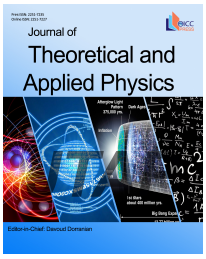

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Effects of topological defect on energy spectra and scattering phase shift of coshine Yukawa potential for nickel monocarbide molecule

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Original Research

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Abstract:

Topological defects generally contribute significant role in shaping the behaviour and interactions of molecular systems, with recognizable influence on their global and local characteristics. This influence often leads to profound changes in the dynamics of the molecules under study. To this end, the analytical eigensolutions of the radial Schrodinger equation with a point-like global monopole under the coshine Yukawa potential has been investigated via the Nikiforov-Uvarov Functional Analysis approach. The Greene-Aldrich approximation was used to overcome the centrifugal barrier which allows for the derivation of the energy and wave function in closed form. The solution of the energy and wave function were applied to investigate the wave function, probability density and scattering phase shift variations with topological defect parameter, dimension number and rotational quantum number for nickel monocarbide diatomic molecule. The results reveal that for the ground and excited states, the wave functions amplitudes were increased with the increase in the topological defect parameters but decreased with the dimension number. The scattering phase shifts were found to be sensitive to the rotational quantum number and topological defect values where the wave form is characterized by a rectangular periodic motion.

Keywords: Bound state energy spectra; Scattering phase shift; Topological defect; Coshine Yukawa potential; Diatomic molecules

1. Introduction

The concept of topological defects and their effects on various quantum systems have been an area of interest for decades now. This concept dates to the early history of the universe during phase transitions, especially in areas of condensed matter physics and theory of particle interactions [1–3]. The major role of these defects is to alter the physical properties of different quantum systems, thereby changing the behaviour of their quantum mechanical particles. This will lead to a shift in the energy eigenstates and eigenfunctions of these particles [4]. Research shows that the topological defects manifest differently in different phenomena. They are known as vortices in semiconductors [5], monopoles, walls and strings in gravitational studies [6, 7]. They are also known as solitons in quasi-one-dimensional polymers [8], dislocations in liquid crystals [9] and domain walls in magnetic materials [10].

Various wave equations with different topological effects including cosmic strings and global monopoles have been widely studied in different areas namely gravitation and cosmology, solid-state physics, general relativity, astrophysics and quantum mechanics [11–17]. The global monopole was investigated with harmonic oscillator within the non-relativistic quantum mechanics [18]. Also, the exact solutions of scalar bosons with Aharonov-Bohm (AB) and Coulomb potentials were obtained in the presence of global monopole [19]. Still in the global monopole space-time environment, the effect of topological defects with Dirac and

Klein-Gordon oscillators were studied [20]. The cosmic strings topological defects have been recently employed in Einstein equation to describe the global monopole point-like defects in solids [21]. In addition, the effect of declination topological defect on the interaction of a spinless electron with radial electric fields was studied within an elastic medium [22]. The effect of screw dislocation on electrons confined in both deformed Kratzer potential and pseudoharmonic quantum dot, respectively, was considered under the influence of an external magnetic field [23, 24]. Nwabuzor et al. [25] X-rayed the impacts of the topological defects on the energy spectra and thermal properties of generalized Morse potential for selected diatomic molecules. Specifically, the specific heat capacity exhibited quasi-saturation tendency as the deformation parameter and topological defects approached unity. Okon and Ikot [26] considered the confinement effects of the AB flux and magnetic fields with topological defect on carbon monoxide (CO) diatomic molecule (DM), which was modelled using screened modified Kratzer potential. The modelled system was seen to exhibit paramagnetic and diamagnetic tendencies for weak and strong magnetic fields, respectively. Most recently, Ikot et al. [27] studied the impacts of topological defects and AB fields on the energy spectra, thermal properties and persistent currents on exponential-type pseudoharmonic oscillator, using extended Nikiforov-Uvarov (ENU) method. The dependence of the thermal properties of the exponential-type pseudoharmonic oscillator on the topological defects and magnetic field flux was clearly established.

In recent times, the studies of the scattering state phase shift of selected confining potential models have attracted much attention, in relation to some DMs. It has been established that a conventional diatomic confining potential model is defined in terms of dissociation energy, equilibrium bond length, inter-atomic separation and screening parameter [28]. The solutions of Klein-Gordon equation (KGE) with Deng-Fan potential in higher dimensions were obtained for hydrogen chloride (HCl) and lithium hydride (LiH) DMs, both in relativistic and nonrelativistic regimes [29]. Here, the scattering state phase shift results and effects on the different quantum states on the eigensolutions were studied, both numerically and graphically for the selected diatomic molecules. By employing the Nikiforov-Uvarov Functional Analysis (NUFA) formalism, the solutions of the KGE with shifted Tietz-Wei potential in higher dimensions and their scattering state phase shift results were discussed elaborately for chlorine dimer (Cl_2) iodine monochloride (ICl) DMs [30]. By using the functional analysis approach (FAA), the scattering state phase shift of generalized Mobius square potential have been obtained [31]. The effects of rotational and vibrational quantum numbers on the obtained results for nitrogen monoiodide (NI) were also considered. Nickel carbide (NiC), being the DM of interest in this study; have in the last few decades drawn considerable and increasing attention due to the puzzling effects displayed in the areas of semiconductor materials science, mechanical and electrical engineering. The stoichiometry of nickel carbides reveals the NiC, Ni_2C and Ni_3C structures as the most prominent, with Ni_3C receiving great attention as the most experimentally relevant carbide [32–34]. Advances in the potential usefulness of nickel carbides have garnered enormous interest resulting from the vital role played in carbon-nanotubes (CNTs) [35], which acts as antennas for radios as well as other electromagnetic devices. Nickel is however a predominant ingredient of aerospace super-alloys, and they are desired also in other scientific applications such as low friction dry lubricant effect [36], high hardness in coatings and enhanced manufacturing of brittle materials [37], as well as electrical components for piezo-resistive sensors [38, 39] which relies on the change in band gap due to deformation changes in resistivity.

