A Python program to draw energy level diagram and to calculate quantum defects, the high lying Rydberg level

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Rydberg atoms have strong and adjustable atomic interactions that can be tweaked by choosing different states with various principal quantum numbers or orbital angular momentum. They are highly used in quantum information applications. Furthermore, these atoms have long lifetimes and many possible energy levels, and their separations enable coupling to electromagnetic fields with frequencies ranging over six orders of magnitude. We studied some properties of these atoms and developed a Python program with two functionalities: Repository available at `https://github.com/AhmedAliRajput/Rydberg-levels-calculation-and-their-graphs.git`. Firstly, it calculates energies of elements in s, p, d, and f orbitals and draws an energy level diagram of the element listed in the program. Secondly, it gives an option for calculating energy and quantum defects of atoms, either listed or not listed in the program. A few user inputs are required, mainly the names of the elements, at least three principal quantum numbers, and their energies. There are 21 elements in the database whose energy level diagrams could be drawn. The database can be extended by adding more elements.

Keywords: Rydberg atoms; Rydberg energy; quantum defects; energy levels; python.

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1. Introduction

In recent years, Rydberg atoms have been the topic of significant research, serving as a testing ground for various quantum mechanical difficulties [1]. Over the last two decades, a series of discoveries in studying highly excited atoms, known as Rydberg atoms, has taken place. As a result, a stirring movement in Rydberg physics has emerged particularly at very low temperatures. The following are the most important areas of research on both the fundamental and applied fields: Rydberg atoms and cold plasma [2], Rydberg atoms blockade [3], Quantum computing with Rydberg atoms [4-5]. Rydberg atoms are gentle giants. They form when a high-energy electron enters an excited state with a high principal quantum number. They were discovered in space for the first time in 1965, though they were predicted in Niels Bohr's first article on hydrogen. Their energy levels are so close together that they do not emit light in the visible spectrum but rather in the terahertz and microwave spectrum, resulting in captivating spectral lines [6]. Quantum defects and Rydberg energy series are investigated in this theoretical study.

2. The Rydberg atoms and quantum defects

Rydberg atom

A Riydberg atom consists of an atom with a single electron in outermost shell which absorbs some energy and transitions from lower to higher energy level. It looks like a hydrogen atom whose electron is excited to a higher energy level. Such an atom is called Rydberg atom. The Rydberg atom shows strong interaction with magnetic and electric field and has long lifetime [1,7-9]. Rydberg atom is very dominant than other simple atoms for being close to continuum. Many experiments including quantum computation cannot be done single electrons, but a Rydberg atom is a good choice for the same. The size of the Rydberg atom is about 100,000 times larger than the simple atom in its ground state [10-12].

Quantum defect

The design of Quantum Defect Theory is based on a single simple fact: when an electron moves far away from its neighbor electrons and the nucleus, it will be under Coulomb force, which is attractive [13-17]. The quantum defect is used for the modification of the Coulomb potential by the inner electrons. Quantum defects δ can be represented by the deflection from hydrogen energy structure in alkali metals atoms. The new energy of Rydberg levels could be estimated by ionization limit if we use quantum defects. We can get the accurate quantum defects with a relative error of 10^{-7} [18-22].

The Rydberg formula for a level with three quantum numbers (principal n, orbital l, and orbital angular j) is given by [23]:

$$I_o - E_{nlj} = \frac{RZ^2}{(n-\delta_{nlj})^2}. \tag{1}$$

Here, E_{nlj} is a excitation energy above the ground state, and I_o is the ionization limit; therefore, the result of $I_o - E_{nlj}$ is the binding energy of the level. δ_{nlj} is the quantum defect, and n is the principal quantum number, then $n - \delta_{nlj}$ is an

effective quantum number, and RZ is the reduced Rydberg constant. The variable Z represents the number of electrons removed and the number of the spectrum, with $Z = 1$ for the neutral atom, $Z = 2$ for the singly charged ion, $Z = 3$ for the doubly charged ion, etc. Thus, a neutral Sodium atom is represented as Na I, whereas the Na+1 ion is represented as Na II, the Na+2 ion by Na III, etc. [24-25].

