

# Xsuite physics manual

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# Chapter 1

## Xtrack

XTrack is a 6D single particle symplectic tracking code used to compute the trajectories of individual relativistic charged particles in circular accelerators. It has been developed based on SixTrack.

The physical models are collected from the main references [1, 2, 3, 4, 5, 6, 7], which contain more details of the derivation of the maps.

### 1.1 Notation and reference frame

The speed, momentum, energy, rest mass, charge of a particle are indicated by  $v$ ,  $P$ ,  $E$ ,  $m$  and  $q$ , respectively. These quantities are related by the following equations:

$$v = \beta c \quad E^2 - P^2 c^2 = m^2 c^4 \quad E = \gamma m c^2 \quad Pc = \beta E \quad (1.1)$$

where  $\beta$  and  $\gamma$  are the relativistic factors.

In a curvilinear reference frame defined by a constant curvature  $h_x$  in the  $\hat{X}, \hat{Z}$  plane and parameterized by  $s$ , the position of the particle at a time  $t$  can be written as:

$$\mathbf{Q}(t) = \mathbf{r}(s) + x \hat{x}(s) + y \hat{y}(s), \quad (1.2)$$

and therefore identified by the coordinates  $s, x, y, t$  in the reference frame defined by  $\hat{x}(s)$  and  $\hat{y}(s)$ . In particle tracking,  $s$  is normally used as independent parameter and  $t$  as a coordinate.

The electromagnetic fields  $\mathbf{E}$  and  $\mathbf{B}$  can be derived in a curvilinear reference frame from the potentials  $V(x, y, s, t)$  and  $\mathbf{A}(x, y, s, t)$ , where

$$\mathbf{A}(x, y, s, t) = A_x(x, y, s, t) \hat{x}(s) + A_y(x, y, s, t) \hat{y}(s) + A_s(x, y, s, t) \hat{z}(s) \quad (1.3)$$

and for which:

$$\mathbf{E} = -\nabla V - \frac{\partial \mathbf{A}}{\partial t} = -\partial_x V \hat{x} - \partial_y V \hat{y} - \frac{1}{1 + hx} \partial_s V \hat{z} - \partial_t \mathbf{A} \quad (1.4)$$

$$\mathbf{B} = \nabla \times \mathbf{A} = \left( \partial_y A_s - \frac{\partial_s A_y}{1 + hx} \right) \hat{x} + \left( \frac{\partial_s A_x - \partial_x (1 + hx) A_s}{1 + hx} \right) \hat{y} \quad (1.5)$$

$$+ (\partial_x A_y - \partial_y A_x) \hat{z}. \quad (1.6)$$

In this reference frame the canonical momenta are:

$$P_x = m\gamma\dot{x} + qA_x, \quad P_y = m\gamma\dot{y} + qA_y, \quad P_s = m\gamma\dot{s}(1 + hx)^2 + q(1 + hx)A_s. \quad (1.7)$$

and the energy of a particle and the field is

$$E = qV + c\sqrt{(mc)^2 + \frac{(P_s - qA_s(1 + hx))^2}{(1 + hx)^2} + (P_x - qA_x)^2 + (P_y - qA_y)^2}. \quad (1.8)$$

## 1.2 Hamiltonian and particle coordinates

If  $s(t)$  is monotonically increasing, it is possible to derive the equations of motion using  $s$  as the independent parameter,  $(-t, E)$  as conjugate coordinates and  $P_s$  as Hamiltonian.

$$P_s = (1 + hx) \left( \sqrt{E^2 - (mc^2)^2 - (P_x - qA_x)^2 - (P_y - qA_y)^2} + qA_s \right) \quad (1.9)$$

Since in accelerators the orbits of the particles are often a perturbation of the reference trajectory followed by a particle with rest mass  $m_0$ , charge  $q_0$ , speed  $\beta_0 c$  and momentum  $P_0$ , one could use the following derived quantities that usually assume small values:

$$p(x, y) = \frac{m_0}{m} \frac{P(x, y)}{P_0} \quad \chi = \frac{q}{q_0} \frac{m_0}{m} \quad a(x, y, s) = \frac{q_0}{P_0} A(x, y, s) \quad (1.10)$$

$$\delta = \frac{P \frac{m_0}{m} - P_0}{P_0} \quad p_t = \frac{E \frac{m_0}{m} - E_0}{P_0 c} \quad p_\sigma = \frac{E \frac{m_0}{m} - E_0}{\beta_0 P_0 c} \quad (1.11)$$

$$\zeta = s \frac{\beta}{\beta_0} - \beta c t \quad \tau = \frac{s}{\beta_0} - c t \quad \sigma = s - \beta_0 c t \quad (1.12)$$

The pairs  $(\zeta, \delta)$ ,  $(\tau, p_\tau)$ ,  $(\sigma, p_\sigma)$  are canonical conjugate and can be generated by the following generating functions <sup>1</sup>

$$F_2 = xp_x + yp_y + \left( \frac{s}{\beta_0} - ct \right) \left( p_\tau + \frac{1}{\beta_0} \right) \quad (1.13)$$

$$F_2 = xp_x + yp_y + (s - ct) \left( \beta_0 p_\sigma + \frac{1}{\beta_0} \right) \quad (1.14)$$

$$F_2 = xp_x + yp_y + (-ct) \left( \sqrt{(1 + \delta)^2 + m^2 c^4} \right) \quad (1.15)$$

$$(1.16)$$

The Hamiltonian is:

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$$^1 F_2(-t, p_{\text{new}}, s), E/(P_0 c) = \frac{\partial F_2}{\partial(-t)}, q_{\text{new}} = \frac{\partial F_2}{\partial p_{\text{new}}}, H_{\text{new}} = H + \frac{\partial F_2}{\partial s},$$

$$H_\delta = \frac{p_t}{\beta_0} - \frac{m_0}{m} \frac{P_s}{P_0} \quad H_\tau = \frac{p_t}{\beta_0} - \frac{m_0}{m} \frac{P_s}{P_0} \quad H_\sigma = p_\sigma - \frac{m_0}{m} \frac{P_s}{P_0} \quad (1.17)$$

$$H_\delta = \frac{p_t}{\beta_0} - (1 + hx) \left( \sqrt{(1 + \delta)^2 - (p_x - \chi a_x)^2 - (p_y - \chi a_y)^2} + \chi a_s \right) \quad (1.18)$$

$$H_\tau = \frac{p_t}{\beta_0} - (1 + hx) \left( \sqrt{(1 + \delta)^2 - (p_x - \chi a_x)^2 - (p_y - \chi a_y)^2} + \chi a_s \right) \quad (1.19)$$

$$H_\sigma = p_\sigma - (1 + hx) \left( \sqrt{(1 + \delta)^2 - (p_x - \chi a_x)^2 - (p_y - \chi a_y)^2} + \chi a_s \right), \quad (1.20)$$

where

$$\delta = \frac{P \frac{m_0}{m} - P_0}{P_0} \quad \chi = \frac{q}{q_0} \frac{m_0}{m}. \quad (1.21)$$

The following identities are useful to derive the equation of motion.

$$\delta = \sqrt{p_t^2 + 2p_t/\beta_0 + 1} - 1 \quad \frac{d\delta}{dp_t} = \frac{p_t + 1/\beta_0}{1 + \delta} = \frac{1}{\beta} \quad (1.22)$$

$$\delta = \sqrt{\beta_0^2 p_\sigma^2 + 2p_\sigma + 1} - 1 \quad \frac{d\delta}{dp_\sigma} = \frac{p_\sigma \beta_0^2 + 1}{1 + \delta} = \frac{\beta_0}{\beta} \quad (1.23)$$

## 1.3 Beam elements

### 1.3.1 Drift

A drift is a straight, field-free region ( $h(x, y) = 0$ ,  $V = 0$  and  $\mathbf{A} = 0$ ). The exact and expanded Hamiltonian for a drift space are

$$H_\tau = \frac{p_t}{\beta_0} - \sqrt{(1 + \delta)^2 - p_x^2 - p_y^2} \approx \frac{p_t}{\beta_0} - \delta + \frac{1}{2} \frac{p_x^2 + p_y^2}{1 + \delta}. \quad (1.24)$$

$$H_\sigma = p_\sigma - \sqrt{(1 + \delta)^2 - p_x^2 - p_y^2} \approx p_\sigma - \delta + \frac{1}{2} \frac{p_x^2 + p_y^2}{1 + \delta}. \quad (1.25)$$

#### 1.3.1.1 Expanded Drift

The map relative to the expanded Hamiltonian is (eq. 3.49 in [3])

$$x_p = \frac{p_x}{1 + \delta} \quad y_p = \frac{p_y}{1 + \delta} \quad (1.26)$$

$$x \leftarrow x + x_p l \quad y \leftarrow y + y_p l \quad (1.27)$$

$$\tau \leftarrow \tau + \frac{l}{\beta_0} - \frac{l}{\beta} - \frac{l}{\beta} \frac{x_p^2 + y_p^2}{2} = \tau + l \left( \frac{\delta}{\beta_0} - \frac{p_t}{1 + \delta} - \frac{x_p^2 + y_p^2}{2\beta} \right) \quad (1.28)$$

$$\sigma \leftarrow \sigma + l - \frac{\beta_0}{\beta} l - \frac{\beta_0}{\beta} l \frac{x_p^2 + y_p^2}{2} = \sigma + l \left( 1 - \frac{\beta_0}{\beta} \left( 1 + \frac{x_p^2 + y_p^2}{2} \right) \right) \quad (1.29)$$

### 1.3.1.2 Exact Drift

The map relative to the exact Hamiltonian is (eq. 3.49 in [3])

$$p_z = \sqrt{(1 + \delta)^2 - p_x^2 - p_y^2} \quad (1.30)$$

$$\frac{dp_z}{dp_t} = \frac{p_t + 1/\beta_0}{p_z} = \frac{1}{\beta_z} \quad (1.31)$$

$$\frac{dp_z}{dp_\sigma} = \frac{\beta_0^2 p_\sigma + 1}{p_z} = \frac{\beta_0}{\beta_z} \quad (1.32)$$

$$x \leftarrow x + \frac{p_x}{p_z} l \quad y \leftarrow y + \frac{p_y}{p_z} l \quad (1.33)$$

$$\tau \leftarrow \tau + \frac{l}{\beta_0} - \frac{l}{\beta_z} = l \left( \frac{1}{\beta_0} - \frac{p_t + 1/\beta_0}{p_z} \right) \quad (1.34)$$

$$\sigma \leftarrow \sigma + l - l \frac{\beta_0}{\beta_z} = l \left( 1 - \frac{\beta_0^2 p_\sigma + 1}{p_z} \right) \quad (1.35)$$

### 1.3.1.3 Polar Drift

It is possible to define a “polar” drift that has the effect of rotating the reference frame [8] for instance in the  $x$ - $z$  plane

$$p_x \leftarrow p_x \cos \theta + p_z \sin \theta \quad p_z \leftarrow -p_x \sin \theta + p_z \cos \theta \quad (1.36)$$

$$z = -x \sin \theta \quad x' = p_x / p_z \quad y' = p_y / p_z \quad (1.37)$$

$$x \leftarrow x \cos \theta - x' z \quad y \leftarrow y - x' z \quad \tau \leftarrow \tau + z / \beta_z. \quad (1.38)$$

where  $\theta$  is the angle bringing the new  $\hat{x}$  towards the old  $\hat{z}$ . The map can be also generated by combining a rotation with a  $-x \sin(\theta)$ -length drift. In case of an  $\hat{x}$  rotation the role of  $x$  and  $y$  are interchanged.



