Xfields
physics manual

Giovanni Iadarola
CERN - Geneva, Switzerland

Contents

1 Space charge

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

$$\rho\left(x,y,s,t\right)=\rho_0\left(x,y,s-\beta_0 ct\right) \tag{1}$$

$$\mathbf{J}\left(x,y,s,t\right)=\beta_0 c\,\rho_0\left(x,y,s-\beta_0 ct\right)\hat{\mathbf{i}}_s \tag{2}$$

We define an auxiliary variable ζ as the position along the bunch:

$$\zeta = s-\beta_0 ct\,. \tag{3}$$

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 [**?**]:

$$ct'=\gamma_0\left(ct-\beta_0 s\right) \tag{4}$$

$$x'=x \tag{5}$$

$$y'=y \tag{6}$$

$$s'=\gamma_0\left(s-\beta_0 ct\right)=\gamma_0\zeta \tag{7}$$

The corresponding inverse transformation is:

$$ct=\gamma_0\left(ct'+\beta_0 s'\right) \tag{8}$$

$$x=x' \tag{9}$$

$$y=y' \tag{10}$$

$$s=\gamma_0\left(s'+\beta_0 ct'\right) \tag{11}$$

The quantities $\left(c\rho, J_x, J_y, J_s\right)$ form a Lorentz 4-vector and therefore they are transformed between K and K' by relationships similar to the Eqs. 4-6 [**?**]:

$$c\rho'\left(\mathbf{r'},t'\right)=\gamma_0\left[c\rho\left(\mathbf{r}\left(\mathbf{r'},t'\right),t\left(\mathbf{r'},t'\right)\right)-\beta_0 J_s\left(\mathbf{r}\left(\mathbf{r'},t'\right),t\left(\mathbf{r'},t'\right)\right)\right] \tag{12}$$

$$J'_s\left(\mathbf{r'},t'\right)=\gamma_0\left[J_s\left(\mathbf{r}\left(\mathbf{r'},t'\right),t\left(\mathbf{r'},t'\right)\right)-\beta_0 c\rho\left(\mathbf{r}\left(\mathbf{r'},t'\right),t\left(\mathbf{r'},t'\right)\right)\right] \tag{13}$$

where the transformations $\mathbf{r}\left(\mathbf{r'},t'\right)$ and $t\left(\mathbf{r'},t'\right)$ are defined by Eqs. 8 and 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 these become:

$$\rho'\left(\mathbf{r'},t'\right)=\frac{1}{\gamma_0}\rho\left(\mathbf{r}\left(\mathbf{r'},t'\right),t\left(\mathbf{r'},t'\right)\right) \tag{14}$$

$$J'_s\left(\mathbf{r'},t'\right)=0 \tag{15}$$

Using Eqs. 1 and 8-10, we obtain:

$$\rho\left(x',y',s(s',t'),t(s',t')\right)=\rho_0\left(x',y',s(s',t')-\beta_0 c\,t(s',t')\right) \tag{16}$$

From Eq. 7 we get:

$$s(s',t')-\beta_0 c\,t(s',t')=\frac{s'}{\gamma_0} \tag{17}$$

where the coordinate t' has disappeared.
We can therefore write:

$$\rho'\left(x', y', s', t'\right) = \frac{1}{\gamma_0}\rho_0\left(x', y', \frac{s'}{\gamma_0}\right) \tag{18}$$

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

$$\frac{\partial^2 \phi'}{\partial x'^2} + \frac{\partial^2 \phi'}{\partial y'^2} + \frac{\partial^2 \phi'}{\partial s'^2} = -\frac{\rho'(x', y', s')}{\varepsilon_0} \tag{19}$$

From Eq. 18 we can write:

$$\frac{\partial^2 \phi'}{\partial x'^2} + \frac{\partial^2 \phi'}{\partial y'^2} + \frac{\partial^2 \phi'}{\partial s'^2} = -\frac{1}{\gamma_0 \varepsilon_0}\rho_0\left(x', y', \frac{s'}{\gamma_0}\right) \tag{20}$$

We now make the substitution:

$$\zeta = \frac{s'}{\gamma_0} \tag{21}$$

obtained from Eq. 7, which allows to rewrite Eq. 20 as:

$$\frac{\partial^2 \phi'}{\partial x^2} + \frac{\partial^2 \phi'}{\partial y^2} + \frac{1}{\gamma_0^2}\frac{\partial^2 \phi'}{\partial \zeta^2} = -\frac{1}{\gamma_0 \varepsilon_0}\rho_0\left(x, y, \zeta\right) \tag{22}$$

