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THEORETICAL STUDY OF THE VIBRATIONAL SPECTRUM OF THE CESIUM DIMER USING A HYBRID INTERACTION MODEL

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The present study investigates the quantum properties of the cesium dimer (Cs_2) using a hybrid interaction model that combines the Möbius square potential with the screened Kratzer potential (MSSKP). The vibrational energy levels are obtained analytically by solving the Schrödinger equation within the framework of the parametric Nikiforov–Uvarov (pNU) method. The calculated spectra exhibit excellent agreement with available experimental Rydberg–Klein–Rees (RKR) data, demonstrating the validity of the proposed model. Comparative analysis with established potential models, namely the Morse and Manning–Rosen potentials, reveals the superior predictive performance of the MSSKP approach. In particular, the MSSKP model achieves a minimum mean absolute error (MAE) of 0.0234 cm^{-1}, compared with 0.2364 cm^{-1} and 0.0517 cm^{-1} for the Morse and Manning–Rosen potentials, respectively. These results highlight the enhanced accuracy and reliability of the MSSKP model in describing the vibrational spectrum of Cs_2. The findings further provide valuable insights into molecular structure, bonding interactions, and quantum behavior, underscoring the potential of the proposed framework for applications in quantum chemistry, molecular spectroscopy, and the theoretical modeling of diatomic molecular systems.
Keywords: *Hybrid interaction model; Mean absolute error; Rydberg–Klein–Rees (RKR) data; Analytical method, Molecular spectroscopy*

1. INTRODUCTION

Accurate theoretical descriptions of molecular systems remain a central pursuit in quantum mechanics and molecular physics, where the interplay between nuclear motion and interatomic forces governs the vibrational, rotational, spectroscopic, and thermodynamic behavior of molecules [1–3]. Among these systems, diatomic molecules serve as fundamental models for understanding molecular interactions due to their relative simplicity and rich physical characteristics [4]. The cesium dimer (Cs_2) is of particular interest because of its unique electronic configuration, large atomic mass, pronounced relativistic effects, and wide applicability across various fields, including atomic physics, molecular spectroscopy, quantum computation, and precision metrology [5]. Cesium dimer (Cs_2) plays a key role in the advancement of atomic clocks, laser cooling technologies, and the exploration of long-range molecular interactions and potential energy surfaces [6]. Despite its importance, achieving a precise theoretical representation of Cs_2 remains challenging due to its highly anharmonic vibrational structure.

Over the years, numerous molecular potential models such as the Morse, Kratzer, Rosen–Morse, and Tietz–Hua potentials have been developed to approximate interatomic interactions in diatomic molecules [7–9]. While these models are analytically convenient and effective for light molecules, their accuracy decreases significantly for heavy diatomic systems such as Cs_2, particularly in higher vibrational and rotational states. This limitation arises because many traditional potentials lack sufficient flexibility to accurately describe the potential energy surface near the dissociation limit, often leading to deviations from experimental data obtained through spectroscopic methods such as Rydberg–Klein–Rees (RKR) analysis [10–12]. A detailed theoretical description of Cs_2 requires potential functions that represent both short- and long-range interactions and incorporate essential molecular parameters, such as the dissociation energy, the equilibrium bond length, and screening effects. An adaptable framework that satisfies these requirements is the Möbius Square–Screened Kratzer Potential (MSSKP) model [13,14]. The Möbius square potential, a relatively recent development in molecular interaction modeling, introduces distinctive geometric features associated with confinement effects in molecular systems. In contrast, the screened Kratzer potential incorporates a screening parameter that effectively modulates long-range intermolecular interactions. The combination of these two forms yields a hybrid potential that simultaneously accounts for short-range confinement and screened long-range behavior, thereby providing a more comprehensive and flexible theoretical framework for the analysis of molecular structure and dynamics.

