Relativistic calculations of pionic and kaonic atoms' hyperfine structure

Martino Trassinelli[1,2,*] and Paul Indelicato[2,†]

[1]*Gesellschaft für Schwerionenforschung, Planckstr. 1, 64291 Darmstadt, Germany*

[2]*Laboratoire Kastler Brossel, École Normale Supérieure, CNRS, Université Pierre et Marie Curie—Paris 6, Case 74, 4 Place Jussieu, 75005 Paris, France*

(Received 27 November 2006; revised manuscript received 20 February 2007; published 20 July 2007)

We present a relativistic calculation of the hyperfine structure in pionic and kaonic atoms. A perturbation method has been applied to the Klein-Gordon equation to take into account the relativistic corrections. The perturbation operator has been obtained via a multipole expansion of the nuclear electromagnetic potential. The hyperfine structure of pionic and kaonic atoms provides an additional term in the quantum electrodynamics calculation of the energy transition of these systems. Such a correction is required for a recent measurement of the pion mass.

DOI: 10.1103/PhysRevA.76.012510 PACS number(s): 36.10.Gv, 03.65.Pm, 31.15.Md, 32.30.Rj

I. INTRODUCTION

In the last few years transition energies in pionic [1] and kaonic atoms [2] have been measured with an unprecedented precision. The spectroscopy of pionic and kaonic hydrogen allows the strong interaction at low energies to be studied [3–5] by measuring the energy and natural width of the ground level with a precision of a few meV [6–8]. Additionally, light pionic atoms can be used to define new low-energy x-ray standards [9] and to evaluate the pion mass using high-accuracy x-ray spectroscopy [10–13]. Similar endeavors are being undertaken using kaonic atoms [2].

In this paper we present a calculation of the hyperfine structure in pionic and kaonic atoms considering the perturbation term due to the interaction between the pion or kaon orbital moment and the magnetic moment of the nucleus. Nonrelativistic calculations for the pionic atom hyperfine structure can be found in Refs. [14–16]. Other theoretical predictions for the hyperfine structure (HFS) including relativistic corrections can be found only for spin-$\frac{1}{2}$ nuclei [17,18]. Contrary to these methods, our technique is not restricted to this case and can be used for an arbitrary value of the nuclear spin while automatically including the relativistic effects. In particular, we calculate the HFS energy splitting for pionic nitrogen, which has been used for a recent measurement of the pion mass aiming at an accuracy of a few ppm [10,11,13,19], and for kaonic nitrogen, which has been proposed for the kaon mass measurement [2].

This paper is organized as follows. In Sec. II we calculate the first energy correction by applying a perturbation method to the Klein-Gordon (KG) equation. In Sec. III we obtain the perturbation term using the multipole expansion of the nuclear electromagnetic potential. Section IV is dedicated to numerical calculations for some pionic and kaonic atoms, and Sec. V is our conclusion.

II. CALCULATION OF THE ENERGY CORRECTION

The relativistic dynamics of a spinless particle is described by the Klein-Gordon equation. The electromagnetic interaction between a negatively charged spin-0 particle with a charge equal to $q=-e$ and the nucleus can be calculated by introducing the nuclear potential A_ν into the KG equation via the minimal coupling $p_\nu \rightarrow p_\nu - qA_\nu$ [20]. In particular, in the case of a central Coulomb potential $(V_0(r),\mathbf{0})$, the KG equation for a particle with mass m is

$$m^2c^2\Psi_0(x) = \left(\frac{1}{c^2}[i\hbar\partial_t + eV_0(r)]^2 + \hbar^2\boldsymbol{\nabla}^2\right)\Psi_0(x), \quad (1)$$

where $\hbar$ is the Planck constant, c is the velocity of light, and the scalar wave function $\Psi_0(x)$ depends on the space-time coordinate $x=(ct,\mathbf{r})$. We consider here the stationary solution of Eq. (1). In this case, we can write

$$\Psi_0(x) = \exp(-iE_0t/\hbar)\varphi_0(\mathbf{r}) \quad (2)$$

and Eq. (1) becomes

$$\left(\frac{1}{c^2}[E_0 + eV_0(r)]^2 + \hbar^2\boldsymbol{\nabla}^2 - m^2c^2\right)\varphi_0(\mathbf{r}) = 0, \quad (3)$$

where E_0 is the total energy of the system (the sum of the mass energy mc^2 and binding energy $\mathcal{E}_0$).

