Nuclear mass correction to the magnetic interaction of atomic systems

Krzysztof Pachucki*

Institute of Theoretical Physics, University of Warsaw, Hoża 69, 00-681 Warsaw, Poland

(Dated: June 11, 2008)

Abstract

The electromagnetic interaction of the atom or ion having an arbitrary spin nucleus is considered. The effective atomic interaction Hamiltonian is derived by a sequence of unitary transformations to separate out the total motion from the internal degrees of freedom. The obtained finite nuclear mass corrections modify the atomic energy levels in the magnetic field. We present resulting contributions to the electron g-factor, the NMR shielding factor and the magnetic susceptibility.

PACS numbers: 31.30.J-, 31.30.js, 32.10.Dk, 31.30.Gs

*krp@fuw.edu.pl; www.fuw.edu.pl/~krp

I. INTRODUCTION

We consider light atomic systems in the homogenous magnetic field including relativistic and finite nuclear mass corrections. While the electromagnetic interactions of electrons is well known, the interaction Hamiltonian of nuclei having an arbitrary spin is not well established. Khriplovich and Pomeransky in Ref. [1] introduced a general form of the interaction of an arbitrary spin with the electromagnetic field and performed noncovariant quasi classical expansion. On the basis of this work, we construct here a general electromagnetic interaction Hamiltonian for an arbitrary spin particle, which is used next to derive magnetic interaction of the atomic system including relativistic corrections. Since the total momentum is not conserved due to the presence of the magnetic field, we perform unitary transformations to separate the internal Hamiltonian of the atomic system from its global motion. With this internal Hamiltonian we obtain several results for finite nuclear mass corrections. Namely, we demonstrate that former result of Hegstrom [2] for relativistic recoil corrections to the atomic g-factor is valid for an arbitrary nuclear spin and to all orders in the electron-nucleus mass ratio. Moreover, we resolve discrepancies for the electron g-factor in hydrogenic ions [3] and obtain results for the NMR shielding factor and the magnetic susceptibility.

II. ELECTROMAGNETIC INTERACTION OF NUCLEI

In the derivation of magnetic interaction of atomic systems, we shall consider at first the effective interaction Hamiltonian of an nucleus with the electromagnetic field. Since there is no general relativistic Hamiltonian for an arbitrary spin particle we assume nonrelativistic expansion including all possible coupling constants, which dimension does not exceed $1/m^3$, where m is the nuclear mass. We find, that the most general effective Hamiltonian is of the form

$$
\begin{aligned}
H_{\rm eff} \;=\; & \frac{\vec\pi^2}{2\,m} + e\,A^0 - \frac{\vec\pi^4}{8\,m^3} \\
& -\frac{e}{2\,m}\,g\,\vec s\cdot\vec B - \frac{e}{4\,m^2}\,(g-1)\,\vec s\cdot(\vec E\times\vec\pi - \vec\pi\times\vec E) \\
& +\frac{e}{8\,m^3}\Big[\{\pi^i\,,\,\{\pi^i\,,\,\vec s\cdot\vec B\}\} + (g-2)\,\{\vec\pi\cdot\vec B\,,\,\vec\pi\cdot\vec s\}\Big] \\
& -\frac{e}{6}\,(s^i\,s^j)^{(2)}\,Q_E\,\Big[E^i_{,j} + \frac{1}{2\,m}\,\{\pi^k\,,\,\delta^{ik}\,\partial_t E^j + \epsilon^{ikl}B^l_{,j}\}\Big] \\
& -\frac{e}{30}\,Q_M\,(s^i\,s^j\,s^k)^{(3)}\,B^i_{,jk}
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{e\,g}{8\,m^3}\Big[(s^i\,s^j)^{(2)}+\frac{1}{3}\,\delta^{ij}\,\vec{s}^{\,2}\Big]\,\epsilon^{ikl}\,\{\pi^k\,,\,B^j_{,l}\}\\
&-\frac{e}{6}\,\langle r_E^2\rangle\,\Big[\vec{\nabla}\cdot\vec{E}+\frac{1}{2\,m}\,\{\vec{\pi}\,,\,\partial_t\vec{E}-\vec{\nabla}\times\vec{B}\}\Big]\\
&+\frac{e}{12\,m}\,\langle r_M^2\rangle\,g\,\vec{s}\cdot(\partial_t^2\vec{B}-\vec{\nabla}^2\vec{B})\\
&-\frac{e^2}{2}\,E^i\,E^j\,[\alpha_E\,\delta^{ij}+\gamma_E\,(s^i\,s^j)^{(2)}]\\
&-\frac{e^2}{2}\,B^i\,B^j\,[\alpha_M\,\delta^{ij}+\gamma_M\,(s^i\,s^j)^{(2)}]+O(1/m^4)
\end{aligned}
\tag{1}
$$

