



Research article

Morse oscillator equation of state: An integral equation theory based with virial expansion and compressibility terms



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ABSTRACT

A number of interaction energy types are employed in the vibrations studies, especially in the spectroscopic analysis, such as the harmonic oscillator and Morse oscillator. In this research, a derivation of an analytical formula of equation of state of Morse oscillator is considered by employing the approximations used in the simple fluids theory. The compressibility formula of the pressure and the virial expansion formula of the pressure using the solutions of the main equation of the simple fluids theory with one of the approximations of the theory are employed for the purpose of the derivation. The virial coefficients of the total Morse oscillator pressure (the first order one, and the second order one) are found for Morse oscillator with respect to the fractional volume of the components, where we conclude that the first order term is proportional to the absolute temperature directly and depends on the diameter of the particles, while we concluded that the second order coefficient term is more complicated than the first order one with temperature, and also, depends on the three Morse oscillator parameters and the diameter of the particles. Besides, we conclude that the total pressure of Morse oscillator, generally, depends on the minimum energy of the well of Morse oscillator, the width parameter of Morse oscillator, and the equilibrium bond distance of the oscillator, in addition to their dependence on the absolute temperature of the components, and the diameter of the particles. The formula of the Morse oscillator equation of state which is found in this research can be applied to multiple materials described using Morse oscillator such as lots of dimers in the vibrations spectroscopy.

1. Introduction

For the study of vibrations in the quantum mechanics and their relations to the spectroscopic results, there are multiple types of the potentials, such as the harmonic oscillator potential an Morse oscillator potential which we focus on in this research. There are multiple used formulas of Morse oscillator, based on the zeros of the energy, such as the formula represented in the following equation (Abebe et al., 2021; Alqannas and Abdel-Khalek, 2019; Ikot et al., 2021; Morse, 1929; Okoia et al., 2020; Rong, 2003):

$$V_{Mo} = E_0 e^{-2(r-r_0)q} [1 - 2e^{(r_0-r)q+2(r-r_0)q}] \quad (1)$$

From equation (1), we note that the formula of Morse oscillator has three different parameters: E_0 which is the minimum energy of the well, q which represents the width parameter of Morse oscillator, and r_0 which represents the equilibrium bond of the oscillator (Pingak et al., 2021; Al-Raei, 2021). In the following, we are going to show a method for deriving an equation of state of Morse oscillator (EOSMO) based

on the integral equations theory using the mean spherical approximation. The integral equations theory is a significant theory for discussing thermodynamics of multiple spectrum of materials such as soft materials and simple fluids. For instance, Zhou et al. (2004) applied the integral equations theory for finding the depletion potential for the colloidal particle, Aguirre-Manzo and González-Mozuelos (2021) discuss the charged colloids with high charges with the salt in suspensions using the theory of the integral equations, Pérez-Molina et al. (2021) used the chaotic data with the theory of the integral equations for the estimation of the virial coefficients of the equation of state, Kalyuzhnyi et al. (2021) applied the theory of the integral equations with the numerical analysis techniques for the study of the mixtures of colloids, Hashimoto et al. (2019) use the theory of the integral equations with the atomic force microscope data for the determination of the number density distribution of colloidal particles on a substrate, Filippov et al. (2019) used the theory of the integral equations for the dusty plasma mixtures, Munaò and Saija (2019) studied the hertzian spheres in case of the low temperatures using the theory of the integral equations in

