_1 x_1 + c_3 x_3)w(d_1 x_1 + d_3 x_3) \quad \text{(C.2)}\]

for \(n = 1, 2, 3\) and we can write

\[\langle F_0^2 \rangle = \frac{\pi}{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})} \left[ P(\sigma, 1, a, a) - 2P(\sigma, 2, a, b) + P(\sigma, 3, b, b) \right] \quad \text{(C.3)}\]
where the coefficients $c$ and $d$ depend on the number $n$. The evaluation of the integral in function $P(\sigma, n, c, d)$ is explicitly done in appendix C.1 and gives the result

$$P(\sigma, n, c, d) = \frac{4}{2n\pi} \frac{1}{\sqrt{S_{11}S_{22} - S_{12}^2}} \left[ \frac{\pi}{2} - \arctan \left( \frac{S_{12}}{\sqrt{S_{11}S_{22} - S_{12}^2}} \right) \right]$$  \hspace{1cm} (C.4)

where $S = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}$ contains the respective matrix elements as a function of $n$, more specifically

$$S(\sigma, n, a, a) = \begin{bmatrix} 1 - \frac{1}{n} & \frac{1}{n} \\ \frac{1}{n} & 1 - \frac{1}{n} \end{bmatrix}$$

$$S(\sigma, n, a, b) = \begin{bmatrix} 1 - \frac{1}{n} & 0 \\ 0 & 1 - \frac{1}{n} \end{bmatrix}$$

$$S(\sigma, n, b, b) = \begin{bmatrix} 1 - \frac{1}{n} & -\frac{1}{n} \\ -\frac{1}{n} & 1 - \frac{1}{n} \end{bmatrix}$$  \hspace{1cm} (C.5)

We show that $\langle F_0^2 \rangle$ and $\langle \bar{F}_0^2 \rangle$ are zero (appendix C.3). Hence, the term $f_3f_1$ vanishes and the two remaining terms are

$$f_3^2 = f_1^2 = \frac{1}{2} \langle F_0\bar{F}_0 \rangle.$$  \hspace{1cm} (C.6)

Consequently, only $\langle F_0\bar{F}_0 \rangle$ must be calculated to cover the quadratic terms. The calculation of $\langle F_0\bar{F}_0 \rangle$ is slightly different from that of $\langle F_0^2 \rangle$. The mixed term is explicitly written as

$$\langle F_0\bar{F}_0 \rangle = \frac{\pi}{\sqrt{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})\sqrt{2(\sigma_{11} - \sigma_{33} - 2i\sigma_{13})}}}$$

$$\frac{1}{2\pi\sqrt{\det\sigma}} \int_{-\infty}^{\infty} d^2x \ e^{-g} \left[ w(z_1) - e^{-g}w(z_2) \right] \left[ w(z_1) - e^{-g}w(z_2) \right].$$  \hspace{1cm} (C.7)

We transform the conjugated complex error functions as in

$$\left[ w(z_1) - e^{-g}w(z_2) \right] = w(z_1) - e^{-g}w(z_2).$$  \hspace{1cm} (C.8)

With the relation $\bar{w}(-z) = w(z)$ [8], we rewrite it to

$$w(z_1) - e^{-g}w(z_2) = w(-z_1) - e^{-g}w(-z_2).$$  \hspace{1cm} (C.9)

Now we use the relation $w(-z) = 2e^{-z^2} - w(z)$ from [8] and transform the term to

