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# Analytical and Computational Study of Bound States in Quantum Systems with Topological Defects under the Morse-Hulthén Interaction Potential

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## Abstract

Approximate solutions of the Schrödinger equation (SE) for the Morse-Hulthén potential (MHP) in cosmic string spacetime were obtained using the Nikiforov–Uvarov (NU) method together with an improved approximation scheme for the centrifugal term. Closed-form expressions for the energy spectra and normalized wave functions were derived. The Hellmann-Feynman theorem (HFT) was used to determine the expectation values of the inverse-squared distance, the kinetic energy and the momentum squared. Numerical investigations were carried out for $H_2$, HCl and LiH diatomic molecules under the influence of the cosmic string topological parameter $\alpha$ and the potential strength $V_0$. The results showed that the topological defect has a significant effect on the rotational–vibrational spectrum of the molecular system through the angular deficit parameter, thereby breaking the usual angular degeneracy of the states. Furthermore, it was observed that an increase in the potential strength deepens the bound states, whereas increasing the quantum numbers reduces the binding energy of the system. The present results reduce to the ordinary flat space in the limit $\alpha \rightarrow 1$. Moreover, the obtained solutions recover the standard Morse and Hulthén potentials as special cases and are consistent with previous studies on exponential-type potentials and quantum systems in curved spacetime geometries reported in the literature. Therefore, the study provides useful insight into the effects of spacetime topology on molecular quantum systems and contributes to the applications of quantum mechanics in curved spacetime and molecular spectroscopy.

**Keywords:** Cosmic string topological defects; Morse-Hulthén potential; Schrödinger equation; Hellmann–Feynman theorem; Diatomic molecules

## 1. Introduction

The search for exact and approximate solutions to the SE remains one of the most permanent and fundamental undertaking in quantum mechanics [1, 2]. The obtained analytical solutions for energy and wave function have led to a deep understanding of the behavior of quantum systems spanning a wide range of physical situations; from the scattering properties of nuclear particles to the vibrational spectra of diatomic molecules [3, 4]. Over the last century, a large number of interaction potentials have been proposed and studied. Among these the Morse potential and the Hulthén potential are particularly significant and versatile, since each encodes crucial physical characteristics that makes them vital tools in theoretical physics and chemical physics [5, 6].

The Morse potential, proposed in 1929 by Philip M. Morse to describe the vibrational spectra of diatomic molecules, represents a significant advance in molecular quantum mechanics [7]. The Morse potential models the vibrational

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structure of diatomic molecules better than the simple harmonic oscillator by incorporating anharmonicity and bond dissociation through its exponential form, accurately representing the potential energy curve of a diatomic molecule from the equilibrium bond length to the bond-breaking limit [8, 9]. The Morse potential is analytical tractable and this property has made it a cornerstone of molecular spectroscopy. Its solutions have been widely investigated using a remarkable variety of mathematical methods, including the asymptotic iteration method (AIM), NU method, supersymmetric quantum mechanics (SUSY QM), hypervirial perturbation methods, and the shifted $1/N$ expansion approach [10, 11, 12, 13]. The importance of the Morse potential rests on the fact that its SE admits closed-form solutions for all bound states, a rare property among anharmonic potentials that has established its status as a fundamental model in quantum mechanics [14].

Similarly, the Hulthén potential formulated by Hulthén in 1942 has been equally invaluable, predominantly in the domains of nuclear and atomic physics [15]. Being a screened Coulomb potential, the Hulthén potential successfully models the interaction between charged particles when the long-range Coulomb tail is partially screened by other charges [16, 17]. This makes it especially apt for characterizing electron-atom scattering, deuteron-proton interactions, and other phenomena where the pure Coulomb potential fails due to screening effects [18, 19]. Like the Morse potential, the Hulthén potential is analytically solvable for s-waves, and considerable literature exists on its exact and approximate solutions using methods such as, the Nikiforov-Uvarov Functional Analysis method, SUSY QM, the shifted $1/N$ expansion, and the NU method [20, 21, 22, 23]. Furthermore, the Hulthén potential has been solved successfully for relativistic wave equations including the Dirac, Klein-Gordon, and Duffin-Kemmer-Petiau equations, indicating its applicability in both relativistic and non-relativistic quantum mechanics [24, 25].

However, the idealized forms of isolated single potentials rarely represent physical reality [26]. Often, different types of interactions coexist and compete in real quantum systems. The combination of the Morse and the Hulthén potentials into a single framework, the Morse- Hulthén potential (MHP), offers a more sophisticated and realistic description of interacting quantum systems, particularly in situations where both molecular bonding and screened Coulomb interactions play dominant roles. Such hybrid potentials have been used to describe complex molecular systems, semiconductor heterostructures, nuclear scattering processes, and even certain cosmological scenarios where multiple interaction scales are present [27, 28, 29]. The combined potential is of the form:

$$V(r) = D_e\left(1-e^{-\delta(r-r_e)}\right)^2 - \frac{V_0 e^{-\delta r}}{1-e^{-\delta r}} \tag{1}$$

Recent investigations have established the advantage of combining these potentials. Considerable interest has been shown in the theoretical study of rotating potentials, including the rotating Morse and Hulthén potentials for non-zero angular momentum states [30, 31]. The range of applicability of these potentials have been significantly extended by these generalizations and enabled their use in three-dimensional problems with nonzero angular momentum quantum numbers. Bayrak and Boztosun [32] have astutely used AIM method to obtain exact analytical solutions of the radial Schrödinger equation for both the Morse and Hulthén potentials for arbitrary quantum numbers. Their method uses a clever approximation to the centrifugal potential which reduces the radial equation to a form convenient for AIM analysis [33].

An important and rapidly developing research area in theoretical physics concerns the influence of topological defects (line-like, point-like, or planar defects in spacetime that arise from symmetry-breaking phase transitions in the early universe) on the behavior of quantum systems [34, 35]. Cosmic strings are one of the most interesting of these defects and they are linear topological defects predicted by various grand unified theories and cosmological models [36]. Cosmic strings produce conical spacetime geometries with non-trivial curvature concentrated along the string axis, characterized by an angular deficit parameter α that changes the local geometry from flat Minkowski space to a cone with deficit angle $2\pi(1-\alpha)$ [37, 38]. Letelier [39] gave fundamental insights into spacetimes with Riemann-Christoffel curvature tensors characterized by directional derivatives of Dirac distributions with support in parallel lines, providing the mathematical framework for understanding cosmic strings with multipolar structure [40].

The line element for a cosmic string spacetime is

$$ds^2 = -dt^2 + dr^2 + \alpha^2 r^2 d\phi^2 + dz^2, \tag{2}$$

where

$0<\alpha<1$ is the topological defect parameter, and $\alpha=1$ corresponds to flat spacetime.

In spite of the extensive work on the analytical solution of the SE for the Morse and Hulthén potentials individually and in combination [41, 42], and the quantum dynamics of particles in cosmic string and other topological defect backgrounds [43, 44], a noteworthy and noticeable gap exists at the intersection of these two research domains. In particular, the problem of analytically solving the SE with a combined MHP in the background of a cosmic string topological defect remains entirely unexplored.