The perturbation correction E_1 can be deduced by introducing an additional operator W in the zeroth-order equation:

$$\left(\frac{1}{c^2}[E + eV_0(r)]^2 + \hbar^2\boldsymbol{\nabla}^2 - m^2c^2 - W(\mathbf{r})\right)\varphi(\mathbf{r}) = 0. \quad (4)$$

In the case of a correction V_1 to the Coulomb potential V_0, we have

$$W(\mathbf{r}) = -\frac{1}{c^2}[2e^2V_0(\mathbf{r})V_1(\mathbf{r}) + 2eEV_1(\mathbf{r}) + e^2V_1^2(\mathbf{r})]. \quad (5)$$

If we consider the interaction with the nuclear magnetic field as a perturbation, we have

$$W(\mathbf{r}) = i\hbar e\{2A_i(\mathbf{r})\partial^i + [\partial_i, A^i(\mathbf{r})]\} - e^2A^i(\mathbf{r})A_i(\mathbf{r}). \quad (6)$$

The correction to the energy due to W can be calculated perturbatively with some manipulation of Eqs. (3) and (4) [21,22], or via a linearization of the KG equation using the Feshbach-Villars formalism [23,24]. In both cases we have

*Electronic address: m.trassinelli@gsi.de

†Electronic address: paul.indelicato@lkb.ens.fr

 ©2007 The American Physical Society

$$E_1 = \frac{c^2\langle W\rangle}{2(E^{nl}_{(0)} + \langle eV_0\rangle)}, \tag{7}$$

where we define for an arbitrary operator A

$$\langle A\rangle = \frac{\int_V \varphi^*(\mathbf{r})A(\mathbf{r},t)\varphi(\mathbf{r})d^3r}{\int_V \varphi^*(\mathbf{r})\varphi(\mathbf{r})d^3r}. \tag{8}$$

Equation (7) is valid for any wave function normalization.

III. CALCULATION OF THE HYPERFINE STRUCTURE OPERATOR

The expression for $W(\mathbf{r})$ in the HFS case is derived using the multipole expansion of the vector potential $\mathbf{A}(\mathbf{r})$ in the Coulomb gauge [25–27]:

$$\mathbf{A}(\mathbf{r}) = -i\frac{\mu_0}{4\pi}\sum_k \left(\frac{k+1}{k}\right)^{1/2} r^{-k-1}\mathbf{C}^{kk}\circ\mathbf{M}^k, \tag{9}$$

where the symbol $\circ$ indicates here the general scalar product between tensor operators, $U^k\circ V^k = \Sigma_q(-1)^q U^k_q V^k_{-q}$.

We neglect here the effect due to the spatial distribution of the nuclear magnetic moment in the nucleus [28] (Bohr-Weisskopf effect), while the effect due to the charge distribution (Bohr-Rosenthal effect) is included in the numerical results of Sec. IV.

The hyperfine structure splitting due to the magnetic dipole interaction is obtained by taking into account only the first magnetic multipole term in Eq. (9) [25,26]:

$$\mathbf{A}(\mathbf{r}) = -i\frac{\mu_0}{4\pi}\sqrt{2}r^{-2}\mathbf{C}^{11}\circ\mathbf{M}^1. \tag{10}$$

$\mathbf{M}^1$ operates only on the nuclear part $|Im_I\rangle$ and $\mathbf{C}^{11}$ is the vector spherical harmonic [26,29] acting on the pion part $|nlm\rangle$ of the wave function. We note that the product between $\mathbf{C}^{11}$ and $\mathbf{M}^1$ is a vector, and thus a tensor of rank 1 $(\mathbf{C}^{11}\circ\mathbf{M}^1)^1$.

We can decompose the perturbation term $W(\mathbf{r})$ as

$$W(\mathbf{r}) = W_1(\mathbf{r}) + W_2(\mathbf{r}), \tag{11}$$

where

$$W_1(\mathbf{r}) = +i\hbar e\{2A_i(\mathbf{r})\partial^i + [\partial_i, A^i(\mathbf{r})]\} \tag{12}$$

is the linear part and

$$W_2(\mathbf{r}) = -e^2A^i(\mathbf{r})A_i(\mathbf{r}) \tag{13}$$

is the quadratic part.

We study first the operator W_1. We note that $[\partial_i, A^i(\mathbf{r})] = \boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{r}) = 0$ since we are using the Coulomb gauge. In this case we have

$$\begin{aligned} W_1(\mathbf{r}) &= +2i\hbar eA_i(\mathbf{r})\partial^i \\ &= -2i\hbar e\mathbf{A}(\mathbf{r})\cdot\boldsymbol{\nabla} \\ &= -e\mu_0\hbar\frac{\sqrt{2}}{2\pi}r^{-2}(\mathbf{C}^{11}\cdot\boldsymbol{\nabla})^1\circ\mathbf{M}^1. \end{aligned} \tag{14}$$

