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Energy Analysis of RbH, NI, And ScI Diatomic Molecules with Position-Dependent Mass

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ABSTRACT

In this study, we analyze the energy level of the diatomic molecules in the case of a non-relativistic quantum system influenced by an external magnetic field and exponential potential. The energy eigenvalue as the solution of the Schrödinger equation in the cosmic-string spacetime was simulated numerically. The energy spectrum was calculated for the three selected diatomic molecules involving RbH, NI, ScI. The influence of the quantum number, potential parameter, and the external magnetic field is considered in this computation to recover the behavior of the particle. The results showed that the energy value depends on the quantum number, potential parameter, mass of the molecule, and magnetic field strength. The magnetic field strength and the potential parameter most apparently affect the change in energy level, followed by the quantum number which also affects the increase in the energy level of the particle considered in this system. In addition, these results may be useful in studying the thermodynamic, optic, and magnetic properties of the atomic interaction of a system particle.

Keywords: Non-relativistic system; Diatomic molecule; Position-dependent mass; External magnetic field; Cosmic string

INTRODUCTION

The study of quantum systems in the presence of external fields has been an interesting area of research due to its significance in atomic, molecular, and condensed matter physics (Abu-Shady et al., 2021; C. O. Edet et al., 2021; Faniandari et al., 2022, 2023; Gu et al., 2022; Karayer, 2020; Sargsian et al., 2021). The quantum behavior of particles in external potentials provides valuable insights into the fundamental nature of interactions within diatomic molecular systems (C. Edet & Ikot, 2022; Morse, 1929; Pekeris, 1934). In particular, the effect of an external magnetic field on molecular systems is crucial for understanding their spectroscopic and thermodynamic properties (Faniandari et al., 2022, 2023). Several studies have explored quantum mechanical models incorporating different potential functions and external fields to analyze the energy spectrum and other physical properties of quantum systems (Greiner & Müller, 2001).

The Schrödinger equation plays a central role in investigating the energy eigenvalues of quantum systems. Various potential models have been proposed to describe interactions in diatomic molecules, including the Morse potential (Khordad et al., 2022; Okoi et al., 2020), Kratzer potential (Ikot et al., 2020; Onyenegecha et al., 2020), and exponential-type potentials (Fu et al., 2019; Ikot et al., 2021; Ovando et al., 2019). In many practical applications, the inclusion of an external magnetic field significantly alters the energy

levels of quantum systems, leading to observable shifts in spectral lines. Previous research has demonstrated that the presence of a cosmic-string spacetime can further modify these energy states, introducing topological effects into the quantum behavior of particles (Cunha & Silva, 2021; C. O. Edet et al., 2022; Mustafa, 2022; Sobhani et al., 2018).

In this study, we analyze the energy spectrum of diatomic molecules within a non-relativistic quantum system subjected to an external magnetic field and an exponential potential within a cosmic-string spacetime. This work aims to understand how different physical parameters influence the energy levels of molecular systems. By incorporating a cosmic string background, we extend the previous findings on molecular energy spectra and contribute to the broader understanding of quantum interactions in curved spacetime scenarios (Mustafa, 2024; Sobhani et al., 2018).

The numerical solution of the Schrödinger equation allows for an accurate evaluation of the energy eigenvalues in such systems (Heidari et al., 2024). To investigate the impact of external parameters, we focus on three selected diatomic molecules: RbH, NI, and ScI. These molecules exhibit interesting spectroscopic properties and serve as ideal candidates for studying the effects of magnetic fields and potential parameters on molecular energy levels (Okorie et al., 2020). The computation considers the influence of the quantum number, potential parameter, and external magnetic field strength to recover the behavior of the particle in different physical settings.

This paper is organized as follows: Section 2 outlines the brief theoretical framework, including the formulation of the Schrödinger equation in the presence of an external magnetic field and an exponential potential. Section 3 presents the materials and methods including the numerical approach and computational methodology. Section 4 discusses the results obtained for the selected diatomic molecules, followed by an analysis of parameter dependencies. Finally, Section 5 concludes with a summary of key findings and potential applications of this study in future research directions.