The existing literature, while considerable, show a clear distinction between studies of exponential-type potentials in flat spacetime and studies of quantum systems in curved or topologically nontrivial backgrounds with simple potentials [45]. Investigations of the Morse potential in curved backgrounds are almost non-existent, and the Hulthén potential has only been considered in curved spacetime in a few cases, usually with significant simplifying assumptions [46,47]. The combined MHP, which would naturally arise in physical scenarios where both molecular bonding and screened Coulomb interactions are present in a topologically defective background, has never been treated analytically. This knowledge gap motivates the present study which seeks to establish the first analytical treatment of the Schrödinger equation for the combined MHP in a cosmic string background. Using the NU method in conjunction with appropriate approximations for the modified centrifugal term, we will derive closed-form expressions for bound state energy eigenvalues and radial wave functions. The influence of the cosmic string's angular deficit parameter $\alpha$ on the energy spectrum will be systematically analyzed, and the interplay between potential parameters and topological parameters will be explored.

This study not only generalizes previous flat-space solutions to a geometrically non-trivial setting but also establishes a foundation for subsequent investigations of quantum information measures, scattering phenomena, and relativistic generalizations in topologically defective spacetimes. The results obtained herein will contribute to a greater understanding of the quantum behavior of particles at the rich interface between potential theory, quantum mechanics, and gravitational topology.

## 2. Solutions of the Schrödinger equation with MHP in the cosmic string topology

We employ the NU method in this study. The details can be found in Ref. [48]. In the spacetime background of a cosmic string, the radial Schrödinger equation with Laplace–Beltrami operator is of the form

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)+\frac{1}{\alpha^2 r^2}\frac{\partial^2}{\partial\phi^2}\right)+V\left(r\right)\right]\Psi\left(r,\phi\right)=E\Psi\left(r,\phi\right) \tag{3}$$

Let the wavefunction ansatz be $\Psi\left(r,\phi\right)=\frac{R(r)}{\sqrt{r}}e^{im\phi}$. Substituting Eq. (1) into Eq. (3) gives

$$\frac{d^2R_{nm}(r)}{dr^2}+\left[\frac{2\mu}{\hbar^2}\left(E_{nm}-\left(D_e+Ae^{-2\delta r}-Be^{-\delta r}-\frac{V_0e^{-\delta r}}{1-e^{-\delta r}}\right)\right)-\frac{\left(\frac{m^2-\frac{1}{4}\alpha^2}{\alpha^2}\right)}{r^2}\right]R_{nm}(r)=0 \tag{4}$$

where the cosmic string modifies the centrifugal term through $\alpha$, $R_{nm}(r)$ is the eigenfunctions, $E_{nm}$ is the energy eigenvalues, $n$ and $m$ represents the principal and magnetic quantum numbers of all possible solutions, $\mu$ is the reduced mass of the system, $\hbar$ is the reduced Planck's constant, $A=D_e e^{2\delta r_e}$, $B=2D_e e^{\delta r_e}$ and $r$ is radial distance from the origin.

With the proposed potential, an exact solution of Eq. (4) cannot be obtained because of the centrifugal barrier. To overcome this difficulty, we use the improved Pekeris-type approximation scheme [49].

$$\frac{1}{r^2} \approx \delta^2 \left[ c_0 + \frac{e^{-\delta r}}{\left(1 - e^{-\delta r}\right)^2} \right] \tag{5}$$

where $c_0 = \frac{1}{12}$ for the Greene–Aldrich-type approximation. Substituting Eq. (5) into Eq. (4) gives

$$\frac{d^2 R_{nm}(r)}{dr^2} + \left[ \frac{2\mu E}{\hbar^2} - \frac{2\mu D_e}{\hbar^2} + \frac{2\mu B}{\hbar^2} e^{-\delta r} - \frac{2\mu A}{\hbar^2} e^{-2\delta r} + \frac{2\mu V_0}{\hbar^2} \frac{e^{-\delta r}}{1 - e^{-\delta r}} - \eta_m \delta^2 c_0 - \eta_m \delta^2 \frac{e^{-\delta r}}{\left(1 - e^{-\delta r}\right)^2} \right] R_{nm}(r) = 0 \tag{6}$$

Changing the variable $s = e^{-\delta r}, \ 0 < s < 1$ in Eq. (6) and simplifying leads to

$$s^2 R''(s) + s R'(s) + \left[ -\varepsilon + \beta s - \gamma s^2 + \frac{\chi s}{1-s} - \frac{\eta_m s}{(1-s)^2} \right] R(s) = 0, \tag{7}$$

where

$$\varepsilon = -\frac{2\mu\left(E - D_e\right)}{\hbar^2 \delta^2} + \eta_m c_0, \ \beta = \frac{2\mu B}{\hbar^2 \delta^2}, \ \gamma = \frac{2\mu A}{\hbar^2 \delta^2}, \ \chi = \frac{2\mu V_0}{\hbar^2 \delta^2}, \ \eta_m = \frac{m^2 - \frac{1}{4}\alpha^2}{\alpha^2}. \tag{8}$$

We reduce Eq. (7) into hypergeometric form after simplification and we have

$$R'' + \frac{1-s}{s(1-s)} R' + \frac{1}{\left[s(1-s)\right]^2} \left[ -\xi_1 s^2 + \xi_2 s - \xi_3 \right] R = 0 \tag{9}$$

where

$$\xi_1 = \varepsilon + \beta + \gamma, \ \xi_2 = 2\varepsilon + \beta - \chi - \eta_m, \ \xi_3 = \varepsilon \tag{10}$$

Now that Eq. (9) and Eq. (1) of Ref. [48] are in the same shape. We have the following parameters:

$$\tau(s) = 1 - s, \ \sigma(s) = s(1-s), \ \tilde{\sigma}(s) = -\xi_1 s^2 + \xi_2 s - \xi_3. \tag{11}$$

Substituting Eq. (11) into Eq. (11) of Ref. [48], we obtain $\pi(s)$ as

$$\pi(s) = -\frac{s}{2} \pm \sqrt{\left(\xi_1 - k + \frac{1}{4}\right)s^2 + \left(k - \xi_2\right)s + \xi_3}\ . \tag{12}$$

where

To find the constant $k$, the discriminant of the expression under the square root of Eq. (11) must be equal to zero. As such we have that for solvability, the expression inside the square root must be a perfect square:

$$\left(\xi_1 - k + \frac{1}{4}\right)s^2 + \left(k - \xi_2\right)s + \xi_3 = \left(As + B\right)^2 \tag{13}$$

Matching coefficients gives $B^2 = \xi_3 = \varepsilon$ therefore, $B = \sqrt{\varepsilon}$ Similarly, $A = \frac{1}{2} + \sqrt{\eta_m + \frac{1}{4}}$