Using the properties of the spherical tensor [26,29], we can show that

$$\mathbf{C}^{11}_q\cdot\boldsymbol{\nabla} = -\frac{r^{-1}}{\sqrt{2}}L_q, \tag{15}$$

where L_q is the dimensionless angular momentum operator in spherical coordinates. The perturbation operator can be written as a scalar product in spherical coordinate of the operator $\mathbf{T}^1$ acting on the pion wave function, and the nuclear operator $\mathbf{M}^1$:

$$W_1(\mathbf{r}) = \frac{e\mu_0\hbar}{2\pi}r^{-3}(\mathbf{L}^1\circ\mathbf{M}^1) = \mathbf{T}^1\circ\mathbf{M}^1 \tag{16}$$

with

$$T^1_q = \frac{e\mu_0\hbar}{2\pi}r^{-3}L_q. \tag{17}$$

The expected value of the operator W_1 can be evaluated by applying the scalar product properties in spherical coordinates [29,30]:

$$\begin{aligned} \langle n'l'IF'm'_F|W_1|nlIFm_F\rangle &= (-1)^{l+I+F}\delta_{FF'}\delta_{m_Fm'_F}\delta_{II'} \\ &\times \begin{Bmatrix} F & I & l' \\ 1 & l & I \end{Bmatrix}\langle n'l'\|T^1\|nl\rangle \\ &\times\langle I\|M^1\|I\rangle, \end{aligned} \tag{18}$$

where $\begin{Bmatrix} a & b & c \\ d & e & f \end{Bmatrix}$ represents a Wigner 6-j symbol. The reduced operator $\langle n'l'\|T^1\|nl\rangle$ is calculated from the matrix elements $\langle n'l'm'|T^1_q|nlm\rangle$ by a particular choice of the quantum numbers m and q and application of the Wigner-Eckart theorem:

$$\begin{aligned} \langle n'l'\|T^1\|nl\rangle &= \delta_{l0}\frac{(-1)^{l-1}}{\begin{pmatrix} l & 1 & l \\ -1 & 0 & 1 \end{pmatrix}}\langle n'l'1|T^1_0|nl1\rangle \\ &= \delta_{l0}\sqrt{l}\sqrt{l+1}\sqrt{2l+1}\frac{e\mu_0\hbar}{2\pi}\langle n'l'1|r^{-3}L_0|nl1\rangle \\ &= \delta_{l0}\delta_{ll'}\sqrt{l}\sqrt{l+1}\sqrt{2l+1}\frac{e\mu_0\hbar}{2\pi}\langle n'l|r^{-3}|nl\rangle, \end{aligned} \tag{19}$$

where $\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix}$ indicates the Wigner 3-j symbol.

The nuclear operator can be related to the magnetic moment of the nucleus by $\langle II|M^1_0|II\rangle = \mu_I\mu_N$ [26,27] where μ_I is the nuclear dipole moment in units of the nuclear magneton $\mu_N = e\hbar/2m_pc$:

$$\langle I\|M^1\|I\rangle = \frac{\mu_I\mu_N}{\begin{pmatrix} I & 1 & I \\ -I & 0 & I \end{pmatrix}}. \tag{20}$$

Using Eq. (17), the total expression for $W_1(\mathbf{r})$ becomes

$$\langle n'l'IF'm'_F|W_1|nlIFm_F\rangle = \delta_{FF'}\delta_{m_F m'_F}\delta_{ll'}\mu_I\mu_N \times \frac{e\mu_0\hbar}{2\pi} \times \frac{F(F+1)-I(I+1)-l(l+1)}{2I}\langle n'l|r^{-3}|nl\rangle, \quad (21)$$

which, as expected, is equal to zero for $l=0$ (and hence $I=F$).

To find the final expression of the HFS energy shift, we have to evaluate the contribution of the operator $W_2(\mathbf{r}) = -e^2A^i(\mathbf{r})A_i(\mathbf{r})$. For this proposal, we use the equivalence of the scalar product (tensor operator of rank 0) between two tensor operators of rank 1 and the standard scalar product between two vectors:

$$W_2(\mathbf{r}) = e^2\mathbf{A}(\mathbf{r})\cdot\mathbf{A}(\mathbf{r}) \equiv e^2\mathbf{A}^1(\mathbf{r})\circ\mathbf{A}^1(\mathbf{r}). \quad (22)$$

The operator W_2 is a scalar product of two tensor operators acting in the same space. In this case we have [29]

$$\langle nlIF\|W_2\|nlIF\rangle = e^2\sum_{F'}\begin{Bmatrix} 1 & 1 & 0 \\ F & F & F' \end{Bmatrix} \times \langle nlIF\|A^1\|nlIF'\rangle \times \langle nlIF'\|A^1\|nlIF\rangle. \quad (23)$$

The reduced matrix element $\langle F'||A^1||F\rangle$ can be calculated by again applying the Wigner-Eckart theorem for the component $q=0$:

$$\langle nlIF'\|A^1\|nlIF\rangle = \frac{\langle nlIF'F'|A^1_0|nlIFF\rangle}{\begin{pmatrix} F' & 1 & F \\ -F' & 0 & F \end{pmatrix}}, \quad (24)$$

where [31]

$$A^1_0(\mathbf{r}) = -i\frac{\mu_0}{4\pi}\sqrt{2}r^{-2}(\mathbf{C}^{11}\circ\mathbf{M}^1)^1_0 = i\frac{\mu_0}{4\pi}r^{-2}\sum_q(-1)^q q C^1_q M^1_{-q}. \quad (25)$$