Our motivation is pivoted on the fact that there is no report on the effect of topological defect on bound state energy spectra and scattering phase shift of coshine Yukawa potential for diatomic molecules, to the best of our knowledge. Hence, we will first obtain the bound state energy, subject to the coshine Yukawa potential (*CYP*) with point-like global monopole (PGM) in higher dimensions, by using the NUFA formalism to solve the higher dimensional nonrelativistic wave equation. Thereafter, the scattering phase shift solutions of the *CYP* with PGM will be obtained in higher dimensions, together with its normalization constant. Numerical results of the bound state energy and scattering phase shift of *CYP* with NiC DM at different dimensions, topological parameters and quantum states are discussed. Also, the effect of the topological defects on the wave function and probability densities of *CYP* with NiC diatomic molecule is evaluated for various quantum states and dimensions. The influence of the different spectroscopic parameters and quantum numbers of NiC on the bound state energy spectra and scattering phase shift of *CYP* is discussed graphically in higher dimensions. *CYP* is defined as [40]

$$V_{CYP}(r) = -4d_e\frac{r_e}{r}\exp(-\delta r)\cosh(\delta r) \tag{1}$$

Here, d_e, r_e and δ represent dissociation energy, equilibrium bond length and screening parameter, respectively. *CYP* combines both the hyperbolic and exponential functions in describing the quantum confinement and dynamics of molecular systems [41]. The *CYP* has been used previously to study the thermodynamic properties of different diatomic molecules [42].

This paper is organized as follows. The framework of the theoretical calculations of the nonrelativistic energy spectra scattering state solutions of the *CYP* with PGM in higher dimensions can be viewed in section 2. In section 3, the graphical and numerical results obtained are presented and discussed accordingly. Section 4 gives the concluding remarks.

2. Theoretical calculations

2.1 Nonrelativistic energy spectra with PGM in higher dimensions

For spacetime with a point-like global monopole (PGM), the line element that explains it is given by [43]

$$ds^2 = -c^2dt^2 + \frac{dr^2}{\alpha^2} + r^2d\theta^2 + r^2\sin^2\theta d\varphi^2 \tag{2}$$

where $0 < \alpha < 1$, $\alpha = 1 - 8\pi G\eta_0^2$. Here, α is the topological effect parameter of the PGM, while depends on the energy scale η_0.
In addition, the metrics given in Eq. (2) describe a spacetime with scalar curvature

$$R = R_{\mu}^{\mu} = \frac{2(1-\alpha^2)}{\alpha^2 r^2} \tag{3}$$

The Schrodinger equation (SE) in this context is defined as

$$-\frac{\hbar^2}{2\mu}\nabla_{LB}^2\psi(\mathbf{r},t) + V(r,t)\psi(\mathbf{r},t) = i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} \tag{4}$$

Here, μ is the reduced mass of the molecular system,

$$\nabla_{LB}^2 = \frac{1}{\sqrt{g}}\partial_i\left(\sqrt{g}g^{ij}\partial_i\right), \;\; g = \det(g_{ij})$$

being the Laplace-Beltrami operator, and $V(r,t) \equiv V(r)$ given in Eq. (1).
Therefore, the SE for the *CYP* in the presence of the PGM is given as

$$-\frac{\mathrm{h}^2}{2\mu r^2}\left[\alpha^2\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial r}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\psi(r,\theta,\varphi,t) + V(r)\psi(r,\theta,\varphi,t) = i\mathrm{h}\frac{\partial\psi(r,\theta,\varphi,t)}{\partial t} \tag{5}$$

Now, we consider a particular solution of Eq. (5) given in terms of eigenvalues of the angular momentum operator $\hat{L}^2$,

$$\psi(r,\theta,\varphi,t) = \exp\left(\frac{-iE_{n,l}t}{\hbar}\right)\frac{R(r)}{r}Y_{l,m}(\theta,\varphi) \tag{6}$$

Here, $Y_{l,m}(\theta,\varphi)$ are spherical harmonics and $R(r)$ is the radial wave function.
By substituting Eqs. (6) and (1) into Eq. (5), we have

$$\frac{-\mathrm{h}^2}{2\mu r^2}\left[\alpha^2\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial r}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\psi(r,\theta,\varphi,t) \tag{7}$$

with $K = l_D + (D-3)/2$, D and l being the dimensionality parameter and angular momentum quantum number, respectively.
Here, the Greene-Aldrich approximation scheme is employed to handle the centrifugal term, due to the presence of the centrifugal term in Eq. (7) which cannot be solved exactly for $l_D = 0$. In addition, this approximation scheme is suitable for both bound and scattering state problems. The Greene-Aldrich approximation scheme used here is defined as [44]

$$\frac{1}{r^2} \approx \frac{4\delta^2}{(1-e^{-2\delta r})^2}; \;\; \frac{1}{r} \approx \frac{2\delta}{(1-e^{-2\delta r})} \tag{8}$$

By inserting Eq. (8) into Eq. (7) and defining a new variable such as $z = e^{-2\delta r}$ with the following dimensionless parameters:

$$-\varepsilon_{n,l_D} = \frac{\mu E_{n,l_D}}{2\hbar\delta^2\alpha^2}; \;\; P = \frac{2\mu d_e r_e}{2\hbar^2\delta\alpha^2}; \;\; Q = \frac{K(K+1)}{\alpha^2} \tag{9}$$

Eq. (7) becomes

$$\frac{d^2R_{n,l_D}(z)}{dz^2} + \frac{(1-z)}{z(1-z)}\frac{dR_{n,l_D}(z)}{dz} + \frac{[-(\varepsilon_{n,l_D}+P)z^2 + 2\varepsilon_{n,l_D}z - (\varepsilon_{n,l_D} - P + Q)]R_{n,l_D}(z)}{z^2(1-z)^2} = 0 \tag{10}$$