Substituting above into Eq. (12), the physically acceptable form of $\pi(s)$ becomes

$$\pi(s) = \sqrt{\varepsilon} - \left(\frac{1}{2} + \sqrt{\varepsilon} + \sqrt{\eta_m + \frac{1}{4}}\right)s \tag{14}$$

and $\tau(s)$ can be written as

$$\tau(s) = 1 + 2\sqrt{\varepsilon} - 2\left(1 + \sqrt{\varepsilon} + 1\sqrt{\eta_m + \frac{1}{4}}\right)s \tag{15}$$

Taking the derivative of Eq. (15), we have

$$\tau'(s) = -2\left(1 + \sqrt{\varepsilon} + \sqrt{\eta_m + \frac{1}{4}}\right) \tag{16}$$

Since $\tau'(s) < 0$ the bound-state condition is satisfied. Referring to Eq. (10) of Ref. [48], we define the constant $\lambda$ as,

$$\lambda = \left(\frac{1}{2} + \sqrt{\varepsilon} + \sqrt{\eta_m + \frac{1}{4}}\right) \tag{17}$$

and taking the derivative of $\sigma(s)$ Eq. (11), we have

$$\sigma''(s) = -2 \tag{18}$$

Substituting Eqs. (16) and (18) into Eq. (13) of Ref. [48], we obtain

$$\lambda_n = 2n\left(1 + \sqrt{\varepsilon} + \sqrt{\eta_m + \frac{1}{4}}\right) + n(n-1). \tag{19}$$

Equating Eqs. (17) and (19) and simplifying yields

$$\sqrt{\varepsilon} = \frac{\beta - \chi - \left(n + \frac{1}{2} + \sqrt{\eta_m + \frac{1}{4}}\right)^2}{2\left(n + \frac{1}{2} + \sqrt{\eta_m + \frac{1}{4}}\right)} \tag{20}$$

Substituting Eq. (8) into Eq. (20) and simplifying yields the energy eigenvalues equation of the MHP in cosmic string topology using the improved approximation scheme as a function of $n$ and $m$ as

$$E_{nm} = D_e + \frac{\hbar^2\delta^2}{2\mu}\left(\frac{m^2-\alpha^2/4}{\alpha^2}\right)c_0 - \frac{\hbar^2\delta^2}{2\mu}\left[\frac{\frac{4\mu D_e e^{\delta r_e}}{\hbar^2\delta^2} - \frac{2\mu V_0}{\hbar^2\delta^2} - \left(n+\frac{1}{2}+\frac{|m|}{\alpha}\right)^2}{2\left(n+\frac{1}{2}+\frac{|m|}{\alpha}\right)}\right]^2 \tag{21}$$

From Eq. (21) we can deduce the following: The degeneracy breaking originates from the modified centrifugal term $\eta_m = \frac{m^2-\alpha^2/4}{\alpha^2}$ which enters the energy equation through $n+\frac{1}{2}+\frac{|m|}{\alpha}$ and therefore causes different angular states to acquire different energies. It must be noted that the effects of cosmic string changes spacetime from flat to conical, modifies angular motion, alters the centrifugal interaction, changes angular quantization, splits formerly degenerate states, and produces topology-induced energy shifts. Thus, the breaking of degeneracy is a direct observable consequence of the spacetime topology.

### 2.1. Special cases:

**Case 1:** If $\alpha = 1$, the centrifugal term becomes $\eta_m = m^2 - \frac{1}{4}$ and we recovered ordinary Euclidean space for the standard MHP.

$$E_{nm} = D_e + \frac{\hbar^2\delta^2}{2\mu}\left(m^2-\frac{1}{4}\right)c_0 - \frac{\hbar^2\delta^2}{2\mu}\left[\frac{\frac{4\mu D_e e^{\delta r_e}}{\hbar^2\delta^2} - \frac{2\mu V_0}{\hbar^2\delta^2} - \left(n+\frac{1}{2}+|m|\right)^2}{2\left(n+\frac{1}{2}+|m|\right)}\right]^2 \tag{22}$$

**Case 2:** If $V_0 = 0$ in Eq. (22), we recovered eigenvalues of Morse Potential

$$E_{nm} = D_e + \frac{\hbar^2\delta^2}{2\mu}\left(m^2-\frac{1}{4}\right)c_0 - \frac{\hbar^2\delta^2}{2\mu}\left[\frac{\frac{4\mu D_e e^{\delta r_e}}{\hbar^2\delta^2} - \left(n+\frac{1}{2}+|m|\right)^2}{2\left(n+\frac{1}{2}+|m|\right)}\right]^2 \tag{23}$$

**Case 3:** If $D_e = 0$ in Eq. (22), we recovered eigenvalues of Hulthén Potential

$$E_{nm} = \frac{\hbar^2\delta^2}{2\mu}\left(m^2-\frac{1}{4}\right)c_0 - \frac{\hbar^2\delta^2}{2\mu}\left[\frac{-\frac{2\mu V_0}{\hbar^2\delta^2} - \left(n+\frac{1}{2}+|m|\right)^2}{2\left(n+\frac{1}{2}+|m|\right)}\right]^2 \tag{24}$$

### 2.2 Wavefunction of MHP in the cosmic string topology

To obtain the wavefunction, we consider Eq. (3) of Ref [48], and upon substituting Eqs. (11) and (14) and integrating, we get

$$\phi(s) = s^{\sqrt{\varepsilon}}(1-s)^{\frac{1}{2}+\sqrt{\eta_m+1/4}} \tag{25}$$

To obtain the hypergeometric function, we first determine the weight function $\rho(x)$. By substituting Eqs. (11) and (14) into Eq. (3) of Ref. [48] and after integrating, we get

$$\rho(s)=s^{2\sqrt{\varepsilon}}(1-s)^{2\sqrt{\eta_m+1/4}} \tag{26}$$

Hence, by substituting Eqs. (11) and (23) into Eq. (2) of Ref. [48], yields the Rodrigues equation given as

$$y_n(s)=\frac{B_{nm}}{s^{2\sqrt{\varepsilon}}(1-s)^{2\sqrt{\eta_m+1/4}}}\times\frac{d^n}{ds^n}\left[s^{n+2\sqrt{\varepsilon}}(1-s)^{n+2\sqrt{\eta_m+1/4}}\right]. \tag{27}$$

where $B_{nm}$ is the normalization constant. Equation (24) is equivalent to

$$y_n(s)=P_n^{\left(2\sqrt{\varepsilon},2\sqrt{\eta_m+1/4}\right)}(1-2s) \tag{28}$$

where $P_n^{(\alpha,\beta)}$ is the Jacobi Polynomials. Hence, combining Eq. (25) and Eq. (28), the wave function is given as

$$R_{nm}(s)=B_{nm}s^{\sqrt{\varepsilon}}(1-s)^{\frac{1}{2}+\sqrt{\eta_m+1/4}}P_n^{\left(2\sqrt{\varepsilon},2\sqrt{\eta_m+1/4}\right)}(1-2s) \tag{29}$$

