Jurnal Fisika Flux: Jurnal Ilmiah Fisika FMIPA Universitas Lambung Mangkurat
Volume 22, Nomor 2, Agustus 2025
1819-796X (p-ISSN); 2541-1713 (e-ISSN)
https://ppjp.ulm.ac.id/journal/index.php/f

Vibrational Mean Energy and Specific Heat Capacity of Nitric Oxide, Nickel Monocarbide, and Scandium Nitride Diatomic Molecule with Screened Modified Pöschl-Teller Potential

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DOI: https://doi.org/doi.org/10.20527/flux.v22i2.22084

Submitted: 08 March 2025; Revised: 16 June 2025; Accepted: 24 June 2025

ABSTRACT

This study explored the energy states of a nonrelativistic system by applying the Schrödinger equation to a particular potential. Specifically, energy levels were examined using a modified Pöschl–Teller potential. This study analyzed the impact of varying quantum numbers on energy levels and investigated the vibrational mean energy and specific heat capacity of diatomic molecules. The focus was on nitric oxide, nickel monocarbide, and scandium nitride molecules to assess their behavior at different temperatures. When the screening parameter is present, the potential becomes weaker and less confining, leading to a lower energy eigenvalue compared to when there is no screening and the potential is deeper or more confining. A screened potential results in a particle having a reduced kinetic energy because it is less confined and less tightly bound to the well. An increase in quantum number leads to a decrease in the energy level of the system. The vibrational mean energy increased at high temperatures and then steadily decreased. The vibrational specific heat capacity decreased to a negative value as the temperature decreased, indicating that the system converted kinetic energy into potential energy within the bonds. These findings offer insights into molecular stability and thermodynamic behavior, which could be beneficial for predicting and managing molecules in high-temperature environments.

KEYWORDS: Schrödinger equation; diatomic molecule; mean energy; specific heat capacity

INTRODUCTION

The exactly solvable relativistic and non-relativistic quantum systems have attracted much attention from many authors since they contain all the necessary information to study quantum models (De Lima et al., 2021; Mahareeq et al., 2025). There are several traditional techniques used to solve Schrödinger-like differential equations with various quantum potentials (Abu-Shady & Khokha, 2021; Heidari et al., 2024; Inyang et al., 2022; Onate & Onyeaju, 2021). Few of these methods include the asymptotic iteration method (AIM) (Das, 2016; López et al., 2024), the Nikiforov–Uvarov (NU) method (Ikot et al., 2021; Karayer, 2020; Karayer & Demirhan, 2021; Okon et al., 2021, 2022; Parmar, 2019), and the Hypergeometric method (Naafi'ah et al., 2023; Nur 'Aini et al., 2023). The algebraic techniques that are related to the inspection of the Hamiltonian of a quantum system as in the supersymmetric quantum mechanics (SUSY QM) which is developed by Witten (Witten, 1981) and the idea of shape-invariant potential (Faniandari et al., 2020, 2022; Gordillo-Núñez et al., 2024; Grandati & Bérard, 2010; Suparmi et al., 2020; Yu et al., 2024; Zhong et al., 2022). This technique is close to the factorization method (Amirkhanov et al., 2000; Dobrogowska & Jakimowicz, 2017; Nigmatullin et al., 2022).

The shape-invariant potential is a special

class of potentials in quantum mechanics where the potential's form remains unchanged under a transformation of parameters. This property allows for solvability of the Schrödinger equation, enabling the determination of energy eigenvalues and eigenfunctions analytically. The SUSY QM method is one of the highly used techniques for computing approximate eigenvalues of the one-dimensional Schrödinger and Schrödinger-like equation (Dutta et al., 2024; Suparmi et al., 2020). The application of semiclassical methods to the study of bound states in SUSY QM gives rise to a modified semiclassical quantization rule. The semiclassical quantization rule, modified in the context of SUSY QM, provides a method for approximating energy levels of bound states by incorporating quantum corrections into classical mechanics. Writing the standard quantum problems in the SUSY form will result in the exact bound state energy spectra for a wide class of solvable potentials (Omugbe et al., 2020; Onate et al., 2021). The structure of SUSY QM motivates a modified semiclassical quantization condition which gives exact energy eigenvalues for a class of shape-invariant potentials, except appropriate Langer-like modifications (Li et al., 2020) are applied. The class of shape-invariant potentials is known to be exactly solvable, where its solution can be written in terms of analytic functions.

In this paper, we investigate the thermodynamic properties of nitric oxide (NO), nickel monocarbide (NiC), and scandium nitride (ScN) diatomic molecules. NO plays a crucial role in atmospheric chemistry and combustion processes (Huber & Herzberg, 1979). NiC is important in astrophysical research and high-temperature materials science (Nuth et al., 1985). ScN has potential applications in semiconductor technology and as a component in high-temperature ceramics (Dismukes et al., 1989). Understanding the thermodynamic properties of these molecules is essential for predicting their behavior and optimizing their use in extreme temperature environments.

The system considered in this study was influenced by the screened modified Pöschl–Teller potential, which has many applications in electrodynamics, interatomic and intermolecular forces, also it can be used to describe molecular vibrations of diatomic molecules (Cari et al., 2022; Sargsian et al., 2021). The generalized Pöschl-Teller potential is also called hyperbolic Scarf II potential (Diaf et al., 2021). Some hyperbolic and trigonometric non-central potentials are exactly solvable within the approximation of centrifugal terms and their bound state solutions have been reported in the previous papers (Faniandari et al., 2022; Ikot et al., 2020; Kasapoglu et al., 2022).

The thermodynamic properties of NO, NiC, and ScN diatomic molecules involving the vibrational mean energy and specific heat capacity are determined by using the energy eigenvalues of a quantum system. A detailed influence of the temperature on the system was simulated and analyzed in the results and discussion to understand the molecular stability and thermodynamic behavior and also to predict and control the molecule in high-temperature systems.