### 1.3.2 Dipole

In a curvilinear reference system with a constant curvature  $h$  in the horizontal plane a uniform magnetic field can be derived by the vector potential:

$$A_x = 0, \quad A_y = 0, \quad A_s = -B_y \left( x - \frac{hx^2}{2(1+hx)} \right). \quad (1.39)$$

With the following normalization  $k_0 = \frac{q_0}{p} B_y$  is the inverse of the bending radius of the reference particle.

The exact and expanded Hamiltonian for a horizontal bending magnet is (eq. 2.12 in [2])

$$H = \frac{p_t}{\beta_0} - (1+hx) \sqrt{(1+\delta)^2 - p_x^2 - p_y^2} + \chi k_0 \left( x + \frac{hx^2}{2} \right) \quad (1.40)$$

$$\simeq \frac{p_t}{\beta_0} + \frac{1}{2} \frac{p_x^2 + p_y^2}{1+\delta} - (1+hx)(1+\delta) + \chi k_0 \left( x + \frac{hx^2}{2} \right) \quad (1.41)$$

#### 1.3.2.1 Thin dipole

The map for a thin dipole kick (horizontal or vertical) from the expanded Hamiltonian is (eq. 4.12 in [4]):

$$p_x \leftarrow p_x + (h_x l - \chi k_0 l) + h_x l \delta - \chi k_0 l h_x x \quad (1.42)$$

$$p_y \leftarrow p_y - (h_y l - \chi \hat{k}_0 l) - h_y l \delta + \chi k_0 l h_y y \quad (1.43)$$

$$\tau \leftarrow \tau - \frac{h_x x - h_y y}{\beta} l. \quad (1.44)$$

#### 1.3.2.2 mad thin dipole

to be checked

$$p_x \leftarrow p_x + (h_x l - \chi k_0 l) + h_x l (p_z - 1) - \chi k_0 l h_x x \quad (1.45)$$

$$p_y \leftarrow p_y - (h_y l - \chi \hat{k}_0 l) - h_y l (p_z - 1) + \chi k_0 l h_y y \quad (1.46)$$

$$\tau \leftarrow \tau - \frac{h_x x - h_y y}{\beta_z} l. \quad (1.47)$$

#### 1.3.2.3 Thick dipole

Defining the following quantities,

$$G_x = \chi \frac{k_0 h_x}{1+\delta}, \quad G_y = \chi \frac{\hat{k}_0 h_y}{1+\delta} \quad (1.48)$$

$$C_{x,y} = \cos(\sqrt{G_{x,y}} L), \quad S_{x,y} = \sin(\sqrt{G_{x,y}} L) \quad (1.49)$$

the map relative to the expanded Hamiltonian is (eq. 4.11 in [2])

$$x \leftarrow C_x \cdot x + \frac{S_x}{\sqrt{G_x}} \frac{1}{1+\delta} \cdot p_x + \frac{\delta}{h_x} (1 - C_x) \quad (1.50)$$

$$p_x \leftarrow -\sqrt{G_x}(1+\delta) \cdot S_x \cdot x + C_x \cdot p_x + \delta\sqrt{1+\delta} \cdot S_x \quad (1.51)$$

$$y \leftarrow C_y \cdot y + \frac{S_y}{\sqrt{G_y}} \frac{1}{1+\delta} \cdot p_y + \frac{\delta}{h_y} (1 - C_y) \quad (1.52)$$

$$p_y \leftarrow -\sqrt{G_y}(1+\delta) \cdot S_y \cdot y + C_y \cdot p_y + \delta\sqrt{1+\delta} \cdot S_y \quad (1.53)$$

$$\sigma \leftarrow \sigma + L \left( 1 - \frac{\beta_0}{\beta} \right) \quad (1.54)$$

$$- \frac{\beta_0}{\beta} \left[ \frac{h_x S_x}{\sqrt{G_x}} \cdot x + \frac{1 - C_x}{h_x} \cdot p_x + \frac{h_y S_y}{\sqrt{G_y}} \cdot y + \frac{1 - C_y}{h_y} \cdot p_y + \delta \left( 2L - \frac{S_x}{\sqrt{G_x}} - \frac{S_y}{\sqrt{G_y}} \right) \right] \quad (1.55)$$

$$- \frac{1}{4} \frac{\beta_0}{\beta} \left[ G_x \left( L - \frac{C_x S_x}{\sqrt{G_x}} \right) \left( x - \frac{\delta}{h_x} \right)^2 + \left( L + \frac{C_x S_x}{\sqrt{G_x}} \right) \frac{p_x^2}{(1+\delta)^2} - \left( x - \frac{\delta}{h_x} \right) \frac{2S_x^2}{1+\delta} \cdot p_x \right. \quad (1.56)$$

$$\left. + G_y \left( L - \frac{C_y S_y}{\sqrt{G_y}} \right) \left( y - \frac{\delta}{h_y} \right)^2 + \left( L + \frac{C_y S_y}{\sqrt{G_y}} \right) \frac{p_y^2}{(1+\delta)^2} - \left( y - \frac{\delta}{h_y} \right) \frac{2S_y^2}{1+\delta} \cdot p_y \right]. \quad (1.57)$$

### 1.3.2.4 Dipole Edge effects

Considering the dipole edge effects from a dipole of length  $L$  and bending angle  $\theta$ , the map is

$$p_x \rightarrow p_x + \frac{1+\delta}{\rho} \tan(\alpha) \cdot x$$

$$p_y \rightarrow p_y - \frac{1+\delta}{\rho} \tan(\alpha) \cdot y,$$

where the bending radius  $\rho$  and  $\alpha$  are defined as

$$\rho^{-1} = \frac{h_x}{\sqrt{1+\delta}} \quad \alpha = \frac{1}{2} \frac{L}{\rho} = \frac{\theta}{2}.$$

### 1.3.3 Combined dipole quadrupole

The following vector potential in curvilinear coordinates

$$A_s = -\frac{g}{1+hx} \left( \frac{x^2}{2} - \frac{y^2}{2} + \frac{hx^3}{3} \right) \quad (1.58)$$

produce a field

$$B_x = g \left( y + \frac{hxy}{1+hx} \right) \quad B_y = gx \quad (1.59)$$

The following vector potential in curvilinear coordinates

$$A_s = -\frac{g}{1+hx} \left( \frac{x^2}{2} - \frac{y^2}{2} + \frac{hx^3}{3} - \frac{hxy^2}{2} \right) \quad (1.60)$$

produce a field

$$B_x = gy \quad B_y = g \left( x + \frac{hy^2}{2+2hx} \right) \quad (1.61)$$

### 1.3.4 Thin Multipole

The effect of a thin multipole can be approximated by the following Hamiltonian  
A longitudinally uniform static magnetic field can be described by the following equations

$$B_y + iB_x = \sum_{n=1} \frac{B_n + iA_n}{r_0^{n-1}} (x + iy)^{n-1} \quad (1.62)$$

$$= B_N \sum_{n=N} \frac{b_n + ia_n}{r_0^{n-1}} (x + iy)^{n-1}. \quad (1.63)$$

Usually multipole are expressed as relative to

A thin multiple idealize the effect of the field by taking the limit of the integration length going to zero while keeping constant the integrated strength. The Hamiltonian is:

$$H = -\delta(s)\chi L \Re \left[ \sum_{n=0} (k_n + i\hat{k}_n)(x + iy)^{n+1} \right]. \quad (1.64)$$

where

$$k_n = n! \frac{q_0}{p_0} \frac{B_{n+1}}{r_0^n} \quad \hat{k}_n = n! \frac{q_0}{p_0} \frac{A_{n+1}}{r_0^n}. \quad (1.65)$$

The corresponding map is:

$$p_x \leftarrow p_x - \chi L \cdot \Re \left[ \sum_{n=0} \frac{1}{n!} (k_n + i\hat{k}_n)(x + iy)^n \right], \quad (1.66)$$

$$p_y \leftarrow p_y + \chi L \cdot \Im \left[ \sum_{n=0} \frac{1}{n!} (k_n + i\hat{k}_n)(x + iy)^n \right], \quad (1.67)$$

In case a curvature  $h$  is the vector potential become:

$$f(x, y) = \int B_x(x, y) dy \quad (1.68)$$

$$g(x, y) = \int \partial_x B_x(x, y) dy \quad (1.69)$$

$$a_s(x, y) = \frac{c_1}{1 + hx} + f(x, y) - \frac{\int_1^x (1 + h\xi)(g(\xi, y) + \xi) + hf(x, y) d\xi}{1 + hx} \quad (1.70)$$

$$\frac{\int_1^x \left( -h\xi (g(x, y)) - \int \mathbf{bx}^{(1,0)}(\xi, y) dy - h \int \mathbf{bx}(\xi, y) dy - h\xi \mathbf{by}(\xi, y) - \mathbf{by}(\xi, y) \right) d\xi}{hx + 1} \quad (1.71)$$

### 1.3.5 Accelerating Cavity

The approximated energy gain of a particle passing through an electric field of frequency  $f = \frac{k}{2\pi c}$  for which:

$$V \sin(\phi - k\tau) = \int_{-l/2}^{l/2} E_s(0, 0, t, s) ds. \quad (1.72)$$

An equivalent vector potential can be derived and normalized as

$$A_s = -\frac{V}{\omega} \cos(\phi - k\tau) \quad V_n = \frac{q_0}{P_0 c} V \quad (1.73)$$

from which one can derive the following map

$$p_t \leftarrow p_t + \chi V_n \sin(\phi - k\tau + k \frac{s - s_0}{\beta_0}), \quad (1.74)$$

where the additional terms in the phase is added in case harmonic number is not exactly integer and the phase is unlocked phase ). The new  $\delta$  can be updated from the new  $p_t$ .