To evaluate the matrix element $\langle nlIF'F'|A^1_0|nlIFF\rangle$ we can explicitly decompose $|nlIFF\rangle$ as a function of the eigenfunctions $|nlm\rangle$ and $|Im_I\rangle$ using the Clebsch-Gordan coefficients. We have

$$\langle nlIF'F'|A^1_0|nlIFF\rangle = i\frac{\mu_0}{4\pi}\frac{1}{r^2}\sum_{m',m'_I,m,m_I}\langle lm'Im'_I|lIF'F'\rangle \times \langle lmIm_I|lIFF\rangle \times [\langle nlm'|r^{-2}C^1_1|nlm\rangle \times \langle Im'_I|M^1_{-1}|Im_I\rangle - \langle nlm'|r^{-2}C^1_{-1}|nlm\rangle \times \langle Im'_I|M^1_1|Im_I\rangle]. \quad (26)$$

Applying the Wigner-Eckart theorem, we obtain

$$\langle nlIF'F'|A^1_0|nlIFF\rangle = i\frac{\mu_0}{4\pi}\frac{1}{r^2}\langle nl\|r^{-2}C^1\|nl\rangle\langle I\|M^1\|I\rangle \times \sum_{m',m'_I,m,m_I}\langle lm'Im'_I|lIF'F'\rangle\langle lmIm_I|lIFF\rangle \times \left[\begin{pmatrix} l & 1 & l \\ -m' & 1 & m \end{pmatrix}\begin{pmatrix} I & 1 & I \\ -m'_I & -1 & m_I \end{pmatrix} - \begin{pmatrix} l & 1 & l \\ -m' & -1 & m \end{pmatrix}\begin{pmatrix} I & 1 & I \\ -m'_I & +1 & m_I \end{pmatrix}\right]. \quad (27)$$

The reduced matrix element $\langle nl\|r^{-2}C^1\|nl\rangle$ can be decomposed into a radial and an angular part:

$$\langle nl\|r^{-2}C^1\|nl\rangle = \langle nl|r^{-2}|nl\rangle\langle l\|C^1\|l\rangle. \quad (28)$$

Due to its symmetry properties, $\langle l\|C^1\|l\rangle$ is equal to zero for any l [29]. This result implies that the reduced matrix elements of A^1 are always equal to zero. As a consequence, the diagonal elements $\langle A^i(\mathbf{r})A_i(\mathbf{r})\rangle=0$ for any wave function, and therefore W_2 does not contribute to the HFS energy shift.

We can now write the final expression for the HFS energy correction:

$$E^{nlF}_1 = \frac{\mu_I\mu_N e\mu_0\hbar c^2}{4\pi[E^{nl}_0 - \langle nl|V_0(r)|nl\rangle]} \times \left(\frac{F(F+1)-I(I+1)-l(l+1)}{2I}\right)\langle nl|r^{-3}|nl\rangle. \quad (29)$$

This formula is obtained by a perturbation approach to the KG equation. For this reason, all the relativistic effects are automatically included in Eq. (29). In the nonrelativistic limit $c\to\infty$, $(E_0-\langle V\rangle)/c^2\to m$ and we find the usual expression of the HFS from the Schrödinger equation [32].

IV. NUMERICAL RESULTS

We present here some calculations for a selection of pionic and kaonic atom transitions. Such calculations are obtained by numerically solving the Klein-Gordon equation using the multiconfiguration Dirac-Fock code developed by one of the author (Indelicato and Desclaux and co-workers [33–36]) that has been modified to include the spin-0 particle case, even in the presence of electrons [37]. The first part is dedicated to the $5\to4$ and $8\to7$ transitions in pionic and kaonic nitrogen, respectively. In the second part we study the dependence of the HFS splitting against the nuclear charge Z to observe the role of the relativistic corrections.

A. Calculation of the energy levels of pionic and kaonic nitrogen

The precise measurement of the $5g\to4f$ transition in pionic nitrogen and the related QED predictions allow for the precise measurement of the pion mass [10–13,19]. In the same way, the transition $8k\to7i$ in kaonic nitrogen can be used for a precise mass measurement of the kaon [2]. For these transitions, strong interaction effects between the meson and nucleus are negligible, and the level energies are, if one excludes relativistic recoil corrections, directly dependent on the reduced mass of the atom. The nuclear spin of the nitrogen isotope ^{14}N is equal to 1, leading to the presence

TABLE I. Energy (in eV) contribution for the selected levels in pionic nitrogen. The first error takes into account neglected higher-order QED corrections. The second is due to the accuracy of the pion mass (±2.5 ppm).

