BINDING ENERGY OF A ONE-DIMENSIONAL IONIC SOLID

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.
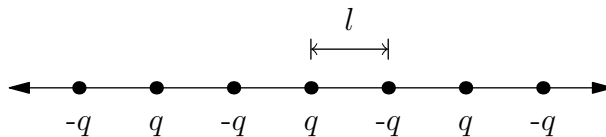

Figure 1: A sketch of a one-dimensional ionic solid.

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

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

Thus, the total energy of an ion is

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

(2)

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

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

(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

$$\varepsilon = \frac{1}{2\pi\epsilon_0} \frac{q^2}{l}$$

(4)

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

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

(5)

What remains is to evaluate the numerical value of the sum

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

(6)

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

2   Euler summation method

The series encountered in physics, typically perturbation expansions, are usually divergent. How can one extract a meaningful number from such series, which represent physical processes and so reflect real processes? On the surface, it would seem impossible to attach any meaning to such obviously divergent series as

$$1 - 1 + 1 - 1 + 1 - \dots$$

(7)

However, as we will now see, perfectly finite numbers can be associated with these series. We are considering (possible diverging) series of the form

$$\sum_{n=0}^{\infty} a_n. \tag{8}$$

Suppose

$$\sum_{n=0}^{\infty} a_n x^n = f(x) \tag{9}$$

converges if $|x| < 1$. Then we **define** the limit of the series Eq. (8) by

$$S = \lim_{x \to 1} f(x) = \lim_{x \to 1} \sum_{n=0}^{\infty} a_n x^n. \tag{10}$$

The algorithm Eq. (10) is called Euler summation.

For example, for the series Eq. (7),

$$S = \sum_{n=0}^{\infty} (-1)^n, \tag{11}$$

$f(x)$ is

$$f(x) = \sum_{n=0}^{\infty} (-1)^n x^n. \tag{12}$$

For $|x| < 1$ the sum Eq. (12) is a convergent geometric series.

$$f(x) = \frac{1}{1+x}, \tag{13}$$

so

$$S = \lim_{x \to 1} \frac{1}{1+x} = \frac{1}{2}. \tag{14}$$

3   Binding energy

Let's consider the following sum:

$$S(x) = \sum_{n=1}^{\infty} \frac{x^n}{n}. \tag{15}$$

The sum of interest,

$$S_0 = S(-1). \tag{16}$$

Also,

$$S(0) = 0. \tag{17}$$

The derivative of S(x) is

$$\frac{\mathrm{d}S}{\mathrm{d}x} = \sum_{n=1}^{\infty} x^{n-1}. \tag{18}$$

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

$$\sum_{n=1}^{\infty} x^{n-1} = \frac{1}{1-x}. \tag{19}$$

Therefore, we obtained the following differential equation:

$$\frac{\mathrm{d}S}{\mathrm{d}x} = \frac{1}{1-x}. \tag{20}$$

Integrating, we get

$$S(x) = -\log(1-x) + C, \tag{21}$$

where C is an integration constant. Using $S(0)$, Eq. (17), we conclude that $C = 0$. Thus,

$$S(x) = -\log(1-x) \qquad \longrightarrow \qquad S_0 = S(-1) = -\log 2. \tag{22}$$

Finally the potential energy of the ion chain per ion is

$$E_o = -\varepsilon \log 2. \tag{23}$$

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.