The Schrodinger equation is one of the eigen value problems which can be solved analytically, numerically or via diagonalization [45–47]. Solving the Schrodinger equation through numeric or diagonalization involves using algorithm to find its solution. In this work, we employ the Nikiforov-Uvarov Functional Analysis (NUFA) method (see Appendix) and also consider the boundary conditions $z \to 0$ as $r \to \infty$ and $z \to 1$ as $r \to 0$, where we propose a wave function of the form

$$R_{nl_D}(z) = z^{\lambda}(1-z)^{\sigma}f_{n,l_D}(z) \tag{11}$$

with

$$\lambda = \pm\sqrt{\left(\frac{K(K+1)}{\alpha^2} - \frac{2\mu d_e r_e}{\hbar^2\delta\alpha^2} - \frac{\mu E_{n,l_D}}{2\hbar^2\delta^2\alpha^2}\right)}; \quad \sigma = \frac{1}{2}\left[1 \pm \sqrt{1 + \frac{4K(K+1)}{\alpha^2}}\right] \tag{12}$$

Hence, the nonrelativistic energy spectra of the *CYP* in higher dimensions are obtained as

$$E_{n,l_D} = -\frac{2\hbar^2\delta^2\alpha^2}{\mu}\left\{\frac{2\mu d_e r_e}{\hbar^2\delta\alpha^2} - \frac{K(K+1)}{\alpha^2} + \left[\frac{\left(\frac{4\mu d_e r_e}{\hbar^2\delta\alpha^2} - \frac{K(K+1)}{\alpha^2}\right)}{2(n+\sigma)} - \frac{(n+\sigma)}{2}\right]^2\right\} \tag{13}$$

2.2 Scattering state solutions of the *CYP* with PGM in higher dimensions

By employing a new transformation scheme $\eta = 1 - e^{-2\delta r}$ and the Greene-Aldrich approximation scheme of Eq. (8), Eq. (7) becomes

$$\eta(1-\eta)\frac{d^2R_{\nu,J_D}(\eta)}{d\eta^2} - \eta\frac{dR_{\nu,J_D}(\eta)}{d\eta} + \frac{[A_1 + A_2\eta + A_3\eta^2]}{\eta(1-\eta)}R_{\nu,J_D}(\eta) = 0 \tag{14}$$

where

$$A_1 = -\frac{K(K+1)}{\alpha^2}; \;\; A_2 = \frac{4\mu d_e r_e}{\hbar^2\delta\alpha^2}; \;\; A_3 = \frac{\mu E_{n,l_D}}{2\hbar^2\delta^2\alpha^2} - \frac{2\mu d_e r_e}{\hbar^2\delta\alpha^2} \tag{15}$$

For the regular solution of scattering states, the wave function is defined as

$$R_{n,l_D}(\eta) = \eta^{w}(1-\eta)^{-\frac{is}{\delta}}\phi_{n,l_D}(\eta) \tag{16}$$

where

$$w = \frac{1}{2}(1 \pm \sqrt{1-4A_1}); \;\; s = \delta\sqrt{A_1 + A_2 + A_3} \tag{17}$$

Substituting Eq. (16) into Eq. (14) gives the hypergeometric Gauss differential equation of the form

$$\eta(1-\eta)\frac{d^2\phi_{n,l_D}(\eta)}{d\eta^2}+\left[2w-\left(1-\frac{2is}{\delta}+2w\right)\eta\right]\frac{d\phi_{n,l_D}(\eta)}{d\eta} -\left(w-\frac{is}{\delta}+G\right)\left(w-\frac{is}{\delta}-G\right)\phi_{n,l_D}(\eta)=0 \tag{18}$$

where

$$G=i\sqrt{A_3} \tag{19}$$

The solutions of Eq. (18) is the hypergeometric function given as

$$\phi_{n,l_D}(\eta) =_2 F_1(a,x,y,\eta) \tag{20}$$

where

$$a=w-\frac{is}{\delta}+G;\ \ x=a-\frac{is}{\delta}-G;\ \ y=2w \tag{21}$$

The general solution of the wave function is obtained as

$$R_{v,J_D}(\eta)=N_{n,l_D}\eta^w(1-\eta)_2^{\frac{-is}{\delta}}F_1(a,x,y,\eta) \tag{22}$$

The scattering state for relativistic energy greater than zero in three dimensions can be defined as [48]

$$\begin{aligned} &U(\eta)\to 0,\ \ \eta\to 0;\\ &U(\eta)\to 2\sin\left[s\eta+\gamma-\frac{l\pi}{2}\right],\ \ \eta\to\infty \end{aligned} \tag{23}$$

For higher dimensions, it can be expressed as [45]

$$\begin{aligned} &U(\eta)\to 0,\ \ \eta\to 0;\\ &U(\eta)\to 2\sin\left[s\eta+\gamma_{l_D}-\frac{\pi}{2}\left(l_D+\frac{(D-3)}{2}\right)\right],\ \ \eta\to\infty \end{aligned} \tag{24}$$

Here, γ and γ_{l_D} are the scattering phase shifts in three dimensions and in higher dimensions, respectively. Also, l_D is the eigenvalues of the vibrational quantum number in higher dimensions.

By using the above recurrence conditions as applicable to Eq. (22) [29], the scattering phase shift relation for the *CYP* in higher dimension and its corresponding normalization constant becomes

$$\gamma_{l_D}=\frac{\pi}{2}[1+K]-\frac{s\ln 2}{\delta}+\arg[\Gamma(y-x-a)]-\arg[\Gamma(y-x)]-\arg[\Gamma(y-a)] \tag{25}$$

$$N_{n,l_D}=\frac{1}{\Gamma(y)}\left|\frac{\Gamma(y-a)\Gamma(y-x)}{\Gamma(y)\Gamma(y-x-a)}\right| \tag{26}$$