The non-relativistic system can be represented by the Schrödinger equation. For the case there is a defect of topology cosmic string, there is declination α in the φ-part. The square of time independent of infinitesimal length given by

$$ds^2 = d\rho^2 + \alpha^2\rho^2 d\varphi^2 + dz^2 \tag{1}$$

The external magnetic field vector and exponential potential are formulated (Eshghi et al., 2017; Hassanabadi et al., 2013)

$$\vec{A} = \left(\frac{Be^{-\sigma\rho}}{2\alpha\rho} + \frac{\Phi_{AB}}{2\pi\rho}\right)\hat{\varphi}_0 \tag{2}$$

$$\tilde{V}(\rho) = \frac{e^{-\sigma\rho}}{\rho} \tag{3}$$

and its position-dependent mass, a function of radial function is given as

$$M(\rho) = \frac{M_0 e^{-\sigma\rho}}{\rho^2} \tag{4}$$

The purpose of using the position-dependent mass is to find out how the mass variable as a function of position affects the quantum mechanical system. For example, the effective mass of electron holes in thin-layered quantum wells varies according to their composition level. In that system, the electron mass can change at a composition rate that depends on its position. The position-dependent mass is useful for studying transport properties in semiconductors. The mass variable as a function of position needs to be used so that the Schrödinger equation that applies Laplacian can be solved analytically. The Schrödinger equation is written as

$$\left\{\left(\bar{p}+\frac{e}{c}\bar{A}\right).\frac{1}{2M}\left(\bar{p}+\frac{e}{c}\bar{A}\right)+(V-E)\right\}f(r,\varphi)=0 \quad (5)$$

MATERIALS & METHODS

The second-order differential of the Schrodinger equation in (5) was already solved using Laplace transform method in our previous publication (Faniandari et al., 2024). The non-relativistic energy is obtained as

$$E=\frac{\hbar^2}{2M_0\sigma}\left[\left(n+\frac{2\kappa+1}{2}\right)\left(2\left\{\left(\frac{M_0}{\hbar}\omega_c\frac{V_0}{2\alpha}\right)^2+\frac{1}{4}-\frac{2M_0}{\hbar^2}V_1\right\}\sigma^2\right)+\frac{3}{2}\sigma-\left\{2\sigma\frac{M_0}{\hbar}\omega_c\frac{V_0}{2\alpha}\left[\left(\frac{m}{\alpha}+\xi\right)+\left(\frac{M_0}{\hbar}\omega_c\frac{V_0}{2\alpha}\right)\right]\right\}-V_1\frac{2M_0\sigma}{\hbar^2}\right] \quad (6)$$

This energy equation becomes the fundamental equation to analyze the energy spectra of the molecules in the system. To examine the behavior of the energy level under the influence of the external magnetic fields in equation (6), we plot it as a function of several parameters for the RbH, NI, and ScI diatomic molecules.

Table 1. ***Model parameter for some diatomic molecules***

Molecules	D_e **(cm^{-1})**	r_e **(Å)**	α **(cm^{-1})**	M_0 **(amu)**
RbH	14580.00	2.3668	0.7070×10^{-1}	0.9961
NI	13227.49	1.9124	2.6400×10^{-3}	12.6114
ScI	23051.34	1.9124	2.5250×10^{-4}	33.1961

The computational methods were used to calculate the energy level of the diatomic molecules in Table 1 using their spectroscopic parameters.

RESULTS & DISCUSSION

In this part, we discuss the theoretical prediction of the energy level for the RbH, NI, and ScI diatomic molecules. The results of the energy level for these three selected diatomic molecules in Table 1 with the variation of quantum number, magnetic quantum number, and external magnetic field are shown in Tables 2-4.

Table 2. ***The energy level for the exponential potential under the influence of external magnetic for the RbH molecule***

m	***n***	***E (eV)***			
		B=12 T	***B=14 T***	***B=16 T***	***B=18 T***
1	0	250512.5	390916.5	575589.8	810556.8
	1	254124.8	395834.0	582013.1	818686.8
	2	257737.2	400751.4	588436.4	826816.7
	3	261349.5	405668.8	594859.7	834946.7
	4	264961.9	410586.3	601283.0	843076.7
2	0	286470.0	439849.8	639502.0	891452.3
	1	290082.3	444767.2	645925.3	899582.3
	2	293694.7	449684.6	652348.6	907712.2
	3	297307.0	454602.1	658771.9	915842.2
	4	300919.4	459519.5	665195.2	923972.2
3	0	322330.2	488690.6	703326.5	972264.6
	1	325942.6	493608.0	709749.8	980394.6
	2	329554.9	498525.5	716173.1	988524.5
	3	333167.3	503442.9	722596.4	996654.5
	4	336779.6	508360.3	729019.7	1004784.5

The theoretical prediction of the energy level for the three selected diatomic molecules with the natural units and the parameters used in our model are listed in Table 1. The computational results are presented in Tables 2-4 sequentially for RbH, NI, and ScI molecules. The energy spectra for the exponential potential under the influence of an external magnetic field for the RbH molecule are shown in Table 2. The presence of the external magnetic field has influenced the energy level to increase with the increase of its value. These results are similar to the NI and ScI diatomic molecules in Table 3 and Table 4.

