Magnetization of diamagnetic atom or molecule in electric field. Notes for the paper "Atomic CP-violating polarizability" by Boris Ravaine, Andrei Derevianko and Mikhail Kozlov

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These are brief notes on the subject. We show that effect disappears in the non-relativistic approximation and, therefore, is suppressed by extra factor $(\alpha Z)^2$. That leads to an overall scaling Z^5R, where R is relativistic enhancement factor for the electron EDM interaction. Similar scaling takes place for the P,T-odd weak neutral currents and there is simple connection between two effects.

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I. CLOSED SHELL ATOM

A. Formalism

It seems obvious that the electric dipole moment (EDM) of the electron d_e should cause magnetization of the atom in the electric field. This effect is similar to the magnetization in the magnetic field. In both cases the external field interacts with electron spins and causes spin polarization of atomic closed shells.

Spin polarization of a closed shell appears in the second order of the many-body perturbation theory (MBPT) in the interaction

$$V_E = -\boldsymbol{D}\cdot\boldsymbol{E} \tag{1}$$

of the atom with the external electric field $\boldsymbol{E}$ and in the interaction of the EDM of the electron with the internal electric field $-\boldsymbol{\nabla}\phi$:

$$H_d = -2d_e \begin{pmatrix} 0 & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} \boldsymbol{\nabla}\phi. \tag{2}$$

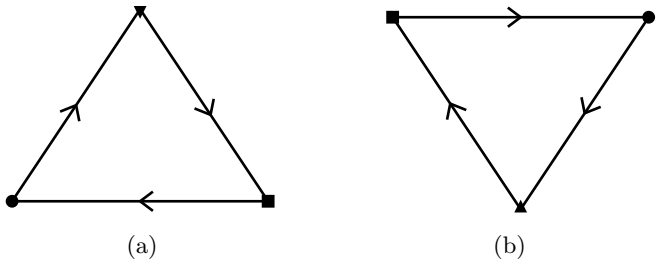
The second order wave function can then be used to calculate expectation value of the magnetic dipole moment

$$\boldsymbol{\mu} = \mu_0(2\boldsymbol{s} + \boldsymbol{l}) \tag{3}$$

of the electrons of the atom. Fig. 1 shows corresponding MBPT diagrams.

Diagram Fig. 1(a) and Fig. 1(b) account for the electron and hole contributions to the spin polarization respectively. Each of these diagrams has mirror partner with circle (H_d) and square (V_E) vertices interchanged. This leads to an extra factor 2 in the expressions below.

Operator (3) is diagonal in the principle quantum number n and orbital quantum number l (but can mix orbitals with different j). Therefore, it can not mix different shells and in the diagrams it can only be placed between operators V_E and H_d. Operator (2) is a scalar and, thus, is diagonal in j. Moreover, its matrix elements decrease very rapidly with j and to a good approximation one can leave only matrix elements between orbitals $s_{1/2}$ and $p_{1/2}$. In this approximation all sums over intermediate states in Fig. 1 run over the orbitals $s_{1/2}$, $p_{1/2}$, and $p_{3/2}$.



(a) (b)

FIG. 1: Diagrams for the induced magnetic moment of the closed shell atom in the electric field $\boldsymbol{E}$. The vertices given by the circle, square, and triangle designate the operators H_d, V_E, and $\boldsymbol{\mu}$ correspondingly. The lines with the arrows directed to the right correspond to the electrons in the excited states. The lines with the arrows directed to the left correspond to the holes in the closed shells.

Now we can write expressions, which correspond to the diagrams Fig. 1:

$$\begin{aligned}\boldsymbol{\mu}\,(\text{Fig. 1(a)}) = &\frac{\langle p_{1/2}|V_E|s'_{1/2}\rangle\langle s'_{1/2}|\boldsymbol{\mu}|s'_{1/2}\rangle\langle s'_{1/2}|H_d|p_{1/2}\rangle}{(\varepsilon_{p_{1/2}}-\varepsilon_{s'_{1/2}})^2}\\ &+\frac{\langle s_{1/2}|V_E|p'_j\rangle\langle p'_j|\boldsymbol{\mu}|p'_{1/2}\rangle\langle p'_{1/2}|H_d|s_{1/2}\rangle}{(\varepsilon_{s_{1/2}}-\varepsilon_{p'_{1/2}})(\varepsilon_{s_{1/2}}-\varepsilon_{p'_j})},\end{aligned} \tag{4a}$$

$$\begin{aligned}\boldsymbol{\mu}\,(\text{Fig. 1(b)}) = &-\frac{\langle p_j|V_E|s'_{1/2}\rangle\langle s'_{1/2}|H_d|p_{1/2}\rangle\langle p_{1/2}|\boldsymbol{\mu}|p_j\rangle}{(\varepsilon_{p_{1/2}}-\varepsilon_{s'_{1/2}})(\varepsilon_{p_j}-\varepsilon_{s'_{1/2}})}\\ &-\frac{\langle s_j|V_E|p'_{1/2}\rangle\langle p'_{1/2}|H_d|s_{1/2}\rangle\langle s_{1/2}|\boldsymbol{\mu}|s_{1/2}\rangle}{(\varepsilon_{s_{1/2}}-\varepsilon_{p'_{1/2}})^2}.\end{aligned} \tag{4b}$$

Note that the signs in (4) are given by the usual MBPT rule: sign $= (-1)^{N_{\rm holes}+N_{\rm loops}}$. We skip the sums in (4) for brevity and use the convention that primed orbitals

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correspond to the excited (electron) states and unprimed orbitals correspond to the occupied (hole) states.