3. Results and discussion

In this work, the equations obtained are applied to the ground electronic state of NiC. Its molecular constants used are given below [49]: $d_e=2.76$ eV, $r_e 1.621$ Å, $\delta=2.25297$ 1/Å, $\mu=9.974265$ amu. The nonrelativistic energy expression of the *CYP* in higher dimensions is presented in equation (13). Also, the scattering phase shift relation for the *CYP* in higher dimension and its corresponding normalization constant are presented in equations (25) and (26), respectively in higher dimensions. Table 1 shows the bound state energies of *CYP* for NiC diatomic molecule at different quantum states in various dimensions and topological defects. At a particular dimension and topological defect, the energies of *CYP* for NiC increases with increase in quantum numbers. Increase in energy levels is also experienced as the dimensions and topological defect increases, for a particular quantum state. This shows that the energy levels of *CYP* for NiC diatomic molecule is greatly influenced by dimensions, topological defect and quantum states. Again, inter-dimensional degeneracy symmetry ($E_l^D=E_{l-1}^{D+2}$) is seen to exist for energy eigenvalues of the *CYP* for NiC diatomic

Table 1. Bound state energy eigenvalues (− eV) of the *CYP* for NiC diatomic molecule at different quantum states in different dimensions and topological defect parameters.

n	l	D = 3			D = 5			D = 6		
		$\alpha=0.2$	$\alpha=0.5$	$\alpha=1.0$	$\alpha=0.2$	$\alpha=0.5$	$\alpha=1.0$	$\alpha=0.2$	$\alpha=0.5$	$\alpha=1.0$
0	0	38207873.76	6113225.936	1528276.245	1618264.805	1152756.775	679184.6092	663351.3994	537461.4348	381998.5044
1	0	9551938.200	1528276.246	382038.8264	1112982.653	560359.4936	244480.6600	517864.8682	319710.2210	169754.7191
2	0	4245283.466	679211.4894	169772.6423	812093.0108	330145.7364	124715.2915	415473.9216	211751.8972	95469.39974
	1	415473.9216	211751.8972	95469.39974	256808.8488	148941.1285	75417.18550	175340.2081	110828.5755	61073.00610
3	0	2387954.312	382038.8262	95479.48344	618563.6962	217354.7216	75429.13748	340697.4604	150494.7267	61085.91522
	1	340697.4604	150494.7267	61085.91522	219353.7720	111420.6041	50472.57110	153786.7937	86069.94230	42399.50608
	2	153786.7937	86069.94230	42399.50608	114014.7930	68569.95714	36116.18248	87982.37844	55945.73022	31130.09690
4	0	1528276.245	244490.3380	61092.37036	486788.9142	153843.3226	50480.57414	284429.5702	112426.3214	42408.47338
	1	284429.5702	112426.3214	42408.47338	189531.8559	86476.21180	36125.73446	135975.5446	68765.59988	31139.98132
	2	135975.5446	68765.59988	31139.98132	102501.0233	56052.50010	27117.25248	80101.90670	46590.60854	23824.55292
	3	80101.90670	46590.60854	23824.55292	64349.11136	39347.81096	21095.32020	52838.29934	33675.88476	18807.92529
5	0	1061290.629	169772.6423	42412.95738	393038.2040	114584.9207	36131.46624	241030.2084	87164.38808	31146.57178
	1	241030.2084	87164.38808	31146.57178	165401.5507	69056.54670	27124.42974	121087.7566	56197.87906	23832.12366
	2	121087.7566	56197.87906	23832.12366	92646.62234	46672.46024	21103.14520	73234.21890	39398.45298	18815.90314
	3	73234.21890	39398.45298	18815.90314	59369.16774	33709.78298	16879.92969	49111.22668	29173.23902	15226.78740
	4	49111.22668	29173.23902	15226.78740	41304.26326	25495.55478	13803.93118	35222.69178	22471.83958	12570.47661

molecule, at a particular topological defect. This shows that the bound state energy eigenvalues of the CYP for NiC diatomic molecule is invariant under a transformation of an increase in the higher dimension by two ($D \to D+2$) and a decrease in the rotational quantum number by one ($l \to l-1$), at each vibrational quantum number considered. The numerical results of the scattering state phase shift of the CYP for NiC diatomic molecule for different dimensions and topological defect are given in Table 2. It is observed that the scattering phase shift of CYP potential increases clearly with increase in rotational quantum number, for each dimension. This increase is also observed for the scattering state phase shift of CYP potential as the dimension increases for each rotational quantum number. In Fig. 1 (a - f), we examined the variations of the wave functions and probability densities for the ground state ($n = 0$) and excited states ($n = 1, 2$) with the topological parameter. The peaks of the wave functions and probability densities are more pronounced as the topological defect parameter increases in strength indicating localization of the molecule. In Fig. 2 (a - f), The wave functions for the ground state ($n = 0$) and first excited state ($n = 1$) are plotted against the radial distance where the amplitudes decreases with an increase in the dimension. The variations of energy with both principal quantum number and orbital quantum number for various dimensions and topological defects are shown in Fig. 3 (a, b) and Fig. 4 (a, b). In these plots, the energy is seen to increase monotonously as the quantum numbers increase. In Fig. 5 (a), we presented the variations of the scattering phase shift with the dimension number for different rotational quantum number. The scattering phase shift increases with the increase in the orbital quantum states with a rectangular periodic wave form. In Fig. 5 (b), the scattering phase shift increases with the dimension number for various topological defect values. The shape is characterized by a rectangular periodic wave form where the amplitudes

Table 2. Scattering Phase Shift of the CYP for NiC diatomic molecules at different dimensions and topological defect parameters.