	$5g$-$4f$	$5f$-$4d$
Coulomb	4054.1180	4054.7189
Finite size	0.0000	0.0000
Self-energy	−0.0001	−0.0003
Vacuum polarization (Uehling)	1.2485	2.9470
Vacuum polarization (Wichman-Kroll)	−0.0007	−0.0010
Vacuum polarization (loop after loop)	0.0008	0.0038
Vacuum polarization (Källén-Sabry)	0.0116	0.0225
Relativistic recoil	0.0028	0.0028
HFS shift	−0.0008	−0.0023
Total	4055.3801	4057.6914
Error	±0.0011	±0.0011
Error due to the pion mass	±0.010	±0.010

of several HFS sublevels. The observed transition is a combination of several different transitions between these sublevels, causing a shift that has to be taken into account to extract the pion mass from the experimental values. Transition probabilities between HFS sublevels can easily be calculated using the nonrelativistic formula [32,38] (the role of the relativistic effects is negligible here). If one neglects the HFS contribution to the transition energy,

$$A_{nlIF\to n'l'IF'} = \frac{(2F+1)(2F'+1)}{2I+1}\begin{Bmatrix} l' & F' & I \\ F & l & 1 \end{Bmatrix}^2 A_{nl\to n'l'}, \tag{30}$$

where

$$A_{nl\to n'l'} = \frac{4(E_{nl}-E_{n'l-1})^3}{3m^2c^4\hbar}\frac{\alpha}{(Z\alpha)^2}\frac{l}{2l+1}(R_{nl}^{n'l-1})^2, \tag{31}$$

with

$$R_{nl}^{n'l'} = \frac{1}{a_0^2}\int_0^\infty \phi_{nl}^*(r)\phi_{n'l'}(r)r^3dr, \tag{32}$$

where $a_0=\hbar/(mcZ\alpha)$ is the Bohr radius and ϕ_{nl} are the nonrelativistic wave functions.

For these calculations, presented in Tables I and II, we used the nitrogen nuclear mass value from Ref. [39]. The *Coulomb* term in Table I includes the nonrelativistic recoil correction using the reduced mass in the KG equation. The pionic and nuclear charge distribution contributions are also included as in [37,40]. For the pion charge distribution radius we take $r_\pi=0.672\pm0.008$ fm [41]. For the nuclei we take values from Ref. [42]. The leading QED correction contribution, due to the vacuum polarization, is calculated self-consistently, thus taking into account the loop-after-loop contribution to all orders, via the Uehling approximation. This is obtained by including the Uehling potential into the KG equation [35]. Other higher-order vacuum polarization contributions are calculated as perturbations to the KG equation: these are the *Wichman-Kroll* and *Källén-Sabry* corrections [43,44]. The self-energy is calculated using the expression in Ref. [45] and it includes the recoil correction. The *relativistic recoil* term has been evaluated by adapting the formulas from Refs. [18,46] (more details can be found in Ref. [13]). The calculations presented here do not take into account second-order recoil effects (Fig. 1 top), or higher QED corrections such as vacuum polarization and self-energy mixed diagrams (Fig. 1 bottom). The contribution from these terms has been estimated using the formula for a spin-$\frac{1}{2}$ particle with a mass equal to the pion mass. For the $5\to4$ pionic nitrogen transitions, vacuum polarization and self-energy mixed diagrams contribute in the order of 1 meV for the diagram with the vacuum polarization loop in the nuclear photon line [47] (Fig. 1 bottom left), and 0.0006 meV for the diagram with the vacuum polarization loop inside the self-energy loop [48] (Fig. 1 bottom right). The second-order recoil contributions are on the order of 0.04 meV [49] (Fig. 1 top). The largest

TABLE II. Hyperfine transition energies and transition rate in pionic nitrogen.

Transition	F-F'	Transition rate (s^{-1})	Transition E (eV)	Shift (eV)
$5f\to4d$	4-3	4.57×10^{13}	4057.6876	−0.00606
	3-2	3.16×10^{13}	4057.6970	0.00341
	3-3	2.98×10^{13}	4057.6845	−0.00910
	2-1	2.13×10^{13}	4057.7031	0.00946
	2-2	2.25×10^{13}	4057.6948	0.00112
	2-3	0.01×10^{13}	4057.6822	−0.01138
$5g\to4d$	5-4	7.13×10^{13}	4055.3779	−0.00304
	4-3	5.47×10^{13}	4055.3821	0.00113
	4-4	5.27×10^{13}	4055.3762	−0.00482
	3-2	4.17×10^{13}	4055.3852	0.00420
	3-3	0.36×10^{13}	4055.3807	−0.00029
	3-4	0.01×10^{13}	4055.3747	−0.00624

TABLE III. Energy (in eV) contribution for the selected levels in kaonic nitrogen. The first error takes into account neglected higher-order QED corrections. The second is due to the accuracy of the kaon mass (±32 ppm).

	$8k$-$7i$	$8i$-$7h$
Coulomb	2968.4565	2968.5237
Finite size	0.0000	0.0000
Self-energy	0.0000	0.0000
Vacuum polarization (Uehling)	1.1678	1.8769
Vacuum polarization (Wichman-Kroll)	−0.0007	−0.0008
Vacuum polarization (loop after loop)	0.0007	0.0016
Vacuum polarization (Källén-Sabry)	0.0111	0.0152
Relativistic recoil	0.0025	0.0025
HFS shift	−0.0006	−0.0008
Total	2969.6374	2970.4182
Error	0.0005	0.0005
Error due to the kaon mass	0.096	0.096

contribution comes from the unevaluated diagram with the vacuum polarization loop in the nuclear photon line [47].

