



Bulk modulus for Morse potential interaction with the distribution function based

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ABSTRACT

The bulk modulus is a significant coefficient for the study of the compressible behaviour of the materials in the bulk case. The bulk moduli can be determined via the experimental method by measuring of the elastic parameters, via the semi-empirical procedures from the equation of state, or from theoretical images as in the theory of the integral equations. In this work we find a relationship of the bulk modulus for the Morse interaction potential employing the Fourier transformation and the mean-spherical approximation for the Morse interaction. We find that the bulk modulus of the Morse potential is composed of two terms, one from the kinetic part, and the other from the internal interaction of the particles composing the described-system. We find that the bulk modulus of the Morse interaction depends on the absolute temperature of the described composition and the compact factor. Besides, we find that the Bulk modulus formula which we derived of Morse potential, depends on the diameter of the particles in the system, and depends on the Morse interaction parameters. The formula which we derive is, in general, applied for the systems described by the Morse interaction in the vibrational case such as the hydrogen chloride and hydrogen fluoride molecules.

Introduction

The bulk moduli are useful coefficients for the study of the elastic states of materials in the bulk case, and these coefficients are found numerically using the semi empirical procedures through the equations of state, or from the theoretical procedures from the theory of the thermodynamics and statistical mechanics, or from direct experimental procedures. There lots of applications and study about the different things of the bulk moduli, for instance, Gupta, R., & Gupta, M [1]. discussed the bulk moduli of the nano-materials in the image of the pressure derivatives of the 2nd order. Hoagland and Fensin [2] discussed some effects of the defects with the bulk moduli in the case of the solids in the crystalline case. Liu and Li [3] applied the computational procedures for the study of tuning of the bulk modulus in a specific case. Blake, et al [4]. discussed the relation between the dynamic and the static bulk modulus for a special case. Weidner, & Li [5] discussed the tuning of the low frequency bulk modulus of a specific molten case. Méndez, et al [6]. discussed the bulk modulus for the water ice transitions using the diffraction of the x ray. Raptakis, et al [7]. studied the finding of the bulk modulus of the layers in a specific state which useful in the study of the modulus in the nano scale cases. In the present procedure, we use the theory of the integral equations for finding a relationship of the bulk modulus in the case of Morse potential. The Morse interaction is a very useful tool for the study of the vibrational cases, especially, in

quantum mechanics and there are important applications of this potential for multiple effects, for instance, Abebe, et al [8]. used the general formalism of the Morse interaction in Dirac equation. Sharma, & Sastri [9] employed the matrices methods and Fourier basis (sine) for the study of the computational solutions of the Schrödinger equation for the rotate Morse potential. Semenov, et al [10]. applied the Morse interaction in the atomistic state of the cobalt and nickel. Gomez, et al [11]. used the operator of the momentum in the relativistic state, in general, for the Morse interaction. Gauti'e, et al [12]. used the Kesten matrix with other procedures for the Morse interaction. Nickabadi, et al [13]. used the DFT procedures for the determination of the Morse interaction parameter of silicene. Ungan, et al [14]. disused the optics effects of the Morse interaction for the quantum dots in the cylindrical state. Peña, et al [15]. derived the Morse interaction formula from the radial potential in general case with multiple parameters. Aldossary [16] applied the Morse interaction versus other potential for the determination of the point of melting and cohesive energies for the nano-materials. Sarathi, and Pathak [17] used the Morse interaction for applying in the study of the negative masses in the complex formalism. Maireche [18] used the modified form of the Morse interaction formula for the study of the bound state using the Schrödinger and Klein Gordon equations. Akanbi, et al [19]. also used the modified form of the Morse interaction for the study of some of the thermodynamic properties for special cases. Nadhira, et al [20]. applied the non-cumulative formalism of the quantum mechanics for the Morse interaction. Ikot, et al [21]. found semi analytical solution of the Klein Gordon equation for the simple Morse interaction. Aldossary, & Al Rsheed [22] discussed the effects of the changing

