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Spectrum Generating Algebra and its role in solvability of Alkali elements

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Abstract Hydrogen atom is always helpful in obtaining data from the other atoms. Revision of the Lie algebraic approach in studying the radial part of the Hydrogen atom and using the Tilting transformation are reasonable means to discuss Alkali elements. The characteristic difference between Alkali elements and Hydrogen atom is the screening effect in Alkali elements which causes much more freedom to the highest electron, valence electron. In this case, these atoms have another terms besides coulomb potential energy; Sentences of the order of inverse square of the distance and above. So, we can consider we have dipole moments, quadruple moments and etc. Therefore, these terms , although they are small, make these elements attractive for applications in quantum information. Also, we can consider them as Rydberg atoms with strong long-range interactions. Here, by considering an inverse square distance potential, Lie algebraic methods help us to obtain energy levels of both bound and excited states and corresponding wave functions too.

1 Introduction

Many physical systems with hidden symmetry in their Hamiltonian are solvable algebraically [1].Keplerian problems with central 2-body potentials, such as Hydrogen-like atoms with Coulomb potential in the non-relativistic: Schrodinger type, or relativistic: Klein-Gordon (K-G) or Dirac types, are some examples [2-5].

On the other hand, using Lie algebraic approach in solving physics problems is custom. Applying the generators of a Lie algebra, Γ_j, one could write the general form of the exact solvable or quasi-exact solvable (QES) Hamiltonian operator as follows [6-7]:

$$H = \sum_{j,k}^{n} C_{jk}\Gamma_j\Gamma_k + \sum_{j=1}^{n} C_j\Gamma_j. \tag{1}$$

Here C_{jk},C_j are coefficients can be found by comparing (1) with the physical Hamiltonian. This Lie algebra is called spectrum generating algebra (SGA), widely used in compact and finite dimensional Lie algebras [8-9]. However, following mathematical tricks, one could extend this method to the non-compact and infinite dimensional Lie algebras too [10-11].

For two reasons, we mainly focus on the Lie algebra $so(2,1)$: firstly, the Tilting transformation is an appropriate proposition in this Lie algebra; then, this Lie algebra is suitable for studying Hydrogen-like atoms such as Alkali elements. To illustrate Tilting transformation in this case, first, one should ,rewrites the Hamiltonian in terms of the generators of Lie algebra $so(2,1)$. Then, a rotation by an angle θ, Tilting angle, can be exerted to take the spectrum of bound and scattering states [12].

Another aspect of Alkali elements is the existence of valence electron makes these atoms Rydberg atoms. Rydberg atoms are those in which the valence electron is in the state of high principal quantum number n. They are of historical interest because of their role in atomic spectroscopy [13] since 1970. The exaggerated properties of Rydberg atoms allow doing experiments that would be difficult or impossible with normal atoms. In this case, applying experimental methods of laser cooling and spectroscopy can be used to study their properties. One of the recent studies of Rydberg atoms has been made by Ryabtsev and his collaborators in the case of Rb element and its role in quantum information [14].

On the other hand, lots of the information from Hydrogen atom is helpful to study Hydrogen-like atoms such as Alkali elements. However, the point is that the valence electron is

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not attracted by nuclear charge Ze, but by a smaller charge than Ze. The electrons in the lower levels of the atom screen the nuclear charge; So, the charge of nuclear decreases to $Z'e = (Z-\mu)e$, where μ is the coefficient of screening effect for any Alkali elements. It is obvious that the valence electron in this case has much more freedom to the other electrons of the atom. Therefore, in a simple model, one can consider the Alkali elements as Rydberg atoms.

Here, in section 2, we review the Lie algebraic investigations of the Hydrogen atom. After that in sec.3, the extension of these results to the Alkali elements by considering the screening effect as an inverse square distance relation is demonstrated. Also, by using SGA in the case of new Lie algebra $so(2,1)$, we obtain the spectrum of Alkali elements in two cases: bound states and scattering states. Finally, in sec.4 the conclusion and discussion are presented.