$$w(-z_1) - e^{-g}w(-z_2) = -w(z_1) + e^{-g}w(z_2) + 2 \left( e^{-z_1^2} - e^{-z_2^2} \cdot e^{-g} \right).$$  \hspace{1cm} (C.10)
We show explicitly in appendix C.4 that
\[ 2 \left( e^{-z_1^2} - e^{-z_2^2} \cdot e^{-g} \right) = 0 \]  
(C.11)
and consequently write
\[ -w(z_1) + e^{-g}w(z_2) = - \left[ w(z_1) - e^{-g}w(z_2) \right] = \left[ w(z_1) - e^{-g}w(z_2) \right]. \]  
(C.12)
We get a global minus sign in front of the integral, but otherwise perform the same calculation we did for \( \langle F_0^2 \rangle \). As a result, the function \( P \) stays the same, but receives complex conjugated arguments. We find the analytic solution of \( \langle F_0 \bar{F}_0 \rangle \) as
\[ \langle F_0 \bar{F}_0 \rangle = \frac{-\pi}{\sqrt{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})}\sqrt{2(\sigma_{11} - \sigma_{33} - 2i\sigma_{13})}} \left[ P(\sigma, 1, a, a^*) - P(\sigma, 2, a, b^*) - P(\sigma, 2, a^*, b) + P(\sigma, 3, b, b^*) \right]. \]  
(C.13)
\[ P(\sigma, n, c, d) \]  
C.1. Evaluation of the function \( P(\sigma, n, c, d) \)
We start from eq. C.2 which reads
\[ P(\sigma, n, c, d) = \frac{1}{2\pi \sqrt{\det \sigma}} \int_{-\infty}^{\infty} d^2 x \ e^{-ngw(c_1x_1 + c_3x_3)w(d_1x_1 + d_3x_3)} \]  
(C.14)
and replace the complex error functions by their integral form [8]
\[ w(z) = \frac{2}{\sqrt{\pi}} \int_{0}^{\infty} d\alpha \ e^{-\alpha^2 + 2i\alpha z} \]  
(C.15)
to obtain
\[ P(\sigma, n, c, d) = \frac{1}{2\pi \sqrt{\det \sigma}} \int_{-\infty}^{\infty} d^2 x \ e^{-ng} \frac{2}{\sqrt{\pi}} \int_{0}^{\infty} d\alpha \ e^{-\alpha^2 + 2i\alpha(c_1x_1 + c_3x_3)} \frac{2}{\sqrt{\pi}} \int_{0}^{\infty} d\beta \ e^{-\beta^2 + 2i\beta(d_1x_1 + d_3x_3)}. \]  
(C.16)
Changing the order of integration, we write the equation as
\[ P(\sigma, n, c, d) = \frac{4}{2\pi \sqrt{\det \sigma \pi}} \int_{0}^{\infty} d\alpha \int_{0}^{\infty} d\beta \ e^{-\alpha^2 - \beta^2} \int_{-\infty}^{\infty} d^2 x \ e^{-ng + 2i\alpha(c_1x_1 + c_3x_3) + 2i\beta(d_1x_1 + d_3x_3)}. \]  
(C.17)
First, solve the spatial part of the integral as done in the linear part.

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\[ \int_{-\infty}^{\infty} d^2x \ e^{-n^2+2i\alpha(c_1x_1+c_3x_3)+2i\beta(d_1x_1+d_3x_3)} = \quad (C.18) \]

\[ \int_{-\infty}^{\infty} d^2x \ e^{-n^2+B_kx_k} = \int_{-\infty}^{\infty} d^2x \ e^{-\frac{n}{2} \sigma_{lm}x_lx_m+B_kx_k}. \]

With \( A = \frac{n}{2} \sigma^{-1} \) and eq. B.16 we get the solution

\[ I = \pi \frac{\sigma_{lm}B_lB_m}{\sqrt{\text{det}(\sigma)}} = 2 \pi \frac{n}{\sqrt{\text{det}(\sigma)}} \left( \sigma_{11}B_1^2 + 2i\alpha c_1 + 2i\beta d_1 \right) = 2 \pi \frac{n}{\sqrt{\text{det}(\sigma)}} \left( \sigma_{33}B_3^2 + 2i\beta c_3 + 2i\alpha d_3 \right) = 2 \pi \frac{n}{\sqrt{\text{det}(\sigma)}} \left( \sigma_{13}B_1B_3 + 2i\alpha c_1c_3 + 2i\beta c_1d_3 + 2i\alpha c_3d_1 + 2i\beta d_1d_3 \right). \]

(C.19)

Now we collect the \( \alpha, \beta \) and \( \alpha\beta \) terms in the exponent \( e^{-\alpha^2-\beta^2} e^{\frac{1}{2n} \sigma_{lm}(2i\alpha c_l + 2i\beta d_l)(2i\alpha c_m + 2i\beta d_m)} \) and write all parts of the sum explicitly:

\[ \sigma_{11}B_1^2 = \sigma_{11}(2i\alpha c_1 + 2i\beta d_1)^2 = -4\sigma_{11}(\alpha^2 c_1^2 + 2\alpha \beta c_1 d_1 + \beta^2 d_1^2) \]

(C.21)

\[ \sigma_{33}B_3^2 = \sigma_{33}(2i\alpha c_3 + 2i\beta d_3)^2 = -4\sigma_{33}(\alpha^2 c_3^2 + 2\alpha \beta c_3 d_3 + \beta^2 d_3^2) \]

(C.22)

\[ \sigma_{13}B_1B_3 = \sigma_{31}B_3B_1 = \sigma_{13}(2i\alpha c_1 + 2i\beta d_1)(2i\alpha c_3 + 2i\beta d_3) = -4\sigma_{13}(\alpha^2 c_1c_3 + \alpha \beta c_1d_3 + \alpha \beta c_3d_1 + \beta^2 d_1d_3). \]

(C.23)

We write the integrand as

\[ e^{-\alpha^2-\beta^2} e^{\frac{1}{2n} \sigma_{lm}B_lB_m} = \]

\[ \exp \left[ -\alpha^2(1 + \frac{2}{n}(\sigma_{11}c_1^2 + \sigma_{33}c_3^2 + 2i\sigma_{13}c_1c_3)) - \beta^2(1 + \frac{2}{n}(\sigma_{11}d_1^2 + \sigma_{33}d_3^2 + 2i\sigma_{13}d_1d_3)) \right. \]

\[ -\alpha \beta(2\frac{1}{n}(2\sigma_{11}c_1d_1 + 2\sigma_{33}c_3d_3 + 2\sigma_{13}c_1d_3 + 2\sigma_{31}c_3d_1)). \]

