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Relativistic calculations of pionic and kaonic atoms hyperfine structure

Martino Trassinelli^{1,2,*} and P. Indelicato^{2,†}

¹*Gesellschaft für Schwerionenforschung, Darmstadt, Germany*

²*Laboratoire Kastler Brossel, École Normale Supérieure; CNRS; Université Pierre et Marie Curie-Paris 6, Paris, France*

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In this article we present a new perturbation method for hydrogen-like systems with a spinless orbiting particle. We apply the perturbation theory to an exact linearized version of the Klein-Gordon equation obtained by a rescaling of the mass and the energy of the system. For this reason, the relativistic corrections are automatically included. The predictions obtained are compared and tested against an other perturbation approach that uses the Feshbach-Villars formalism and with a self-consistent calculation. We use this new perturbation method to calculate the hyperfine structure of pionic and kaonic atoms providing an additional term in the calculation of the energy transition of these systems. Such a correction is required for a recent measurement of the pion mass.

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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 to study the strong interaction at low energies [3, 4, 5] by measuring the energy and natural width of the ground level with a precision of few meV [6, 7, 8]. Besides, light pionic atoms can additionally be used to define new low-energy X-ray standards [9] and to evaluate the pion mass using high accuracy X-ray spectroscopy [10, 11, 12, 13]. Similar endeavour are in progress with kaonic atoms [2]

Strong interaction and mass measurements require precise calculations of the pure electromagnetic contribution of the atomic energy levels. To reach a precision of a few parts per million (ppm), Quantum Electrodynamics (QED) and relativistic corrections have to be calculated accurately. For spinless particles, the Klein-Gordon (KG) equation has to be used to take into account the relativistic effects. Additional contributions as hyperfine structure (HFS) and recoil corrections have to be calculated using perturbation methods. Due to the non-linearity of the KG equation, the usual perturbation theory cannot be directly applied as in the case of the Schrödinger and Dirac equations, and other techniques have to be used. In this paper we present a new perturbation method for the KG equation. One way to do perturbative calculations in the KG equation is to use the Feshbach-Villars formalism, which transforms the second order KG equation into two first order differential equations [14, 15]. An other way is to extract the energy correction manipulating the KG equation with and without perturbation operator [16, 17]. Here we use an alternative method that uses as the starting point an exact linearization of the KG equation obtained via an energy rescaling. All

methods provide similar results taking into account the relativistic effects to all the orders. We test the validity of such methods comparing their predictions for the vacuum polarization with a self-consistent calculation.

Using the formalism presented here, we then calculate the hyperfine structure in pionic and kaonic atoms considering the perturbation term due to the interaction between the pion or kaon orbital magnetic moment with the magnetic momentum of the nucleus. 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 few ppm [10, 11, 13, 18], and for kaonic nitrogen that has been proposed for the kaon mass measurement [2].

This article is organized as follows. In Sec. II we will develop the perturbation method starting from the Klein-Gordon equation. In Sec. III, we calculate and compare the vacuum polarization and nuclear finite size contributions using different methods. Section IV is dedicated to the calculation of the hyperfine structure term and includes numerical results for some pionic and kaonic atoms.

II. CALCULATION OF THE ENERGY CORRECTION

The relativistic dynamic 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 taken into account introducing the nuclear quadrivector potential A_ν in the KG equation via the minimal coupling $p_\nu \rightarrow p_\nu - qA_\nu$ [19]. In particular, in the case of a central Coulomb potential $(V_0(r), \mathbf{0})$, the KG equation for a particle with a mass μ is:

$$\mu^2 c^2 \Psi_{(0)}(x) = \left\{ \frac{1}{c^2} [i\hbar\partial_t + eV_0(r)]^2 + \hbar^2 \nabla^2 \right\} \Psi_{(0)}(x), \quad (1)$$

