One dimensional ionic crystal

We consider a straight chain of $2N \gg 1$ ions with alternating electric charges regularly spaced with an interatomic distance $r$. Because of the electrostatic potential, each ion interact with all the others. Additionally, there is a repulsive interaction between nearest neighbors only with a potential energy of the form $a/r^n$.

![One dimensional ionic crystal](image_url)

**FIG. 1:** One dimensional ionic crystal

(a) Express the total cohesion energy $E$ of the crystal. (*Note: Using the Taylor development of $\ln(1 + x)$ around $x = 0$, you can verify that $\sum_{k=1}^{\infty} (-1)^{k-1} \frac{1}{k} = \ln(2)$.*)

(b) Express the equilibrium interatomic distance $r_0$.

(c) Compute the work $W(\eta)$ required to stretch the string by a factor $1 + \eta$ with $\eta \ll 1$, starting from equilibrium. Expressing the work as $W = \frac{Nq^2}{4\pi\epsilon_0 r_0} f(n)\eta^2$ and specify $f(n)$.
Cubic crystal with first neighbor Morse potential interaction

We now consider a three dimensional crystal with \( N \) atoms at sites \( R_{n_x,n_y,n_z} = r (n_x \hat{x} + n_y \hat{y} + n_z \hat{z}) \) where \( r \) is the interatomic distance used as a scale factor for the crystal. Each atom interacts only with its nearest neighbor through a Morse potential \( U(r) = U_0 \left( e^{-2a(r-d)} - 2e^{-a(r-d)} \right) \) with \( U_0, a \) and \( d \) parameters which are established experimentally.

![Cubic crystal](image)

**FIG. 2: Cubic crystal**

(a) Assuming the kinetic energy is zero, express the total cohesion energy \( E(r) \) of the crystal.

(b) Express the equilibrium interatomic distance \( r_e \).

(c) Express the equilibrium bulk modulus \( B \)

**[3] Relation between elastic constants.** The bulk modulus is defined as \( B = -V \frac{dP}{dV} \) where \( V \) is the volume and \( P \) is the pressure. The Young modulus is defined as \( Y = \frac{\tau}{\epsilon} \) where \( \tau \) is the stress, a tensile or compressive force per unit area, and \( \epsilon \) is the resulting strain. The Poisson ratio \( \nu \) is defined as \( \epsilon_y = -\nu \epsilon_x \) where \( \epsilon_x \) is the stress along direction \( x \) and \( \epsilon_y \) is the relative change in dimension in any direction \( y \) perpendicular to \( x \). Finally, the modulus of rigidity is defined as \( G = \frac{\sigma}{\alpha} \) where \( \sigma \) is a shear stress and \( \alpha \) is the resulting shear angle.

In the following two questions you are going to establish relations between \( B, Y, \eta \) and \( G \). For this, you may consider a cube of side \( l \) made of an isotropic solid material.

(a) Establish the relation \( Y = 3B(1-2\nu) \) *(Hint: Write in terms of the pressure the strain along one direction resulting from the compressive stress and the Poisson ratio. Then express the relative change in volume. Finally, use your results in the bulk modulus definition.)*

(b) Establish the relation \( Y = 2G(1+\nu) \) *(Hint: Express the relative increase in length of a diagonal of the side of the cube. Then identify this change to that resulting from the combined effect of an equivalent compressive and tensile stress along the two diagonals of the same side of the cube.)*