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of the Morse interaction parameters to the cohesive energy. Kozlovskii, & Dobush [23] used a modified formalism of the Morse interaction for the study of the model of cell-fluids in the case of the phase change. The potential formula of the Morse interaction can be written in multiple forms such as the following form [25]:

$$U_M(r) = D_0 [e^{-2a(r-r_0)} - 2e^{-a(r-r_0)}] \quad (1)$$

Where D_0 represents the equilibrium energy of the potential, a is the parameter which determines the width of the potential well and r_0 is equilibrium bond distance. In the following, we are going to show a method for deriving a formula of the Bulk modulus of the Morse potential based on the integral equations theory using the mean spherical approximation. In the second section of this work, we show the theoretical method of the derivation of the equation of the bulk modulus, and in the third section, we illustrate some discussion of the derived formula, and in the last one, we illustrate the conclusions of the work.

The method

We use the statistical mechanics principles in the image of the theory of the integral equations for the deriving of the bulk modulus formula of Morse interaction. One of the most important equations in the integral equation theory is the Ornstein Zernike equation which describes the correlation between the particles in the system as direct correlation and indirect correlation and this equation is given as follows [24]:

$$h(r) = n \int d\vec{r}' h(r') c(|\vec{r} - \vec{r}'|) + c(r) \quad (2)$$

Where r is the distance between the particles of the system, n is number of the density, $c(r)$ is the direct correlation function, while $h(r)$ is the total correlation function. As we see from the previous equation, if we need to find a solution of the equation, we need another approximation for this purpose where there are multiple approximations in the integral equations theory can be applied such as the mean-spherical-approximation that states that the direct correlation function is proportional to the interaction potential between the particle in the system, the Percus-Yevick approximation which states that the direct correlation function is related to the interaction potential via exponential function, the random phase approximation which states that the direct correlation function is composed of two parts, the first part is from the long range interaction and the other is from the short range interaction, and the hyper-netted chain approximation which states that the radial-distribution-function is related to the potential of the interaction via an exponential function.

In this work, we apply the first approximation for deriving the formula of the bulk modulus of the Morse potential. We start from the general formula of the statistic structure factor which can be derived from the radial distribution function via Fourier analysis which is written as:

$$B^{-1}(T, n) = \lim_{q \rightarrow \infty} S_C(q) \quad (3)$$

$$B(T, n) = \left[1 - \rho \lim_{q \rightarrow \infty} c(q) \right] k_B n T \quad (4)$$

Or in another form:

$$B(T, n) = k_B \left[1 - 4\pi\rho \int_0^\infty r^2 c(r) dr \right] n T \quad (5)$$

We treat each term of the previous formula using the mean spherical approximation and the boundary condition of the correlation functions, where we have for the Morse interaction:

$$B(T, n) = k_B n T + 4\pi k_B n^2 T \int_0^d r^2 dr + 8\pi k_B n^2 T \beta D_e \int_d^\infty r^2 e^{-a(r-r_0)} dr - 4\pi k_B n^2 T \beta D_e \int_d^\infty r^2 e^{-2a(r-r_0)} dr \quad (6)$$

The previous formula can be written in simpler form using the following reduced Morse parameters:

$$ar^{**} = r^* \quad (7)$$

$$r - r_0 = r^{**} \quad (8)$$

$$ar^{**} = r^{***} \quad (9)$$

$$B(T, n) = k_B n T + 4\pi k_B n^2 T I_1 + 8\pi n^2 D_e I_2 - 4\pi n^2 D_e I_3 \quad (10)$$

Where:

$$I_1 = C_2(a, r_0) \int_0^d r^{*2} dr^* \quad (11)$$

$$I_2 = C_2(a, r_0) \int_d^\infty r^{*2} e^{-r^*} dr^* \quad (12)$$

$$I_3 = C_3(a, r_0) \int_d^\infty r^{*2} e^{-2r^*} dr^* \quad (13)$$

We can find the first integral in the previous three equations directly as a power integral to the reduced parameter, while we can find the other two integrals by applying the partition multiple times for each one, so if we apply the partition procedure and if we use the first two equations of the reduced parameter, i. e Eqs. (7), (8), and (9) we find that:

$$I_1 = \frac{d^3}{3} \quad (14)$$

$$I_2 = \frac{e^{-a(d-r_0)}}{a} \left(d^2 + \frac{2d}{a} + \frac{2}{a^3} \right) \quad (15)$$

$$I_3 = \frac{e^{-2a(d-r_0)}}{2a} \left(d^2 + \frac{d}{a} + \frac{1}{2a^2} \right) \quad (16)$$