Now we direct quantization axis along electric field: $\boldsymbol{E} = E\hat{\boldsymbol{z}}$ and evaluate matrix elements in (4). Obviously, only z-component of the vector $\boldsymbol{mu}$ will contribute to (4), corresponding matrix elements being:

$$\langle s_{1/2},\omega|\boldsymbol{\mu}|s_{1/2},\omega\rangle = 2\omega\mu_0\hat{\boldsymbol{z}}, \tag{5a}$$

$$\langle p_{1/2},\omega|\boldsymbol{\mu}|p_{1/2},\omega\rangle = \frac{2\omega}{3}\mu_0\hat{\boldsymbol{z}}, \tag{5b}$$

$$\langle p_{3/2},\omega|\boldsymbol{\mu}|p_{3/2},\omega\rangle = \frac{4\omega}{3}\mu_0\hat{\boldsymbol{z}}, \tag{5c}$$

$$\langle p_{1/2},\omega|\boldsymbol{\mu}|p_{3/2},\omega\rangle = -\frac{\sqrt{2}}{3}\mu_0\hat{\boldsymbol{z}}. \tag{5d}$$

Matrix elements of the dipole operator $\boldsymbol{D} = -e\boldsymbol{r}$ in atomic units can be reduced to the radial integrals $R_{s,p} = \int(P_sP_p+Q_sQ_p)rdr$: (the overall sign has to be checked!)

$$\langle s_{1/2},\omega|\boldsymbol{D}|p_{1/2},\omega\rangle = -\frac{2\omega}{3}R_{s,p_{1/2}}\hat{\boldsymbol{z}}, \tag{6a}$$

$$\langle s_{1/2},\omega|\boldsymbol{D}|p_{3/2},\omega\rangle = \frac{\sqrt{2}}{3}R_{s,p_{3/2}}\hat{\boldsymbol{z}}. \tag{6b}$$

Finally, we use the following shorthand notation for the matrix element of the operator (2):

$$\langle s_{1/2}|H_d|p_{1/2}\rangle \equiv h_d^{sp}. \tag{7}$$

Substitution of Equations (5) — (7) into (4) gives the following expression for the induced magnetic moment of the atom in the electric field:

$$\begin{aligned}\boldsymbol{\mu}_{\rm ind} &= \boldsymbol{\mu}\,(\text{Fig. 1(a)}) + \boldsymbol{\mu}\,(\text{Fig. 1(b)})\\ &= \frac{4}{9}\mu_0 E\hat{\boldsymbol{z}}\left\{\frac{h_d^{s'p}}{\varepsilon_{p_{1/2}}-\varepsilon_{s'_{1/2}}}\left(\frac{R_{p_{1/2}s'}}{\varepsilon_{p_{1/2}}-\varepsilon_{s'_{1/2}}}-\frac{R_{p_{3/2}s'}}{\varepsilon_{p_{3/2}}-\varepsilon_{s'_{1/2}}}\right)\right.\\ &\left.-\frac{h_d^{p's}}{\varepsilon_{s_{1/2}}-\varepsilon_{p'_{1/2}}}\left(\frac{R_{s,p'_{1/2}}}{\varepsilon_{s_{1/2}}-\varepsilon_{p'_{1/2}}}-\frac{R_{s,p'_{3/2}}}{\varepsilon_{s_{1/2}}-\varepsilon_{p'_{3/2}}}\right)\right\}.\end{aligned} \tag{8}$$

In Eq. (8) we assume again that there are sums over core and excited (primed) orbitals.

B. Scaling with Z and order of magnitude estimates

Eq. (8) can be used for numerical calculations and for the order of magnitude estimates. It follows from the structure of expression (8) that there are significant cancellations. Indeed, in the non-relativistic approximation the terms in each parentheses exactly cancel each other. This cancellation can be understood in a following way. Diagram Fig. 1(a) and (b) describe contributions to the magnetization from the virtual electron and the hole respectively. It is natural that these two contributions have opposite signs. Because electron EDM is coupled to the electron spin, in the non-relativistic approximation magnetization is caused by the spin-polarization only. That means that g-factors for both contributions are equal to 2 and there is complete cancellation. When relativistic corrections are taken into account, the spin couples to the orbital angular momentum, which leads to non-zero orbital polarization. Because of that g-factors for the excited electron and for the hole become different and no complete cancellation takes place.

