

Relativistic energy calculations for Modified Hulthén Potential

Rachna Joshi

Department of Physics, Acharya Narendra Dev College,
University of Delhi, Delhi 110019, INDIA

Email: rachnajoshi@andc.du.ac.in

ABSTRACT

Under the Modified Hulthén Potential, relativistic corrections are found in the energy eigenvalues of the hydrogen atom. In the context of time independent perturbation theory, the relativistic correction to the kinetic energy, spin orbit term, and Darwin term is determined. The sum of these three gives the total relativistic energy corrections for a particular state of the atom. The variation of the relativistic energy levels with potential parameters is investigated. The Schrodinger problem is numerically solved using the very efficient Numerov technique, which is frequently used to solve second-order ordinary differential equations without a first-order component.

Keywords— Relativistic energy corrections; Numerov Method; Modified Hulthén Potential

I. INTRODUCTION

When dealing with objects travelling at speeds close to the speed of light (c), or when extreme precision is needed in computations and experiments, relativistic corrections are crucial in several branches of physics. Relativistic corrections are required in the field of quantum mechanics, particularly when particles are travelling at speeds that are close to the speed of light. Relativistic phenomena like time dilation and length contraction are not taken into account by the non-relativistic Schrödinger equation, which explains the behaviour of particles in non-relativistic quantum mechanics. The Dirac equation and the Klein-Gordon equation were created as a result to account for relativistic effects for spin-1/2 and spin-less particles, respectively. Understanding the behaviour of particles at high energies, as seen in accelerators like the Large Hadron Collider (LHC), or when researching processes like pair creation and annihilation, requires relativistic adjustments [1].

Atomic physics relies heavily on relativistic energy adjustments, particularly when working with heavy atoms or very accurate spectroscopic observations. Due to the powerful electric fields generated by the positively charged nucleus in atoms with high atomic numbers (Z), electrons may move at speeds that are almost equal to the speed of light. As a result, in order to make correct predictions of atomic characteristics, relativistic effects must be considered as they have a considerable impact on the behaviour of electrons. Relativistic energy corrections are crucial in explaining fine structure in atomic spectra. The fine structure arises from the interaction between the electron's orbital angular momentum and its intrinsic spin. The spin-orbit coupling, which results from relativistic effects, causes the energy levels of electrons with different orbital angular momentum quantum numbers (l) to split into multiple sublevels. This splitting is observable in atomic spectral lines and must be accounted for in high-precision spectroscopy [2].

The hydrogen spectrum exhibits a little energy adjustment known as the Lamb shift. According to quantum electrodynamics (QED), it develops as a result of the interaction between the electron's magnetic moment and the magnetic field produced by the electron's own motion around the nucleus. The Lamb shift, a relativistic adjustment to the energy levels of hydrogen, was crucial in the creation of QED [3]. Relativistic corrections are relevant in understanding hyperfine structure in atomic spectra. Hyperfine structure arises from the interaction between the electron's magnetic dipole moment and the nuclear magnetic moment. The Dirac equation and relativistic corrections are used to describe the hyperfine splitting in the energy levels of atoms with non-zero nuclear spin [4]. Due to the strong electric fields emanating from the nucleus, relativistic corrections for electrons travelling at high speeds become important for heavy metals with large atomic numbers (Z). To precisely compute transition energies and spectroscopic data for heavy ions, these adjustments are necessary [5].

The interaction between an electron and the nucleus in an atom is modelled mathematically using the

modified Hulthén potential, which is frequently used in atomic physics. It is an expansion of the original Hulthén potential, which was developed to roughly represent the nuclear potential that an electron in an atom experiences when it is attracted to it. The modified Hulthén potential is a useful tool in a variety of atomic physics applications because it has a number of benefits over the original Hulthén potential. The modified Hulthén potential is a helpful model to investigate the energy levels and wave functions of electrons in atoms because it contains analytically solvable bound-state solutions for the Schrödinger equation. A deeper knowledge of atomic structure is made possible by the analytical solutions, which offer insights into the behaviour of electrons in the presence of a screened Coulomb potential [6-7].