Table 3. ***The energy level for the exponential potential under the influence of an external magnetic for the NI molecule***

m	***n***	***E (eV)***			
		B=12 T	***B=14 T***	***B=16 T***	***B=18 T***
1	0	16093.4	26586.4	40561.3	58499.3
	1	16376.9	26973.0	41066.8	59139.6
	2	16660.4	27359.5	41572.3	59779.9
	3	16943.8	27746.1	42077.8	60420.2
	4	17227.3	28132.7	42583.3	61060.5
2	0	19441.4	30954.1	46112.3	65394.4
	1	19724.8	31340.6	46617.8	66034.6
	2	20008.3	31727.2	47123.3	66674.9
	3	20291.8	32113.7	47628.8	67315.2
	4	20575.3	32500.3	48134.3	67955.5
3	0	22637.4	35192.0	51548.6	72185.9
	1	22920.9	35578.5	52054.1	72826.2
	2	23204.4	35965.1	52559.6	73466.5
	3	23487.9	36351.6	53065.1	74106.8
	4	23771.3	36738.2	53570.6	74747.1

Table 4. ***The energy level for the exponential potential under the influence of external magnetic for the ScI molecule***

m	***n***	***E (eV)***			
		B=12 T	***B=14 T***	***B=16 T***	***B=18 T***
1	0	2211.4	6384.0	11484.5	17992.5
	1	2317.9	6529.6	11675.3	18234.5
	2	2424.3	6675.3	11866.1	18476.5
	3	2530.8	6820.9	12056.9	18718.5
	4	2637.2	6966.5	12247.7	18960.6
2	0	4645.9	8740.5	14157.9	21113.9
	1	4752.3	8886.1	14348.7	21355.9
	2	4858.8	9031.7	14539.5	21597.9
	3	4965.2	9177.3	14730.3	21839.9
	4	5071.7	9323.0	14921.1	22081.9
3	0	6365.9	10778.0	16616.1	24068.8
	1	6472.4	10923.6	16806.9	24310.8
	2	6578.8	11069.2	16997.7	24552.8
	3	6685.3	11214.8	17188.5	24794.8
	4	6791.8	11360.5	17379.3	25036.8

Figure 1 shows the energy as a function of the quantum number n for the RbH, NI, and ScI diatomic molecules. Figures 2-3 show the energy as a function of the potential parameters σ and V_0 for the RbH, NI, and ScI diatomic molecules. Figures 4 show the energy as a function of the magnetic field strength B with the variation of the diatomic molecules.

In Figure 1, the energy was plotted as a function of quantum number n for the three diatomic molecules, RbH, NI, and ScI. The

energy eigenvalue for each molecule has a positive value and it was increased linearly with an increase in quantum number. As we know from Table 1, the mass of ScI is the biggest and then followed by NI and RbH. It is shown that the larger mass of the molecule also caused the energy eigenvalue to decrease. The change of the energy level for the small molecule (in this case RbH) is the biggest compared to the NI and ScI diatomic molecules.