where $\{X\,,\,Y\}\equiv X\,Y+Y\,X$, $\vec{\pi}=\vec{p}-e\,\vec{A}$, e is the charge of the considered particle, g is the gyromagnetic factor [4], Q_E and Q_M electric quadrupole and magnetic octupole constants respectively, $\langle r_E^2\rangle$ and $\langle r_M^2\rangle$ charge and magnetic radii respectively, α_E, γ_E, α_M, γ_M electric (magnetic) scalar and tensor polarizabilities. There are no further constants involved, as the requirements of Lorentz symmetry fixes the form of interaction of the spin to the electromagnetic field. In particular all terms which are linear in spin can be obtained from the Bargman-Michel-Telegdi (BMT) equation, and such derivation was presented in Ref. [1]. The terms quadratic in spin were obtained following Ref. [1], from the general form of the relativistic interaction using the nonrelativistic expansion. The irreducible second $(s^i\,s^j)^{(2)}$ and third order $(s^i\,s^j\,s^k)^{(3)}$ tensors in Eq. (1) are, by definition, symmetric with respect to all indeces and traceless, for example

$$
(s^i\,s^j)^{(2)}=\frac{s^i\,s^j+s^j\,s^i}{2}-\frac{\delta^{ij}}{3}\,s^k\,s^k\,. \tag{2}
$$

The Hamiltonian of Eq. (1) can be regarded as the definition of the nuclear charge radius and nuclear polarizabilities. In fact, there are several different definitions of nuclear charge radii in the literature [5], depending on the nuclear spin and there is no a uniquely accepted one. Moreover, there is no precise definition of the electric polarizability for nuclei, because α_E depends on the form of the other interaction terms in the Hamiltonian, namely one can use unitary transformation to eliminate $\vec{\pi}\cdot\partial_t\vec{E}$ at the expense of appearance of an additional $\vec{E}^2$ term. We will justify below the Hamiltonian of Eq. (1) by considering two examples of the scalar and the minimally coupled $s=1/2$ particle. For the scalar point particle $s=0$ the effective Hamiltonian is unique and reads

$$
H=e\,A^0+\frac{\vec{\pi}^{\,2}}{2\,m}-\frac{\vec{\pi}^{\,4}}{8\,m^3} \tag{3}
$$

Inclusion of the finite size corresponds to the replacement $A^\mu \to \tilde{A}^\mu$, where

$$\tilde{A}^\mu(q) = \rho(q)\, A^\mu(q) \approx \left(1 + \frac{\langle r_E^2\rangle}{6}\, q^2\right) A^\mu(q) = A^\mu + \frac{\langle r_E^2\rangle}{6}\left(\vec{\nabla}^2 - \frac{\partial^2}{\partial t^2}\right) A^\mu \tag{4}$$

The Hamiltonian $\tilde{H}$ including the finite size is therefore

$$\begin{aligned} \tilde{H} &= H + e\,(\tilde{A}^0 - A^0) - \frac{e}{2\,m}\,\{\pi^i\,,\,\tilde{A}^i - A^i\} \\ &= H - \frac{e\,\langle r_E^2\rangle}{6}\,\vec{\nabla}\cdot\vec{E} - \frac{e\,\langle r_E^2\rangle}{6}\left[\vec{\nabla}\cdot\frac{\partial\vec{A}}{\partial t} + \frac{\partial^2 A^0}{\partial t^2} - \frac{1}{2\,m}\left\{\pi^i, \left(\vec{\nabla}^2 - \frac{\partial^2}{\partial t^2}\right) A^i\right\}\right] \end{aligned} \tag{5}$$