A screening parameter that takes into consideration the screening effect brought on by other electrons in the atom is introduced by the modified Hulthén potential. In a multi-electron atom, the interaction between the nucleus and an electron is effectively described by this effect. Particularly for atoms with many electrons, the screening parameter makes it possible to describe the atomic potential in a more accurate manner [8]. The modified Hulthén potential can also be used to model the nuclear-nuclear interaction in atomic collisions, where two atomic nuclei interact with each other. In these scenarios, the potential parameters can be adjusted to describe the nuclear interaction accurately [9]. The modified Hulthén potential is a useful approximation for a variety of practical uses, while not being a completely accurate depiction of the atomic potential. It is frequently used in theoretical research as a more basic potential that yet effectively captures certain crucial elements of the interaction between an electron and a nucleus [10]. Due to its clarity, analytical solvability, and capacity to represent key facets of electron-nucleus interactions in atoms, the modified Hulthén potential is useful in atomic physics. It is a useful resource for comprehending atomic structure and behaviour in both single- and multi-electron systems.

In the current work, the relativistic energy corrections are presented for the Modified Hulthén potential and hence the relativistic energies are determined for the same. Accurate and fast Numerov method is employed for the solution of the radial part of the Schrodinger equation.

II. THEORY

The Hamiltonian for Hydrogen atom under Modified Hulthén Potential (in Rydberg units) is given by:

$$H_0 = -\nabla^2 + V_{MHP}(r) \quad (1)$$

where $V_{MHP}(r)$ is the Modified Hulthén Potential and is given by:

$$V_{MHP}(r) = -\frac{2Z\mu}{\exp(\mu r) - 1} \text{Cos}(b\mu r) + \frac{2a}{r^2} \quad (2)$$

Here μ , a and b are the parameters of Modified Hulthén Potential. The first step involves determining the energies and wave functions of the stationary states, denoted as E and $\Psi(r)$. To find energies and wavefunctions one needs to solve the time independent Schrodinger equation:

$$H \Psi(r) = E \Psi(r) \quad (3)$$

The Numerov method finds application in solving the Time-Independent Schrödinger Equation (TISE). This technique, pioneered by B. V. Numerov, is tailor-made for tackling second-order ordinary differential equations without a first-order differential term [11-12]. As a result, it proves highly beneficial when solving the one-dimensional Schrödinger equation or the radial Schrödinger equation in three dimensions. The method enables a simple elimination of the first-order derivative term through a minor substitution, making the solution process more manageable. This method enables the solution of differential equations in the following form:

$$\frac{d^2y}{dx^2} = P(x) - Q(x)y(x) \quad (4)$$

The application of centered difference equation gives:

$$y_{n+1} - 2y_n + y_{n-1} \approx 2 \left(\frac{h^2}{2} \frac{d^2y}{dx^2} + \frac{h^4}{4!} \frac{d^4y}{dx^4} + O(h^6) \right) \quad (5)$$

with $y_n = y(x_n)$ the Numerov expression is:

$$y_{n+1} \left[1 + \frac{Q_{n+1}h^2}{12} \right] = 2y_n \left[1 - \frac{5Q_n h^2}{12} \right] - y_{n-1} \left[1 + \frac{Q_{n-1}h^2}{12} \right] + \frac{h^2}{12} (P_{n+1} + 10P_n + P_{n-1}) + O(h^6) \quad (6)$$

While solving Schrödinger's equation, a problem arises due to a singularity occurring at $r = 0$, which presents a significant challenge. To overcome this obstacle, researchers can use a variable step grid instead of the conventional constant step grid. In this particular investigation, a logarithmic grid is chosen as the approach to handle the singularity effectively. Moreover, the introduction of a new variable, t , ensures that the grid maintains uniform spacing for all r values throughout the study. Here

$$t = \log(Zr) \quad \text{and} \quad \Delta t = \frac{\Delta r}{r} \quad (7)$$

with $t_{\min} = -8$ which gives $Z r_{\min} = 0.0034$. Δt is equivalent to the “h” in the equations (5) and (6).

As t_{\min} becomes increasingly negative, r_{\min} decreases but does not become zero. The number of grid points is given by:

$$N = \frac{\log(Z * r_{\max}) - t_{\min}}{\Delta t} \quad (8)$$

Unlike the Runge-Kutta method, where functions P and Q must be evaluated six times per step, the Numerov method is remarkably efficient. Despite evaluating P and Q only once per step, it allows us to achieve an error of $O(h^6)$, making it highly accurate.

