Study on the Energy Level Splitting of the Francium Atom (Fr) in an External Magnetic Field

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ABSTRACT

In This paper the normal Francium atom is considered with the use of nonrelativistic quantum mechanical approach and the Bohr's atomic model. We study the energy shift values of a Francium atom by the external magnetic fields effect; we considered the two cases; that effect without external magnetic fields and those of with the external magnetic fields.

KEYWORDS: energy shift, energy level splitting, magnetic field effect on the atom

INTRODUCTION

Atom is a Greek word which means "indivisible". The Greek believed that matter can be broken down into very small invisible particles called atom. Greek philosophers such as Democritus and John Dalton put forward the concept of the atom, Democritus explained the nature of matter; He also proposed that all substances are made up of matter. He stated that atoms are constantly moving invisible, minuscule particles that are different in shape, size, and temperature and cannot be destroyed.

Later in the year 1808, John Dalton proposed the atomic theory and explained the law of chemical combination. By the end of the 18th and the early 20th centuries, many scientists such as J. J Thomson, Gold Stein, Rutherford, Bohr among other developed and proposed several concept on the "atom"

J. J Thomson was the first and one of the many scientists who proposed models for the structure of an atom. J. J Thomson discovered negatively charged particles by cathode ray tube experiment in the year 1897. The particles were named "electrons".

Development

In the year 1904, J. J Thomson suggested a model of the atom as a sphere of positive matter in which electrons as positioned by electrostatic force. J. J. Thomson believed electrons to be two-thousand times lighter than a proton. He assumed that an atom is composed of a cloud of negative charge in a sphere of positive charge. The positive and negative charge is equal in magnitude and therefore an atom has no charge as a whole and is electrically neutral.

In each element, the ground state of the atom contains a fixed and equal number of protons and electrons. An atom characterized by an atomic number Z has a nucleus which carries almost the entire mass of the atom and a positive electric charge (Ze) surrounded by Z electrons each of which carries a negative charge (-e). The orbital motion of the electron is characterized by an orbital momentum quantum number 1 and its projection $m_i = -1, -1 + 1, -1 + 2, ..., +1$

with reference to the axis of quantization, which is usually chosen as the z-axis. The electron has also an intrinsic spin quantum numbers = 1/2, its projection $m_s = -1/2$, +1/2 with reference to the same axis. Thus the total number of electrons with the same angular momentum 1 are 2 (21 +1) which are filled, following the Pauli's exclusion principle. The orbital and spin angular momentum of the electron add up quantum mechanically to yield a totalangular momentum quantum number J and its

projection m_j where $m_j = -J, -J + 1, -J + 2, \dots, +J$ along the z-axis.

When an atom with angular momentum J is in the absence of external fields and when the atom is not interacting with other particles, all the (2J+1) sub-levels are completely degenerate with respect to energy. When the external magnetic field is applied, the energy levels are split into the possible numbers of (2J+1) and this is called the Zeeman Effect.

The Ground State Energy of Single-Electron Hydrogen Atom

In 1913, Bohr proposed his quantized shell model of the atom to explain how electrons can have stable orbits around the nucleus. The motion of the electrons in the Rutherford model was unstable because according to classical mechanics and electromagnetic theory; thus, the electron would lose energy and spiral into the nucleus. The energy of an electron depends on the size of the orbit and is lower for smaller orbits. The atom will be completely stable in the state with smallest orbit, since there is no orbit of lower energy into which the electron can jump. Bohr assumed that an electron in an atom moves in an orbit about the nucleus under the influence of the electrostatic attraction of the nucleus. Circular or elliptical orbits are allowed by classical mechanics, and Bohr selected to consider circular orbits for simplicity. He then, postulated that instead of the infinity of orbits which are possible in classical mechanics, only a

certain set of stable orbits, which he called stationary states are allowed. As a result, atom can only exist in certain allowed energy levels with energies $E_a, E_b, E_c, ...$

If the orbits are quantized, the amount of energy absorbed or emitted is also quantized, producing discrete spectra. Photon absorption and emission are among the primary methods of transferring energy into and out of the atoms. The energies of the photons are quantized, and their energy is explained as being equal to the change in energy of electron when it moves from one orbit to another.