Transforming back to $r$ -space using $s=e^{-\delta r}$, $v=\sqrt{\eta_m+\frac{1}{4}}$ the physical radial wavefunction becomes

$$R_{nm}(r)=B_{nm}e^{-\delta r\sqrt{\varepsilon}}(1-e^{-\delta r})^{\frac{1}{2}+v}P_n^{\left(2\sqrt{\varepsilon},2v\right)}(1-2e^{-\delta r}). \tag{30}$$

Using the normalization condition, we obtain the normalization constant as follows:

$$\int_0^\infty\left|R_{nm}(r)\right|^2dr=1 \tag{31}$$

Substitute the wavefunction into Eq. (31)

$$B_{nm}^2\int_0^\infty e^{-2\delta r\sqrt{\varepsilon}}(1-e^{-\delta r})^{1+2v}\times\left[P_n^{\left(2\sqrt{\varepsilon},2v\right)}(1-2e^{-\delta r})\right]^2dr=1 \tag{32}$$

By letting, $y=1-2s$ we have

$$\frac{B_{nm}^2}{\delta}\int_0^1 s^{2\sqrt{\varepsilon}-1}(1-s)^{1+2v}\times\left[P_n^{\left(2\sqrt{\varepsilon},2v\right)}(1-2s)\right]^2ds=1. \tag{33}$$

After simplifying Eq. (33), we have

$$\frac{B_{nm}^2}{\delta}\frac{1}{2^{2\sqrt{\varepsilon}+2v+1}}\times\int_{-1}^1(1-x)^{2\sqrt{\varepsilon}-1}(1+x)^{2v+1}\times\left[P_n^{\left(2\sqrt{\varepsilon},2v\right)}(x)\right]^2dx=1. \tag{34}$$

Recall the Jacobi orthogonality formula is equivalent to our expression as

$$\int_{-1}^{1}(1-x)^{a}(1+x)^{b}\left[P_{n}^{(a,b)}(x)\right]^{2}dx=\frac{2^{a+b+1}}{n!(2n+a+b+1)}\frac{\Gamma\left(n+a+1\right)\Gamma\left(n+b+1\right)}{\Gamma\left(n+a+b+1\right)}. \quad (35)$$

where

$$a=2\sqrt{\varepsilon}-1,\ \ b=2v+1 \quad (36)$$

Hence

$$a+b+1=2\sqrt{\varepsilon}+2v+1 \quad (37)$$

Hence, by comparing Eq. (31) with the standard integral of Eq. (35), we obtain the normalization constant as

$$B_{nm}^{2}=\delta\frac{n!(2n+a+b+1)\Gamma\left(n+a+b+1\right)}{\Gamma\left(n+a+1\right)\Gamma\left(n+b+1\right)} \quad (38)$$

The normalized radial wavefunction is obtained by combining Eqs. (29) and (38) as

$$R_{nm}(r)=\sqrt{\delta\frac{n!(2n+a+b+1)\Gamma\left(n+a+b+1\right)}{\Gamma\left(n+a+1\right)\Gamma\left(n+b+1\right)}}e^{-\delta r\sqrt{\varepsilon}}(1-e^{-\delta r})^{\frac{1}{2}+v}P_{n}^{\left(2\sqrt{\varepsilon},2v\right)}(1-2e^{-\delta r}) \quad (40)$$

Thus, the cosmic string topology affects the normalization amplitude, probability density, spatial localization and orthogonality structure of the quantum system under study. As $\alpha\to 1$, the flat-space normalization is recovered.

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## 3. Application of Hellmann-Feynman theorem (HFT) to the MHP

One dependable method for determining the expectation values of quantum mechanical observables for any quantum numbers is by applying the HFT [50-52]. This approach involves considering that the Hamiltonian of a specific quantum mechanical system is dependent on a parameter $\eta_m$ . Let $E(\eta_m)$ and $\Psi\left(\eta_m\right)$ represent the eigenvalues and eigenfunctions of the Hamiltonian, respectively.

$$H(\eta_m)\Psi=E\left(\eta_m\right)\Psi \quad (41)$$

then:

$$\frac{\partial E}{\partial\eta_m}=\left\langle\frac{\partial H}{\partial\eta_m}\right\rangle \quad (42)$$

This allows us to obtain expectation values directly from derivatives of the energy. The effective Morse-Hulthen radial Hamiltonian is expressed as

$$H=-\frac{\hbar^{2}}{2\mu}\frac{d^{2}}{dr^{2}}+D_{e}-2D_{e}e^{\delta r_{e}}e^{-\delta r}+D_{e}e^{2\delta r_{e}}e^{-2\delta r}-\frac{V_{0}e^{-\delta r}}{1-e^{-\delta r}}+\frac{\hbar^{2}\eta_{m}}{2\mu r^{2}} \quad (43)$$

### 3.1. Expectation values of inverse square radial separation $\left\langle \frac{1}{r^2} \right\rangle$

By taking the partial derivative of Eqs. (21) and (43) we obtain the expectation values of the $\left\langle \frac{1}{r^2} \right\rangle$ as

$$\left\langle \frac{1}{r^2} \right\rangle = \delta^2 c_0 + \frac{\delta^2 \left[ \frac{4\mu D_e e^{\delta r_e}}{\hbar^2 \delta^2} - \frac{2\mu V_0}{\hbar^2 \delta^2} - \left( n + \frac{1}{2} + \frac{|m|}{\alpha} \right)^2 \right]}{4\left( n + \frac{1}{2} + \frac{|m|}{\alpha} \right)\frac{|m|}{\alpha}} \left[ \frac{\frac{4\mu D_e e^{\delta r_e}}{\hbar^2 \delta^2} - \frac{2\mu V_0}{\hbar^2 \delta^2}}{\left( n + \frac{1}{2} + \frac{|m|}{\alpha} \right)^2} + 1 \right] \quad (44)$$

### 3.2. Expectation values for kinetic energy $\langle T \rangle$ and momentum squared $\langle p^2 \rangle$

Recall that the kinetic energy of the system under study is of the form

$$\langle T \rangle = E_{nm} - \left( D_e - 2D_e e^{\delta r_e} \left\langle e^{-\delta r} \right\rangle + D_e e^{2\delta r_e} \left\langle e^{-2\delta r} \right\rangle - V_0 \left\langle \frac{e^{-\delta r}}{1 - e^{-\delta r}} \right\rangle \right) - \frac{\hbar^2 \eta_m}{2\mu} \left\langle \frac{1}{r^2} \right\rangle \quad (45)$$

By substituting $\eta_m = \mu$ into Eq. (42) and taking the partial derivative of Eq. (45) for $\mu$ leads to

$$\langle T \rangle = E_{nm} - D_e + 2D_e e^{\delta r_e} \left\langle e^{-\delta r} \right\rangle - D_e e^{2\delta r_e} \left\langle e^{-2\delta r} \right\rangle - V_0 \frac{F}{\Lambda_n} - \frac{\hbar^2 \eta_m}{2\mu} \left[ \delta^2 c_0 + \frac{\delta^2 \left( A - B - \Lambda_n^2 \right)}{4\Lambda_n \left( |m| / \alpha \right)} \left( \frac{A - B}{\Lambda_n^2} + 1 \right) \right] \quad (46)$$