The following is the equation for the relativistic adjustment to kinetic energy:

$$\Delta E_1 = -\frac{1}{2mc^2} \left[E_n^2 + 2E_n \left(\frac{Ze^2}{4\pi\epsilon_0} \right) \left\langle \frac{1}{r} \right\rangle + \left(\frac{Ze^2}{4\pi\epsilon_0} \right)^2 \left\langle \frac{1}{r^2} \right\rangle \right] \quad (9)$$

Spin-orbit term is:

$$\Delta E_2 = \frac{\hbar^2}{2} \langle \xi(r) \rangle \left[j(j+1) - l(l+1) - \frac{3}{4} \right] \quad (10)$$

$$\text{with } \xi(r) = \frac{1}{2m^2c^2} \frac{1}{r} \frac{dV}{dr} \quad (11)$$

and the Darwin's term is:

$$\Delta E_3 = \frac{\pi \hbar^2}{2m^2c^2} \left(\frac{Ze^2}{4\pi\epsilon_0} \right) |\Psi_{n00}(0)|^2 \quad (12)$$

Hence the total relativistic correction in energy eigenvalue is given by:

$$\Delta E = \Delta E_1 + \Delta E_2 + \Delta E_3 \quad (13)$$

The relativistic energy is obtained by adding the relativistic energy correction to the non-relativistic energy

$$E_{rel} = E_{NR} + \Delta E \quad (14)$$

The detailed formulation of these relativistic correction terms to the energy eigenvalues can be found in the standard textbook of atomic physics [13]

III. RESULTS AND DISCUSSION

The Numerov method is a powerful numerical technique used to solve the Schrödinger equation, which describes the behavior of quantum systems such as atoms and molecules. It was originally developed by Boris Numerov in 1927. The Numerov algorithm is a second-order accurate algorithm, which implies that it yields results that are somewhat accurate while using less computer power than higher-order algorithms like Runge-Kutta. Because of this, it strikes an excellent balance between accuracy and effectiveness. The approach may be used to solve many kinds of quantum systems since it is stable over a broad variety of potentials and energy levels. It is immune to the numerical instability that can develop in other numerical techniques. The method can handle a variety of boundary conditions, including both open and closed boundary conditions. This versatility makes it adaptable to different physical scenarios. Both confined states (discrete energy levels) and scattered states (continuous energy spectrum) may be calculated using the Numerov approach. Due to its adaptability, it can be used with many different quantum systems.

The potential energy in quantum mechanics may take on a large range of values, which causes the wave function to behave quite differently in various locations. By use of a logarithmic grid, more points may be focused in areas where the potential energy varies quickly, allowing for improved resolution of these areas without squandering computing resources in areas where the potential energy changes slowly. Also, certain quantum systems, such as Coulombic potentials, include singularities or regions where the potential energy changes quickly. Such scenarios can be handled better by a logarithmic grid since it enables the placement of additional grid points around these singularities, better reflecting the behaviour of the wave function.

The method has been tried and tested by the author and co-workers in many problems [14-17]. The numerical simulation for the present study is conducted using a logarithmic grid, with a fixed step size of $\Delta r = 0.01$. In the present simulation, the minimum value of r (r_{\min}) is set to 0.00034 a.u. corresponding to $Z=1$ and $t_{\min}=-8$, while the maximum value of r (r_{\max}) varies till 2000 a.u., depending on the specific combination of the MHP parameters. This range is chosen to guarantee the proper convergence of the obtained results. In the current calculations, we present precise outcomes, where the energy eigenvalues and wavefunctions exhibit convergence up to 8 decimal places in all cases. The process of finding the correct energy eigenvalues in Numerov method involves an iterative numerical approach, adjusting the initial guess for energy until you find the wavefunction that satisfies the boundary conditions or has certain convergence properties. Once we have the energy eigenvalues, the corresponding wavefunctions are normalized using standard normalization techniques. The implementation details of the Numerov method varies depending on the specific problem under

study and we have to optimize various parameters as per the numerical problem under study. The Numerov method is based on the second-order Taylor expansion of the solution $\psi(x)$ around a grid point. The process usually involves setting up a trial energy value, integrating the differential equation using the Numerov method, and then comparing the calculated value of ψ at the other boundary with the desired boundary condition. The energy is then adjusted (usually using root-finding methods like the bisection method or Newton's method) until the desired boundary condition is satisfied, yielding the energy eigenvalue.

