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Investigation of Some Elements In nP^2- Configuration by Zeeman Effect

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Abstract

Calculation of the relativistic and diamagnetic corrections of the g_J-factors have been performed in order to find evidence of configuration interaction in 3P-configuration elements. The comparison between the experimental and calculated g_J-factors of the ground configuration showed no evidence of configuration in C, Si and Ge. In Sn, however, there is an indication that configuration interaction is present. In Pb evidence of configuration interaction was found.

Introduction

In Zeeman effect, if we apply an external magnetic field (B), it will interacted with the total magnetic moment (μ) of the atom, and we can obtain the magnetic moment of the spin angular moment (μ_s) as.

$$\mu_s = -\, g_e .\, \mu_B .\, S \qquad \dots (1)$$

Where (μ_B) is the Bohr magneton, and (g_e) is the (g) factor of the electron spin. In the same way we can obtain the magnetic moment (μ_L) due to the orbital angular momenta (L).

$$\mu_L = -\, \mu_B .\, L \qquad \dots (2)$$

The total magnetic moment of the atom is then:

$$\mu = \mu_L + \mu_s = -\, \mu_B\, (L + g_e .\, S) \qquad \dots (3)$$

The operator for the interaction with external magnetic field (Zeeman Hamiltonian, H_Z) will be:

$$H_z = -\, \mu_\beta .\, B\, (L + g_e .\, S) \qquad \dots (4)$$

Where ($g_e = 2.002319288$) (Inguscio *et al.*, 1984) and (B) is the external magnetic field. When we apply this magnetic field, we will obtain an energy splitting of a given energy level into (2J +1) sub- levels. The energy of these sub-levels (E_Z) will then be:

$$E_z = \mu_B .\, B .\, g_J .\, M_J \qquad \dots (5)$$

M_J is the magnetic quantum number and the atomic g_J-factor can be given by following expression (Veseth, 1980)

$$g_J = 1 + (g_e - 1)\, \frac{J(J+1) - (L+1) + S(S+1)}{2J(J+1)} \qquad \dots (6)$$

The experimental g_J-factors can deviate from this simple expression. There are several effects which account for these discrepancies, namely the relativistic and diamagnetic corrections and a correction due to the motion of the nucleus. These corrections have been treated extensively by Abragam and Vleck (Abragam *et al.*, 1963) they calculated theoretically g_J-factors for oxygen with an excellent agreement with experimental data.

The g_J-factors are also sensitive for the break-down of LS-coupling. These can be used as a way to analyze the break-down of LS-coupling and to obtain eigenvectors.

The relativistic and diamagnetic corrections can be divided into two parts, the spin-other-orbit and orbit-orbit corrections. These corrections depend mainly on the electron density of the core.

Briet and Margenau (Briet, 1928, Margenau, 1940) has expressed the corrections of relativistic and diamagnetic as δ_{z1} and δ_{z2}. Judd and Lindgren (Judd et al, 1961) has been shown that the total relativistic and diamagnetic correction operator can be written as

$$\delta_z = \delta_{z1} + \delta_{z2} = -\alpha^2 \mu_o \,.\, H. \sum\{(1+2s)(T+Y) - [s-(s.r).r/r^2]\,(T+U) \quad \ldots(7)$$

Where
$$\left.\begin{aligned} Y_{(r)} &= \frac{1}{3}\left[\frac{1}{r^3}\int_0^r r'^2 \rho'_{(r')}\, dr' + \int_0^\infty \frac{\rho(r')}{r'}\, dr'\right] \\ U_{(r)} &= \frac{1}{r^3}\int_0^r r'^2 \rho'_{(r')}\, dr' \end{aligned}\right\} \quad \ldots (8)$$

T is the kinetic ener gy of the electron and, $\mu_o = 1.3996241842 \times 10^4$ MH_z/T (Cohen *et al.*, 1986). In the case of equivalent electrons outside closed shells, the correction of the g_J-value is given by

$$\delta g = -\alpha^2 \,[\, g(T+Y) - h(T+U)] \quad \ldots(9)$$

Where (g) is the classical value of Landé-factor and (h) is written by Conway and Wybourne (Conway *et al.*, 1953) as

$$h = \frac{2}{3}\,[(g-1) - \varsigma] \quad \ldots (10)$$

Where(ς) is the correction factor.

