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Calculation of the Zeeman-Fine Energies and the Spectrum with Doppler-Shift Correction of Atomic Lithium

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Abstract

We have calculated the Zeeman-fine energies of atomic Lithium (Li) by using the varying effective Landé g-factor method. We take the principle quantum number in the range; ($2 \le n \le 10$). For this range we find 26 different energy values and 325 wavelengths some of which are the same. The Doppler shift is found to be $\left(\Delta\lambda = \pm 0.004\lambda\right)$. The Doppler shift-corrected wavelengths are in perfect agreement with the observed (NIST) values for atomic Li.

Keywords: Hydrogen-Like Atoms, Effective Landé G-Factor, Quantum Entanglement, Zeeman-Fine Energies, Photonic Transitions, Quantum Flux of Photon

1. Introduction

The investigation of hydrogen-like atoms with their low ionization potential and relative simplicity of their outer shell structure, have attracted a lot of attention. During the last two decades with the advent of laser cooling [1-4] and magnetic trapping [5], as well as spin polarization related to quantum entanglement [6], lithium and sodium have been the focus of a number of theoretical and experimental studies. Moreover with the realization of Bose Einstein condensation [7,8], they have attracted further attention.

Recently Saglam *et al.* [9] calculated the Zeeman-fine energy expression of hydrogen-like atoms given by:

$$E\left(n, m_l, g^*\right) = -C/n^2 - m_l \hbar\omega_c^*/2 \pm g^* \hbar\omega_c^*/4$$

corresponding to the eigenstates $\left|n, l, m_j >\right.$. Here the constant C is a characteristic for each atom and determined from the ionization energy, ω_c^* is the cyclotron angular frequency corresponding to the effective magnetic field, B^* inside the atom and g^* is the effective Landé g-factor, which is treated as a varying parameter. As was discussed by Saglam *et al.* [9] the effective magnetic field, B^* can be very high so that this leads to the spin-flip energies of the order of (eV). For the case of atomic Cesium, the spin-flip energy was shown to be 1.38 eV. Saglam *et al.* [9] defined a dimensionless function:

$$f\left(n, m_l, g^*\right) = \left[E\left(n, m_j, g^*\right) + C/n^2\right] \Big/ \hbar\omega_c^*$$

which takes the form:

$$f\left(n, m_l, g^*\right) = \left(-m_l/2 \pm g^*/4\right)$$

and depends on m_l and g^* directly and depends on n indirectly as the range of m_l is determined by $\left[-\left(n-1\right) \le m_l \le \left(n-1\right)\right]$. They used the plots of $f\left(n, m_l, g^*\right)$ (as a function of g^*) to study the

$$(ns^2S_{1/2}) \rightarrow (np^2P_{3/2}) \rightarrow (n's^2S_{1/2})$$

transitions in hydrogen-like atoms and showed that the entanglements of s and p states, occur at $g^* = 1$. The aim of the present study is to calculate the Zeeman-fine energies and the spectrum of the atomic Lithium by using the above mentioned varying effective Landé g-factor method. The outline of the present study is as follows: In Section 2.1 the energy levels of Hydrogen-like atoms in the presence of a uniform magnetic field is studied. In Section 2.2 we calculate the Zeeman-fine energies of Li atom. In Section 2.3 we establish the connection between the Zeeman-fine energies, effective Landé-g factors, and the quantum flux of both photon and the electronic orbits corresponding to the entangled states. Section 2.4 gives the detailed calculation of the Zeeman-fine energies of Li atom. The calculation of the Doppler shift is given in Section 2.5. Section 3 is the conclusions.