*Electronic address: m.trassinelli@gsi.de

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

where \hbar is the Planck constant, c the velocity of the light and the scalar wavefunction $\Psi_{(0)}(x)$ depends on the quadrivector coordinate $x = (ct, \mathbf{r})$. The perturbation correction can be deduced introducing an additional operator W in the zeroth order equation (Eq. (1)):

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

where we used

$$\Psi(x) = \exp(-iE^{nl}t/\hbar) \varphi^{nl}(\mathbf{r}) \quad (3)$$

for the exact solution of the perturbed equation. $W(\mathbf{r})$ is in general non-linear. In the case of a correction V_1 to the Coulomb potential V_0 , we have:

$$W(\mathbf{r}) = -\frac{1}{c^2} (2e^2 V_0(\mathbf{r}) V_1(\mathbf{r}) + 2eE V_1(\mathbf{r})), \quad (4)$$

where E is the total energy of the system (sum of the mass and binding energy). If we consider the interaction with the nuclear magnetic field as a perturbation, we have:

$$W(\mathbf{r}) = i\hbar e [2A_i(\mathbf{r})\partial^i + [\partial_i, A^i(\mathbf{r})]] - e^2 A^i(\mathbf{r}) A_i(\mathbf{r}). \quad (5)$$

To solve Eq. (2) using perturbation methods, we can apply a variable change to obtain an equation linear in the energy. For this purpose, we consider the new variables E_r , the relativistic energy, and μ_r the relativistic reduced mass [20]:

$$\begin{cases} E_r = \frac{E^2 - \mu^2 c^4}{2\mu_r c^2}, \\ \mu_r = \frac{E}{c^2}. \end{cases} \quad (6)$$

With this new set of variables, Eq. (1) becomes:

$$\left[E_r^{nl}{}_{(0)} + eV_0(r) + \frac{e^2 V_0^2(r)}{2\mu_r c^2} + \frac{\hbar^2 \nabla^2}{2\mu_r} \right] \varphi_{(0)}^{nl}(\mathbf{r}) = 0, \quad (7)$$

where $\varphi_{(0)}^{nl}(\mathbf{r})$ is the solution of the KG equation without perturbation. Similarly, Eq. (2) becomes:

$$\left[E_r^{nl} + eV_0(r) + \frac{e^2 V_0^2(r)}{2\mu_r c^2} + \frac{\hbar^2 \nabla^2}{2\mu_r} - \frac{W(\mathbf{r})}{2\mu_r} \right] \varphi^{nl}(\mathbf{r}) = 0. \quad (8)$$

This equation can be written in the usual form for perturbation expansion:

$$[H_0(r) + \mathcal{W}(\mathbf{r})] \varphi^{nl}(\mathbf{r}) = E_r^{nl} \varphi^{nl}(\mathbf{r}), \quad (9)$$

where

$$H_0(r) = -\frac{\hbar^2 \nabla^2}{2\mu_r} - \frac{e^2 V_0^2(r)}{2\mu_r c^2} - eV_0(r), \quad (10)$$

is the zeroth order Hamiltonian with solution:

$$H_0 \varphi_{(0)}^{nl} = E_r^{nl}{}_{(0)} \varphi_{(0)}^{nl}, \quad (11)$$

and

$$\mathcal{W}(\mathbf{r}) = \frac{W(\mathbf{r})}{2\mu_r} \quad (12)$$

is the perturbation operator.

The first correction term to the energy can be calculated from the KG equation solutions with the perturbation term (Eq. (9)) and without (Eq. (11)). Eigenvalues and eigenfunctions of Eq. (9) can be written as a function of the solutions of Eq. (11): $E_r^{nl} = E_r^{nl}{}_{(0)} + E_r^{nl}{}_{(1)} + \dots$ and $\varphi^{nl} = \varphi_{(0)}^{nl} + \varphi_{(1)}^{nl} + \dots$, where $E_r^{nl}{}_{(1)}$ and $\varphi_{(1)}^{nl}$ are the corrections due to $W(\mathbf{r})$.