In order to simplify $\tilde{H}$, one performs the unitary transformation

$$H \to e^{-i\,\phi}\,H\,e^{i\,\phi} + \partial_t\phi \tag{6}$$

with

$$\phi = \frac{e\,\langle r_E^2\rangle}{6}\,(\vec{\nabla}\cdot\vec{A} + \partial_t\,A^0) \tag{7}$$

and obtains

$$\tilde{H} = H - \frac{e}{6}\,\langle r_E^2\rangle\left(\vec{\nabla}\cdot\vec{E} + \frac{1}{2\,m}\,\{\vec{\pi}\,,\,\partial_t\vec{E} - \vec{\nabla}\times\vec{B}\}\right) \tag{8}$$

what exactly corresponds to $\langle r_E^2\rangle$ contribution in Eq. (1). The next example is the minimally coupled $s = 1/2$ particle, for which Hamiltonian is

$$H = \vec{\alpha}\cdot\vec{\pi} + \beta\,m + e\,A^0 \tag{9}$$

The Foldy-Wouthuysen transformation S [6] leads to a new Hamiltonian

$$\tilde{H} = e^{i\,S}\,(H - i\,\partial_t)\,e^{-i\,S}\,, \tag{10}$$

which does not couple upper and lower components of the Dirac wave function up to a specified order in $1/m$, which is here $1/m^3$. The Hamiltonian $\tilde{H}$ is expanded in a power series in S

$$\tilde{H} = H + [i\,S\,;\,H - i\,\partial_t] + \frac{1}{2!}\,[i\,S\,;\,[i\,S\,;\,H - i\,\partial_t]] + \frac{1}{3!}\,[i\,S\,;\,[i\,S\,;\,[i\,S\,;\,H - i\,\partial_t]]] + \ldots \tag{11}$$

As a result of these multiple commutations with adequately chosen S one obtains a nonrelativistic expansion of the Dirac Hamiltonian H [7]

$$\tilde{H} = e\,A^0 + \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{2\,m} - \frac{(\vec{\sigma}\cdot\vec{\pi})^4}{8\,m^3} - \frac{i\,e}{8\,m^2}\,[\vec{\sigma}\cdot\vec{\pi}, \vec{\sigma}\cdot\vec{E}] - \frac{e}{16\,m^3}\left\{\vec{\sigma}\cdot\vec{\pi}\,,\,\vec{\sigma}\cdot\partial_t\vec{E}\right\} + O(1/m^4), \tag{12}$$

One notes that $\tilde{H}$ is not unique. Different S may lead to a different Hamiltonian but equivalent up to some transformation ϕ. Hamiltonian $\tilde{H}$ can be further simplified using

$$(\vec{\sigma}\cdot\vec{\pi})^2 = \vec{\pi}^{\,2} - e\,\vec{\sigma}\cdot\vec{B} \tag{13}$$

namely

$$\begin{aligned}\tilde{H} \;=&\; e\,A^0 + \frac{\vec{\pi}^2}{2\,m} - \frac{\vec{\pi}^4}{8\,m^3} - \frac{e}{2\,m}\,\vec{\sigma}\cdot\vec{B} - \frac{e}{8\,m^2}\,\vec{\sigma}\cdot(\vec{E}\times\vec{\pi} - \vec{\pi}\times\vec{E}) + \frac{e}{8\,m^3}\,\{\vec{\pi}^2\,,\,\vec{\sigma}\cdot\vec{B}\}\\ &-\frac{e}{8\,m^2}\Big[\nabla\cdot\vec{E} + \frac{1}{2\,m}\{\vec{\pi}\,,\,\partial_t\vec{E}\}\Big] + \frac{e}{16\,m^3}\,\vec{\sigma}\cdot\partial_t^2\vec{B} - \frac{e^2}{8\,m^3}\,\vec{B}^2 + O(1/m^4),\end{aligned} \tag{14}$$

This Hamiltonian is equal to the one in Eq. (1) when $g = 2$, $\langle r_E^2\rangle = \langle r_M^2\rangle = 3/(4\,m^2)$, $\alpha_M = 1/(4\,m^3)$, $\gamma_M = \alpha_E = \gamma_E = 0$. We observe that even the point charge particle has nonvanishing charge and magnetic radii according to Eq. (1).