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addition to the Monte-Carlo simulation, Herrera (2018) found some structural and thermodynamic properties of fluids described by hard sphere and Yukawa potential using the theory of the integral equations, Arauz-Lara showed some application of the integral equations theory to the colloidal fluids, Pizio et al. (2011) discussed a model for the simple fluids using the second order of the integral equations theory, Lukšič et al. (2011) applied the integral equations theory for the mixtures of the electrolytes and non-charged hard spheres for purpose of the determination of the structural properties and thermodynamics of these mixtures, Fukudome et al. (2014) showed a new formula for the direct correlation function for the hard sphere fluids, Wu et al. (2014) calculated the static structure factor for the charged spheres using the integral equations theory, Lomba et al. (2015) used the three dimensional integral equations approximation for discussing of fluids with confinement and applied in the case of the argon in zeolites, Miyata and Miyazaki (2016) discussed the one component fluids interacting via Lennard-Jones interaction for the study of the temperature derivative of the radial distribution function using the integral equations theory, Melnyk et al. (2016) found the structure factor of the fluids of the hard core type interacting via short range Yukawa potential using the integral equations theory and the simulation methods, Al-Raei (2022a) derived a state equation for London interaction. Also, Al-Raei (2021) applied the theory for the study of some soft materials, Zhou (2010) discussed the fluids with the honeycomb interaction with the integral equations theory. In the second section of this work, theoretical method of the derivation of the equation of state is illustrated, and in the third section, some discussions of the derived formula are illustrated, and in the last one, conclusions of the work are illustrated.

2. The method

The main equation in the study of the simple fluids using the integral equation theory is Ornstein-Zernike equation (OZE) which has two different terms: the first term is resulted from the direct correlation and the other is resulted from the indirect one, the OZE is worded via following formula (Al-Raei, 2022b,c):

$$h_r^T \equiv c_r^O + \tau \int d\vec{r}' c^O(|\vec{r}' - \vec{r}|) h_{|\vec{r}'|}^T \tag{2}$$

Where the distance of the particles is r , the particle density number is τ , c^O and h^T are correlation functions. From the formula of the equation (2), it is clear that the finding of solutions of this equation needs another equation which is resulted from multiple types of the approximations used in the simple fluids theory where some have linear form, some have exponential form, and others have natural logarithmic form. In this work, we employ the approximation namely MSA (mean spherical approximation) where this approximation is the basic approximation of this study for finding the solutions and from these solutions, we derive our equation of state for Morse oscillator. The starting point of deriving the equation of state of Morse oscillator is from the general form of the pressure which has two terms as in the equation (3):

$$P_{tot}(\tau, T) \equiv \frac{1}{3}(2P_{Vir} + P_{Com}) \tag{3}$$

where the first term returns to the virial case, and the other returns to the compressibility one. Firstly, the treating of the virial terms is done, where this term is illustrated in the equation (4):

$$P_{Vir}(\tau, T) \equiv P_k + P_l = k_B \tau T - \frac{2\pi}{3} \tau^2 \int_0^\infty r^3 V'_{M_o} g^r dr \tag{4}$$

where Boltzmann constant is k_B , the temperature is T , the radial distribution function is g^r , and V'_{M_o} is the Morse potential derivation with respect to the distance which can be found in the following equation:

$$V'_{M_o} = 2qE_0 e^{-2q(r-r_0)} [e^{q(r_0-r)} + 2q(r-r_0) - 1] \tag{5}$$

and by using the solutions of the equation (2) in the virial pressure equation, we find:

$$P_{Vir}(\tau, T) = k_B \tau T - \frac{1}{3} 2\pi \tau^2 \int_0^\infty dr V'_{M_o} g_1^r r^3 - \frac{1}{3} 2\pi \tau^2 dr \int_d^\infty V'_{M_o} g_2^r r^3 \tag{6}$$

$$P_{Vir}(\tau, T) = k_B \tau T - \frac{2\pi q E_0}{3} \tau^2 \int_d^\infty \frac{[e^{-q(r-r_0)} - \beta D_e e^{-q(r-r_0)} + 2\beta D_e e^{-2q(r-r_0)} - e^{-2q(r-r_0)} - 2\beta D_e e^{-3q(r-r_0)} + \beta D_e e^{-4q(r-r_0)}]}{r^3} dr \tag{7}$$

and by other form:

$$P_{Vir}(\tau, T) = k_B \tau T - \frac{2\pi q E_0}{3} \tau^2 [(1 - \beta E_0) \int_d^\infty r^3 e^{-q(r-r_0)} dr + (2\beta E_0 - 1) \int_d^\infty r^3 e^{-2q(r-r_0)} dr - 2\beta E_0 \int_d^\infty r^3 e^{-3q(r-r_0)} dr + \beta E_0 \int_d^\infty r^3 e^{-4q(r-r_0)} dr] \tag{8}$$