In the past, researchers have successfully determined the non-relativistic energy levels of the Modified Hulthén potential through their investigations [18-20]. However, it is important to note that, as of the current knowledge available to the author, there has been no prior determination of the relativistic energy levels for the Modified Hulthén potential. This present study represents the first attempt to explore and determine the relativistic energy levels associated with this specific potential. The research conducted by the author focuses on analyzing the behavior of relativistic energy levels concerning various potential parameters. This exploration involves investigating the impact of different factors on the relativistic energies within the framework of the Modified Hulthén potential. By studying the relativistic energy levels, the research aims to gain a deeper understanding of the quantum behavior of particles subjected to this potential. Relativistic effects become significant at high energies or for particles moving at velocities close to the speed of light. As a result, investigating relativistic energy levels is crucial in accurately describing and predicting the behavior of particles in scenarios where relativistic effects cannot be ignored. The findings of this study are expected to contribute valuable insights to the field of quantum mechanics, especially in understanding the behavior of particles in the presence of the Modified Hulthén potential.

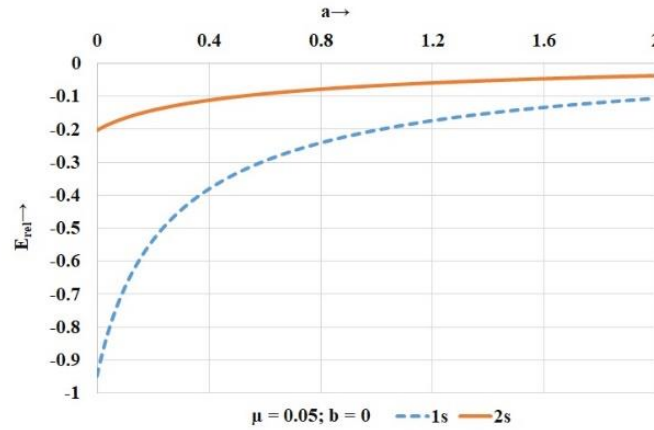


Figure 1: Variation of relativistic energy for the 1s $^2S_{1/2}$ and 2s $^2S_{1/2}$ states as a function of the parameter "a" of the Modified Hulthén Potential for $\mu=0.05$; $b=0$

Figure 1 presents a plot illustrating the dependence of relativistic energies for the 1s $^2S_{1/2}$ and 2s $^2S_{1/2}$ states on the parameter "a" of the Modified Hulthén potential. The plotted curves demonstrate how relativistic energies change as "a" varies. Notably, there is a general trend of increasing relativistic energies with an increase in the parameter "a". When "a" is small, the increase in relativistic energies is steep, indicating that even small variations in "a" lead to significant changes in the energy levels. As "a" increases, the slope of the curve decreases, resulting in less increase in energies for larger values of "a." Consequently, for large values of "a," the curve approaches a state of flattening out, implying that further increases in "a" have diminishing effects on the relativistic energies. Additionally, it is evident that the parameter "a" has a more pronounced impact on the ground state (1s $^2S_{1/2}$) compared to the first excited state (2s $^2S_{1/2}$). This observation indicates that changes in "a" have a greater influence on the lower energy state, which is the ground state, while the higher energy state, the first excited state, is relatively less sensitive to variations in "a." Overall, Figure 1 provides valuable insights into the behaviour of relativistic energies in the Modified Hulthén potential as a function of the parameter "a." It shows how the energy levels respond to changes in "a" and highlights the relative importance of this parameter on the ground and excited states

In Figure 2, the behavior of relativistic energies for the 1s $^2S_{1/2}$ state is depicted concerning the parameter "b" of the Modified Hulthén potential. As "b" varies, the relativistic energy demonstrates an increasing trend, indicating that an increase in the value of "b" leads to higher energy levels. When "b" is small, the increase in relativistic energy is relatively modest. In this region, even substantial changes in "b" result in relatively small variations in energy levels. However, as the value of "b" increases, the slope of the curve also increases, signifying that the increase in relativistic energy becomes more pronounced with larger values of "b." Consequently, the energy levels rise more steeply for higher values of "b."