III. BREIT-PAULI HAMILTONIAN WITH THE HOMOGENOUS MAGNETIC FIELD

The Hamiltonian in Eq. (1) describes interaction of nucleus and other arbitrary particle as well, with the electromagnetic field. It is used below to obtain the Breit-Pauli Hamiltonian H_{BP} for atomic systems [8] including interaction with the external homogenous magnetic field. Hamiltonian H_{BP} includes a sum of $H_{\rm eff}$ for all electrons and nuclei, static Coulomb interactions, and corrections to the electric as well as magnetic interactions between electrons and nuclei, namely

$$H_{BP} \;=\; \sum_a H_a + \sum_{a>b,b} H_{ab}\,, \tag{15}$$

$$\begin{aligned}H_a \;=&\; \frac{\vec{\pi}_a^2}{2\,m} - \frac{\vec{\pi}_a^4}{8\,m^3} - \frac{e_a}{2\,m_a}\,g_a\,\vec{s}_a\cdot\vec{B}_a - \frac{e_a^2}{2}\,B_a^i\,B_a^j\,[\alpha_a^M\,\delta^{ij} + \gamma_a^M\,(s_a^i\,s_a^j)^{(2)}]\\ &+\frac{e_a}{8\,m_a^3}\Big[4\,\vec{\pi}_a^2\,\vec{s}_a\cdot\vec{B}_a + (g_a-2)\,\{\vec{\pi}_a\cdot\vec{B}_a\,,\,\vec{\pi}_a\cdot\vec{s}_a\}\Big]\,,\end{aligned} \tag{16}$$

$$\begin{aligned}H_{ab} \;=&\; \frac{e_a\,e_b}{4\,\pi}\bigg\{\frac{1}{r_{ab}} - \frac{1}{2\,m_a\,m_b}\,\pi_a^i\left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^3}\right)\pi_b^j - \frac{2\,\pi}{3}\,\langle r_{Ea}^2 + r_{Eb}^2\rangle\,\delta^3(r_{ab})\\ &-\frac{2\,\pi\,g_a\,g_b}{3\,m_a\,m_b}\,\vec{s}_a\cdot\vec{s}_b\,\delta^3(r_{ab}) + \frac{g_a\,g_b}{4\,m_a\,m_b}\,\frac{s_a^i\,s_b^j}{r_{ab}^3}\left(\delta^{ij} - 3\,\frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^2}\right)\\ &+\frac{1}{2\,r_{ab}^3}\Big[\frac{g_a}{m_a\,m_b}\,\vec{s}_a\cdot\vec{r}_{ab}\times\vec{\pi}_b - \frac{g_b}{m_a\,m_b}\,\vec{s}_b\cdot\vec{r}_{ab}\times\vec{\pi}_a + \frac{(g_b-1)}{m_b^2}\,\vec{s}_b\cdot\vec{r}_{ab}\times\vec{\pi}_b\\ &-\frac{(g_a-1)}{m_a^2}\,\vec{s}_a\cdot\vec{r}_{ab}\times\vec{\pi}_a\Big] + \frac{1}{6}\Big[Q_{Ea}\,(s_a^i\,s_a^j)^{(2)} + Q_{Eb}\,(s_b^i\,s_b^j)^{(2)}\Big]\,\frac{(3\,r_{ab}^i\,r_{ab}^j - \delta^{ij}\,r_{ab}^2)}{r_{ab}^5}\bigg\}\,.\end{aligned} \tag{17}$$

This Hamiltonian will be transformed to the form, where the coupling of external degrees of freedom, momentum and spin, is separated out from the internal Hamiltonian to the maximal possible degree. For this, we introduce center of mass variables

$$\vec{R} = \sum_a \frac{m_a}{M}\,\vec{r}_a\,, \tag{18}$$

$$\vec{\Pi} = \sum_a [\vec{p}_a - e_a\,\vec{A}(\vec{R})] \equiv \vec{P} - e\,\vec{A}(\vec{R})\,, \tag{19}$$

and relative coordinates

$$\vec{x}_a = \vec{r}_a - \vec{R}\,, \tag{20}$$

$$\vec{q}_a = \vec{p}_a - \frac{m_a}{M}\,\vec{P}\,, \tag{21}$$

such that

$$[x^i_a\,,\,q^j_b] = i\,\delta^{ij}\left(\delta_{ab} - \frac{m_b}{M}\right), \tag{22}$$

$$[R^i\,,\,P^j] = i\,\delta^{ij}\,, \tag{23}$$

$$[x^i_a\,,\,P^j] = [R^i\,,\,q^j_a] = 0\,. \tag{24}$$

In Eq. (19) we introduced the total charge of the system $e \equiv \sum_a e_a$. We next perform a sequence of unitary transformations ϕ of Eq. (6), to transform the Hamiltonian to the form where the coupling of internal degrees of freedom to the total momentum is simplified. The first transformation ϕ_1 is the Power-Zienau-Wooley transformation which for an arbitrary electromagnetic field is