(C.24)

By replacing the coefficients \( c \) and \( d \) with our coefficients \( a \) and \( b \) in the arguments of the complex error functions, we find the three terms reducing to
\[ e^{-\alpha^2 - \beta^2} \cdot e^{\frac{1}{n^2} \sigma_{lm} B_l B_m} = \exp \left[-\left(1 + \frac{1}{n}\right)\alpha^2 - \left(1 + \frac{1}{n}\right)\beta^2 - \left(2 \frac{1}{n}\right)\alpha\beta\right]; \quad n = 1. \] (C.25)

\[ e^{-\alpha^2 - \beta^2} \cdot e^{\frac{1}{n^2} \sigma_{lm} B_l B_m} = \exp \left[-\left(1 + \frac{1}{n}\right)\alpha^2 - \left(1 - \frac{1}{n}\right)\beta^2 - 0\alpha\beta\right]; \quad n = 2. \] (C.26)

\[ e^{-\alpha^2 - \beta^2} \cdot e^{\frac{1}{n^2} \sigma_{lm} B_l B_m} = \exp \left[-\left(1 - \frac{1}{n}\right)\alpha^2 - \left(1 - \frac{1}{n}\right)\beta^2 + \left(2 \frac{1}{n}\right)\alpha\beta\right]; \quad n = 3. \] (C.27)

We write this generally in matrix form

\[ e^{-\alpha^2 - \beta^2} \cdot e^{\frac{1}{n^2} \sigma_{lm} B_l B_m} = e^{-S_{11}\alpha^2 - 2S_{12}\alpha\beta - S_{22}\beta^2} \] (C.28)

where

\[
S = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}
\]

with the respective matrix elements given by

\[
S(\sigma, n, a, a) = \begin{bmatrix} 1 + \frac{1}{n} & \frac{1}{n} \\ \frac{1}{n} & 1 + \frac{1}{n} \end{bmatrix}
\]

\[
S(\sigma, n, a, b) = \begin{bmatrix} 1 + \frac{1}{n} & 0 \\ 0 & 1 - \frac{1}{n} \end{bmatrix}
\]

\[
S(\sigma, n, b, b) = \begin{bmatrix} 1 - \frac{1}{n} & -\frac{1}{n} \\ -\frac{1}{n} & 1 - \frac{1}{n} \end{bmatrix}
\]

We now write the function \(P\) as

\[ P(\sigma, n, c, d) = 4 \frac{1}{n\pi} \int_0^\infty d\alpha \int_0^\infty d\beta \ e^{-S_{11}\alpha^2 - 2S_{12}\alpha\beta - S_{22}\beta^2} \] (C.30)

where we define \(A = \frac{4}{n\pi}\). We rearrange and write

\[ P(\sigma, n, c, d) = A \int_0^\infty d\alpha \ e^{-S_{11}\alpha^2} \int_0^\infty d\beta \ e^{-2S_{12}\alpha\beta - S_{22}\beta^2}. \] (C.31)

Now, substitute \(\gamma = \sqrt{S_{22}}\beta\) and restore the integral form of the complex error function:

\[ P(\sigma, n, c, d) = A \int_0^\infty d\alpha \ e^{-S_{11}\alpha^2} \int_0^\infty d\gamma \ \frac{1}{\sqrt{S_{22}}} e^{-\gamma^2 + 2i\left(\frac{S_{12}}{\sqrt{S_{22}}}\right)\gamma}. \] (C.32)

We solve the second integral:
\[ P(\sigma, n, c, d) = A \int_0^\infty d\alpha \ e^{-S_{11}\alpha^2} \frac{\sqrt{\pi}}{2} w \left( i \frac{S_{12}\alpha}{\sqrt{S_{22}}} \right). \quad (C.33) \]

Repeat the same for the first integral, substitute \( \delta = \sqrt{S_{11}} \alpha \):

\[ P(\sigma, n, c, d) = A \frac{1}{\sqrt{S_{11}S_{22}}} \frac{\sqrt{\pi}}{2} \int_0^\infty d\delta \ e^{-\delta^2} w \left( i \frac{S_{12}\delta}{\sqrt{S_{22}}} \right). \quad (C.34) \]

We can now substitute \( r = \frac{S_{12}}{\sqrt{S_{11}S_{22}}} \) and write

\[ P(\sigma, n, c, d) = A \frac{1}{\sqrt{S_{11}S_{22}}} \frac{\sqrt{\pi}}{2} \int_0^\infty d\delta \ e^{-\delta^2} w(\delta). \quad (C.35) \]

