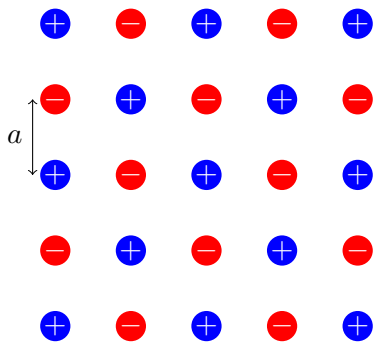
Cohesive Energy of Ionic Crystal

In 2 dimensions, a simple cubic ionic crystal is an arrangement of positive and negative point charges $\pm q$, separated on a square lattice by a distance a, and arranged as shown below:



What is the electrostatic energy per unit charge of this crystal? Naïvely we write down the formula

$$u = \frac{q^2}{4\pi\epsilon_0 a}\alpha$$

where we define the **Madelung constant**

$$\alpha = \sum_{(n_x,n_y)\neq(0,0)} \frac{(-1)^{n_x+n_y}}{\sqrt{n_x^2+n_y^2}}.$$

Unfortunately, this is what mathematicians call a conditionally convergent sum – by changing the order in which we perform the sum, we can obtain any value we want. One very simple way to see this is to sum all of the positive terms first, and then all the negative terms, in which case we get $+\infty - \infty$.

What is the physical reason for this conditionally convergent sum? The basic idea is that depending on the order in which we "build" the crystal, we may build up very large surface charges, for example, which never die off at any finite size, and therefore do not cancel as we take the limit of infinite crystal size. As we will see in this problem, it is not entirely trivial to find a proper ordering of the sum which will converge.

On the other hand, physically it is hard to imagine that this is a problem. One obvious way to see this is that if we place one of these crystals in water, we may generically expect it to dissolve. Since we do not generically expect such a crystal to absorb an "infinite" amount of energy from the water to dissolve, we expect u should be a finite quantity. Therefore, we must evaluate α by choosing a physically reasonable order in which to perform the sum.

(a) Let us begin with a "simple" choice of ordering for the sum. Suppose that we order the sum as follows:

$$\alpha = \sum_{n=1}^{\infty}(-1)^n \sum_{|n_x|+|n_y|=n} \frac{1}{\sqrt{n_x^2+n_y^2}}.$$

Show explicitly that this sum will not converge.[1]

[1] I would do this by finding upper and lower bounds for the sums at fixed n.

(b) A more physically motivated ordering would be to order the sum such that we sum over terms in the order of increasing $\sqrt{n_x^2 + n_y^2}$. Write some computer code to evaluate this sum, and provide a numerical estimate of α to 3 significant digits.

(c) Comment on whether this model is reasonable when compared to experimental data, which typically gives $|u| \sim 10^{-18}$ J. You may use that $q = 1.6 \times 10^{-19}$ C is the charge of an electron will be the charge on the ions in the crystal, and that the lattice spacing $a \sim 10^{-10}$ m.