2 Review of so(2,1) Lie algebraic method in Hydrogen atom

Hamiltonian of Hydrogen atom is:

$$H = \frac{P^2}{2m_e} - k\frac{e^2}{r}, \tag{2}$$

where: m_e (electron mass), r (distance from nuclear to valence electron), P (momentum), e (charge of electron) and k (Coulomb constant). Since, the Coulomb potential is radial, the Hamiltonian is solvable in the spherical polar system and the radial part of it, namely,

$$r(H-E)|R(r)>= \Pi|R(r)>= 0, \tag{3}$$

is

$$(r\frac{d^2}{dr^2} + 2\frac{d}{dr} - \frac{l(l+1)}{r^2} + (ke^2 - Er)\frac{2m_e}{\hbar^2})R(r) = 0. \tag{4}$$

For simplicity, we work in the atomic units (a.u.) where we have $e = \hbar = k = m_e = 1$. The parameter $l(l+1)$ is the eigenvalue of the angular momentum operator [15]. This solvable equation could be written by the generators of $so(2,1)$ Lie algebra:

$$\begin{aligned} \Gamma_1 &= \frac{1}{2}(rP^2 + r - a\frac{\alpha^2}{r} - bi\alpha\frac{\vec{\gamma}.\vec{r}}{r^2}), \\ \Gamma_2 &= \frac{1}{2}(rP^2 - r - a\frac{\alpha^2}{r} - bi\alpha\frac{\vec{\gamma}.\vec{r}}{r^2}), \\ \Gamma_3 &= \vec{r}.\vec{P}, \end{aligned} \tag{5}$$

and commutation relations:

$$[\Gamma_1,\Gamma_2] = i\Gamma_3, \ \ [\Gamma_2,\Gamma_3] = -i\Gamma_1, \ \ [\Gamma_3,\Gamma_1] = i\Gamma_2. \tag{6}$$

Table 1 Coefficients of the equation (8) in three cases

Coefficients	Schrodinger	K-G	Dirac
C_1	$\frac{1}{2m}$	1	1
C_2	$-E$	$-(E^2 - {E_0}^2)$	$-(E^2 - {E_0}^2)$
C_3	$-\alpha$	$-2\alpha E$	$-2\alpha E$

Here a, b are constant parameters and $\alpha = \frac{e^2}{\hbar c} = 7.29 \times 10^{-3}$ is the fine structure constant and $\gamma_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}$ in which σ_i are the Pauli matrices. Following Eq.(1) general Hamiltonian of $so(2,1)$ Lie algebra is:

$$\Pi = C_1\Gamma_1 + C_2\Gamma_2 + C_0. \tag{7}$$

This is a second order differential equation and hermitian operator. It is obviously possible to write

$$\Pi = C_1(\Gamma_1 + \Gamma_2) + C_2(\Gamma_1 - \Gamma_2) + C_0. \tag{8}$$

Choosing an appropriate expression for C_1, C_2 and C_0 we obtain the Hamiltonians both in the non relativistic and relativistic cases. If we have $a = b = 0$ Eq.(8) is the non relativistic Schrodinger equation of Hydrogen atom. For $a = 1, b = 0$ Eq.(8) concludes K-G and by substitution $a = b = 1$ we have the second order Dirac equation [5].

The casimir operator of this Lie algebra is:

$$C^2 = \Gamma_3^2 - \Gamma_1^2 - \Gamma_2^2 = -a\alpha^2 - b\alpha. \tag{9}$$

This operator has a negative sign, which means the non-compactness character of $so(2,1)$ Lie algebra. On the other hand, the radial wave function $R(r) = |\Psi\rangle$ depends on two quantum numbers n, l and is independent of angular momentum orientation; i.e., it is invariant under rotation. Therefore, we could establish Tilting transformation for solving Eq.(8), written by the generators of $so(2,1)$ Lie algebra. In this transformation Γ_1, Γ_2 generators are rotated by an angle θ around the operator Γ_3, which does not appear in the radial Hamiltonian (8):

$$e^{i\theta\Gamma_3}(\Gamma_1 \pm \Gamma_2)e^{-i\theta\Gamma_3} = e^{\pm\theta}(\Gamma_1 \pm \Gamma_2), \tag{10}$$

and the transformed wave function $|\widetilde{\Psi}\rangle = e^{i\theta\Gamma_3}|\Psi\rangle$; Following these receptions, the eigenvalue equations $\Pi|\widetilde{\Psi}\rangle = 0$ for any suitable angle θ conclude the spectrum of bound states and scattering states [16].