Now, use the relation \[8\]
\[ w(iz) = e^{z^2} (1 - \text{erf}(z)) \quad (C.36) \]

and write

\[ P(\sigma, n, c, d) = A \frac{1}{\sqrt{S_{11}S_{22}}} \frac{\sqrt{\pi}}{2} \int_0^\infty d\delta \ e^{-\delta^2} e^{r^2\delta^2} [1 - \text{erf}(r\delta)] \quad (C.37) \]

and

\[ P(\sigma, n, c, d) = A \frac{1}{\sqrt{S_{11}S_{22}}} \frac{\sqrt{\pi}}{2} \int_0^\infty d\delta \ e^{-(1-r^2)\delta^2} [1 - \text{erf}(r\delta)]. \quad (C.38) \]

Now, we substitute \( \epsilon = \sqrt{(1-r^2)} \delta \) and write

\[ P(\sigma, n, c, d) = A \frac{1}{\sqrt{S_{11}S_{22}(1-r^2)}} \frac{\sqrt{\pi}}{2} \int_0^\infty d\epsilon \ e^{-\epsilon^2} \left[ 1 - \text{erf} \left( \frac{r\epsilon}{\sqrt{1-r^2}} \right) \right] \quad (C.39) \]

and

\[ P(\sigma, n, c, d) = A \frac{1}{\sqrt{S_{11}S_{22}(1-r^2)}} \frac{\sqrt{\pi}}{2} \left[ \int_0^\infty d\epsilon \ e^{-\epsilon^2} - \int_0^\infty d\epsilon \ e^{-\epsilon^2} \text{erf} \left( \frac{r\epsilon}{\sqrt{1-r^2}} \right) \right]. \quad (C.40) \]

With \( \int_0^\infty d\epsilon \ e^{-\epsilon^2} = \frac{\sqrt{\pi}}{2} \), we write

\[ P(\sigma, n, c, d) = A \frac{1}{\sqrt{S_{11}S_{22}(1-r^2)}} \frac{\sqrt{\pi}}{2} \left[ \frac{\sqrt{\pi}}{2} - \int_0^\infty d\epsilon \ e^{-\epsilon^2} \text{erf} \left( \frac{r\epsilon}{\sqrt{1-r^2}} \right) \right]. \quad (C.41) \]
Now, we use the relation (see app. C.2)

\[
\int_0^\infty dt \ e^{-t^2} \text{erf}(at) = \frac{\arctan(a)}{\sqrt{\pi}}
\]

(C.42)

and obtain

\[
P(\sigma, n, c, d) = A \frac{1}{\sqrt{S_{11}S_{22}(1-\tau^2)}} \frac{\sqrt{\pi}}{2} \left[ \frac{\sqrt{\pi}}{2} - \frac{1}{\sqrt{\pi}} \arctan \left( \frac{r}{1-\tau^2} \right) \right].
\]

(C.43)

After restoring A and r, we write

\[
P(\sigma, n, c, d) = \frac{4}{n\pi} \frac{1}{\sqrt{S_{11}S_{22} - S_{12}^2}} \frac{\sqrt{\pi}}{2} \left[ \frac{\sqrt{\pi}}{2} - \frac{1}{\sqrt{\pi}} \arctan \left( \frac{S_{12}}{\sqrt{S_{11}S_{22} - S_{12}^2}} \right) \right].
\]

(C.44)

We now move \(\sqrt{\pi}\) into the brackets and obtain

\[
P(\sigma, n, c, d) = \frac{4}{2n\pi} \frac{1}{\sqrt{S_{11}S_{22} - S_{12}^2}} \left[ \frac{\pi}{2} - \arctan \left( \frac{S_{12}}{\sqrt{S_{11}S_{22} - S_{12}^2}} \right) \right].
\]

(C.45)

which is the analytical solution for the function \(P(\sigma, n, c, d)\).

### C.2. \texttt{arctan} in Function \(P\)

Here, we show that eq. C.42 is valid. We begin with

\[
I(\alpha) = \int_0^\infty \text{erf}(at) e^{-t^2} \ dt.
\]

(C.46)

Now we calculate the derivative

\[
\frac{dI}{d\alpha} = \frac{2}{\sqrt{\pi}} \int_0^\infty t e^{-(at)^2-t^2} \ dt = \frac{2}{\sqrt{\pi}} \int_0^\infty t e^{-(1+\alpha^2)t^2} \ dt
\]

(C.47)

where we used the error function’s definition of its derivative

\[
\frac{d}{dz} \text{erf}(z) = \frac{2}{\sqrt{\pi}} e^{-z^2} \ dt.
\]

(C.48)

Now substitute \(s = t^2\), leading to \(ds = 2t \ dt\) and giving the equation

\[
\frac{dI}{d\alpha} = \frac{1}{\sqrt{\pi}} \int_0^\infty e^{-(1+\alpha^2)s} \ ds = \frac{1}{\sqrt{\pi}} \int_0^\infty e^{-gs} \ ds.
\]

(C.49)

Solving the above integral, we obtain
\[
\frac{dI}{d\alpha} = \frac{1}{\sqrt{\pi}} \frac{1}{(1 + \alpha^2)} \tag{C.50}
\]

and with
\[
\frac{d}{d\alpha} \arctan(\alpha) = \frac{1}{1 + \alpha^2} \tag{C.51}
\]

we finally reach
\[
I(\alpha) = \int_{0}^{\infty} \text{erf}(\alpha t) e^{-t^2} \, dt = \frac{\arctan(\alpha)}{\sqrt{\pi}} \tag{C.52}
\]

which is eq. C.42.