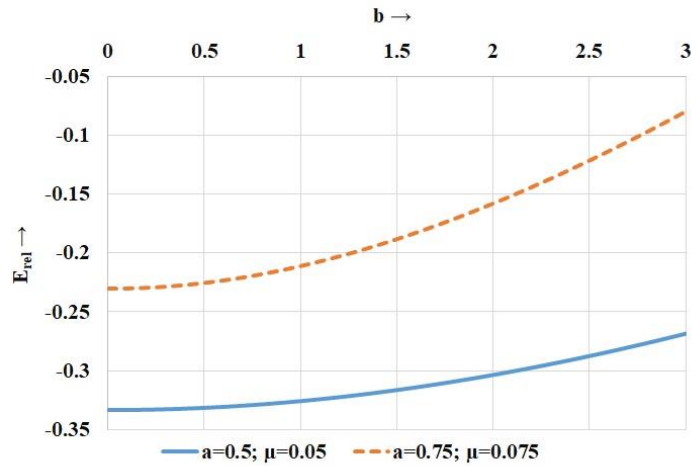


Figure 2: Variation of relativistic energy for the $1s\ 2S_{1/2}$ state as a function of the parameter “b” of the Modified Hulthén Potential.

Two different combinations of the parameters "a" and "μ" are plotted, and interestingly, the trend of the variation in relativistic energy with "b" remains consistent for both combinations. The increase in energy with an increase in "b" is observed in both cases, indicating that this relationship holds true regardless of specific values for "a" and "μ." Notably, when the values of the parameters "a" and "μ" are large, the effect of the parameter "b" on the relativistic energies becomes more pronounced. In this scenario, even small changes in "b" lead to significant alterations in the energy levels. On the contrary, when the values of "a" and "μ" are relatively small, the impact of the parameter "b" on the relativistic energies is less pronounced, meaning that variations in "b" result in smaller changes in energy levels.

Overall, Figure 2 provides valuable insights into how relativistic energies for the $1s\ 2S_{1/2}$ state respond to changes in the parameter "b" of the Modified Hulthén potential. The increasing trend of energy with increasing "b" is consistent for different combinations of "a" and "μ." Moreover, the effect of "b" on energy levels is more significant when "a" and "μ" are large and less pronounced when "a" and "μ" are small.

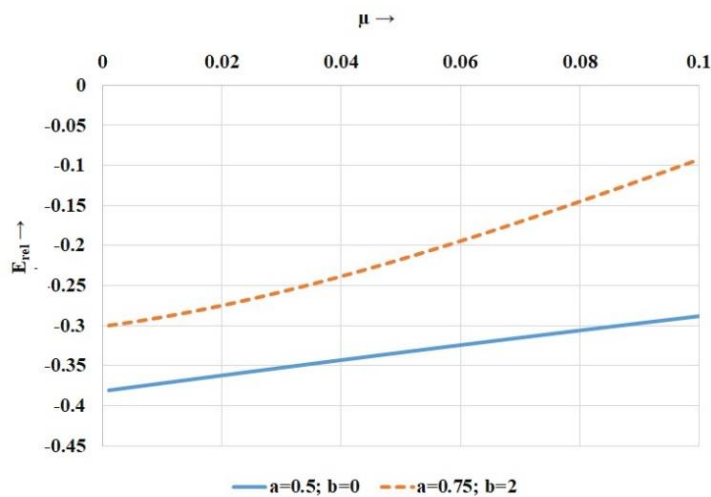


Figure 3: Variation of relativistic energy for the $1s\ 2S_{1/2}$ state as a function of the parameter “μ” of the Modified Hulthén Potential.