Bohr was clever enough to find a way, to calculate the electron orbital energies in hydrogen atom. This was an important first step that has been improved upon, but it is well worth repeating here, because it does correctly describe many characteristic of hydrogen atom in the next portion. The simplest example of the Bohr model is for the hydrogen atom (Z=1) or for a hydrogen-like ion (Z >1), in which a negatively-charged electron orbits a small positively-charged nucleus; electromagnetic energy will be absorbed or emitted if an electron moves from one orbit to another. Only certain electron orbits are permitted.

Bohr explained how electrons could jump from one orbit to another only by emitting or absorbing energy. When the electron jumps to a larger orbit, it must absorb a equal in energy to the difference in orbits.

Electrons in an atom are held their orbits by the forces of electrical attraction acting between them and the nucleus, the higher is its energy, although with an increase in this distance its bound with the nucleus naturally, weakens, However, no two electrons can be in the same energy state and therefore electrons are arranged in layer in the shell. There may be only strictly limited number of electrons in each level, 2 in the first innermost shell, 8 in the second and so on these shells are denoted by the symbols K, L, M, N respectively.

Each shell can contain only a fixed number of electrons. The first shell can hold up to two electrons, the second shell can hold up to eight (2+6) electrons, the third shell can hold up to 18 (2+6+10) and so on. The general formula is that the nth shell can in principle hold up to $2n^2$ electrons.

For the case of the one electron atom, Bohr's was able to modify the classical model to obtain the quantization of energy levels by making the additional postulate that the angular momentum of the electron moving in circular orbit

can only take one of the value $L = \frac{nh}{2\pi} = nh$, when n is a

positive integer, n= 1, 2, 3, 4,... and the common occurring $h/2\pi$ is conventionally denoted by \hbar .

Calculation of the Ground State Energy of the Simplest Single- Electron Hydrogen Atom

The hydrogen atom is the simplest atom in nature and therefore a good starting point to study atom and atomic structure. The hydrogen atom consists of a single negatively charged electron that moves about a positively charged proton. In Bohr's model, the electron is pulled around the proton in a perfectly circular orbit by an attractive Coulomb force. The proton is approximately 1840 times more massive than the electron, so the proton moves very little in response to the force on the proton by the electron. Consider an electron of charge e and mass m, it will be taken to be moving with a velocity v in a circular orbit of radius r in an atom.

The Coulomb force between a stationary nucleus with the nucleus of charge +Ze and orbiting electron with charge 'e' is

$$F = K \frac{Ze^2}{r^2}$$
(1)

From the Newton's second law of motion, the electron mass m times the centripetal acceleration $\frac{v^2}{r}$ called centripetal

force
$$F_c = \frac{mv^2}{r}$$
, It can be expressed as follow;
 $K \frac{Ze^2}{r^2} = \frac{mv^2}{r}$
 $v = K \frac{Ze^2}{mvr}$
(2)

N. Bohr proposed that the angular momentum (L) of the allowed orbit takes the integral values of $h = \frac{h}{2\pi}$.

From Bohr's postulate (3), the angular momentum (m v r) of the allowed orbits takes the integral values of $h/2\pi$. Hence, Bohr's postulate that the angular momentum is given by

By using the above equations (2) and (3), we get the value of v and r as

$$\mathbf{v}^2 = \left(\frac{\mathrm{K}\,\mathrm{Z}\mathrm{e}^2}{\mathrm{n}\mathrm{h}}\right)^2 \tag{4}$$

Substituting equation (4) into the equation (3), we get the radius of the orbit

$$r = \frac{(n h)^2}{m K Z e^2} .$$

where, $\frac{(h)^2}{Kme^2} = 0.529 \stackrel{\circ}{A}$ called Bohr's radius.

