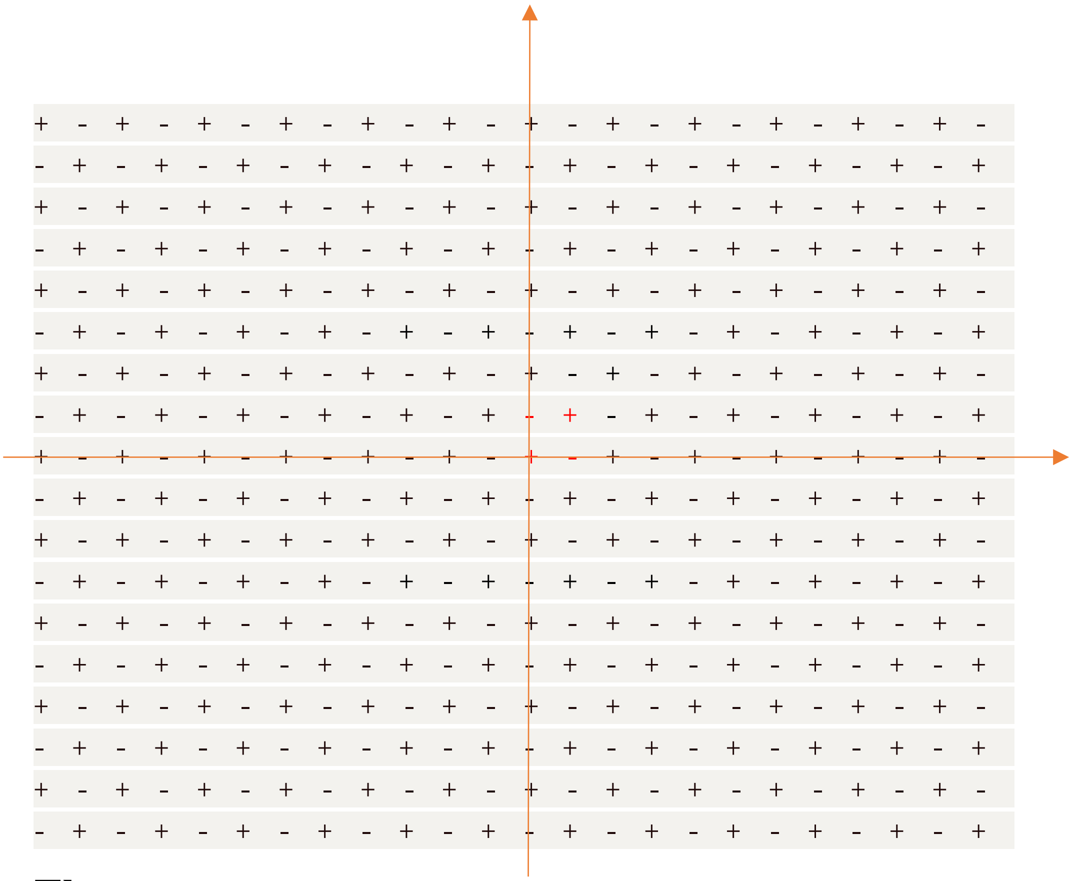


Theory

1. square unit cell

The electric potential is defined as follows:

$$\varphi(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \sum \frac{q_{ij}}{|\vec{r} - \overrightarrow{r_{ij}}|}$$

Obviously, Electric potentials are summed by unit cells in real space:

$$\varphi(\vec{r}) = \frac{q}{4\pi\varepsilon_0} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \sum_{k} \frac{q_k}{\sqrt{(mL + x_k - x)^2 + (nL + y_k - y)^2 + (z_k - z)^2}}$$

$$= \frac{q}{4\pi\varepsilon_0 L} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \sum_{k} \frac{q_k}{\sqrt{\left(m + \frac{x_k}{L} - \frac{x}{L}\right)^2 + \left(n + \frac{y_k}{L} - \frac{y}{L}\right)^2 + \left(\frac{z_k}{L} - \frac{z}{L}\right)^2}}$$

Another form: Because $\overrightarrow{r_{ij}}$ is periodic in the xy plane, we can take the Fourier expansion of the above equation as follows:

$$\varphi(\vec{r}) = \sum_{n_1} \sum_{n_2} f_{n_1,n_2}(\vec{r}) e^{i\frac{2\pi}{L}(n_1 x + n_2 y)}$$

And the Fourier expansion of the charge:

$$\rho = \sum_{l,m} \rho_{l,m} \cdot e^{i\frac{2\pi}{L}(lx + my)}$$

And then we can plug this into Poisson's equation $\nabla^2 \varphi(\vec{r}) = 0$, and the boundary conditions: $(\frac{\partial\varphi}{\partial z})_{z=0} = -\frac{\rho}{2\varepsilon_0}$

For the Poisson's equation: $\nabla^2\varphi(\vec{r}) = 0$, we can know that the z part of the potential should be an exponential term (A.Steele, 1973; T.H.M. Van Den Berg,A. Van Der Avoird, 1989).

For example, we can use explain it by separation of variables as below:

We can set $\varphi(\vec{r}) = \sum R(x,y)\cdot Z(z)$, and because of the periodic charge distribution, R(x,y) can be written as a plane wave form:

$$R(x,y) = re^{i\frac{2\pi}{L}(n_1x+n_2y)}$$

We plug it into the Poisson equation:

$$\sum r(-(\frac{2\pi}{L})^2\cdot({n_1}^2+{n_2}^2)+\frac{\partial^2}{\partial z^2}Z) = 0$$

So we must have $-(\frac{2\pi}{L})^2\cdot({n_1}^2+{n_2}^2)+\frac{\partial^2}{\partial z^2}Z = 0$

We can easily know that $Z(z)\sim e^{-\frac{2\pi}{L}\cdot\sqrt{{n_1}^2+{n_2}^2}\cdot z}$ (In order to facilitate, we set z>0)

Then we use the boundary conditions: $(\frac{\partial\varphi}{\partial z})_{z=0} = -\frac{\rho}{2\varepsilon_0}$, and we know that

$$\rho = \sum_{l,m}\rho_{l,m}\cdot e^{i\frac{2\pi}{L}(lx+my)}, \varphi(\vec{r}) = \sum f\cdot e^{i\frac{2\pi}{L}(lx+my)}\cdot e^{-\frac{2\pi}{L}\cdot\sqrt{l^2+m^2}\cdot z}$$

So combine these two equations, we can get $f = \frac{L}{4\pi\varepsilon_0}\frac{\rho_{l,m}}{\sqrt{l^2+m^2}}$

So $\varphi(\vec{r}) = \sum\frac{L}{4\pi\varepsilon_0}\frac{\rho_{l,m}}{\sqrt{l^2+m^2}}\cdot e^{i\frac{2\pi}{L}(lx+my)}\cdot e^{-\frac{2\pi}{L}\cdot\sqrt{l^2+m^2}\cdot z}$

Another simpler and cruder method to get this formula is to use the electrostatic potential expansion formula in unbounded space:

$$\rho(x',y',z') = \sum_{l,m}\rho_{l,m}\cdot e^{i\frac{2\pi}{L}(lx'+my')}\cdot\delta(z')$$

$$\varphi(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\rho(x',y',z')\cdot dx'dy'dz'}{[(x'-x)^2+(y'-y)^2+(z'-z)^2]^{1/2}}$$

The potential produced by each term of the Fourier expansion of the charge density can be calculated as:

$$I_{lm}(x,y,z) = \frac{1}{4\pi\varepsilon_0}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dx'dy'\exp\left\{\frac{i2\pi}{L}[mx'+ly']\right\}}{[(x'-x)^2+(y'-y)^2+z^2]^{1/2}}$$

The double integral can be evaluated to yield (Edgar A. Kraut, 1972):

$$I_{lm} = \frac{L}{4\pi\varepsilon_0}\frac{1}{\sqrt{l^2+m^2}}\cdot e^{i\frac{2\pi}{L}(lx+my)}\cdot e^{-\frac{2\pi}{L}\cdot\sqrt{l^2+m^2}\cdot z}$$

According to the principle of superposition of potentials, the total potential is easily obtained:

$$\varphi(\vec{r}) = \sum \frac{L}{4\pi\varepsilon_0} \frac{\rho_{l,m}}{\sqrt{l^2+m^2}} \cdot e^{i\frac{2\pi}{L}(lx+my)} \cdot e^{-\frac{2\pi}{L}\cdot\sqrt{l^2+m^2}\cdot z}$$

For an array of point charges q_k at points $r_k(x_k, y_k, 0)$, and it's a periodic array.
So the potential can be written as below:

$$\varphi(\vec{r}) = \frac{L}{4\pi\varepsilon_0 L^2} \sum_{l,m} \sum_{k} q_k \frac{e^{-\frac{2\pi z}{L}\cdot\sqrt{l^2+m^2}}}{\sqrt{l^2+m^2}} \cdot e^{i\frac{2\pi}{L}(l(x-x_k)+m(y-y_k))}$$

We can expand this by using Euler's formula, note that the factor l and m can go from minus infinity to infinity, so we could just keep the $\cos(\frac{2\pi}{L}(l\cdot(x-x_k)+m\cdot(y-y_k)))$ term.
So the final form of the potential is:

$$\varphi(\vec{r}) = \frac{1}{4\pi\varepsilon_0 L} \sum_{l,m} \frac{e^{-\frac{2\pi z}{L}\cdot\sqrt{l^2+m^2}}}{\sqrt{l^2+m^2}} \sum_{k} q_k cos(\frac{2\pi}{L}(l\cdot(x-x_k)+m\cdot(y-y_k)))$$

2.Other shape unit cells

Note that if this is a rectangle charge distribution, the potential will be:

$$\varphi(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \sum_{l,m} \frac{e^{-2\pi z\cdot\sqrt{(\frac{l}{L_1})^2+(\frac{m}{L_2})^2}}}{\sqrt{(l\cdot L_2)^2+(m\cdot L_1)^2}} \sum_{k} q_k cos(\frac{2\pi l}{L_1}\cdot(x-x_k)+\frac{2\pi m}{L_2}\cdot(y-y_k))$$

$$\varphi(\vec{r}) = \frac{q}{4\pi\varepsilon_0} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \sum_{k} \frac{q_k}{\sqrt{(mL_1+x_k-x)^2+(nL_2+y_k-y)^2+(z_k-z)^2}}$$

And if this is a parallelogram cell, the potential will be:

$$\varphi(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \sum_{l,m} \frac{e^{-2\pi z\cdot\sqrt{(\frac{l}{L_1})^2+(\frac{m}{L_2 sin\theta}-\frac{l}{L_1 tan\theta})^2}}}{\sqrt{(l\cdot L_2 sin\theta)^2+(m\cdot L_1-l\cdot L_2 cos\theta)^2}} \sum_{k} q_k cos(\frac{2\pi l}{L_1}\cdot(x-x_k) + 2\pi(\frac{m}{L_2 sin\theta}-\frac{l}{L_1 tan\theta})\cdot(y-y_k))$$

$$\varphi(\vec{r}) = \frac{q}{4\pi\varepsilon_0} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \sum_{k} \frac{q_k}{\sqrt{(mL_1+nL_2\cos\theta+x_k-x)^2+(nL_2\sin\theta+y_k-y)^2+(z_k-z)^2}}$$

For a regular hexagon, the inverted lattice vector is:

$$\overrightarrow{b_1} = \frac{2\pi}{3L}(\vec{i}+\sqrt{3}\vec{j}), \overrightarrow{b_2} = \frac{2\pi}{3L}(\vec{i}-\sqrt{3}\vec{j})$$

So as the above deduction, we can get:

$$\varphi(\vec{r}) = \frac{1}{4\pi\varepsilon_0 L}\cdot\frac{2}{\sqrt{3}}\sum_{l,m}\frac{e^{-\frac{2\pi z}{3L}\cdot\sqrt{(l+m)^2+3(l-m)^2}}}{\sqrt{(l+m)^2+3(l-m)^2}}\sum_k q_k cos(\frac{2\pi}{3L}((l+m)\cdot(x-x_k)$$

$$+\sqrt{3}(l-m)\cdot(y-y_k)))$$

$$\varphi(\vec{r}) = \frac{q}{4\pi\varepsilon_0}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\sum_k\frac{q_k}{\sqrt{(mL_1+x_k-x)^2+(nL_2+y_k-y)^2+(z_k-z)^2}}$$

3. Detailed formula

1. We assume a positive charge at the origin, then for the charge distribution, we have (x_k, y_k, q_k)=(0,0,e),(0.5L,0.5L,e),(0.5L,0,-e),(0,0.5L,-e)

We substitute the charge distribution into the formula for electric potential and get the following equation:

$$\varphi(\vec{r}) = \frac{q}{4\pi\varepsilon_0 L}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\left(\frac{1}{\sqrt{\left(m-\frac{x}{L}\right)^2+\left(n-\frac{y}{L}\right)^2+\left(\frac{z}{L}\right)^2}}+\frac{1}{\sqrt{\left(m+0.5-\frac{x}{L}\right)^2+\left(n+0.5-\frac{y}{L}\right)^2+\left(\frac{z}{L}\right)^2}}\right.$$

$$\left.-\frac{1}{\sqrt{\left(m+0.5-\frac{x}{L}\right)^2+\left(n-\frac{y}{L}\right)^2+\left(\frac{z}{L}\right)^2}}-\frac{1}{\sqrt{\left(m-\frac{x}{L}\right)^2+\left(n+0.5-\frac{y}{L}\right)^2+\left(\frac{z}{L}\right)^2}}\right)$$

$$\varphi(\vec{r}) = \frac{e}{4\pi\varepsilon_0 L}\cdot 4\sum_{l,m\ is\ odd}\frac{e^{-\frac{2\pi z}{L}\cdot\sqrt{l^2+m^2}}}{\sqrt{l^2+m^2}}cos(\frac{2\pi}{L}(lx+my))$$

2. If we separate the positive and negative charges, and shift the negative charge down a distance d, from the equation above in **Theory**, we can make a mathematical equivalent. Change the charge of the negative charge to $-e\cdot exp[-\frac{2\pi d}{L}\cdot\sqrt{l^2+m^2}]$, and think that the positive and negative charges are also in the same plane.