Assuming a statistical population distribution of the HFS sublevels, we can use Eq. (30) to calculate the mean value of the transitions using the results in Table II. Comparing this calculation with the one without the HFS, we obtain a value for the HFS shift. For the transitions $5g \rightarrow 4f$ and $5f \rightarrow 4d$ we obtain shifts of 0.8 and 2.2 meV, respectively. These values correspond to a correction to the pion mass of between 0.2 and 0.6 ppm.

The transition energies for the $8 \rightarrow 7$ transitions in kaonic nitrogen are presented in Tables III and IV. As for pionic nitrogen, the error contribution due to the QED correction not considered here is dominated by the unevaluated diagram with the vacuum polarization loop in the nuclear photon line [47], the associated correction is estimated as to be on the order of 0.5 meV. For the $8k \rightarrow 7i$ and $8i \rightarrow 7h$ transitions we have a HFS shift of 0.6 and 0.8 meV, respectively, which correspond to a correction to the kaon mass of between 0.2 and 0.3 ppm.

As a general note, we remark that, if we assume a statistical distribution of the population of the initial state sublevels, transitions $nl \rightarrow n's$ with the s orbital as the final state have an average HFS shift equal to zero, because of an exact cancellation between the weighted excited sublevels' energy shifts as seen from Eq. (30).

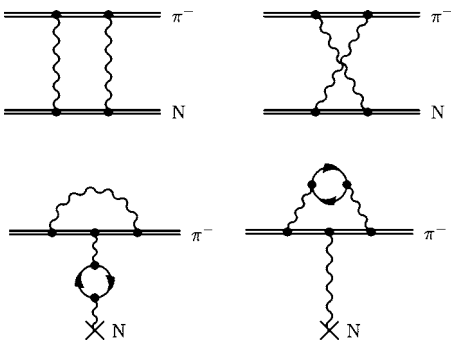

FIG. 1. Diagrams relative to the unevaluated QED contributions: second-order recoil correction (top), and vacuum polarization and self-energy mixed diagrams (bottom). Their effects are estimated using the available formulas for spin-1/2 particles.

B. General behavior of the hyperfine structure correction over Z

For the nonrelativistic case, the HFS splitting normalized to the binding energy and to the nuclear magnetic moment depends linearly on $Z\alpha$. Any deviation from this linear dependence in the Klein-Gordon HFS can be attributed only to relativistic effects.

To study the behavior of the normalized HFS splitting $(E^{9p}_{F=1/2} - E^{9p}_{F=3/2})/(\mathcal{E}_0 \mu_I)$ for the relativistic case, we calculated the HFS for a selected choice of pionic atoms with a stable nucleus of spin 1/2. The orbital $9p$ has been chosen to minimize the effect of the finite nuclear size and strong in-

TABLE IV. Hyperfine transition energies and transition rate in kaonic nitrogen.

Transition	F-F'	Transition rate (s^{-1})	Transition E (eV)	Shift (eV)
$8i \rightarrow 7h$	7-6	1.19×10^{13}	2970.4169	−0.00216
	6-5	1.00×10^{13}	2970.4196	0.00050
	6-6	0.98×10^{13}	2970.4145	−0.00453
	5-4	0.84×10^{13}	2970.4217	0.00265
	5-5	0.03×10^{13}	2970.4175	−0.00154
	5-6	0.00×10^{13}	2970.4125	−0.00656
$8k \rightarrow 7i$	8-7	1.54×10^{13}	2969.6365	−0.00149
	7-6	1.33×10^{13}	2969.6383	0.00029
	7-7	1.31×10^{13}	2969.6347	−0.00326
	6-5	1.15×10^{13}	2969.6398	0.00178
	6-6	0.03×10^{13}	2969.6367	−0.00126
	6-7	0.00×10^{13}	2969.6332	−0.00480

TABLE V. HFS separation of the $F=1/2$ and $F=3/2$ levels for the $9p$ orbital for pionic atoms with spin-1/2 nucleus.

Element	Z	$9p$ energy (eV)	HFS splitting (eV)
H	1	−39.93816	0.0001
^{3}He	2	−174.8370	−0.0009
^{13}C	6	−1633.402	0.0060
^{15}N	7	−2226.813	−0.0039
^{19}F	9	−3689.435	0.0767
^{31}P	15	−10286.63	0.1544
^{57}Fe	26	−31023.63	0.0643
^{77}Se	34	−53146.21	0.8293
^{89}Y	39	−69987.00	−0.3143
^{107}Ag	47	−101681.2	−0.4266
^{129}Xe	54	−134178.0	−4.1295
^{183}W	74	−250634.4	1.2629
^{202}Pb	82	−306731.6	7.8662

teraction shifts, particularly for high values of Z. The results are summarized in Table V. For these calculations we used the nuclear mass values from Ref. [39], the nuclear radii from Refs. [42,50], and the nuclear magnetic moments from Ref. [51].