For nth state,
$$r_n = \frac{0.529 n^2}{Z} \mathring{A}$$
. (n=1, 2, 3, 4, ...) (5)

From which the total energy $E_0\ \mbox{of}$ the electron in the Hydrogen atom is

$$E_0 = T + V$$

$$E_0 = \frac{m}{2h^2} \left(\frac{K Z e^2}{n}\right)^2 - \frac{m}{h^2} \left(\frac{K Z e^2}{n}\right)^2$$

$$E_0 = -13.6 \frac{Z^2}{n^2} eV$$
(6)

The ground state energy for the hydrogen atom is obtained

$$n=1, Z=1$$
 then
 $E_0 = -13.6 \,\text{eV}$ (7)

$$E_n = -13.6 \frac{Z^2}{n^2} eV$$
 for Hydrogen like atom (8)

The above equation (8) is also true for all the simplest one electron hydrogen like atom and so it is very useful to calculate the ground state energy of the chosen hydrogen like Francium atom.

Basic Concept of Alkali Metals

The group(I) in the periodic table consisting of the chemical elements lithium (Li), sodium (Na), potassium (K), rubidium (Rub), cesium (Cs) and francium (Fr). They are collectively known as the alkali metals. This group lies in the S-block of the periodic table is all alkali. All alkali metals have their outermost electron in an s-orbital. Indeed, the alkali metal provides the best example of group trends in properties in the periodic table. The alkali metals, halogen and novel gases are their important group in the periodic table. The alkali metals are soft, reactive metals.

The outer electron of an atom determines the chemical and optical properties of their atom. The electron in the closed inner orbits do not take part in the emission of spectral lines, and thus atoms are divided into two main categories which are one electron system and many electrons system. The alkali metals (such as lithium, sodium and potassium) have a single electron in the outermost shell. The alkali metals therefore behave much like the hydrogen atom. Hence, the alkali metals have hydrogen–like spectra. Each alkali atom contains, in addition to the completed sub-shells of electron, one single electron in the outer shell. The complete electron configurations are written out in the below table.

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Sr. No	Element	Atomic No	symbol	Electrons Configuration
1	Francium	87	Fr	$1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s^25p^66s^24f^{14}5d^{10}6p^67s^1$

The chemical element Francium is classed as an alkali metal. Francium is a chemical with symbol Fr and atomic number 87. In 1939, it was discovered by Marguerite Perey in France. It was the last element. Outside the laboratory, Francium is extremely rare, with trace amounts found in uranium and thorium ores, where the isotope Francium-223 continually forms and decays.

Francium used to be known as eka-caesium. It is extremely radioactive, its most stable isotope, Francium-223 has a maximum half-life of only 22 minutes. It is the second-most electropositive element, behind only Caesium, and is the second rarest naturally occurring element. The isotope of Francium decay quickly into astatine, radium and radon. The electronic structure of a Francium atom is 7s¹ and so the element is classed as an alkali metal. A heavy element with a single valence electron, it has the highest equivalent weight of any element.

A Francium atom has 87 electrons. The electron configuration of the Francium atom is $(1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^6 6s^2 4f^{14} 5d^{10} 6p^6 7s^1)$. The 86th out

of the 87th electrons of the Francium atom are interlocked in closed shells. We focused considered only the state of 87th optical electron in discussing the spectrum of natural Francium atom. The electron configuration shows that the outermost shell is (7s). Therefore, the orbital angular momentum is l = 0 and spin angular momentum is s = 1/2 for electron. The total angular momentum J can take J = (l + s), L, |l - s|. Then, the total angular momentum of the ground state of Francium atom will be J = 1/2.

If the valence electron in the s-shell can jump to the excited state due to various physical mechanisms and reach to the 5f-state, the orbital angular momentum of the excited electron is I = 3 and the spin angular momentum is s = 1/2. Thus the total angular momentum may be J = 7/2 and J = 5/2.

The term symbol of the first excited state and ground state of ⁸⁷Fr with their corresponding quantum numbers are as shown in below table.

Table- The first excited state and ground state of the 87Fr atom with their corresponding quantum numbers.