**C.3. Show** \( \langle F_0^2 \rangle, \langle \bar{F}_0^2 \rangle = 0 \)

Here we show that the terms \( \langle F_0^2 \rangle \) and \( \langle \bar{F}_0^2 \rangle \) are always zero by showing that the sum of the functions \( P(\sigma, c, d, n) \) is zero

\[
\langle F_0^2 \rangle = \frac{(\tilde{K})^2 \pi}{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})} \left[ P(\sigma, 1, a, a) - 2P(\sigma, 2, a, b) + P(\sigma, 3, b, b) \right] = 0. \tag{C.53}
\]

For that, we evaluate eq. C.28 at the respective values for \( S \) and \( n \) in accordance to eq. C.5 and obtain the equation set

\[
P(\sigma, 1, a, a) = \frac{4 \sqrt{\det(\sigma)}}{\sqrt{3}} \left[ \frac{\pi}{2} - \arctan\left( \frac{1}{\sqrt{3}} \right) \right];
\]

\[
2P(\sigma, 2, a, b) = \frac{4 \sqrt{\det(\sigma)} \pi}{\sqrt{0.75} \cdot 2} = \frac{4 \sqrt{\det(\sigma)} \pi}{\sqrt{3}};
\]

\[
P(\sigma, 3, b, b) = \frac{4 \sqrt{\det(\sigma)} \sqrt{3}}{3} \left[ \frac{\pi}{2} - \arctan\left( \frac{-1/3}{1/\sqrt{3}} \right) \right] = \frac{4 \sqrt{\det(\sigma)}}{\sqrt{3}} \left[ \frac{\pi}{2} + \arctan\left( \frac{1}{\sqrt{3}} \right) \right]. \tag{C.54}
\]

Finally, we take the sum of the and write

\[
\frac{4 \sqrt{\det(\sigma)} \pi}{2 \sqrt{3}} - \arctan\left( \frac{1}{\sqrt{3}} \right) + \frac{4 \sqrt{\det(\sigma)} \pi}{2 \sqrt{3}} + \arctan\left( \frac{1}{\sqrt{3}} \right) - \frac{4 \sqrt{\det(\sigma)} \pi}{\sqrt{3}} = 0. \tag{C.55}
\]
C.4. Show \((e^{-z_1^2} - e^{-z_2^2} \cdot e^{-g}) = 0\)

We show that \((e^{-z_1^2} - e^{-z_2^2} \cdot e^{-g}) = 0\). It is sufficient to show that the difference of the exponents is zero. Therefore, we test for

\[ z_2^2 = z_2^2 + g; \]

\[ \frac{x_1^2 + 2ix_1x_3 - x_3^2}{2(s_3 - s_1 + 2i\sigma_{13})} = \frac{(s_{33} - i\sigma_{13}x_1 + i(\sigma_{11} + i\sigma_{13}))^2}{\text{det}(\sigma) \cdot 2(s_{33} - s_{11} + 2i\sigma_{13})} = \frac{(s_{33}x_1^2 - 2\sigma_{13}x_1x_3 + \sigma_{11}x_3^2)}{2 \text{det}(\sigma)}. \]

(C.56)

For a better overview, we denote the numerators and denominators in the equation as in

\[ \frac{N_1}{D} = \frac{N_2}{\text{det}(\sigma)D} + \frac{N_3}{2 \text{det}(\sigma)} \]  

(C.57)

with \(N_1 = x_1^2 + 2ix_1x_3 - x_3^2\), \(N_2 = s_{33} - i\sigma_{13}x_1 + i(\sigma_{11} + i\sigma_{13})^2\), \(N_3 = (s_{33}x_1^2 - 2\sigma_{13}x_1x_3 + \sigma_{11}x_3^2)\) and \(D = 2(s_{33} - s_{11} + 2i\sigma_{13})\) and manipulate the right-hand-side of the equation until we get the numerator \(N_1\). First we bring the R.H.S. to a common denominator so that we obtain

\[ \frac{N_1}{D} = \frac{N_2}{\text{det}(\sigma)D} + \frac{\tilde{N}_3}{2 \text{det}(\sigma)}. \]

(C.58)