From Eq. (1) the Rydberg energy is given by

$$E_{nlj} = I_o - \frac{RZ^2}{(n - \delta_{nlj})^2}. \quad (2)$$

Rearranging (2), for quantum defects,

$$\delta_{nlj} = n - \sqrt{\frac{RZ^2}{(I_o - E_{nlj})}}. \quad (3)$$

Equation (3) is used to map the measured data into quantum defects, subsequently fitted to a Ritz expansion [26]:

$$\delta_{nlj} = a_o + \frac{a_1}{(n - \delta_o)^2} + \frac{a_2}{(n - \delta_o)^4} + \frac{a_1}{(n - \delta_o)^6}. \quad (4)$$

A least-square adjustment can be used to determine the fitting parameters a_o, a_1 and a_2 for a given Rydberg series (different values for n and fixed values for l and j).

3. Methodology

The present theoretical study uses a Python program based on Quantum defects and the Rydberg energy series. Under this investigation, the upper-level energies of low principal quantum numbers n listed at NIST [27] are taken out, for the following neutral atoms Li I, Na I, K I, Rb I, Cs I, Fr I, Cr I, Ag I, Cu I, Zn I, Fe I, Cd I, B I, Al I, GA I, In I, C I, Ge I, S I, Mg I, Be I, and Cl I . Ionization energies of all elements are also extracted from NIST [27].

3.1. Calculation of quantum defects and Rydberg energy

After obtaining upper energy levels data from NIST, the energy levels are sorted and rearranged in ascending order based on their principal quantum numbers n. As a result, the Rydberg energy series is formed by all energy levels with the same configuration and spectral term but different n values at NIST [27]. The energies of low n values, *i.e.*, for $n < 10$, are presented at NIST as the low-lying Rydberg energy series. Using these low-lying Rydberg energies, we calculated the high-lying Rydberg energy series up to $n = 50$ by using the Python program. The quantum defects are computed primarily using Eq. (3), and the coefficients a_o, a_1, and a_3, are calculated with the help of low-lying Rydberg energy series taken from NIST by the least-square fitting followed by determination of Quantum defects using Ritz Expansion in Eq. (4). Therefore, we can make graphs between quantum defects and n values of different elements. The high-lying Rydberg series obtained from Eq. (2) was evaluated only when the quantum defects were accurately determined.

3.2. Energy level graph

The energy level graph of each element was plotted using the Python program taken their various n values and fixed values of *l* and *j* to determine the attractive energy levels.

4. Result and discussion

The present theoretical study provides details about quantum defects and Rydberg energies by using a Python program. There are two functionalities in the developed Python program: Firstly, this program uses a variety of selective neutral atoms such as Li I, Na I, K I, Rb I, Cs I, Fr I, Cr I, Ag I, Cu I, Zn I, Fe I, Cd I, B I, Al I, GA I, In I, C I, Ge I, S I, Mg I, Be I, and Cl I, to calculate energies in s, p, d and f orbital and plot energy levels graphs for various n values as well as fixed l and j values for each atom listed in program. Secondly, it provides an option for determining quantum defects and Rydberg

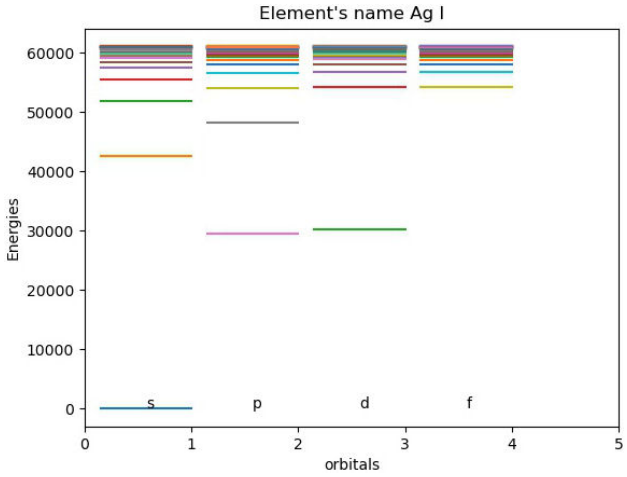

FIGURE 1. Energy level diagram of Ag I.

