Electrostatic energy of a crystal

\[
\frac{k e^2}{a} = 1
\]

\[
U = 4 \left( -\frac{1}{4} \right) = -4
\]

\[
= 4 \left( -1 + \frac{1}{\sqrt{2}} + \frac{1}{2} \right) = 0.83...
\]

\[
= 4 \left( -1 + \left( \frac{1}{\sqrt{2}} + \frac{1}{2} \right) - \left( \frac{1}{3} + \frac{2}{\sqrt{5}} \right) \right) = -4.08...
\]

\[
= 4 \left( \ldots + \left( \frac{1}{4} + \frac{2}{\sqrt{10}} + \frac{1}{2\sqrt{2}} \right) \right) = 0.86...
\]

So we see that adding shells of positive and negative charge does not seem to converge.

Now let's consider a molecule of four ions.

\[
U = -\frac{4}{1} + \frac{2}{\sqrt{2}} = -2.59...
\]
Now just considering the interactions between two molecules. I’ve only drawn the unique pair to consider. The rest can be accounted for by symmetry.

\[
U_{20} = 4 \left( \frac{1}{2} \right) + 2 \left( \frac{1}{\sqrt{2}} \right) + 2 \left( \frac{1}{\sqrt{10}} \right) - 4 \left( \frac{1}{\sqrt{5}} \right) - 2 \left( \frac{1}{1} \right) - 2 \left( \frac{1}{3} \right) = -0.409\ldots
\]

Now for the diagonal case.

\[
U_{22} = 4 \left( \frac{1}{2\sqrt{2}} \right) + \left( \frac{1}{\sqrt{2}} \right) + \left( \frac{1}{3\sqrt{2}} \right) + 2 \left( \frac{1}{\sqrt{10}} \right) - 4 \left( \frac{1}{\sqrt{5}} \right) - 4 \left( \frac{1}{\sqrt{13}} \right)
\]

\[
= 0.091\ldots
\]

Now for the partial sums...

\[
U_{oo} = -2.59\ldots
\]

\[
U_{oo} + \frac{4}{2} U_{20} = -3.40\ldots
\]

\[
U_{oo} + \frac{4}{2} U_{20} + \frac{4}{2} U_{22} = -3.22\ldots
\]

So this does seem to be converging.

\[
U \text{ per ion} = -0.805\ldots
\]
Lastly we consider the energy in one mole of NaCl.

\[ a = 2.8 \times 10^{-10} \text{ m} \]

\[ U = \frac{ke^2}{a} = \frac{9 \times 10^9 \text{ J} \cdot \text{m}}{C^2} \left( \frac{1.6 \times 10^{-19} \text{ C}}{2.8 \times 10^{-10} \text{ m}} \right)^2 = 8.23 \times 10^{-9} \text{ J} \]

\[ 2 \times N_a \times -0.874 \times 8.23 \times 10^{-19} \text{ J} = -8.6 \times 10^5 \text{ J/mol} \]

\[ U = -8.6 \times 10^5 \text{ J/mol} \]

**Electrostatics in a spherical world**

As always, we should choose our Gaussian boundary based on the symmetry. In this case we can choose lines of "latitude" on our sphere which will yield an electric field of the form shown.

\[ |E| \frac{2\pi R \sin \theta}{2\pi \varepsilon} = \frac{q}{\varepsilon} \]

\[ \hat{E}(\theta) = \frac{1}{2\pi \varepsilon} \frac{q}{R \sin \theta} \hat{\theta} \]
Something to note about this form of an electric field is that it has singularities at both the north and south poles (i.e. $\Theta = 0$ and $\Theta = \pi$). These can be thought of as a source and a sink for electric field or, in other words, a pair of charges of opposite sign. This can also be seen by considering the ambiguity of a boundary on a sphere.

Thus the total charge in sphere world is always zero.

To determine the energy of a pair of charges, $q_1$ and $q_2$, in sphere world, we should do the work integral.

$$U = -\frac{1}{2\pi \varepsilon'} \int_{\pi/2}^{\Theta_{1z}} \frac{q_1 q_2}{R \sin \Theta} R \, d\Theta = \frac{1}{2\pi \varepsilon'} \left. q_1 q_2 \ln(\cot \Theta + \csc \Theta) \right|_{\pi/2}^{\Theta_{1z}}$$

$$U(\Theta_{1z}) = \frac{q_1 q_2}{2\pi \varepsilon'} \ln \left( \cot \Theta_{1z} + \csc \Theta_{1z} \right)$$