

Simple Elastic Force and its relation with intermolecular Force-Potential



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(Recibido el 16 de octubre de 2021, aceptado el 27 de noviembre de 2021)

Abstract

Elastic force of material is demonstrated through some kind of potential and consequently derivable force of interaction within a diatomic molecule and the like along with the experiment for finding the spring constant of a spring. Theoretical preliminaries discussed here are mainly of pedagogic value.

Keywords: Elastic forcé, molecule.

Resumen

La fuerza elástica del material se demuestra a través de algún tipo de fuerza de interacción potencial y, en consecuencia, derivable dentro de una molécula diatómica y similar, junto con el experimento para encontrar la constante elástica de un resorte. Los preliminares teóricos discutidos aquí son principalmente de valor pedagógico.

Palabras clave: Fuerza elástica, molécula.

I. INTRODUCCIÓN

We know that the elastic force of materials comes into play as a restoring forcé while external force tends to deform the material body and that is simply given by

$$F=Kx.$$

This gives the restoring force for a longitudinal deformation by a small displacement 'x' where 'K' the proportionality constant, called the force-constant is a positive parameter. Now this force is shown to have a potential root of evolution in case of intermolecular force. As all real forces having some material-source must be derivable from a potential function here also the force is considered to have been derived from a potential. The graphical plot of force and the corresponding potential against intermolecular distance have been shown with explanation for both of tensile and compressive strain and stress. And finally the basic elasticity-equation (Eq. 1) in terms of force constant is derived in this pedagogic article. Some more trials have been made to find something more.

II. THEORETICAL DERIVATION OF THE FORMULA

Let the potential function corresponding to interatomic force of a diatomic molecule be given by,

$$U(x) = \frac{b}{x^2} - \frac{a}{x} \quad (i)$$

$U(x)$ being zero at $x = b/a$ and $x = \infty$.

For this potential to have an extremum at $x = 2b/a$ and $x = \infty$ meaning that the force is equal to zero at those points too because the force is usually given by,

$$F(x) = -\frac{dU(x)}{dx} = \frac{2b}{x^3} - \frac{a}{x^2} \quad (iii)$$

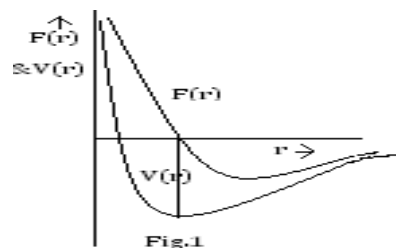


FIGURA 1. The potential function corresponding to interatomic force of a diatomic molecule.

The force is zero at $x = 2b/a$ and at $x = \infty$. The graphical nature of the force and the potential against the interatomic distance is shown in the figure (Fig.1) aside. For $x < (b/a)$ both $U(x)$ and $F(x)$ are positive while for $(b/a) < x < (2b/a)$ the $F(x)$ is positive and $U(x)$ is negative. And of-course for $x > (2b/a)$ both are negative. The interatomic distance $x =$

($2b/a$) is called the mean-equilibrium distance. As an external compressive force tends to decrease down the value of x a positive internal force i.e. of repulsion of reaction as well as restoration comes into play. Contrariwise while a tensile force tends to increase x a negative force i.e. of attraction type comes into play as the internal force of reaction and restoration. Now the derivation of Eq. (i) from Eq. (iii) is as follows. Let us consider that due to external stress a small elongation ' ϵ ' has taken place. Then it can be written as

$$F(x) = F(d_0 + \epsilon) = \frac{2b}{(d_0 + \epsilon)^3} - \frac{a}{(d_0 + \epsilon)^2},$$

where d_0 is the mean equilibrium distance. Now as $\epsilon \ll d_0$ by means of Binomial expansion and neglecting higher powered terms with (ϵ/d_0) one gets

$$F(x) = \frac{2b}{d_0^3} \left\{ 1 - \frac{3\epsilon}{d_0} \right\} - \frac{a}{d_0^2} \left\{ 1 - \frac{2\epsilon}{d_0} \right\} \quad \left[\frac{2b}{d_0^3} = \frac{a}{d_0^2} \text{ for} \right. \\ \left. = \frac{2b}{d_0^3} \left[-\frac{\epsilon}{d_0} \right] = \left(\frac{2b}{d_0^4} \right) \epsilon. \right. \quad \text{(iv)}$$

Hence $\{F(x)\} = F(d_0 + \epsilon) \propto \epsilon$. Now for this extra force if we replace ϵ by x as the small elongation then one gets Eq. (i) with force-constant being equal to

$$K = \frac{2b}{d_0^4} = \frac{a^4}{8b^3} \text{ giving } b = \frac{a^{\frac{4}{3}}}{2K^{\frac{1}{3}}}. \text{ Putting this value of 'b'}$$

in Eq. (iii) it is obtained that

$$F(x) = \frac{a^{\frac{4}{3}}}{K^{\frac{1}{3}} x^3} - \frac{a}{x^2}. \quad \text{(v)}$$

The average interatomic force in the state of vibration under such a potential may be calculated for a range of value of ' x ' from $(+b/a)$ to $(+3b/a)$ about the mean equilibrium position and then (b/a) may be regarded as the amplitude of oscillation.

$$\bar{F} = \frac{a}{2b} \int_{+\frac{b}{a}}^{+\frac{3b}{a}} F(x) dx = \frac{a^3}{9b^2}.$$