Solving the radial Schrödinger equation within this hybrid potential framework provides valuable insight into bound-state energy eigenvalues and the corresponding wavefunctions—quantities that are essential for predicting

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vibrational spectra, molecular stability, and related physical properties [15,16]. Analytical techniques such as the Nikiforov–Uvarov (NU) method [17] are particularly advantageous in this context, as they enable exact or approximate solutions of second-order differential equations derived from the Schrödinger equation, even for complex potential forms. Recent studies have continued to investigate Cs_2 using a variety of potential models and solution techniques. Approaches based on the Tietz–Hua, improved Rosen–Morse, generalized Pöschl–Teller, Manning–Rosen, and deformed exponential-type potentials have been employed to determine the rovibrational spectra of Cs_2 with varying degrees of agreement with experimental observations [18–20]. For example, the Tietz–Hua potential has demonstrated improved consistency with spectroscopic data compared to the Morse potential, particularly at higher vibrational levels. Similarly, the improved Rosen–Morse potential has proven effective in modeling the rotational–vibrational spectra of heavy dimers, showing enhanced agreement with experimental measurements.

Building on these developments, the present work investigates the quantum bound states described by the Möbius Square plus Screened Kratzer Potential (MSSKP) [21]. This hybrid potential is particularly well suited for analyzing vibrational and rotational spectra, as well as the discrete energy levels of diatomic molecules such as Cs_2, where an accurate representation of interatomic interactions is essential. Owing to its well-resolved vibrational structure, Cs_2 provides a valuable benchmark for evaluating theoretical models and validating spectroscopic predictions. Although both the Möbius square potential and the screened Kratzer potential have been extensively studied in isolation, their combined formulation has not yet been systematically explored. This study addresses that gap by solving the Schrödinger equation within the MSSKP framework for the Cs_2 molecule. The resulting energy eigenvalues are compared with experimental data obtained from Rydberg–Klein–Rees (RKR) analysis to assess the accuracy and reliability of the proposed potential. The findings align with ongoing efforts to develop more refined potential energy models in quantum chemistry and molecular physics. Ultimately, this work contributes to a deeper understanding of heavy diatomic molecules and strengthens the theoretical foundation for future experimental and computational investigations.

The interaction potential adopted in this study is written in the following form [21].

$$V(r_z) = Y_0\left(\frac{A_0 + B_0 e^{-\alpha_z r_z}}{1-e^{-\alpha_z r_z}}\right)^2 - 2D_e\left(\frac{r_e}{r_z} - \frac{r_e^2}{2r_z^2}\right)e^{-\alpha_z r_z}\,. \tag{1}$$

The dissociation energy is denoted by D_e, whereas r_e represent the equilibrium bond length parameter. Furthermore, $A_0, B_0,$ and Y_0 corresponds to the strength of the Möbius square potential, while α_z are the screening parameter.

2 THE THEORY

The quantum dynamics of a particle confined within a potential field are described by the time-independent Schrödinger equation. For the hybrid potential examined in this study, the corresponding radial equation can be written as [22]:

$$\frac{d^2\psi_{nl}}{dr_z^2} + \left(\frac{2\mu_z}{\hbar^2}E_{nl} - \frac{2\mu_z}{\hbar^2}V(r_z) - \frac{l(l+1)}{r_z^2}\right)\psi_{nl}(r_z) = 0\,. \tag{2}$$

Here, l represents the angular momentum quantum number, μ_z is the reduced mass, r_z denotes the particle distance, and $\hbar$ is the reduced Planck constant.

Inserting Equation (1) into Equation (2) gives

$$\frac{d^2\psi_{nl}(r_z)}{dr_z^2} + \left(\frac{2\mu_z}{\hbar^2}E_{nl} - \frac{2\mu_z}{\hbar^2}\left(Y_0\left(\frac{A_0 + B_0 e^{-\alpha_z r_z}}{1-e^{-\alpha_z r_z}}\right)^2 - 2D_e\left(\frac{r_e}{r_z} - \frac{r_e^2}{2r_z^2}\right)e^{-\alpha_z r_z}\right) - \frac{l(l+1)}{r_z^2}\right)\psi_{nl}(r_z) = 0\,, \tag{3}$$