State	Term symbol	n	1	S	J	mj	Lande's g-factor
Ground state	${}^{2}\mathbf{S}_{\frac{1}{2}}$	7	0	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}, -\frac{1}{2}$	2

The Effective Nuclear Charge (Z_{eff}) and the Screening Constant (σ)

The screening constant describes the decrease in attraction between the negatively charged electron and the positively charged nucleus in any atom with more than one electron. Electrons in an atom can shield each other from the pull of the nucleus. It is also referred to as the screening effect or atomic shielding. The more electron shells there are, the greater the shielding effect experienced by the outermost electrons. The screening effect depends only on the number of electron orbit inside the valence shell. The screening effect is due to the repulsion by other electrons. Each new electron that is pulled on by the positive charge of the nucleus is repelled by the electrons. The shielding effect can be defined as reduction in the attractive nuclear charge on the electron cloud, due to a difference in the attraction forces on the electrons in the atom. In hydrogen-like atoms (those with

only one electron), the net force on the electron is just as large as the electric attraction from the nucleus. However, when more electrons are involved, each electron (in the nshell) feels not only the electromagnetic attraction from the positive nucleus, but also repulsion forces from other electrons in shells from 1 to n. This causes the net force on electrons in outer shells to be significantly smaller in magnitude; therefore, these electrons are not as strongly bonded to the nucleus as electrons closer to the nucleus.

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The shielding effect explains why valence shell electrons are more easily removed from the atom. The effect also explains atomic size. The more shielding, the further the valence shell can spread out and atom will be larger.

The values of the screening constant can estimate the effective nuclear charge on each electron. The effective nuclear charge (often symbolized as $Z_{\rm eff}\,$ or Z^*) is the net positive charge or full experienced by an electron in a multi-electron atom due to the protons in the nucleus. The term "effective" is used because the shielding effect of negatively charged electrons prevents higher orbital electrons from experiencing the full nuclear charge by the repelling effect of inner-layer electrons. The effective nuclear charge experienced by the outer shell electron is also called the core charge. It is possible to determine the strength of the nuclear charge by looking at the oxidation number of the atom.

Outer shell electrons are the electron located farthest from the nucleus. These electrons have the least attraction to the nucleus due to the distance. Therefore, these outer shell electrons have minimum effect from the nucleus. Electrons in the outermost shell are known as valence electrons. In an atom with one electron, that electron experiences the full charge of the positive nucleus. In this case, the effective nuclear charge can be calculated from Coulomb's law. However, in an atom with many electrons the outer electrons are simultaneously attracted to the positive nucleus and repelled by the negatively charged electrons. The effective nuclear charge on such an electron is given by the following equation:

$$Z_{\rm eff} = Z - \sigma \tag{9}$$

where Z is the number of protons in the nucleus (atomic number), and σ is the average number of electrons between the nucleus and the electron in question (the number of non-valence electrons) called screening parameter or screening parameter.

For 7s electron of the Francium atom, the parameter of the screening constant is σ = 83.205 obtained from the reference web page of the www.nuclear-power.net.

Therefore, the effective nuclear charge $\rm \,Z_{eff}\,$ of the chosen Francium atom is

 $Z_{eff} = 87 - 83.205 = 3.795$

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Electron	Hydrogen	Lithium	Sodium	Potassium	Rubidium	Caesium	Francium		
Identity	Н	Li	Na	K	Rb	Cs	Fr		
1s	0	0.9377	2.1277	2.7962	4.2963	6.0612	9.3942		
2s	E	1.7410	6.5954	018.4330	a 12.5160	4.800	17.3510		
2p	E	L'n	<mark>7.8610</mark>	9.6577	13.9140	16.603	20.8280		
3s	E	0	9.1 <mark>563</mark>	14.0570	22 <mark>.3510</mark>	26.798	32.9190		
3p			Deve	15.4200	24.2880	29.098	37.0660		
3d	4				28.3140	33.028	42.3270		
4s		N 33.	ISSN:	16.7410	30.8290	38.505\	50.5100		
4p		N.C.			32.5930	41.055	54.9390		
4d		J.	14 2		° Z	45.412	60.8370		
4f		L.			5		69.5630		
5s			all	m	34.2300	48.382	66.4440		
5p						50.255	70.1400		
5d							76.5060		
6s						51.790	77.6590		
6p							80.5800		
7s							83.2050		

Table-Hydrogen and Alkali Metals Group I (Η to Fr) Shielding Constant (σ)

The Ground State Energy of the Normal Francium Atom Next to the Hydrogen, the alkali metals Li, Na, K ...have the simplest spectra. Each alkali atom contains in addition to the complete sub-shells of electrons, one single electron in an outer shell. Therefore, the alkali metals are hydrogen-like atoms.