### 3.3. Expectation values for momentum squared $\langle p^2 \rangle$

The kinetic energy operator is

$$T = \frac{p^2}{2\mu} \quad (47)$$

Therefore,

$$\langle p^2 \rangle = 2\mu \langle T \rangle \quad (48)$$

Substituting Eq. (46) yield,

$$\langle p^2 \rangle = 2\mu E_{nm} - 2\mu D_e + 4\mu D_e e^{\delta r_e} \left\langle e^{-\delta r} \right\rangle - 2\mu D_e e^{2\delta r_e} \left\langle e^{-2\delta r} \right\rangle - 2\mu V_0 \frac{F}{\Lambda_n} - \hbar^2 \eta_m \left[ \delta^2 c_0 + \frac{\delta^2 \left( A - B - \Lambda_n^2 \right)}{4\Lambda_n \left( |m| / \alpha \right)} \left( \frac{A - B}{\Lambda_n^2} + 1 \right) \right] \quad (49)$$

where

$$\eta_m = \frac{m^2 - \alpha^2 / 4}{\alpha^2}, \quad \Lambda_n = n + \frac{1}{2} + \frac{|m|}{\alpha}, \quad A = \frac{4\mu D_e e^{\delta r_e}}{\hbar^2 \delta^2}, \quad B = \frac{2\mu V_0}{\hbar^2 \delta^2}, \quad F = \frac{A - B - \Lambda_n^2}{2\Lambda_n}, \quad (50)$$

$$F=\frac{\frac{4\mu D_e e^{\delta r_e}}{\hbar^2\delta^2}-\frac{2\mu V_0}{\hbar^2\delta^2}-\left(n+\frac{1}{2}+\frac{|m|}{\alpha}\right)^2}{2\left(n+\frac{1}{2}+\frac{|m|}{\alpha}\right)} \tag{51}$$

## 4. Results and discussion

The analytical solution of the SE under a MHP were obtained for the selected molecules using the NU method. The energy spectra were obtained using experimentally established spectroscopic constants in **Table 1** [53].

**Table 1** Spectroscopic data for the various diatomic molecules Inyang et al. [53]

| **Molecule** | $D_e(eV)$ | $\mu(amu)$ | $r_e(\overset{0}{\mathrm{A}})$ | $\delta(\overset{0}{\mathrm{A}}^{-1})$ |
|---|---|---|---|---|
| $H_2$ | 4.744 | 0.5039 | 0.741 | 1.942 |
| HCl | 4.619 | 0.980 | 1.275 | 1.867 |
| LiH | 2.515 | 0.880 | 1.595 | 1.799 |

Tables 2, 3 and 4 present the numerical energy eigenvalues of the selected diatomic molecules; $H_2$, HCl and LiH for different values of the principal quantum number $n$, magnetic quantum number $m$, cosmic string topological parameter $\alpha$, and potential strength $V_0$. It is observed that all the obtained energy eigenvalues are negative. This confirms the existence of bound states for the Morse–Hulthén interaction in cosmic string spacetime. Also, the energy eigenvalues increase gradually with increasing n. Stated differently, the energies become less negative as $n$ increases. Physically, this behavior is expected since higher quantum states correspond to larger average internuclear separation and weaker binding interaction between the constituent particles of the molecule. Therefore, the particle moves toward the continuum region as the vibrational excitation increases. The results further show that as $m$ increases, the magnitude of the energy eigenvalues decreases. This effect originates from the modified centrifugal contribution induced by the cosmic string geometry. The increase in m enhances the effective centrifugal interaction, thereby reducing the binding strength of the system. Furthermore, a decrease in $\alpha$ produces stronger shifts in the energy spectrum. Since $\alpha$ measures the angular deficit in spacetime, its smaller values correspond to stronger topological deformation. This modifies the rotational structure of the system and removes the ordinary angular degeneracy of the molecular states. Hence, the topology of spacetime directly affects the bound-state energies of the molecules. The tables additionally reveal that increasing $V_0$ leads to more negative energy eigenvalues, signifying stronger confinement and deeper bound states. Physically, this indicates that the attractive Hulthén interaction becomes stronger, thereby increasing the binding energy of the molecular system. Overall, the numerical results show that the combined MHP together with the cosmic string topology significantly modifies the rotational-vibrational structure of diatomic molecules. The interaction between molecular dynamics and spacetime topology produces observable shifts in the energy spectrum, indicating that topological defects can strongly influence quantum molecular systems.

**Table 2** Energy eigenvalues $(eV)$ of $H_2$ molecules

| | | $V_0=0.10eV$ | | | $V_0=2(eV)$ | | |
|---|---|---|---|---|---|---|---|
| $m$ | $n$ | $\alpha=0.1$ | $\alpha=0.5$ | $\alpha=1$ | $\alpha=0.1$ | $\alpha=0.5$ | $\alpha=1$ |
| 2 | 0 | -36.98704589 | -1232.210788 | -4047.514637 | -32.30749841 | -1116.330303 | -3669.933863 |
| | 1 | -31.64863597 | -816.7624468 | -2052.994840 | -27.48058875 | -739.5036098 | -1860.816895 |
| | 2 | -27.03530256 | -577.8426303 | -1232.226431 | -23.31208314 | -522.7969538 | -1116.345946 |
| | 3 | -23.02759757 | -427.9678750 | -816.7780900 | -19.69363682 | -386.8589004 | -739.5192530 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | 4 | -19.52994130 | -327.8304019 | -577.8582735 | -16.53855466 | -296.0355256 | -522.8125970 |
| 3 | 0 | -5.127231292 | -577.8165583 | -2052.988322 | -3.534025347 | -522.7708818 | -1860.810377 |
| | 1 | -3.660161222 | -427.9418030 | -1232.219913 | -2.225865602 | -386.8328284 | -1116.339428 |
| | 2 | -2.356275627 | -327.8043299 | -816.7715720 | -1.066448572 | -296.0094536 | -739.5127350 |
| | 3 | -1.197303532 | -257.6167283 | -577.8517555 | -0.039201657 | -232.3526859 | -522.8060790 |
| | 4 | -0.1675829420 | -206.5370687 | -427.9770002 | -0.870081273 | -186.0284081 | -386.8680256 |