2. Formalism

2.1. Energy Levels of Hydrogen-Like Atoms in the Presence of a Uniform Magnetic Field

As was discussed by Saglam *et al.* [9], when an atom is subject to a laser beam, because of the photon's magnetic moment [10] and hence the large intrinsic magnetic field along the propagation direction [11], we will have diamagnetic and paramagnetic effects which is associated with a large magnetic field inside the atom. This field is called the effective field, B^*. The Landé-g factor is also replaced by the effective value, g^* which is treated as a varying parameter [12,13]. With these replacements [9] the energy eigenvalues corresponding to the eigenstates $|n,l,m_j>$ reads:

$$E\left(n,m_l,m_s,g^*,B^*\right)=-\frac{C}{n^2}-\mu_B B^*\left(m_l+g^*m_s\right) \qquad (1)$$

Here the constant C is the characteristic of each atom and determined from the ionization energy. Substituting the value of $\mu_B=\frac{e\hbar}{2mc}$ and $m_s=\pm\frac{1}{2}$ in Equation (1), we find:

$$E\left(n,m_l,B^*,g^*\right)=-\frac{C}{n^2}-\frac{m_l\hbar\omega_c^*}{2}\mp\frac{g^*\hbar\omega_c^*}{4} \qquad (2)$$

where $\omega_c^*=\frac{eB^*}{mc}$ is the cyclotron angular frequency corresponding to B^*. As was discussed by Saglam *et al.* [9] the effective magnetic field, B^* inside the atom can be very high so that this leads to the spin flip energies at the order of a few electron volts (eV). For the case of atomic Cesium, the spin flip energy is taken to be 1.38 eV. To proceed further, following Saglam *et al.* [9] we define a dimensionless function, $f\left(n,m_l,g^*\right)$ which is given by the relation:

$$f\left(n,m_l,g^*\right)=\left[E\left(n,m_j,g^*\right)+C/n^2\right]\Big/\hbar\omega_c^* \qquad (3a)$$

or

$$f\left(n,m_l,g^*\right)=-m_l/2\pm g^*/4 \qquad (3b)$$

which depends on m_l and g^* directly and depends on n indirectly as the range of m_l is determined by $\left[-(n-1)\le m_l\le(n-1)\right]$. The plot of these $f\left(n,m_l,g^*\right)$ functions with respect to g^* gives us the possible g^* values in the energy expression given by (1). At the first glance we see that the crossing of these lines correspond to integer values of g^* such as: $g^*=0,1,2,3,\cdots$. However in the following section we will see that for Li atom the allowed values of g^* are restricted only with the three odd integers. These are: $g^*=1,3,5$. In the present study we will consider only n values up to 10. We will see that in the range of ($2\le n\le 10$) we get 26 different energy values which produce 325 wavelengths some of which are the same. For each λ value we also calculate the Doppler shift and find that it is equal to: $\Delta\lambda=\pm 0.004\lambda$. The Doppler shift-corrected wavelengths are in perfect agreement with the observed (NIST) values [14] for atomic Li.

2.2. Calculation of the Effective Landé G-Factors of the Zeeman-Fine Energies of Li Atom

In Li atom we have 3 electrons altogether. Therefore it will be easy to study $f\left(n,m_l,g^*\right)$ as a function of g^*. The plots for $n=1$ and $n=2$ are given in (**Figure 1(a)**) and (**Figure 2(a)**) respectively; For $n=1$ we have $l=0$ and hence $m_l=0$, so from Equation (3) we get two lines crossing at $g^*=0$. Therefore the first two electrons occupy the entangled state, with the energy corresponding to the crossing energies of $1s\uparrow$ and $1s\downarrow$ states, which is the $s-s$ entanglement at $g^*=0$ (**Figure 1(a)**). For $n=2$ we have $l=0,\ 1$ and hence $m_l=0,\ \pm1$, so from Equation (3), the plots of $f\left(2,m_l,g^*\right)$ gives us the diamond shaped parallelogram whose corners correspond to $s-s$ entanglement at $g^*=0$, $s-p$ and $p-s$ entanglements at $g^*=1$ and $p-p$ entanglement at $g^*=2$ (**Figure 2(a)**). Therefore the third electron (the so called 2*s* electron) occupies the entangled state at crossing of $2s\uparrow$ and $2p\downarrow$ states [($s-p$) entanglements at $g^*=1$] which corresponds to the lowest energy, the ground state energy, for $n=2$. The plots of energy expression (2) for $n=1$ and $n=2$ are given in **Figure 1(b)** and **Figure 2(b)** respectively. In order to find the excited states we go to the higher values of n. The plots of $f\left(n,m_l,g^*\right)$ and $E\left(n,m_l,g^*\right)$ for $n=3$ and $n=4$ are given in **Figure 3** and **Figure 4** respectively. We see that although the crossings of these lines occur at the integer values of g^* such as: $g^*=0,1,2,3,\cdots$, however, as far as the photonic transitions are concerned, in the following section we will see that for Li atom the allowed values of g^* are restricted only with the three odd integers. These are: $g^*=1,3,5$. The reason for this is that: First, The energy values given by (2) are limited to the range: $-5.3917\text{ eV}\le E<0$. Secondly, the value of the spin-flip energy which is equal to 1.848328 eV for Li atom and finally, the photonic transitions occur between the points satisfying the condition: ($\Delta g^*=$ even integer). In passing we note that for a given n, although the maximum value of g^* is equal to ($g^*_{\max}=2n-2$), any energy value corresponding to $5\le g^*\le(2n-2)$ can be obtained by the