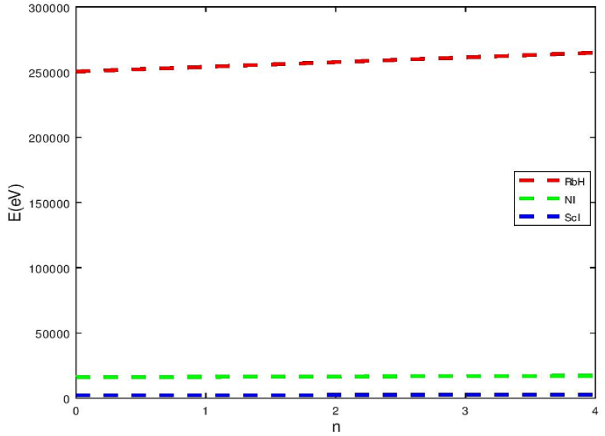

Figure 1. The graph of energy versus n for RbH, NI, and ScI

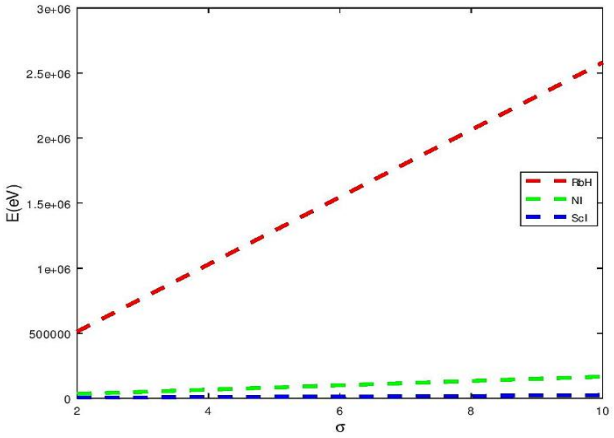

Figure 2. The graph of energy versus σ for RbH, NI, and ScI

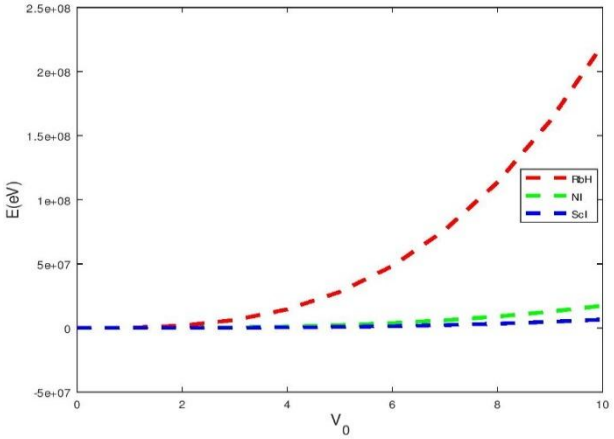

Figure 3. The graph of energy versus V_0 for RbH, NI, and ScI

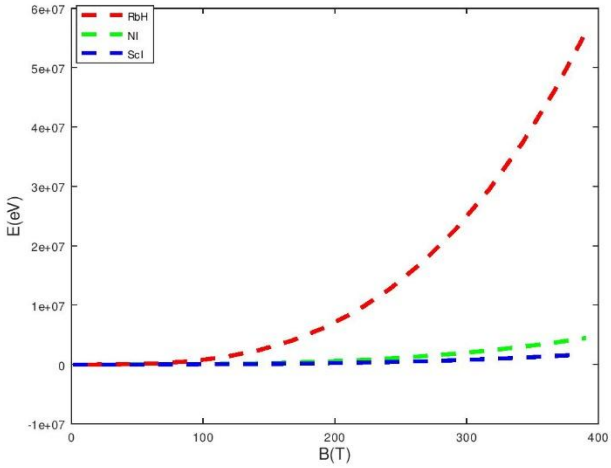

Figure 4. The graph of energy versus magnetic field strength B for RbH, NI, and ScI.

The energy as a function of potential parameter σ is plotted for the three diatomic molecules in Figure 2 when B = 12 T. The energy tends to increase with the increase of σ, respectively for RbH, NI, and ScI. The particle is more bound with small values of σ, while less bound with the increasing values of α. The molecule's mass change has a non-linear effect on the plot of the energy level. The weigher particle has a smaller energy level for the fixed value of external magnetic field strength *B*.

In Figure 3, the energy as a function of potential parameter V_0 is plotted for the three selected molecules, when B is fixed to be 12 T. It is obvious that the increasing value of potential parameter V_0 caused the energy to increase exponentially. The molecule's mass change has a negative effect on the plot of the energy. The weigher particle has a smaller energy level for the fixed value of external magnetic field strength *B*. Furthermore, it tends to be more bound with an increasing value of M_0.

In Figure 4, we plotted the energy level against the magnetic field strength *B* with the variation of the diatomic molecules, when the potential parameters are constant. The energy decays exponentially as the magnetic field strength *B* grows, respectively for the RbH, NI, and ScI molecules. The weigher mass of the diatomic molecule will decrease the energy level of the particle. The particle becomes more bound for ScI, then followed by NI and RbH.

Our results indicate that the energy eigenvalues strongly depend on the quantum number, potential parameter, mass of the molecule, and strength of the magnetic field. Specifically, the external magnetic field and potential parameter exhibit the most significant influence on the energy spectrum, leading to observable shifts in energy levels. Additionally, the quantum number plays a crucial role in determining the overall increase in energy values within the system.

The implications of our findings extend beyond theoretical quantum mechanics, as the results are relevant for understanding the thermodynamic, optical, and magnetic properties of molecular systems. Investigating the influence of external parameters on energy levels aids in refining models used in spectroscopy, quantum computing, and material sciences. Furthermore, the study of energy spectra in a cosmic-string spacetime provides new perspectives on quantum interactions in the presence of topological defects.

CONCLUSION

The analysis of the behavior of the bound state energy levels for the RbH, NI, and ScI diatomic molecules was carried out in the non-relativistic system. The various values of the potential parameter, mass parameter, and external magnetic force were employed.

It showed that the energy value depends on the quantum number, potential parameter, mass of the molecule, and magnetic field strength. The magnetic field strength and the potential parameter most apparently affect the change in energy level, then followed by the quantum number which also affects the increase in the energy level of the particle considered in this system. These results can motivate the further study of molecular physics for several molecules.

Declaration by Authors

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