**Table 3** Energy eigenvalues $(eV)$ of $HCl$ molecules

| | | $V_0 = 0.10eV$ | | | $V_0 = 2(eV)$ | | |
|---|---|---|---|---|---|---|---|
| $m$ | $n$ | $\alpha = 0.1$ | $\alpha = 0.5$ | $\alpha = 1$ | $\alpha = 0.1$ | $\alpha = 0.5$ | $\alpha = 1$ |
| 2 | 0 | -742.3679662 | -16471.88958 | -53490.91688 | -713.2728272 | -15849.31021 | -51471.63173 |
| | 1 | -670.0913037 | -11008.64874 | -27264.60688 | -643.7260632 | -10592.19478 | -26234.82466 |
| | 2 | -607.2495682 | -7866.488698 | -16471.89702 | -583.2583937 | -7568.587343 | -15849.31765 |
| | 3 | -552.2721337 | -5895.086238 | -11008.65618 | -530.3584487 | -5671.565663 | -10592.20222 |
| | 4 | -503.9022182 | -4577.581966 | -7866.496132 | -483.8168668 | -4403.771141 | -7568.594777 |
| 3 | 0 | -306.4248934 | -7866.476307 | -27264.60378 | -293.8016929 | -7568.574952 | -26234.82156 |
| | 1 | -284.0613229 | -5895.073847 | -16471.89392 | -272.2862336 | -5671.553272 | -15849.31455 |
| | 2 | -263.7443418 | -4577.569575 | -11008.65308 | -252.7402874 | -4403.758750 | -10592.19912 |
| | 3 | -245.2337036 | -3653.778108 | -7866.493034 | -234.9326724 | -3514.822627 | -7568.591679 |
| | 4 | -228.3234690 | -2981.138530 | -5895.090574 | -218.6652188 | -2867.562728 | -5671.569999 |

**Table 4** Energy eigenvalues $(eV)$ of $LiH$ molecules

| | | $V_0 = 0.10eV$ | | | $V_0 = 4eV$ | | |
|---|---|---|---|---|---|---|---|
| $m$ | $n$ | $\alpha = 0.1$ | $\alpha = 0.5$ | $\alpha = 1$ | $\alpha = 0.1$ | $\alpha = 0.5$ | $\alpha = 1$ |
| 2 | 0 | -36.98704589 | -1232.210788 | -4047.514637 | -32.30749841 | -1116.330303 | -3669.933863 |
| | 1 | -31.64863597 | -816.7624468 | -2052.994840 | -27.48058875 | -739.5036098 | -1860.816895 |
| | 2 | -27.03530256 | -577.8426303 | -1232.226431 | -23.31208314 | -522.7969538 | -1116.345946 |
| | 3 | -23.02759757 | -427.9678750 | -816.7780900 | -19.69363682 | -386.8589004 | -739.5192530 |
| | 4 | -19.52994130 | -327.8304019 | -577.8582735 | -16.53855466 | -296.0355256 | -522.8125970 |
| 3 | 0 | -5.127231292 | -577.8165583 | -2052.988322 | -3.534025347 | -522.7708818 | -1860.810377 |
| | 1 | -3.660161222 | -427.9418030 | -1232.219913 | -2.225865602 | -386.8328284 | -1116.339428 |
| | 2 | -2.356275627 | -327.8043299 | -816.7715720 | -1.066448572 | -296.0094536 | -739.5127350 |
| | 3 | -1.197303532 | -257.6167283 | -577.8517555 | -0.039201657 | -232.3526859 | -522.8060790 |
| | 4 | -0.1675829420 | -206.5370687 | -427.9770002 | -0.870081273 | -186.0284081 | -386.8680256 |