Here, the using of the dimensionless form of the parameters of the Morse oscillator those are given in the following equation:

$$\rho^* \equiv q r^{**} \tag{9}$$

$$\rho^{**} \equiv -(r_0 - r) \tag{10}$$

$$\rho^{***} \equiv q r^{***} \tag{11}$$

gives the virial term of the pressure as:

$$P_{Vir}(\tau, T) = k_B \tau T - \frac{2\pi q E_0}{3} \tau^2 [(1 - \beta E_0) u_4 + (2\beta E_0 - 1) u_3 - 2\beta E_0 u_2 + \beta E_0 u_1] \tag{12}$$

where:

$$u_1 = K_1(q, r_0) \int_d^\infty \rho^{*3} e^{-4\rho^*} d\rho^* \tag{13}$$

$$u_2 = K_2(q, r_0) \int_d^\infty \rho^{*3} e^{-3\rho^*} d\rho^* \tag{14}$$

$$u_3 = K_3(q, r_0) \int_d^\infty \rho^{*3} e^{-2\rho^*} d\rho^* \tag{15}$$

$$u_4 = K_4(q, r_0) \int_d^\infty \rho^{*3} e^{-\rho^*} d\rho^* \tag{16}$$

The integrating of the previous four equations can be done using the power-n with the exponential function integral which gives the following four results:

$$u_1 = e^{4(r_0-r)q} \left[-\frac{r^3}{4q} - \frac{3r^2}{16q^2} - \frac{6r}{64q^3} - \frac{6}{256q^4} \right] \Big|_d^\infty \tag{17}$$

$$u_2 = e^{3(r_0-r)q} \left[-\frac{r^3}{3q} - \frac{r^2}{3q^2} - \frac{2r}{9q^3} - \frac{2}{27q^4} \right] \Big|_d^\infty \tag{18}$$

$$u_3 = e^{2(r_0-r)q} \left[-\frac{r^3}{2q} - \frac{3r^2}{4q^2} - \frac{3r}{4q^3} - \frac{3}{8q^4} \right] \Big|_d^\infty \tag{19}$$

$$u_4 = e^{(r_0-r)q} \left[-\frac{r^3}{q} - \frac{3r^2}{q^2} - \frac{6r}{q^3} - \frac{6}{q^4} \right] \Big|_d^\infty \tag{20}$$

which gives the virial term of the pressure equation after returning to the dimensionless parameters as follows:

$$\begin{aligned}
 P_{Vir}(\tau, T) = & k_B \tau T - \frac{2\pi E_0}{3} \tau^2 [(1 - \beta E_0) (\frac{d^3}{1} + \frac{3d^2}{q} + \frac{6d}{q^2} + \frac{6}{q^3}) e^{-\delta^*} \\
 & + (2\beta E_0 - 1) (\frac{d^3}{2} + \frac{3d^2}{4q} + \frac{3d}{4q^2} + \frac{3}{8q^3}) e^{-2\delta^*} \\
 & - 2\beta E_0 (\frac{d^3}{3} + \frac{d^2}{3q} + \frac{2d}{9q^2} + \frac{2}{27q^3}) e^{-3\delta^*} \\
 & + \beta E_0 (\frac{d^3}{4} + \frac{3d^2}{16q} + \frac{3d}{32q^2} + \frac{3}{128q^3}) e^{-4\delta^*}]
 \end{aligned} \tag{21}$$

where:

$$\delta^* = (d)\rho^{***} \tag{22}$$

Then, the treating of the compressibility pressure is done, where this term is given in the following equation: is given as follows:

$$P_{Com}(\tau, T) \equiv \int_0^\tau \frac{1}{\tau \chi} d\tau \tag{23}$$

with helping of the static structure factor as:

$$\chi_T(k_B \tau T) = S_{Co}(k_\lambda \rightarrow 0) \Rightarrow (k_B \tau T \chi_T) = \frac{1}{1 - \tau c(k_\lambda \rightarrow 0)} \tag{24}$$