In Equation (3), the centrifugal contribution is handled through the Greene–Aldrich approximation [23], a procedure that has been effectively employed in several recent studies [24,25]. This approach yields a reliable treatment of the centrifugal term for $\alpha_z << 1,$, leading to the following expression:

$$r_z^{-2} \approx \alpha_z^2\left(1-e^{-\alpha_z r_z}\right)^{-2}, r_z^{-1} \approx \alpha_z\left(1-e^{-\alpha_z r_z}\right)^{-1}. \tag{4}$$

To facilitate the solution, an appropriate change of variable, $y_z = e^{-\alpha_z r_z}$, is introduced. By applying this transformation in conjunction with Equation (4) to Equation (3), and carrying out the required algebraic simplifications, the radial equation is reduced to the standard Schrödinger form, expressed as follows:

$$\frac{d^2\psi(y_z)}{dy_z^2} + \frac{1-y_z}{y_z(1-y_z)}\frac{d\psi(y_z)}{dy_z} + \frac{1}{y_z^2(1-y_z)^2}\begin{bmatrix} -\left(\varepsilon_z^2+\delta^2+\kappa_1\right)y_z^2 + \\ \left(2\varepsilon_z^2 - 2\delta^2 + \kappa_1 - \kappa_2\right)y_z \\ -\left(\varepsilon_z^2+\delta^2+\lambda\right)\end{bmatrix}\psi(y_z) = 0, \tag{5}$$

where

$$\left.\begin{aligned} -\varepsilon_z^2 &= \frac{2\mu_z E_{nl}}{\alpha_z^2\hbar^2}, \quad \delta^2 = \frac{8\mu_z A_0^2 Y_0}{\alpha_z\hbar^2}, \quad \kappa_1 = \frac{4\mu_z A_0 B_0 D_e r_e}{\alpha_z\hbar^2}, \\ \kappa_2 &= \frac{4\mu_z B_0^2 D_e r_z^2}{\hbar^2}, \quad \lambda = l(l+1) \end{aligned}\right\}. \tag{6}$$

Tezcan and Sever [26] demonstrated that the parametric Nikiforov–Uvarov (pNU) method provides a more straightforward and efficient procedure for determining both energy eigenvalues and the corresponding wavefunctions. Compared with the conventional Nikiforov–Uvarov approach [17], the pNU technique offers greater implementation simplicity and improved computational efficiency. Its principal advantage lies in its direct applicability and the high accuracy of solutions obtained for wave equations associated with a wide range of potential energy functions. Based on their formulation, the standard form of the equation is written as follows:

$$\psi''(t) + \frac{(b_1 - b_2 t)}{t(1-b_3 t)}\psi'(t) + \frac{1}{t^2(1-b_3 t)^2}\left[-T_0 t^2 + T_1 t - T_2\right]\psi(t) = 0\,. \tag{7}$$

Using Equation (7), the expressions for the energy eigenvalues and their corresponding wavefunctions were derived and are presented as follows:

$$b_2 n - (2n+1)b_5 + \left[2b_8 + n(n+1)\right]b_3 + b_7 + (2n+1)\sqrt{b_9} + \sqrt{b_8}\left[2\sqrt{b_9} + b_3(2n+1)\right] = 0\,. \tag{8}$$

$$\psi(t) = N_{nl} t^{b_{12}} (1-b_3 t)^{-b_{12} - \frac{b_{13}}{b_3}} p_n^{\left(b_{10}-1, \frac{b_{11}}{b_3} - b_{10} - 1\right)}(1-2b_3 t)\,. \tag{9}$$

The parametric constants featured in Equations (8) and (9) are calculated using the following expressions:

$$\left.\begin{aligned} &b_1 = b_2 = b_3 = 1, b_4 = 0.5(1-b_1), b_5 = 0.5(b_2 - 2b_3), \\ &b_6 = b_5^2 + T_0, b_7 = 2b_4 b_5 - T_1, \\ &b_8 = b_4^2 + T_2, b_9 = b_3(b_7 + b_3 b_8) + b_6, \\ &b_{10} = b_1 + 2b_4 + 2\sqrt{b_8}, \\ &b_{11} = b_2 - 2b_5 + 2\left(\sqrt{b_9} + b_3\sqrt{b_8}\right), \\ &b_{12} = b_4 + \sqrt{b_8}, \\ &b_{13} = b_5 - \left(\sqrt{b_9} + b_3\sqrt{b_8}\right) \end{aligned}\right\} \tag{10}$$