$$\begin{aligned}\phi_1 &= \sum_a e_a \int_0^1 du\,\vec{x}_a\cdot\vec{A}(\vec{R}+u\,\vec{x}_a)\\ &= \sum_a e_a\Big[x^i_a\,A^i + \frac{1}{2!}\,x^i_a\,x^j_a\,A^i_{,j} + \frac{1}{3!}\,x^i_a\,x^j_a\,x^k_a\,A^i_{,jk} + \ldots\Big]\,. \end{aligned}\tag{25}$$

where for homogenous magnetic field, only the first two terms do not vanish. The corresponding transformation of the kinetic momentum is

$$e^{-i\,\phi_1}\,\pi^j_a\,e^{i\,\phi_1} = \tilde{\pi}^j_a + \frac{m_a}{M}\,\Pi^j \tag{26}$$

$$\tilde{\pi}_a = q_a + \frac{1}{2}\left(e_a\,\vec{x}_a + \frac{m_a}{M}\,\vec{D}\right)\times\vec{B}, \tag{27}$$

and of the kinetic energy is

$$e^{-i\,\phi_1}\sum_a \pi^2_a\,e^{i\,\phi_1} = \frac{\Pi^2}{2M} + \sum_a \frac{\tilde{\pi}^2_a}{2\,m_a} + \frac{\vec{\Pi}}{M}\cdot\vec{D}\times\vec{B} \tag{28}$$

where $\vec{B} \equiv \vec{B}(\vec{R})$ and $\vec{D} = \sum_a e_a\,\vec{x}_a$. The transformed Hamiltonian is decomposed into nonrelativistic H_0, relativistic H_R and the motional parts H_Π

$$
\begin{aligned}
H' &= H_0 + H_R + H_\Pi && (29)\\
H_0 &= \sum_a \frac{\tilde{\pi}_a^2}{2\,m_a} + \sum_{a>b,b} \frac{e_a\,e_b}{4\,\pi\,r_{ab}} - \sum_a \frac{e_a}{2\,m_a}\,g_a\,\vec{s}_a\cdot\vec{B} + \frac{\vec{\Pi}^2}{2\,M} + \frac{\vec{\Pi}}{M}\cdot\vec{D}\times\vec{B} && (30)\\
H_R &= \sum_a \biggl\{-\frac{\tilde{\pi}_a^4}{8\,m^3} + \frac{e_a}{8\,m_a^3}\left[4\,\vec{\pi}_a^2\,\vec{s}_a\cdot\vec{B}_a + (g_a-2)\,\{\vec{\pi}_a\cdot\vec{B}_a\,,\,\vec{\pi}_a\cdot\vec{s}_a\}\right] && (31)\\
&\quad -\frac{e_a^2}{2}\,B_a^i\,B_a^j\left[\alpha_a^M\,\delta^{ij} + \gamma_a^M\,(s_a^i\,s_a^j)^{(2)}\right]\biggr\}\\
&\quad + \sum_{a>b,b}\frac{e_a\,e_b}{4\,\pi}\biggl\{-\frac{1}{2\,m_a\,m_b}\,\tilde{\pi}_a^i\left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^3}\right)\tilde{\pi}_b^j - \frac{2\,\pi}{3}\,\langle r_{Ea}^2 + r_{Eb}^2\rangle\,\delta^3(r_{ab})\\
&\quad -\frac{2\,\pi\,g_a\,g_b}{3\,m_a\,m_b}\,\vec{s}_a\cdot\vec{s}_b\,\delta^3(r_{ab}) + \frac{g_a\,g_b}{4\,m_a\,m_b}\,\frac{s_a^i\,s_b^j}{r_{ab}^3}\left(\delta^{ij} - 3\,\frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^2}\right)\\
&\quad +\frac{1}{2\,r_{ab}^3}\biggl[\frac{g_a}{m_a\,m_b}\,\vec{s}_a\cdot\vec{r}_{ab}\times\tilde{\pi}_b - \frac{g_b}{m_a\,m_b}\,\vec{s}_b\cdot\vec{r}_{ab}\times\tilde{\pi}_a + \frac{(g_b-1)}{m_b^2}\,\vec{s}_b\cdot\vec{r}_{ab}\times\tilde{\pi}_b\\
&\quad -\frac{(g_a-1)}{m_a^2}\,\vec{s}_a\cdot\vec{r}_{ab}\times\tilde{\pi}_a\biggr] + \frac{1}{6}\Bigl[Q_{Ea}\,(s_a^i\,s_a^j)^{(2)} + Q_{Eb}\,(s_b^i\,s_b^j)^{(2)}\Bigr]\,\frac{(3\,r_{ab}^i\,r_{ab}^j - \delta^{ij}\,r_{ab}^2)}{r_{ab}^5}\biggr\}
\end{aligned}
$$