Now, if we use the previous three equations in the equation of the bulk modulus, we find the following form of the bulk modulus for Morse potential:

$$B(T, n) = k_B n T + \frac{4\pi k_B d^3}{3} n^2 T + \frac{8\pi n^2 D_e}{a} \left(d^2 + \frac{2d}{a} + \frac{2}{a^3} \right) e^{-a(d-r_0)} - \frac{2\pi n^2 D_e}{a} \left(d^2 + \frac{d}{a} + \frac{1}{2a^2} \right) e^{-2a(d-r_0)} \quad (17)$$

Results and discussion

The formula (17) is the main formula which we derived in this study for the bulk modulus of the Morse interaction. We see from the formula that the bulk modulus, in general, is function to the well depth of the Morse interaction, the parameter of the width of the well of the Morse interaction, the bond distance of the Morse interaction, the diameter of the particles composing the system, the numerical density and the absolute temperature of the described system.

Besides, as we see from that formula, the bulk modulus is composed of two main terms, the first one is the kinetic one which is:

$$B_1(T, n) = k_B n T \quad (18)$$

and the other term is resulted from the Morse interaction which is:

$$B_2(T, n) = \frac{4\pi k_B d^3}{3} n^2 T + \frac{8\pi n^2 D_e}{a} \left(d^2 + \frac{2d}{a} + \frac{2}{a^3} \right) e^{-a(d-r_0)} - \frac{2\pi n^2 D_e}{a} \left(d^2 + \frac{d}{a} + \frac{1}{2a^2} \right) e^{-2a(d-r_0)} \quad (19)$$

We can write the formula of the bulk modulus with respect to the fractional volume which is defined as:

$$\varphi = \frac{\pi}{6} \rho d^3 \quad (20)$$

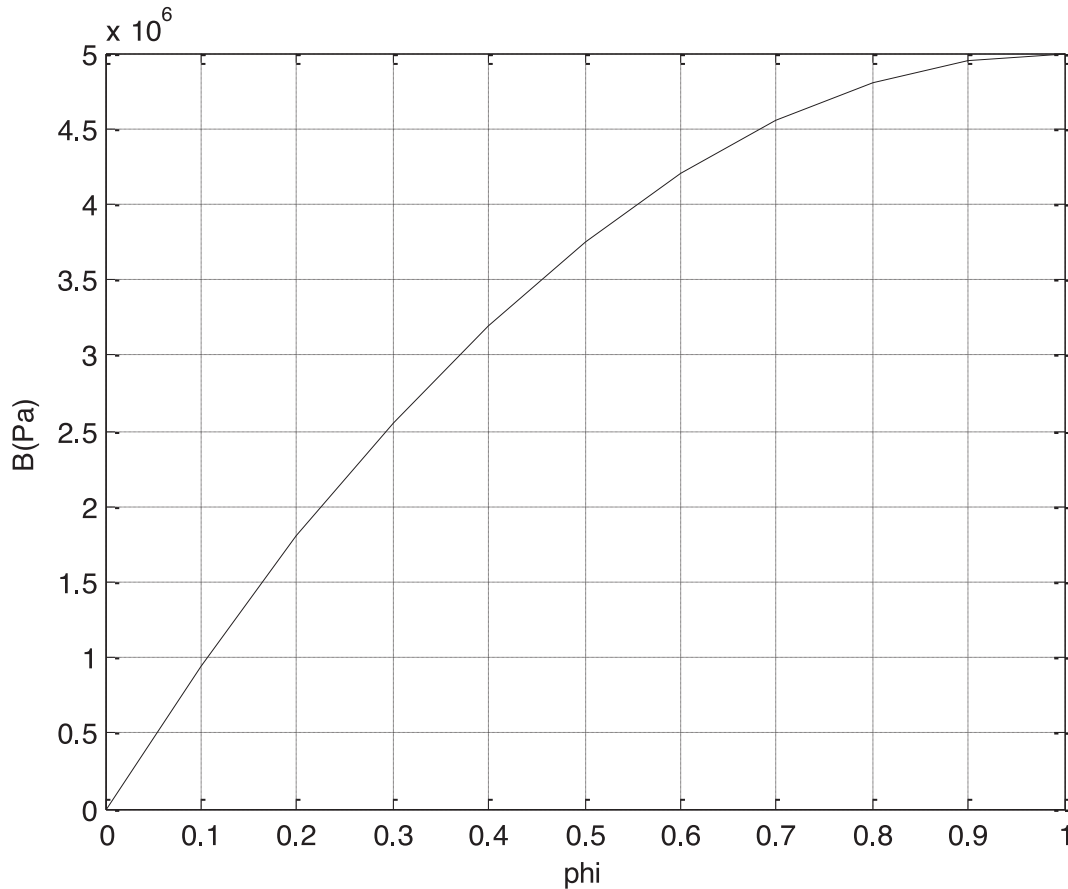


Fig. 1. The bulk modulus versus the compact factor.

In the following form:

$$B(T, \varphi) = \mu_1(T)\varphi + \mu_2(T)\varphi^2 \quad (21)$$

Where:

$$\mu_1(T) = \frac{6k_B}{\pi d^3} T \quad (22)$$

$$\mu_2(T) = \frac{144k_B}{\pi d^6} \left[\frac{1}{3}d^3 + \frac{D_0}{k_B a T} \left[\frac{1}{2} \left(d^2 + \frac{d}{a} + \frac{1}{2a^2} \right) e^{-2a(d-r_0)} - \left(d^2 + \frac{2d}{a} + \frac{2}{a^3} \right) e^{-a(d-r_0)} \right] \right] \quad (23)$$

In Fig. 1, we plotted the bulk modulus for $\mu_1=10^7$ Pa and $\mu_2=-0.5 \times 10^7$ Pa.

In addition, we can write the formula of the bulk modulus of the Morse interaction with respect to the absolute temperature as follows:

$$B(T, \varphi) = \eta_1(\varphi) + \eta_2(\varphi)T \quad (24)$$

Where:

$$\eta_1(\varphi) = \frac{144D_0\varphi^2}{\pi ad^3} \left[\frac{1}{2} \left(d^2 + \frac{d}{a} + \frac{1}{2a^2} \right) e^{-2a(d-r_0)} - \left(d^2 + \frac{2d}{a} + \frac{2}{a^3} \right) e^{-a(d-r_0)} \right] \quad (25)$$

$$\eta_2(\varphi) = \frac{6k_B\varphi + 48k_B\varphi^2}{\pi d^3} \quad (26)$$

In Fig. 2, we represents the bulk modulus versus the absolute temperature.

We see from the previous formulas that the bulk modulus for the Morse interaction is a square function to the fractional volume and a

linear function to the absolute temperature. Other calculations based on the equation which we derived for the bulk modulus can be done and all we need: the bond distance of the Morse potential for the system, the parameter of the width of Morse potential, the diameter of the particles in the considered system and the depth of the well, however, in this work, we focused on the derivation of the formula rather than the computational calculations. In addition to that, The results in this study can be applied further to some important systems such as phosphorus dimer as in the study by Jia et al. [26], and Peng et al. [27] where they studied the enthalpy and the Gibbs free energy of the gaseous phosphorus where they used the Tietz with the fitting parameters similar to the Morse one. Also, such as the gaseous nitrogen as in the study by Jia et al. [28] where they studied the entropy and Gibbs free energy for nitrogen. Also, some diatomic molecules as in the study by Jiang et al. [29] where they studied the enthalpy for the carbon monoxide, the hydrogen chloride, and the Bohr fluoride. Also, such as the carbon dioxide with the thermodynamic properties as in the study by Wang et al. [30]. Also, as the hydrogen sulfide with the same properties as in the study by Jia et al. [31]. In addition to the study to the three atomic molecules such the water as in the study by Wang et al. [32] where they studied the ideal gas thermodynamic properties for water. The importance of the previous studies that these studies include the fitting parameter of the potential and this can be applied for some numerical calculations based on the formula of the bulk modulus of the Morse potential which we derived in this work.