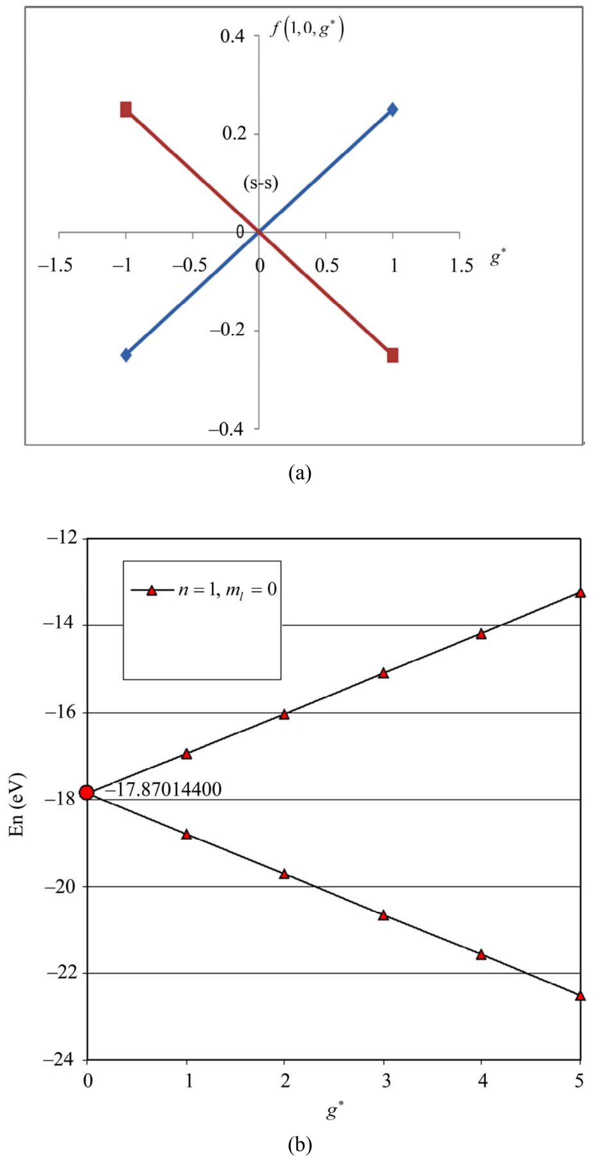

Figure 1. (a) $f(1, m_l, g^*)$ **as a function** g^***; (b)** $E(1, m_l, g^*)$ **as a function of** g^*

values in the range: $g^* = 1, 3, 5$ as well. Therefore the g^* values in this reduced zone ($g^* = 1, 3, 5$) will give us all the possible energy values.

2.3. Flux Quantization Argument

Let us assume that the ground state electron [the electron occupying the ($s - p$) entangled state at $g^* = 1$] is excited to a higher level by the absorption of a single photon. Now we ask: What is quantum flux difference between the final and initial states? Recently Saglam and Sahin [10,11] showed that, depending on its helicity photon carries an intrinsic magnetic moment and hence a quantum flux of $\pm\Phi_0$ where $\Phi_0 = (hc/e)$ is the flux quantum. Therefore in the end of a one photon absorption process the quantum flux difference between the final and initial quantum states of electron must be equal to the intrinsic quantum flux of the absorbed photon which is equal to $\pm\Phi_0$. On the other hand Saglam *et al.* [15] also calculated the quantized magnetic flux through the electronic orbits of Dirac hydrogen atom corresponding to the $|n, l, m_j >$. It is shown that the quantum flux is given by: $\Phi(n, l, m_j) = (n - l - m_j)\Phi_0$. For the present case we have the entangled states with the energies given by (1) where we have ($m_l + g^* m_s$) which stands for m_j. Therefore for the present case the quan-