### 1.3.6 RF-Multipole

The RF-multipole generalizes the interaction of a particle with an electromagnetic field by assuming that

$$\Delta E(x, y, \tau) = q \int_{-L/2}^{L/2} E_z(x, y, t) ds \quad (1.75)$$

$$\Delta P_x(x, y, \tau) = q \int_{-L/2}^{L/2} E_x(x, y, t) + \beta c B_y(x, y, t) ds \quad (1.76)$$

$$\Delta P_y(x, y, \tau) = q \int_{-L/2}^{L/2} E_y(x, y, t) - \beta c B_x(x, y, t) ds. \quad (1.77)$$

are harmonic in  $x, y$  and periodic in  $\tau$  of frequency  $f = \frac{k}{2\pi c}$  such that:

$$a_s(x, y, \tau) = \Re \left[ \sum_{n=1}^N \left( k_n \cos(\phi_n - k\tau) + i\hat{k}_n \cos(\hat{\phi}_n - k\tau) \right) (x + iy)^n \right], \quad (1.78)$$

The map then follows:

$$\Delta p_x = - \sum_{n=1}^N \frac{\chi}{n!} \Re \left[ (k_n C_n + i\hat{k}_n \hat{C}_n) (x + iy)^{(n-1)} \right], \quad (1.79)$$

$$\Delta p_y = \sum_{n=1}^N \frac{\chi}{n!} \Im \left[ (k_n C_n + i\hat{k}_n \hat{C}_n) (x + iy)^{(n-1)} \right], \quad (1.80)$$

$$\Delta p_t = -\chi k \sum_{n=1}^N \Re \left[ (k_n S_n + i\hat{k}_n \hat{S}_n) (x + iy)^n \right], \quad (1.81)$$

where

$$C_n = \cos(\phi_n - \omega \Delta t) \quad \hat{C}_n = \cos(\hat{\phi}_n - \omega \Delta t) \quad (1.82)$$

$$S_n = \sin(\phi_n - \omega \Delta t) \quad \hat{S}_n = \sin(\hat{\phi}_n - \omega \Delta t). \quad (1.83)$$

### 1.3.7 Solenoid

The expanded Hamiltonian for a particle in a solenoid is

$$H = p_\sigma + \frac{1}{2} \frac{(p_x + R \cdot y)^2 + (p_y - R \cdot x)^2}{1 + \delta},$$

where  $R = \frac{1}{2} \frac{q}{P_{0c}} \mathbf{B}(0, 0, s)$ . The map for a solenoid of length  $L$  in the thin lens approximation with the expanded Hamiltonian (eq. 4.35 in [4])

$$\begin{aligned} x &\rightarrow C \cdot x + S \cdot y \\ p_x &\rightarrow -\theta R \cdot C \cdot x + C \cdot p_x - \theta R \cdot S \cdot y + S \cdot p_y \\ y &\rightarrow -S \cdot x + C \cdot y \\ p_y &\rightarrow \theta R \cdot S \cdot x - S \cdot p_x - \theta R \cdot C \cdot y + C \cdot p_y \\ \sigma &\rightarrow \sigma - \frac{\beta_0}{\beta} \frac{\theta}{1 + \delta} \left( \frac{1}{2} R(x^2 + y^2) + (p_x y - p_y x) \right) \end{aligned}$$

where  $R \equiv R(s_0)$ ,  $\theta = \frac{R}{1 + \delta}$ ,  $C = \cos(\theta)$  and  $S = \sin(\theta)$ .

The map for a thick solenoid is (eq. 3.47, 3.48 in [1])

$$\begin{aligned}
x &\rightarrow C^2 \cdot x + \frac{1}{R} \cdot S \cdot C \cdot p_x + S \cdot C \cdot y + \frac{1}{R} \cdot S^2 \cdot p_y \\
p_x &\rightarrow -R \cdot S \cdot C \cdot x + C^2 \cdot p_x - R \cdot S^2 \cdot y + S \cdot C \cdot p_y \\
y &\rightarrow -S \cdot C \cdot x - \frac{1}{R} \cdot S^2 \cdot p_x + C^2 \cdot y + \frac{1}{R} \cdot S \cdot C \cdot p_y \\
p_y &\rightarrow R \cdot S^2 \cdot x - S \cdot C \cdot p_x - R \cdot S \cdot C \cdot y + C^2 \cdot p_y \\
\sigma &\rightarrow \sigma - \frac{L}{2} \left[ R^2(x^2 + y^2) + 2R \left( \frac{p_x}{1+\delta} y - \frac{p_y}{1+\delta} x \right) + \frac{p_x^2 + p_y^2}{(1+\delta)^2} \right]
\end{aligned}$$

where  $\theta = R \cdot L$ ,  $C = \cos \theta$  and  $S = \sin \theta$ .

### 1.3.8 AC-dipole

The excitation amplitude of the AC-dipole is denoted by  $A$  [Tm], the excitation frequency by  $q_d$  [ $2\pi$ ] and the phase of the excitation by  $\phi$ . The map presented here is for a purely horizontal dipole, the map for a vertical dipole is obtained by replacing  $p_x \rightarrow p_y$ .

The effect of the AC-dipole is split into four stages. The turn number is denoted by  $n$ .

1. A number of free turns  $n_{\text{free}}$ , in which the AC-dipole has no effect on the motion.
2. Ramp-up of the voltage from 0 to the excitation amplitude  $A$  for  $n_{\text{ramp-up}}$  turns.

$$\begin{aligned}
n' &= \frac{n - n_{\text{free}}}{n_{\text{ramp-up}}} \\
p_x &\rightarrow p_x + n' \cdot \frac{A}{pc} \cdot (1 + \delta) \sin(2\pi q_d \cdot (n - n_{\text{free}}) + \phi)
\end{aligned}$$

3. Constant excitation amplitude for  $n_{\text{flat}}$  turns.

$$p_x \rightarrow p_x + \frac{A}{pc} \cdot (1 + \delta) \sin(2\pi q_d \cdot (n - n_{\text{free}}) + \phi)$$

4. Ramp-down of the voltage from the excitation amplitude  $A$  to 0 for  $n_{\text{ramp-down}}$  turns.

$$\begin{aligned}
n' &= \frac{n - n_{\text{free}} - n_{\text{ramp-up}} - n_{\text{flat}} - n_{\text{ramp-down}}}{n_{\text{ramp-down}}} \\
p_x &\rightarrow p_x + n' \cdot \frac{A}{p} \cdot (1 + \delta) \sin(2\pi q_d \cdot (n - n_{\text{free}}) + \phi)
\end{aligned}$$

### 1.3.9 Wire

For each part we define  $p_z = \sqrt{(1 + \delta)^2 - x'^2 - y'^2}$ , using the current values for  $x'$  and  $y'$ .

Step 1. Initial backwards drift of length  $L = \frac{emb l}{2}$ .

$$\begin{aligned} x &\rightarrow x - L \cdot \frac{x'}{p_z} \\ y &\rightarrow y - L \cdot \frac{y'}{p_z} \end{aligned}$$

Step 2.

$$\begin{aligned} y &\rightarrow y - \frac{x \cdot \sin(t_x)}{\cos\left(\arctan\left(\frac{x'}{p_z}\right) - t_x\right)} \cdot \frac{y'}{\sqrt{(1+\delta)^2 - y'^2}} \\ x &\rightarrow x \cdot \left[ \cos(t_x) - \sin(t_x) \cdot \tan\left(\arctan\left(\frac{x'}{p_z}\right) - t_x\right) \right] \\ x' &\rightarrow \sqrt{(1+\delta)^2 - y'^2} \cdot \sin\left(\arctan\left(\frac{x'}{p_z}\right) - t_x\right) \\ x &\rightarrow x - \frac{y \cdot \sin(t_y)}{\cos\left(\arctan\left(\frac{y'}{p_z}\right) - t_y\right)} \cdot \frac{x'}{\sqrt{(1+\delta)^2 - x'^2}} \\ y &\rightarrow y \cdot \left[ \cos(t_y) - \sin(t_y) \cdot \tan\left(\arctan\left(\frac{y'}{p_z}\right) - t_y\right) \right] \\ y' &\rightarrow \sqrt{(1+\delta)^2 - x'^2} \sin\left(\arctan\left(\frac{y'}{p_z}\right) - t_y\right) \end{aligned}$$

Step 3. Drift part of length  $L = lin$ .

$$\begin{aligned} x &\rightarrow x + L \cdot \frac{x'}{p_z} \\ y &\rightarrow y + L \cdot \frac{y'}{p_z} \end{aligned}$$

Step 4. Here  $x_i = x - r_x$  and  $y = y - r_y$ .

$$\begin{aligned} x' &\rightarrow x' - \frac{\frac{cur \cdot 10^{-7}}{chi} \cdot x_i}{x_i^2 + y_i^2} \left[ \sqrt{(lin + l)^2 + x_i^2 + y_i^2} - \sqrt{(lin - l)^2 + x_i^2 + y_i^2} \right] \\ y' &\rightarrow y' - \frac{\frac{cur \cdot 10^{-7}}{chi} \cdot y_i}{x_i^2 + y_i^2} \left[ \sqrt{(lin + l)^2 + x_i^2 + y_i^2} - \sqrt{(lin - l)^2 + x_i^2 + y_i^2} \right] \end{aligned}$$

Step 5. Drift of length  $L = leff - lin$ .

$$\begin{aligned} x &\rightarrow x + L \frac{x'}{p_z} \\ y &\rightarrow y + L \frac{y'}{p_z} \end{aligned}$$

Step 6.

$$\begin{aligned}
 x &\rightarrow x - \frac{y \cdot \sin(-t_y)}{\cos\left(\arctan\left(\frac{y'}{p_z}\right) + t_y\right)} \cdot \frac{x'}{\sqrt{(1+\delta)^2 - x'^2}} \\
 y &\rightarrow y \cdot \left[ \cos(-t_y) - \sin(-t_y) \cdot \tan\left(\arctan\left(\frac{y'}{p_z}\right) + t_y\right) \right] \\
 y' &\rightarrow \sqrt{(1+\delta)^2 - x'^2} \cdot \sin\left(\arctan\left(\frac{y'}{p_z}\right) + t_y\right) \\
 y &\rightarrow y - \frac{x \cdot \sin(-t_x)}{\cos\left(\arctan\left(\frac{x'}{p_z}\right) + t_x\right)} \cdot \frac{y'}{\sqrt{(1+\delta)^2 - y'^2}} \\
 x &\rightarrow x \cdot \left[ \cos(-t_x) - \sin(-t_x) \cdot \tan\left(\arctan\left(\frac{x'}{p_z}\right) + t_x\right) \right] \\
 x' &\rightarrow \sqrt{(1+\delta)^2 - y'^2} \cdot \sin\left(\arctan\left(\frac{x'}{p_z}\right) + t_x\right)
 \end{aligned}$$