For higher Z values a nonlinear dependence on $Z\alpha$ appears as can be seen in Fig. 2. This nonlinearity originates in the two different parts of Eq. (29): the nontrivial dependence on $\mathcal{E}_0$ in the denominator and the expectation value $\langle nl|r^{-3}|nl\rangle$.

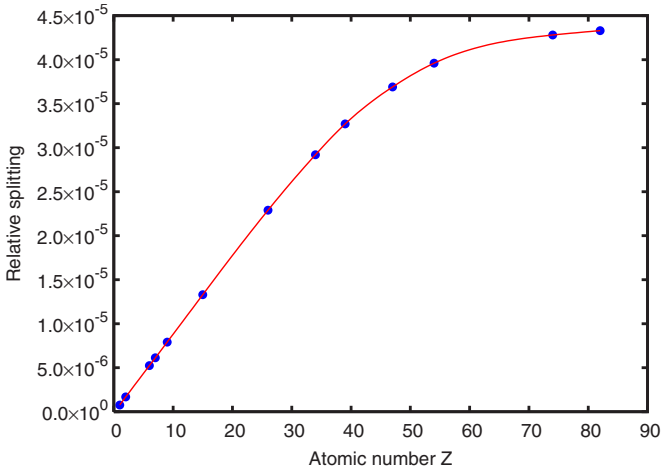

FIG. 2. (Color online) Value of relative splitting $(E^{9p}_{F=1/2} - E^{9p}_{F=3/2})/(\mathcal{E}_0\mu_I)$ for pionic atoms with different values of Z. Nuclear masses, radii, and magnetic moment values have been obtained from Refs. [39,42,50,51].

V. CONCLUSIONS

We have presented a relativistic calculation of the hyperfine structure in pionic and kaonic atoms. The precise evaluation of the specific case of pionic and kaonic nitrogen is particularly important for the new measurement of the pion and kaon mass. The small error in the theoretical predictions, of the order of 1 meV for the $5\rightarrow 4$ transition, corresponds to a systematic error of $\approx$0.2 ppm for the pion mass evaluation, considerably smaller than the error of previous theoretical predictions [52].

The formalism presented in this paper can be applied for other effects such as the quadrupole nuclear moment, which cannot be negligible for mesonic atoms with high Z. In this case, HFS due to the quadrupole moment can be predicted using the next multipole in the expansion of the electric potential of the nucleus to evaluate the corresponding perturbation operator. This application is particularly important for the calculation of the atomic levels in heavy pionic ions, where relativistic and nuclear deformation effects can be taken into account at the same time.

ACKNOWLEDGMENTS

We thank B. Loiseau, T. Ericson, D. Gotta, and L. M. Simons for interesting discussions about pionic atoms. We thank A. Surzhykov for confirming some calculations in the manuscript. One of the authors (M.T.) was partially sponsored by the Alexander von Humboldt Foundation. Laboratoire Kastler Brossel is Unité Mixte de Recherche du CNRS No. 8552.

[1] D. Gotta, Prog. Part. Nucl. Phys. **52**, 133 (2004).
[2] G. Beer, A. M. Bragadireanu, W. Breunlich, M. Cargnelli, C. Curceanu (Petrascu), J.-P. Egger, H. Fuhrmann, C. Guaraldo, M. Giersch *et al.*, Phys. Lett. B **535**, 52 (2002).
[3] J. Gasser and H. Leutwyler, Ann. Phys. (N.Y.) **158**, 142 (1984).
[4] V. E. Lyubovitskij and A. Rusetsky, Phys. Lett. B **494**, 9 (2000).
[5] J. Gasser, M. A. Ivanov, E. Lipartia, M. Mojzis, and A. Rusetsky, Eur. Phys. J. C **26**, 13 (2002).
[6] Pionic Hydrogen Collaboration, PSI Experiment Proposal No. R-98.01, 1998 (unpublished), URL http://pihydrogen.web.psi.ch
[7] D. F. Anagnostopoulos *et al.*, Nucl. Phys. A **721**, 849c (2003).
[8] DEAR Collaboration, G. Beer *et al.*, Phys. Rev. Lett. **94**, 212302 (2005).
[9] D. F. Anagnostopoulos, D. Gôtta, P. Indelicato, and L. M. Simons, Phys. Rev. Lett. **91**, 240801 (2003).
[10] S. Lenz *et al.*, Phys. Lett. B **416**, 50 (1998).
[11] Pion Mass Collaboration, PSI Experiment Proposal No. R-97.02, 1997 (unpublished).
[12] N. Nelms *et al.*, Nucl. Instrum. Methods Phys. Res. A **477**, 461 (2002).