The first order energy correction $E_r^{nl}{}_{(1)}$ can easily be calculated by multiplying Eq. (9) with $(\varphi_{(0)}^{nl})^*$ and Eq. (11) with $(\varphi^{nl})^*$. Integrating the two equations over the space coordinates and subtracting one to the other, we obtain:

$$\begin{aligned} E_r^{nl}{}_{(1)} &= \frac{\int_V (\varphi_{(0)}^{nl})^*(\mathbf{r}) \mathcal{W}(\mathbf{r}) \varphi^{nl}(\mathbf{r}) d^3r}{\int_V (\varphi_{(0)}^{nl})^*(\mathbf{r}) \varphi_{(0)}^{nl}(\mathbf{r}) d^3r} \\ &= \frac{\int_V (\varphi_{(0)}^{nl})^*(\mathbf{r}) \frac{W(\mathbf{r})}{2\mu_r} \varphi_{(0)}^{nl}(\mathbf{r}) d^3r}{\int_V (\varphi_{(0)}^{nl})^*(\mathbf{r}) \varphi_{(0)}^{nl}(\mathbf{r}) d^3r}, \end{aligned} \quad (13)$$

or, with a more synthetic notation,

$$E_r^{nl}{}_{(1)} = \langle nl | \mathcal{W} | nl \rangle = \frac{\langle nl | W | nl \rangle}{2\mu_r}. \quad (14)$$

We can now calculate the correction to the energy $E = E_{(0)} + E_{(1)} + \dots$. Using Eq. (6) we obtain:

$$E_{(1)}^{nl} = \frac{c^2 \langle W \rangle}{E_{(0)}^{nl} \left(1 + \frac{\mu^2 c^4}{E_{(0)}^{nl}} \right)}. \quad (15)$$

The zeroth order energy includes the mass energy of the orbiting particle and its binding energy: $E_{(0)} = \mu c^2 + \mathcal{E}_{(0)}$. In the limit $c \rightarrow \infty$, Eq. (15) reproduces the non-relativistic perturbation theory correction

$$E_{(1)}^{nl} = \langle nl | \mathcal{W} | nl \rangle = \frac{\langle nl | W | nl \rangle}{2\mu_r}, \quad (16)$$

as we will see in a particular case in Sec. IV.

This results can be compared to the Feshbach-Villars perturbation formalism [14, 15] or perturbation theory for quadratic equations [16, 17] that predict a first energy correction similar to Eq. (13):

$$E_{FV}^{nl}{}_{(1)} = \frac{c^2 \langle W \rangle}{2E_{(0)}^{nl} \left(1 + \frac{\langle eV_0 \rangle}{E_{(0)}^{nl}} \right)}. \quad (17)$$

Both equations. (15) and (17) include relativistic corrections but have a different form. If we make a development in $Z\alpha$ of the denominator of the two equations we

obtain

$$E_{(1)}^{nl} = \frac{c^2 \langle W \rangle}{E_{(0)}} \left\{ 1 - \frac{(Z\alpha)^2}{2n^2} + \mathcal{O}[(Z\alpha)^4] \right\}, \quad (18)$$

and

$$E_{FV(1)}^{nl} = \frac{c^2 \langle W \rangle}{E_{(0)}} \left\{ 1 - 2 \frac{(Z\alpha)^2}{2n^2} + \mathcal{O}[(Z\alpha)^4] \right\}, \quad (19)$$

where we used the virial theorem in the relativistic approximation:

$$\langle eV_0 \rangle = -\frac{(Z\alpha)^2}{n^2} + \mathcal{O}[(Z\alpha)^4] \quad (20)$$

The two expressions differ already in order of $(Z\alpha)^2$ with a term proportional to $(Z\alpha)^2/n^2$. Such a difference comes from the different approach of the perturbation methods and cannot be explained from the formulas above. However, the two perturbation techniques can be compared to each other and with a self-consistent calculation, where all order perturbation terms are included. The most probable is that this difference is canceled out by higher order terms. Equation (15) is very suitable for implementation in our code, as it does not require evaluation of new quantities. As an example we take the perturbation due to the vacuum polarization which will be calculated in the next section using both formalisms.