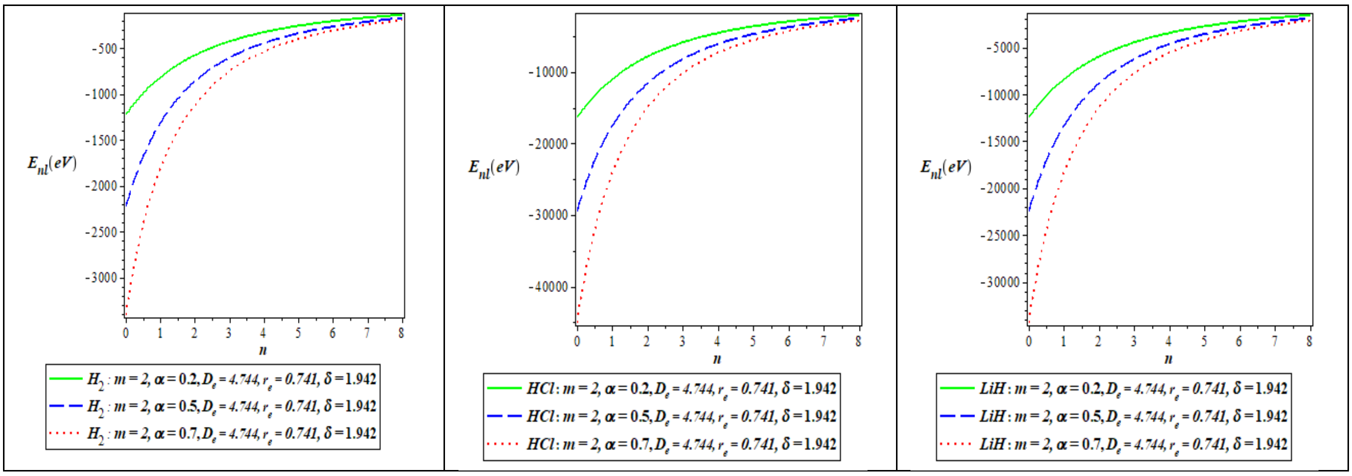


**Figure 1** Variation of energy vs $n$ for various topological parameter for the selected molecules

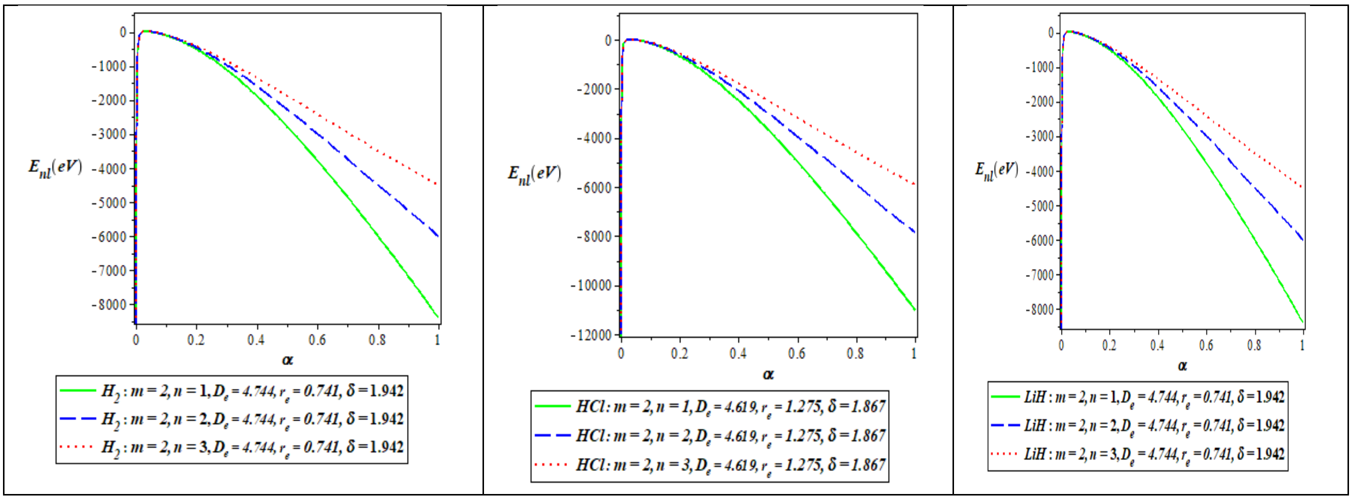


**Figure 2** Variation of energy vs topological parameter for the selected molecules

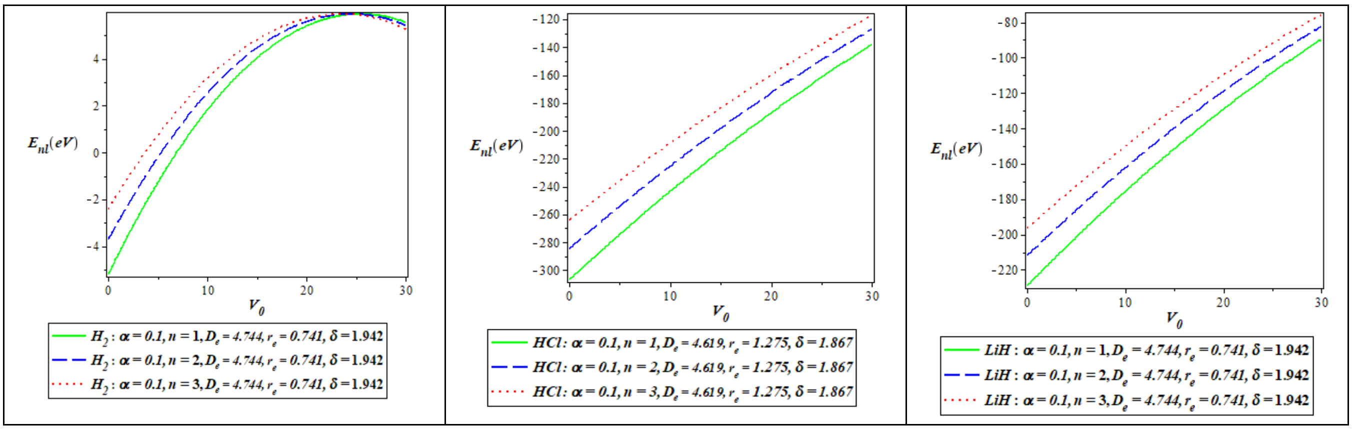


**Figure 3** Variation of energy vs potential parameter for the selected molecules

**Figure 1** shows that the energy eigenvalues increase monotonically with increasing principal quantum number $n$. This means that the energy levels become less negative as the quantum state increases. Physically, higher values of $n$ correspond to excited vibrational states where the particle is less tightly bound to the molecular potential well. **Figure 2** illustrates the direct influence of spacetime topology on the molecular energy spectrum. The energy eigenvalues vary significantly with the cosmic string parameter $\alpha$, confirming that the topological defect modifies the rotational-vibrational motion of the particle. As $\alpha$ approaches unity, the system gradually recovers the ordinary flat spacetime behavior. However, for smaller values of $\alpha$, the angular deficit becomes stronger and the energy levels shift considerably. The figure therefore demonstrates that the cosmic string breaks the ordinary angular degeneracy of the molecular states. Different angular momentum states experience different energy shifts under the influence of the topological defect. This provides clear evidence that spacetime geometry plays a significant role in determining the quantum properties of the molecular system. In **Fig. 3** as $V_0$ increases gradually, the energy eigenvalues are lowered. Physically, increasing $V_0$ reinforces the short-range attractive component of the Hulthén interaction. As a result, the effective potential well becomes deeper, leading to increased confinement of the quantum particle and lower bound-state energies. The figure further indicates that the response of the energy levels to variations in $V_0$ is nonlinear. This nonlinear dependence comes from the combined effects of exponential molecular interaction, centrifugal distortion and cosmic string topology.

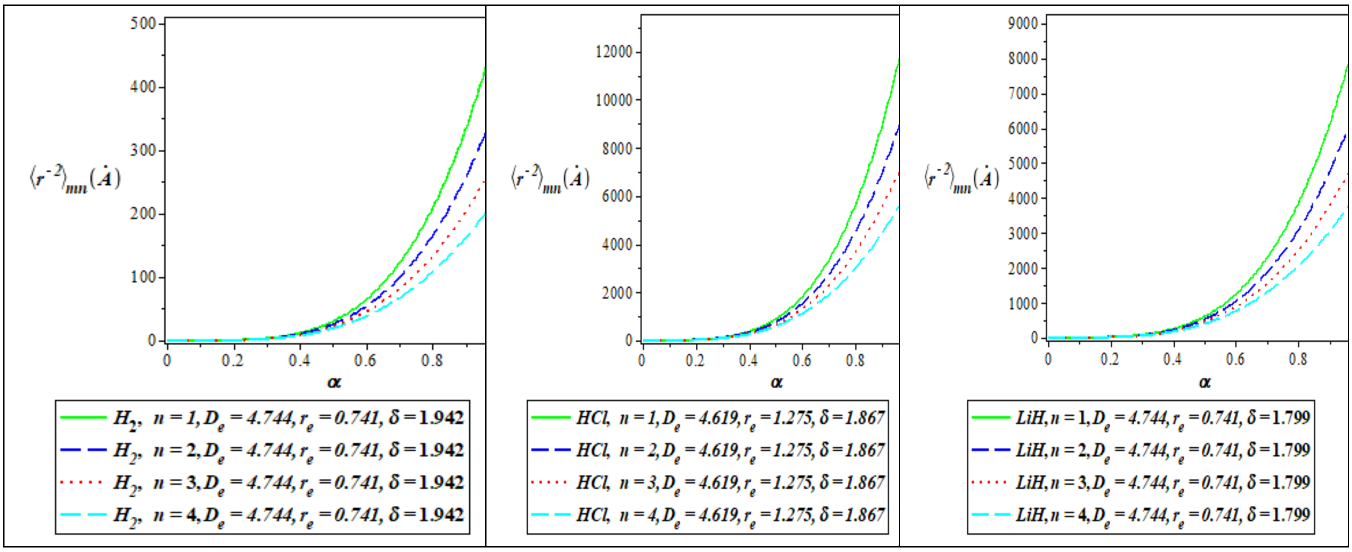


**Figure 4** Variation of expectation values of inverse squared radial separation vs topological parameter for the selected molecules

From **Fig. 4**, $\left\langle \frac{1}{r^2} \right\rangle$ increases as topological defect decreases, which demonstrates low quantum states are more localized as the particle experiences stronger angular repulsion and the cosmic string geometry modifies the special confinement of the molecular system considered in this study. In **Fig. 5**, $\langle T \rangle$ increases as $n$ and $m$ increases. Also, for stronger topological defect, the angular deficit becomes stronger causing distortion in the confinement geometry leading to increase in effective rotational interaction of the diatomic molecules under study. In **Fig. 6**, $\langle p^2 \rangle$ increases as the cosmic string parameter become stronger, hence, the cosmic string topology modifies the momentum distribution through the angular deficit factor. However, for decreasing cosmic string topology, the topology-induced confinement becomes stronger leading to effective angular interaction increase as the momentum fluctuations become larger.