BASIC THEORY

The SUSY Hamiltonians that are defined from the SUSY charge operators proposed by Witten (Witten, 1981) are

$$H_{-}(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_{-}(x) \quad \text{for } V_{-}(x) = \phi^2(x) - \frac{\hbar}{\sqrt{2m}}\phi'(x) \tag{1}$$

and

$$H_{+}(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_{+}(x) \quad \text{for } V_{+}(x) = \phi^2(x) + \frac{\hbar}{\sqrt{2m}}\phi'(x) \tag{2}$$

Here H_{-} and H_{+}, are supersymmetry partners of the Hamiltonian, $V_{-}(x)$ and $V_{+}(x)$ are the SUSY partner potential. The new operators are initiated to shorten the determination of the energy level and wave function, given as

$$A^{+} = -\frac{\hbar}{\sqrt{2m}}\frac{d}{dx} + \phi(x) \text{ , and } A = \frac{\hbar}{\sqrt{2m}}\frac{d}{dx} + \phi(x) \tag{3}$$

where A^{+} is the raising operator and A is the lowering operator. The SUSY partner Hamiltonian can be defined from equation (3) with the relation

$$H_{-}(x) = A^{+}A = \left(-\frac{\hbar}{\sqrt{2m}}\frac{d}{dx} + \phi(x)\right)\left(\frac{\hbar}{\sqrt{2m}}\frac{d}{dx} + \phi(x)\right) \quad (4a)$$

$$H_{+}(x) = AA^{+} = \left(\frac{\hbar}{\sqrt{2m}}\frac{d}{dx} + \phi(x)\right)\left(-\frac{\hbar}{\sqrt{2m}}\frac{d}{dx} + \phi(x)\right) \quad (4b)$$

Thus, the multiplication of the operator results in the final SUSY partner Hamiltonian below

$$H_{-}(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \phi^2(x) - \frac{\hbar}{\sqrt{2m}}\phi'(x) \quad (4c)$$

$$H_{+}(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \phi^2(x) + \frac{\hbar}{\sqrt{2m}}\phi'(x) \quad (4d)$$

Eqs. (4c)-(4d) was similar to eqs. (1)-(2), with the substitution of $V_{-}(x)$ and $V_{+}(x)$. The ordinary Hamiltonian was recovered from the original Schrödinger potential which is used in standard (non-SUSY) quantum mechanics and eq. (1), given by

$$H(x) = H_{-}(x) + E_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - V_{-}(x) + E_0 \quad (8)$$

Respectively, the effective potential $V(x)$ can be defined with a similar form

$$V(x) = V_{-}(x) + E_0 = \phi^2(x) - \frac{\hbar}{\sqrt{2m}}\phi'(x) + E_0 \quad (9)$$

The super-potential $\phi(x)$ is determined hypothetically from eq. (8) based on the shape of effective potential from the associated system.

To determine the energy spectrum, Gendenshtein introduced the shape invariance condition (Gendenshtein, 1983). Accordingly, if the pair of supersymmetric partner potentials defined in eq. (9) are similar in shape and differ only in the parameters that appear in them, then they are said to be shape invariant. More specifically, if $V(x)$ satisfy the requirement that

$$V_{+}(x, a_j) = V_{-}(x, a_{j+1}) + R(a_{j+1}) \quad (10)$$

with

$$V_{+}(x, a_j) = \phi^2(x, a_j) + \frac{\hbar}{\sqrt{2m}}\phi'(x, a_j) \quad (11)$$

and

$$V_{-}(x, a_{j+1}) = \phi^2(x, a_{j+1}) - \frac{\hbar}{\sqrt{2m}}\phi'(x, a_{j+1}) \quad (12)$$

where $j = 0,1,2, \ldots$, and a is a parameter in the original potential $V_{-}(x)$, whose ground state energy is zero, $a_j = f_j(a_0)$ where f_j is a function applied j times, the remainder $R(a_j)$ is a's dependence but is independent of x, then $V(x)$ is said to be shaped-invariant. The remainder $R(a_j)$ and $R(a_{j+1})$ is the residual energy and represents the energy shift between the partner potentials when the shape parameter changes from a_j to a_{j+1}.

The energy eigenvalue of the Hamiltonian is given by

$$E_n{}^{(-)} = \sum_{k=1}^{n} R\,(a_k) \quad (13)$$

and by using eqs. (11), (12) and (13), the total energy spectra is given by

$$E_n = E_n{}^{(-)} + E_0 \quad (14)$$

Solution Of Schrödinger Equation For Screened Modified Pöschl-Teller Potential

The Schrödinger Equation of screened modified Pöschl-Teller Potential is proposed (Pöschl & Teller, 1933).

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\left\{\frac{\partial}{\partial r}\left(r^2\frac{\partial \Psi}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial \Psi}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial}{\partial}\right. + \frac{\hbar^2}{2m}\alpha^2\left\{\frac{\delta(\delta-1)}{\sinh^2\alpha r} - \frac{\mu(\mu+1)}{\cosh^2\alpha r}\right\}e^{-2\alpha r}(V_0 + e^{2\alpha r})\Psi = E\Psi \quad (15)$$

The Pöschl-Teller potential itself lies in the second term

$$V(r) = \frac{\hbar^2}{2m}\alpha^2\left\{\frac{\delta(\delta-1)}{\sinh^2\alpha r} - \frac{\mu(\mu+1)}{\cosh^2\alpha r}\right\}e^{-2\alpha r}(V_0 + e^{2\alpha r}) \quad (13a)$$

with V_0 as a screening parameter that represents the strength of the interaction between particles. It effectively controls the range and depth of the potential well, influencing the behavior of particles within the system and the overall shape of the potential energy curve. The other parameters involving δ, μ, and α were constant, the value is determined to shape the desired potential well.