For Francium atom, a small requires correction term to equation (8) was made by Hertz's formula, with the screening constant, denoted by (σ). Therefore this equation (8) can also be written as in the following form,

$$E_0 = -13.6 \frac{Z_{eff}^2}{n^2}$$
(10)

where Z_{eff} is the effective nuclear charge and which can be obtained by using the following equation, which is in the form of

$$Z_{\rm eff} = Z - \sigma \tag{11}$$

In equation (10) Z_{eff} is used instead of Z, because of, in an atom with many electrons, the outer electron are simultaneously attracted to the positive nucleus and repelled by the negatively charged electrons. The effective

nuclear charge on such electron is given by the above equation (11).

For Francium atom, the screening constant for the 7s state

electron is σ =83.205, this value is obtained from the previous table. Then, equation (10) can be written as follow;

$$E_0 = -13.6 \frac{(Z - \sigma)^2}{n^2} eV$$
 (12)

By using this equation (12), we can calculate the ground state (n=7) energy of the Francium and its energy values is $E_0 = -3.98 \text{ eV}$ (13)

The value which is our calculated for the ground state energy of the Francium is nearly equal to the the value of references data which is -4.0 eV.

THE EFFECT OF UNIFORM MAGNETIC FIELD ON AN ATOM

The Interaction between an Atom and External Magnetic Field

If the atom is placed in the magnetic field, the total angular momentum vector J processes about the direction of magnetic field B as axis. In classical electrodynamics, the interaction energy of an external magnetic field B with total magnetic moment is given by

$$\mathbf{H}_{\rm int} = -\boldsymbol{\mu}_{\rm j} \cdot \mathbf{B} \ . \tag{14}$$

The Schrödinger equation for an atom in a uniform magnetic field is $H \Psi = E \Psi$ (15)

where H is the total Hamiltonian and in the form of $H = H_0 + H_{int}$ (16)

 $\mathbf{H} = \mathbf{H}_{0} + (\boldsymbol{\mu}_{B} \mathbf{g} \mathbf{J} \cdot \mathbf{B}).$

The unperturbed Hamiltonian H_0 satisfies the equation $H_0\Psi = E_0\Psi$ (18)

(17)

(20)

where E_0 is the unperturbed energy eigenvalue.

To find the energy value corresponding to the complete Hamiltonian H, the magnetic field is conveniently chosen along the z-axis so that

 $\mathbf{J} \cdot \mathbf{B} = \mathbf{J}_{z} \mathbf{B}_{z} = \mathbf{J}_{z} \mathbf{B}.$ (19)

The eigenvalue E of the Hamiltonian ${\rm H}_{\rm int}$ on the $\left| {\ Jm} \right\rangle$ basis

are

 $E = E_0 + (\mu_B g m_I B)$

where m_{I} is the projection of vector **J** on the direction of the

magnetic field and it can take (2J + 1) values from -J to + J.

The Shifting of Energy Levels by the Presence Magnetic Field

When the external magnetic field is applied, the energy levels are split into the possible numbers of (2J+1) and this is called the Zeeman Effect.

Since the external magnetic field removes the degeneracy, the total angular momentum quantum number J = 7/2 level splits into eight sub-levels with

 $m_{\rm i}{=}7\!/2,\,5\!/2,\,3\!/2,\,1\!/2,\,-1\!/2,\,-3\!/2,\,-5\!/2,\,-7\!/2$ and the total angular

momentum quantum number J = 5/2 level into six sublevels with $m_i = 5/2$, 3/2, 1/2, -1/2, -3/2, -5/2.