Step 7. Shift.

$$\begin{aligned}
 x &\rightarrow x + embl \cdot \tan(t_x) \\
 y &\rightarrow y + embl \cdot \frac{\tan(t_y)}{\cos(t_x)}
 \end{aligned}$$

Step 8. Negative drift of length  $L = \frac{embl}{2}$ .

$$\begin{aligned}
 x &\rightarrow x - L \cdot \frac{x'}{p_z} \\
 y &\rightarrow y - L \cdot \frac{y'}{p_z}
 \end{aligned}$$

### 1.3.10 Misalignment

Misalignments of elements affects the coordinates at the entrance of an element as follows

$$\begin{aligned}
 x &\rightarrow (x - x_s) \cdot t_c + (y - y_s) \cdot t_s \\
 y &\rightarrow -(x - x_s) \cdot t_s + (y - y_s) \cdot t_c,
 \end{aligned}$$

where  $x_s$  and  $y_s$  are the displacements in the horizontal and vertical directions, respectively.  $t_c$  and  $t_s$  are the cosine and sine of the tilt angle for the element.

### 1.3.11 Electron Lens

#### 1.3.11.1 Hollow electron lens - uniform annular profile

For a uniform distribution of the electron beam between  $R_1$  and  $R_2$ , the radial kick can be described by a shape function  $f(r)$  and a maximum kick strength  $\theta_{\max}$ :

$$\theta(r) = \frac{f(r)}{(r/R_2)} \cdot \theta_{\max} \tag{1.84}$$



with  $r = \sqrt{x^2 + y^2}$  and  $\theta_{\max}$  independent of  $r$ . The shape function  $f(r)$  is defined as

$$f(r) = \frac{I(r)}{I_T} = \frac{2\pi}{I_T} \int_0^r r \rho(r) dr \quad (1.85)$$

where  $I_T$  is the total electron beam current,  $I(r)$  is the current enclosed in a radius  $r$  and  $\rho(r)$  is the electron beam density distribution.

For a uniform profile one then obtains:

$$\begin{cases} 0 & , \quad r < R_1 \\ \frac{r^2 - R_1^2}{R_2^2 - R_1^2} & , \quad R_1 \leq r < R_2 \\ 1 & , \quad R_2 \leq r \end{cases} \quad (1.86)$$

and

$$\theta_{\max} = \theta(R_2) = \frac{2LI_T(1 \pm \beta_e \beta_p)}{4\pi\epsilon_0 (B\rho)_p \beta_e \beta_p c^2} \cdot \frac{1}{R_2} \quad (1.87)$$

where  $L$  is the length of the e-lens,  $I_T$  the total electron beam current,  $\beta_{e/p}$  the relativistic  $\beta$  of electron/proton beam,  $B\rho$  the magnetic rigidity,  $c$  the speed of light and  $\epsilon_0$  the vacuum permittivity. The  $\pm$ -sign represents the two cases of the electron beam traveling in the direction of the proton beam (+) or in the opposite direction (-). For hollow electron beam collimation, electron and proton beam travel in the same direction.

The kick in  $(x', y')$  can then be expressed as (note  $\frac{x}{r} = \cos(\phi)$ ,  $\frac{y}{r} = \sin(\phi)$ ):

$$x' = x' - \theta_{\max} \cdot \frac{r_2}{r^2} \cdot f(r) \cdot x \quad (1.88)$$

$$y' = y' - \theta_{\max} \cdot \frac{r_2}{r^2} \cdot f(r) \cdot y \quad (1.89)$$

If the electron lens is offset by  $(x_{\text{offset}}, y_{\text{offset}})$ , the coordinates  $(x, y)$  are simply transferred to:

$$\tilde{x} = x + x_{\text{offset}} \quad (1.90)$$

$$\tilde{y} = y + y_{\text{offset}} \quad (1.91)$$

$$\tilde{r} = \sqrt{\tilde{x}^2 + \tilde{y}^2} \quad (1.92)$$

and the kick is then given by:

$$x' = x' - \theta_{\max} \cdot \frac{r_2}{\tilde{r}^2} \cdot f(\tilde{r}) \cdot \tilde{x} \quad (1.93)$$

$$y' = y' - \theta_{\max} \cdot \frac{r_2}{\tilde{r}^2} \cdot f(\tilde{r}) \cdot \tilde{y} \quad (1.94)$$



# Chapter 2

## Xfields

### 2.1 Fields generated by a bunch of particles

We assume that the bunch travels rigidly along  $s$  with velocity  $\beta_0 c$ :

$$\rho(x, y, s, t) = \rho_0(x, y, s - \beta_0 c t) \quad (2.1)$$

$$\mathbf{J}(x, y, s, t) = \beta_0 c \rho_0(x, y, s - \beta_0 c t) \hat{\mathbf{i}}_s \quad (2.2)$$

We define an auxiliary variable  $\zeta$  as the position along the bunch:

$$\zeta = s - \beta_0 c t. \quad (2.3)$$

We call  $K$  the lab reference frame in which we have defined all equations above, and we introduce a boosted frame  $K'$  moving rigidly with the reference particle. The coordinates in the two systems are related by a Lorentz transformation [?]:

$$ct' = \gamma_0 (ct - \beta_0 s) \quad (2.4)$$

$$x' = x \quad (2.5)$$

$$y' = y \quad (2.6)$$

$$s' = \gamma_0 (s - \beta_0 c t) = \gamma_0 \zeta \quad (2.7)$$

The corresponding inverse transformation is:

$$ct = \gamma_0 (ct' + \beta_0 s') \quad (2.8)$$

$$x = x' \quad (2.9)$$

$$y = y' \quad (2.10)$$

$$s = \gamma_0 (s' + \beta_0 c t') \quad (2.11)$$

The quantities  $(c\rho, J_x, J_y, J_s)$  form a Lorentz 4-vector and therefore they are transformed between  $K$  and  $K'$  by relationships similar to the Eqs. 2.4-2.6 [?]:

$$c\rho'(\mathbf{r}', t') = \gamma_0 [c\rho(\mathbf{r}(\mathbf{r}', t'), t(\mathbf{r}', t')) - \beta_0 J_s(\mathbf{r}(\mathbf{r}', t'), t(\mathbf{r}', t'))] \quad (2.12)$$

$$J'_s(\mathbf{r}', t') = \gamma_0 [J_s(\mathbf{r}(\mathbf{r}', t'), t(\mathbf{r}', t')) - \beta_0 c\rho(\mathbf{r}(\mathbf{r}', t'), t(\mathbf{r}', t'))] \quad (2.13)$$

where the transformations  $\mathbf{r}(\mathbf{r}', t')$  and  $t(\mathbf{r}', t')$  are defined by Eqs. 2.8 and 2.11 respectively. The transverse components  $J_x$  and  $J_y$  of the current vector are invariant for our transformation, and are anyhow zero in our case.

Using Eq. 2.2 these become:

$$\rho'(\mathbf{r}', t') = \frac{1}{\gamma_0} \rho(\mathbf{r}(\mathbf{r}', t'), t(\mathbf{r}', t')) \quad (2.14)$$

$$J'_s(\mathbf{r}', t') = 0 \quad (2.15)$$

Using Eqs. 2.1 and 2.8-2.10, we obtain:

$$\rho(x', y', s(s', t'), t(s', t')) = \rho_0(x', y', s(s', t') - \beta_0 c t(s', t')) \quad (2.16)$$

From Eq. 2.7 we get:

$$s(s', t') - \beta_0 c t(s', t') = \frac{s'}{\gamma_0} \quad (2.17)$$

where the coordinate  $t'$  has disappeared.

We can therefore write:

$$\rho'(x', y', s', t') = \frac{1}{\gamma_0} \rho_0\left(x', y', \frac{s'}{\gamma_0}\right) \quad (2.18)$$

The electric potential in the bunch frame is solution of Poisson's equation:

$$\frac{\partial^2 \phi'}{\partial x'^2} + \frac{\partial^2 \phi'}{\partial y'^2} + \frac{\partial^2 \phi'}{\partial s'^2} = -\frac{\rho'(x', y', s')}{\epsilon_0} \quad (2.19)$$

From Eq. 2.18 we can write:

$$\frac{\partial^2 \phi'}{\partial x'^2} + \frac{\partial^2 \phi'}{\partial y'^2} + \frac{\partial^2 \phi'}{\partial s'^2} = -\frac{1}{\gamma_0 \epsilon_0} \rho_0\left(x', y', \frac{s'}{\gamma_0}\right) \quad (2.20)$$

We now make the substitution:

$$\zeta = \frac{s'}{\gamma_0} \quad (2.21)$$

obtained from Eq. 2.7, which allows to rewrite Eq. 2.20 as:

$$\frac{\partial^2 \phi'}{\partial x^2} + \frac{\partial^2 \phi'}{\partial y^2} + \frac{1}{\gamma_0^2} \frac{\partial^2 \phi'}{\partial \zeta^2} = -\frac{1}{\gamma_0 \epsilon_0} \rho_0(x, y, \zeta) \quad (2.22)$$

Here we have dropped the "'" sign from  $x$  and  $y$  as these coordinates are unaffected by the Lorentz boost.

The quantities  $\left(\frac{\phi}{c}, A_x, A_y, A_s\right)$  form a Lorentz 4-vector, so we can write:

$$\phi = \gamma_0 (\phi' + \beta_0 c A'_s) \quad (2.23)$$

$$A_s = A'_s + \beta_0 \frac{\phi'}{c} \quad (2.24)$$

In the bunch frame the charges are at rest therefore  $A'_x = A'_y = A'_s = 0$  therefore:

$$\phi = \gamma_0 \phi' \quad (2.25)$$

$$A_s = \beta_0 \frac{\phi'}{c} = \frac{\beta_0}{\gamma_0 c} \phi \quad (2.26)$$

Combining Eq. 2.25 with Eq. 2.22 we obtain the equation in  $\phi$ :

$$\boxed{\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{1}{\gamma_0^2} \frac{\partial^2 \phi}{\partial \zeta^2} = -\frac{1}{\epsilon_0} \rho_0(x, y, \zeta)} \quad (2.27)$$

### 2.1.1 2.5D approximation

For large enough values of  $\gamma_0$ , Eq. 2.22 can be approximated by:

$$\boxed{\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = -\frac{1}{\epsilon_0} \rho_0(x, y, \zeta)} \quad (2.28)$$

which means that we can solve a simple 2D problem for each beam slice (identified by its coordinate  $\zeta$ ).