By using the identity of $e^{-2\alpha r} = \mathrm{sech}^2\,\alpha r$ and multiplying the term of V_0 into the bracket,

the screened Modified Pöschl-Teller potential was reduced to

$$V(r)=\frac{\hbar^2}{2m}\alpha^2\begin{Bmatrix}\frac{\delta(\delta-1)(1+V_0)}{\sinh^2\alpha r}\\-2V_0\delta(\delta-1)\coth\alpha r\\+2V_0\delta(\delta-1)+\frac{\mu(\mu+1)(V_0-1)}{\cosh^2\alpha r}\\-2V_0\mu(\mu+1)\\+2V_0\mu(\mu+1)\tanh\alpha r\end{Bmatrix} \quad (16b)$$

Eq. (16b) was employed in eq. (15), resulting

$$\begin{pmatrix}-\frac{\hbar^2}{2m}\frac{1}{r^2}\begin{Bmatrix}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi}{\partial r}\right)\\+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right)\\+\frac{1}{\sin^2\theta}\frac{\partial^2\Psi}{\partial\varphi^2}\end{Bmatrix}\\+\frac{\hbar^2}{2m}\alpha^2\begin{Bmatrix}\frac{\delta(\delta-1)(1+V_0)}{\sinh^2\alpha r}\\-2V_0\delta(\delta-1)\coth\alpha r\\+2V_0\delta(\delta-1)\\+\frac{\mu(\mu+1)(V_0-1)}{\cosh^2\alpha r}\\-2V_0\mu(\mu+1)\\+2V_0\mu(\mu+1)\tanh\alpha r\end{Bmatrix}\Psi\end{pmatrix}=E\Psi \quad (17)$$

The Schrödinger equation which is expressed in eq. (17) is solved using the variable separation method by setting

$$\psi_n(\vec{r})=\frac{R(r)}{r}P(\theta)\Phi(\varphi) \quad (18)$$

then eq. (17) reduces to 3 parts:

$$\begin{pmatrix}\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial\frac{R}{r}}{\partial r}\right)\\-\frac{2m}{\hbar^2}\frac{\hbar^2}{2m}\alpha^2r^2\begin{Bmatrix}\frac{\delta(\delta-1)(1+V_0)}{\sinh^2\alpha r}\\-2V_0\delta(\delta-1)\coth\alpha r\\+2V_0\delta(\delta-1)\\+\frac{\mu(\mu+1)(V_0-1)}{\cosh^2\alpha r}\\-2V_0\mu(\mu+1)\\+2V_0\mu(\mu+1)\tanh\alpha r\end{Bmatrix}\\+\frac{2m}{\hbar^2}r^2E-l(l+1)=0\end{pmatrix} \quad (19)$$

$$\frac{1}{P\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial \mathrm{P}}{\partial\theta}\right)+l(l+1)-\frac{m^2}{\sin^2\theta}=0 \quad (20)$$

$$\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\varphi^2}+m^2=0 \quad (21)$$

The polar part of the Schrödinger equation is just associated Legendre second-order differential that has solution given as Associated Legendre Polynomial given as

$$\mathrm{P}_l^m(\theta)=N_\theta(1-w^2)^{m/2}\frac{d^mP_{l(w)}}{dw^m} \quad (22)$$

with $w=\cos\theta$ and the azimuthal wave function is $\Phi=\mathrm{N}_\varphi e^{im\varphi}$. The solution radial part of Schrödinger using SUSY QM is solved from the equation

$$\begin{aligned}&-\frac{\hbar^2}{2m}\frac{\partial^2R}{\partial r^2}\\&+\frac{\hbar^2}{2m}\alpha^2\begin{Bmatrix}\frac{\delta(\delta-1)(1+V_0)}{\sinh^2\alpha r}\\-2V_0\delta(\delta-1)\coth\alpha r\\+2V_0\delta(\delta-1)\\+\frac{\mu(\mu+1)(V_0-1)}{\cosh^2\alpha r}-2V_0\mu(\mu+1)\\+2V_0\mu(\mu+1)\tanh\alpha r\end{Bmatrix}R-ER\\&+\frac{\hbar^2}{2m}\frac{l(l+1)R}{r^2}=0\end{aligned} \quad (23)$$

The centrifugal term $\frac{1}{r^2}$ in eq. 20 diverges as $r\to\infty$ and making analytical solutions very difficult. To deal with the singular centrifugal term, the hyperbolic approximation $\frac{1}{r^2}\approx\frac{\alpha^2}{\sinh^2\alpha r}$ is used. This approximation replaces the centrifugal term $\frac{1}{r^2}$ with a smooth function that behaves similarly but remains finite as $r\to0$. By using this approximation, eq. 20 can be rewritten as

$$\begin{aligned}&-\frac{\hbar^2}{2m}\frac{\partial^2R}{\partial r^2}\\&+\frac{\hbar^2}{2m}\alpha^2\begin{Bmatrix}\frac{\delta(\delta-1)(1+V_0)+l(l+1)}{\sinh^2\alpha r}\\-2V_0\delta(\delta-1)\coth\alpha r\\+2V_0\delta(\delta-1)\\+\frac{\mu(\mu+1)(V_0-1)}{\cosh^2\alpha r}-2V_0\mu(\mu+1)\\+2V_0\mu(\mu+1)\tanh\alpha r\end{Bmatrix}R\\&-ER=0\end{aligned} \quad (24)$$

and setting the effective potential as

$$V_{eff}(r)=\frac{\hbar^2}{2m}\alpha^2\begin{Bmatrix}\frac{\delta(\delta-1)(1+V_0)+l(l+1)}{\sinh^2\alpha r}\\-2V_0\delta(\delta-1)\coth\alpha r\\+\frac{\mu(\mu+1)(V_0-1)}{\cosh^2\alpha r}\\+2V_0\mu(\mu+1)\tanh\alpha r\end{Bmatrix} \quad (25)$$