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:

$$\phi = \gamma_0\left(\phi' + \beta_0 c A_s'\right) \tag{23}$$

$$A_s = A_s' + \beta_0 \frac{\phi'}{c} \tag{24}$$

In the bunch frame the charges are at rest therefore $A_x' = A_y' = A_s' = 0$ therefore:

$$\phi = \gamma_0 \phi' \tag{25}$$

$$A_s = \beta_0 \frac{\phi'}{c} = \frac{\beta_0}{\gamma_0 c}\phi \tag{26}$$

Combining Eq. 25 with Eq. 22 we obtain the equation in ϕ:

$$\boxed{\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{1}{\gamma_0^2}\frac{\partial^2 \phi}{\partial \zeta^2} = -\frac{1}{\varepsilon_0}\rho_0\left(x, y, \zeta\right)} \tag{27}$$

We now compute the Lorentz force on the particles. We stay in the thin lens approximation so we approximate the velocity vector of the particle as:

$$\mathbf{v} = \beta c\, \hat{\mathbf{i}}_s \tag{28}$$

The Lorenz force can be written as:

$$\begin{aligned}\mathbf{F} &= q\left(-\nabla\phi - \frac{\partial \mathbf{A}}{\partial t} + \beta c\,\hat{\mathbf{i}}_s \times (\nabla \times \mathbf{A})\right) \\ &= q\left(-\nabla\phi - \frac{\beta_0}{\gamma_0 c}\frac{\partial \phi}{\partial t}\hat{\mathbf{i}}_s + \beta c\,\hat{\mathbf{i}}_s \times (\nabla \times \mathbf{A})\right)\end{aligned} \tag{29}$$

We compute the vector product:

$$\begin{aligned}\hat{\mathbf{i}}_s \times (\nabla \times \mathbf{A}) &= \left(\frac{\partial A_s}{\partial x} - \frac{\partial A_x}{\partial s}\right)\hat{\mathbf{i}}_x + \left(\frac{\partial A_s}{\partial y} - \frac{\partial A_y}{\partial s}\right)\hat{\mathbf{i}}_y \\ &= \left(\frac{\partial A_s}{\partial x} - \frac{\partial A_x}{\partial s}\right)\hat{\mathbf{i}}_x + \left(\frac{\partial A_s}{\partial y} - \frac{\partial A_y}{\partial s}\right)\hat{\mathbf{i}}_y + \underbrace{\left(\frac{\partial A_s}{\partial s} - \frac{\partial A_s}{\partial s}\right)}_{=0}\hat{\mathbf{i}}_s \\ &= \nabla A_s - \frac{\partial \mathbf{A}}{\partial s}\end{aligned} \tag{30}$$

We replace:

$$\mathbf{F} = q\left(-\nabla\phi - \frac{\beta_0}{\gamma_0 c}\frac{\partial \phi}{\partial t}\hat{\mathbf{i}}_s + \beta\beta_0\nabla\phi - \frac{\beta\beta_0}{\gamma_0}\frac{\partial \phi}{\partial s}\hat{\mathbf{i}}_s\right) \tag{31}$$

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

$$\phi(x, y, s, t) = \phi\left(x, y, t - \frac{s}{\beta_0 c}\right) \tag{32}$$

For a function in this form we can write:

$$\frac{\partial \phi}{\partial s} = \frac{\partial}{\partial \zeta} = -\frac{1}{\beta_0 c}\frac{\partial \phi}{\partial t} \tag{33}$$

obtaining:

$$\mathbf{F} = q\left(-\nabla\phi + \frac{\beta_0^2}{\gamma_0}\frac{\partial \phi}{\partial \zeta}\hat{\mathbf{i}}_s + \beta\beta_0\nabla\phi - \frac{\beta\beta_0}{\gamma_0}\frac{\partial \phi}{\partial \zeta}\hat{\mathbf{i}}_s\right) \tag{34}$$

Reorganizing:

$$\mathbf{F} = -q(1 - \beta\beta_0)\nabla\phi - \frac{\beta_0(\beta - \beta_0)}{\gamma_0}\frac{\partial \phi}{\partial \zeta}\hat{\mathbf{i}}_s \tag{35}$$