III. THE VACUUM POLARIZATION AND NUCLEAR FINITE SIZE CORRECTIONS

In this section we calculate the energy correction due to the vacuum polarization and the finite size of the nucleus in several pionic atoms with different atomic number Z to compare the perturbative results with a self-consistent calculation. This calculation has been performed using the multi-configuration Dirac-Fock (MCDF) code developed by one of the author (P.I.) and J.-P. Desclaux [21, 22, 23, 24] that has been modified to include spin-0 particles case, even in the presence of electrons [25]. In this code, the vacuum polarization and the finite size of the nucleus can be taken into account self-consistently introducing a correction $V_1(\mathbf{r})$ of the Coulomb potential into the Klein-Gordon equation, and solving it numerically to find the eigenvalues and eigenfunctions [23, 25].

In the perturbation method, the vacuum polarization and nuclear finite size energy corrections are obtained by adding a perturbation V_1 to the Coulomb potential in Eq. (1) and deriving the corresponding perturbation operator W . Considering only the first order correction, we have:

$$W(\mathbf{r}) = -\frac{1}{c^2} (2e^2 V_0(\mathbf{r}) V_1(\mathbf{r}) + 2eE V_1(\mathbf{r})). \quad (21)$$

Equation (15) becomes:

$$E_{(0)} = -2 \frac{e \langle V_1 \rangle + \frac{\langle e^2 V_0 V_1 \rangle}{E_{(0)}}}{1 + \frac{\mu^2 c^4}{E_{(0)}^2}}. \quad (22)$$

In our case, V_1 consist in two independent contribution: $V_1(\mathbf{r}) = \delta V_{VP}(\mathbf{r}) + \delta V_{FS}(\mathbf{r})$ with $\delta V_{VP}(\mathbf{r})$ is due to the vacuum polarization and $\delta V_{FS}(\mathbf{r})$ to the nuclear finite size.

For the vacuum polarization contribution, we use the well known expression [26, 27]:

$$\delta V_{VP}(r) = -\frac{Z\alpha}{r} \frac{2\alpha}{3\pi} \int_1^\infty e^{-2m_e r \zeta} \left(1 + \frac{1}{2\zeta^2} \right) \frac{\sqrt{\zeta^2 - 1}}{\zeta^2} d\zeta. \quad (23)$$

For the nuclear finite size we use the model with a sphere of radius R with constant charge density for $r \leq R$:

$$\delta V_{FS}(r) = \begin{cases} \frac{Z\alpha}{2R} \left[\left(\frac{r}{R} \right)^2 + \frac{2R}{r} - 3 \right] & \text{for } r \leq R, \\ 0 & \text{for } r > R. \end{cases} \quad (24)$$

We consider here only the first order correction for the vacuum polarization and nuclear finite size. Mixed effects of vacuum polarization and finite size and vacuum polarization have not been taken into account in the perturbation method. For this reason, we restrict our study to a few orbitals with a characteristic radius r_n much larger than the mean square radius $\langle r_N^2 \rangle^{1/2}$ of the nucleus charge distribution. In particular we studied the orbital $5g$, $7i$ and $9l$, where we chose the highest quantum number ℓ to minimize the effect of the finite size of the nucleus.

We compare in addition these relativistic calculations to the non-relativistic ones, obtained using the classical perturbation theory to the Schrödinger equation (Eq. (16)). Nuclear masses and radii and pion mass value are obtained from Refs. [28, 29, 30].

The results are presented in Tables I, II and III and Figs. 1 and 2. As expected, there is a noticeable difference between the non-relativistic and relativistic perturbation predictions. The values provided by the linerized and non-linerized KG equation perturbation approaches are very close to the self-consistent prediction. These differences can be compared with estimated error considering the second order non-relativistic perturbation correction and the numerical calculation accuracy represented in the error bars.