So that

$$E'=E-2\frac{\hbar^2}{2m}\alpha^2V_0\delta(\delta-1)+2\frac{\hbar^2}{2m}\alpha^2V_0\mu(\mu+1) \quad (26)$$

then the main equation became

$$\begin{aligned}&-\frac{\hbar^2}{2m}\frac{\partial^2R}{\partial r^2}\\&+\frac{\hbar^2}{2m}\alpha^2\begin{Bmatrix}\frac{\delta(\delta-1)(1+V_0)+l(l+1)}{\sinh^2\alpha r}\\-2V_0\delta(\delta-1)\coth\alpha r\\+\frac{\mu(\mu+1)(V_0-1)}{\cosh^2\alpha r}\\+2V_0\mu(\mu+1)\tanh\alpha r\end{Bmatrix}R-E'R\\&=0\end{aligned} \quad (27)$$

From the energy potential function expressed in eq. (25) then the hypothetical superpotential was proposed to match with the hyperbolic function, involving $\frac{1}{\sinh^2\alpha r}$, $\coth\alpha r$, $\frac{1}{\cosh^2\alpha r}$, and $\tanh\alpha r$. From the table of potential and superpotential pairs (Suparmi, 2011), all those terms are reproduced in a linear combination below

$$\phi = \frac{\hbar\alpha}{\sqrt{2m}}(A\coth\alpha r\ + B\tanh\alpha r + C) \quad (28)$$

and by using the relations of

$$V_{eff}(r) = \phi^2 - \frac{\hbar}{\sqrt{2m}}\phi' + \varepsilon_0 \quad (29)$$

the hypothetical superpotential in eq. (28) was became

$$\begin{aligned}&\phi^2 - \frac{\hbar}{\sqrt{2m}}\phi' + \varepsilon_0\\ &= \frac{\hbar^2}{2m}\alpha^2\begin{pmatrix} A^2\coth^2\alpha r + A\mathrm{csch}^2\alpha r + 2AB \\ +2AC\coth\alpha r + B^2\tanh^2\alpha r \\ -B\,\mathrm{sech}^2\alpha r\ + 2BC\tanh\alpha r + C^2\end{pmatrix} + \varepsilon_0\end{aligned} \quad (30)$$

Substituting the effective potential from eq. (22) to the left side of eq. (26) and substituting eq. (30) into the right side of eq. (29), the equal relation is become

$$\begin{aligned}&\frac{\hbar^2}{2m}\alpha^2\begin{Bmatrix}\frac{\delta(\delta-1)(1+V_0)+l(l+1)}{\sinh^2\alpha r} \\ -2V_0\delta(\delta-1)\coth\alpha r \\ +\frac{\mu(\mu+1)(V_0-1)}{\cosh^2\alpha r} \\ +2V_0\mu(\mu+1)\tanh\alpha r\end{Bmatrix}\\ &= \frac{\hbar^2}{2m}\alpha^2\begin{pmatrix}(A^2+A)\,\mathrm{csch}^2\alpha r + A^2 + 2AB \\ +2AC\coth\alpha r - (B^2+B)\,\mathrm{sech}^2\alpha r \\ +B^2 \\ +2BC\tanh\alpha r + C^2\end{pmatrix}\\ &+ \varepsilon_0\end{aligned} \quad (31)$$

Equating the coefficient of the same term on the left and right sides in eq. (28), it can be inferred the relations of:

The coefficient of $\frac{1}{\sinh^2\alpha r}$:

$$(\delta(\delta-1)(1+V_0) + l(l+1)) = (A^2 + A) \quad (32)$$

the coefficient of $\coth\alpha r$:

$$2\delta(\delta-1)V_0 = -2AC \quad (33)$$

the coefficient of $\frac{1}{\cosh^2\alpha r}$:

$$-\mu(\mu+1)(-1+V_0) = (B^2+B) \quad (34)$$

the coefficient of $\tanh\alpha r$:

$$2\mu(\mu+1)V_0 = 2BC \quad (35)$$

and the constant:

$$\frac{\hbar^2}{2m}\alpha^2(2AB + A^2 + B^2 + C^2) + \varepsilon_0 = 0 \quad (36)$$

So that, with the substitution and elimination method, resulting

$$A = -\left[\frac{1}{2} + \sqrt{\left(\delta(\delta-1)(1+V_0) + \left(l+\frac{1}{2}\right)^2\right)}\right] \quad (37)$$

$$B = -\left[\frac{1}{2} - \sqrt{\frac{1}{4} - \mu(\mu+1)(-1+V_0)}\right] \quad (38)$$

$$C = \frac{\mu(\mu+1)V_0 - \delta(\delta-1)V_0}{\left[-\sqrt{\left(\delta(\delta-1)(1+V_0) + \left(l+\frac{1}{2}\right)^2\right)} + \sqrt{\frac{1}{4} - (-1+V_0)\mu(\mu+1)} - 1\right]} \quad (39)$$

and the ground state energy was given by

$$\begin{aligned}\varepsilon_0 = &-\frac{\hbar^2}{2m}\alpha^2\left(\frac{\mu(\mu+1)V_0 - \delta(\delta-1)V_0}{B+A}\right)^2\\ &-\frac{\hbar^2}{2m}\alpha^2(A+B)^2\end{aligned} \quad (40)$$

The superpartner potential is defined by

$$\begin{aligned}V_- = &\frac{\hbar^2}{2m}\alpha^2 A(A+1)\,\mathrm{csch}^2\alpha r + 2\frac{\hbar^2}{2m}\alpha^2 AC\coth\alpha r\\ &-\frac{\hbar^2}{2m}\alpha^2 B(B+1)\,\mathrm{sech}^2\alpha r\\ &+2\frac{\hbar^2}{2m}\alpha^2 BC\tanh\alpha r\\ &+\frac{\hbar^2}{2m}\alpha^2(C^2 + (A+B)^2)\end{aligned} \quad (41)$$

and

$$\begin{aligned}V_+ = &\frac{\hbar^2}{2m}\alpha^2 A(A-1)\,\mathrm{csch}^2\alpha r + 2\frac{\hbar^2}{2m}\alpha^2 AC\coth\alpha r\\ &-\frac{\hbar^2}{2m}\alpha^2 B(B-1)\,\mathrm{sech}^2\alpha r\\ &+2\frac{\hbar^2}{2m}\alpha^2 BC\tanh\alpha r\\ &+\frac{\hbar^2}{2m}\alpha^2 C^2 + \frac{\hbar^2}{2m}\alpha^2(A+B)^2\end{aligned} \quad (42)$$