Writing the dependencies explicitly:

$$F_x(x, y, \zeta(t)) = -q(1 - \beta\beta_0)\frac{\partial \phi}{\partial x}(x, y, \zeta(t)) \tag{36}$$

$$F_y(x, y, \zeta(t)) = -q(1 - \beta\beta_0)\frac{\partial \phi}{\partial y}(x, y, \zeta(t)) \tag{37}$$

$$F_z(x, y, \zeta(t)) = -q\left(1 - \beta\beta_0 - \frac{\beta_0(\beta - \beta_0)}{\gamma_0}\right)\frac{\partial \phi}{\partial \zeta}(x, y, \zeta(t)) \tag{38}$$

Over the single interaction we neglect the particle slippage[1]:

$$\beta = \beta_0 \tag{39}$$
$$\zeta(t) = \zeta \tag{40}$$

This gives the following simplification:

$$F_x(x, y, \zeta) = -q(1 - \beta_0^2)\frac{\partial \phi}{\partial x}(x, y, \zeta) \tag{41}$$
$$F_y(x, y, \zeta) = -q(1 - \beta_0^2)\frac{\partial \phi}{\partial y}(x, y, \zeta) \tag{42}$$
$$F_z(x, y, \zeta) = -q(1 - \beta_0^2)\frac{\partial \phi}{\partial \zeta}(x, y, \zeta) \tag{43}$$

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

$$\Delta \mathbf{P} = \frac{L}{\beta_0 c}\mathbf{F} \tag{44}$$

from which we can compute the kicks on the normalized momenta (recalling that $P_0 = m_0\beta_0\gamma_0 c$):

$$\boxed{\Delta p_x = \frac{m_0}{m}\frac{\Delta P_x}{P_0} = -\frac{qL(1-\beta_0^2)}{m\gamma_0\beta_0^2c^2}\frac{\partial \phi}{\partial x}(x, y, \zeta)} \tag{45}$$

$$\boxed{\Delta p_y = \frac{m_0}{m}\frac{\Delta P_y}{P_0} = -\frac{qL(1-\beta_0^2)}{m\gamma_0\beta_0^2c^2}\frac{\partial \phi}{\partial y}(x, y, \zeta)} \tag{46}$$

$$\boxed{\Delta \delta \simeq \Delta p_z = \frac{m_0}{m}\frac{\Delta P_z}{P_0} = -\frac{qL(1-\beta_0^2)}{m\gamma_0\beta_0^2c^2}\frac{\partial \phi}{\partial \zeta}(x, y, \zeta)} \tag{47}$$

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

1.1 2.5D approximation

For large enough values of γ_0, Eq. 22 can be approximated by:

$$\boxed{\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = -\frac{1}{\varepsilon_0}\rho_0(x, y, \zeta)} \tag{48}$$

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

[1] In any case one would need to take into account also the dispersion in order to have the right slippage.

1.2 Modulated 2D

Often the beam distribution can be factorized as:

$$\rho_0(x, y, \zeta) = N q_0 \lambda_0(\zeta) \rho_\perp(x, y) \tag{49}$$

where:

$$\int \lambda_0(z)\, dz = 1 \tag{50}$$

$$\int \rho_\perp(x, y)\, dx\, dy = 1 \tag{51}$$

In this case the potential can be factorized as:

$$\phi(x, y, \zeta) = q_0 \lambda_0(\zeta) \phi_\perp(x, y) \tag{52}$$

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

$$\frac{\partial^2 \phi_\perp}{\partial x^2} + \frac{\partial^2 \phi_\perp}{\partial y^2} = -\frac{1}{\varepsilon_0} \rho_\perp(x, y) \tag{53}$$

The kick can be expressed as:

$$\boxed{\Delta p_x = \frac{m_0}{m} \frac{\Delta P_x}{P_0} = -\frac{q q_0 N L (1 - \beta_0^2)}{m \gamma_0 \beta_0^2 c^2} \lambda_0(\zeta) \frac{\partial \phi}{\partial x}(x, y)} \tag{54}$$

$$\boxed{\Delta p_y = \frac{m_0}{m} \frac{\Delta P_y}{P_0} = -\frac{q q_0 N L (1 - \beta_0^2)}{m \gamma_0 \beta_0^2 c^2} \lambda_0(\zeta) \frac{\partial \phi}{\partial y}(x, y)} \tag{55}$$

$$\boxed{\Delta \delta \simeq \Delta p_z = \frac{m_0}{m} \frac{\Delta P_z}{P_0} = -\frac{q q_0 N L (1 - \beta_0^2)}{m \gamma_0 \beta_0^2 c^2} \frac{d\lambda_0}{d\zeta}(\zeta)\, \phi(x, y)} \tag{56}$$