RESULTS AND CONCLUSIONS

The Energy Shift Value for Francium Atom by External Magnetic Field

In this chapter, it is calculated the energy shift value of the Francium atom when it is exposed to magnetic fields and without external magnetic fields.

Atom in magnetic field was a very long history starting from the discovered by Zeeman in 1896 of the splitting spectral lines into components in a magnetic field. All the energy levels of the valence electron in an alkali metal are split into two, one level corresponding to a total angular momentum quantum number J = 1 + 1/2 and the other J = 1 - 1/2

The interaction causing this splitting is the spin-orbit interaction, which was discussed in detail, in connection with one electron atom. The energy shift value due to this effect was calculated by details.

The Energy Shift Value for $^2\mathrm{S}_{1/2}$ level without External Magnetic Field

By using the previous obtained equation, we calculated the energy value for ${}^{2}S_{1/2}$. This equation can also be written as follow;

(21)

where, $\Delta E = \mu_B g m_J B$ is the energy shift value from the E₀.

The energy shift value for this level will be degenerated. **Develop** field strength is 0 T, therefore the energy value is equal to E_0 and it can be express as,

 $E_0 = -3.98 \text{ eV}$

The Energy Shift Value for ²S_{1/2} level with External Magnetic Field Strength of 5.0 T

(22)

When the external magnetic field strength of 5.0T is applied on the Francium atom. The energy shift value between the upper sub-level m_j =+1/2 and E_0 can be obtained by the following equation

 $\Delta E = \mu_B g m_J B$

 $E = E_0 + \Delta E$

$$\Delta E = +5.79625 \times 10^{-5} \text{ eV } \text{T}^{-1} \times 2 \times \frac{1}{2} \times 5.0 \text{ T}$$

 $\Delta E = +2.898125 \times 10^{-4} \text{ eV}$

where g = Lande's g-factor and its value is 2 for s-state electron taken from previous table.

Therefore, the energy value of the upper sub-levels for $m_j \mbox{=} + 1/2$ is

$$E = E_0 + \Delta E$$

 $E = -3.98 \,\text{eV} + 2.898125 \times 10^4 \,\text{eV}$ (23)

Similarly, the energy value for the lower sub-level m_j =-1/2 is the same amount of the upper shift values and thus we can be express as

 $\Delta E = -2.898125 \times 10^{-4} \, eV$ and

 $E = E_0 + \Delta E$

 $E = -3.98 \,\text{eV} - 2.898125 \times 10^4 \,\text{eV}$ (24)

The energy values for external magnetic field strength B=0.0T, B=5.0T, B=10.0T, B=15.0T, B=20.0T and B=25.0T are calculated and the detail values are shown in below figure(1) to figure(6).

In this paper, the ground state energy and energy shift values of a Francium atom without the external magnetic field and with the external magnetic field are calculated, From the calculation, the position of the ground state energy of the Francium atom can be presented in figure(1) to figure(6) for various magnetic field strengths. These figures show the Francium atom will not have energy shift value when there is not present external magnetic field strength. When the magnetic field applies to the Francium atom, the energy shift values are appeared.

We can also be seen from all figures that the unperturbed ground state energy level E_0 is split into two sub levels when the magnetic field is applied and they shift symmetrically around the ground state energy level E_0 with equal spacing in all figures. The difference shift level is depends only on the strength of the magnetic field strength B, but independent of the principal quantum number 'n' of the valence electron. We found that the larger amount of energy shift values is observed for the greater the magnetic field strengths.



Fig (1) The energy shift value for ${}^{2}S_{1/2}$ of the Francium atom without the external magnetic field and Fig (2) with 5.0 T



Fig (3) The energy shift value for ${}^{2}S_{1/2}$ of the Francium atom with the external magnetic field strength of 10.0 T and Fig (4) 15.0 T.



Fig (5) The energy shift value for ${}^{2}S_{1/2}$ of the Francium atom with the external magnetic field strength of 20.0 T and Fig (6) 25.0 T.

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