By using eqs. (10), (11), (12), (41), and (42) the shape-invariant parameters can be obtained by

$$\begin{aligned}&a_0 = A;\ a_1 = A-1;\ \ a_2 = A-2, \ldots\\ &b_0 = B;\ b_1 = B-1;\ b_2 = B-2\,, \ldots\end{aligned} \quad (43)$$

a_0 and b_0 are the initial parameter, so that it is set to be constant and similar (requisite the shape-invariance). Following by a_j with j = 1,2,3, ... are the shifted parameters, reduced from the initial parameter with an integer. By applying parameters in equation (43), the new superpartner potential was given by

$$\begin{aligned}&V_-(a_1, b_1)\\ &= \frac{\hbar^2}{2m}\alpha^2 A(A-1)\mathrm{csch}^2\alpha r + 2\frac{\hbar^2}{2m}\alpha^2 AC\coth\alpha r\\ &-\frac{\hbar^2}{2m}\alpha^2 B(B-1)\,\mathrm{sech}^2\alpha r + 2\frac{\hbar^2}{2m}\alpha^2 BC\tanh\alpha r\\ &+\frac{\hbar^2}{2m}\alpha^2\left\{\frac{\mu(\mu+1)V_0 - \delta(\delta-1)V_0}{[A+B\ -\ 2]}\right\}^2 + \frac{\hbar^2}{2m}\alpha^2(A\\ &+B-2)^2\end{aligned} \quad (44)$$

The energy spectra associated with $H_$that are obtained from eq. (13) was defined by

$$\begin{aligned}&E_n^{(-)}\\ &= \frac{\hbar^2}{2m}\alpha^2\left\{\alpha^2\frac{\mu(\mu+1)V_0 - \delta(\delta-1)V_0}{[A+B\,]}\right\}^2\\ &+\frac{\hbar^2}{2m}\alpha^2(A\\ &+B)^2 - \frac{\hbar^2}{2m}\alpha^2\left\{\alpha^2\frac{\mu(\mu+1)V_0 - \delta(\delta-1)V_0}{[A+B\ -\ 2n]}\right\}^2\\ &-\frac{\hbar^2}{2m}\alpha^2(A+B-2n)^2\end{aligned} \quad (45)$$

$$\begin{aligned}E'_n = &\frac{\hbar^2}{2m}\alpha^2\left(-\left\{\alpha^2\frac{\mu(\mu+1)V_0 - \delta(\delta-1)V_0}{[A+B\ -\ 2n]}\right\}^2\right.\\ &\left.-\frac{\hbar^2}{2m}\alpha^2(A+B-2n)^2\right)\end{aligned} \quad (46)$$

Finally, the energy spectra of the system from eqs. (28) and (46) were obtained as

$$E = \left(-\frac{\hbar^2}{2m}\alpha^2 \left\{ \frac{\mu(\mu+1)V_0 - \delta(\delta-1)V_0}{[A+B-2n]} \right\}^2 - \frac{\hbar^2}{2m}\alpha^2(A+B-2n)^2 \right) + 2\frac{\hbar^2}{2m}\alpha^2\mu(\mu+1)V_0 - 2\frac{\hbar^2}{2m}\alpha^2\delta(\delta-1)V_0 \quad (47)$$

that gives

$$E_n = \left(-\frac{\hbar^2}{2m}\alpha^2 \left\{ \frac{\mu(\mu+1)V_0 - \delta(\delta-1)V_0}{-2\left[\frac{1}{2}\sqrt{\begin{pmatrix}(\delta(\delta-1)\\(1+V_0))\end{pmatrix} + \left(l+\frac{1}{2}\right)^2} - \frac{1}{2}\sqrt{\frac{1}{4} - (\mu(\mu+1)\\(-1+V_0))} + n + \frac{1}{2} \right]} \right\}^2 \right) + 2\frac{\hbar^2}{2m}\alpha^2\{\mu(\mu+1)V_0 - \delta(\delta-1)V_0\} - \frac{\hbar^2}{2m}\alpha^2 4 \left\{ \frac{1}{2}\sqrt{\frac{1}{4} - \mu(\mu+1)(-1+V_0)} - \frac{1}{2}\sqrt{\begin{pmatrix}\delta(\delta-1)(1+V_0)\\ +\left(l+\frac{1}{2}\right)^2\end{pmatrix}} + n + \frac{1}{2} \right. \quad (48)$$

By setting a new parameter

$$4\eta = \mu(\mu+1)V_0 - \delta(\delta-1)V_0 \quad (49)$$

$$\kappa = \frac{1}{2}\left(\sqrt{\delta(\delta-1)(1+V_0) + \left(l+\frac{1}{2}\right)^2} - \sqrt{\frac{1}{4} - \mu(\mu+1)(-1+V_0)} + 1 \right) \quad (50)$$

then energy eigenvalue in eq. (48) was rewritten as

$$E_n = -\frac{16\hbar^2\alpha^2}{2m}\left\{ \left(\frac{\eta}{2(\kappa+n)} - \frac{(\kappa+n)}{2} \right)^2 \right\} \quad (51)$$

If the modified Pöschl-Teller potential is without screening parameter ($V_0 = 0$), the energy spectra in eq. (51) was reduced to

$$E_n = -\frac{\hbar^2}{2m}\alpha^2 \left\{ \sqrt{\frac{1}{4} + \mu(\mu+1)} - \sqrt{\left(\delta(\delta-1) + \left(l+\frac{1}{2}\right)^2 \right)} - 2n - 1 \right\}^2 \quad (52)$$

and can be rewritten as

$$E_n = A\{\eta' - n\}^2 \quad (53)$$

with

$$\eta' = \frac{1}{2}\left(\sqrt{\frac{1}{4} + \mu(\mu+1)} - \sqrt{\left(\delta(\delta-1) + \left(l+\frac{1}{2}\right)^2 \right)} - 1 \right) \quad (54)$$

and

$$A = -\frac{4\hbar^2}{2m}\alpha^2 \quad (55)$$

The energy eigenvalue with and without screening parameters is shown in eqs. (51) and (52) were numerically calculated with various values of the radial quantum number n and orbital quantum number ℓ.