They calculated the values of (h) for ($3P_1$, $3P_2$, $1D_2$) states as (1/2, 3/10, 0) respectively. They have done extensive studies of the ground states, and their results show a fair agreement with experimental results.

Because the nucleus has a finite mass, the orbital gyromagnetic ratio deviates from unity. The general theory of the nuclear motion on the orbital, g_J-factors has been developed by Phillips (Phillips, 1949). It should be noted that this effect decreases rapidly with increasing nuclear mass, and can be neglected for heavier elements.

Many investigations of relativistic and diamagnetic effect of g_J-factors has been done in several elements. In the alkalines, which have been studied by Veseth (Veseth, 1980, 1987) using many body perturbation theory, he has also made investigation of the halogenides and the second row elements. An analysis of energy-levels in $6P^2$ configuration performed by Gil and Heldt (Gil *et al.,* 1983) including configuration interaction effects, which can serve as an estimate of the configuration mixing. The g_j-factors (Yan, 2002), are calculated for $2p^2$ and $3p^2$ states of lithium and lithiumlike ions including relativistic correction of order α^2. A recent experimenta determination (Verdu *et al.,* 2004 ;Vogel *et al.,* 2005) has been done by means of a penning trap in which a spin flip is directly excited, reached an accuracy of 10^{-9}. The g_{j-} factor of the bound electron in the hydrogenlike ion has been found to be within the predicated theoretical value (Yerokhin *et al.*, 2002). The second order corrections to the Breit-Rabi formula are calculated (Briet *et al.*, 1931) and the results can be used for a precise determination of nuclear magnetic moments from g_{j-} factor experiment. It is desirable to calculate the g_j-factors (Moskovkhin et al, 2006, Castillega *et al.*, 2000 and George *et al.*, 2001) definitively using high-quality wave function. The precisely measured atomic g_j-factors are of special interest, allowing a sensitive test for calculation of corrected wave function. Shabaev et al (Shabaev *et al.*, 2006) proposed that the measurement of a specific difference of g_j-factors in the H-and B- like charge state of some heavy element may lead to a new determination of the fine-structure constant. Very recently, the Zeeman spectral line profiles of magnetic dipole transitions in (Ar) has been measured in the large helical device (Lwamae *et al.*, 2007). The fully relativistic theory of Zeeman splitting of the hyperfine-structure levels in lithiumlike ions and hydrogenlike ions with strong magnetic field of range from (1-10 T) has been investigated (Moskovkhin *et al.*, 2008; 2006). Experiments were performed to investigate the g-factor of hydrogenlike carbon and oxygen (Verdu *et al.*, 2004) which reached an accuracy of about $7x10^{-10}$ using a penning trap with a strong magnetic field (B= 3.8T). Some authors (Quint et al, 2008) present a laser-microwave double-resonance technique for the precise determination of g-factors in heavy, highly charged ions confined in a penning trap. The determination of the Landé g-factor of $3d^2\ D_{5/2}$ has found to be $g_{5/2}$ = 1.0003340 (Chwalla *et al.*, 2009). The expression for nonperturbative Landé g-factor and Bohr magneton obtained (Efrain *et al.*, 2009) possible applications of effect was outlined

In the current-voltage characteristic for Si the two Zeeman splittings are resolved (Jouault *et al*, 2009) which allows to estimate the Landé g-factor for impurity $g = 1.96 \pm 0.16$. Landé g-factor and diamagnetic coefficient γ was measured (Abbarchi *et al.*, 2010), the dependence of g and γ on quantum dot size and shape was discussed.

Results and discussion

The application of atomic magnetic resonance and laser magnetic resonance has led to very precise measurement of atomic g_j-value in most of the metastable states in the IV elements.The experimental g_j-factors differ from the classical Lande' g_j-value due to relativistic and diamagnetic effects, the electrons anomalous spin and departure from pure LS-coupling. If the relativistic and diamagnetic corrections can be calculated accurately and many-body effects can be neglected, it is possible to obtain the breakdown of LS-coupling more accurately from the g_j-values than from an analysis of the energy levels. Since it is not always possible to include all interactions in the energy matrix, the use of g_j-factors to obtain the breakdown of LS-coupling is however limited to a few configurations, were the number of states with the same (J) value is not larger than 2.To obtain the relativistic and diamagnetic correction (eq. 9), the expectation values of the integrals Y and U (eq. 8) and the kinetic energy T were calculated using nonrelativistic self-consistent-field wave function of Hartree-Fock type (Froese, 1977).The results of the calculations are presented in table (1).