### 2.1.2 Modulated 2D

Often the beam distribution can be factorized as:

$$\rho_0(x, y, \zeta) = q_0 \lambda_0(\zeta) \rho_{\perp}(x, y) \quad (2.29)$$

where:

$$\int \rho_{\perp}(x, y) dx dy = 1 \quad (2.30)$$

and  $\lambda_0(z)$  is therefore the bunch line density.

For a bunched beam:

$$\int \lambda_0(z) dz = N \quad (2.31)$$

where  $N$  is the bunch population.

In this case the potential can be factorized as:

$$\phi(x, y, \zeta) = q_0 \lambda(\zeta) \phi_{\perp}(x, y) \quad (2.32)$$

where  $\phi_{\perp}(x, y)$  is the solution of the following 2D Poisson equation:

$$\frac{\partial^2 \phi_{\perp}}{\partial x^2} + \frac{\partial^2 \phi_{\perp}}{\partial y^2} = -\frac{1}{\epsilon_0} \rho_{\perp}(x, y) \quad (2.33)$$

## 2.2 Lorentz force

We now compute the Lorentz force on the particles moving in the longitudinal directions, including particles of the bunch itself (space charge forces) and particles of a colliding bunch moving in the opposite directions (beam-beam forces). The angles of such test particles are neglected as done in the usual thin-lens approximation. Therefore the velocity of a test particle can be written as:

$$\mathbf{v} = \beta c \hat{\mathbf{i}}_s \quad (2.34)$$

The Lorenz force can be written as:

$$\begin{aligned} \mathbf{F} &= q \left( -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t} + \beta c \hat{\mathbf{i}}_s \times (\nabla \times \mathbf{A}) \right) \\ &= q \left( -\nabla\phi - \frac{\beta_0}{\gamma_0 c} \frac{\partial \phi}{\partial t} \hat{\mathbf{i}}_s + \beta c \hat{\mathbf{i}}_s \times (\nabla \times \mathbf{A}) \right) \end{aligned} \quad (2.35)$$

We compute the vector product:

$$\begin{aligned} \hat{\mathbf{i}}_s \times (\nabla \times \mathbf{A}) &= \left( \frac{\partial A_s}{\partial x} - \frac{\partial A_x}{\partial s} \right) \hat{\mathbf{i}}_x + \left( \frac{\partial A_s}{\partial y} - \frac{\partial A_y}{\partial s} \right) \hat{\mathbf{i}}_y \\ &= \left( \frac{\partial A_s}{\partial x} - \frac{\partial A_x}{\partial s} \right) \hat{\mathbf{i}}_x + \left( \frac{\partial A_s}{\partial y} - \frac{\partial A_y}{\partial s} \right) \hat{\mathbf{i}}_y + \underbrace{\left( \frac{\partial A_s}{\partial s} - \frac{\partial A_s}{\partial s} \right)}_{=0} \hat{\mathbf{i}}_s \\ &= \nabla A_s - \frac{\partial \mathbf{A}}{\partial s} \end{aligned} \quad (2.36)$$

We replace:

$$\mathbf{F} = q \left( -\nabla\phi - \frac{\beta_0}{\gamma_0 c} \frac{\partial \phi}{\partial t} \hat{\mathbf{i}}_s + \beta \beta_0 \nabla\phi - \frac{\beta \beta_0}{\gamma_0} \frac{\partial \phi}{\partial s} \hat{\mathbf{i}}_s \right) \quad (2.37)$$

The potentials will have the same form as the sources (this can be shown explicitly using the Lorentz transformations):

$$\phi(x, y, s, t) = \phi \left( x, y, t - \frac{s}{\beta_0 c} \right) \quad (2.38)$$

For a function in this form we can write:

$$\frac{\partial \phi}{\partial s} = \frac{\partial}{\partial \zeta} = -\frac{1}{\beta_0 c} \frac{\partial \phi}{\partial t} \quad (2.39)$$

obtaining:

$$\mathbf{F} = q \left( -\nabla\phi + \frac{\beta_0^2}{\gamma_0} \frac{\partial \phi}{\partial \zeta} \hat{\mathbf{i}}_s + \beta \beta_0 \nabla\phi - \frac{\beta \beta_0}{\gamma_0} \frac{\partial \phi}{\partial \zeta} \hat{\mathbf{i}}_s \right) \quad (2.40)$$

Reorganizing:

$$\mathbf{F} = -q(1 - \beta \beta_0) \nabla\phi - \frac{\beta_0(\beta - \beta_0)}{\gamma_0} \frac{\partial \phi}{\partial \zeta} \hat{\mathbf{i}}_s \quad (2.41)$$

Writing the dependencies explicitly:

$$F_x(x, y, \zeta(t)) = -q(1 - \beta\beta_0) \frac{\partial\phi}{\partial x}(x, y, \zeta(t)) \quad (2.42)$$

$$F_y(x, y, \zeta(t)) = -q(1 - \beta\beta_0) \frac{\partial\phi}{\partial y}(x, y, \zeta(t)) \quad (2.43)$$

$$F_z(x, y, \zeta(t)) = -q \left( 1 - \beta\beta_0 - \frac{\beta_0(\beta - \beta_0)}{\gamma_0} \right) \frac{\partial\phi}{\partial \zeta}(x, y, \zeta(t)) \quad (2.44)$$

where  $\zeta(t)$  is the position of the particle within the bunch.

## 2.3 Space charge

Over the single interaction we neglect the particle slippage<sup>1</sup>:

$$\beta = \beta_0 \quad (2.45)$$

$$\zeta(t) = \zeta \quad (2.46)$$

This gives the following simplification of Eqs. (2.42) - (2.44):

$$F_x(x, y, \zeta) = -q(1 - \beta_0^2) \frac{\partial\phi}{\partial x}(x, y, \zeta) \quad (2.47)$$

$$F_y(x, y, \zeta) = -q(1 - \beta_0^2) \frac{\partial\phi}{\partial y}(x, y, \zeta) \quad (2.48)$$

$$F_z(x, y, \zeta) = -q(1 - \beta_0^2) \frac{\partial\phi}{\partial \zeta}(x, y, \zeta) \quad (2.49)$$

In this way the force over the single interaction becomes independent on time and therefore we can compute the kicks simply as:

$$\Delta \mathbf{P} = \frac{L}{\beta_0 c} \mathbf{F} \quad (2.50)$$

where  $L$  is the portion of the machine on which we want to compute the e-cloud interaction.

The kicks on the normalized momenta can be expressed as (recalling that  $P_0 = m_0\beta_0\gamma_0c$ ):

$$\Delta p_x = \frac{m_0}{m} \frac{\Delta P_x}{P_0} = -\frac{qL(1 - \beta_0^2)}{m\gamma_0\beta_0^2c^2} \frac{\partial\phi}{\partial x}(x, y, \zeta) \quad (2.51)$$

$$\Delta p_y = \frac{m_0}{m} \frac{\Delta P_y}{P_0} = -\frac{qL(1 - \beta_0^2)}{m\gamma_0\beta_0^2c^2} \frac{\partial\phi}{\partial y}(x, y, \zeta) \quad (2.52)$$

$$\Delta \delta \simeq \Delta p_z = \frac{m_0}{m} \frac{\Delta P_z}{P_0} = -\frac{qL(1 - \beta_0^2)}{m\gamma_0\beta_0^2c^2} \frac{\partial\phi}{\partial \zeta}(x, y, \zeta) \quad (2.53)$$

---

<sup>1</sup>In any case one would need to take into account also the dispersion in order to have the right slippage.

If the beam includes particles of different species (tracking of fragments), note that here  $q$  and  $m$  refer to the individual particle while  $m_0$  is the mass of the reference particle.

In the modulated 2D case (see Sec. 2.1.2 and in particular Eq. 2.32), the kick can be expressed as:

$$\Delta p_x = \frac{m_0}{m} \frac{\Delta P_x}{P_0} = -\frac{qq_0 L(1 - \beta_0^2)}{m\gamma_0 \beta_0^2 c^2} \lambda_0(\zeta) \frac{\partial \phi_\perp}{\partial x}(x, y) \quad (2.54)$$

$$\Delta p_y = \frac{m_0}{m} \frac{\Delta P_y}{P_0} = -\frac{qq_0 L(1 - \beta_0^2)}{m\gamma_0 \beta_0^2 c^2} \lambda_0(\zeta) \frac{\partial \phi_\perp}{\partial y}(x, y) \quad (2.55)$$

$$\Delta \delta \simeq \Delta p_z = \frac{m_0}{m} \frac{\Delta P_z}{P_0} = -\frac{qq_0 L(1 - \beta_0^2)}{m\gamma_0 \beta_0^2 c^2} \frac{d\lambda_0}{d\zeta}(\zeta) \phi_\perp(x, y) \quad (2.56)$$

## 2.4 Beam-beam interaction

We consider a test particle moving in the opposite direction with velocity:

$$\mathbf{v}_W = -\beta_{0W} c \hat{\mathbf{i}}_s \quad (2.57)$$

$$s_W(t) = -\beta_{0W} c t \quad (2.58)$$

Equations (2.42) - (2.44) become:

$$F_x(x, y, \zeta_W(t)) = -q(1 + \beta_{0W}\beta_{0S}) \frac{\partial \phi}{\partial x}(x, y, \zeta_W(t)) \quad (2.59)$$

$$F_y(x, y, \zeta_W(t)) = -q(1 + \beta_{0W}\beta_{0S}) \frac{\partial \phi}{\partial y}(x, y, \zeta_W(t)) \quad (2.60)$$

$$F_z(x, y, \zeta_W(t)) = -q \left( 1 + \beta_{0W}\beta_{0S} - \frac{\beta_{0S}(\beta_{0W} + \beta_{0S})}{\gamma_0} \right) \frac{\partial \phi}{\partial \zeta}(x, y, \zeta_W(t)) \quad (2.61)$$

where we have used the the subscript  $S$  (strong) for the bunch generating the fields, and the subscript  $W$  (weak) for the test particle.