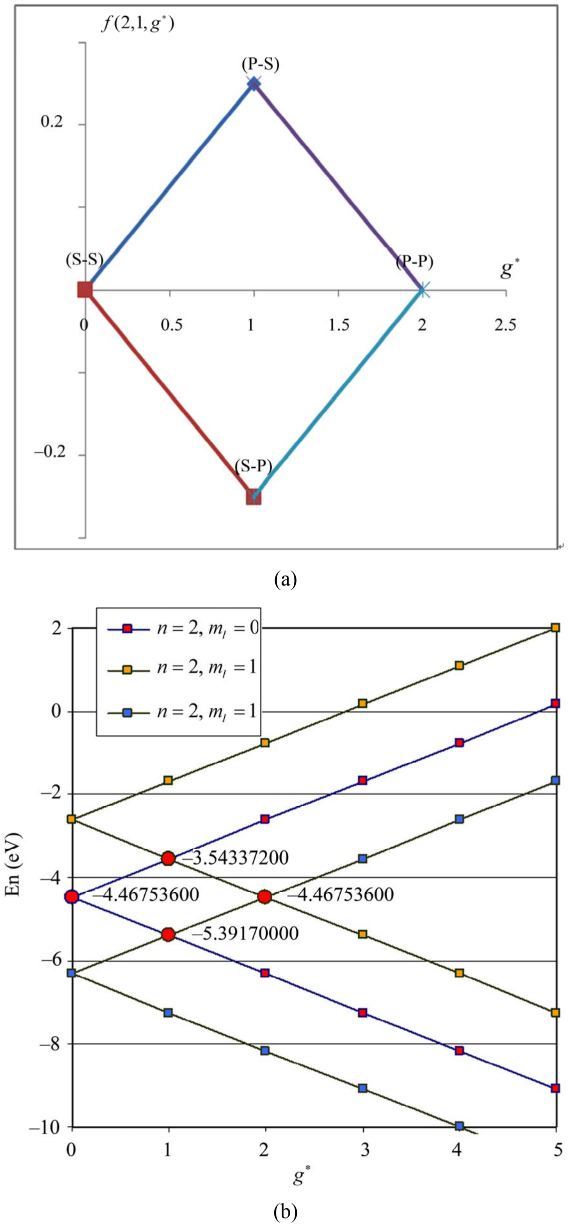

Figure 2. (a) $f(2, m_l, g^*)$ **as a fuction of** g^* **; (b)** $E(2, m_l, g^*)$ **as a function** g^***.**