As we can observe in Fig. 2, non-relativistic and relativistic approaches differ significantly for high values of Z . In contrast, the relativistic prediction of the linear equation and quadratic equation perturbations are very close as expected from Eqs. (18) and (19). For levels like $5g$ and $7i$ we can observe a consistent systematic deviation from the all-order treatment that can be justified

TABLE I: Calculation of the vacuum polarization and nuclear finite size contributions for $5g$ level in pionic atoms with different values of Z . The third and fourth columns are obtained solving the KG equation numerically with and without the correction of the Coulomb potential. In the fifth column contains the energy correction values using the self-consistent method. In the sixth, seventh and eight columns, the same correction via perturbation method using non-relativistic equation, the method presented here (Eq. 15) and other relativistic methods (Eq. 17). The errors are estimated considering the second order non-relativistic perturbation correction and the numerical calculation accuracy. All the energies are in eV.

Z	A	Self-consistent method			Perturbation methods			Estimated error
		KG point-like	KG with VP and FS	Difference	Non-relativistic equation	This work	Other methods	
1	1	-66.01929	-66.01929	0.00000	0.00000	0.00000	0.00000	-0.00002
6	12	-2696.58773	-2696.58905	-0.00132	-0.00131	-0.00131	-0.00131	0.00821
10	20	-7527.81474	-7527.86693	-0.05219	-0.05215	-0.05218	-0.05217	0.01297
14	27	-14783.52908	-14783.92736	-0.39828	-0.39788	-0.39821	-0.39817	0.01692
18	40	-24483.09997	-24484.63739	-1.53742	-1.53515	-1.53703	-1.53676	0.01975
24	52	-43566.94797	-43573.12527	-6.17730	-6.16341	-6.17516	-6.17323	0.02668
30	64	-68117.95088	-68134.47802	-16.52714	-16.47570	-16.52050	-16.51240	0.01577
36	84	-98158.34020	-98193.39920	-35.05900	-34.91720	-35.04450	-35.01980	-0.00167
54	132	-221127.11088	-221289.10783	-161.99695	-160.82100	-161.97300	-161.71700	-0.17107
68	166	-350944.01571	-351304.29187	-360.27616	-356.59200	-360.38800	-359.48800	-0.49383
70	174	-371943.45060	-372340.62147	-397.17087	-392.92800	-397.32700	-396.27500	-0.55850
82	208	-510802.11815	-511470.97918	-668.86103	-659.79900	-669.55100	-667.12400	-1.05531
92	238	-643443.65188	-644410.68941	-967.03753	-951.32600	-968.57900	-964.16800	-1.63385

TABLE II: Same as Table I for the $7i$ level.

Z	A	Self-consistent method			Perturbation methods			Estimated error
		KG point-like	KG with VP and FS	Difference	Non-relativistic equation	This work	Other methods	
1	1	-129.39786	-129.39786	0.00000	0.00000	0.00000	0.00000	0.00003
6	12	-5285.39072	-5285.48550	-0.09478	-0.09473	-0.09477	-0.09476	0.01612
10	20	-14755.12768	-14756.50027	-1.37259	-1.37100	-1.37206	-1.37191	0.02581
14	27	-28978.06835	-28984.33004	-6.26169	-6.25008	-6.25822	-6.25691	0.03640
18	40	-47993.31445	-48010.91916	-17.60471	-17.55820	-17.59240	-17.58630	0.05187
24	52	-85411.59441	-85464.00965	-52.41524	-52.21100	-52.37440	-52.34230	0.09682
30	64	-133560.98902	-133676.58146	-115.59244	-114.98000	-115.50400	-115.39400	0.18443
36	84	-192493.76030	-192707.78300	-214.02270	-212.55600	-213.88200	-213.58800	0.33220
54	132	-433934.66658	-434710.47673	-775.81015	-766.15500	-775.92900	-773.53500	1.32185
70	174	-730499.27884	-732187.04239	-1687.76355	-1656.16000	-1689.98000	-1681.27000	3.15465
82	208	-1003988.59321	-1006661.60628	-2673.01307	-2608.55000	-2679.91000	-2661.03000	5.34115
92	238	-1265627.98781	-1269342.57978	-3714.59197	-3605.80000	-3728.14000	-3695.20000	7.73467

TABLE III: Same as Table I for the $9l$ level.

