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$_f$-factors have been performed in order to find evidence of configuration interaction in 3P-configuration elements. The comparison between the experimental and calculated g$_f$-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 ($\mu$) of the atom, and we can obtain the magnetic moment of the spin angular moment ($\mu_s$) as:

$$\mu_s = - g_e \cdot \mu_B \cdot S$$  

Where ($\mu_B$) 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 ($\mu_L$) due to the orbital angular momenta ($L$):

$$\mu_L = - \mu_B \cdot L$$  

The total magnetic moment of the atom is then:

$$\mu = \mu_L + \mu_s = - \mu_B (L + g_e \cdot S)$$

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

$$H_Z = - \mu_B \cdot B \cdot (L + g_e \cdot S)$$

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:

$$E_Z = \mu_B \cdot B \cdot g_J \cdot M_J$$

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

$$g_J = 1 + (g_e - 1)$$

$$f \left( J+1 \right) - (L+1) + S(S+1)$$

$$2f(J+1)$$

$$\ldots \ (6)$$
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 $\delta z_1$ and $\delta z_2$. Judd and Lindgren (Judd et al, 1961) has been shown that the total relativistic and diamagnetic correction operator can be written as

$$\delta z = \delta z_1 + \delta z_2 = -\alpha^2 \mu_0 \cdot H \cdot \sum \{(1+2s)(T+Y) - [s- (s.r).r/r^2] (T + U) \} \ldots (7)$$

Where

$$Y(r) = \frac{1}{3} \left[ \frac{1}{r^2} \int_0^r r'^2 \rho'(r') \, dr' + \int_0^\infty \frac{p(r)}{r} \, dr \right]$$

$$U(r) = \frac{1}{r} \int_0^r r'^2 \rho'(r') \, dr$$

$T$ is the kinetic energy of the electron and $\mu_0 = 1.3996241842 \times 10^4 \text{MH}_z/T$ (Cohen et al., 1986). In the case of equivalent electrons outside closed shells, the correction of the $g_J$-value is given by

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

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

$$h = \frac{2}{3} \left[ (g - 1) - \xi \right] \ldots (10)$$

Where $\xi$ 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 ± 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 Landé \( g_J \)-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)

<table>
<thead>
<tr>
<th>Atom</th>
<th>( Z )</th>
<th>( T )</th>
<th>( Y )</th>
<th>( U )</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>6</td>
<td>1.00060</td>
<td>0.55147</td>
<td>0.61115</td>
</tr>
<tr>
<td>Si</td>
<td>14</td>
<td>0.81236</td>
<td>0.51706</td>
<td>0.72456</td>
</tr>
<tr>
<td>Ge</td>
<td>32</td>
<td>1.06354</td>
<td>0.82040</td>
<td>1.40440</td>
</tr>
<tr>
<td>Sn</td>
<td>50</td>
<td>1.16076</td>
<td>0.96009</td>
<td>1.74033</td>
</tr>
<tr>
<td>Pb</td>
<td>82</td>
<td>1.33620</td>
<td>1.18228</td>
<td>2.23839</td>
</tr>
</tbody>
</table>

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 \( \mu_0 \).

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**

<table>
<thead>
<tr>
<th>Atom</th>
<th>Level</th>
<th>Landè value with correction for the anomalous moment of free electron</th>
<th>Relativistic and diamagnetic corrections ($x10^{-6}$)</th>
<th>Theoretical $g_J$ - value</th>
<th>Experimental $g_J$ - value</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>$3P_1$</td>
<td>1.5011596</td>
<td>1.5011596</td>
<td>1.5010785</td>
<td>1.501091 (a)</td>
</tr>
<tr>
<td></td>
<td>$3P_2$</td>
<td>1.5011596</td>
<td></td>
<td>1.501061</td>
<td>1.501061 (a)</td>
</tr>
<tr>
<td></td>
<td>$1D_2$</td>
<td>1.0</td>
<td></td>
<td>0.9999173</td>
<td></td>
</tr>
<tr>
<td>Si</td>
<td>$3P_1$</td>
<td>1.5011596</td>
<td>1.5011596</td>
<td>1.5010943</td>
<td>1.5008307 (b)</td>
</tr>
<tr>
<td></td>
<td>$3P_2$</td>
<td>1.5011596</td>
<td></td>
<td>1.5010779</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$1D_2$</td>
<td>1.0</td>
<td></td>
<td>0.9999291</td>
<td></td>
</tr>
<tr>
<td>Ge</td>
<td>$3P_1$</td>
<td>1.5011596</td>
<td>1.5011596</td>
<td>1.5010748</td>
<td>1.5011780 (c)</td>
</tr>
<tr>
<td></td>
<td>$3P_2$</td>
<td>1.5011596</td>
<td></td>
<td>1.5010485</td>
<td>1.4946410 (c)</td>
</tr>
<tr>
<td></td>
<td>$1D_2$</td>
<td>1.0</td>
<td></td>
<td>0.9998996</td>
<td>1.0064390 (c)</td>
</tr>
<tr>
<td>Sn</td>
<td>$3P_1$</td>
<td>1.5011596</td>
<td>1.5011596</td>
<td>1.5010674</td>
<td>1.5011240 (d)</td>
</tr>
<tr>
<td></td>
<td>$3P_2$</td>
<td>1.5011596</td>
<td></td>
<td>1.5010365</td>
<td>1.4487560 (d)</td>
</tr>
<tr>
<td></td>
<td>$1D_2$</td>
<td>1.0</td>
<td></td>
<td>0.9998870</td>
<td>1.0523340 (d)</td>
</tr>
<tr>
<td>Pb</td>
<td>$3P_1$</td>
<td>1.5011596</td>
<td>1.5011596</td>
<td>1.5010536</td>
<td>1.5007552 (e)</td>
</tr>
<tr>
<td></td>
<td>$3P_2$</td>
<td>1.5011596</td>
<td></td>
<td>1.5010155</td>
<td>1.2751778 (e)</td>
</tr>
<tr>
<td></td>
<td>$1D_2$</td>
<td>1.0</td>
<td></td>
<td>0.9998658</td>
<td>1.2263100 (e)</td>
</tr>
</tbody>
</table>

- (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.
References


Yan, Z-C., (2002): Relativistic corrections to the Zeeman effect of lithium and lithium-like ions in the \( 22\text{P}_{J} \) and \( 32\text{P}_{J} \) states, Physical Review A66, pp.022502-5.

دراسة بعض العناصر في ترتيب الألكتروني $np^2$ باستخدام ظاهرة Zeeman

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الخلاصة

تم حساب التصحيح النسبي و الدايامغناطيسي (الأنفاذية المغناطيسية) لعامل $g$ وذلك لإيجاد وسيلة للتفاعل الترتبي في مجموعة العناصر 3P. نجد من المقارنة بين النتائج النظرية و العملية لعامل $g$ للتشكيلية الأساسية غير هناك إشارة لوجود التفاعل للعناصر Ge, Si, C، أما في حالة Sn، نجد أن التفاعل الترتبي ظاهر بشكل واضح.

في حالة Pb، حيث أن التفاعل الترتبي ظاهر بشكل واضح.