By comparing Equations (5) and (7), the parametric constants in Equation (10) are obtained as follows:

$$\left.\begin{aligned} &T_0 = \varepsilon_z^2 + \delta^2 + \kappa_1 \\ &T_1 = 2\varepsilon_z^2 - 2\delta^2 + \kappa_1 - \kappa_2 \\ &T_2 = \varepsilon_z^2 + \delta^2 + \lambda \\ &\textit{and} \\ &b_1 = b_2 = b_3 = 1, b_4 = 0, b_5 = -0.5, \\ &b_6 = \frac{1}{4} + \varepsilon_z^2 + \delta^2 + \kappa_1, b_7 = -2\varepsilon_z^2 + 2\delta^2 - \kappa_1 + \kappa_2 \\ &b_8 = \varepsilon_z^2 + \delta^2 + \lambda, b_9 = \frac{1}{4} + \delta^2 + \delta^2 + 2\delta^2 + \kappa_2 + \lambda, \\ &b_{10} = 1 + 2\sqrt{\varepsilon_z^2 + \delta^2 + \lambda}, \\ &b_{11} = 2 + \sqrt{8\delta^2 + 4\kappa_2 + 1 + 4\delta^2 + 4\delta^2 + 4\lambda} + 2\sqrt{\varepsilon_z^2 + \delta^2 + \lambda}, \\ &b_{12} = \sqrt{\varepsilon_z^2 + \delta^2 + \lambda}, \\ &b_{13} = -\frac{1}{2} - \left[\frac{1}{2}\sqrt{8\delta^2 + 4\kappa_2 + 1 + 4\delta^2 + 4\delta^2 + 4\lambda} + \sqrt{\varepsilon_z^2 + \delta^2 + \lambda}\right] \end{aligned}\right\} \tag{11}$$

By substituting Equations (6) and (11) into (8) and (9), the resulting expressions for the energy eigenvalues and their corresponding wavefunctions are obtained as:

$$E_{nl} = Y_0 A_0^2 + \frac{\alpha_z^2 \hbar^2 l(l+1)}{2\mu_z} - \frac{\alpha_z^2 \hbar^2}{8\mu_z} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu_z D_e r_e^2}{\hbar^2} + \frac{2\mu_z Y_0}{\alpha_z^2 \hbar^2} \left(A_0 + B_0 \right)^2} \right)^2 + \frac{4\mu_z D_e r_e}{\alpha_z \hbar^2} + + \frac{2\mu_z Y_0 \left(A_0^2 - B_0^2 \right)}{\alpha_z^2 \hbar^2} + l(l+1)}{n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu_z D_e r_e^2}{\hbar^2} + \frac{2\mu_z Y_0}{\alpha_z^2 \hbar^2} \left(A_0 + B_0 \right)^2}} \right]^2 . \tag{12}$$

and

$$\psi(t) = N_{nl} t^{\sqrt{\varepsilon^2 + \delta^2 A_0^2 + l(l+1)}} (1-t)^{\frac{1}{2} + \left(\sqrt{\delta^2 (A_0 + B_0)^2 + \kappa_2 + \left(\frac{1}{2} + l \right)^2} \right)} p_n^{\left(2\sqrt{\varepsilon^2 + \delta^2 A_0^2 + l(l+1)}, \left(2\sqrt{\delta^2 (A_0 + B_0)^2 + \kappa_2 + \left(\frac{1}{2} + l \right)^2} \right) \right)} (1-2t) \tag{13}$$

where N_{nl} represents the normalization constant, as obtained from Equation (14).