Therefore, we multiply

\[ \tilde{N}_3 = N_3 \ast (s_{33} - s_{11} + 2i\sigma_{13}) \]

\[ = s_{11}s_{33}x_1^2 + 2i\sigma_{13}s_{33}x_1^2 - s_{33}x_1^2 - 2s_{11}s_{13}x_1x_3 - 4i\sigma_{13}x_1x_3 \]

(C.59)

From here on, we only care about the numerators and have in mind that our result must be a factor \(\text{det}(\sigma)\) larger than the numerator \(N_1\). Now, taking the sum of the numerators of the R.H.S:

\[ N_2 + \tilde{N}_3 = -s_{11}s_{33}x_1^2 + 2s_{11}s_{13}x_1x_3 - 2i\sigma_{11}s_{13}x_1x_3 - s_{13}x_1^2 + 2i\sigma_{13}x_1x_3 \]

\[ + s_{33}x_1^2 + 2i\sigma_{11}s_{33}x_1x_3 - 2i\sigma_{13}s_{33}x_1x_3 - s_{33}x_1^2 + 2i\sigma_{13}s_{33}x_1x_3 \]

\[ + s_{11}s_{33}x_1^2 + 2i\sigma_{13}s_{33}x_1^2 - 2i\sigma_{13}s_{33}x_1x_3 - 2s_{11}s_{13}x_1x_3 - 4i\sigma_{13}x_1x_3 \]

\[ + 2s_{13}s_{33}x_1x_3 + s_{11}s_{33}x_1x_3 - 2i\sigma_{13}s_{33}x_1x_3 - 2s_{13}s_{33}x_1x_3 \]

\[ = s_{11}s_{33}x_1^2 - s_{13}x_1^2 + 2s_{11}s_{13}x_1x_3 + 2i\sigma_{13}s_{33}x_1x_3 - 2s_{13}s_{33}x_1x_3 - 2s_{13}s_{33}x_1x_3 \]

\[ - 2s_{11}s_{13}x_1x_3 - 2i\sigma_{13}x_1x_3 - 2s_{13}s_{33}x_1x_3 - 2s_{13}s_{33}x_1x_3 - s_{11}s_{33}x_3 + s_{13}x_3^2. \]

(C.60)

Now we factor out \(x_1^2, -x_3^2\) and \(2ix_1x_3\) and obtain

\[ N_2 + \tilde{N}_3 = x_1^2(s_{33}s_{11} - s_{13}^2) + 2ix_1x_3(s_{33}s_{11} - s_{13}^2) - x_3^2(s_{33}s_{11} - s_{13}^2) \]

\[ = N_1 \text{ det } \sigma. \]

(C.61)

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Thus, we conclude that
\[ \frac{N_1}{D} = \frac{N_2 + \tilde{N}_3}{\det(\sigma)D} \] (C.62)
and the difference \( z_1^2 - z_2^2 - g = 0 \).

## D. Round Beams

In this section of the appendix, we show how the singularity occurring for a round beam cross-section can be removed and how a round beam can be treated in a numerical simulation.

### D.1. Round Beam - Linear Term

Basis is the elliptical solution of the generalized linear term (eq. 2.13)
\[
\langle x_k F_0 \rangle = \frac{i}{2(\sigma_{11} + \sigma_{33} + 2i\sigma_{13})} \left[ \sigma_{k1} + i\sigma_{k3} - \left( \frac{\sigma_{k1}(\sigma_{33} - i\sigma_{13}) + i\sigma_{k3}(\sigma_{11} + i\sigma_{13})}{\sqrt{\sigma_{11}\sigma_{33} - \sigma_{13}^2}} \right) \right].
\] (D.1)

For a round beam cross-section, singularities in denominator must be avoided. A round beam is characterized by \( \sigma_{11} = \sigma_{33} \) and \( \sigma_{13} = 0 \). In order to circumvent the singularity, we redefine
\[
\sigma_{11} = (\sigma + \epsilon)^2 = \sigma^2 + 2\sigma\epsilon + \epsilon^2 \quad \text{and} \quad \sigma_{33} = (\sigma - \epsilon)^2 = \sigma^2 - 2\sigma\epsilon + \epsilon^2.
\] (D.2)

where \( \epsilon \) is an infinitesimal small number. Inserting the new definitions into equation D.1 and omitting \( \epsilon^2 \) we get
\[
\langle x_k F_0 \rangle = \frac{i}{8\sigma\epsilon} \left[ \sigma_{k1} + i\sigma_{k3} - \left( \frac{\sigma_{k1}(\sigma^2 - 2\sigma\epsilon) + i\sigma_{k3}(\sigma^2 + 2\sigma\epsilon)}{\sigma^2} \right) \right]
= \frac{i}{8\sigma\epsilon} \left( \frac{(\sigma_{k1}2\sigma\epsilon - \sigma_{k3}2\sigma\epsilon)}{\sigma^2} \right)
= \frac{i}{4\sigma^2} (\sigma_{k1} - i\sigma_{k3}).
\] (D.3)

Note that \( \langle x_k F_0 \rangle = 0 \) for \( k=2,4 \).

