Previous (March 1 – March 12)

First, we deal a single beam bunch in turns, consider ACE methods:

$$\varphi(\boldsymbol{r})=\sum_{i=1}^{k}q_i\psi\left(\boldsymbol{r}-\boldsymbol{r}_i'\right)=\sum_{n=0}^{\infty}\sum_{i=1}^{k}(-1)^n\frac{q_i}{n!}\boldsymbol{r}_i'^n\cdot n\cdot\nabla^n\psi\left(\boldsymbol{r}\right)$$

If no particle losing in turns, can we treat the potential as following in a lattice?

$$\Phi(r)=\Phi_{Fourier}(r)+\Phi_{\mathrm{Re}al}(r)$$

$$\Phi_{Fourier}(r)=\frac{4\pi}{\Omega}\sum_{I}\sum_{G\neq0}Q_I\frac{e^{-(|G|^2+\kappa^2)/4\alpha^2}e^{iG.(r-R_I)}}{|G|^2+\kappa^2}$$ where Ω is the cubic volume occupied

$$\Phi_{\mathrm{Re}al}(r)=\sum_{I}Q_I\frac{\left[erfc\left(\alpha|r-R_I|+\frac{\kappa}{2\alpha}\right)e^{\kappa|r-R_I|}+erfc\left(\alpha|r-R_I|-\frac{\kappa}{2\alpha}\right)e^{-\kappa|r-R_I|}\right]}{2|r-R_I|}$$

So, if we use ACE, we need calculate the following interactions:

$\nabla^n\psi_F\left(r\right)$ where $\psi_F(r)=e^{i\boldsymbol{G}\cdot\boldsymbol{r}}$

$\nabla^n\psi_R\left(r\right)$ where $\psi_R\left(r\right)=\frac{e^{-\kappa r}}{r}erfc\left(\alpha r-\frac{\kappa}{2\alpha}\right)$

For $\nabla^{\boldsymbol{n}}\boldsymbol{\psi_F}\left(\boldsymbol{r}\right)$:

$$\partial_x\psi_F\left(r\right)=\partial_x e^{iG_xr_x}e^{iG_yr_y}e^{iG_zr_z}=iG_x\psi_F\left(r\right)$$

So, we have

$$\partial_x^{n_x}\partial_y^{n_y}\partial_z^{n_z}\psi_F\left(r\right)=i^{n_x+n_y+n_z}G_x^{n_x}G_y^{n_y}G_z^{n_z}\psi_F\left(r\right)$$

For $\nabla^{\boldsymbol{n}}\boldsymbol{\psi_R}\left(\boldsymbol{r}\right)$:

$$\because\quad\partial_x^{n_x}\psi_R\left(r\right)=\sum_{m_x}\binom{n_x}{m_x}\partial_x^{m_x}\left(\frac{e^{-\kappa r}}{r}\right)\partial_x^{n_x-m_x}\left[erfc\left(\alpha r-\frac{\kappa}{2\alpha}\right)\right]$$

$\therefore$ So we have

$$\partial_x^{n_x}\partial_y^{n_y}\partial_z^{n_z}\psi_R\left(r\right)$$
$$=\sum_{m_x,m_y,m_z}\binom{n_x}{m_x}\binom{n_x}{m_x}\binom{n_x}{m_x}\partial_x^{m_x}\partial_y^{m_y}\partial_z^{m_z}\left(\frac{e^{-\kappa r}}{r}\right)\partial_x^{n_x-m_x}\partial_y^{n_y-m_y}\partial_z^{n_z-m_z}\left[erfc\left(\alpha r-\frac{\kappa}{2\alpha}\right)\right]$$

where $\begin{bmatrix} n \\ m \end{bmatrix} = \frac{n!}{2^m m!(n-2m)!}$, suppose there is no screening effect, we can let $\kappa = 1$.

Next (March 15 – March 26)

Continue working on CASA project.