2 FFT Poisson solver

2.1 Discrete Fourier Transform

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

$$\hat{a}_k = \mathrm{DFT}_M(a_m) = \sum_{m=0}^{M-1} a_m\, e^{-j 2\pi \frac{km}{M}} \quad \text{for } k \in 0, ..., M \tag{57}$$

The corresponding inverse transform is defined as:

$$a_n = \mathrm{DFT}_M^{-1}(\hat{a}_k) = \frac{1}{M} \sum_{k=0}^{M-1} \hat{a}_k\, e^{j 2\pi \frac{km}{M}} \quad \text{for } m \in 0, ..., M \tag{58}$$

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

$$
\begin{aligned}
\hat{a}_{k_x k_y} &= \mathrm{DFT}_{M_x M_y}\left\{a_{m_x m_y}\right\} = \mathrm{DFT}_{M_y}\left\{\mathrm{DFT}_{M_x}\left\{a_{m_x m_y}\right\}\right\} \\
&= \sum_{m_x=0}^{M_x-1} e^{-j2\pi\frac{k_x m_x}{M_x}} \sum_{m_y=0}^{M_y-1} e^{-j2\pi\frac{k_y m_y}{M_y}} a_{m_x m_y}
\end{aligned} \tag{59}
$$

$$
\begin{aligned}
a_{n_x n_y} &= \mathrm{DFT}^{-1}_{M_x M_y}\left\{a_{k_x k_y}\right\} = \mathrm{DFT}^{-1}_{M_y}\left\{\mathrm{DFT}^{-1}_{M_x}\left\{\hat{a}_{k_x k_y}\right\}\right\} \\
&= \frac{1}{M_x M_y} \sum_{k_x=0}^{M_x-1} e^{j2\pi\frac{k_x m_x}{M_x}} \sum_{k_y=0}^{M_y-1} e^{j2\pi\frac{k_y m_y}{M_y}} \hat{a}_{k_x k_y}
\end{aligned} \tag{60}
$$

2.2 FFT convolution - 1D case

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

$$
\phi(x) = \int_{-\infty}^{+\infty} \rho(x')\, G(x - x') dx' \tag{61}
$$

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

$$
\rho(x) = \rho(x)\, \Pi_{[0,L]}\,(x) \tag{62}
$$

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

$$
\Pi_{[a,b]}(x) = \begin{cases} 1 & \text{for } x \in [a, b] \\ 0 & \text{elsewhere} \end{cases} \tag{63}
$$

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

$$
\phi_L(x) = \phi(x)\Pi_{[0,L]}\left(\frac{x}{L}\right) \tag{64}
$$

We replace Eq. (62) and Eq. (64) into Eq.(61), obtaining:

$$
\phi_L(x) = \Pi_{[0,L]}\,(x) \int_{-\infty}^{+\infty} \Pi_{[0,L]}\,(x')\, \rho(x')\, G(x - x') dx' \tag{65}
$$

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

$$
\phi_L(x) = \int_{-\infty}^{+\infty} \Pi_{[0,L]}\,(x)\, \Pi_{[0,L]}\,(x - x'')\, \rho(x - x'')\, G(x'')\, dx'' \tag{66}
$$

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

$$
\begin{cases} 0 < x < L \\ 0 < (x - x'') < L \end{cases} \tag{67}
$$

We flip the signs in the second equation, obtaining:

$$\begin{cases} 0 < x < L \\ -L < (x'' - x) < 0 \end{cases} \tag{68}$$

Combining the two equations we obtain:

$$-L < -L + x < x'' < x < L \tag{69}$$

i.e. the integrand is zero for $-L < x'' < L$. Therefore in Eq. (66) we can replace $G(x'')$ with its truncated version:

$$G_{2L}(x'') = G(x'')\,\Pi_{[-L,L]}\left(x''\right) \tag{70}$$

obtaining:

$$\phi_L(x) = \int_{-\infty}^{+\infty} \Pi_{[0,L]}\left(\frac{x}{L}\right) \Pi_{[0,L]}\left(\frac{x - x''}{L}\right) \rho(x - x'')\, G_{2L}(x'')dx'' \tag{71}$$

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:

$$G_{2LR}(x'') = \sum_{n=-\infty}^{+\infty} G_{2L}(x'' - 2nL) = \sum_{n=-\infty}^{+\infty} G(x'' - 2nL)\,\Pi_{[-L,L]}\left(\frac{x'' - 2nL}{2L}\right) \tag{72}$$

obtaining:

$$\phi_L(x) = \int_{-\infty}^{+\infty} \Pi_{[0,L]}\left(\frac{x}{L}\right) \Pi_{[0,L]}\left(\frac{x - x''}{L}\right) \rho(x - x'')\, G_{2LR}(x'')dx'' \tag{73}$$