Then we can change the charge distribution like:

(x_k, y_k, q_k)=(0,0,e),(0.5L,0.5L,e),(0.5L,0, $-e\cdot exp[-\frac{2\pi d}{L}\cdot\sqrt{l^2+m^2}]$),(0,0.5L, $-e\cdot exp[-\frac{2\pi d}{L}\cdot\sqrt{l^2+m^2}]$)

Note that (l,m)=(0,0) is a singularity, let's talk about it separately.

For z>0, for example, we set a path $m=0, and\ l\to 0$, then

$$\lim_{l\to 0}\frac{2e^{-\frac{2\pi lz}{L}}}{l}\cdot(1-e^{-\frac{2\pi ld}{L}}) = \frac{2\cdot\frac{2\pi ld}{L}}{l} = 4\pi\frac{d}{L}$$

Then finally we can get:

$$\varphi(\vec{r}) = \frac{e}{4\pi\varepsilon_0 L}(\sum_{l,m\neq(0,0)}\{\frac{e^{-\frac{2\pi z}{L}\cdot\sqrt{l^2+m^2}}}{\sqrt{l^2+m^2}}\cdot cos(\frac{2\pi}{L}(lx+my))\cdot[(1+(-1)^{l+m})$$

$$-((-1)^l+(-1)^m)\cdot e^{-\frac{2\pi d}{L}\cdot\sqrt{l^2+m^2}}]\}+4\pi\frac{d}{L})$$

We find that in this equation, we have a constant term, this is the same as the literature

(Edgar A. Kraut, 1972) says "If charge plane is not neutral, there will be a constant term".

For -d<z<0 and z<-d, we can make the same discussion. And finally we get:

$$\varphi(\vec{r}) = \frac{e}{4\pi\varepsilon_0 L}\Big(\sum_{l,m\neq(0,0)}\{\frac{e^{-\frac{2\pi z}{L}\cdot\sqrt{l^2+m^2}}}{\sqrt{l^2+m^2}}\cdot cos(\frac{2\pi}{L}(lx+my))\cdot[(1+(-1)^{l+m}) - ((-1)^l+(-1)^m)\cdot e^{-\frac{2\pi d}{L}\cdot\sqrt{l^2+m^2}}]\} + 4\pi\frac{d}{L}\Big), \qquad z>0$$

$$\varphi(\vec{r}) = \frac{e}{4\pi\varepsilon_0 L}\Big(\sum_{l,m\neq(0,0)}\{\frac{e^{-\frac{2\pi z}{L}\cdot\sqrt{l^2+m^2}}}{\sqrt{l^2+m^2}}\cdot cos(\frac{2\pi}{L}(lx+my))\cdot[(1+(-1)^{l+m}) - ((-1)^l+(-1)^m)\cdot e^{-\frac{2\pi d}{L}\cdot\sqrt{l^2+m^2}}]\} + 4\pi\frac{d+2z}{L}\Big), \qquad -\mathrm{d}<\mathrm{z}<0$$

$$\varphi(\vec{r}) = \frac{e}{4\pi\varepsilon_0 L}\Big(\sum_{l,m\neq(0,0)}\{\frac{e^{-\frac{2\pi z}{L}\cdot\sqrt{l^2+m^2}}}{\sqrt{l^2+m^2}}\cdot cos(\frac{2\pi}{L}(lx+my))\cdot[(1+(-1)^{l+m}) - ((-1)^l+(-1)^m)\cdot e^{-\frac{2\pi d}{L}\cdot\sqrt{l^2+m^2}}]\} - 4\pi\frac{d}{L}\Big), \qquad z<-d$$

$$\varphi(\vec{r}) = \frac{q}{4\pi\varepsilon_0 L}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\Big(\frac{1}{\sqrt{\left(m-\frac{x}{L}\right)^2+\left(n-\frac{y}{L}\right)^2+\left(\frac{z}{L}\right)^2}} + \frac{1}{\sqrt{\left(m+0.5-\frac{x}{L}\right)^2+\left(n+0.5-\frac{y}{L}\right)^2+\left(\frac{z}{L}\right)^2}} - \frac{1}{\sqrt{\left(m+0.5-\frac{x}{L}\right)^2+\left(n-\frac{y}{L}\right)^2+\left(\frac{z+d}{L}\right)^2}} - \frac{1}{\sqrt{\left(m-\frac{x}{L}\right)^2+\left(n+0.5-\frac{y}{L}\right)^2+\left(\frac{z+d}{L}\right)^2}}\Big)$$

3. We can also align the positive and negative charges up and down,

(x_k, y_k, q_k)=(0,0,e),(0.5L,0.5L,e),(0,0, $-e\cdot exp[-\frac{2\pi d}{L}\cdot\sqrt{l^2+m^2}]$),(0.5L,0.5L, $-e\cdot exp[-\frac{2\pi d}{L}\cdot\sqrt{l^2+m^2}]$)

The same as **Situation 2** discusses, then the electric potential will be like:

$$\varphi(\vec{r}) = \frac{e}{4\pi\varepsilon_0 L}\Big(\sum_{l,m\neq(0,0)}\{\frac{e^{-\frac{2\pi z}{L}\cdot\sqrt{l^2+m^2}}}{\sqrt{l^2+m^2}}\cdot cos(\frac{2\pi}{L}(lx+my))\cdot(1+(-1)^{l+m})\cdot(1-e^{-\frac{2\pi d}{L}\cdot\sqrt{l^2+m^2}})\} + 4\pi\frac{d}{L}\Big) \qquad z>0$$

$$\varphi(\vec{r}) = \frac{e}{4\pi\varepsilon_0 L}\Big(\sum_{l,m\neq(0,0)}\{\frac{e^{-\frac{2\pi z}{L}\cdot\sqrt{l^2+m^2}}}{\sqrt{l^2+m^2}}\cdot cos(\frac{2\pi}{L}(lx+my))\cdot(1+(-1)^{l+m})\cdot(1-e^{-\frac{2\pi d}{L}\cdot\sqrt{l^2+m^2}})\} + 4\pi\frac{d+2z}{L}\Big) \qquad -\mathrm{d}<\mathrm{z}<0$$

$$\varphi(\vec{r}) = \frac{e}{4\pi\varepsilon_0 L}\Big(\sum_{l,m\neq(0,0)} \{\frac{e^{-\frac{2\pi z}{L}\cdot\sqrt{l^2+m^2}}}{\sqrt{l^2+m^2}}\cdot cos(\frac{2\pi}{L}(lx+my))\cdot(1+(-1)^{l+m})$$

$$\cdot(1-e^{-\frac{2\pi d}{L}\cdot\sqrt{l^2+m^2}})\} - 4\pi\frac{d}{L}\Big) \qquad z < -d$$

$$\varphi(\vec{r}) = \frac{q}{4\pi\varepsilon_0 L}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\Bigg(\frac{1}{\sqrt{\left(m-\frac{x}{L}\right)^2+\left(n-\frac{y}{L}\right)^2+\left(\frac{z}{L}\right)^2}} + \frac{1}{\sqrt{\left(m+0.5-\frac{x}{L}\right)^2+\left(n+0.5-\frac{y}{L}\right)^2+\left(\frac{z}{L}\right)^2}}$$

$$-\frac{1}{\sqrt{\left(m-\frac{x}{L}\right)^2+\left(n-\frac{y}{L}\right)^2+\left(\frac{z+d}{L}\right)^2}} - \frac{1}{\sqrt{\left(m+0.5-\frac{x}{L}\right)^2+\left(n+0.5-\frac{y}{L}\right)^2+\left(\frac{z+d}{L}\right)^2}}\Bigg)$$

4. For the average potential, because of periodicity, $\bar{\varphi}(z) = \frac{1}{|\vec{\tau}|}\iint_{\tau\ is\ a\ unit\ cell}\varphi(\vec{r})\,d\vec{\tau}$

For the situation that $l^2+m^2>0$, $\int_{y=0}^{L}\int_{x=0}^{L} cos(\frac{2\pi}{L}(lx+my))\,dxdy \equiv 0$, so only $l=m=0$, it contributes to the average potential.

So the average potential is:

$$\bar{\varphi}(z) = \frac{e}{4\pi\varepsilon_0 L}\cdot 4\pi\frac{d}{L} = \frac{ed}{\varepsilon_0 L^2} \qquad z>0$$

$$\bar{\varphi}(z) = \frac{e}{4\pi\varepsilon_0 L}\cdot 4\pi\frac{d+2z}{L} = \frac{e(d+2z)}{\varepsilon_0 L^2} \qquad -\mathrm{d}<\mathrm{z}<0$$

$$\bar{\varphi}(z) = \frac{e}{4\pi\varepsilon_0 L}\cdot(-4\pi\frac{d}{L}) = -\frac{ed}{\varepsilon_0 L^2} \qquad z<-d$$

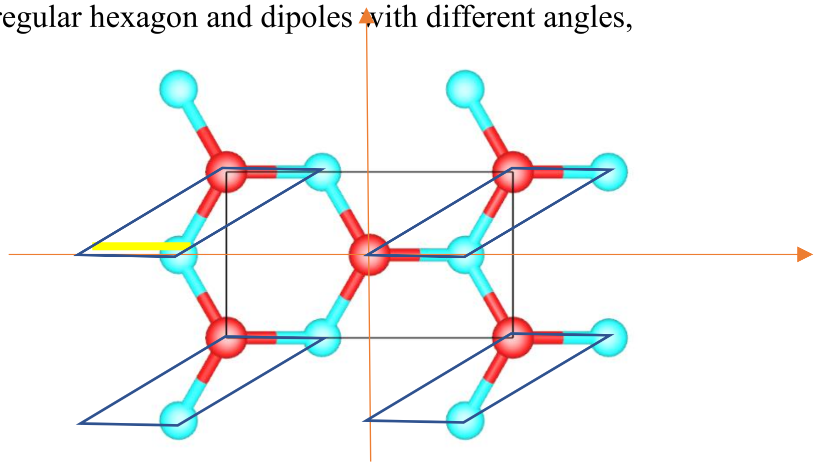
Note that if this is a rectangle charge distribution, the average potential will be:

$$\bar{\varphi}(z) = \frac{e}{4\pi\varepsilon_0 L_1 L_2}\cdot 4\pi d = \frac{ed}{\varepsilon_0 L_1 L_2} \qquad z>0$$

$$\bar{\varphi}(z) = \frac{e}{4\pi\varepsilon_0 L_1 L_2}\cdot 4\pi(d+2z) = \frac{e(d+2z)}{\varepsilon_0 L_1 L_2} \qquad -d<z<0$$

$$\bar{\varphi}(z) = \frac{e}{4\pi\varepsilon_0 L_1 L_2}\cdot(-4\pi d) = -\frac{ed}{\varepsilon_0 L_1 L_2} \qquad z<-d$$

5. For the regular hexagon and dipoles with different angles,



(x_k, y_k, q_k)=(0,0, e), $(\frac{3}{2}L, \frac{\sqrt{3}}{2}L, e)$, $(\frac{3}{2}L, -\frac{\sqrt{3}}{2}L, e)$,

$$(\frac{1}{2}cos\theta \cdot L, \frac{\sqrt{3}}{2}cos\theta \cdot L, -e \cdot e^{-\frac{2\pi sin\theta}{3} \cdot \sqrt{(l+m)^2+3(l-m)^2}}),$$

$$(\left(\frac{3}{2}+\frac{1}{2}cos\theta\right) \cdot L, \frac{\sqrt{3}}{2}(cos\theta - 1) \cdot L, -e \cdot e^{-\frac{2\pi sin\theta}{3} \cdot \sqrt{(l+m)^2+3(l-m)^2}}),$$