With k_λ is the amplitude of the wave vector, and the previous formula becomes:

$$(\chi_T k_B \tau T)^{-1} = -4\pi\tau \int_0^\infty r^2 c^O dr + 1 \tag{25}$$

using the solutions of the equation (2) in the compressibility equation, we find

$$\begin{aligned}
 (\chi_T k_B \tau T)^{-1} = & 4\pi\tau \int_0^d dr r^2 + 8\pi\beta\tau E_0 \int_d^\infty dr r^2 e^{-q(r-r_0)} \\
 & - 4\pi\beta\tau E_0 \int_d^\infty dr r^2 e^{-2q(r-r_0)} + 1
 \end{aligned} \tag{26}$$

and if we use the Morse oscillator dimensionless parameters, the equation (26) is worded as:

$$(\chi_T k_B \tau T)^{-1} = \frac{4\pi d^3 \tau}{3} + 8\pi\beta\tau E_0 u_6 - 4\pi\beta\tau E_0 u_5 + 1 \tag{27}$$

where:

$$u_5 = K_5(q, r_0) \int_d^\infty \rho^{*2} e^{-2\rho^*} d\rho^* \tag{28}$$

$$u_6 = K_6(q, r_0) \int_d^\infty \rho^{*2} e^{-\rho^*} d\rho^* \tag{29}$$

The integrating of the previous two equations can be done using the power-n with the exponential function integral which gives the following two results:

$$u_5 = e^{2(r_0-r)q} \left[-\frac{r^2}{2q} - \frac{r}{2q^2} - \frac{1}{4q^3} \right]_d^\infty \tag{30}$$

$$u_6 = e^{(r_0-r)q} \left[-\frac{r^2}{q} - \frac{2r}{q^2} - \frac{2}{q^3} \right]_d^\infty \tag{31}$$

By substituting the integrals in the equation (27), we find the compressibility in the following equation:

$$\begin{aligned}
 (\chi_T k_B \tau T)^{-1} = & 1 + \frac{4}{3} \pi \tau d^3 - 8\pi\beta\tau E_0 e^{-(d-r_0)q} (\frac{d^2}{q} + \frac{2r}{q^2} + \frac{2}{q^3}) \\
 & + 4\pi\beta\tau E_0 e^{-2(d-r_0)q} (\frac{d^2}{2q} + \frac{d}{2q^2} + \frac{1}{4q^3})
 \end{aligned} \tag{32}$$

And we find that the compressibility term of the pressure is given in the following equation:

$$P_{Com}(\tau, T) = T k_B \int_0^\rho [1 + \frac{4\pi\tau d^3}{3} - 8\pi\beta\tau E_0 e^{-(d-r_0)q} (\frac{d^2}{q} + \frac{2r}{q^2} + \frac{2}{q^3}) + 4\pi\beta\tau E_0 e^{-2q(d-r_0)} (\frac{d^2}{2q} + \frac{d}{2q^2} + \frac{1}{4q^3})] d\tau \tag{33a}$$

By using the power-n integrals, we find:

$$\begin{aligned}
 P_C(\tau, T) = & k_B \tau T + [\frac{2\pi d^3 k_B T}{3} - 4\pi E_0 e^{-\delta^*} (\frac{d^2}{q} + \frac{2r}{q^2} + \frac{2}{q^3}) \\
 & + 2\pi E_0 e^{-2\delta^*} (\frac{d^2}{2q} + \frac{d}{2q^2} + \frac{1}{4q^3})] \tau^2
 \end{aligned} \tag{33b}$$