$$\int_0^\infty |\psi_{nl}(r_z)|^2 \, dr_z = 1 . \tag{14}$$

3. RESULTS AND DISCUSSION

This research focuses on the vibrational energy states of Cs_2. Using the spectrum, the energy levels were determined via Equation (12), which was then employed to examine the system's quantum characteristics. All computations utilized the conversion factors $1\ \text{amu} = 931.494028\ \text{MeV}/c^2$ and $\hbar c = 1973.29\ \text{eVÅ}$, as specified in reference [27]. In molecular spectroscopy, the force constant k_e plays a crucial role because it characterizes the curvature of the potential energy curve at the equilibrium bond distance. Mathematically, it is obtained by taking the second derivative of the potential energy with respect to the internuclear separation r, evaluated at the equilibrium position $k_e = \left. \frac{d^2 V(r)}{dr^2} \right|_{r=r_e}$.

For a diatomic molecule, this constant is directly connected to the harmonic vibrational frequency ω_e at equilibrium (C). The relationship is expressed as $k_e = \mu_z \omega_e^2$, where μ_z denotes the reduced mass of the molecule.

When applying the Möbius square plus screened Kratzer potential (MSSKP), the value of the force constant is obtained through the Varshni conditions. These conditions ensure that the minimum of the proposed potential corresponds properly to the experimentally observed spectroscopic equilibrium configuration [28,29]. The analysis of the $3^3\sum_g^+$ electronic state of the Cs_2 molecule is based on the experimental molecular constants $D_e = 2722.28\ cm^{-1}$, $r_e = 5.3474208 \dot{A}$, $\mu_z = 66.38\, amu$ and $\omega_e = 28.8918\ cm^{-1}$ reported in references [18,20]. From these parameters, the quantity $\alpha_z = \left(\frac{\mu_z \omega_e^2}{2D_e} \right)$ is evaluated, forming the basis for calculating the vibrational energy levels of the cesium dimer.

To assess the accuracy of the model, the mean absolute error (MAE) is computed using the expression $MAE = \frac{1}{v} \sum_{n=0}^{10} \left| E_n^{Com.} - E_n^{RKR} \right|$. In this formulation, E_n^{RKR} represents the theoretical energy obtained from the model, E_n^{RKR} corresponds to the reference energy derived from the Rydberg–Klein–Rees (RKR) data, and v denotes the total number of available experimental data points. The vibrational energy levels obtained for Cs_2, expressed in cm^{-1}, are presented in Table 1.

The Rydberg–Klein–Rees (RKR) method is fundamentally grounded in experimental spectroscopic data and is widely regarded as a reliable benchmark because it reconstructs the molecular potential energy curve directly from observed transition frequencies. In contrast, analytical potential models such as the Morse and Manning–Rosen functions are commonly used to describe anharmonic vibrational motion. The Morse potential provides a reasonable

representation of bond stretching, whereas the Manning–Rosen potential introduces an additional shape parameter that improves its flexibility.

Despite their usefulness, both models have limitations in accurately describing molecular behavior at very short internuclear distances as well as in the asymptotic long-range region. These shortcomings become more pronounced at higher vibrational quantum numbers, where noticeable deviations from expected trends occur.

To address these limitations, the Möbius square plus screened Kratzer potential (MSSKP) proposed in this study incorporates features that effectively capture both short-range confinement and long-range screening effects. For Cs_2, the model achieves a mean absolute error (MAE) of 0.0234 cm^{-1}, which is significantly lower than the values obtained using the Morse (0.2364 cm^{-1}) and Manning–Rosen (0.0517 cm^{-1}) potentials. Moreover, the vibrational energy levels predicted by the MSSKP are in excellent agreement with experimental RKR results, demonstrating its superior accuracy and reliability in modeling the vibrational behavior of heavy diatomic molecules.