### D.2. Round Beam - Quadratic Term

As basis, we use the covariant form of Bassetti’s and Erskine’s formula for beam deflection angles which is valid for bi-Gaussian beams with a round cross-section [7]
\( (f_3 + if_1) = i \left( \frac{1 - e^{-r^2/2\sigma^2}}{x_1 + ix_3} \right) = i \left( \frac{1 - e^{-r^2/2\sigma^2}}{r^2} \right) (x_1 - ix_3) \) \hspace{1cm} (D.4)

with \( x_1 + x_3 = r \). After expanding eq. D.4, we obtain

\[
\begin{bmatrix}
x_3 \left( \frac{1 - e^{-r^2/2\sigma^2}}{r^2} \right) + ix_1 \left( \frac{1 - e^{-r^2/2\sigma^2}}{r^2} \right)
\end{bmatrix} = f_3 + if_1. \hspace{1cm} (D.5)
\]

Now follows the exemplary calculation of \( f_1^2 \):

\[
f_1^2 = \left[ x_1 \left( \frac{1 - e^{-r^2/2\sigma^2}}{r^2} \right) \right]^2 = \frac{x_1^2}{r^4} \left( 1 - 2e^{-r^2/2\sigma^2} + e^{-3r^2/2\sigma^2} \right). \hspace{1cm} (D.6)
\]

Note that to obtain \( f_3^2 \) we simply have to replace the index of the variable \( x \).

We have to integrate over the interacting distribution now in order to obtain \( \langle (f_3^2 + f_1^2) \rangle \). We have shown earlier that \( \langle f_1 \rangle = \langle f_3 \rangle \). Thus we can write

\[
\langle f_3^2 + f_1^2 \rangle = \frac{1}{2\pi\sigma^2} \int_0^\infty \int_0^\infty dx_1 dx_3 \ x_1^2 + x_3^2 \left( \frac{1}{r^4} \left( e^{r^2/2\sigma^2} - 2e^{-r^2/2\sigma^2} + e^{-3r^2/2\sigma^2} \right) \right) \hspace{1cm} (D.7)
\]

where we used \( x_1 + x_3 = r \) in the second step. For the simplicity of the calculation we move to polar coordinates in the following step and write

\[
\langle f_3^2 + f_1^2 \rangle = \frac{1}{2\pi\sigma^2} \int_0^{2\pi} \int_0^\infty d\theta \ dr \ r \ \frac{1}{r^2} \left( e^{r^2/2\sigma^2} - 2e^{-r^2/2\sigma^2} + e^{-3r^2/2\sigma^2} \right) \hspace{1cm} (D.8)
\]

In order to solve the remaining integral, we substitute \( s = \frac{r^2}{2\sigma^2} \rightarrow dr = \frac{2\sigma^2}{r^2} ds \) and write

\[
\langle f_3^2 + f_1^2 \rangle = \frac{2\pi}{2\pi\sigma^2} \int_0^\infty ds \ \frac{2\sigma^2}{2r^2} \left( e^{-s} - 2e^{-2s} + e^{-3s} \right) \hspace{1cm} (D.9)
\]

We see now that we have to solve an integral of the form

\[
I = \lim_{\epsilon \to 0} \int_\epsilon^{\infty} ds \ \frac{e^{-ns}}{s}. \hspace{1cm} (D.10)
\]
The solution to this integral is provided in [8] and given by
\[ \int_z^{\infty} \frac{e^{-t}}{t} \, dt = -\gamma - \ln(z) - \sum_{n=1}^{\infty} \frac{-(1)^n z^n}{n!}. \] (D.11)
We cut off the above solution after the first non-trivial term \( \ln(z) \) and apply it to our case. Thus, we can write
\[
\lim_{\epsilon \to 0} \int_{\epsilon}^{\infty} ds \left( e^{-s} - 2e^{-2s} + e^{-3s} \right) = -\gamma - \ln(\epsilon) + 2\ln(2) - \gamma - \ln(3)
= 2\ln(2) - \ln(3)
\] (D.12)
and conclude that the round-beam-solution for the quadratic part of the space charge force is
\[
(f_3^2 + f_1^2) = \frac{1}{2\sigma_{11}} \left( 2\ln(2) - \ln(3) \right).
\] (D.13)