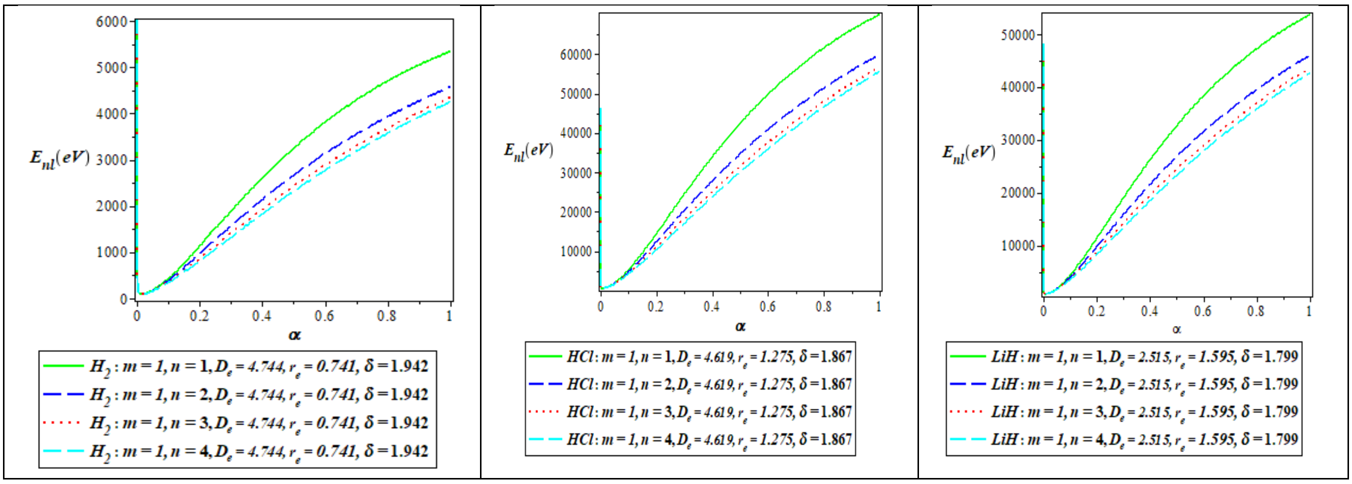


**Figure 5 Variati**on of expectation values of kinetic energy vs topological parameter for the selected molecules

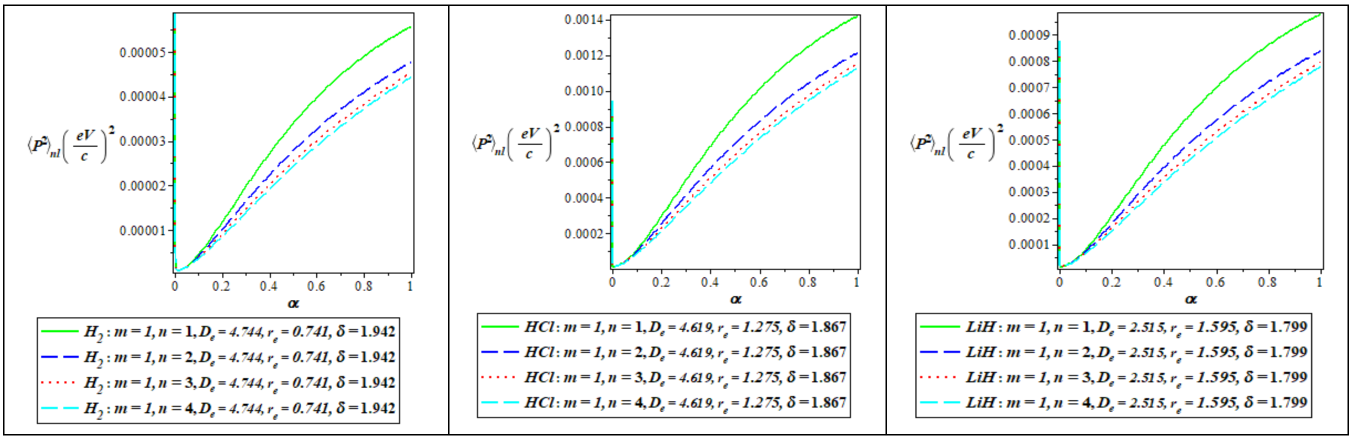


**Figure 6** Variation of expectation values of momentum squared vs topological parameter for the selected molecules

## 5. Conclusion

In this work, the bound-state solutions of the SE with the MHP in cosmic string spacetime were successfully derived using the NU method. An improved approximation scheme was employed to handle the centrifugal interaction term, leading to closed-form expressions for the energy eigenvalues and normalized radial wavefunctions. Analytical expressions for the expectation values of the inverse-squared distance, the kinetic energy and the momentum squared were derived using the Hellmann–Feynman theorem. The numerical results obtained for $H_2$, $HCl$ and $LiH$ molecules showed that the cosmic string topological parameter $\alpha$ has a significant influence on the rotational–vibrational energy spectrum of the system. In particular, the topological defect modifies the angular momentum contribution and breaks the ordinary angular degeneracy. The results further showed that increasing the potential strength parameter $V_0$ increases the confinement of the quantum particle and produces deeper bound states, while increasing the principal quantum number reduces the binding strength of the system. An important feature of the present model is that it contains several physically meaningful special cases. In the limit $V_0 = 0$, the interaction reduces to the standard Morse potential which is extensively used in molecular vibrational spectroscopy. Similarly, when the Morse interaction is removed, the system reduces to the Hulthén potential which has important applications in nuclear and atomic physics. Furthermore, in the flat-space limit $\alpha \to 1$, the obtained results recover the conventional Schrödinger solutions in ordinary Euclidean spacetime. These limiting cases validate the correctness and consistency of the study. The obtained results are in good agreement with existing studies on exponential-type potentials, molecular systems and quantum systems in topologically nontrivial spacetimes reported in the literature. The present investigation therefore extends previous works by combining the MHP interaction with cosmic string topology and by providing explicit analytical expressions for both the spectral properties and expectation values of the system. The results may find useful applications in molecular spectroscopy, condensed matter physics, quantum field theory in curved spacetime and the study of topological defects in quantum systems.

## Compliance with ethical standards


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### *Disclosure of conflict of interest*

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

### *Author contributions statement*

E. S. William and S. O. Inyang: Conceptualization, Methodology, Writing - Original Draft, Formal Analysis, Investigation, Writing-Review & Editing. E P Inyang and O. A. Akinde: Software, Validation, Visualization, Writing - Review & Editing, M. C. Bede: Resources, Project Administration. I. D. Ekpa: Supervision, Validation.


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