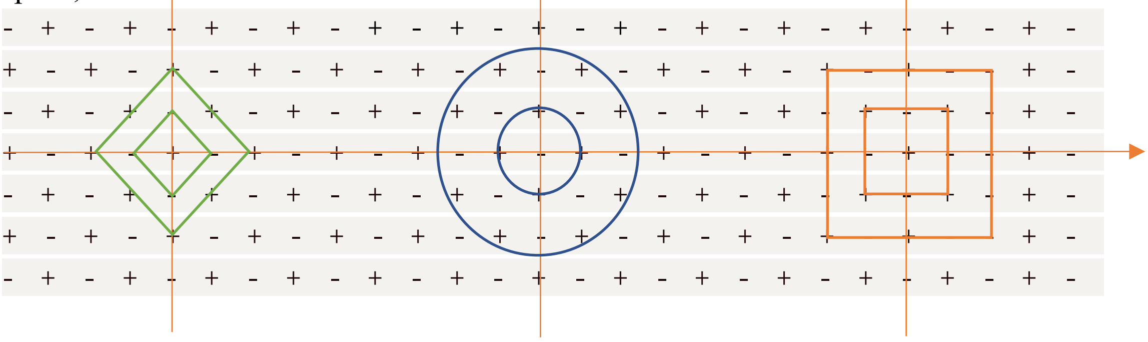
$$(\frac{1}{2}cos\theta \cdot L, \ \frac{\sqrt{3}}{2}(cos\theta - 2) \cdot L, -e \cdot e^{-\frac{2\pi sin\theta}{3} \cdot \sqrt{(l+m)^2+3(l-m)^2}})$$

$$\varphi(r) = \frac{e}{4\pi\varepsilon_0 L} \cdot \frac{2}{\sqrt{3}} \sum_{l,m\neq(0,0)} \frac{e^{-\frac{2\pi z}{3L} \cdot \sqrt{(l+m)^2+3(l-m)^2}}}{\sqrt{(l+m)^2+3(l-m)^2}} \left\{ \cos\left[\frac{2\pi}{3L}\left((l+m)x + \sqrt{3}(l-m)y\right)\right] - e^{-\frac{2\pi sin\theta}{3} \cdot \sqrt{(l+m)^2+3(l-m)^2}} \cdot \cos\left[\frac{2\pi}{3L}\left((l+m)x + \sqrt{3}(l-m)y\right) - \frac{2\pi}{3}(2l-m)cos\theta\right]\right\} + \frac{esin\theta}{3\sqrt{3}\varepsilon_0 L}$$

$$\varphi(\vec{r}) = \frac{q}{4\pi\varepsilon_0 L} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \left(\frac{1}{\sqrt{\left(3m - \frac{x}{L}\right)^2 + \left(\sqrt{3}\,n - \frac{y}{L}\right)^2 + \left(\frac{z}{L}\right)^2}} + \frac{1}{\sqrt{\left(3m + \frac{3}{2} - \frac{x}{L}\right)^2 + \left(\sqrt{3}\,n + \frac{\sqrt{3}}{2} - \frac{y}{L}\right)^2 + \left(\frac{z}{L}\right)^2}} - \frac{1}{\sqrt{\left(3m + \cos\theta - \frac{x}{L}\right)^2 + \left(\sqrt{3}\,n - \frac{y}{L}\right)^2 + \left(\sin\theta - \frac{z}{L}\right)^2}} - \frac{1}{\sqrt{\left(3m + \frac{3}{2} + \cos\theta - \frac{x}{L}\right)^2 + \left(\sqrt{3}\,n + \frac{\sqrt{3}}{2} - \frac{y}{L}\right)^2 + \left(\sin\theta - \frac{z}{L}\right)^2}} \right)$$

Convergence Analysis

In addition to summing by primitive cells, there are different summation forms in real space, such as:



Consider (0,0,z) in the first case (one plane), the corresponding summation formulas of above are:

$$\varphi(\vec{r}) = \frac{2q}{4\pi\varepsilon_0 L} \sum_{m=-s}^{s} \sum_{n=|m|-s}^{s-|m|} \frac{(-1)^{m+n}}{\sqrt{\left(m - \frac{2x}{L}\right)^2 + \left(n - \frac{2y}{L}\right)^2 + \left(\frac{2z}{L}\right)^2}}$$

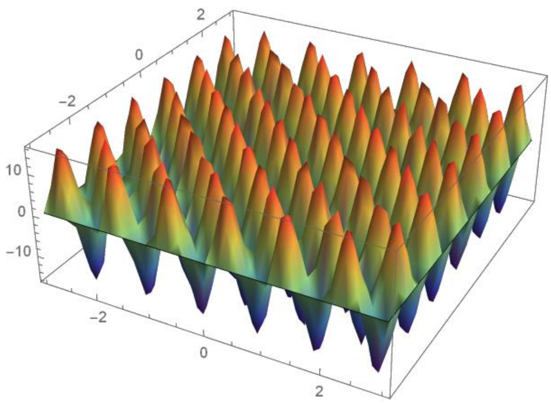
$$\varphi(\vec{r}) = \frac{2q}{4\pi\varepsilon_0 L} \sum_{m=-s}^{s} \sum_{n=-\sqrt{s^2-m^2}}^{\sqrt{s^2-m^2}} \frac{(-1)^{m+n}}{\sqrt{\left(m-\frac{2x}{L}\right)^2+\left(n-\frac{2y}{L}\right)^2+\left(\frac{2z}{L}\right)^2}}$$

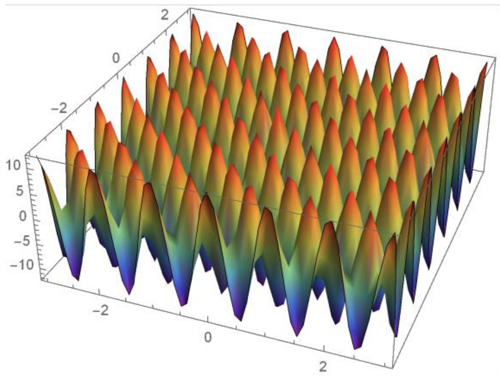
$$\varphi(\vec{r}) = \frac{2q}{4\pi\varepsilon_0 L} \sum_{m=-s}^{s} \sum_{n=-s}^{s} \frac{(-1)^{m+n}}{\sqrt{\left(m-\frac{2x}{L}\right)^2+\left(n-\frac{2y}{L}\right)^2+\left(\frac{2z}{L}\right)^2}}$$

These summation forms all have the same C4 symmetry as the plane, but differ in the speed of convergence. The simulation results found that the convergence is faster when the summation process can maintain the neutral condition.

For example, the square summation minus 1/4 of the contribution of the four corner charges, the convergence is faster.

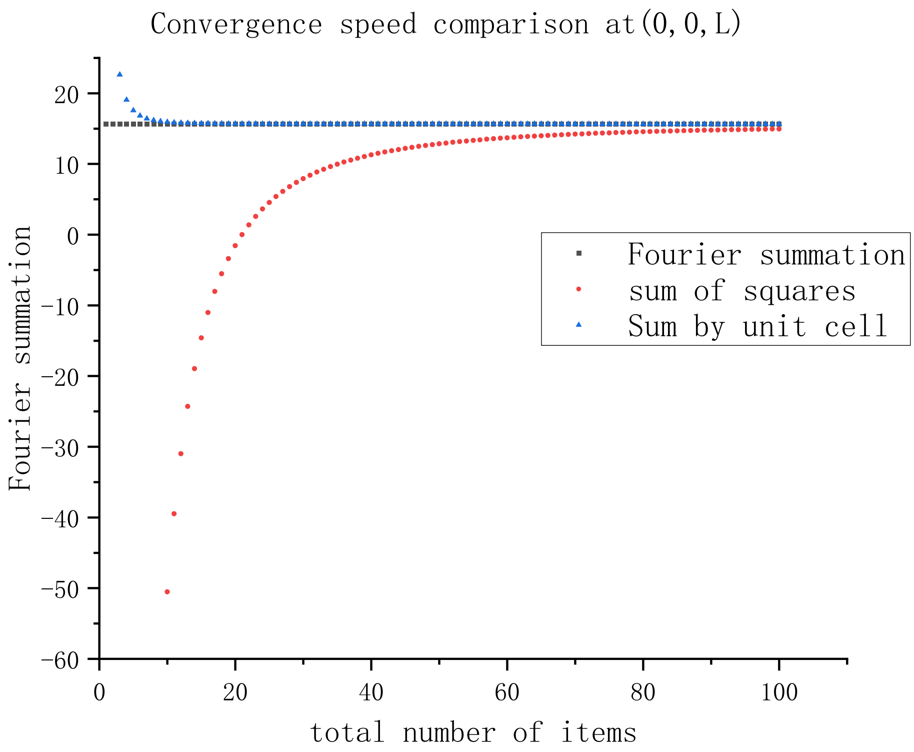
If we set z=L, and we plot the distribution of potential in the z=L plane, and compare with the result given by cell summation (The ordinate is enlarged by a factor of 10,000 to reduce the effects of computer rounding errors):

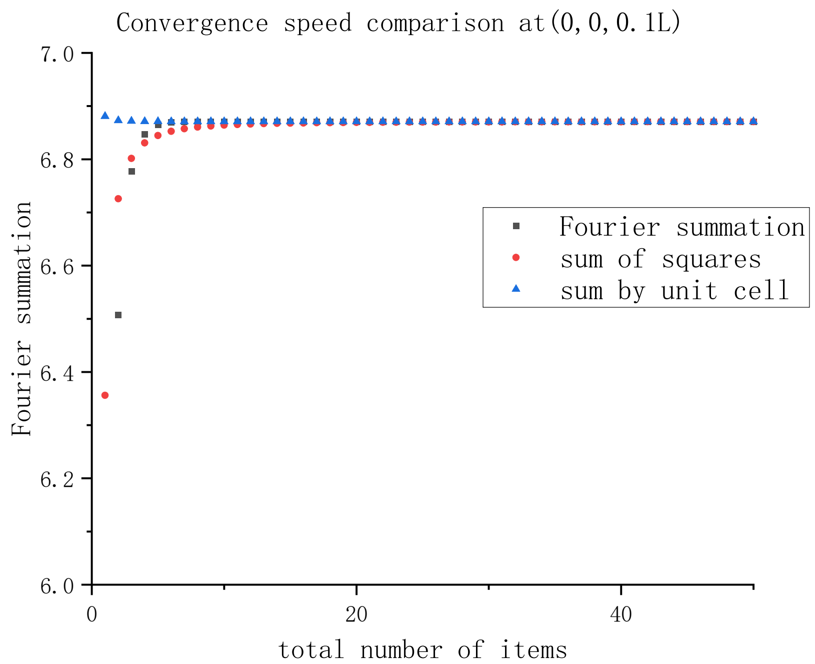




It can be found that the results given by the two summation methods are very similar, and the error does not exceed 1%, and it matches the result of the Fourier summation.

To illustrate this more clearly, we took two specific field points and compared the convergence speed of the above three summation methods:





It is not difficult to find that when z is large, the Fourier series summation converges very quickly, but when z<<L, the real space summation converges faster. This is because the ratio of the adjacent two terms of the former is a power function of z, while the latter is the relationship of the square root.

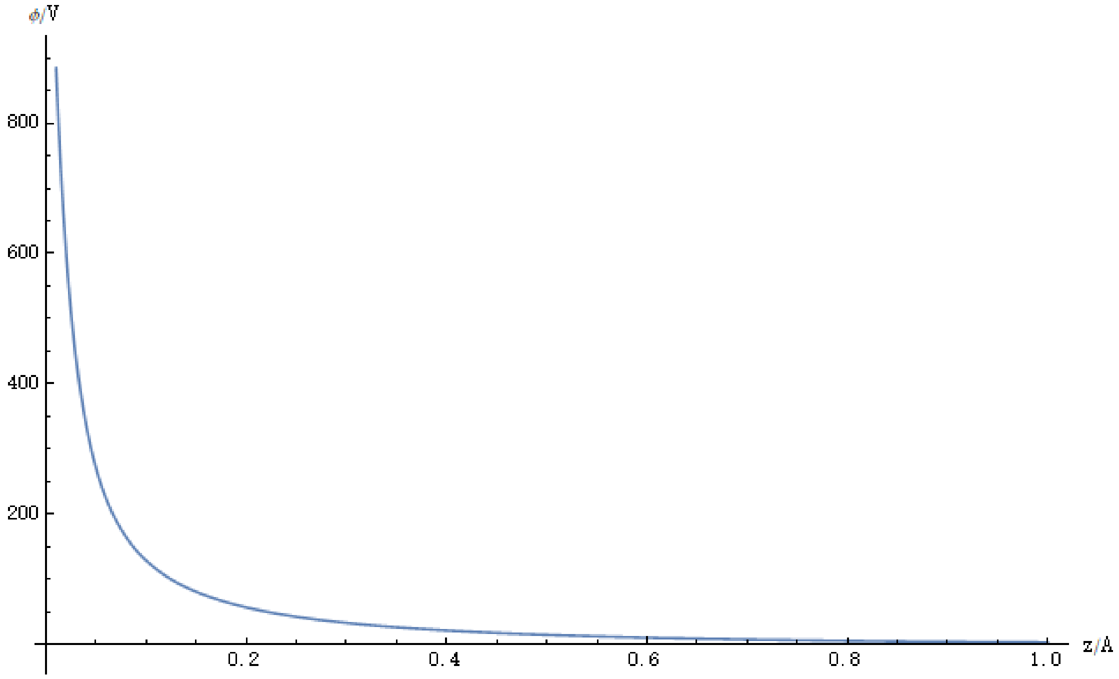
Another significant advantage of Fourier summation over real space summation is that there are no edge effects, and the summation is always a periodic function of the x, y plane. With real space summation, if you consider very large x, y, more terms are needed to sum to approximate the exact value. However, since the real distribution of the electric potential in the x, y plane is periodic, we only need to solve the electric potential in the unit cell near the origin, so the real space summation is still a good method when z<<L.

Numerical Results

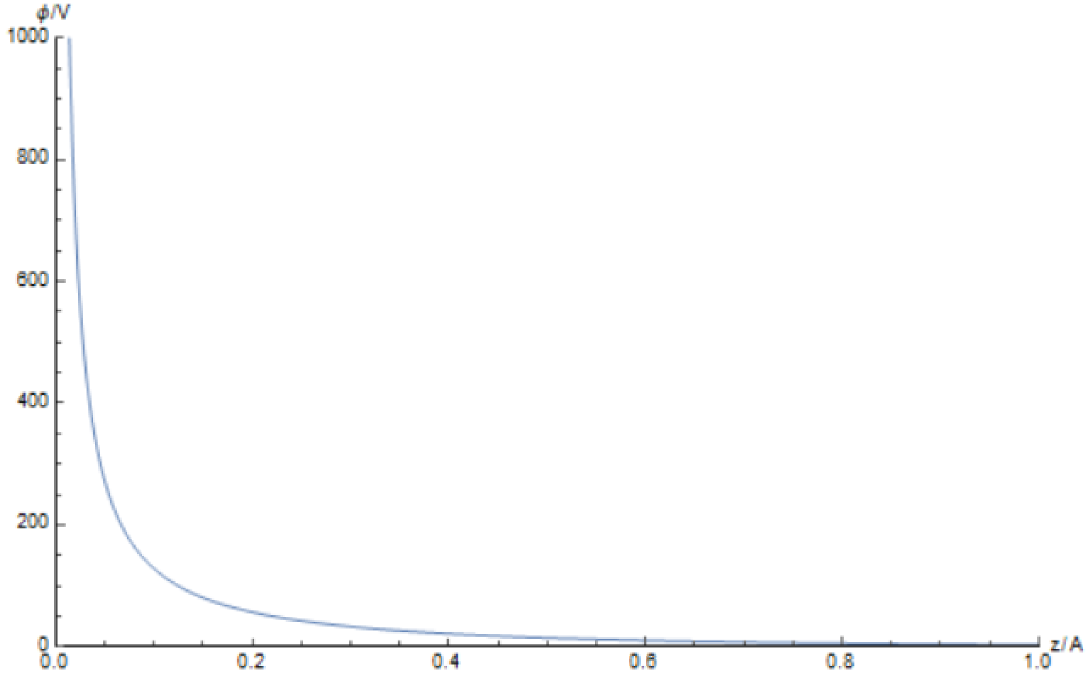
We set L=0.3A, and q is the electron charge.