Further the dependence of the relativistic energy on the parameter “μ” of the Modified Hulthén potential is shown in Figure-3 which depicts a rise in the relativistic energy on increasing the parameter “μ”. Two curves are plotted wherein the first one is at the lower values of the “a” and “b” parameter and the second one is at the higher values of these parameters. The trend is same in both the curves i.e. there is a monotonic increase in the relativistic energy with the parameter “μ”. However, the slope of the curve which corresponds to the rate of increase of the relativistic energy with parameter “μ” is found to be more in the second case. The effect of “μ”

on the relativistic energy is more pronounced when the other parameters are also strong. Also in contrast to the other two cases i.e. corresponding to the variation of relativistic energy with “a” and “b” parameters, wherein the slope was found to be steeper either for the low values or the high values of other parameters, it is observed in this case that the slope is nearly uniform for the entire range of the parameter “ μ ” considered in the present study. This means there is no flat region in the curves.

Towards the end of the study, a set of benchmark values are presented for relativistic energy corrections. These benchmark values are provided for a range of parameters that have not been explored previously, as well as for higher values of specific parameters, including Z, μ , a, and b, for both the $1s\ ^2S_{1/2}$ and $1s\ ^2S_{1/2}$ states.

Table 1: Relativistic energy corrections for the $1s\ ^2S_{1/2}$ state at some selected values of the parameters of the Modified Hulthén potential

Z	μ	a	b	E_{NR}	ΔE	E_{REL}
1	0.05	0.5	0	-0.33339433	-0.00000592	-0.33340025
1	0.05	0.5	2	-0.30355178	-0.00000673	-0.30355851
1	0.05	1	0	-0.2020849	-0.00000227	-0.20208717
1	0.05	1	2	-0.16147563	-0.00000299	-0.16147862
1	0.1	0.5	0	-0.28768387	-0.00000639	-0.28769026
1	0.1	0.5	2	-0.18664813	-0.00000926	-0.18665738
1	0.1	1	0	-0.15835888	-0.00000257	-0.15836144
1	0.1	1	2	-0.03117158	-0.00000493	-0.0311765
2	0.05	0.5	0	-1.4292921	-0.00009068	-1.42938278
2	0.05	0.5	2	-1.39710009	-0.00009411	-1.3971942
2	0.05	1	0	-0.90208372	-0.00003373	-0.90211746
2	0.05	1	2	-0.85655262	-0.00003679	-0.85658941
2	0.1	0.5	0	-1.33357733	-0.00009466	-1.33367199
2	0.1	0.5	2	-1.21420712	-0.00010766	-1.21431478
2	0.1	1	0	-0.80833962	-0.00003632	-0.80837594
2	0.1	1	2	-0.64590254	-0.00004778	-0.64595032
3	0.05	0.5	0	-3.28912212	-0.00045229	-3.28957441
3	0.05	0.5	2	-3.25618894	-0.0004601	-3.25664904
3	0.05	1	0	-2.10208351	-0.00016631	-2.10224982
3	0.05	1	2	-2.05494673	-0.00017331	-2.05512004
3	0.1	0.5	0	-3.14340657	-0.00046584	-3.14387241
3	0.1	0.5	2	-3.01771859	-0.00049615	-3.01821474
3	0.1	1	0	-1.95833612	-0.00017519	-1.95851131
3	0.1	1	2	-1.78279911	-0.00020215	-1.78300126
4	0.05	0.5	0	-5.91288421	-0.00141867	-5.91430288
4	0.05	0.5	2	-5.87959568	-0.00143265	-5.88102833
4	0.05	1	0	-3.80208343	-0.00051856	-3.80260199
4	0.05	1	2	-3.75417539	-0.00053111	-3.7547065
4	0.1	0.5	0	-5.71716838	-0.00145094	-5.71861932
4	0.1	0.5	2	-5.58840037	-0.0015057	-5.58990607
4	0.1	1	0	-3.6083349	-0.00053972	-3.60887462
4	0.1	1	2	-3.42621047	-0.00058861	-3.42679908

Table 2: Relativistic energy corrections for the $2s\ ^2S_{1/2}$ state at some selected values of the parameters of the Modified Hulthén potential