Table 1: The radial integrals (in atomic units)

Atom	Z	T	Y	U
C	6	1.00060	0.55147	0.61115
Si	14	0.81236	0.51706	0.72456
Ge	32	1.06354	0.82040	1.40440
Sn	50	1.16076	0.96009	1.74033
Pb	82	1.33620	1.18228	2.23839

The theoretical and experimental g_J-factors is compared as showing in the table (2). The experimental value has been corrected to the new value using μ_0.

The corrections in C are so large, since it seems like the radial integrals are too large compared with the integrals in the other elements. In Si the corrections are too small. If the experimental g_J-factors of the $3P_1$ state in all P^2 elements compared, it seems that the g_J-value in Si is somewhat smaller than expected. Veseth (Veseth, 1987) made the accuracy of the experimental value, since a systematic reduction of the observed magnetic field, made by him-self, gave a result in agreement with his calculations and the experimental results of the P^2 elements.

In Ge and Sn, the agreement is better. We can conclude that in Ge the configuration interactions are negligible, since the theoretical g_J-factors for the J=2 states are within the experimental errors. In Sn there is a significant difference indicating a possibility that the configuration interactions are present.

In the case of Pb, the agreement is rather poor both in $3P_1$ and the J=2 states, if one neglects configuration mixing as presented in table 2.

Table 2: The values of g_J-factors

Atom	**Level**	**Landè value with correction for the anomalous moment of free electron**	**Relativistic and diamagnetic corrections ($x10^{-6}$)**	**Theoretical g_J - value**	**Experimental g_J - value**
C	$3P_1$	1.5011596	– 81.1	1.5010875	1.5011091 (a)
	$3P_2$	1.5011596	– 98.3	1.501061	1.5010961 (a)
	$1D_2$	1.0	– 82.7	0.9999173	
Si	$3P_1$	1.5011596	– 65.3	1.5010943	1.5008307 (b)
	$3P_2$	1.5011596	– 81.7	1.5010779	
	$1D_2$	1.0	– 70.8	0.9999291	
Ge	$3P_1$	1.5011596	– 84.8	1.5010748	1.5011780 (c)
	$3P_2$	1.5011596	– 111.1	1.5010485	1.4946410 (c)
	$1D_2$	1.0	–100.4	0.9998996	1.0064390 (c)
Sn	$3P_1$	1.5011596	– 92.2	1.5010674	1.5011240 (d)
	$3P_2$	1.5011596	– 123.1	1.5010365	1.4487560 (d)
	$1D_2$	1.0	– 113.0	0.9998870	1.0523340 (d)
Pb	$3P_1$	1.5011596	– 106.0	1.5010536	1.5007552 (e)
	$3P_2$	1.5011596	– 144.1	1.5010155	1.2751778 (e)
	$1D_2$	1.0	– 134.2	0.9998658	1.2263100 (e)

a- (Inguscio et al, 1984), b- (Wolber et al, 1970), c- (Childs et al, 1964), d- (Childs, 1971), e- (Lurio et al, 1970).

Conclusion

The determination of relativistic and diamagnetic correction of g_J-factors can be used to find the configuration interaction of the elements. These calculations are so simple, but can be improved by including many-body effects. There are still needs for accurate measurements of the g_J-factors in state of the P^2 elements and also for improved theoretical calculations in order to study the configuration interaction and other effects.

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دراسة بعض العناصر في ترتيب الالكتروني np^2 باستخدام ظاهرة Zeeman

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الخلاصة

تم حساب التصحيح النسبي و الدايامغنطيسي (الأنفاذية المغنطيسية) لعامل g_j وذلك لإيجاد وسيلة للتفاعل الترتيبي في مجموعة العناصر 3P. نجد من المقارنة بين النتائج النظرية و العملية لعامل g_j للتشكيلة الأساسية عدم وجود دليل قاطع للتفاعل الترتيبي للعناصر Ge, Si, C, أما في حالة Sn فهناك إشارة لوجود التفاعل الترتيبي, حيث في حالة Pb نجد أن التفاعل الترتيبي ظاهر بشكل واضح.