1. We take the point (x,y)=(0,0) and calculate the potential distribution in the z direction, because (x,y) only affects the magnitude of the cosine factor behind it and not the z-direction distribution（if z/L is not too small）, it makes sense.

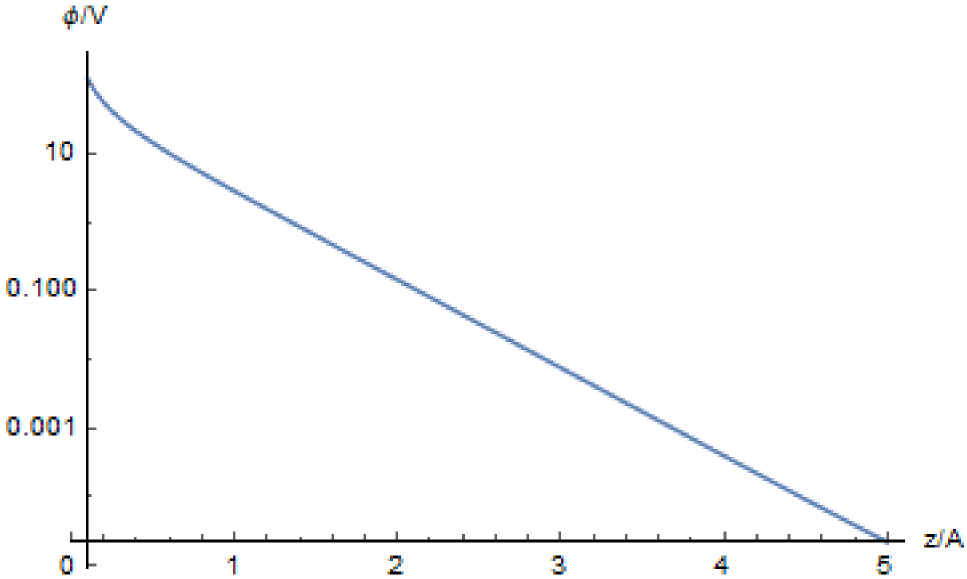
For $z = (0.01,1)A$, we plot the potential (φ)



As a comparison, verify it with real space summation:

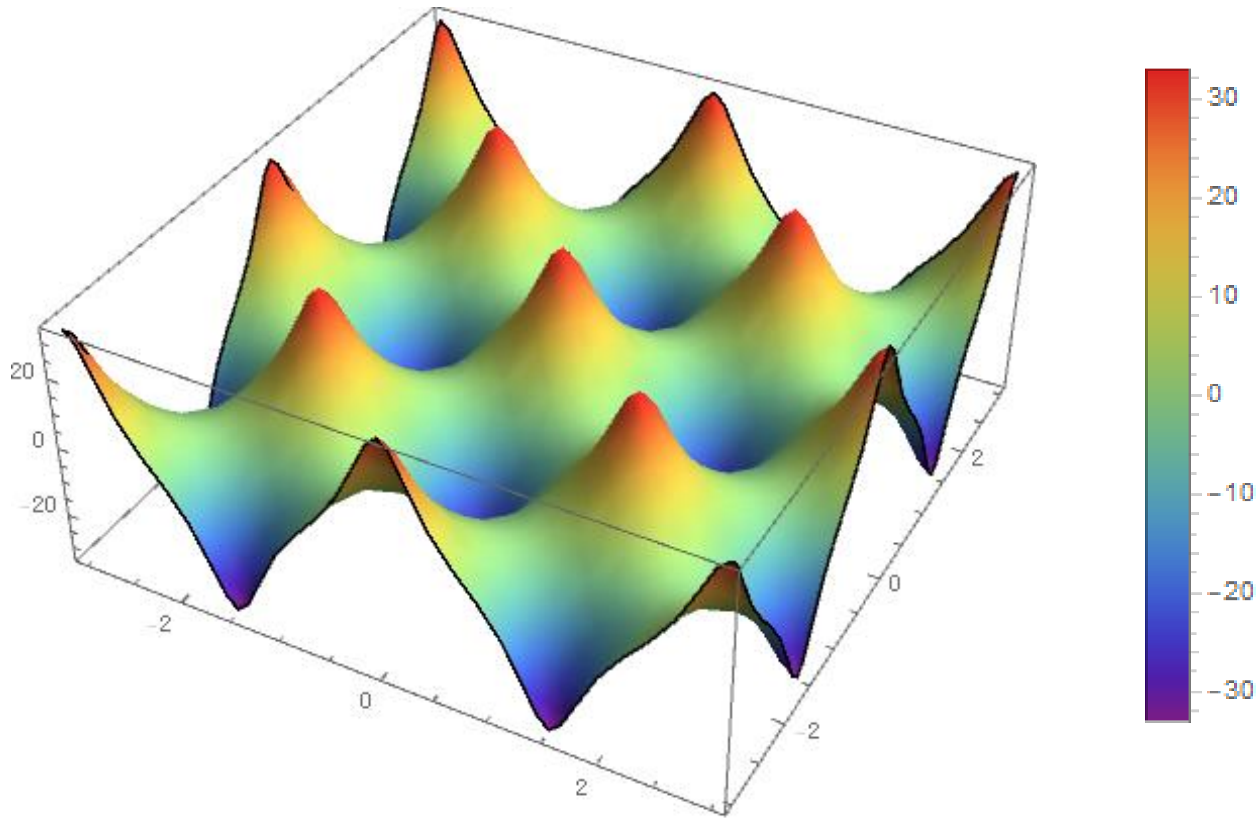


For $z = (0.1A, 5A)$, we plot the potential (φ) and the logplot as below:

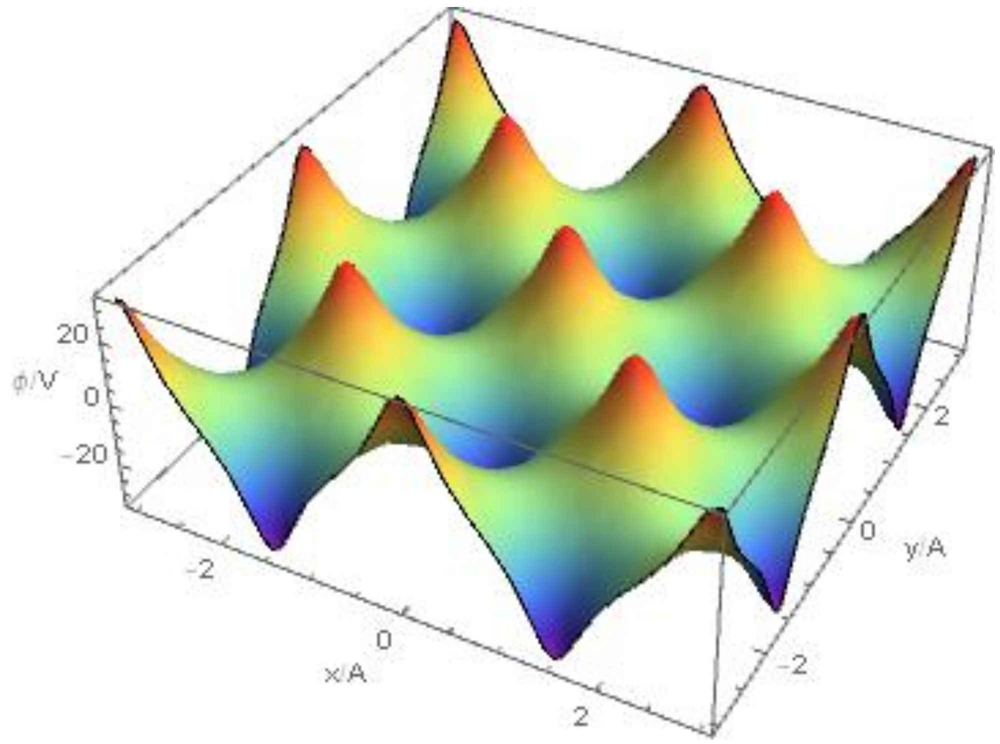


We find that when z is large(z>0.1L), the graph is a straight line, which indicates that the electric potential decays exponentially. From the form of the Fourier summation above, we can also see that when z is relatively large, only the term (l,m)=(1,1),(1,-1),(-1,1),(-1,-1) plays a major role, and $\varphi(\vec{r}) \approx \frac{e}{4\pi\varepsilon_0 L} \cdot 8\sqrt{2} \cdot e^{-\frac{2\sqrt{2}\pi z}{L}} cos(\frac{2\pi x}{L}) cos(\frac{2\pi y}{L})$

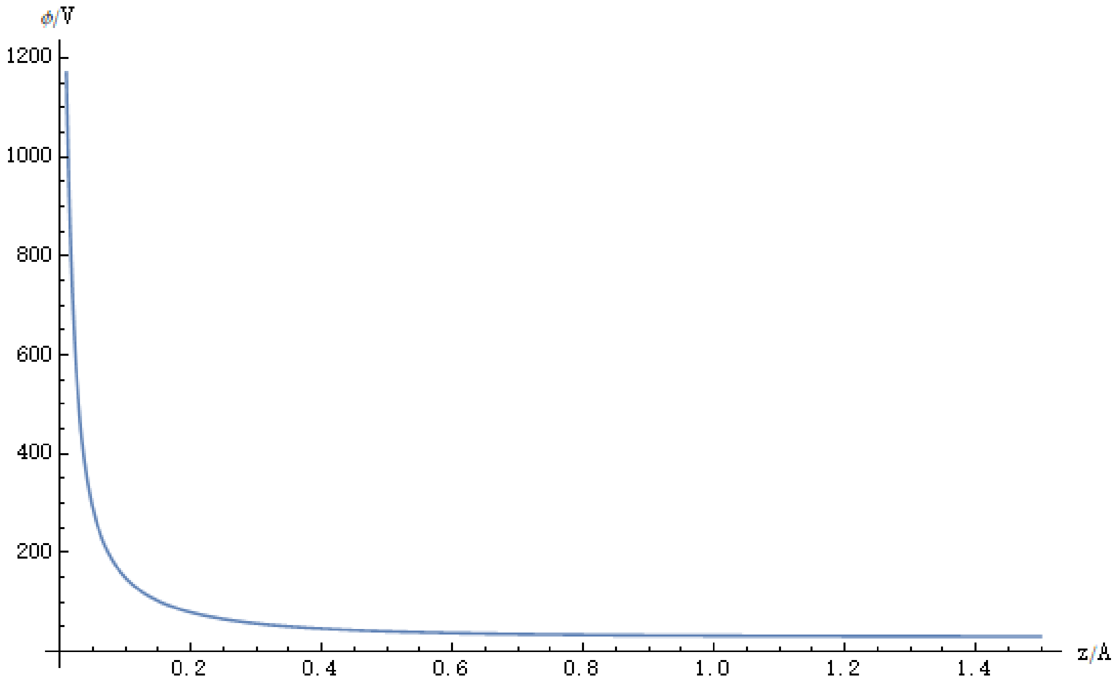
If we set z=0.1L=0.3A, and we plot the distribution of potential in the z=0.1L plane by Fourier summation:



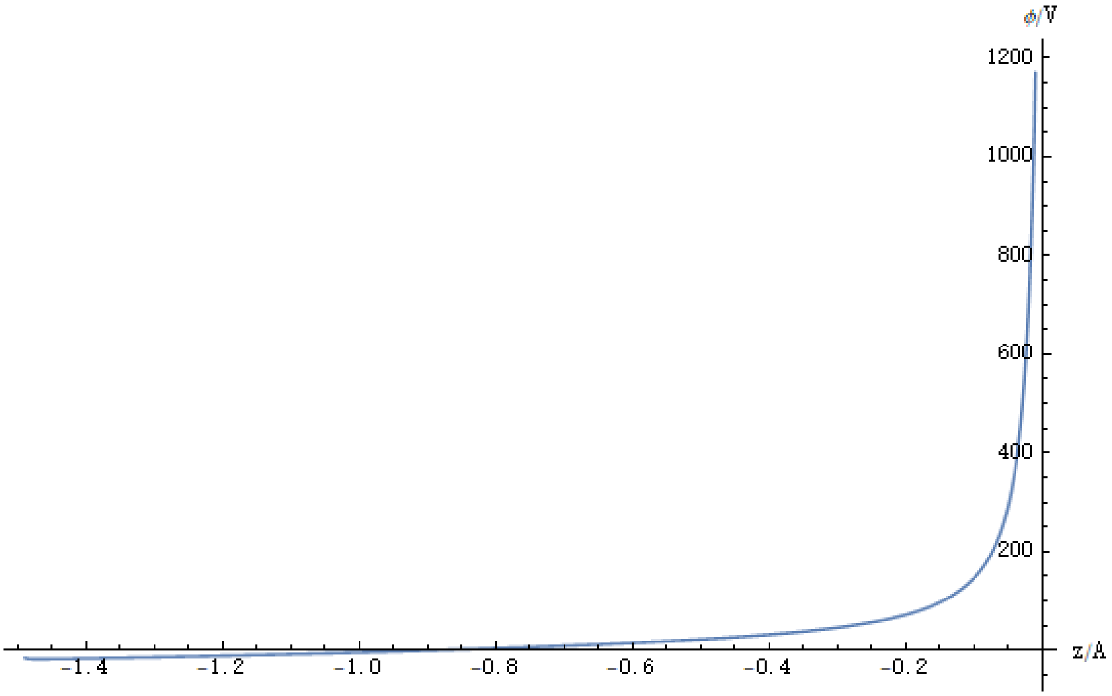
verify it with real space summation:

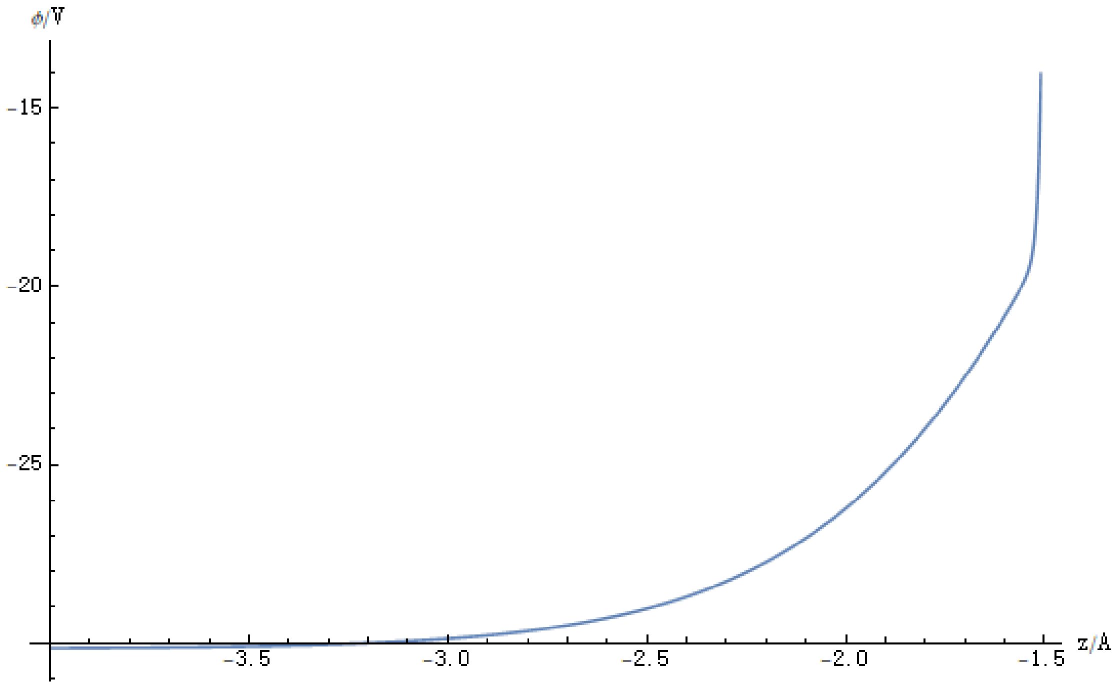


2. We set d=1.5A, L=3A, (x,y)=(0,0), and z/A ranges from 0.01 to 1.5,-1.49 to -0.01,-4 to -1.51, also we plot the potential (φ).



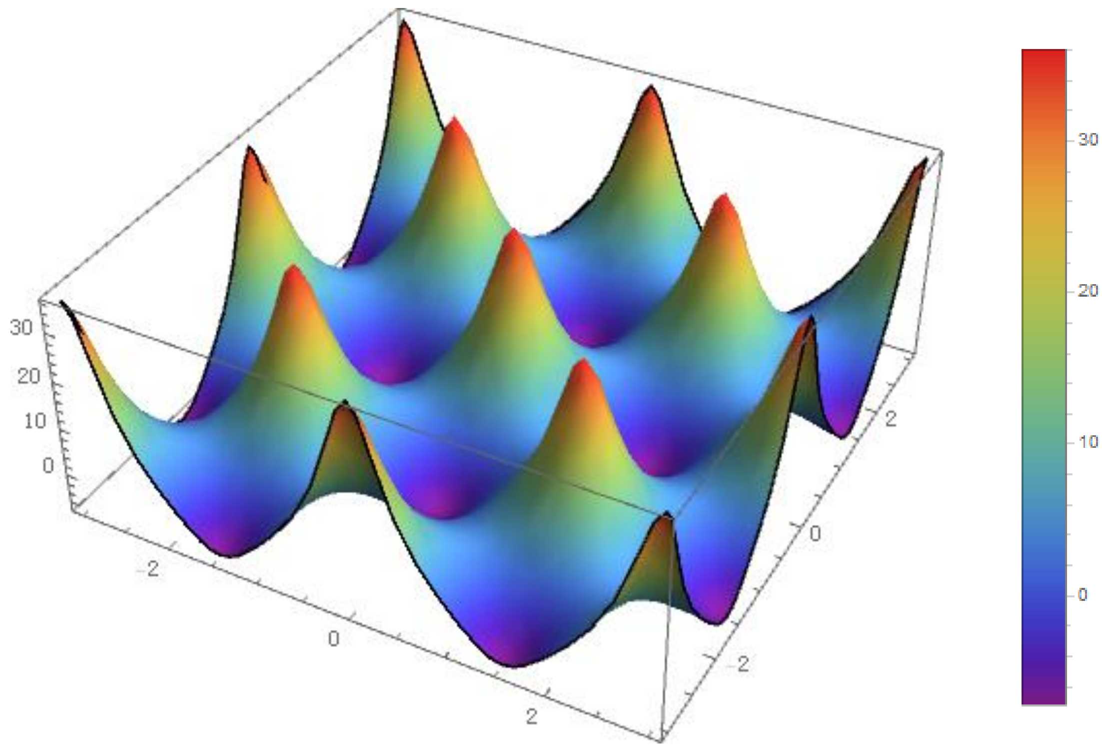
We can see that in this figure, for about z>0.6A, the potential tends to a constant value (30.2V).



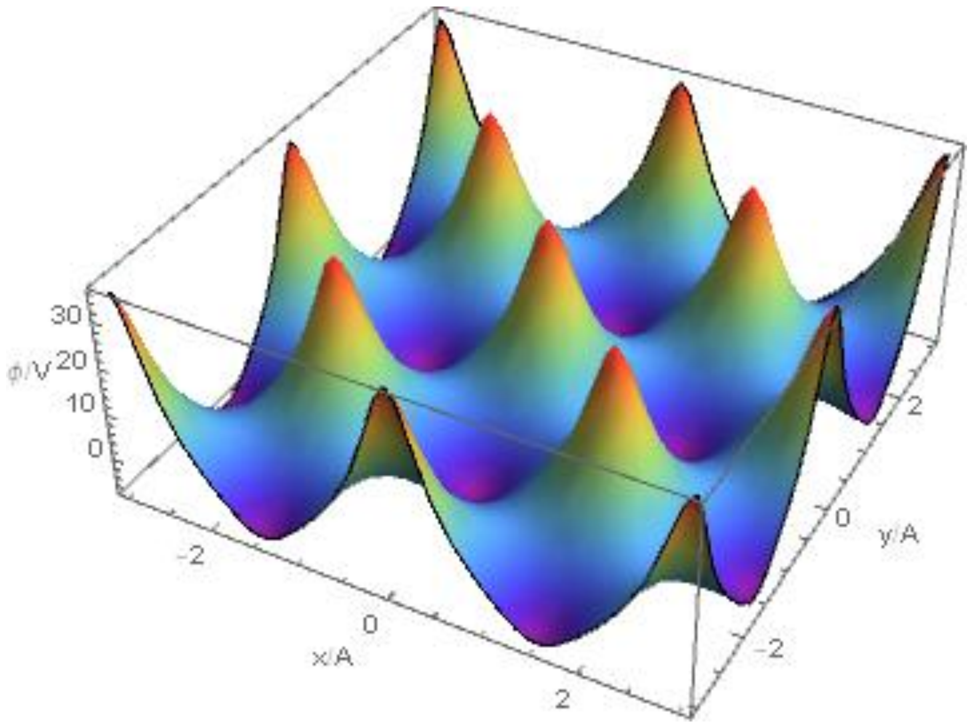


We could find the same thing as the situation when z>0.6A does when z<-3.5A, the potential tends to be a constant value (-30.2V) when z<-3.5A.

We set d=z=0.1L=0.3A, and we plot the distribution of the potential.

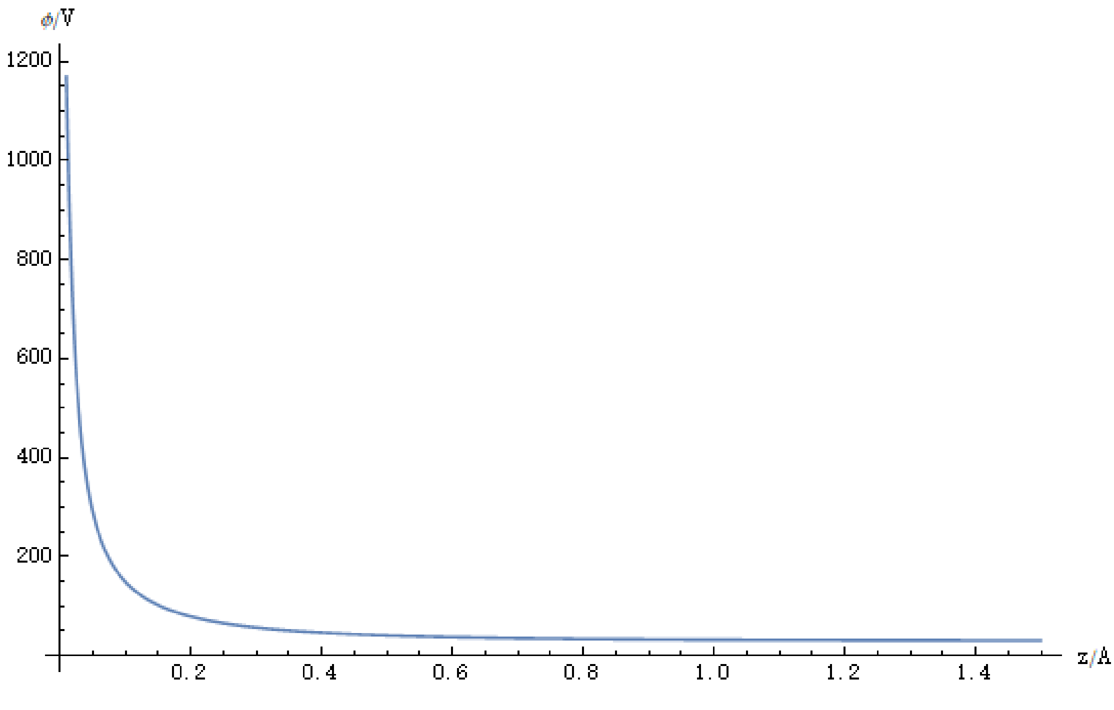


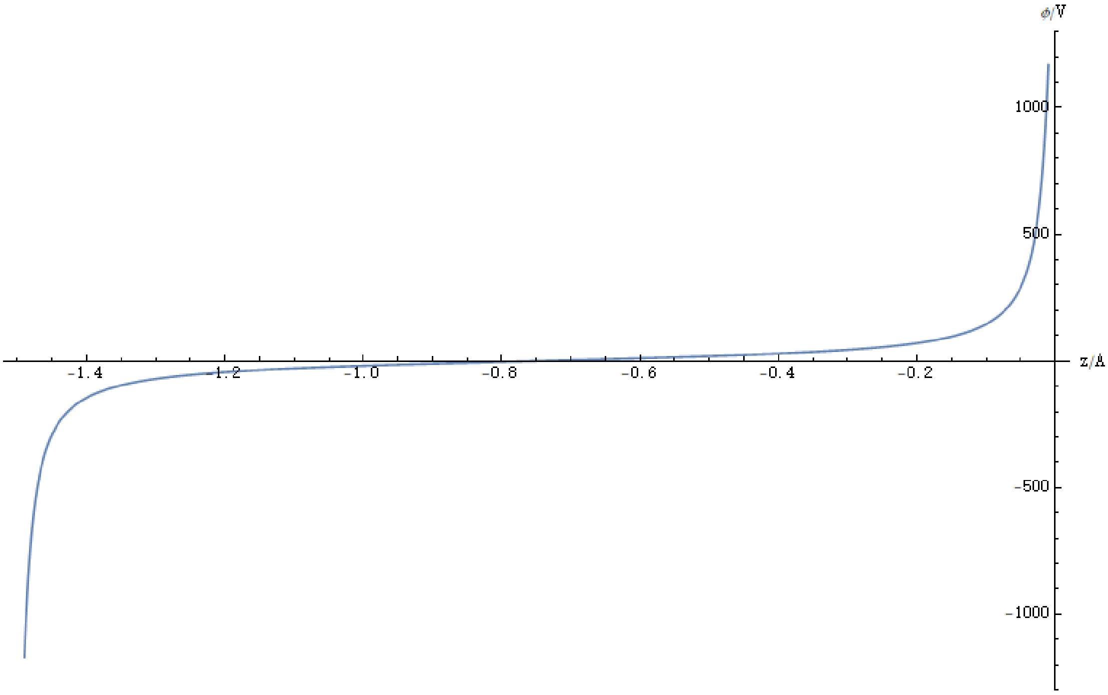
As a comparison, verify it with real space summation:



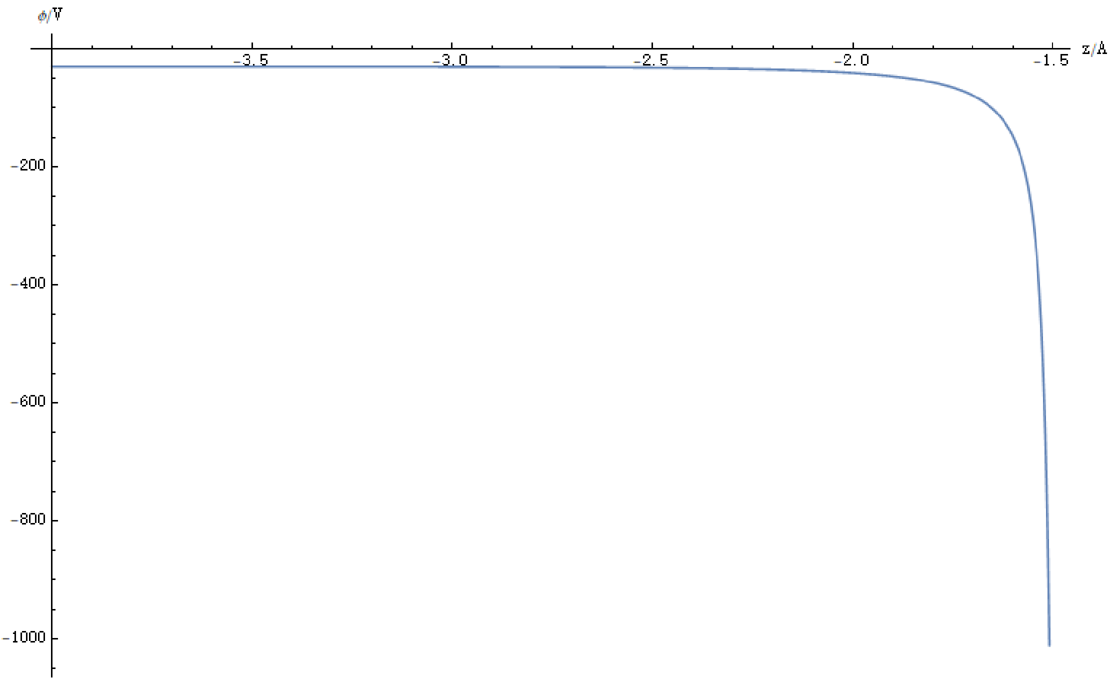
3. In situation **3**, all parameters are the same as in situation **2**, except that the plane of negative charge is moved to align with the plane of positive charge. The results are as follows:

We set d=0.5L=1.5A, (x,y)=(0,0), and z/A ranges from 0.01 to 1,-1.49 to -0.01,-3 to -1.51, also we plot the potential (φ).



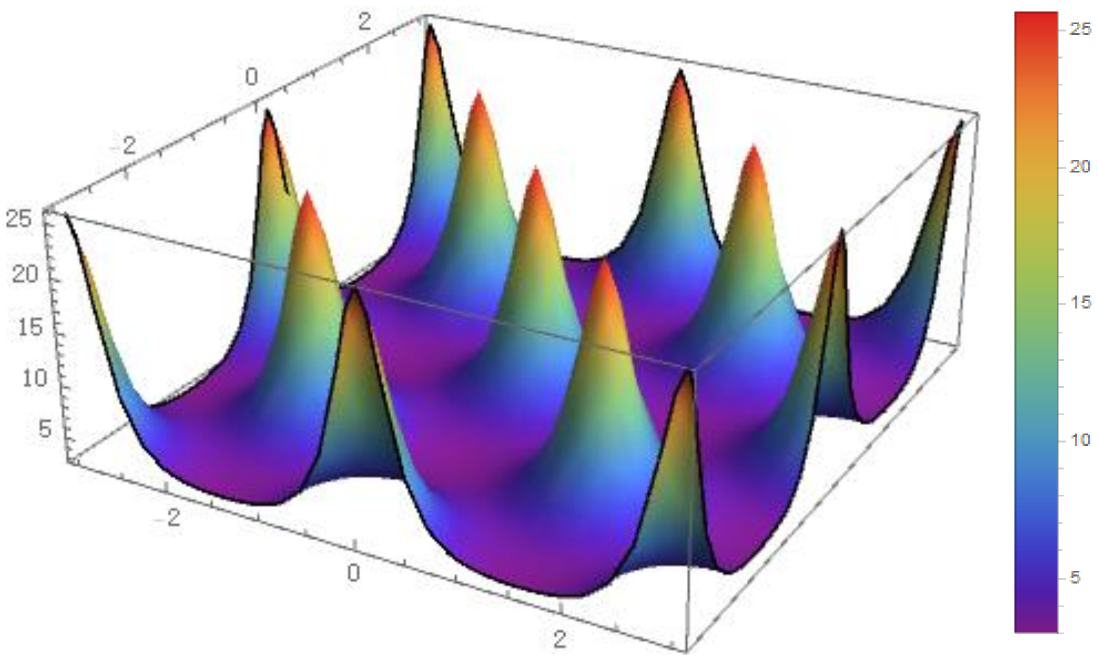


In this range, the graph is symmetric about z=0.5L because the positive and negative charges are planar symmetric.

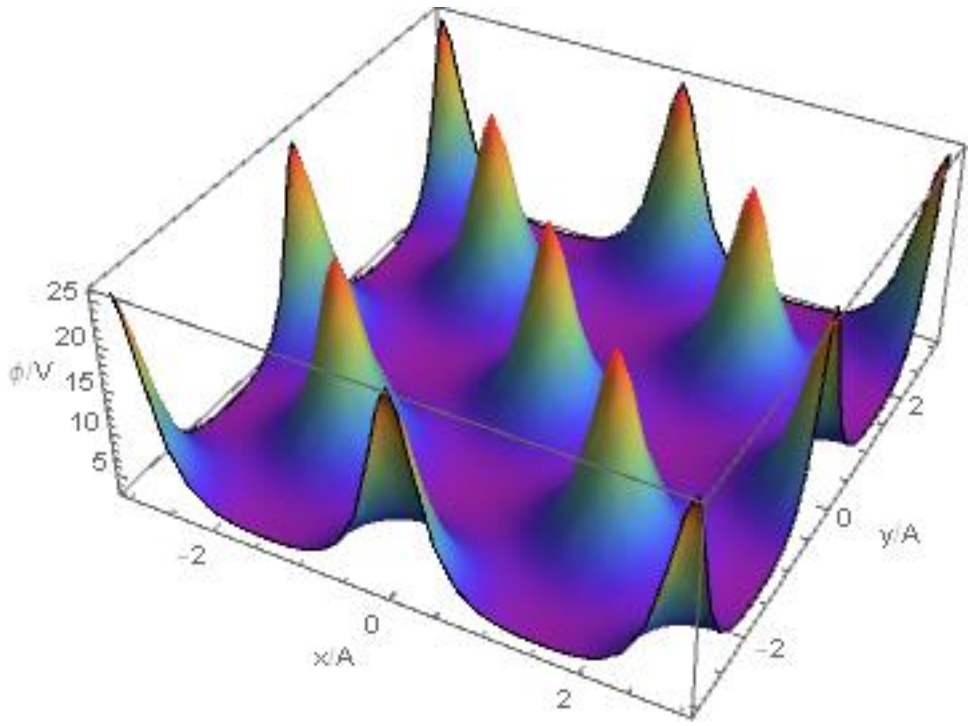


Situation 3 is almost the same as Situation 2 when z>0, and because of the symmetry of positive and negative charges, the potential distribution is odd-function symmetric with z=-0.5L as the origin.

We set d=z=0.1L=0.3A, and we plot the distribution of the potential.



As a comparison, verify it with real space summation:



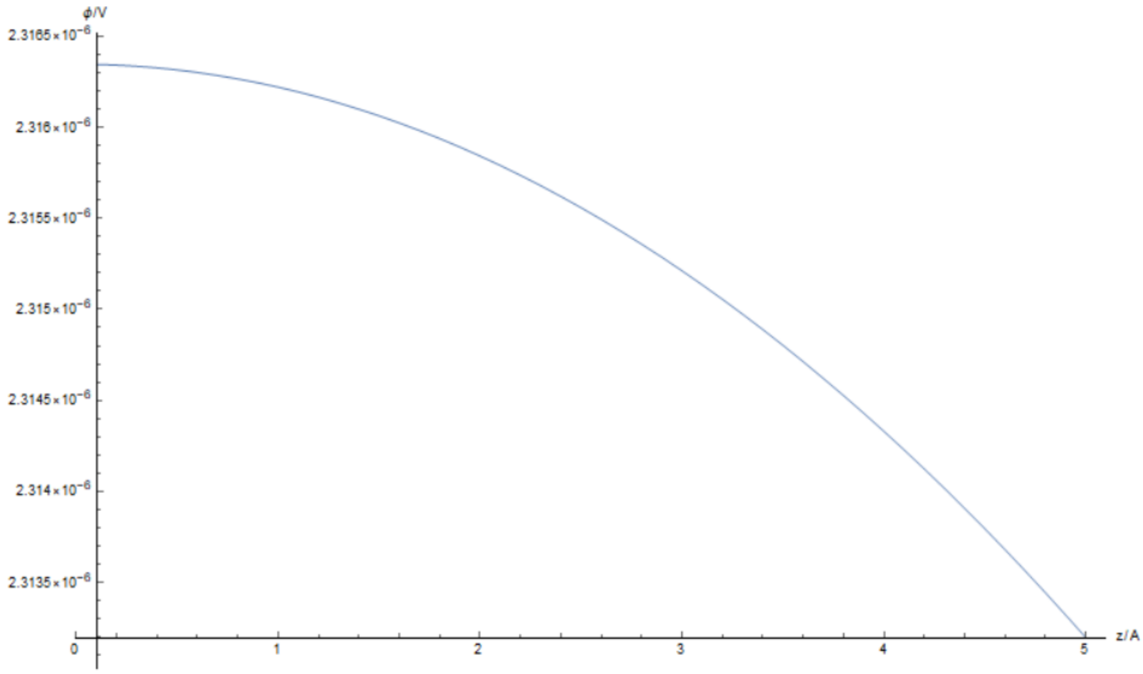
4. Average Potential

From the Fourier summation formula, it can be found that the average potential on any z-plane depends only on the l=0, m=0 term, which is a piecewise function. First, we use real space summation to verify this interesting conclusion.

$$\bar{\varphi}(z)=\frac{q}{4\pi\varepsilon_0 L^3}\int_0^L\int_0^L dxdy\sum_{m=-s}^{s}\sum_{n=-s}^{s}\left(\frac{1}{\sqrt{\left(m-\frac{x}{L}\right)^2+\left(n-\frac{y}{L}\right)^2+\left(\frac{z}{L}\right)^2}}+\frac{1}{\sqrt{\left(m+0.5-\frac{x}{L}\right)^2+\left(n+0.5-\frac{y}{L}\right)^2+\left(\frac{z}{L}\right)^2}}-\frac{1}{\sqrt{\left(m+0.5-\frac{x}{L}\right)^2+\left(n-\frac{y}{L}\right)^2+\left(\frac{z+d}{L}\right)^2}}-\frac{1}{\sqrt{\left(m-\frac{x}{L}\right)^2+\left(n+0.5-\frac{y}{L}\right)^2+\left(\frac{z+d}{L}\right)^2}}\right)$$

We set L=3A, $\frac{q}{4\pi\varepsilon_0 L^3}\approx 0.5333201797\ V\cdot A^{-2}$. For simplicity, we ignore this coefficient in the following calculations.

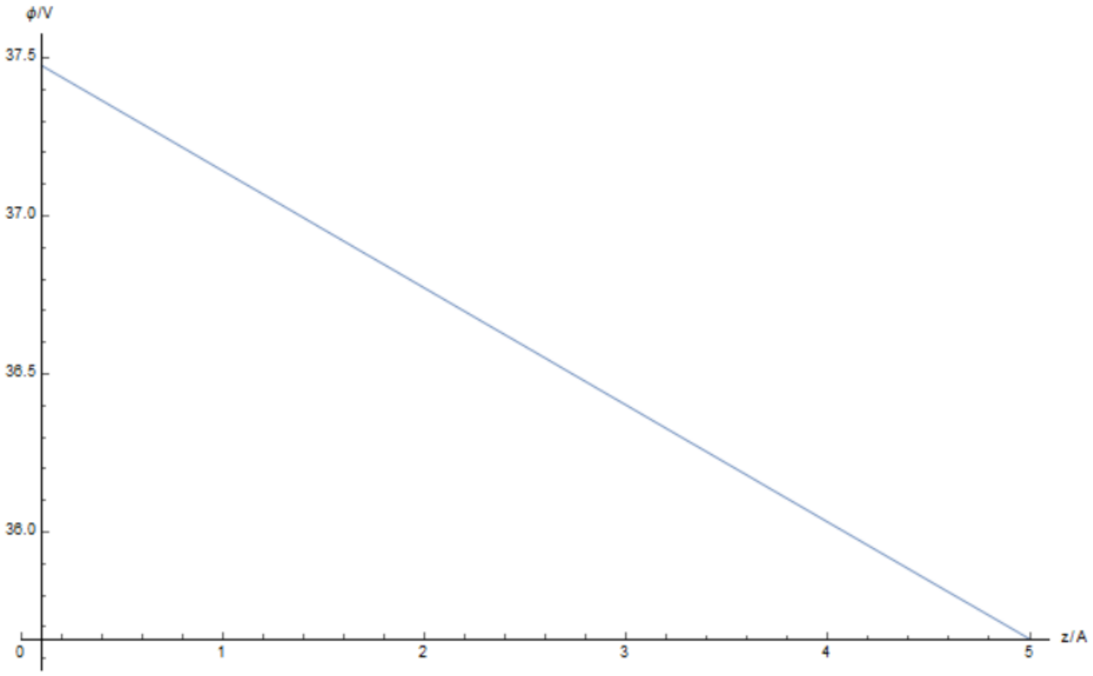
If d=0, integrate the real space summation formula to find the average potential of z from 0.1A to 5A:



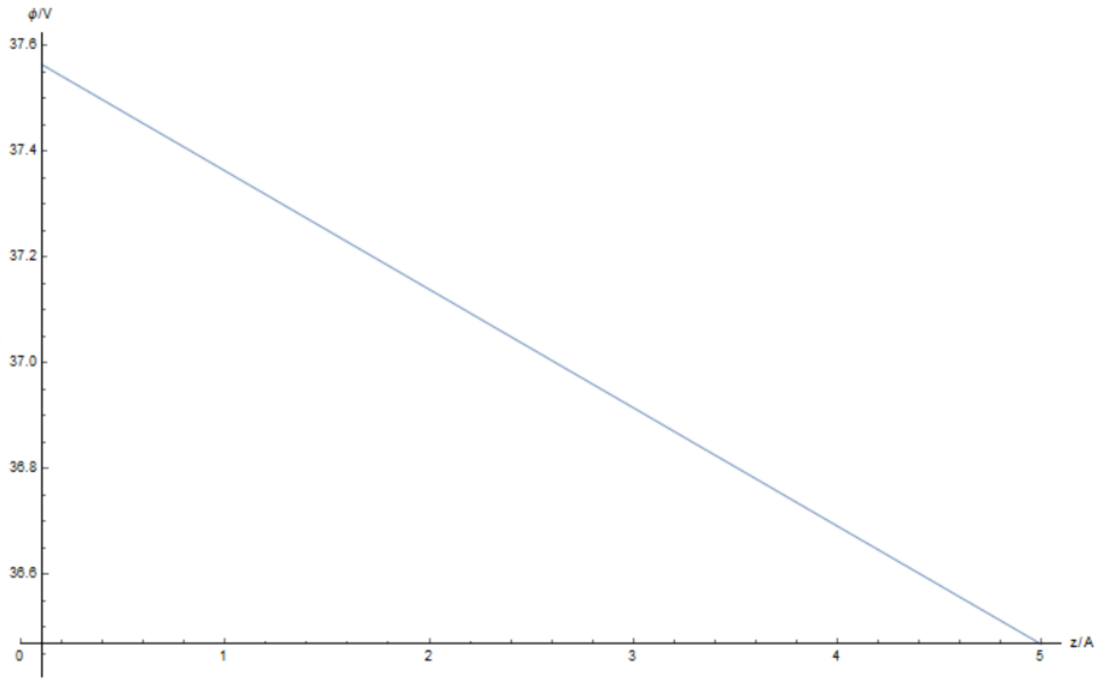
Due to the high symmetry when d=0, the average potential of any z-plane is 0, so this result is in line with expectations.

If we set L=3A, d=1A, integrate the real space summation formula to find the average potential of z from 0.1A to 5A:

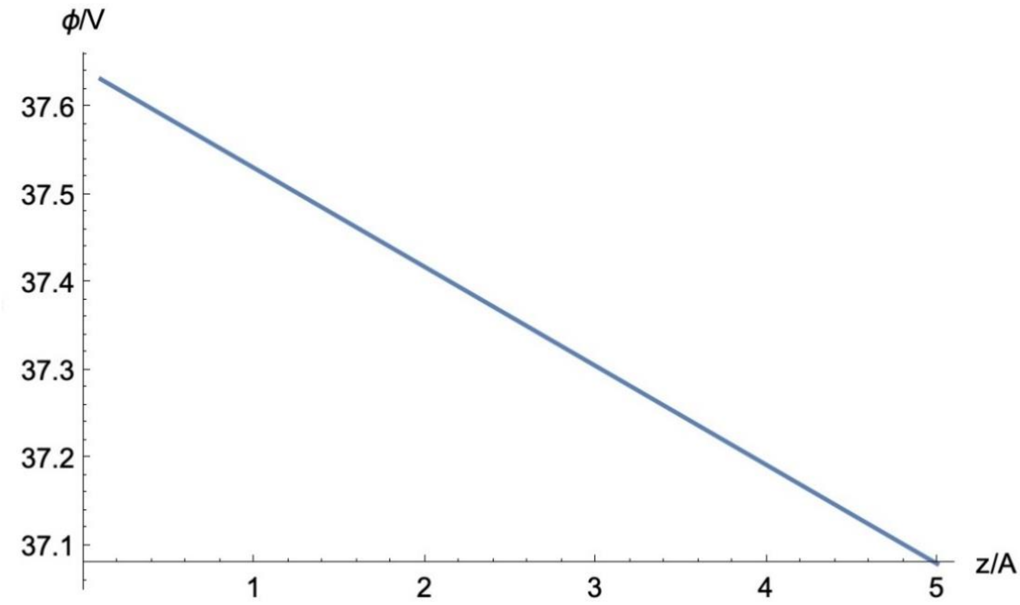
① $s=30,\ which\ means\ m,n\in[-30,30]$



② $s = 50,\ which\ means\ m, n \in [-50,50]$

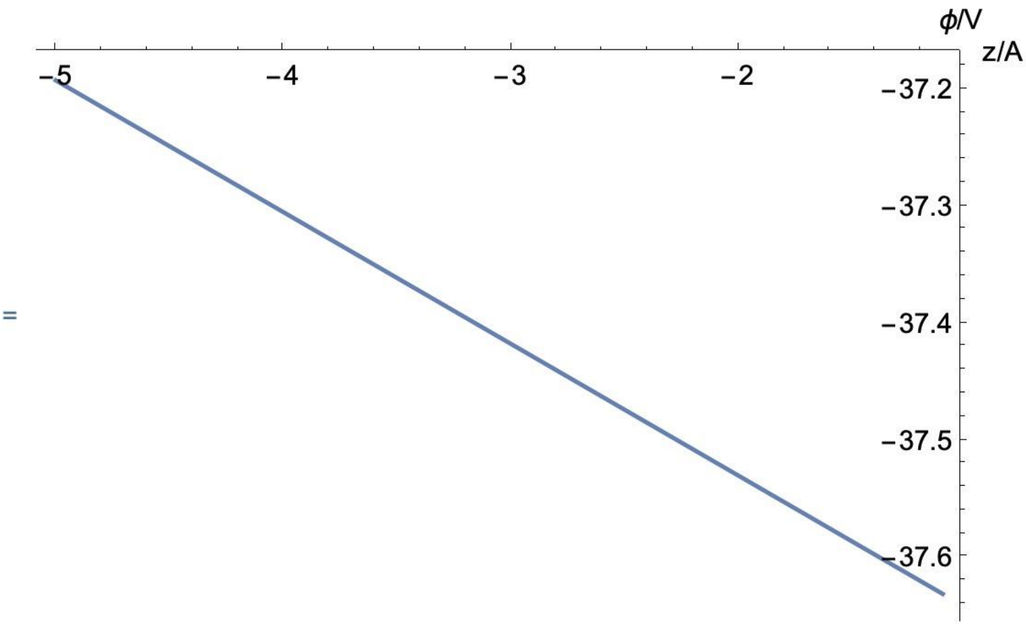


③ $s = 100,\ which\ means\ m, n \in [-100,100]$



We can find that as s increases, while the decrease is decreasing. This is because the real space summation is slow to converge when z is large, and the larger s, the smaller the error. So we can reasonably infer that when s is large enough, the average potential of z > 0 is a constant (but currently beyond our computing power), about $0.5333201797 \times 37.6V \approx 20.0V$, almost the same as the result using Fourier transform.

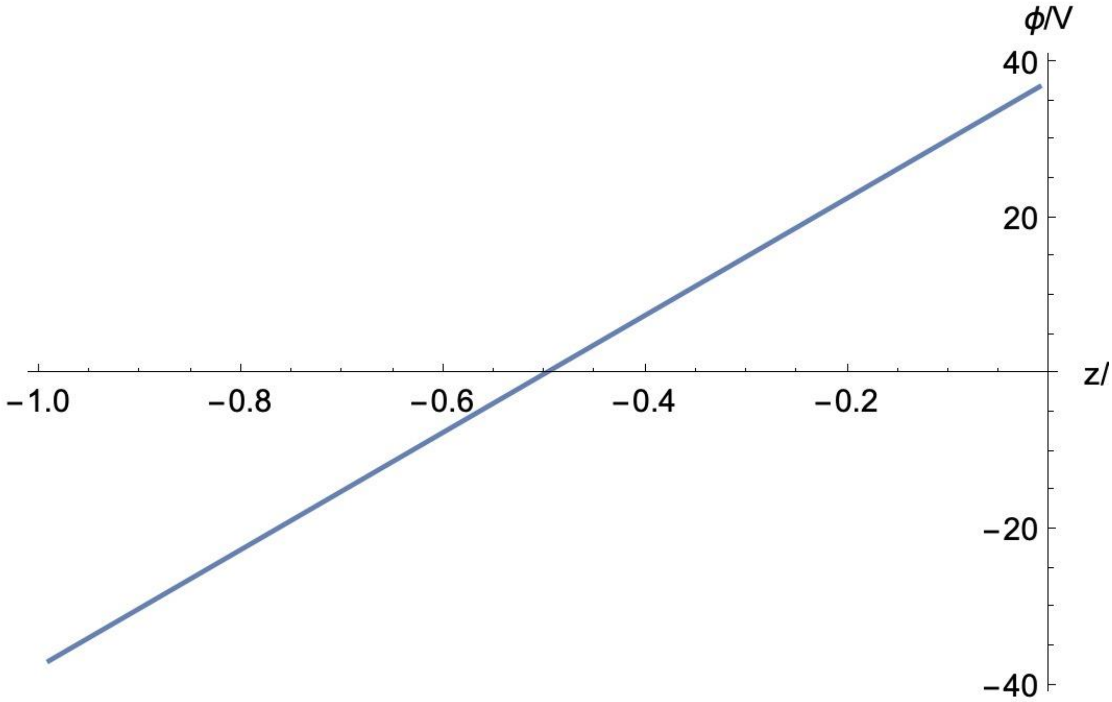
Now we set L=3A, d=1A, s=100, integrate the real space summation formula to find the average potential of z from -5A to -1.1A:



we can reasonably infer that when s is large enough, the average potential of z < -d is a constant (but currently beyond our computing power), about

$0.5333201797 \times -37.6V \approx -20.0V$

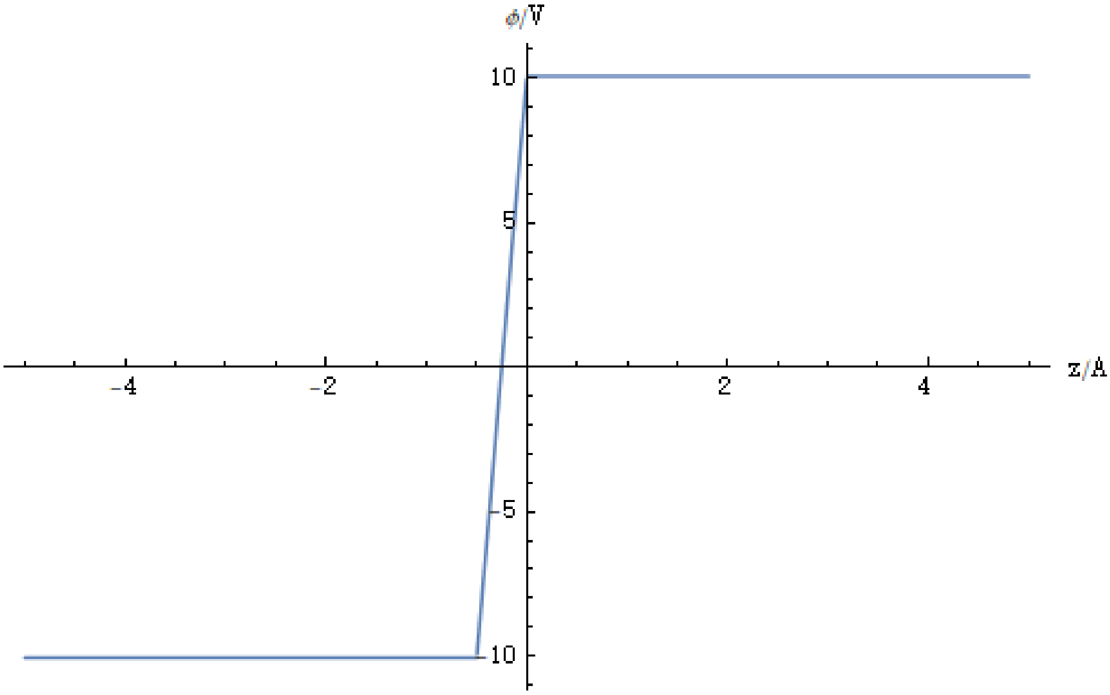
-0.99A to -0.01A:



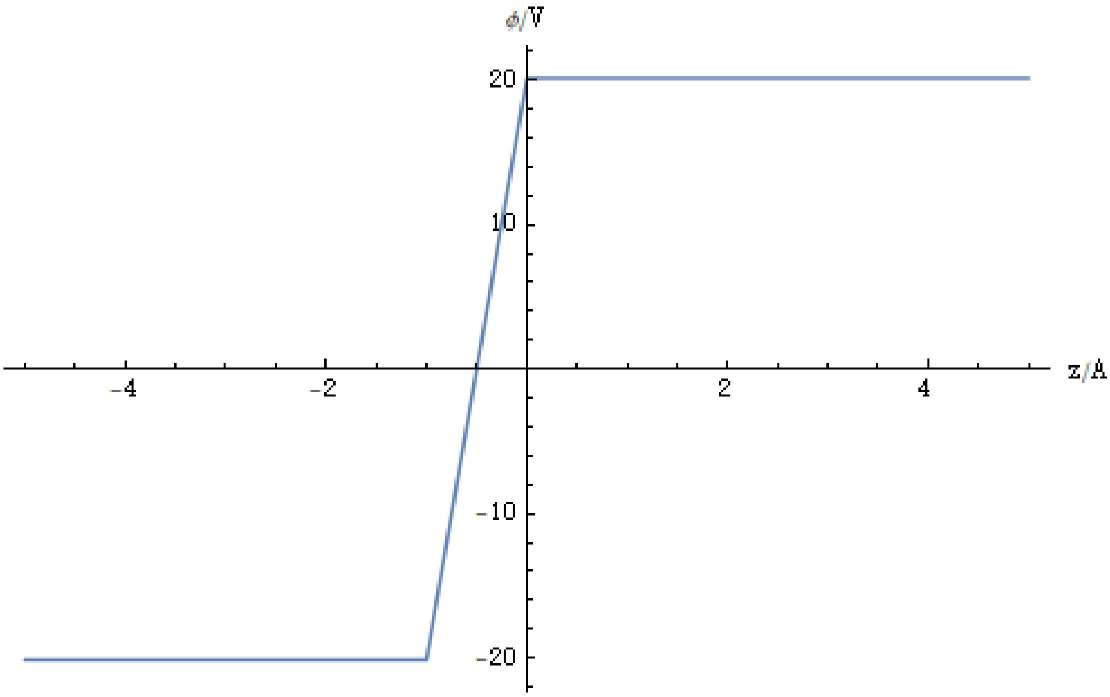
Between the positive and negative charge layers, the result of the real-space summation converges faster, resulting in a linear change in potential, which is also in line with our previous expectations.