1	$\gamma_{D=3}$			$\gamma_{D=4}$			$\gamma_{D=5}$		
	$\alpha = 0.2$	$\alpha = 0.5$	$\alpha = 1.0$	$\alpha = 0.2$	$\alpha = 0.5$	$\alpha = 1.0$	$\alpha = 0.2$	$\alpha = 0.5$	$\alpha = 1.0$
0	4.712592654	− 1.570592654	4.712592654	5.344263002	2.202670348	5.344263002	5.975933351	− 0.3072519573	2.834340697
1	5.975933351	− 0.3072519573	2.834340697	3.466011045	3.466011045	3.466011045	4.097681393	0.9560887394	7.239274047
2	4.097681393	0.9560887394	7.239274047	7.870944396	4.729351742	7.870944396	8.502614744	2.219429436	5.361022090
3	8.502614744	2.219429436	5.361022090	5.992692434	5.992692438	5.992692434	9.765955437	3.482770133	9.765955437
4	9.765955437	3.482770133	9.765955437	10.39762579	7.256033135	10.39762579	7.887703479	4.746110829	7.887703479
5	7.887703479	4.746110829	7.887703479	8.519373832	8.519373832	8.519373832	12.29263683	6.009451526	12.29263683
6	12.29263683	6.009451526	12.29263683	12.92430718	9.782714528	12.92430718	10.41438488	7.272792223	10.41438488
7	10.41438488	7.272792223	10.41438488	11.04605523	11.04605523	11.04605523	14.81931822	8.536132924	14.81931822
8	14.81931822	8.536132924	14.81931822	15.45098857	12.30939592	15.45098857	12.94106627	9.799473621	12.94106627
9	12.94106627	9.799473621	12.94106627	13.57273662	13.57273662	13.57273662	17.34599962	11.06281432	17.34599962
10	17.34599962	11.06281432	17.34599962	17.97766997	14.83607732	17.97766997	15.46774766	12.32615501	15.46774766
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
20	29.97940658	23.69622128	29.97940658	30.61107693	27.46948428	30.61107693	28.10115463	24.95956198	28.10115463
30	42.61281355	36.32962825	42.61281355	43.24448390	40.10289125	43.24448390	40.73456159	37.59296894	40.73456159
40	55.24622052	48.96303522	55.24622052	55.87789087	52.73629822	55.87789087	53.36796856	50.22637591	53.36796856
50	67.87962748	61.59644218	67.87962748	68.51129784	65.36970519	68.51129784	66.00137553	62.85978288	66.00137553
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
80	102.6382557	99.49666304	102.6382557	106.4115188	103.2699261	106.4115188	107.0431891	100.7600037	107.0431891
90	115.2716627	112.1300700	115.2716627	119.0449258	115.9033331	119.0449258	119.6765961	113.3934107	119.6765961
100	127.9050697	124.7634770	127.9050697	131.6783327	128.5367400	131.6783327	132.3100031	126.0268177	132.3100031

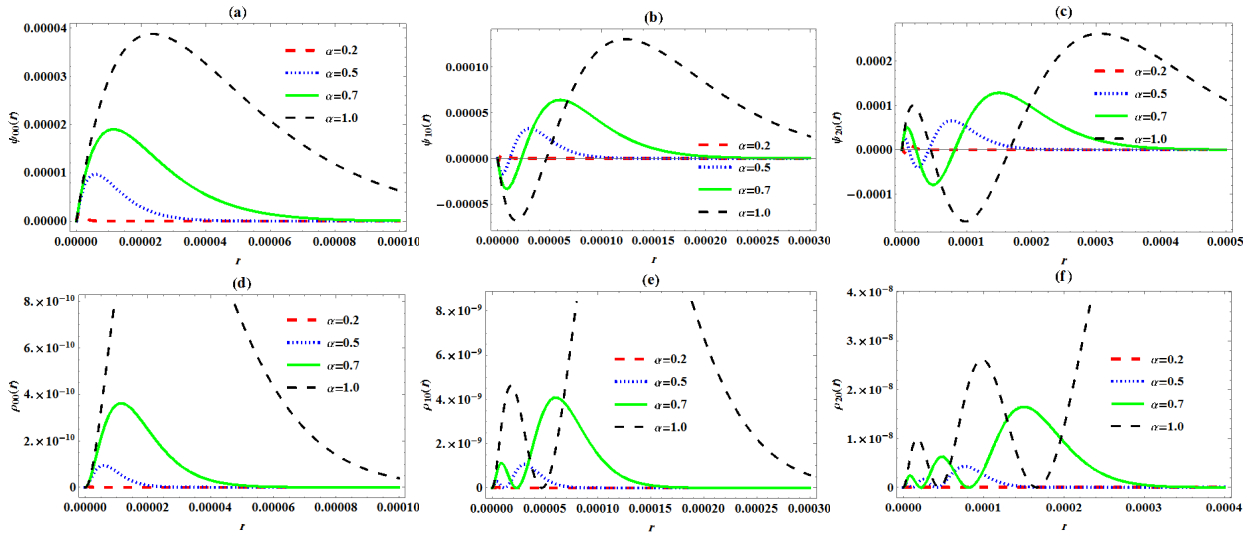

Figure 1. Variations of wave functions and Probability densities in 3D for NiC diatomic molecule at various topological defect parameters.

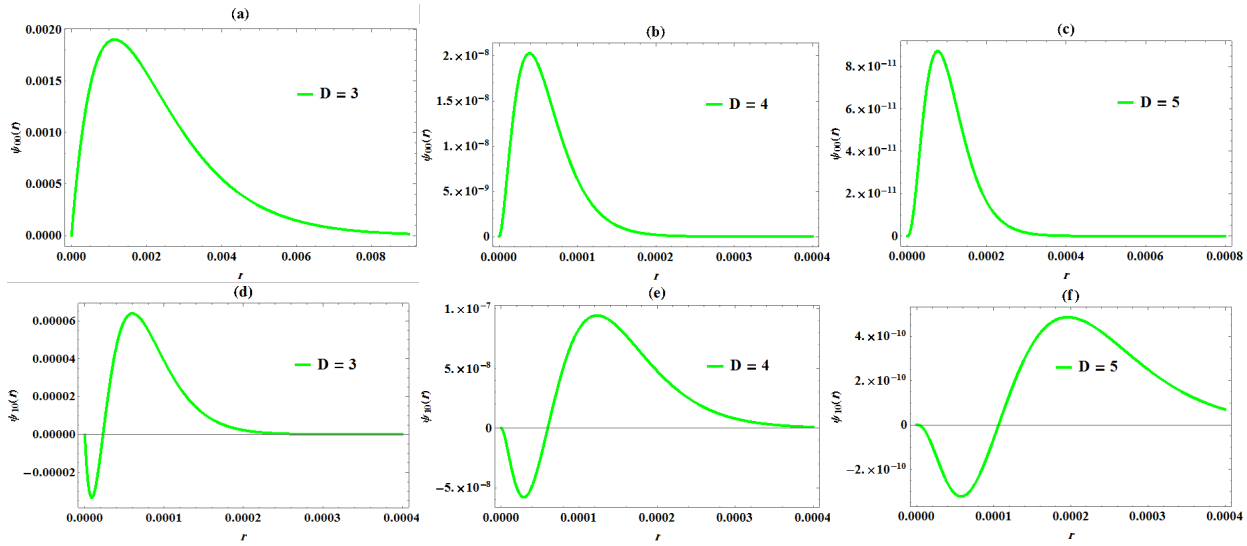

Figure 2. Variations of wave functions for the ground and first excited states of CYP for NiC diatomic molecule at various dimensions.