In the case of there being no screening parameter, the vibrational partition function, vibrational mean energy, and specific heat are obtained from the non-relativistic energy equation in eq. (53). The vibrational partition function is defined as (Onate et al., 2021)

$$Z(\eta', \beta) = \sum e^{-\beta E_{nl}}, \beta = \frac{1}{kT} \quad (56)$$

with k as the Boltzmann constant, and E_{nl} as the non-relativistic energy spectrum of the system. By eq. (53) and by setting $\frac{1}{\tau^2} = \beta A$ then the partition function in eq. (56) became

$$Z(\eta', \beta) = \sum_0^{\frac{\eta'}{\tau}} e^{-\left\{\frac{\eta'-n}{\tau}\right\}^2} \quad (57)$$

In the classical regime when the temperature T, is high enough, then the value of η' is high, and β is small therefore eq. (57) could be written in integral form as

$$Z(\eta', \beta) = \tau\frac{\sqrt{\pi}}{2} erf\left(\frac{\eta'}{\tau}\right) \quad (58)$$

with $y = \frac{n-\eta'}{\tau}$ and erf is the error function given as

$$erf(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2} dt \quad (59)$$

The vibrational specific heat and the vibrational mean energy are defined as (Ikhdair & Falaye, 2013)

$$U(\beta, \eta') = -\frac{\partial}{\partial\beta}\ln Z(\eta', \beta) \quad (60)$$

$$C = -\frac{\partial}{\partial T}U = -k\beta^2\frac{\partial}{\partial\beta}U \quad (61)$$

RESULTS AND DISCUSSION

In the numerical calculations, the natural unit parameters $\hbar = 1,\ \alpha = 0.01,\ m = 1fm^{-1}$ were used. The energy of the system with the variation of l ($\delta = 0{,}001;\ \mu = 0{,}002$) is shown in Table 1. Energy spectra En with the variation of n and ℓ quantum numbersTable 1 and Figure 1.

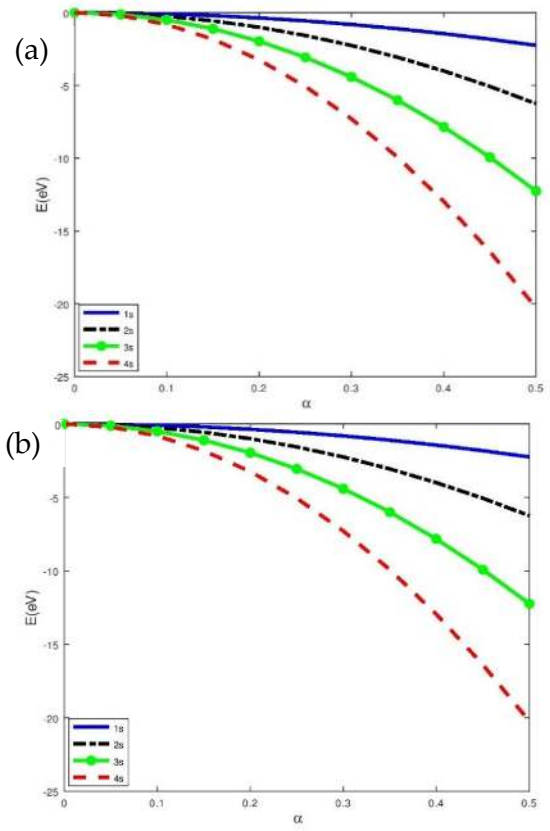

Figure 1. The variation of the energy eigenvalues as a function of potential parameter α: (a) with screening parameter, (b) without screening parameter.

From Table 1 and Figure 1, the energy spectra have a negative value for the selected quantum number. The increase of the quantum number will affect the decrease of the energy spectra of the system. There is no significant change in the energy eigenvalue for the case with the screening parameter and without the screening parameter. Compared to the computational research conducted by (Oluwadare & Oyewumi, 2018), for the system with diatomic molecule NiC and ScN, also had a negative value of energy spectra. The energy level at *l=0* and *n*=1 of ScN is −4.511606254 eV, and −2.704420808 eV for NiC. They considered a system confined by the shifted Deng-Fan potential. The different confining potentials cause the energy of the system to be different.

Table 1. Energy spectra E_n with the variation of n and ℓ quantum numbers.

ℓ	n	E_n (eV) with screening parameter	E_n (eV) without screening parameter
0	1	-0.0008983	-0.0008982
	2	-0.0025013	-0.0024970
	3	-0.0049042	-0.0048958
	4	-0.0081071	-0.0080946
	5	-0.0121100	-0.0120930

It can be only seen in the numerical results, that the energy eigenvalue without the screening parameter is lower (in a small number) than the energy eigenvalue with the screening parameter. The potential that is screened causes the particle to have less kinetic energy because the particle is less confined by the well and the particle is less tightly bound to the well. Physically, the particle's wavefunction extends further out and the energy eigenvalue decreases. Thus, when the screening parameter is present, the potential is weaker (less confining), which results in a lower energy eigenvalue compared to the case where there is no screening, and the potential is deeper (more confining).

In the case there is no screening parameter, the vibrational mean energy from the eq. (60) and specific heat from the eq. (61) were simulated for the diatomic molecule, namely NO, NiC, and ScN with the parameters in Table 2. Despite slight differences in mass, these molecules are expected to exhibit similar trends, so that the energy spectra, vibrational mean energy, and specific heat capacity can be figured out.