The initial expression for H_Π is somewhat complicated,

$$
\begin{aligned}
H_\Pi &= -\frac{1}{8\,M^3}\,\Pi^4 - \frac{1}{2\,M^3}\,\Pi^2\,\vec{\Pi}\cdot\vec{D}\times\vec{B} - \frac{\Pi^2}{2\,M^2}\left(\sum_a\frac{\tilde{\pi}^2}{2\,m_a} + \sum_{a>b,b}\frac{e_a\,e_b}{4\,\pi\,r_{ab}}\right)\\
&\quad -\frac{\Pi^i\,\Pi^j}{2\,M^2}\left(\sum_a\frac{\tilde{\pi}_a^i\,\tilde{\pi}_a^j}{m_a} + \sum_{a>b,b}\frac{e_a\,e_b}{4\,\pi}\,\frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^3}\right) - \sum_a\frac{1}{2\,M\,m_a^2}\,\tilde{\pi}_a^2\,\tilde{\pi}_a\cdot\vec{\Pi}\\
&\quad +\sum_a\frac{e_a}{4\,M^2\,m_a}\left[2\,\Pi^2\,\vec{s}_a\cdot\vec{B} + (g_a-2)\,\vec{\Pi}\cdot\vec{B}\,\vec{\Pi}\cdot\vec{s}_a\right]\\
&\quad +\sum_a\frac{e_a}{4\,M\,m_a^2}\left[4\,\tilde{\pi}_a\cdot\vec{\Pi}\,\vec{s}_a\cdot\vec{B} + (g_a-2)\,\vec{\Pi}\cdot\vec{B}\,\tilde{\pi}_a\cdot\vec{s}_a + (g_a-2)\,\vec{\Pi}\cdot\vec{s}_a\,\tilde{\pi}_a\cdot\vec{B}\right]\\
&\quad +\sum_{a>b,b}\frac{e_a\,e_b}{4\,\pi}\left[\frac{1}{2\,M\,m_a\,r_{ab}^3}\,\vec{s}_a\cdot\vec{r}_{ab}\times\vec{\Pi} - \frac{1}{2\,M\,m_b}\,\Pi^i\left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^3}\right)\tilde{\pi}_b^j\right] && (32)
\end{aligned}
$$

In order to simplify H_Π we perform several unitary transformations ϕ similar to that in Ref. [9] such that H_Π becomes

$$
H_\Pi = -\frac{\Pi^4}{8\,M^3} - \frac{\Pi^2}{2\,M^2}\left(\sum_a\frac{\tilde{\pi}^2}{2\,m_a} + \sum_{a>b,b}\frac{e_a\,e_b}{4\,\pi\,r_{ab}}\right) + \frac{e}{2\,M^3}\left[\Pi^2\,\vec{s}\cdot\vec{B} + \frac{(\hat{g}-2)}{2}\,\vec{s}\cdot\vec{\Pi}\,\vec{B}\cdot\vec{\Pi}\right] \quad (33)
$$

where we neglected odd (with respect to the inversion) higher order terms, because their expectation value is of higher order than $O(1/M^3)$. Moreover, we expressed the sum of angular momenta by the $\hat{g}$-operator

$$
\sum_a \frac{e_a}{m_a}\,(\vec{l}_a + g_a\,\vec{s}_a) \equiv \frac{e}{M}\,\hat{g}\,\vec{s} \quad (34)
$$

with $\vec{l}_a = \vec{x}_a \times \vec{q}_a$ and $\vec{s} = \sum_a (\vec{l}_a + \vec{s}_a)$. For states with the definite angular momentum, $\hat{g}$ can be replaced by the g-factor of the total system.