Similarly the average value of the potential within the same range may thus be found as

$$\bar{U} = \frac{a}{2b} \int_{+\frac{b}{a}}^{+\frac{3b}{a}} U(x) dx = \frac{a^2}{b} \left(\frac{1}{3} - \frac{\ln 3}{2} \right) \approx -0.216 \left\{ \frac{a^2}{b} \right\}.$$

This average energy may be related to the internal energy of the material concerned via absolute temperature. The minimum force and the minimum potential also may thus be found out to be $(-a^3/27b^2)$ and $(-a^2/4b)$ respectively meaning exactly this amount of positive energy is at least

required to break the inter molecular bonding. Now let us investigate which difference could be observed if instead of the potential function as mentioned above in Eq. (i) would be considered. The newer potential is as follows;

$$U(x) = \frac{b}{x^3} - \frac{a}{x^2}. \quad \text{(vi)}$$

With this potential the corresponding graphical plots for both potential and the force against inter-atomic distance are exactly similar to those of the previous one. Only the values of the constant parameters such as the inter-atomic mean distance of equilibrium, the zeros of the functions and the ranges are different. Here the mean equilibrium distance becomes $(3b/2a)$ and the range becomes from (b/a) to $(2b/a)$, with amplitude of oscillation equals to $(3b/2a)$. In this case the average force and the average potential within the above-mentioned range of oscillation are found to be as given below;

$$\bar{F} = \frac{a^4}{8b^3} \quad \text{and} \quad \bar{U} = \frac{a^3}{8b^2}.$$

Here the point is to be noted that with the same coefficients but different powers of the single variable ' x ' (the one dimensional inter-atomic distance) changes in a few physical properties such as the inter-atomic mean distance of equilibrium, the mean values of force and energy can be observed. With the higher power of the inverse function of distance the force becomes stronger and the energy-state becomes higher revealing somewhat a way the Van der Waal state undergoes transition from one state to another.

III. ABOUT THE SPRING CONSTANT

Knowledge on the geometry of a spring is primary requirement for understanding the physics of elastic property of a spring. A spring may be regarded as a helix or a helicoids [1] which may be thought to be generated by winding around a cylinder of uniform radius the hypotenuse of a rectangular triangle with its base-vertex at a peripheral point on the cylinder-surface. The equation of a helix is given in a pair as follows.

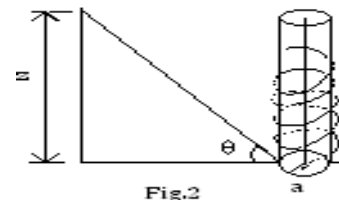


FIGURA 2. A spring as a hélix or a helicoids.

$$x^2 + y^2 = a^2, \quad (y/x) = \tan\left(\frac{z}{am}\right) \text{ where } m = \tan \theta$$

A small increase or an element of length of helix or spring is related to the corresponding small change in vertical height 'z' in the following way;

$$\frac{ds}{dz} = \frac{\sqrt{1+m^2}}{m}$$



Fig.3

Figure 3. Consideration of a small increase or an element of length of helix or spring related to the corresponding small change in vertical height 'z'.

Each point on the spring /helix has its own counter point where the horizontal component of the tension in the spring material are equal and opposite and thereby cancel each other. The vertical components being all in the same common vertical direction adds up to a total force balancing the weight 'W'. But the horizontal components being equal and opposite in direction produce no translational motion yet being noncollinear produce a net torque due to which the spring gets twisted a little until torsional rigidity balances the external torque.

$$W = \sum \Delta T_i \sin \theta_i.$$

In the language of calculus $dT = c_0 K ds =$

$$c_0 K \left(\frac{\sqrt{1+m^2}}{m} \right) dz \text{ and } W = \int_0^h dT \sin \theta = c_0 K h.$$

'ds' is the small element of actual length of the spring-wire in balanced condition whereas 'c₀ds' is the small expansion of it and 'c₀h' is the total expansion. Thus the well known equation used in experiment with spring in undergraduate course is obtained;

$$W = c_0 K h = Ky \text{ [} c_0 h = y = \text{total expansion].}$$

The horizontal components on the other hand yields a torque as follows; $adT \cos \theta = d\tau = cd\phi$ where 'c' is the torsional rigidity modulus.

$$\text{or } \phi = \left\{ \frac{ac_0Kh}{c} \right\} \cot \theta = \left(\frac{aW}{c} \right) \cot \theta.$$

Thus as 'W' increases 'φ' the angle of twist also increases proportionally but not exactly linearly 'θ' then increases producing a decrease in the 'cot θ' value.

IV. CONCLUSION

The whole article is based on the well known elementary theory of elasticity and undergraduate experiment with a spring for finding out the spring constant. The experiment is easy both to perform and understand theoretically while the theoretical. At least even in brief escapes the undergraduate syllabus. It is considered here and has been tried to be made clear. Some important revelations have been made here regarding the average force and average energy in the oscillating state of a diatomic molecule and even their strength of interaction varying from state to state. Moreover depression of a spring is found to linearly depend on the weight hanged from the spring. But simultaneously the free end of the spring undergoes a twist around by some angle 'φ' which is usually observed in the experiment too has been accounted for.

ACKNOWLEDGEMENTS

The author would like to gratefully acknowledge the kind help provided by the School Education Department, West Bengal by ordering extension of the closure of school due to extended lockdown for Covid19 scare which gave time to think of and write this article.

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