Table 2. Parameters for the diatomic molecules (Oluwadare & Oyewumi, 2018; Sever et al., 2007)

Molecule	***m* (in amu)**
NO	7.4684410
NiC	9.9742650
ScN	10.682771

For the given value of η' and unit of τ, the dependence of the vibrational partition function Z on β is shown for NO, NiC, and ScN diatomic molecules. It is found that the Z increases when β and η' increase for the three molecules. This

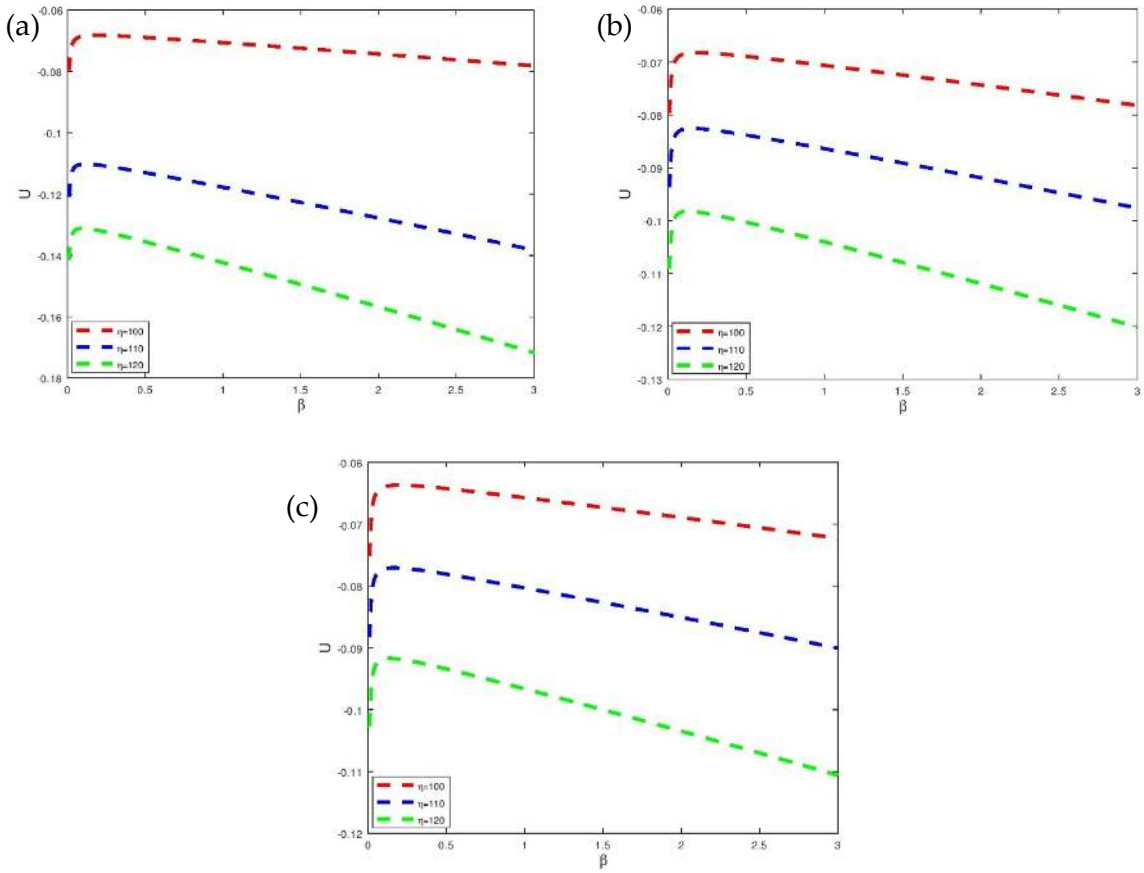

Figure 2. Vibrational mean energy (U) of diatomic molecules as a function of β for different η': (a) NO, (b) NiC, (c) ScN.

means that the diatomic molecules are sensitive to the various values of the temperature parameters β and η'. It is shown in Figure 2 that the vibrational mean energy U first increases for the small value of β and η', and then decreases monotonically with the increasing parameters β and η', respectively. At very high temperatures (small value of β), the system approaches the classical limit, so that it behaves classically and many vibrational modes are fully excited. As the temperature decreases from extremely high levels, anharmonic effects and the shift from classical to quantum behavior lead to an apparent increase in the vibrational mean energy, as the system reorganizes and adjusts to a more thermally stable state. After reaching the peak, the vibrational mean energy decreases with temperature because as the temperature drops, the population of higher-energy vibrational states diminishes. At lower temperatures (high value of β), fewer states are thermally excited, and the system predominantly occupies lower energy states, leading to a decrease in the vibrational mean energy.

Figure 3 shows the vibrational specific heat of the system C ($k = 1$) that decreases with the increasing value of temperature parameters β and η' to the negative value. Heat capacity is defined as the change in heat compared with temperature changes, then if in this case, C is negative it can mean that the system loses energy, for example by radiating energy when vibrating. Heat capacity is also defined as the energy absorbed when the system temperature rises by one degree Celsius. This process can explained due to the thermal conductivity of molecules that arises through lattice vibrations, so it can be concluded that the thermal conductivity of diatomic molecules is selected according to the phonon heat capacity (Zhao et al., 2017).