3 so(2,1) Lie algebra and SGA in Alkali elements

One of the most traditional methods of using Lie algebra in physics is that the Hamiltonian and other physical operators could be written in terms of the generators of this Lie algebra. In this case, this Lie algebra is called SGA [1]. But, sometimes, all of the generators do not appear in the algebraic form of the Hamiltonian, whereas all of them are in the Casimir operator. In this case, we can obtain the spectrum using a unitary transformation and then rotating the Hamiltonian by an angle θ around the missing generator. This trick concludes the solvability of the system.

Interaction of an electron with an electromagnetic field, i.e., $(\overrightarrow{E},\overrightarrow{B})$, the ordinary atom, can be expressed in terms of the Lie algebra $so(4,2)$. The operators of this Lie algebra are [5]:

$$\overrightarrow{J} = \overrightarrow{r}\times\overrightarrow{P},\quad \overrightarrow{M} = \frac{1}{2m}(\overrightarrow{P}\times\overrightarrow{L}-\overrightarrow{L}\times\overrightarrow{P})-\frac{Ze^2}{r^2}\overrightarrow{r}$$
$$\overrightarrow{A} = \frac{1}{2m}(\overrightarrow{P}\times\overrightarrow{L}-\overrightarrow{L}\times\overrightarrow{P})+\frac{Ze^2}{r^2}\overrightarrow{r},\quad A_4=\overrightarrow{r}.\overrightarrow{P}-\frac{3}{2}i\hbar,$$
$$\Gamma_i = rP_i,\quad \Gamma_4=\frac{1}{2}(r\overrightarrow{P}.\overrightarrow{P}-r),\quad \Gamma_5=\frac{1}{2}(r\overrightarrow{P}.\overrightarrow{P}+r). \tag{11}$$

However, some of these operators are needed in the radial equation of Alkali elements with screening effect. In fact, only A_4,Γ_4 and Γ_5 by adding a new term are sufficient. In this case, the effective potential energy for (valence electron)+(nuclear+rest of the electrons) is:

$$U_{eff} = -\frac{Z}{r}+\frac{l(l+1)}{2r^2}+\frac{\mu}{2r^2}. \tag{12}$$

By summarizing two terms 2,3 as follows:

$$l(l+1)+\mu = l'(l'+1). \tag{13}$$

The quantum level l goes up to l' where $l' > l$:

which means the freedom of the valence electron is now more than the other electrons of atom. Also, we see from table.2 that by increasing the atomic number of Alkali elements, this effect is much series. In this case, the generators of $so(2,1)$ Lie algebra become:

$$\Gamma_1 = \frac{1}{2}(rP^2+r+\frac{l'(l'+1)}{r}),$$
$$\Gamma_2 = \frac{1}{2}(rP^2-r+\frac{l'(l'+1)}{r}),$$
$$\Gamma_3 = \vec{r}.\vec{P}. \tag{14}$$

Therefore, in the case of relativistic Hamiltonian of $so(2,1)$ Lie algebra by using Eq.(8) and table 1:

$$\Pi|\Psi(r)\rangle =$$
$$[(\Gamma_1+\Gamma_2)-(E^2-E_0^2)(\Gamma_1-\Gamma_2)-2\alpha ZE]|\Psi(r)\rangle = 0. \tag{15}$$