Since components of the total momentum do not commute with each other

$$[\Pi^i\,,\,\Pi^j] = i\,e\,\epsilon^{ijk}\,B^k \tag{35}$$

and couple to internal degrees of freedom, one can not assume that the wave function is a product of atomic internal and the global wave function, as long as the magnetic field does not vanish or the total charge is zero. The presence of the coupling of spin to the total motion, indicates that magnetic interaction depends to some extend on the state of ion in the trap. Therefore, when the precision measurement is performed, the magnitude of the coupling of global motion to the spin should be estimated, including the following spin dependent interaction with the electric field [9]

$$\delta H = \frac{e}{2\,M}\,(\hat{g}-1)\,\vec{s}\cdot\frac{(\vec{\Pi}\times\vec{E}-\vec{E}\times\vec{\Pi})}{2\,M} \tag{36}$$

Therefore the relation between the cyclotron and the Larmor frequencies is not exact, and we expect corrections of the order the ratio of the potential depth to the atomic mass, which can be significant for the g-factor measurement in hydrogen-like carbon [10]. Precise estimate however, requires detailed knowledge about the trapping potential.

IV. MAGNETIC INTERACTIONS OF ATOMIC SYSTEMS

The magnetic interaction resulting from the nonrelativistic Hamiltonian H_0 in Eq. (30) is

$$H_0 \approx -\sum_a \frac{e_a}{2\,m_a}\,(\vec{l}_a + g_a\,\vec{s}_a)\cdot\vec{B} + \sum_a \frac{e_a^2}{8\,m_a}\,(\vec{x}_a\times\vec{B})^2 + \frac{3}{8\,M}\,(\vec{D}\times\vec{B})^2 \tag{37}$$

The last two terms are responsible for the magnetic susceptibility while the first term gives the magnetic moment including finite nuclear mass corrections. If we assume a spinless nucleus, this first term can be rewritten for states with vanishing total momentum, using standard coordinates to the form

$$-\sum_a \frac{e_a}{2\,m_a}\,(\vec{l}_a + g_a\,\vec{s}_a)\cdot\vec{B} = -\frac{e_e}{2\,m_e}\left[\left(1-\frac{m_e}{m_N}\right)\vec{L} + g\,\vec{S}\right] + \frac{e_e}{2\,m_N}\sum_{a\neq b,b}\vec{r}_a\times\vec{p}_b\cdot\vec{B} \tag{38}$$

where $r_a \equiv r_{aN}$, in agreement with the result of Philips in [11]. It so happens that the second term also contributes to the magnetic susceptibility

$$\delta E = \left(\frac{e_e}{2\,m_N}\right)^2 \left\langle \sum_{a\neq b,b} \vec{r}_a \times \vec{p}_b \cdot \vec{B}\, \frac{1}{(E-H)'} \sum_{a\neq b,b} \vec{r}_a \times \vec{p}_b \cdot \vec{B} \right\rangle \tag{39}$$

although the resulting correction is quadratic in the electron-nucleus mass ratio, and therefore is small if not negligible.

Consider now the relativistic interaction with the magnetic field resulting from H_R in Eq. (31), and neglect the terms quadratic in $\vec{B}$.

$$\begin{aligned}
\delta H \;=\; & \sum_a \frac{1}{4\,m_a^3} \Big[q_a^2\, \vec{D}_a \times \vec{q}_a \cdot \vec{B} + 2\, e_a\, q_a^2\, \vec{s}_a \cdot \vec{B} + e_a\,(g_a-2)\, \vec{q}_a \cdot \vec{s}_a\, \vec{q}_a \cdot \vec{B}\Big] \\
& + \sum_{a\neq b,b} \frac{e_a\, e_b}{4\,\pi} \Big[-\frac{1}{4\,m_a\, m_b}\, q_a^i \left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i\, r_{ab}^j}{r_{ab}^3}\right) (\vec{D}_b \times \vec{B})^j \\
& + \frac{1}{4\,r_{ab}^3}\, \frac{g_a}{m_a\, m_b}\, (\vec{s}_a \times \vec{r}_{ab}) \cdot (\vec{D}_b \times \vec{B}) - \frac{1}{4\,r_{ab}^3}\, \frac{(g_a-1)}{m_a^2}\, (\vec{s}_a \times \vec{r}_{ab}) \cdot (\vec{D}_a \times \vec{B})\Big]
\end{aligned} \tag{40}$$

where

$$\vec{D}_a = e_a\, \vec{x}_a + \frac{m_a}{M}\, \vec{D} \tag{41}$$

Eq. (40) agrees with the former result of Hegstrom [2], which was derived with the assumption that nucleus has spin 1/2. Therefore we have shown here, that his result is valid for an arbitrary spin of nuclei.