E. Linear Mapping - Defocusing Space Charge Quadrupoles

In this section of the appendix, we show a linear approximation of the space charge force and treat it as a quadrupole that defocuses in both planes. For that we need the space charge focusing lengths from which the transfer functions of the quadrupoles are generated. We recall the kick function
\[ F_0(x_1, x_3, \sigma) = \sqrt{\pi} \left[ w(z_1) + e^{-g}w(z_2) \right]. \] (E.1)
where \( D_+ = \sqrt{2(\sigma_{11} - \sigma_{33} + 2i\sigma_{13})} \) and \( g = \frac{1}{2} \sigma_{ij}^{-1} x_i x_j \). In order to find the focal lengths, we calculate the gradient in the origin of the kick function
\[
\left. \frac{\partial F_0}{\partial x_1} \right|_{x_1,x_3=0} = \sqrt{\pi} \left[ w'(z_1) \frac{dz_1}{dx_1} - \left( \frac{\partial}{\partial x_1} e^{-g}w(z_2) + w'(z_2) \frac{dz_2}{dx_1} e^{-g} \right) \right]. \] (E.2)
For the sake of a better overview, we calculate the three terms in the rectangular brackets separately
\[
\left. w'(z_1) \frac{dz_1}{dx_1} \right|_{x_1,x_3=0} = \left. w'(a_1 x_1 + a_3 x_3) \frac{dz_1}{dx_1} \right|_{x_1,x_3=0} = \left. \left( -2(a_1 x_1 + a_3 x_3) \cdot w(z_1) + \frac{2i}{\sqrt{\pi}} \right) a_1 \right|_{x_1,x_3=0}
= \frac{2i}{\sqrt{\pi}} \cdot a_1.
\] (E.3)
\[
\frac{\partial}{\partial x_1} e^{-g}\bigg|_{x_1,x_3=0} = \frac{\partial}{\partial x_1} e^{-\frac{1}{2}\left(\sigma_{11}^{-1} x_1^2 + \sigma_{33}^{-1} x_3^2 + 2\sigma_{13}^{-1} x_1 x_3\right)}\bigg|_{x_1,x_3=0}
\]
\[
= \left(-\frac{x_1}{\sigma_{11} - \frac{\sigma_{11}}{\sigma_{13}}}\right) \cdot e^{-\frac{1}{2}\left(\sigma_{11}^{-1} x_1^2 + \sigma_{33}^{-1} x_3^2 + 2\sigma_{13}^{-1} x_1 x_3\right)}\bigg|_{x_1,x_3=0}
\]
\[
= 0
\]  
(E.4)

\[
\left. w'(z_2) \frac{dz_2}{dx_1} e^{-g}\right|_{x_1,x_3=0} = \left( -2 z_2 \cdot w(z_2) + \frac{2i}{\sqrt{\pi}} \right) \cdot b_1 \cdot e^{-\frac{1}{2}\left(\sigma_{11}^{-1} x_1^2 + \sigma_{33}^{-1} x_3^2 + 2\sigma_{13}^{-1} x_1 x_3\right)}\bigg|_{x_1,x_3=0}
\]
\[
= \frac{2i}{\sqrt{\pi}} \cdot b_1.
\]  
(E.5)

We assemble all the terms and obtain

\[
\left. \frac{\partial F_0}{\partial x_1}\right|_{x_1,x_3=0} = \frac{2i}{D_+} \cdot (a_1 - b_1).
\]  
(E.6)

Repeating the calculation for \( \frac{\partial F_0}{\partial x_3}\bigg|_{x_1,x_3=0} \) yields

\[
\left. \frac{\partial F_0}{\partial x_3}\right|_{x_1,x_3=0} = \frac{2i}{D_+} \cdot (a_3 - b_3).
\]  
(E.7)

Putting both solutions together, we find

\[
\tilde{K} \left[ \left. \frac{\partial F_0}{\partial x_1}\right|_{x_1=0} + \left. \frac{\partial F_0}{\partial x_3}\right|_{x_3=0} \right] = \tilde{K} \frac{2i}{D_+} \cdot [(a_1 - b_1)x_1 + (a_3 - b_3)x_3]
\]  
(E.8)

and the inverse focusing lengths we find as

\[
\frac{1}{f_{x_1}} = \text{Im} \left[ \frac{2i}{D_+} (a_1 - b_1) \right]
\]  
(E.9)

and

\[
\frac{1}{f_{x_3}} = \text{Re} \left[ \frac{2i}{D_+} (a_3 - b_3) \right].
\]  
(E.10)

For the case of a beam with a round cross-section, we need a special treatment. We start with the round kick function

\[
F_0(r, \sigma) = \frac{1 - e^{-\frac{r^2}{\sigma_{11}}}}{r}
\]  
(E.11)

and calculate the derivative \( \frac{\partial F_0}{\partial r} \) which gives us the gradient as a function of the radius \( r \).
\[
\frac{\partial F_0}{\partial r} = \frac{r}{2\sigma_r^2}.
\] (E.12)

We can argue that for small \( r \), the inverse focusing length for round beams is proportional to \( \sigma_{11} \) or \( \sigma_{33} \), respectively, and we find the inverse focusing lengths as

\[
\frac{1}{f_{x_1}} = \frac{1}{f_{x_3}} = \tilde{K} \frac{\partial F_0}{\partial r} \bigg|_{x_1=x_3=0} = \tilde{K} \frac{1}{2\sigma_{11}} = \tilde{K} \frac{1}{2\sigma_{33}}.
\] (E.13)