Conclusions

In this work, we derived an analytical-formula of the bulk modulus for systems described by Morse potential in the vibrational case. We applied the mean spherical approximation in the integral equation theory

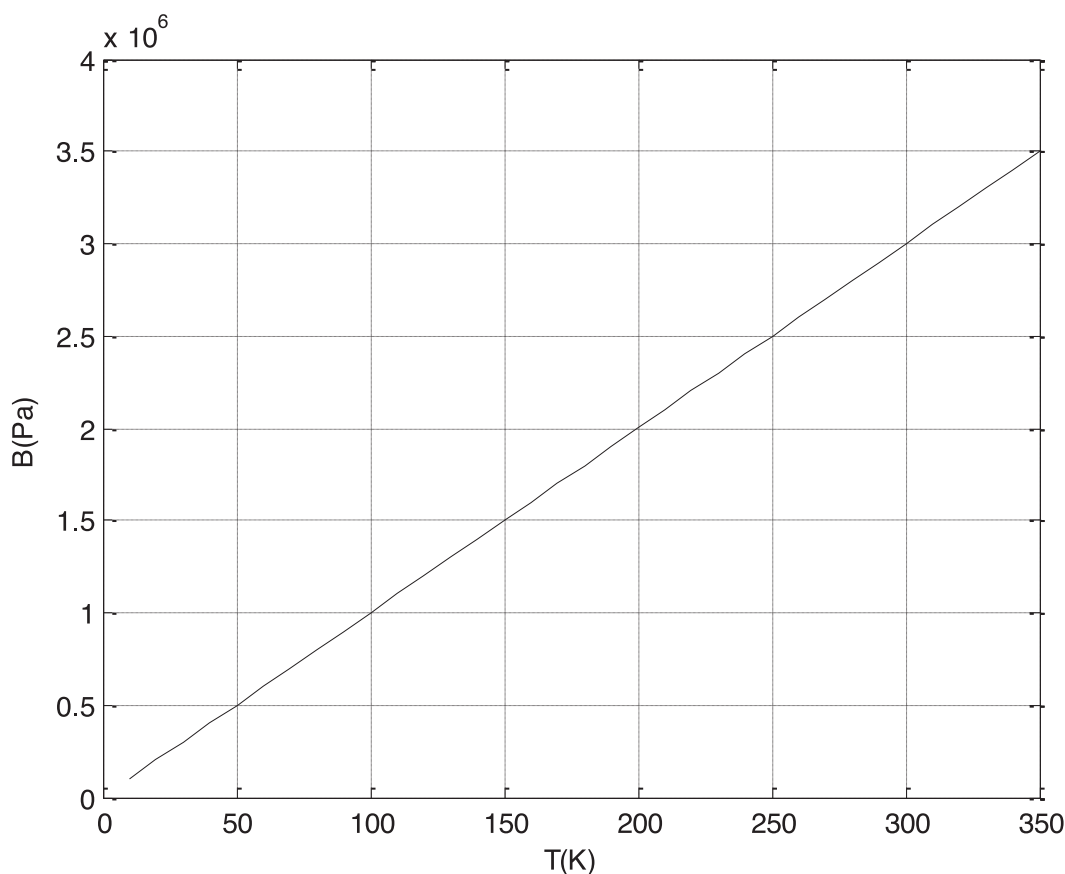


Fig. 2. The bulk modulus versus temperature.

of low density systems for purpose of finding the formula. We applied the general formula of the compressibility which includes the kinetic term and the internal interaction of the particles term.

We found that the bulk modulus for the Morse interaction depends on the absolute temperature of the system, and is function to the well potential width, the bond distance of Morse potential, the diameter of particle of the described system, and the compact factor. We found that the bulk modulus increases with the absolute temperature of the described system via a linear type increasing.

We believe that formula of the bulk modulus for Morse potential which we derived in this study is general and can be applied for the study of some systems described by Morse potential interaction such as the diatomic molecules such as the hydrogen chloride and the hydrogen fluoride. Also, the formula method which we derived in this work can be expanded to other type of important potentials such as Tietz potential [13,27] and the screening potential [33] in the electrical form.

Declaration of Competing Interest

No conflict of interests.

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