[13] M. Trassinelli, Ph.D. thesis, Université Pierre et Marie Curie, Paris, France, 2005, URL http://tel.ccsd.cnrs.fr/tel-00067768
[14] P. Ebersold, B. Aas, W. Dey, R. Eichler, H. J. Leisi, W. W. Sapp, and F. Scheck, Nucl. Phys. A **296**, 493 (1978).
[15] J. Koch and F. Scheck, Nucl. Phys. A **340**, 221 (1980).
[16] F. Scheck, *Leptons, Hadrons, and Nuclei*, 1st ed. (Elsevier, North-Holland, 1983).
[17] G. J. M. Austen and J. J. de Swart, Phys. Rev. Lett. **50**, 2039 (1983).
[18] D. A. Owen, Found. Phys. **24**, 273 (1994).
[19] M. Trassinelli *et al.* (unpublished).
[20] J. Bjorken and S. Drell, *Relativistic Quantum Mechanics*, 1st ed. (McGraw-Hill, San Francisco, 1964).
[21] R. Decker, H. Pilkuhn, and A. Schlageter, Z. Phys. D: At., Mol. Clusters **6**, 1 (1987).
[22] R. N. Lee, A. I. Milstein, and S. G. Karshenboim, Phys. Rev. A **73**, 012505 (2006).
[23] J. L. Friar, Z. Phys. A **297**, 147 (1980).
[24] M. Leon and R. Seki, Nucl. Phys. A **352**, 477 (1981).
[25] C. Schwartz, Phys. Rev. **97**, 380 (1955).
[26] I. Lindgren and A. Rosén, Case Stud. At. Phys. **4**, 93 (1974).
[27] K. T. Cheng and W. J. Childs, Phys. Rev. A **31**, 2775 (1985).
[28] A. Bohr and V. F. Weisskopf, Phys. Rev. **77**, 94 (1950).
[29] A. R. Edmonds, *Angular Momentum in Quantum Mechanics*, 3rd ed. (Princeton University Press, Princeton, NJ, 1974).
[30] I. Lindgren and J. Morrison, *Atomic Many-Body Theory, Atoms and Plasmas*, 2nd ed. (Springer, Berlin, 1982).
[31] D. A. Varshalovich, A. N. Moskalev, and V. K. Khersonskii, *Quantum Theory of Angular Momentum*, 1st ed. (World Scientific, Singapore, 1988).
[32] H. B. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms*, 1st ed. (Springer-Verlag, Berlin, 1957).
[33] J. P. Desclaux, Comput. Phys. Commun. **9**, 31 (1975).
[34] J. P. Desclaux, in *Methods and Techniques in Computational Chemistry*, edited by E. Clementi (STEF, Cagliari, 1993), Vol. A, p. 253; URL http://dirac.spectro.jussieu.fr/mcdf
[35] S. Boucard and P. Indelicato, Eur. Phys. J. D **8**, 59 (2000).
[36] J. Desclaux, J. Dolbeault, M. Esteban, P. Indelicato, and E. Séré, in *Computational Chemistry*, edited by P. Ciarlet (Elsevier, Amsterdam, 2003), Vol. X, p. 1032.
[37] J. P. Santos, F. Parente, S. Boucard, P. Indelicato, and J. P. Desclaux, Phys. Rev. A **71**, 032501 (2005).
[38] V. Béretetski, E. Lifchitz, and L. Pitayevsky, *Électrodynamique Quantique*, Physique Theorique, 2nd ed. (Éditions MIR, Moscou, 1989).
[39] G. Audi, A. Wapstra, and C. Thibault, Nucl. Phys. A **729**, 337 (2003).
[40] S. Boucard, Ph.D. thesis, Université Pierre et Marie Curie, Paris, France, 2000, URL http://tel.ccsd.cnrs.fr/tel-00067768
[41] S. Eidelman, K. Hayes, K. Olive, M. Aguilar-Benitez, C. Amsler, D. Asner, K. Babu, R. Barnett, J. Beringer, P. Burchat *et al.*, Phys. Lett. B **592**, 1 (2004); URL http://pdg.lbl.gov
[42] I. Angeli, At. Data Nucl. Data Tables **87**, 185 (2004).
[43] L. W. Fullerton and G. A. Rinker, Phys. Rev. A **13**, 1283 (1976).
[44] K. N. Huang, Phys. Rev. A **14**, 1311 (1976).
[45] B. Jeckelmann, ETHZ-IMP Technical Report No. 1B-85-03, 1985 (unpublished).
[46] W. A. Barker and F. N. Glover, Phys. Rev. **99**, 317 (1955).
[47] K. Pachucki, Phys. Rev. A **53**, 2092 (1996).
[48] M. I. Eides, H. Grotch, and V. A. Shelyuto, Phys. Rep. **342**, 63 (2001).
[49] J. R. Sapirstein and D. R. Yennie, in *Quantum Electrodynamics*, edited by T. Kinoshita, Directions in High Energy Physics Vol. 7 (World Scientific, Singapore, 1990), p. 560.
[50] P. J. Mohr and B. N. Taylor, Rev. Mod. Phys. **77**, 1 (2005).
[51] P. Raghavan, At. Data Nucl. Data Tables **42**, 189 (1989).
[52] H. C. Schröder *et al.*, Eur. Phys. J. C **21**, 473 (2001).