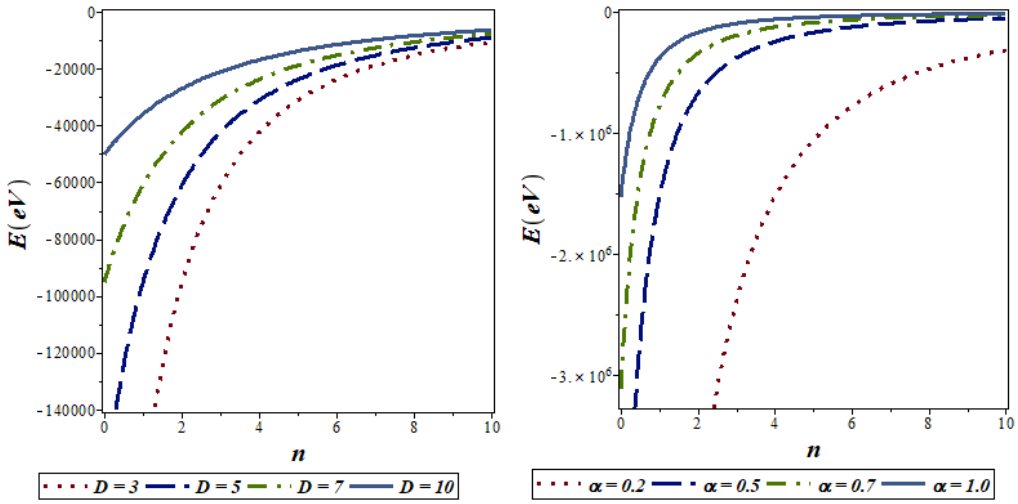

Figure 3. Variation of energy eigenvalues of NiC diatomic molecule with vibrational quantum number at various dimensions and topological defect parameters.

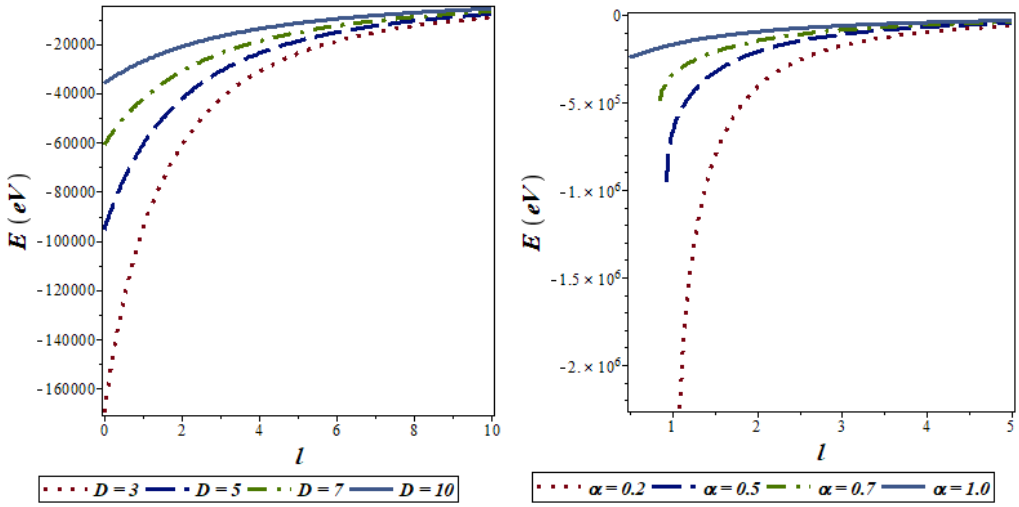

Figure 4. Variation of energy eigenvalues of NiC diatomic molecule with rotational quantum number at various dimensions and topological defect parameters.

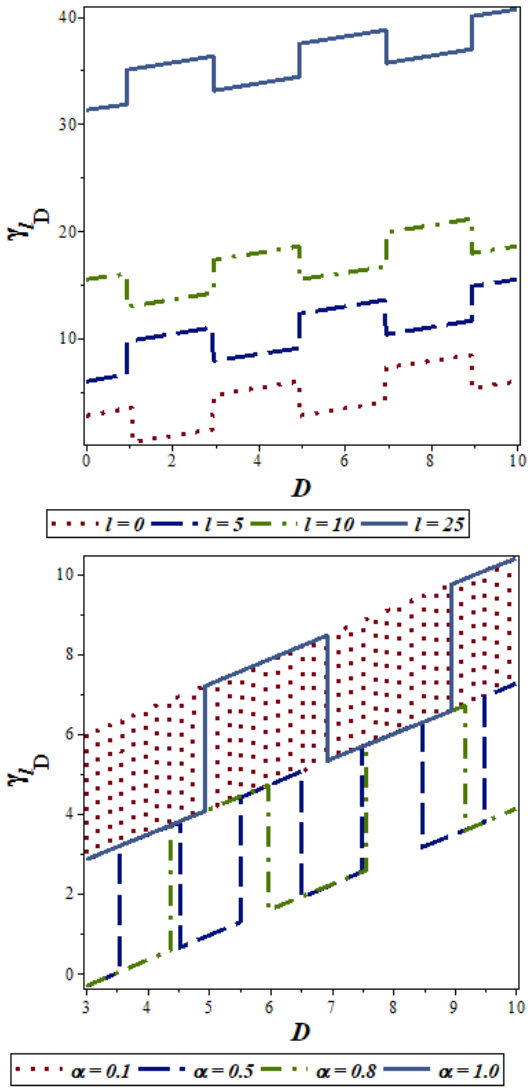

Figure 5. Variation of scattering phase shift of NiC diatomic molecule with dimensions at various rotational quantum number and topological defect parameters.