$\zeta_W(t)$  is the position of the test particle within the bunch generating the fields:

$$\zeta_W(t) = s_W(t) - \beta_{0S} c t = -(\beta_{0W} + \beta_{0S}) c t \quad (2.62)$$

In modulated-2D case (Eq. 2.32), Eqs. (2.59) - (2.60) become:

$$F_x(x, y, \zeta_W(t)) = -qq_{0S}(1 + \beta_{0W}\beta_{0S}) \lambda_{0S}(\zeta_W(t)) \frac{\partial \phi_\perp}{\partial x}(x, y) \quad (2.63)$$

$$F_y(x, y, \zeta_W(t)) = -qq_{0S}(1 + \beta_{0W}\beta_{0S}) \lambda_{0S}(\zeta_W(t)) \frac{\partial \phi_\perp}{\partial y}(x, y) \quad (2.64)$$

$$F_z(x, y, \zeta_W(t)) = -qq_{0S} \left( 1 + \beta_{0W}\beta_{0S} - \frac{\beta_{0S}(\beta_{0W} + \beta_{0S})}{\gamma_0} \right) \frac{d\lambda_{0S}}{d\zeta}(\zeta_W(t)) \phi_\perp(x, y) \quad (2.65)$$



The change in momentum for the test particle is given by:

$$\Delta \mathbf{P} = \int_{-\infty}^{+\infty} \mathbf{F}(t) dt \quad (2.66)$$

Therefore:

$$\Delta P_x(x, y, \zeta_W(t)) = -qq_{0S}N_S(1 + \beta_{0W}\beta_{0S}) \frac{\partial \phi_{\perp}}{\partial x}(x, y) \int_{-\infty}^{+\infty} \lambda_{0S}(\zeta_W(t)) dt \quad (2.67)$$

$$\Delta P_y(x, y, \zeta_W(t)) = -qq_{0S}N_S(1 + \beta_{0W}\beta_{0S}) \frac{\partial \phi_{\perp}}{\partial y}(x, y) \int_{-\infty}^{+\infty} \lambda_{0S}(\zeta_W(t)) dt \quad (2.68)$$

$$\Delta P_z(x, y, \zeta_W(t)) = -qq_{0S} \left( 1 + \beta_{0W}\beta_{0S} - \frac{\beta_{0S}(\beta_{0W} + \beta_{0S})}{\gamma_0} \right) \phi_{\perp}(x, y) \int_{-\infty}^{+\infty} \frac{d\lambda_{0S}}{d\zeta}(\zeta_W(t)) dt \quad (2.69)$$

Using Eq. (2.62) and Eq. (2.31) we can write:

$$\int_{-\infty}^{+\infty} \lambda_{0S}(\zeta_W(t)) dt = \frac{1}{(\beta_{0W} + \beta_{0S})c} \int_{-\infty}^{+\infty} \lambda_{0S}(\zeta) d\zeta = \frac{N_S}{(\beta_{0W} + \beta_{0S})c} \quad (2.70)$$

Similarly, for a bunched beam:

$$\int_{-\infty}^{+\infty} \frac{d\lambda_{0S}}{d\zeta}(\zeta_W(t)) dt = \frac{1}{(\beta_{0W} + \beta_{0S})c} \int_{-\infty}^{+\infty} \frac{d\lambda_{0S}}{d\zeta} d\zeta = \frac{\lambda_{0S}(+\infty) - \lambda_{0S}(-\infty)}{(\beta_{0W} + \beta_{0S})c} = 0 \quad (2.71)$$

From which we can write:

$$\Delta p_x = \frac{m_0}{m} \frac{\Delta P_x}{P_0} = -\frac{qq_{0S}N_S}{m\beta_{0W}\gamma_{0W}c^2} \frac{(1 + \beta_{0W}\beta_{0S})}{(\beta_{0W} + \beta_{0S})} \frac{\partial \phi_{\perp}}{\partial x}(x, y) \quad (2.72)$$

$$\Delta p_y = \frac{m_0}{m} \frac{\Delta P_y}{P_0} = -\frac{qq_{0S}N_S}{m\beta_{0W}\gamma_{0W}c^2} \frac{(1 + \beta_{0W}\beta_{0S})}{(\beta_{0W} + \beta_{0S})} \frac{\partial \phi_{\perp}}{\partial y}(x, y) \quad (2.73)$$

$$\Delta p_z = \frac{m_0}{m} \frac{\Delta P_z}{P_0} = 0 \quad (2.74)$$

## 2.5 Longitudinal profiles

### 2.5.1 Gaussian profile

The profile is in the form:

$$\lambda_0(z) = \frac{N}{\sqrt{2\pi}\sigma} e^{-\frac{(z-z_0)^2}{2\sigma^2}} \quad (2.75)$$

### 2.5.2 q-Gaussian

The profile is in the form:

$$\lambda_0(z) = \frac{N\sqrt{\beta}}{C_q} e_q \left( -\beta(z - z_0)^2 \right) \quad (2.76)$$

where  $e_q$  is the  $q$ -exponential function:

$$e_q(x) = [1 + (1 - q)x]_+^{\frac{1}{1-q}} \quad (2.77)$$

$C_q$  is a normalization factor dependent on  $q$  alone:

$$C_q = \frac{\sqrt{\pi}\Gamma\left(\frac{3-q}{2(q-1)}\right)}{\sqrt{q-1}\Gamma\left(\frac{1}{q-1}\right)} \quad (2.78)$$

The parameter beta defines the standard deviation of the distribution:

$$\sigma = \sqrt{\frac{1}{\beta(5-3q)}} \iff \beta = \frac{1}{\sigma^2(5-3q)} \quad (2.79)$$

These expressions are valid for values of the parameter  $q$  is the range of interest:

$$1 < q < \frac{5}{3} \quad (2.80)$$

In general the  $q$ -Gaussian is defined outside this range, but for smaller values it has a limited support (not of interest) and for larger values has a not defined standard deviation.

## 2.6 FFT Poisson solver

### 2.6.1 Notation for Discrete Fourier Transform

We will use the following notation for the Discrete Fourier Transform of a sequence of length  $M$ :

$$\hat{a}_k = \text{DFT}_M(a_m) = \sum_{m=0}^{M-1} a_m e^{-j2\pi \frac{km}{M}} \quad \text{for } k \in 0, \dots, M \quad (2.81)$$

The corresponding inverse transform is defined as:

$$a_n = \text{DFT}_M^{-1}(\hat{a}_k) = \frac{1}{M} \sum_{k=0}^{M-1} \hat{a}_k e^{j2\pi \frac{km}{M}} \quad \text{for } m \in 0, \dots, M \quad (2.82)$$

Multidimensional Discrete Fourier Transforms are obtained by applying sequentially 1D DFTs.. For example, in two dimensions:

$$\begin{aligned} \hat{a}_{k_x k_y} &= \text{DFT}_{M_x M_y} \{a_{m_x m_y}\} = \text{DFT}_{M_y} \left\{ \text{DFT}_{M_x} \{a_{m_x m_y}\} \right\} \\ &= \sum_{m_x=0}^{M_x-1} e^{-j2\pi \frac{k_x m_x}{M_x}} \sum_{m_y=0}^{M_y-1} e^{-j2\pi \frac{k_y m_y}{M_y}} a_{m_x m_y} \end{aligned} \quad (2.83)$$

$$\begin{aligned} a_{n_x n_y} &= \text{DFT}_{M_x M_y}^{-1} \{a_{k_x k_y}\} = \text{DFT}_{M_y}^{-1} \left\{ \text{DFT}_{M_x}^{-1} \{\hat{a}_{k_x k_y}\} \right\} \\ &= \frac{1}{M_x M_y} \sum_{k_x=0}^{M_x-1} e^{j2\pi \frac{k_x m_x}{M_x}} \sum_{k_y=0}^{M_y-1} e^{j2\pi \frac{k_y m_y}{M_y}} \hat{a}_{k_x k_y} \end{aligned} \quad (2.84)$$

### 2.6.2 FFT convolution - 1D case

The potential can be written as the convolution of a Green function with the charge distribution:

$$\phi(x) = \int_{-\infty}^{+\infty} \rho(x') G(x - x') dx' \quad (2.85)$$

We assume that the source is limited to the region  $[0, L]$ :

$$\rho(x) = \rho(x) \Pi_{[0,L]}(x) \quad (2.86)$$

where  $\Pi_{[a,b]}(x)$  is a rectangular window function defined as:

$$\Pi_{[a,b]}(x) = \begin{cases} 1 & \text{for } x \in [a, b] \\ 0 & \text{elsewhere} \end{cases} \quad (2.87)$$

We are interested in the electric potential only the region occupied by the sources, so we can compute:

$$\phi_L(x) = \phi(x) \Pi_{[0,L]} \left( \frac{x}{L} \right) \quad (2.88)$$

We replace Eq. (2.86) and Eq. (2.88) into Eq.(2.85), obtaining:

$$\phi_L(x) = \Pi_{[0,L]}(x) \int_{-\infty}^{+\infty} \Pi_{[0,L]}(x') \rho(x') G(x - x') dx' \quad (2.89)$$

We apply the change of variable  $x'' = x - x'$ :

$$\phi_L(x) = \int_{-\infty}^{+\infty} \Pi_{[0,L]}(x) \Pi_{[0,L]}(x - x'') \rho(x - x'') G(x'') dx'' \quad (2.90)$$

The integrand vanishes outside the set of the  $(x, x'')$  defined by:

$$\begin{cases} 0 < x < L \\ 0 < (x - x'') < L \end{cases} \quad (2.91)$$

We flip the signs in the second equation, obtaining:

$$\begin{cases} 0 < x < L \\ -L < (x'' - x) < 0 \end{cases} \quad (2.92)$$

Combining the two equations we obtain:

$$-L < -L + x < x'' < x < L \quad (2.93)$$

i.e. the integrand is zero for  $-L < x'' < L$ . Therefore in Eq.(2.90) we can replace  $G(x'')$  with its truncated version:

$$G_{2L}(x'') = G(x'') \Pi_{[-L,L]}(x'') \quad (2.94)$$

obtaining:

$$\phi_L(x) = \int_{-\infty}^{+\infty} \Pi_{[0,L]} \left( \frac{x}{L} \right) \Pi_{[0,L]} \left( \frac{x-x''}{L} \right) \rho(x-x'') G_{2L}(x'') dx'' \quad (2.95)$$