Z	μ	a	b	E_{NR}	ΔE	E_{REL}
1	0.05	0.5	0	-0.09997642	-0.00000195	-0.09997838
1	0.05	0.5	0.5	-0.09541986	-0.00000202	-0.09542188
1	0.05	1	0	-0.066329	-0.00000093	-0.06632994
1	0.05	1	0.5	-0.06097415	-0.00000099	-0.06097513
1	0.075	0.5	0	-0.08008279	-0.00000199	-0.08008478
1	0.075	0.5	0.5	-0.07130278	-0.0000021	-0.07130488
1	0.075	1	0	-0.04787949	-0.00000095	-0.04788045
1	0.075	1	0.5	-0.03806087	-0.00000103	-0.0380619
2	0.05	0.5	0	-0.48766834	-0.00003026	-0.4876986
2	0.05	0.5	0.5	-0.48237722	-0.00003059	-0.48240782
2	0.05	1	0	-0.34965513	-0.00001422	-0.34966936
2	0.05	1	0.5	-0.34316085	-0.00001449	-0.34317534
2	0.075	0.5	0	-0.44276564	-0.00003082	-0.44279646
2	0.075	0.5	0.5	-0.43171124	-0.0000315	-0.43174274
2	0.075	1	0	-0.30617519	-0.00001464	-0.30618983
2	0.075	1	0.5	-0.2928925	-0.00001518	-0.29290768
3	0.05	0.5	0	-1.16715812	-0.00015102	-1.16730914
3	0.05	0.5	0.5	-1.16160262	-0.00015182	-1.16175444
3	0.05	1	0	-0.85520938	-0.00007035	-0.85527973
3	0.05	1	0.5	-0.84829596	-0.00007101	-0.84836697
3	0.075	0.5	0	-1.09725377	-0.00015319	-1.09740696
3	0.075	0.5	0.5	-1.08534875	-0.00015489	-1.08550363
3	0.075	1	0	-0.78672405	-0.00007201	-0.78679606
3	0.075	1	0.5	-0.77211191	-0.00007337	-0.77218528
4	0.05	0.5	0	-2.13844422	-0.00047364	-2.13891786
4	0.05	0.5	0.5	-2.13275285	-0.00047511	-2.13322795
4	0.05	1	0	-1.5829867	-0.00021955	-1.58320625
4	0.05	1	0.5	-1.575856	-0.00022076	-1.57607676
4	0.075	0.5	0	-2.0435393	-0.00047908	-2.04401839
4	0.075	0.5	0.5	-2.03119023	-0.00048224	-2.03167248
4	0.075	1	0	-1.4894995	-0.00022371	-1.48972322
4	0.075	1	0.5	-1.47418442	-0.00022629	-1.47441071

These benchmark values serve as reference points and provide crucial insights into the behavior of relativistic energy corrections across different sets of parameters. By presenting these benchmark values, the aim is to offer a comprehensive understanding of how the relativistic effects evolve as the potential parameters take on unexplored values or are pushed to higher values. Moreover, the inclusion of benchmark values for the $1s\ ^2S_{1/2}$ and $2s\ ^2S_{1/2}$ states provides a comprehensive view of relativistic energy corrections for both the ground state and the first excited state. This comprehensive analysis enables a more complete understanding of the impact of relativistic effects on the entire energy spectrum of the system under consideration.

In summary, the presentation of benchmark values for relativistic energy corrections represents a crucial aspect of the study. It not only allows for comparisons and validations but also enhances the applicability and significance of the research findings in the context of quantum systems described by the Modified Hulthén

potential with varying parameter values, including previously unexplored regions and higher values of Z , μ , a , and b .

IV CONCLUSIONS

The modified Hulthén potential is a fascinating quantum mechanical conundrum that may be used to test different theoretical hypotheses and mathematical procedures. The determination of accurate energy levels and characteristics of this potential can be useful for the researchers in atomic physics to improve or create new theories. The Hulthén potential may be used to investigate interactions between charged particles, such as electrons and nuclei in atoms and molecules, in both its original and modified forms. It is possible to get insight into the stability and characteristics of atomic and molecular systems by comprehending the energy levels in this potential. Quantum mechanical systems with certain potentials can be used to simulate some of the physical and chemical characteristics of materials. Understanding the behaviour of particles inside specific materials, which may have an influence on their general characteristics, may be accomplished using the modified Hulthén potential.

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