If we work in the center of mass system, we should consider reduced mass m_{red}:

$$m_{red} = \frac{Mm_e}{M+m_e}\simeq 1, \tag{16}$$

and for the rest energy in a.u. we have:

$$E_0 = m_{red}c^2 = \frac{1}{\alpha^2}. \tag{17}$$

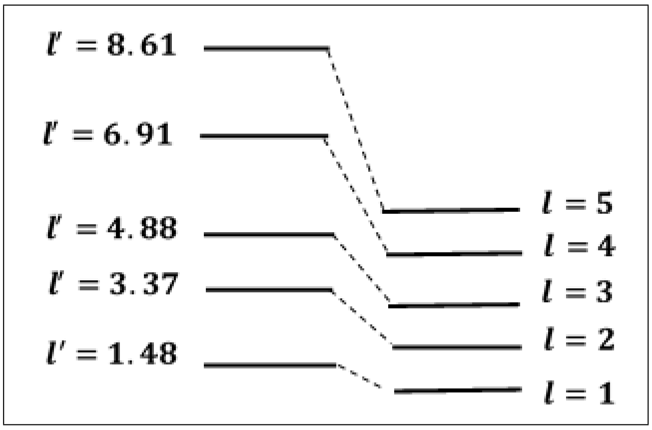

Fig. 1 Comparing the level of valence electron without and with the screening effect

Now, by using Tilting transformation

$$[(e^{-\theta}-(E^2-\frac{1}{\alpha^4})e^{\theta})\Gamma_1+$$
$$(e^{-\theta}+(E^2-\frac{1}{\alpha^4})e^{\theta})\Gamma_2-2\alpha ZE]|\widetilde{\Psi}(r)\rangle = 0, \tag{18}$$

the generators Γ_1,Γ_2 obey:

$$\Gamma_1|N,l\rangle = N'|N,l\rangle,\quad \Gamma_2|N,l\rangle = \lambda|N,l\rangle, \tag{19}$$

where $N' = N+l'+1$ is real and discrete value, whereas λ is imaginary and continues value. The rotation angle θ must be chosen for the bound states to eliminate the non-compact generator Γ_1, so that $e^{-\theta} = k = \pm\sqrt{-(E^2-\frac{1}{\alpha^4})}$ and:

$$E = \frac{-N'}{\alpha^2\sqrt{N'^2+Z^2\alpha^2}},$$
$$\Psi(r) = e^{-\theta}\sqrt{\frac{2r}{N'^3}}\bigwedge_{N'-l'-1}^{2l'+1}(\frac{2r}{N'}), \tag{20}$$

where $\bigwedge_n^l(r)$ is the generalized Laugurre function [17]. If we choose $e^{-\theta} = K = \pm\sqrt{E^2-\frac{1}{\alpha^4}}$, so that the compact generator Γ_2 can be eliminated:

$$E = \frac{\lambda}{\alpha^2\sqrt{\lambda^2+Z^2\alpha^2}},$$
$$\Psi(r) = \frac{e^{-\theta}}{r}\sqrt{\frac{2}{\pi}}\sin(Kr-\frac{\pi}{2}l'+\frac{Z\alpha}{K}(\log(2Kr)+\delta(l'))), \tag{21}$$

where $\delta(l') = arg(\Gamma(l'+1-i\frac{Z\alpha}{K}))$ and $\Gamma(l)$ shows Gamma function[18].

Table 2 Some of the quantum numbers of Alkali elements

Alkali elements	l	Z	μ	l'	Z'	$\Delta l'$
Li	1	3	1.7	0.68	1.3	0.32
Na	2	11	8.8	0.86	2.9	1.14
K	3	19	16.8	1.46	2.9	1.54
Rb	4	37	34.8	1.18	2.9	2.82
Cs	5	55	52.8	1.46	2.9	3.54

4 Conclusion and Discussion

The radial part of the Hydrogen atom is solvable algebraically in both non-relativistic and relativistic cases. The underlying Lie algebra is $so(2,1)$. Typically, this part of the Hamiltonian for specified angular momentum l is only dependent on the principal quantum number n and this is the reason for using Tilting transformation. Using this method, we could obtain the spectrum of bound states and scattering states for a certain angle θ. Here we extend this method to Alkali elements which are Hydrogen-like and we see that by considering the screening effect as an inverse square distance potential, we obtain the new expression for the principal quantum number in bound states and a new term in the scattering phase shift.

Actually, the screening effect causes the Alkali element to be considered as a dipole moment where its negative charge is the valence electron and the positive part of it is the (nuclear+rest electrons of the atom). This pattern is similar to Rydberg atoms, which we consider here for Alkali elements.

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