Since the two window functions force the integrand to zero outside the region  $|x''| < L$  we can replace  $G_{2L}(x'')$  with its replicated version:

$$G_{2LR}(x'') = \sum_{n=-\infty}^{+\infty} G_{2L}(x'' - 2nL) = \sum_{n=-\infty}^{+\infty} G(x'' - 2nL) \Pi_{[-L,L]} \left( \frac{x'' - 2nL}{2L} \right) \quad (2.96)$$

obtaining:

$$\phi_L(x) = \int_{-\infty}^{+\infty} \Pi_{[0,L]} \left( \frac{x}{L} \right) \Pi_{[0,L]} \left( \frac{x-x''}{L} \right) \rho(x-x'') G_{2LR}(x'') dx'' \quad (2.97)$$

We can go back to the initial coordinate by substituting  $x'' = x - x'$ :

$$\phi_L(x) = \Pi_{[0,L]} \left( \frac{x}{L} \right) \int_{-\infty}^{+\infty} \rho(x') G_{2LR}(x - x') dx' \quad (2.98)$$

This is a cyclic convolution, so we can proceed as follows. We split the integral:

$$\phi_L(x) = \Pi_{[0,L]} \left( \frac{x}{L} \right) \sum_{n=-\infty}^{+\infty} \int_{2nL}^{2(n+1)L} \rho(x') G_{2LR}(x - x') dx' \quad (2.99)$$

In each term we replace  $x''' = x' + 2nL$ :

$$\phi_L(x) = \Pi_{[0,L]} \left( \frac{x}{L} \right) \sum_{n=-\infty}^{+\infty} \int_0^{2L} \rho(x''' - 2nL) G_{2LR}(x - x''' - 2nL) dx''' \quad (2.100)$$

We use the fact that  $G_{2LR}(x)$  is periodic:

$$\begin{aligned} \phi_L(x) &= \Pi_{[0,L]} \left( \frac{x}{L} \right) \sum_{n=-\infty}^{+\infty} \int_0^{2L} \rho(x''' - 2nL) G_{2LR}(x - x''') dx''' \\ &= \Pi_{[0,L]} \left( \frac{x}{L} \right) \int_0^{2L} \sum_{n=-\infty}^{+\infty} \rho(x''' - 2nL) G_{2LR}(x - x''') dx''' \end{aligned} \quad (2.101)$$

We can define a replicated version of  $\rho(x)$ :

$$\rho_{2LR}(x) = \sum_{n=-\infty}^{+\infty} \rho(x - 2nL) \quad (2.102)$$

noting that this implies:

$$\rho_{2LR}(x) = 0 \quad \text{for } x \in [L, 2L] \quad (2.103)$$

We obtain:

$$\phi_L(x) = \Pi_{[0,L]} \left( \frac{x}{L} \right) \int_0^{2L} \rho_{2LR}(x') G_{2LR}(x - x') dx' \quad (2.104)$$

The function:

$$\phi_{2LR}(x) = \int_0^{2L} \rho_{2LR}(x') G_{2LR}(x - x') dx' \quad (2.105)$$

is periodic of period  $2L$ . From it the potential of interest can be simply calculated by selecting the first half period  $[0, L]$ :

$$\phi_L(x) = \Pi_{[0,L]} \left( \frac{x}{L} \right) \phi_{2LR}(x) \quad (2.106)$$

To compute the convolution in Eq. 2.105 we expand  $\phi_{2LR}(x)$  in Fourier series:

$$\phi_{2LR}(x) = \sum_{k=-\infty}^{+\infty} \tilde{\phi}_k e^{j2\pi k \frac{x}{2L}} \quad (2.107)$$

where the Fourier coefficients are given by:

$$\tilde{\phi}_k = \frac{1}{2L} \int_0^{2L} \phi_{2LR}(x) e^{-j2\pi k \frac{x}{2L}} dx \quad (2.108)$$

We replace Eq. (2.105) into Eq. (2.108) obtaining:

$$\hat{\phi}_k = \frac{1}{2L} \int_0^{2L} \int_0^{2L} \rho_{2LR}(x') G_{2LR}(x - x') e^{-j2\pi k \frac{x}{2L}} dx' dx \quad (2.109)$$

With the change of variable  $x'' = x - x'$  we obtain:

$$\tilde{\phi}_k = \frac{1}{2L} \int_0^{2L} \rho_{2LR}(x') e^{-j2\pi k \frac{x'}{2L}} dx' \int_0^{2L} G_{2LR}(x'') e^{-j2\pi k \frac{x''}{2L}} dx'' \quad (2.110)$$

where we recognize the Fourier coefficients of  $\rho_{2LR}(x)$  and  $G_{2LR}(x)$ :

$$\tilde{\rho}_k = \frac{1}{2L} \int_0^{2L} \rho_{2LR}(x) e^{-j2\pi k \frac{x}{2L}} dx \quad (2.111)$$

$$\tilde{G}_k = \frac{1}{2L} \int_0^{2L} G_{2LR}(x) e^{-j2\pi k \frac{x}{2L}} dx \quad (2.112)$$

obtaining simply:

$$\hat{\phi}_k = 2L \hat{G}_k \hat{\rho}_k \quad (2.113)$$

I assume to have the functions  $\rho_{2LR}(x)$  and  $G_{2LR}(x)$  sampled (or averaged) with step:

$$h_x = \frac{2L}{M} = \frac{L}{N} \quad (2.114)$$

I can approximate the integrals in Eqs. (2.111) and (2.112) as:

$$\tilde{\rho}_k = \frac{1}{M} \sum_{n=0}^{M-1} \rho_{2LR}(x_n) e^{-j2\pi \frac{kn}{M}} = \frac{1}{M} \hat{\rho}_k \quad (2.115)$$

$$\tilde{G}_k = \frac{1}{M} \sum_{n=0}^{M-1} G_{2LR}(x_n) e^{-j2\pi \frac{kn}{M}} = \frac{1}{M} \hat{G}_k \quad (2.116)$$

where we recognize the Discrete Fourier Transforms:

$$\hat{\rho}_k = \text{DFT}_M \{ \rho_{2LR}(x_n) \} \quad (2.117)$$

$$\hat{G}_k = \text{DFT}_M \{ G_{2LR}(x_n) \} \quad (2.118)$$

Using Eq. (2.107) we can obtain a sampled version of  $\phi(x)$ :

$$\phi_{2LR}(x_n) = \sum_{n=0}^{M-1} \tilde{\phi}_k e^{j2\pi \frac{kn}{M}} \quad (2.119)$$

where we have assumed that  $\phi(x)$  is sufficiently smooth to allow truncating the sum. Using Eqs. (2.113), (2.115) and (2.116) we obtain:

$$\phi_{2LR}(x_n) = 2L \sum_{n=0}^{M-1} \tilde{G}_k \tilde{\rho}_k e^{j2\pi \frac{kn}{M}} = \frac{2L}{M^2} \sum_{n=0}^{M-1} \hat{G}_k \hat{\rho}_k e^{j2\pi \frac{kn}{M}} \quad (2.120)$$

This can be rewritten as:

$$\phi_{2LR}(x_n) = \frac{1}{M} \sum_{n=0}^{M-1} (h_x \hat{G}_k) \hat{\rho}_k e^{j2\pi \frac{kn}{M}} = \text{DFT}_M^{-1} \{ \phi_k \} \quad (2.121)$$

where

$$\hat{\phi}_k = h_x \hat{G}_k \hat{\rho}_k \quad (2.122)$$

We call “Integrated Green Function” the quantity:

$$G_{2LR}(x_n) = h_x G_{2LR}(x_n) \quad (2.123)$$

we introduce the corresponding Fourier transform:

$$\hat{G}_k^{\text{int}} = \text{DFT}_M \{ G_{2LR}^{\text{int}}(x_n) \} \quad (2.124)$$

Eq. (2.122) can be rewritten as:

$$\boxed{\hat{\phi}_k = \hat{G}_k^{\text{int}} \hat{\rho}_k} \quad (2.125)$$

In summary the potential at the grid nodes can be computed as follows:

1. We compute the Integrated Green function at the grid points in the range  $[0, L]$ :

$$G_{2LR}^{\text{int}}(x_n) = \int_{x_n - \frac{h_x}{2}}^{x_n + \frac{h_x}{2}} G(x) dx \quad (2.126)$$

2. We extend to the interval  $[L, 2L]$  using the fact that in this interval:

$$G_{2LR}^{\text{int}}(x_n) = G_{2LR}^{\text{int}}(x_n - 2L) = G_{2LR}^{\text{int}}(2L - x_n) \quad (2.127)$$

where the first equality comes from the periodicity of  $G_{2LR}^{\text{int}}(x)$  and the second from the fact that  $G(x)$  is an even function (i.e.  $G(x) = G(-x)$ ). Note that for  $x_n \in [L, 2L]$  we have that  $2L - x_n \in [0, L]$  so we can reuse the values computed at the previous step.

3. We transform it:

$$\hat{G}_k^{\text{int}} = \text{DFT}_{2N} \{G_{2LR}(x_n)\} \quad (2.128)$$

4. We assume that we are given  $\rho(x_n)$  in the interval  $[0, L]$ . From this we can obtain  $\rho_{2LR}(x_n)$  over the interval  $[0, 2L]$  simply extending the sequence with zeros (see Eq. (2.103)).