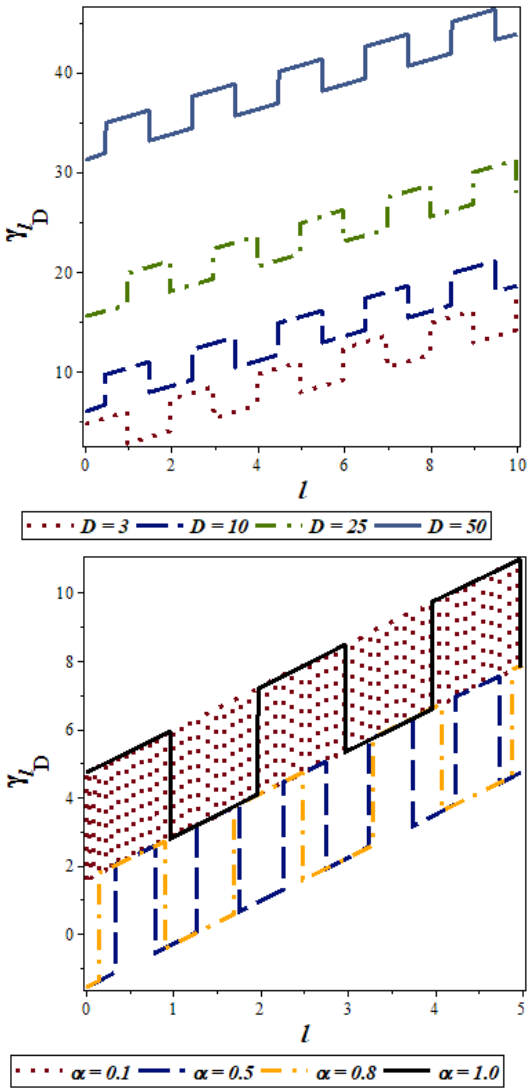

Figure 6. Variation of scattering phase shift of NiC diatomic molecule with rotational quantum number at various dimensions and topological defect parameters.

overlap. Similar trends are observed for the scattering phase shift plotted in Fig. 6 (a, b). These results are new, and they promise to be very relevant in different areas of applied physics.

4. Conclusion

The eigensolutions of the nonrelativistic radial Schrödinger equation with PGM in higher dimensions for a diatomic substance confined in a CYP function has been obtained via the Nikiforov-Uvarov functional analysis approach. The analytical equation for the energy spectra and wave function were obtained in closed form. These equations were applied to investigate the variation of the energy spectra, wave function, probability density and scattering phase shift of NiC with the dimension number and the topological defect parameter. The wave functions amplitudes for the ground and excited states were found to increase with the increase in the topological defect parameters but decrease with the dimension number. The scattering phase shifts were found to be sensitive to the rotational quantum number and topological defect parameter where the wave form is characterized by a rectangular periodic motion.
we can conclude that the present study will have meaningful impact in areas of chemical physics, condensed matter physics, atomic physics, especially in quantum dots studies with exponential-type potentials [50–55], potential energy functions applicability [56–60] and most recently in studies involving non-commutative phase space [61].

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Authors contributions
U.S. Okorie: Conceptualization, Writing – Original draft, Formal Analysis. A.N. Ikot: Methodology, Investigation. G.J. Rampho: Validation, Writing – Review and Editing. E. Omugbe: Software, Visualization. R. Horchani: Formal Analysis, Resources. All the authors read and approved the submission of the manuscript.

Availability of data and materials
This manuscript has no associated data, or the data will not be deposited. Hence, all data included are available on request by contacting the corresponding author.

Conflict of interests
The authors declare no conflict of interest.

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Appendix
Review of Nikiforov-Uvarov-Functional Analysis (NUFA) Method

Using the concepts of NU method [62], parametric NU method [63] and the functional analysis method [64], we proposed a simple and elegant method for solving a second order differential equation of the hypergeometric type called Nikiforov-Uvarov-Functional Analysis (NUFA) method. As it is well-known, the NU is used to solve a second-order differential equation of the form [62]

$$\frac{d^2\psi(s)}{ds^2}+\frac{\tilde{\tau}(s)}{\sigma(s)}\frac{d\psi(s)}{ds}+\frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s)=0 \tag{27a}$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials, at most of second degree, and $\tilde{\tau}(s)$ is a first-degree polynomial. Tezcan and Sever [63] latter introduced the parametric form of NU method in the form

$$\frac{d^2\psi(s)}{ds^2}+\frac{\alpha_1-\alpha_2 s}{s(1-\alpha_3 s)}\frac{d\psi(s)}{ds}+\frac{1}{s^2(1-\alpha_3 s)^2}[-\xi_1 s^2+\xi_2 s-\xi_3]\psi(s)=0 \tag{27b}$$

where α_i and $\xi_i (i=1,\ 2,\ 3)$ are all parameters. It can be observed in Eq. (3) that the differential equation has two singularities at $s\to 0$ and $s\to 1$, thus we take the wave function in the form,

$$\psi(s)=s^{\lambda}(1-s)^{\nu}f(s) \tag{27c}$$

Substituting Eq. (27c) into Eq. (27b) leads to the following equation,

$$s(1-\alpha_3 s)\frac{d^2f(s)}{ds^2}+[\alpha_1+2\lambda-(2\lambda\alpha_3+2\nu\alpha_3+\alpha_2)s]\frac{df(s)}{ds}-\alpha_3\left(\lambda+\nu+\frac{1}{2}(\frac{\alpha_2}{\alpha_3}-1)+\sqrt{\frac{1}{4}(\frac{\alpha_2}{\alpha_3}-1)^2+\frac{\xi_1}{\alpha_3^2}}\right)\left(\lambda+\nu+\frac{1}{2}(\frac{\alpha_2}{\alpha_3}-1)-\sqrt{\frac{1}{4}(\frac{\alpha_2}{\alpha_3}-1)^2+\frac{\xi_1}{\alpha_3^2}}\right)+\left[\frac{\lambda(\lambda-1)+\alpha_1\lambda-\xi_3}{s}+\frac{\nu(\nu-1)\alpha_3+\alpha_2\nu-\alpha_1\alpha_3\nu-\frac{\xi_1}{\alpha_3}+\xi_2-\xi_3\alpha_3}{(1-\alpha_3 s)}\right]f(s)=0 \tag{27d}$$