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

$$\phi_L(x) = \Pi_{[0,L]}\left(\frac{x}{L}\right) \int_{-\infty}^{+\infty} \rho(x')\, G_{2LR}(x - x')dx' \tag{74}$$

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

$$\phi_L(x) = \Pi_{[0,L]}\left(\frac{x}{L}\right) \sum_{n=-\infty}^{+\infty} \int_{2nL}^{2(n+1)L} \rho(x')\, G_{2LR}(x - x')\, dx' \tag{75}$$

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

$$\phi_L(x) = \Pi_{[0,L]}\left(\frac{x}{L}\right) \sum_{n=-\infty}^{+\infty} \int_{0}^{2L} \rho(x''' - 2nL)\, G_{2LR}(x - x''' - 2nL)\, dx''' \tag{76}$$

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

$$\begin{aligned} \phi_L(x) &= \Pi_{[0,L]}\left(\frac{x}{L}\right) \sum_{n=-\infty}^{+\infty} \int_{0}^{2L} \rho(x''' - 2nL)\, G_{2LR}(x - x''')dx''' \\ &= \Pi_{[0,L]}\left(\frac{x}{L}\right) \int_{0}^{2L} \sum_{n=-\infty}^{+\infty} \rho(x''' - 2nL)\, G_{2LR}(x - x''')dx''' \end{aligned} \tag{77}$$

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

$$\rho_{2LR}(x) = \sum_{n=-\infty}^{+\infty} \rho(x - 2nL) \tag{78}$$

noting that this implies:

$$\rho_{2LR}(x) = 0 \quad \text{for } x \in [L, 2L] \tag{79}$$

We obtain:

$$\phi_L(x) = \Pi_{[0,L]}\left(\frac{x}{L}\right) \int_0^{2L} \rho_{2LR}(x')\, G_{2LR}(x - x')dx' \tag{80}$$

The function:

$$\phi_{2LR}(x) = \int_0^{2L} \rho_{2LR}(x')\, G_{2LR}(x - x')dx' \tag{81}$$

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

$$\phi_L(x) = \Pi_{[0,L]}\left(\frac{x}{L}\right) \phi_{2LR}(x) \tag{82}$$

To compute the convolution in Eq. 81 we expand $\phi_{2LR}(x)$ in Fourier series:

$$\phi_{2LR}(x) = \sum_{k=-\infty}^{+\infty} \tilde{\phi}_k\, e^{j2\pi k \frac{x}{2L}} \tag{83}$$

where the Fourier coefficients are given by:

$$\tilde{\phi}_k = \frac{1}{2L} \int_0^{2L} \phi_{2LR}(x)\, e^{-j2\pi k \frac{x}{2L}}\, dx \tag{84}$$

We replace Eq. (81) into Eq. (84) obtaining:

$$\hat{\phi}_k = \frac{1}{2L} \int_0^{2L} \int_0^{2L} \rho_{2LR}(x')\, G_{2LR}(x - x')\, e^{-j2\pi k \frac{x}{2L}}\, dx'\, dx \tag{85}$$

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

$$\tilde{\phi}_k = \frac{1}{2L} \int_0^{2L} \rho_{2LR}(x') e^{-j2\pi k \frac{x'}{2L}} dx' \int_0^{2L} G_{2LR}(x'') e^{-j2\pi k \frac{x''}{2L}}\, dx'' \tag{86}$$

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

$$\tilde{\rho}_k = \frac{1}{2L} \int_0^{2L} \rho_{2LR}(x)\, e^{-j2\pi k \frac{x}{2L}}\, dx \tag{87}$$

$$\tilde{G}_k = \frac{1}{2L} \int_0^{2L} G_{2LR}(x)\, e^{-j2\pi k \frac{x}{2L}}\, dx \tag{88}$$

obtaining simply:

$$\hat{\phi}_k = 2L\, \hat{G}_k\, \hat{\rho}_k \tag{89}$$

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

$$h_x = \frac{2L}{M} = \frac{L}{N} \tag{90}$$

I can approximate the integrals in Eqs. (87) and (88) as:

$$\tilde{\rho}_k = \frac{1}{M} \sum_{n=0}^{M-1} \rho_{2LR}(x_n)\, e^{-j2\pi \frac{kn}{M}} = \frac{1}{M} \hat{\rho}_k \tag{91}$$

$$\tilde{G}_k = \frac{1}{M} \sum_{n=0}^{M-1} G_{2LR}(x_n)\, e^{-j2\pi \frac{kn}{M}} = \frac{1}{M} \hat{G}_k \tag{92}$$

where we recognize the Discrete Fourier Transforms:

$$\hat{\rho}_k = \mathrm{DFT}_M \left\{\rho_{2LR}(x_n)\right\} \tag{93}$$

$$\hat{G}_k = \mathrm{DFT}_M \left\{G_{2LR}(x_n)\right\} \tag{94}$$

Using Eq. (83) we can obtain a sampled version of $\phi(x)$:

$$\phi_{2LR}(x_n) = \sum_{n=0}^{M-1} \tilde{\phi}_k\, e^{j2\pi \frac{kn}{M}} \tag{95}$$

where we have assumed that $\phi(x)$ is sufficiently smooth to allow truncating the sum. Using Eqs. (89), (91) and (92) we obtain:

$$\phi_{2LR}(x_n) = 2L \sum_{n=0}^{M-1} \tilde{G}_k\, \tilde{\rho}_k\, e^{j2\pi \frac{kn}{M}} = \frac{2L}{M^2} \sum_{n=0}^{M-1} \hat{G}_k\, \hat{\rho}_k\, e^{j2\pi \frac{kn}{M}} \tag{96}$$

This can be rewritten as:

$$\phi_{2LR}(x_n) = \frac{1}{M} \sum_{n=0}^{M-1} (h_x \hat{G}_k)\, \hat{\rho}_k\, e^{j2\pi \frac{kn}{M}} = \mathrm{DFT}_M^{-1} \left\{\phi_k\right\} \tag{97}$$

where

$$\hat{\phi}_k = h_x \hat{G}_k\, \hat{\rho}_k \tag{98}$$

We call "Integrated Green Function" the quantity:

$$G_{2LR}(x_n) = h_x G_{2LR}(x_n) \tag{99}$$

we introduce the corresponding Fourier transform:

$$\hat{G}_k^{\mathrm{int}} = \mathrm{DFT}_M \left\{ G_{2LR}^{\mathrm{int}}(x_n) \right\} \tag{100}$$

Eq. (98) can be rewritten as:

$$\boxed{\hat{\phi}_k = \hat{G}_k^{\mathrm{int}}\, \hat{\rho}_k} \tag{101}$$

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 $[0, L]$:

$$G^{\text{int}}_{2LR}(x_n) = \int_{x_n - \frac{h_x}{2}}^{x_n + \frac{h_x}{2}} G(x)dx \tag{102}$$

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

$$G^{\text{int}}_{2LR}(x_n) = G^{\text{int}}_{2LR}(x_n - 2L) = G^{\text{int}}_{2LR}(2L - x_n) \tag{103}$$

   where the first equality comes from the periodicity of $G^{\text{int}}_{2LR}(x)$ 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:

$$\hat{G}^{\text{int}}_k = \text{DFT}_{2N}\left\{G_{2LR}(x_n)\right\} \tag{104}$$

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. (79)).

5. We transform it:

$$\hat{\rho}_k = \text{DFT}_{2N}\left\{\rho_{2LR}(x_n)\right\} \tag{105}$$

6. We compute the potential in the transformed domain:

$$\hat{\phi}_k = \hat{G}^{\text{int}}_k \hat{\rho}_k \quad \text{for } k \in [0, 2N] \tag{106}$$

7. We inverse-transform:

$$\phi_{2LR}(x_n) = \text{DFT}^{-1}_{2N}\left\{\hat{\phi}_k\right\} \tag{107}$$

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

$$\phi(x_n) = \phi_{2LR}(x_n) \quad \text{for } x_n \in [0, L] \tag{108}$$

2.3 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 $[0, L_x] \times [0, L_y] \times [0, L_z]$:

$$G^{\text{int}}_{2LR}(x_{n_x}, y_{n_y}, z_{n_z}) = \int_{x_{n_x} - \frac{h_x}{2}}^{x_{n_x} + \frac{h_x}{2}} dx \int_{y_{n_y} - \frac{h_y}{2}}^{y_{n_y} + \frac{h_y}{2}} dy \int_{z_{n_z} - \frac{h_z}{2}}^{z_{n_z} + \frac{h_z}{2}} dz\, G(x, y, z) \tag{109}$$

