

Binding energy of a one-dimensional ionic solid¹

1 Introduction

Consider a one-dimensional ionic solid consisting of alternating positive and negative ions (with charges $\pm q$) with nearest neighbours connected by rigid links of length l (see Fig 1). Are the links compressed or extended? When allowed to move, do the ions explode or collapse? The first step to answer those questions is to calculate the electrostatic energy of the chain per ion.

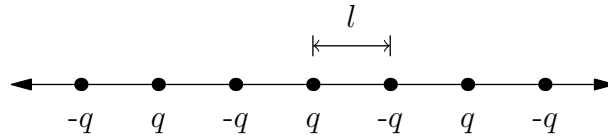


Figure 1: A sketch of a one-dimensional ionic solid.

We compute the electrostatic energy of interaction between the arbitrary chosen ion and all other ions in the chain.

The energy of two charges, q_1 and q_2 , separated by a distance r is

$$E(r) = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r}. \quad (1)$$

Thus, the total energy of an ion is

$$E_0 = \frac{1}{4\pi\epsilon_0} \frac{q^2}{l} \sum_{\substack{n=-\infty \\ n \neq 0}}^{\infty} \frac{(-1)^n}{|n|}, \quad (2)$$

where the term with $n = 0$ – the self-interaction of the ion – is excluded from the summation.

$$E_0 = \frac{1}{2\pi\epsilon_0} \frac{q^2}{l} \sum_{n=1}^{\infty} \frac{(-1)^n}{n}, \quad (3)$$

where we used the fact the terms in the series are even functions of n and left the summation over positive n .

The factor in front of the summation sign

$$\varepsilon = \frac{1}{2\pi\epsilon_0} \frac{q^2}{l} \quad (4)$$

¹The physics problem in this note is “borrowed” from: [H. Reid, Invitation to Numerical Analysis, MIT, 2014.](#)

has the dimension of energy and “absorbs” all dimensional parameters of the problem. It is the double energy of interaction of two neighboring ions.

$$E_o = \varepsilon \sum_{n=1}^{\infty} \frac{(-1)^n}{n}. \quad (5)$$

What remains is to evaluate the numerical value of the sum

$$S_0 = \sum_{n=1}^{\infty} \frac{(-1)^n}{n}. \quad (6)$$

We are going to use the Euler summation method and differentiation by a parameter.

Let's consider the following sum:

$$S(x) = \sum_{n=1}^{\infty} \frac{x^n}{n}. \quad (7)$$

The sum of interest,

$$S_0 = S(-1). \quad (8)$$

Also,

$$S(0) = 0. \quad (9)$$

The derivative of $S(x)$ is

$$\frac{dS}{dx} = \sum_{n=1}^{\infty} x^{n-1}. \quad (10)$$

The sum on the right is a geometric series. Assuming it is convergent,

$$\sum_{n=1}^{\infty} x^{n-1} = \frac{1}{1-x}. \quad (11)$$

Therefore, we obtained the following differential equation:

$$\frac{dS}{dx} = \frac{1}{1-x}. \quad (12)$$

Integrating, we get

$$S(x) = -\log(1-x) + C, \quad (13)$$

where C is an integration constant. Using $S(0)$, Eq. (9), we conclude that $C = 0$. Thus,

$$S(x) = -\log(1-x) \quad \longrightarrow \quad S_0 = S(-1) = -\log 2. \quad (14)$$

Finally the potential energy of the ion chain per ion is

$$E_o = -\varepsilon \log 2. \quad (15)$$

This value is negative, i.e it is less than the energy of the “exploded chain” configuration when all ions are at the infinity, i.e. the periodic configuration is more energetically favorable.