So far, we have verified the interesting conclusion that the average potential is a piecewise function, and now show the whole image for d=0.5A,1.0A and 1.5A:

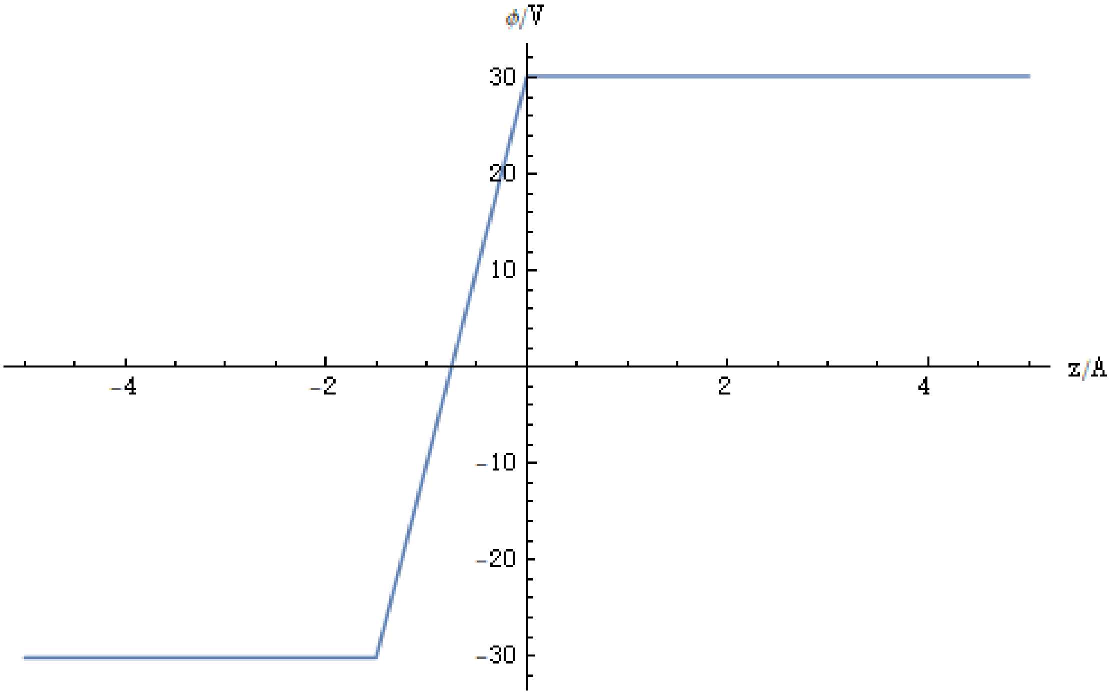
① d=0.5A



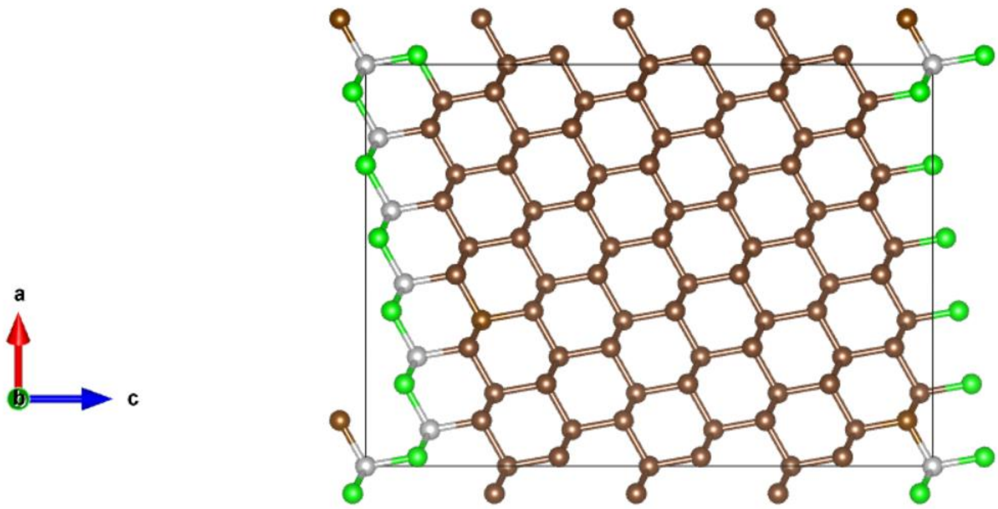
②d=1.0A



③d=1.5A



Offset



Schematic diagram of the (3,3,2) crystal plane along the b-axis

Assuming a B atom and a N atom connected to form a pair, their average potential on the

crystal plane is easy to calculate, similar to a pair of plate capacitors.
Our formula for calculating the average potential drop is:

$$\Delta V_{average} = n\frac{\sigma e}{\varepsilon_0}d$$

In order to determine the total average potential of a certain crystal plane (h, k, l), we need to determine the following three parameters:

(1) n:How many pairs of "capacitors" are in this layer of atoms

There are four different atoms in a face-centered cube. C1(p,q,m), C2(p,q+0.5,m+0.5), C3(p+0.5,q,m+0.5), C4(p+0.5,q+0.5,m). p, q, m are all natural numbers.

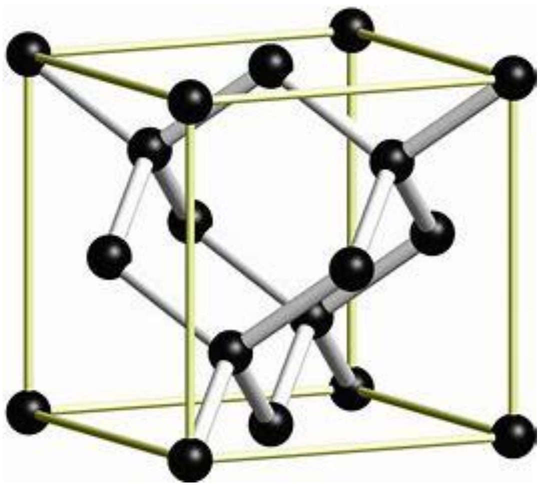
Since we always make the [h, k, l] direction (that is, the c-axis direction) periodic when taking the atomic layer, and the total length of this period is $\frac{(h+k)a}{2\sqrt{h^2+k^2+l^2}}$ (we suppose h,k,l is sorted from largest to smallest), so we can get:

$$n = \frac{(h+k)a}{2d_{hkl}\sqrt{h^2+k^2+l^2}}$$

where d_{hkl} is the spacing of N atoms in adjacent layers in the [h,k,l] direction, i.e. the spacing of the (h,k,l) planes of a face-centered cubic(fcc) lattice:

$$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}} \qquad \text{when h, k, l are all odd numbers;}$$

$$d_{hkl} = \frac{a}{2\sqrt{h^2+k^2+l^2}} \quad \text{other situation}$$



(2)σe: Surface charge density per "plate capacitor"

σ is the atomic density of the fcc lattice in the (h, k, l) plane. Let the average area occupied by each atom on the (h, k, l) crystal plane be A, then we can get:

$$\sigma=\frac{1}{A}=\frac{d_{hkl}}{Ad_{hkl}}=\frac{d_{hkl}}{V_{cell}}$$

V_{cell} is the average volume occupied by each atom, independent of the crystal plane, and for the fcc lattice:

$$V_{cell}=\frac{a^3}{4}$$

(3) d:Plate spacing for each "plate capacitor"

Each N atom will be connected to 4 B atoms to form a regular tetrahedron. The relative positions of these 4 B atoms relative to the N atom are(Under the primitive cell-based vector): (0.25a,0.25a,0.25a); (0.25a,-0.25a,-0.25a); (-0.25a,0.25a,-0.25a); (-0.25a,-0.25a,0.25a)

Since the equation for the (h,k,l) crystal plane can be written as:$hx+ky+lz=0$

Therefore, the distances of the 4 B atoms from the (h,k,l) crystal plane are respectively:

$$\frac{|h+k+l|a}{4\sqrt{h^2+k^2+l^2}};\quad \frac{|-h+k+l|a}{4\sqrt{h^2+k^2+l^2}};\quad \frac{|h-k+l|a}{4\sqrt{h^2+k^2+l^2}};\quad \frac{|h+k-l|a}{4\sqrt{h^2+k^2+l^2}};$$

For the distance d, we should consider the smallest distance between B and N atoms of the whole space.

If we consider the closest fcc, we could get:

$$c_{min}=\frac{a}{4\sqrt{h^2+k^2+l^2}}\cdot\min\{|h+k-l|,|h-k-l|,|h-k+l|\}$$

If we consider the first B fcc and the second N fcc, then:

$$c_{min}=\frac{a}{4\sqrt{h^2+k^2+l^2}}\cdot\min\{|-h\pm 3k+l|,|h-k\pm 3l|,|\pm 3h+k-l|\}$$

$$\cdots$$

If we consider the first B fcc and the Number p N fcc:

$$c_{min}=\frac{a}{4\sqrt{h^2+k^2+l^2}}\cdot\min\{|-h\pm(2p-1)k+l|,|h-k\pm(2p-1)l|,|\pm(2p-1)h+k-l|\}$$

So, from what we discussed above, we could get:

$$c_{min}=\frac{a}{4\sqrt{h^2+k^2+l^2}}\cdot\min\{|-h\pm(2p-1)k+l|,|h-k\pm(2p-1)l|,|\pm(2p-1)h+k-l|\}$$

And p could be all positive integers. (1,2,3,4,⋯)

In order not to make each "capacitor" overlap, we might as well take:

$$d=c_{\min}$$

Substitute the above parameters into our formula for calculating the average potential drop:

$$\Delta V_{average} = n\frac{\sigma e}{\varepsilon_0}d$$

$$= n\frac{d_{hkl}e}{V_{cell}\varepsilon_0}c_{\min}$$

$$= \frac{(h+k)a}{2d_{hkl}\sqrt{h^2+k^2+l^2}} \cdot \frac{d_{hkl}e}{\frac{a^3}{4}\varepsilon_0}c_{\min}$$

It can be seen from the formula that when $d = c_{\min} = 0$, the total average potential is 0, (if we consider that h,k,l are all positive numbles, that is, the sum of two of h,k,l is equal to the other)

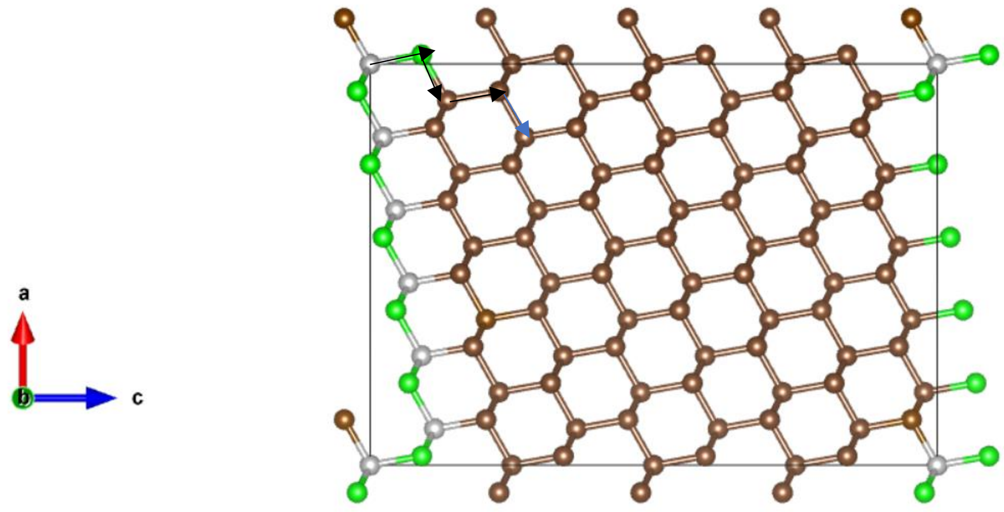
We get the final formula:

$$\Delta V_{average} = \frac{2(h+k)ec_{\min}}{a^2\varepsilon_0\sqrt{h^2+k^2+l^2}}$$

Where

$$c_{min} = \frac{a}{4\sqrt{h^2+k^2+l^2}} \cdot \min\{|-h \pm (2p-1)k + l|, |h - k \pm (2p-1)l|, |\pm(2p-1)h + k - l|\}$$

And p could be all positive integers. (1,2,3,4,⋯)



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