Relativistic corrections to the dipole radial integrals and to the energies are of the order of $(\alpha Z)^2$. Matrix elements (7) scale as $\alpha^2Z^3R_d$, where R_d is relativistic enhancement factor,

$$R_d = \frac{3}{\gamma(4\gamma^2-1)} = \begin{cases}1, & Z=1,\\ 1.4, & Z=55,\\ 2.3, & Z=80,\end{cases} \tag{9}$$

where $\gamma = \sqrt{1-(\alpha Z)^2}$. An analytical expression for (7), which is accurate to 20% can be found in [1]:

$$h_d^{sp} = \frac{16}{3}\frac{\alpha^2Z^3R_d}{(\nu_s\nu_p)^{3/2}}d_e, \tag{10}$$

where R_d is given by (9) and the effective quantum number $\nu = (-2\varepsilon)^{-1/2}$.

To estimate relativistic suppression in (8) we neglect the difference in radial integrals $R_{s,p_{1/2}}$ and $R_{s,p_{3/2}}$ and use the following expression for the fine splitting [2]:

$$\varepsilon_{p_{3/2}} - \varepsilon_{p_{1/2}} = \frac{(\alpha Z)^2}{4\nu_p^3}. \tag{11}$$

Substituting (10) and (11) into (8) we get the following approximate expression for the induced magnetic moment:

$$\frac{\mu_{\rm ind}}{\mu_0 E} = \frac{16}{27}\alpha^4Z^5R\left(\frac{R_{p,s'}}{\nu_{s'}\nu_p^4(\varepsilon_p-\varepsilon_{s'})}-\frac{R_{s,p'}}{\nu_s\nu_{p'}^4(\varepsilon_s-\varepsilon_{p'})}\right). \tag{12}$$

This equation can be used for the semiempirical estimates of the effect. To a first approximation we can say that everything in the parentheses is of the order of one atomic unit. A better approximation should include experimental energies and effective quantum numbers and some estimate of the radial integrals. The dominant contribution should be from the last occupied and the first vacant shells.

Eq. (12) shows that even after we take into account cancellations in the non-relativistic limit, there are still two similar terms with opposite signs. To a first approximation $\nu_{s'} \approx \nu_{p'} \gg \nu_s \approx \nu_p$. Also, for a noble gas atom $(\varepsilon_p - \varepsilon_{s'}) < (\varepsilon_s - \varepsilon_{p'})$ (the shells go in a following order: s, p, s', p'). Because of that we can expect that the first term in the parentheses in (12) should be significantly larger then the second and there is no cancellation.

C. P,T-odd weak neutral currents

Recently there was a renewed interest to the P,T-odd weak neutral current interactions of electrons with nucleons [3]. It is known that in atomic experiments EDM of the electron is indistinguishable from the scalar P,T-odd weak neutral currents [1]:

$$H_{P,T} = \mathrm{i}\frac{G_\mathrm{F}}{\sqrt{2}}(Zk_1^p + Nk_1^n)\gamma_0\gamma_5\rho(\boldsymbol{r}), \tag{13}$$

where $G_\mathrm{F} = 2.2225 \times 10^{-14}$ a.u. is the Fermi constant, $k_1^{p,n}$ are dimensionless constants of the scalar P,T-odd weak neutral currents for proton and neutron, Z, N are the numbers of protons and neutrons in the nucleus, $\gamma_{0,5}$ are Dirac matrices and $\rho(\boldsymbol{r}) \approx \Theta(r_\mathrm{N} - r)$ is the nuclear density, r_N being nuclear radius.

Operator (13) mixes only levels $s_{1/2}$ with $p_{1/2}$, corresponding matrix elements being:

$$\langle s_{1/2}|H_{P,T}|p_{1/2}\rangle \equiv h^{sp}_{P,T} = \frac{G_\mathrm{F}}{2\sqrt{2}\pi}\frac{\alpha Z^2 R_1}{(\nu_s\nu_p)^{3/2}}(Zk_1^p + Nk_1^n), \tag{14}$$

where R_1 is relativistic enhancement factor, similar to (9) [1]:

$$R_1 = \frac{4\gamma(2Zr_\mathrm{N})^{2\gamma-2}}{\Gamma^2(2\gamma+1)} = \begin{cases} 1, & Z = 1, \\ 2.6, & Z = 55, \\ 6.6, & Z = 80, \end{cases} \tag{15}$$

where we use the following approximation: $r_\mathrm{N} = 1.2(Z + N)^{1/3}$ Fm.

Because of the similarity between operators H_d and $H_{P,T}$, there is no need in calculating μ_ind for P,T-odd weak neutral currents. It is sufficient to substitute h_d^{sp} in (8) with $h_{P,T}^{sp}$. Comparing (10) with (14) we find that to get μ_ind induced by the P,T-odd weak neutral currents we need to make following substitution:

$$\frac{d_e}{er_0} \Longleftrightarrow 1.3 \times 10^{-13}\frac{R_1}{R_d}(k_1^p + \frac{N}{Z}k_1^n), \tag{16}$$

where r_0 is Borh radius and R_d and R_1 are given by (9) and (15).

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