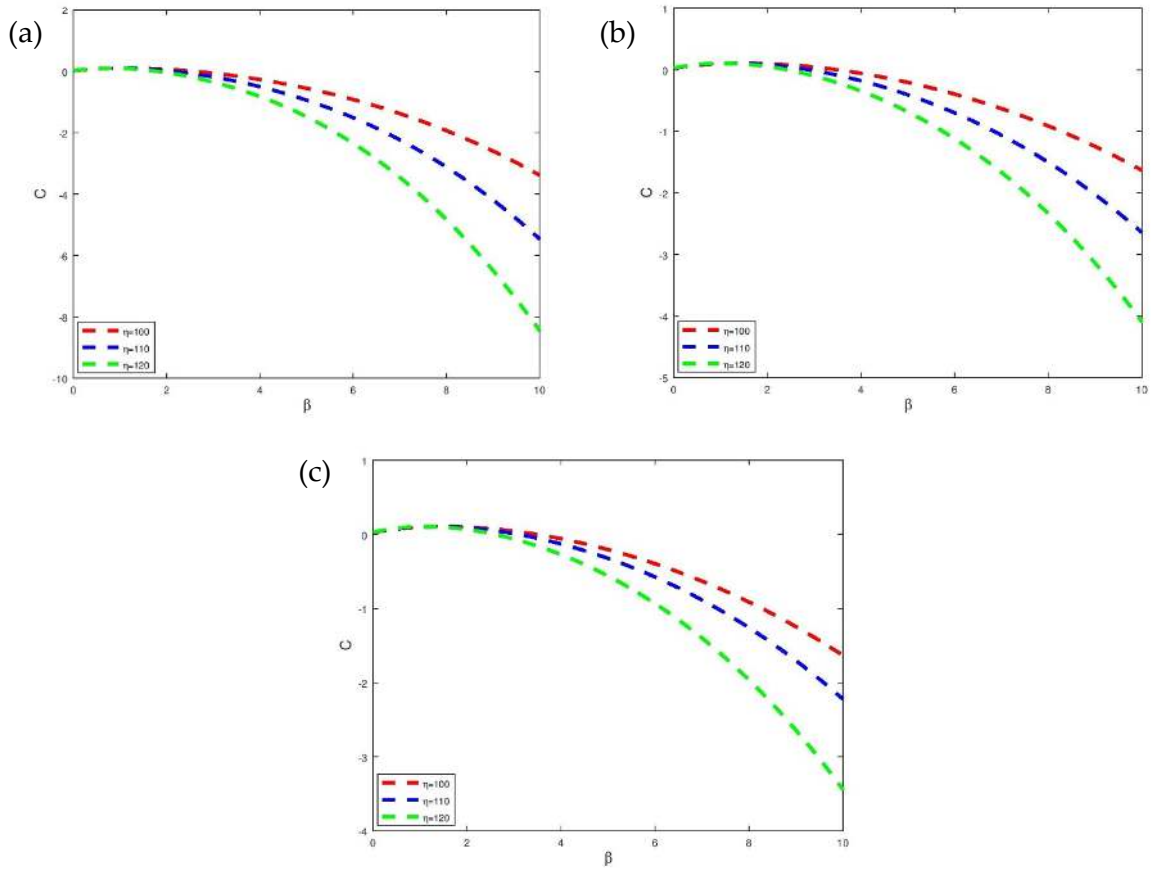

Figure 3. Vibrational specific heat (*C*) of diatomic molecules as a function of β for different : (a) NO, (b) NiC, (c) ScN.

The curves for different η' are splitting away from each other at higher values of β. The vibrational specific heat capacity decreases with decreasing temperature due to quantum mechanical effects, specifically the behavior of vibrational energy levels in solids. As the temperature decreases, fewer vibrational states are thermally accessible due to quantum restrictions, leading to a decrease in vibrational-specific heat capacity. This phenomenon is related to the modified Pöschl-Teller potential that influenced the system. The potential of introducing anharmonic effects reduces the rate of decrease in heat capacity at low temperatures (high value of β) compared to a purely harmonic oscillator. However, at very low temperatures, quantum effects still dominate, leading to a decrease in heat capacity as expected.

Overall, the NO, NiC, and ScN diatomic molecules have slightly different energy levels, vibrational mean energy, and specific heat capacity. This is due to their mass which are close to each other. So, mathematically the differences in the numerical calculation of the three molecules are not much different and can be figured in one graph.

CONCLUSION

The vibrational mean energy and specific heat capacity have been obtained for modified Pöschl-Teller potential. The solution of the Schrödinger equation has been obtained by applying the SUSY QM method to find the eigenvalues. By varying the existence of screening parameters and quantum number, the energy level shows a change and shift to lower energies. The screening parameter has a small effect on the energy spectra. The analysis of the vibrational partition function and vibrational mean energy for NO, NiC, and ScN diatomic molecules demonstrates their

temperature sensitivity. The vibrational mean energy initially increases at small values of temperature, reaching a peak, and then decreasing as the parameters continue to grow. At high temperatures, the system behaves classically and as the temperature decreases, quantum effects and anharmonicity lead to a temporary increase in vibrational mean energy as the system reorganizes. The vibrational specific heat capacity decreases as temperature increases, even reaching negative values, suggesting a conversion of kinetic energy into potential energy within molecular bonds. This decline in heat capacity is primarily due to quantum mechanical restrictions, which limit thermal access to higher vibrational states at low temperatures. The modified Pöschl-Teller potential influences this behavior by introducing anharmonicity, which slows the rate of decrease in heat capacity compared to a purely harmonic system.

This study's findings have significant implications for materials science and astrophysics. In materials science, understanding the vibrational properties and thermodynamic behavior of diatomic molecules like NO, NiC, and ScN is crucial for developing new materials with specific thermal characteristics. The observed decrease in vibrational specific heat capacity at low temperatures could be exploited in the design of cryogenic materials or applications requiring precise thermal management at extreme conditions. In astrophysics, these results provide insights into the behavior of molecules in various cosmic environments. The temperature-dependent properties of diatomic molecules could help explain spectral observations of cool stars or planetary atmospheres, where these molecules may be present.

However, this study has several limitations. The use of the modified Pöschl-Teller potential, while providing valuable insights, is an approximation of real molecular interactions. Additionally, the study focuses on isolated diatomic molecules and does not account for intermolecular interactions or external fields that may be present in real-world scenarios. Future work could address these limitations by incorporating more complex potential models to better approximate real molecular interactions, extending the analysis to polyatomic molecules and molecular clusters, and investigating the effects of external fields or high-pressure environments on molecular vibrational properties. These extensions would further enhance our understanding of molecular behavior across various temperature regimes.

ACKNOWLEDGEMENT

This research was supported by the High Reputable of International Scientific Publication (RPIBT), Universitas Diponegoro with contract number 222-681/UN7.D2/PP/IV/2025.

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