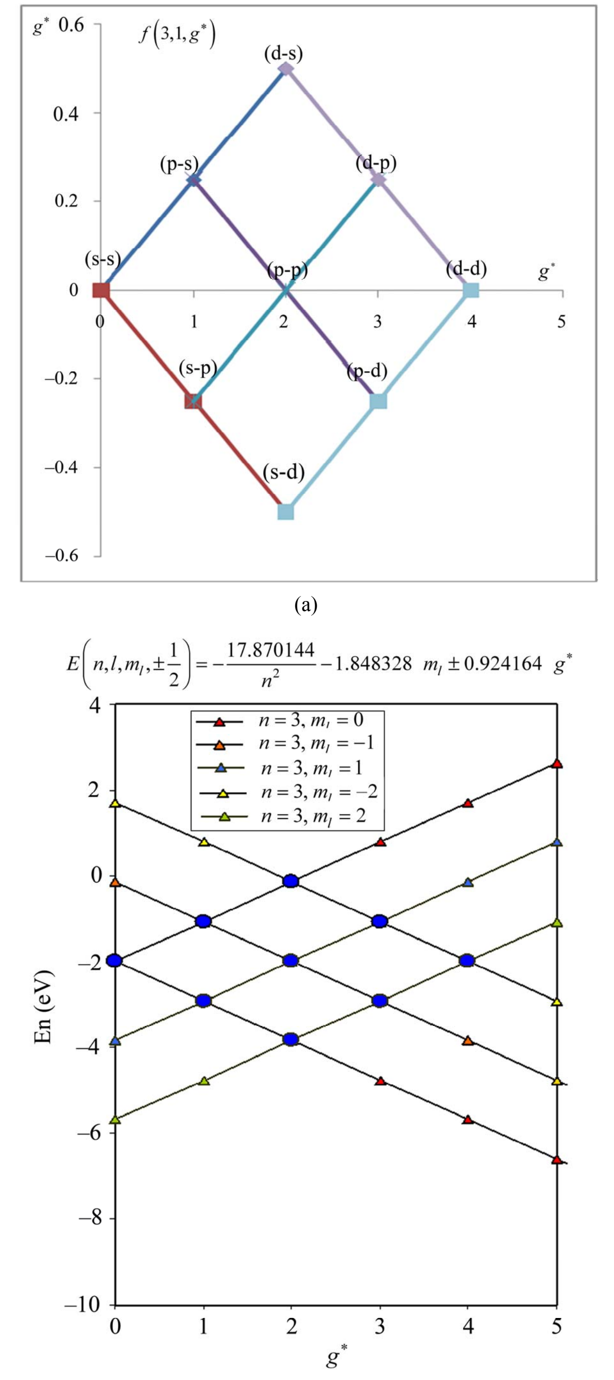

Figure 3. (a) $f(3,m_l,g^*)$ **as a function** g^***; (b)** $E(3,m_l,g^*)$ **as a function** g^***.**

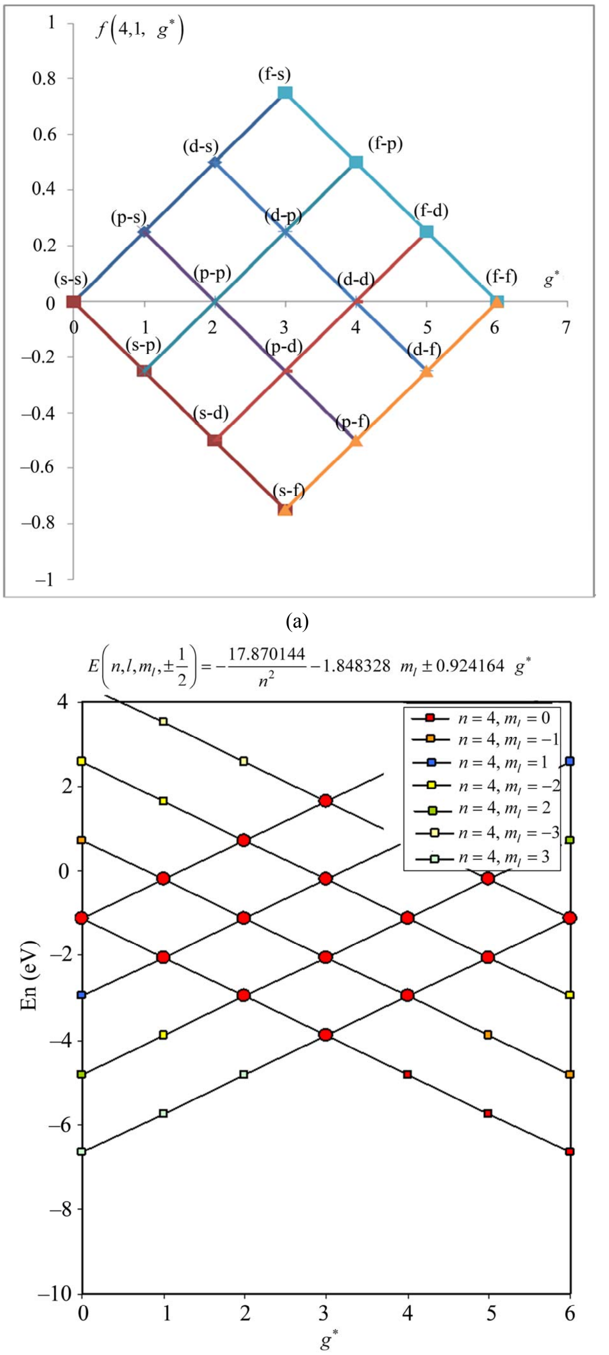

Figure 4. (a) $f(4,m_l,g^*)$ **as a function** g^***; (b)** $E(4,m_l,g^*)$ **as a function** g^***.**