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

$$G^{\text{int}}_{2LR}(x_n, y_n, z_n) = G^{\text{int}}_{2LR}(x_n - 2L_x, y_n, z_n) = G^{\text{int}}_{2LR}(2L_x - x_n, y_n, z_n) \quad \text{for } x_n \in [L_x, 2L_x], y_n \in [0, 2L_y], z_n \in [0, 2L_z] \tag{110}$$

$$G^{\text{int}}_{2LR}(x_n, y_n, z_n) = G^{\text{int}}_{2LR}(x_n, y_n - 2L_y, z_n) = G^{\text{int}}_{2LR}(x_n, 2L_y - y_n, z_n) \quad \text{for } y_n \in [L_y, 2L_y], x_n \in [0, 2L_x], z_n \in [0, 2L_z] \tag{111}$$

$$G^{\text{int}}_{2LR}(x_n, y_n, z_n) = G^{\text{int}}_{2LR}(x_n, y_n, z_n - 2L_z) = G^{\text{int}}_{2LR}(x_n, y_n, 2L_z - z_n) \quad \text{for } z_n \in [L_z, 2L_z], x_n \in [0, 2L_x], y_n \in [0, 2L_y] \tag{112}$$

This allows reusing the values computed at the previous step.

3. We transform it:

$$\hat{G}^{\text{int}}_{k_x k_y k_z} = \text{DFT}_{2N_x 2N_y 2N_z} \{G_{2LR}(x_n, y_n, z_n)\} \tag{113}$$

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. (79)).

5. We transform it:

$$\hat{\rho}^{\text{int}}_{k_x k_y k_z} = \text{DFT}_{2N_x 2N_y 2N_z} \{\rho_{2LR}(x_n, y_n, z_n)\} \tag{114}$$

6. We compute the potential in the transformed domain:

$$\hat{\phi}_{k_x k_y k_z} = \hat{G}^{\text{int}}_{k_x k_y k_z} \hat{\rho}_{k_x k_y k_z} \quad \text{for } k_{x/y/z} \in [0, 2N_{x/y/z}] \tag{115}$$

7. We inverse-transform:

$$\phi_{2LR}(x_n, y_n, z_n) = \text{DFT}^{-1}_{2N_x 2N_y 2N_z} \left\{ \hat{\phi}_{k_x k_y k_z} \right\} \tag{116}$$

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

$$\phi(x_n, y_n, z_n) = \phi_{2LR}(x_n, y_n, z_n) \text{ for } (x_n, y_n, z_n) \in [0, L_x] \times [0, L_y] \times [0, L_z] \tag{117}$$

2.4 Green functions for 2D and 3D Poisson problems

3D Poisson problem, free space boundary conditions

For the equation:

$$\nabla^2 \phi(x, y, z) = -\frac{1}{\varepsilon_0} \rho(x, y, z) \tag{118}$$

where:

$$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) \tag{119}$$

the solution can be written as

$$\phi(x,y,z) = \iiint_{-\infty}^{+\infty} \rho(x',y',z')\, G(x-x',y-y',z-z')\, dx'\, dy'\, dz' \tag{120}$$

where:

$$G(x,y,z) = \frac{1}{4\pi\varepsilon_0} \frac{1}{\sqrt{x^2+y^2+z^2}} \tag{121}$$

The corresponding integrated Green function can be written as:

$$G_{2LR}^{\text{int}}(x_{n_x}, y_{n_y}, z_{n_z}) = \int_{x_{n_x}-\frac{h_x}{2}}^{x_{n_x}+\frac{h_x}{2}} dx \int_{y_{n_y}-\frac{h_y}{2}}^{y_{n_y}+\frac{h_y}{2}} dy \int_{z_{n_z}-\frac{h_z}{2}}^{x_{n_z}+\frac{h_z}{2}} dz\, G(x,y,z) \tag{122}$$

$$= + F\left(x_{n_x} + \frac{h_x}{2}, y_{n_x} + \frac{h_y}{2}, z_{n_x} + \frac{h_z}{2}\right) \tag{123}$$

$$- F\left(x_{n_x} + \frac{h_x}{2}, y_{n_x} + \frac{h_y}{2}, z_{n_x} - \frac{h_z}{2}\right) \tag{124}$$

$$- F\left(x_{n_x} + \frac{h_x}{2}, y_{n_x} - \frac{h_y}{2}, z_{n_x} + \frac{h_z}{2}\right) \tag{125}$$