We will study below in more details two special cases, NMR shielding constant for closed shell atoms and g-factors of hydrogenic ions. For the closed shell atoms, the interaction of the nuclear spin with the magnetic field is obtained from Eq. (40)

$$\begin{aligned}
\delta H \;=\; & -\frac{e_N}{2\,m_N}\, g_N\, \vec{s}_N \cdot \vec{B} + \frac{e_N}{4\,m_N^3} \Big[2\, q_N^2\, \vec{s}_N \cdot \vec{B} + (g_N-2)\, \vec{q}_N \cdot \vec{s}_N\, \vec{q}_N \cdot \vec{B}\Big] \\
& + {\sum_b}' \frac{e_N\, e_b}{4\,\pi}\, \frac{(\vec{s}_N \times \vec{r}_{Nb})}{4\,r_{Nb}^3} \cdot \Big[\frac{g_N}{m_N\, m_b}\, \vec{D}_b \times \vec{B} - \frac{(g_N-1)}{m_N^2}\, \vec{D}_N \times \vec{B}\Big]
\end{aligned} \tag{42}$$

There is also indirect contribution through second order interaction coming from the Hamiltonian

$$\delta H = -\sum_a \frac{e_a}{2\,m_a}\, \vec{l}_a \cdot \vec{B} + {\sum_b}' \frac{e_N\, e_b}{4\,\pi}\, \frac{(\vec{s}_N \times \vec{r}_{Nb})}{2\,m_N\, r_{Nb}^3} \cdot \Big[g_N\, \frac{\vec{q}_b}{m_b} - (g_N-1)\, \frac{\vec{q}_N}{m_N}\Big] \tag{43}$$

The resulting energy shift in the magnetic field can be represented as

$$\delta E = -\frac{e_N}{2\,m_N}\, g_N\, \vec{s}_N \cdot \vec{B}\, (1-\sigma) \tag{44}$$

with the shielding constant σ equal to

$$\sigma = \frac{\alpha}{3\,m_e}\left\langle\sum_a{}' \frac{1}{r_a}\right\rangle + \frac{\langle p_N^2\rangle}{m_N}\left(\frac{2+3\,g_N}{6\,g_N}\,\frac{1}{m_N} - \frac{(g_N-1)}{3\,g_N}\,\frac{1}{Z\,m_e}\right) \\ +\frac{\alpha}{3\,m_N}\left\langle\sum_{a\neq b,b}{}' \vec{r}_a\times\vec{p}_b\,\frac{1}{(E-H)'}\sum_c{}'\frac{\vec{r}_c}{r_c^3}\times\left[\frac{\vec{p}_c}{m_e} - \frac{(g_N-1)}{g_N}\,\frac{\vec{p}_N}{m_N}\right]\right\rangle \tag{45}$$

where $\vec{p}_N = -\sum'_a \vec{p}_a$ and prime denotes the sum over electrons, but not nuclei. The finite nuclear mass corrections, together with higher order relativistic corrections can be important when nuclear magnetic moment is obtained from NMR type of measurement.

The second case is the electron g-factor in the S-state of hydrogenic ion, like in C^{5+} The interaction Hamiltonian from Eq. (40) is

$$\delta H = -\sum_a \frac{e_a}{2\,m_a}\,\vec{s}_a\cdot\vec{B}\left[g_a - \frac{q_a^2}{m_a^2}\left(\frac{2}{3}+\frac{g_a}{6}\right) + \frac{2}{3}\sum_{b\neq a}\frac{e_b}{4\,\pi}\,\frac{\vec{r}_{ab}}{r_{ab}^3}\cdot\left(\frac{g_a}{m_b}\,\vec{D}_b - \frac{(g_a-1)}{m_a}\,\vec{D}_a\right)\right] \tag{46}$$

The resulting relativistic finite nuclear mass correction to the electron g-factor

$$\delta g_e = \frac{(Z\,\alpha)^2}{n^2}\left[\frac{1}{(1+x)^2}\left(\frac{g_e}{6} - 1 - \frac{1}{3}\,\frac{x}{1+x}\right) - \frac{Z}{3}\,\frac{x^2}{(1+x)^2}\left(g_e + \frac{1}{1+x}\right)\right] \tag{47}$$

with $x = m_e/m_N$, is in agreement with the former result obtained by Eides and Grotch in [12], and indicates that the later result of Martynenko and Faustov [13] is not correct.

In summary, we obtain finite nuclear mass corrections to magnetic interactions of atomic (ionic) systems and indicate possible significance of the coupling of the electron and nuclear spins to the motion of the whole atomic system in the precise experimental determination of the electron g-factor in hydrogen-like ions [10].

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