tum flux through the orbits corresponding to the entangled states in hydrogen-like atoms will be given by:

$$\Phi\left(n,l,m_j\right)=\left[n-l-\left(m_l+g^*m_s\right)\right]\Phi_0 \tag{4}$$

We have stated that when the ground state electron is excited to a higher level with an absorption of one photon (or more photons) the flux difference between two quantum orbits must be equal to integer multiples of ($\pm\Phi_0$). Therefore the difference of the flux in (4) must be equal to integer multiples of ($\mp\Phi_0$). In (4), since we have $m_s=\pm\left(1/2\right)$, the above requirement is possible only when the change of g^* between two states is equal to an even integer number:

$$\Delta g^{*} = 0, 2, 4, \ldots \tag{5}$$

We have said that in Li atom the ground state electron (2s electron) occupies the entangled state of $2s\uparrow$ and $2p\downarrow$ at $g^{*}=1$. Therefore a photonic transition occurs either to the entangled states with $g^{*}=3$ or $g^{*}=5$. In the present study we will consider only n values up to 10. We will see that in this range ($2 \le n \le 10$) we get 26 different energy values which produce 325 wavelengths some of which are the same.

2.4. Detailed Calculation of the Zeeman-Fine Energies of Li Atom

From the (NIST) values, the ionization energy of Li atom is $5.3917\ \text{eV}$, while the smallest amount of energy that allows a transition from the ground state to the nearest excited state ($2s^{2}S_{1/2} \rightarrow 2p^{2}P_{3/2}$) is equal to 1.848328 eV which corresponds to $6707.91A^{o}$. In this transition the initial and the final value of g^{*} is the same and equal to unity: $g^{*}=1$. Therefore we can write $m_j = m_l + g^{*} m_s = m_l + m_s$ Therefore from (2) the energies of the initial and final states are:

$$E\left(n=2, m_j = 1/2, B^{*}\right) = -\frac{C}{2^2} - \frac{\hbar\omega_c^{*}}{4} = -5.3917 \tag{6}$$

and

$$E\left(n=2, m_j = 3/2, B^{*}\right) = -\frac{C}{2^2} - \frac{\hbar\omega_c^{*}}{2} - \frac{\hbar\omega_c^{*}}{4} = -3.5434 \tag{7}$$

respectively. The solutions of (6) and (7) gives us that $C = 17.870144$ eV and $\left(\hbar\omega_c^{*}/2\right) = 1.848328$ eV . Substitution of these values in (2) gives the Zeeman-fine energies of Li atom:

$$E\left(n, m_l, B*\right) = -\frac{17.840144}{n^2} - \left(1.848328\right) m_l \mp \left(0.924164\right) g^{*} \tag{8}$$

In the present study we will take n values in the range ($2 \le n \le 10$). For each value of n substituting the values of m_l and taking $g^{*} = 1,3,5$ we get 26 different energy values which are given in **Table 1**. These 26 different energy values give us 325 wavelengths some of which are the same. The Doppler shift-corrected wavelengths are in perfect agreement with the observed (NIST) values [14] for atomic Li (**Figure 5**). In **Table 2**, we give the comparison between the observed values and the corresponding calculated values which have Doppler shift-correction as well. The Doppler shift-corrected wavelengths are in perfect agreement with the observed (NIST) values for atomic Li.