$$+ F\left(x_{n_x} + \frac{h_x}{2}, y_{n_x} - \frac{h_y}{2}, z_{n_x} - \frac{h_z}{2}\right) \tag{126}$$

$$- F\left(x_{n_x} - \frac{h_x}{2}, y_{n_x} + \frac{h_y}{2}, z_{n_x} + \frac{h_z}{2}\right) \tag{127}$$

$$+ F\left(x_{n_x} - \frac{h_x}{2}, y_{n_x} + \frac{h_y}{2}, z_{n_x} - \frac{h_z}{2}\right) \tag{128}$$

$$+ F\left(x_{n_x} - \frac{h_x}{2}, y_{n_x} - \frac{h_y}{2}, z_{n_x} + \frac{h_z}{2}\right) \tag{129}$$

$$- F\left(x_{n_x} - \frac{h_x}{2}, y_{n_x} - \frac{h_y}{2}, z_{n_x} - \frac{h_z}{2}\right) \tag{130}$$

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

$$F(x,y,z) = \int_{x_0}^{x} dx \int_{y_0}^{y} dy \int_{z_0}^{x} dz\, G(x,y,z) \tag{131}$$

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

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

$$F(x,y,z) = \frac{1}{4\pi\varepsilon_0} \iiint \frac{1}{\sqrt{x^2+y^2+z^2}} dxdydz \tag{132}$$

$$= \frac{1}{4\pi\varepsilon_0} \left[-\frac{z^2}{2} \arctan\left(\frac{xy}{z\sqrt{x^2+y^2+z^2}} \right) - \frac{y^2}{2} \arctan\left(\frac{xz}{y\sqrt{x^2+y^2+z^2}} \right) \right. \tag{133}$$

$$- \frac{x^2}{2} \arctan\left(\frac{yz}{x\sqrt{x^2+y^2+z^2}} \right) + yz \ln\left(x + \sqrt{x^2+y^2+z^2} \right) \tag{134}$$

$$\left. + xz \ln\left(y + \sqrt{x^2+y^2+z^2} \right) + xy \ln\left(z + \sqrt{x^2+y^2+z^2} \right) \right] \tag{135}$$

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.

2D Poisson problem, free space boundary conditions

For the equation:

$$\nabla_\perp^2 \phi(x,y) = -\frac{1}{\varepsilon_0} \rho(x,y) \tag{136}$$

where:

$$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right) \tag{137}$$

the solution can be written as

$$\phi(x,y) = \iiint_{-\infty}^{+\infty} \rho(x',y')\, G(x-x', y-y')\, dx'\, dy' \tag{138}$$

where:

$$G(x,y) = -\frac{1}{4\pi\varepsilon_0} \log\left(\frac{x^2+y^2}{r_0^2} \right) \tag{139}$$

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:

$$
\begin{aligned}
G_{2LR}^{\text{int}}(x_{n_x}, y_{n_y}) &= \int_{x_{n_x}-\frac{h_x}{2}}^{x_{n_x}+\frac{h_x}{2}} dx \int_{y_{n_y}-\frac{h_y}{2}}^{y_{n_y}+\frac{h_y}{2}} dy\, G(x,y,z) && (140) \\
&= + F\left(x_{n_x} + \frac{h_x}{2}, y_{n_x} + \frac{h_y}{2}\right) && (141) \\
&\quad - F\left(x_{n_x} + \frac{h_x}{2}, y_{n_x} - \frac{h_y}{2}\right) && (142) \\
&\quad - F\left(x_{n_x} - \frac{h_x}{2}, y_{n_x} + \frac{h_y}{2}\right) && (143) \\
&\quad + F\left(x_{n_x} - \frac{h_x}{2}, y_{n_x} - \frac{h_y}{2}\right) && (144) \\
& && (145)
\end{aligned}
$$

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

$$
F(x,y) = \int_{x_0}^{x} dx \int_{y_0}^{y} dy\, G(x,y) \qquad (146)
$$

where (x_0, y_0) is an arbitrary starting point.
An expression for $F(x,y,z)$ is the following (where we have chosen $r_0 = 1$:

$$
\begin{aligned}
F(x,y,z) &= -\frac{1}{4\pi\varepsilon_0} \iint \ln\left(x^2 + y^2\right) dx/, dy && (147) \\
&= \frac{1}{4\pi\varepsilon_0} \left[3xy - x^2 \arctan(y/x) - y^2 \arctan(x/y) - xy \ln\left(x^2 + y^2\right)\right] && (148)
\end{aligned}
$$

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.