5. We transform it:

$$\hat{\rho}_k = \text{DFT}_{2N} \{\rho_{2LR}(x_n)\} \quad (2.129)$$

6. We compute the potential in the transformed domain:

$$\hat{\phi}_k = \hat{G}_k^{\text{int}} \hat{\rho}_k \quad \text{for } k \in [0, 2N] \quad (2.130)$$

7. We inverse-transform:

$$\phi_{2LR}(x_n) = \text{DFT}_{2N}^{-1} \{\hat{\phi}_k\} \quad (2.131)$$

which provides the physical potential in the range  $[0, L]$ :

$$\phi(x_n) = \phi_{2LR}(x_n) \quad \text{for } x_n \in [0, L] \quad (2.132)$$

### 2.6.3 Extension to multiple dimensionss

The procedure described above can be extended to multiple dimensions by applying the same reasoning for all coordinates. This gives the following procedure:

1. We compute the Integrated Green function at the grid points in the volume  $[0, L_x] \times [0, L_y] \times [0, L_z]$ :

$$G_{2LR}^{\text{int}}(x_{n_x}, y_{n_y}, z_{n_z}) = \int_{x_{n_x} - \frac{h_x}{2}}^{x_{n_x} + \frac{h_x}{2}} dx \int_{y_{n_y} - \frac{h_y}{2}}^{y_{n_y} + \frac{h_y}{2}} dy \int_{z_{n_z} - \frac{h_z}{2}}^{z_{n_z} + \frac{h_z}{2}} dz G(x, y, z) \quad (2.133)$$

2. We extend to the region  $[0, 2L_x] \times [0, 2L_y] \times [0, 2L_z]$  using the fact that:

$$G_{2LR}^{\text{int}}(x_n, y_n, z_n) = G_{2LR}^{\text{int}}(x_n - 2L_x, y_n, z_n) = G_{2LR}^{\text{int}}(2L_x - x_n, y_n, z_n) \\ \text{for } x_n \in [L_x, 2L_x], y_n \in [0, 2L_y], z_n \in [0, 2L_z] \quad (2.134)$$

$$G_{2LR}^{\text{int}}(x_n, y_n, z_n) = G_{2LR}^{\text{int}}(x_n, y_n - 2L_y, z_n) = G_{2LR}^{\text{int}}(x_n, 2L_y - y_n, z_n) \\ \text{for } y_n \in [L_y, 2L_y], x_n \in [0, 2L_x], z_n \in [0, 2L_z] \quad (2.135)$$

$$G_{2LR}^{\text{int}}(x_n, y_n, z_n) = G_{2LR}^{\text{int}}(x_n, y_n, z_n - 2L_z) = G_{2LR}^{\text{int}}(x_n, y_n, 2L_z - z_n) \\ \text{for } z_n \in [L_z, 2L_z], x_n \in [0, 2L_x], y_n \in [0, 2L_y] \quad (2.136)$$

This allows reusing the values computed at the previous step.

3. We transform it:

$$\hat{G}_{k_x k_y k_z}^{\text{int}} = \text{DFT}_{2N_x 2N_y 2N_z} \{ G_{2LR}(x_n, y_n, z_n) \} \quad (2.137)$$

4. We assume that we are given  $\rho(x_n, y_n, z_n)$  in the region  $[0, L_x] \times [0, L_y] \times [0, L_z]$ . From this we can obtain  $\rho_{2LR}(x_n)$  over the region  $[0, 2L_x] \times [0, 2L_y] \times [0, 2L_z]$  simply extending the matrix with zeros (see Eq. (2.103)).

5. We transform it:

$$\hat{\rho}_{k_x k_y k_z}^{\text{int}} = \text{DFT}_{2N_x 2N_y 2N_z} \{ \rho_{2LR}(x_n, y_n, z_n) \} \quad (2.138)$$

6. We compute the potential in the transformed domain:

$$\hat{\phi}_{k_x k_y k_z} = \hat{G}_{k_x k_y k_z}^{\text{int}} \hat{\rho}_{k_x k_y k_z} \quad \text{for } k_x/y/z \in [0, 2N_x/y/z] \quad (2.139)$$

7. We inverse-transform:

$$\phi_{2LR}(x_n, y_n, z_n) = \text{DFT}_{2N_x 2N_y 2N_z}^{-1} \{ \hat{\phi}_{k_x k_y k_z} \} \quad (2.140)$$

which provides the physical potential in the region  $[0, L_x] \times [0, L_y] \times [0, L_z]$ :

$$\phi(x_n, y_n, z_n) = \phi_{2LR}(x_n, y_n, z_n) \quad \text{for } (x_n, y_n, z_n) \in [0, L_x] \times [0, L_y] \times [0, L_z] \quad (2.141)$$

## 2.6.4 Green functions for 2D and 3D Poisson problems

### 2.6.4.1 3D Poisson problem, free space boundary conditions

For the equation:

$$\nabla^2 \phi(x, y, z) = -\frac{1}{\epsilon_0} \rho(x, y, z) \quad (2.142)$$

where:

$$\nabla = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \quad (2.143)$$

the solution can be written as

$$\phi(x, y, z) = \iiint_{-\infty}^{+\infty} \rho(x', y', z') G(x - x', y - y', z - z') dx' dy' dz' \quad (2.144)$$

where:

$$G(x, y, z) = \frac{1}{4\pi\epsilon_0} \frac{1}{\sqrt{x^2 + y^2 + z^2}} \quad (2.145)$$



The corresponding integrated Green function can be written as:

$$G_{2LR}^{\text{int}}(x_{n_x}, y_{n_y}, z_{n_z}) = \int_{x_{n_x} - \frac{h_x}{2}}^{x_{n_x} + \frac{h_x}{2}} dx \int_{y_{n_y} - \frac{h_y}{2}}^{y_{n_y} + \frac{h_y}{2}} dy \int_{z_{n_z} - \frac{h_z}{2}}^{z_{n_z} + \frac{h_z}{2}} dz G(x, y, z) \quad (2.146)$$

$$= + F\left(x_{n_x} + \frac{h_x}{2}, y_{n_y} + \frac{h_y}{2}, z_{n_z} + \frac{h_z}{2}\right) \quad (2.147)$$

$$- F\left(x_{n_x} + \frac{h_x}{2}, y_{n_y} + \frac{h_y}{2}, z_{n_z} - \frac{h_z}{2}\right) \quad (2.148)$$

$$- F\left(x_{n_x} + \frac{h_x}{2}, y_{n_y} - \frac{h_y}{2}, z_{n_z} + \frac{h_z}{2}\right) \quad (2.149)$$

$$+ F\left(x_{n_x} + \frac{h_x}{2}, y_{n_y} - \frac{h_y}{2}, z_{n_z} - \frac{h_z}{2}\right) \quad (2.150)$$

$$- F\left(x_{n_x} - \frac{h_x}{2}, y_{n_y} + \frac{h_y}{2}, z_{n_z} + \frac{h_z}{2}\right) \quad (2.151)$$

$$+ F\left(x_{n_x} - \frac{h_x}{2}, y_{n_y} + \frac{h_y}{2}, z_{n_z} - \frac{h_z}{2}\right) \quad (2.152)$$

$$+ F\left(x_{n_x} - \frac{h_x}{2}, y_{n_y} - \frac{h_y}{2}, z_{n_z} + \frac{h_z}{2}\right) \quad (2.153)$$

$$- F\left(x_{n_x} - \frac{h_x}{2}, y_{n_y} - \frac{h_y}{2}, z_{n_z} - \frac{h_z}{2}\right) \quad (2.154)$$

where  $F(x, y, z)$  is a primitive of  $G(x, y, z)$ , which can be obtained as:

$$F(x, y, z) = \int_{x_0}^x dx \int_{y_0}^y dy \int_{z_0}^z dz G(x, y, z) \quad (2.155)$$

with  $(x_0, y_0, z_0)$  being an arbitrary starting point.

An expression for  $F(x, y, z)$  is the following

$$F(x, y, z) = \frac{1}{4\pi\epsilon_0} \iiint \frac{1}{\sqrt{x^2 + y^2 + z^2}} dx dy dz \quad (2.156)$$

$$= \frac{1}{4\pi\epsilon_0} \left[ -\frac{z^2}{2} \arctan\left(\frac{xy}{z\sqrt{x^2 + y^2 + z^2}}\right) - \frac{y^2}{2} \arctan\left(\frac{xz}{y\sqrt{x^2 + y^2 + z^2}}\right) \right] \quad (2.157)$$

$$- \frac{x^2}{2} \arctan\left(\frac{yz}{x\sqrt{x^2 + y^2 + z^2}}\right) + yz \ln\left(x + \sqrt{x^2 + y^2 + z^2}\right) \quad (2.158)$$

$$+ xz \ln\left(y + \sqrt{x^2 + y^2 + z^2}\right) + xy \ln\left(z + \sqrt{x^2 + y^2 + z^2}\right) \quad (2.159)$$

Note that we need to choose the first cell center to be in (0,0,0) for evaluation of the integrated Green function. Therefore the cell edges have non zero coordinates and the denominators in the formula will always be non-vanishing.

### 2.6.4.2 2D Poisson problem, free space boundary conditions

For the equation:

$$\nabla_{\perp}^2 \phi(x, y) = -\frac{1}{\varepsilon_0} \rho(x, y) \quad (2.160)$$

where:

$$\nabla = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right) \quad (2.161)$$

the solution can be written as

$$\phi(x, y) = \iiint_{-\infty}^{+\infty} \rho(x', y') G(x - x', y - y') dx' dy' \quad (2.162)$$

where:

$$G(x, y) = -\frac{1}{4\pi\varepsilon_0} \log \left( \frac{x^2 + y^2}{r_0^2} \right) \quad (2.163)$$

where  $r_0$  is arbitrary constant which has no effect on the evaluated fields (changes the potential by an additive constant).

The corresponding integrated Green function can be written as:

$$G_{2LR}^{\text{int}}(x_{n_x}, y_{n_y}) = \int_{x_{n_x} - \frac{h_x}{2}}^{x_{n_x} + \frac{h_x}{2}} dx \int_{y_{n_y} - \frac{h_y}{2}}^{y_{n_y} + \frac{h_y}{2}} dy G(x, y, z) \quad (2.164)$$

$$= + F \left( x_{n_x} + \frac{h_x}{2}, y_{n_y} + \frac{h_y}{2} \right) \quad (2.165)$$

$$- F \left( x_{n_x} + \frac{h_x}{2}, y_{n_y} - \frac{h_y}{2} \right) \quad (2.166)$$

$$- F \left( x_{n_x} - \frac{h_x}{2}, y_{n_y} + \frac{h_y}{2} \right) \quad (2.167)$$

$$+ F \left( x_{n_x} - \frac{h_x}{2}, y_{n_y} - \frac{h_y}{2} \right) \quad (2.168)$$

$$(2.169)$$

where  $F(x, y)$  is a primitive of  $G(x, y)$ , which can be obtained as:

$$F(x, y) = \int_{x_0}^x dx \int_{y_0}^y dy G(x, y) \quad (2.170)$$

where  $(x_0, y_0)$  is an arbitrary starting point.

An expression for  $F(x, y, z)$  is the following (where we have chosen  $r_0 = 1$ ):

$$F(x, y, z) = -\frac{1}{4\pi\varepsilon_0} \iint \ln(x^2 + y^2) dx / , dy \quad (2.171)$$

$$= \frac{1}{4\pi\varepsilon_0} \left[ 3xy - x^2 \arctan(y/x) - y^2 \arctan(x/y) - xy \ln(x^2 + y^2) \right] \quad (2.172)$$

Note that we need to choose the first cell center to be in (0,0) for evaluation of the integrated Green function. Therefore the cell edges have non zero coordinates and the denominators in the formula will always be non-vanishing.

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