Table 1. Zeeman-fine Energies and related g^{*} values for $n = 2,3,4,5,6,7,8,9,10$. (Here $l = 0,1,2,3,4,5,\ldots$ states are denoted by s,p,d,f,g,h,… respectively.)

n	$\left(-\frac{C}{n^2} - \frac{m_l \hbar\omega_c^{*}}{2} \mp \frac{g^{*}\hbar\omega_c^{*}}{4}\right)$/ eV		
10	−1.10286544	→	$(10s\text{-}10p)_{g^{*}=1}$
	−2.95119344	→	$(10s\text{-}10f)_{g^{*}=3}$
	−4.79952144	→	$(10s\text{-}10h)_{g^{*}=5}$
9	−1.14478310	→	$(9s\text{-}9p)_{g^{*}=1}$
	−2.99311100	→	$(9s\text{-}9f)_{g^{*}=3}$
	−4.84143910	→	$(9s\text{-}9h)_{g^{*}=5}$
8	−1.20338500	→	$(8s\text{-}8p)_{g^{*}=1}$
	−3.05171300	→	$(8s\text{-}8f)_{g^{*}=3}$
	−4.90004100	→	$(8s\text{-}8h)_{g^{*}=5}$
7	−1.28886082	→	$(7s\text{-}7p)_{g^{*}=1}$
	−3.13718882	→	$(7s\text{-}7f)_{g^{*}=3}$
	−4.98551682	→	$(7s\text{-}7h)_{g^{*}=5}$
6	−1.42055689	→	$(6s\text{-}6p)_{g^{*}=1}$
	−3.26888489	→	$(6s\text{-}6f)_{g^{*}=3}$
	−5.11721289	→	$(6s\text{-}6h)_{g^{*}=5}$
5	−1.63896976	→	$(5s\text{-}5p)_{g^{*}=1}$
	−3.48729776	→	$(5s\text{-}5f)_{g^{*}=3}$
	−5.33562576	→	$(5s\text{-}5h)_{g^{*}=5}$
4	−0.19272000	→	$(4s\text{-}4p)_{g^{*}=1}$
	−2.04104800	→	$(4s\text{-}4f)_{g^{*}=3}$
	−3.88937600	→	$(4s\text{-}4h)_{g^{*}=5}$
3	−1.06140760	→	$(3p\text{-}3s)_{g^{*}=1}$
	−2.90973560	→	$(3s\text{-}3p)_{g^{*}=1}$
	−4.75806360	→	$(3s\text{-}3f)_{g^{*}=3}$
2	−3.54337200	→	$(2p\text{-}2s)_{g^{*}=1}$
	−5.39170000	→	$(2s\text{-}2p)_{g^{*}=1}$

2.5. Calculation of the DopplerShift for Li Atom

The above calculations are based on the assumption that the center of mass of the Li atom is at rest, but only the outermost electron is moving. But since the experimental results are taken from the moving Li atom, there will be a small difference coming from the Doppler shift. To calculate the Doppler shift we take two different repeated wavelengths from the (NIST) database. For example if we $\lambda_1 = 5271.00A^{o}$ and $\lambda_2 = 4971.75A^{o}$. The corresponding calculated values are $\left(\lambda_1\right)_{cal} = 5292.78A^{o}$ and $\left(\lambda_2\right)_{cal} = 4995.78A^{o}$ respectively. Now we can calculate