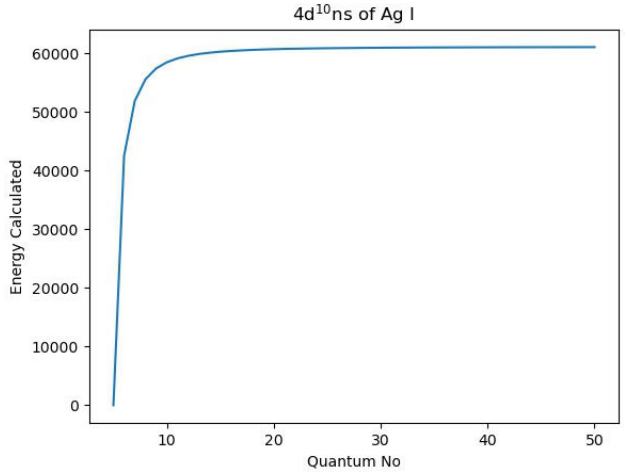

FIGURE 2. Rydberg energies of orbital 's' of Ag I.

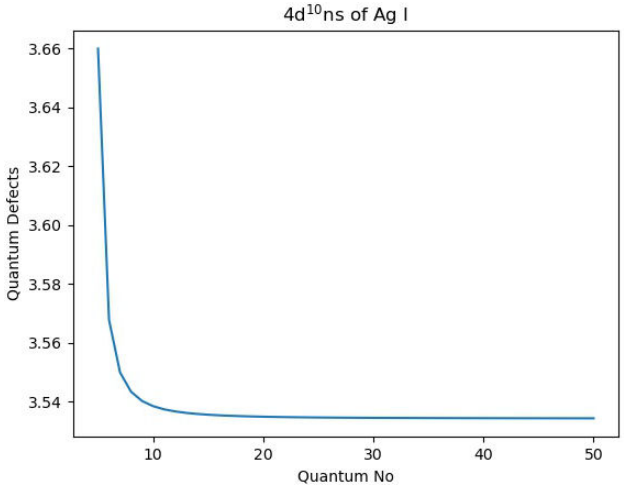

FIGURE 3. Quantum defects of orbital 's' of AgI.

berg energies for any atom and ion that are listed or not listed in the program. Only a few user inputs are needed, namely, at least three principal quantum numbers, their energies, and the names of the constituent elements. Equation (3) is used to calculate quantum defects of low lying Rydberg energies, and then coefficients are determined using least square fitting using Eq. (4). These low-lying energies are used as an input to estimate high lying Rydberg energies up to $n = 50$. Figure 1 shows energy levels of s, p, d, and f orbitals. All energies with higher principal quantum numbers cluster near ionization energy of 61106.45 and make manifold of highly excited states. Figure 2 shows that as the quantum number increases, the value of energy is also increased and after $n = 10$ the energy of the s orbital remains constant. The graph between the calculated quantum defects and the principle quantum number shows the irrational behavior because of the perturbation among the neighboring energy levels in the given element. In some cases it decreases rapidly while in fewer cases it goes steeply down (see Fig. 3).

5. Conclusion

We developed a Python program to calculate energies and quantum defects of atoms and ions. The program also draws an energy level diagram of Rydberg atoms and ions. It uses a database (NIST database) of atoms in which the energy of the first four levels is present. The program asks one of the options (i) to calculate energy and quantum defects and (ii) to draw the energy level diagram. The program can also calculate Rydberg energies for atoms not listed in the data base. To calculate energy of such atoms and ions, the program asks for some initial data.

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