Eq. (27d) can be reduced to a Gauss hypergeometric equation if and only if the following functions vanished,

$$\lambda(\lambda-1)+\alpha_1\lambda-\xi_3=0 \tag{27e}$$

$$\nu(\nu-1)\alpha_3+\alpha_2\nu-\alpha_1\alpha_3\nu-\frac{\xi_1}{\alpha_3}+\xi_2-\xi_3\alpha_3=0 \tag{27f}$$

Thus, Eq. (27d) now becomes

$$s(1-\alpha_3 s)\frac{d^2f(s)}{ds^2}+[\alpha_1+2\lambda-(2\lambda\alpha_3+2\nu\alpha_3+\alpha_2)s]\frac{df(s)}{ds}-\alpha_3\left(\lambda+\nu+\frac{1}{2}(\frac{\alpha_2}{\alpha_3}-1)+\sqrt{\frac{1}{4}(\frac{\alpha_2}{\alpha_3}-1)^2+\frac{\xi_1}{\alpha_3^2}}\right)\left(\lambda+\nu+\frac{1}{2}(\frac{\alpha_2}{\alpha_3}-1)-\sqrt{\frac{1}{4}(\frac{\alpha_2}{\alpha_3}-1)^2+\frac{\xi_1}{\alpha_3^2}}\right)f(s)=0 \tag{27g}$$

Solving Eqs. (27f) and (27g) completely give,

$$\lambda=\frac{1}{2}\left((1-\alpha_1)\pm\sqrt{(1-\alpha_1)^2+4\xi_3}\right) \tag{27h}$$

$$\nu=\frac{1}{2\alpha_3}\left((\alpha_3+\alpha_1\alpha_3-\alpha_2)\pm\sqrt{(\alpha_3+\alpha_1\alpha_3-\alpha_2)^2+4(\frac{\xi_1}{\alpha_3}+\alpha_3\xi_3-\xi_2)}\right) \tag{27i}$$

Eq. (27g) is the hypergeometric equation type of the form,

$$x(1-x)\frac{d^2f(x)}{dx^2}+[c+(a+b+1)x]\frac{df(x)}{dx}-[ab]f(x)=0 \tag{27j}$$

where a, b, c are given as follows,

$$a=\sqrt{\alpha_3}\left(\lambda+\nu+\frac{1}{2}(\frac{\alpha_2}{\alpha_3}-1)+\sqrt{\frac{1}{4}(\frac{\alpha_2}{\alpha_3}-1)^2+\frac{\xi_1}{\alpha_3^2}}\right) \tag{27k}$$

$$b=\sqrt{\alpha_3}\left(\lambda+\nu+\frac{1}{2}(\frac{\alpha_2}{\alpha_3}-1)-\sqrt{\frac{1}{4}(\frac{\alpha_2}{\alpha_3}-1)^2+\frac{\xi_1}{\alpha_3^2}}\right) \tag{27l}$$

$$c=\alpha_1+2\lambda \tag{27m}$$

Setting either a or b equal to a negative integer $-n$, the hypergeometric function $f(s)$ turns to a polynomial of degree n. Hence, the hypergeometric function $f(s)$ approaches finite in the following quantum condition i.e. $a=-n$, where $n=0,\,1,\,2,\,3,\cdots,n_{\max}$.
Using the above quantum condition,

$$\sqrt{\alpha_3}\left(\lambda+\nu+\frac{1}{2}(\frac{\alpha_2}{\alpha_3}-1)+\sqrt{\frac{1}{4}(\frac{\alpha_2}{\alpha_3}-1)^2+\frac{\xi_1}{\alpha_3^2}}\right)=-n \tag{27n}$$

$$\lambda+\nu+\frac{1}{2}(\frac{\alpha_2}{\alpha_3}-1)+\frac{n}{\sqrt{\alpha_3}}=-\sqrt{\frac{1}{4}(\frac{\alpha_2}{\alpha_3}-1)^2+\frac{\xi_1}{\alpha_3^2}} \tag{27o}$$

Squaring both sides of Eq. (27o) and rearranging, we obtain the energy equation for the NUFA method as

$$\lambda^2+2\lambda\left(\nu+\frac{1}{2}(\frac{\alpha_2}{\alpha_3}-1)+\frac{n}{\sqrt{\alpha_3}}\right)+\left(\nu+\frac{1}{2}(\frac{\alpha_2}{\alpha_3}-1)+\frac{n}{\sqrt{\alpha_3}}\right)^2-\frac{1}{4}(\frac{\alpha_2}{\alpha_3}-1)^2-\frac{\xi_1}{\alpha_3^2}=0 \tag{27p}$$

By substituting Eqs. (27h) and (27i) into Eq. (27c), we obtain the corresponding wave equation for the NUFA method as

$$\psi(s)=\xi s^{\frac{(1-\alpha_1)+\sqrt{(\alpha_1-1)^2+4\xi_3}}{2}}(1-\alpha_3 s)^{\frac{(\alpha_3+\alpha_1\alpha_3-\alpha_2)+\sqrt{(\alpha_3+\alpha_1\alpha_3-\alpha_2)^2+4(\frac{\xi_1}{\alpha_3^2}+\alpha_3\xi_3-\xi_2)}}{2\alpha_3}}{}_2F_1(a,b,c;s) \tag{27q}$$

where ξ is the normalization constant.