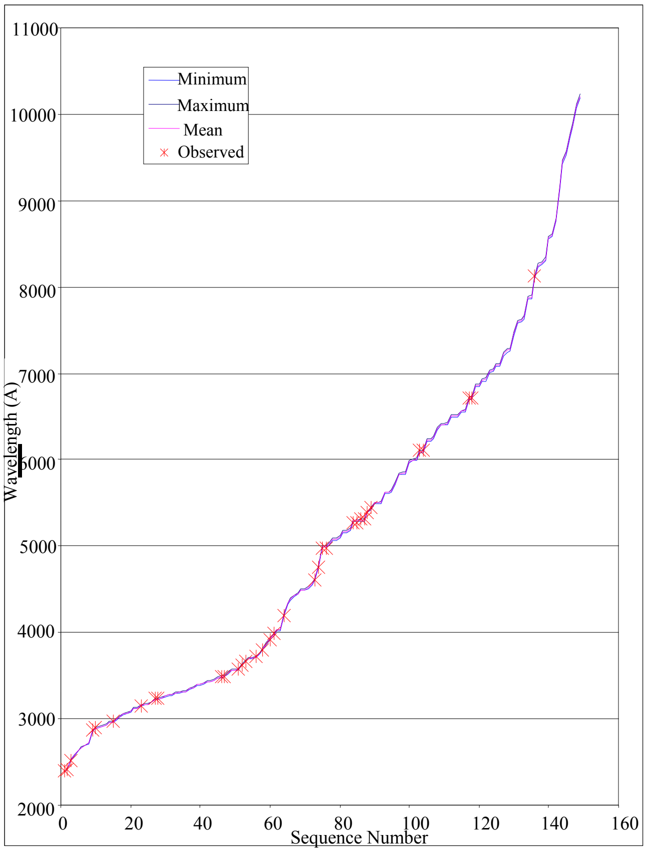

Figure 5. A comparison between Doppler-shift corrected wavelengths (A^o) and observed values.

Table 2. Comparision between the observed and Doppler shift-corrected calculated wavelengths.

$\lambda_{calculated}$ A^o	$\lambda_{observed}$ A^o
2384.78 ± 9.58	2394.39
2410.78 ± 9.64	2410.84
2517.70 ± 10.07	2518.00
2863.18 ± 11.47	2868.00
2890.86 ± 11.58	2895.00
2960.24 ± 11.87	2968.00
3159.55 ± 12.58	3144.00
3228.14 ± 12.93	3232.66
3229.90 ± 12.93	3232.66
3487.92 ± 13.95	3488.00
3489.98 ± 13.95	3488.00
3573.5 ± 14.32	3579.80
3624.33 ± 14.47	3618.00
3669.30 ± 14.65	3662.00
3714.88 ± 14.88	3718.70
3801.95 ± 15.18	3794.72
3922.87 ± 15.66	3915.35
3975.01 ± 15.94	3985.48
4210.75 ± 16.78	4196.00
4616.00 ± 18.41	4602.83
4767.68 ± 19.04	4760.00
4995.00 ± 19.89	4971.66
4995.41 ± 19.99	4971.75
5292.48 ± 21.08	5271.00
5292.78 ± 21.08	5271.00
5298.00 ± 21.26	5315.00
5298.50 ± 21.26	5315.00
5428.59 ± 21.76	5440.00
5428.59 ± 21.76	5440.00
6094.62 ± 24.41	6103.54
6094.62 ± 24.42	6103.65
6707.9 ± 26.83	6707.76
6707.91 ± 26.83	6707.91

the average Doppler shift by using the above values:

$$\frac{\Delta\lambda}{\lambda} = \frac{1}{2}\left(\frac{\Delta\lambda_1}{\lambda_1} + \frac{\Delta\lambda_2}{\lambda_2}\right) \cong 0.004 \qquad (9)$$

So the magnitude of the Doppler shift is found to be

$$\left|\Delta\lambda\right| = 0.004\lambda\ . \qquad (10)$$

3. Conclusions

We have calculated the effective Landé g-factors, g^*, related to the Zeeman-fine energies and the spectrum of the atomic Lithium (Li) by using the varying effective Landé g-factor method. It is shown the allowed values of g^* are restricted only with three odd integers ($g^* = 1,3,5$) and this result is independent of the limit of the principle quantum number, n. In the present study we take the principle quantum number in the range; $(2 \le n \le 10)$. For this range we find 26 different energy values and 325 wavelengths some of which are the same. The present calculations are based on the assumption that the center of mass of the Li atom is at rest, but only the outermost electron is moving. But since the experimental results are taken from the moving Li atom, there will be a small difference coming from the Doppler shift. The Doppler shift is found to be $\Delta\lambda = \pm 0.004\lambda$. The Doppler shift-corrected wavelengths are in perfect agreement with the observed (NIST) values for atomic Li. The present results suggest new wavelengths such as

$$3301.62 \pm 13.21 A^o, \; 3166.85 \pm 12.67 A^o \; \text{and} \; 3353.96 \pm 13.42 A^o$$

should be observed. Applications of the above treatment can give access to the production of new laser lights from atomic Lithium as well. Extending the range of n to $(2 \le n \le 32)$ will allow us to calculate all the observed wavelengths for Li atom. A more detailed study will be presented in the future.

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