Table 1. Calculated vibrational energies for the $3^3\sum_g^+$ state of Cs_2 compared with Rydberg–Klein–Rees (RKR) data and earlier theoretical results (units in cm^{-1}).

n	RKR [10-12]	Manning–Rosen Potential [20]	Morse Potential [20]	Present Study (MSSKP)
0	14.4248	14.4266	14.4267	14.4255
1	43.1680	43.1756	43.1652	43.1712
2	71.7657	71.7818	71.7504	71.7700
3	100.2211	100.2448	100.1822	100.2305
4	128.5375	128.5645	128.4608	128.5450
5	156.7182	156.7409	156.5860	156.7258
6	184.7663	184.7737	184.5579	184.7692
7	212.6851	212.6628	212.3765	212.6760
8	240.4778	240.4080	240.0418	240.4430
9	268.1477	268.0091	267.5537	268.0805
10	295.6980	295.4661	294.9123	295.5872
		MAE = 0.05170	MAE = 0.23640	MAE = 0.02340

4. CONCLUSIONS

In this work, the Möbius square plus screened Kratzer potential (MSSKP) model has been successfully employed to describe quantum bound states, with analytical solutions obtained through the parametric Nikiforov–Uvarov (pNU) method. Application of the model to the cesium dimer (Cs_2) demonstrates its remarkable ability to accurately reproduce the vibrational energy spectrum. The calculated results exhibit excellent agreement with available experimental Rydberg–Klein–Rees (RKR) data, yielding a minimum mean absolute error of 0.0234 cm^{-1} and outperforming conventional potentials such as the Morse and Manning–Rosen models. These findings confirm the reliability, accuracy, and predictive strength of the MSSKP framework in modeling molecular vibrational dynamics. Furthermore, the proposed potential provides a valuable theoretical basis for understanding molecular structure, bonding characteristics, and quantum behavior. Owing to its effectiveness and versatility, the MSSKP model may serve as a powerful tool in molecular spectroscopy and quantum chemistry, with potential applications to more complex systems, including polyatomic molecules, excited electronic states, nanostructured materials, and related quantum-mechanical problems [30–39].

Data Availability Statement
All results presented in this study were obtained through the numerical evaluation of analytically derived expressions. No external datasets were used or generated in this work.

Disclosure Statement
The authors declare that there are no conflicts of interest regarding the publication of this article.

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Author Contributions
E. P. Inyang: Conceptualization, resources, investigation, and funding acquisition.
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ТЕОРЕТИЧНЕ ДОСЛІДЖЕННЯ КОЛИВАЛЬНОГО СПЕКТРА ЦЕЗІЄВОГО ДИМЕРУ ЗА ВИКОРИСТАННЯМ ГІБРИДНОЇ МОДЕЛІ ВЗАЄМОДІЇ

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У цьому дослідженні вивчаються квантові властивості димеру цезію (Cs_2) за допомогою гібридної моделі взаємодії, яка поєднує потенціал квадратів Мебіуса з екранованим потенціалом Кратцера (MSSKP). Рівні коливальної енергії отримані аналітично шляхом розв'язання рівняння Шредінгера в рамках параметричного методу Нікіфорова-Уварова (pNU). Розраховані спектри демонструють чудову відповідність з доступними експериментальними даними Ридберга-Клейна-Ріса (RKR), що демонструє валідність запропонованої моделі. Порівняльний аналіз з усталеними моделями потенціалів, а саме з потенціалами Морзе та Маннінга-Розена, показує вищу прогностичну ефективність підходу MSSKP. Зокрема, модель MSSKP досягає мінімальної середньої абсолютної похибки (MAE) 0,0234 $см^{-1}$ порівняно з 0,2364 $см^{-1}$ та 0,0517 $см^{-1}$ для потенціалів Морзе та Маннінга-Розена відповідно. Ці результати підкреслюють підвищену точність та надійність моделі MSSKP в описі коливального спектру Cs_2. Отримані дані також надають цінне розуміння молекулярної структури, взаємодій і зв'язків, а також квантової поведінки, підкреслюючи потенціал запропонованої моделі для застосування в квантовій хімії, молекулярній спектроскопії та теоретичному моделюванні двохатомних молекулярних систем.

Ключові слова: *гібридна модель взаємодії; середня абсолютна похибка; дані Ридберга-Кляйна-Ріса (RKR); аналітичний метод, молекулярна спектроскопія*