By substituting the equation (21) and the equation (33b) in the general formula of pressure, we find that:

$$\begin{aligned}
 P(\tau, T) \equiv & \frac{2}{3} [k_B \tau T - \frac{2\pi E_0}{3} [(1 - \beta E_0) (\frac{d^3}{1} + \frac{3d^2}{q} + \frac{6d}{q^2} + \frac{6}{q^3}) e^{-\delta^*} \\
 & + (2\beta E_0 - 1) (\frac{d^3}{2} + \frac{3d^2}{4q} + \frac{3d}{4q^2} + \frac{3}{8q^3}) e^{-2\delta^*} \\
 & - 2\beta E_0 (\frac{d^3}{3} + \frac{d^2}{3q} + \frac{2d}{9q^2} + \frac{2}{27q^3}) e^{-3\delta^*} \\
 & + \beta E_0 (\frac{d^3}{4} + \frac{3d^2}{16q} + \frac{3d}{32q^2} + \frac{3}{128q^3}) e^{-4\delta^*}] \tau^2 \\
 & + \frac{1}{3} [k_B \tau T + [\frac{2\pi d^3 k_B T}{3} - 4\pi E_0 e^{-\delta^*} (\frac{d^2}{q} + \frac{2r}{q^2} + \frac{2}{q^3}) \\
 & + 2\pi E_0 e^{-2\delta^*} (\frac{d^2}{2q} + \frac{d}{2q^2} + \frac{1}{4q^3})] \tau^2]
 \end{aligned} \tag{34}$$

and in simpler form:

$$\begin{aligned}
 P(\tau, T) \equiv & k_B \tau T - [\frac{4\pi E_0}{9} [(1 - \beta E_0) (\frac{d^3}{1} + \frac{3d^2}{q} + \frac{6d}{q^2} + \frac{6}{q^3}) e^{-\delta^*} \\
 & + (2\beta E_0 - 1) (\frac{d^3}{2} + \frac{3d^2}{4q} + \frac{3d}{4q^2} + \frac{3}{8q^3}) e^{-2\delta^*} \\
 & - 2\beta E_0 (\frac{d^3}{3} + \frac{d^2}{3q} + \frac{2d}{9q^2} + \frac{2}{27q^3}) e^{-3\delta^*} \\
 & + \beta E_0 (\frac{d^3}{4} + \frac{3d^2}{16q} + \frac{3d}{32q^2} + \frac{3}{128q^3}) e^{-4\delta^*}] \\
 & + [\frac{2\pi d^3 k_B T}{9} - \frac{4\pi E_0}{3} e^{-\delta^*} (\frac{d^2}{q} + \frac{2r}{q^2} + \frac{2}{q^3}) \\
 & + \frac{\pi E_0}{3} e^{-2\delta^*} (\frac{d^2}{q} + \frac{d}{q^2} + \frac{1}{2q^3})] \tau^2
 \end{aligned} \tag{35}$$

3. Results and discussion

The equation (35) is the basic equation of this study where that equation can be reworded using the fractional volume of the components, which is illustrated in the following equation:

$$v = d^3 \tau \frac{\pi}{6} \tag{36}$$

and the equation (35) becomes:

$$P_{tot}(v, T) = \Gamma_2 v^2 + \Gamma_1 v \tag{37}$$

where:

$$\Gamma_1 = k_B \frac{6d^{-3}}{\pi} T \tag{38}$$

$$\begin{aligned}
\Gamma_2(T) = & -\frac{16E_0}{\pi d^6} \left[(1 - \beta E_0) \left(\frac{d^3}{1} + \frac{3d^2}{q} + \frac{6d}{q^2} + \frac{6}{q^3} \right) e^{-\delta^*} \right. \\
& + (2\beta E_0 - 1) \left(\frac{d^3}{2} + \frac{3d^2}{4q} + \frac{3d}{4q^2} + \frac{3}{8q^3} \right) e^{-2\delta^*} \\
& - 2\beta E_0 \left(\frac{d^3}{3} + \frac{d^2}{3q} + \frac{2d}{9q^2} + \frac{2}{27q^3} \right) e^{-3\delta^*} \\
& \left. + \beta E_0 \left(\frac{d^3}{4} + \frac{3d^2}{16q} + \frac{3d}{32q^2} + \frac{3}{128q^3} \right) e^{-4\delta^*} \right] \\
& + \frac{8k_B T}{\pi d^3} - \frac{48E_0}{\pi d^6} e^{-\delta^*} \left(\frac{d^2}{q} + \frac{2r}{q^2} + \frac{2}{q^3} \right) \\
& + \frac{12E_0}{\pi d^6} e^{-2\delta^*} \left(\frac{d^2}{q} + \frac{d}{q^2} + \frac{1}{2q^3} \right)
\end{aligned} \tag{39}$$

It is noted from the equation (35), and the equation (37) that the total pressure of Morse oscillator is function to the fractional volume via square function. Also, we see from the two equations ((35), and (37)) that the total pressure of Morse oscillator depends on the absolute temperature, the fractional volume of the components, the depth of Morse potential, the bond distance of Morse potential, the components' diameter, and the well width parameter. Besides, it can be seen that the pressure is proportional to the square of the Morse potential well depth. In addition to that it is seen from the equation (38) that the first order virial expansion coefficient of the Morse potential does not depend on the three Morse oscillator parameters, and this first order coefficient is function to the inverse of the cube of the diameter of the components and to the linear function of the temperature. While the second order virial coefficient of Morse oscillator (from the equation (39)), depends on the Morse bond distance, the well depth of Morse potential, and the width parameter of Morse potential, and also to the diameter of the components, and temperature. Besides, it can be seen from the equation (39) that the second order virial coefficient is function to an exponential function with the width of the Morse potential and the bond distance of Morse oscillator, while this coefficient is a square function to the depth of the Morse potential. Further applications of the equation of the total pressure derived from this work can be applied to significant molecules and dimers, for instance: the dimer of phosphorus (Jia et al., 2018; Peng et al., 2018), the nitrogen gaseous, hydrogen chloride, carbon monoxide, hydrogen sulphide, and Bohr fluoride (Jia et al., 2019; Jiang et al., 2019; Wang et al., 2019, and Jia et al., 2020), and for water (Wang et al., 2021), where we can use the fittings parameters resulted from the previous studies for simulating our equation of state of Morse oscillator for further numerical results.

4. Conclusions

In this research, an analytical formula of the Morse oscillator equation of state for systems described by Morse potential in the vibrational case was derived. The mean spherical approximation for low density simple fluid for deriving the Morse oscillator equation of state. The general formula of pressure which includes the virial expansion term and the compressibility term was applied.

Based on the Morse oscillator equation of state derived in this research, it is shown that the Morse oscillator pressure depends on the absolute temperature of the components, the depth of the Morse oscillator potential well, the bond distance of Morse potential, the diameter of particle of the described system, and the compact factor. We found that the pressure of the Morse oscillator depends on the fractional volume via square function. In addition and based on the Morse oscillator equation of state derived in this research. The first two order terms of the virial Morse oscillator pressure were found, where, it was shown that the first order virial coefficient does not depend on the three Morse oscillator parameters, while only the second order virial coefficient is dependent on the three Morse oscillator parameters in addition to its dependence on the absolute temperature of the components and the diameter of the components.

We believe that the Morse oscillator equation of state which was derived in this research can be applied generally for the study for lots of systems described by the Morse oscillator interaction such as the diatomic molecules, for instance: the hydrogen chloride and the hydrogen fluoride, where this equation can be applied for the numerical calculations, however, in this work we focus on the finding of the equation of state of Morse oscillator rather than the calculating of the numerical values.

Declarations

Author contribution statement

Marwan Al-Raei: Conceived and designed the experiments; performed the experiments; analyzed and interpreted the data; contributed reagents, materials, analysis tools or data; wrote the paper.

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