Z	A	Self-consistent method			Perturbation methods			Estimated error
		KG point-like	KG with VP and FS	Difference	Non-relativistic equation	This work	Other methods	
1	1	-39.93759	-39.93759	0.00000	0.00000	0.00000	0.00000	0.00001
6	12	-1631.26018	-1631.26019	-0.00001	-0.00001	-0.00001	-0.00001	0.00497
10	20	-4553.79390	-4553.79548	-0.00158	-0.00158	-0.00158	-0.00158	0.00785
14	27	-8942.85561	-8942.87772	-0.02211	-0.02210	-0.02212	-0.02211	0.01027
18	40	-14810.03338	-14810.15802	-0.12464	-0.12451	-0.12462	-0.12461	0.01220
24	52	-26353.00196	-26353.71952	-0.71756	-0.71648	-0.71748	-0.71735	0.01459
30	64	-41201.50547	-41203.92789	-2.42242	-2.41731	-2.42206	-2.42134	0.01644
36	84	-59368.00967	-59374.06286	-6.05319	-6.03645	-6.05212	-6.04954	0.01794
54	132	-133708.75011	-133746.21596	-37.46585	-37.27810	-37.46190	-37.42610	0.03660
70	174	-224834.43411	-224940.55071	-106.11660	-105.33700	-106.13200	-105.96132	0.10296
82	208	-308686.03304	-308878.57298	-192.53994	-190.75600	-192.63300	-192.20900	0.22746
92	238	-388739.34149	-389031.55931	-292.21782	-288.99100	-292.44900	-291.64000	0.38309

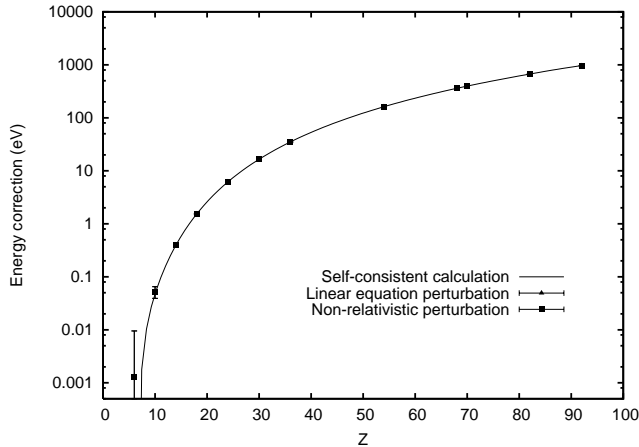


FIG. 1: Comparison between self-consistent and perturbation calculation for different pionic atoms. The error bars of the values are estimated considering the second order non-relativistic perturbation correction and the numerical calculation error.

by the existence of a non-negligible contribution of the nuclear charge distribution radius, and higher-order vacuum polarization contribution. The large contribution of the neglected higher order perturbation terms (represented by error bars in the figures) doesn't allow us to draw any clear cut conclusion: both predictions do not differ by more than two standard deviations from the all-order calculation. We can only suppose that this systematic deviation between the two relativistic perturbation methods will be canceled by the contribution of the higher order perturbation terms not considered here.

IV. THE HYPERFINE STRUCTURE IN PIONIC AND KAONIC ATOMS

The hyperfine structure in pionic and kaonic atoms arises from the interaction between the nuclear magnetic moment and the orbital magnetic moment of the particle that can be taken into account by introducing a new term in the KG equation.

This term is obtained from the multipole development of the nuclear electromagnetic field [31, 32, 33]. Non-relativistic calculations for the pionic atom hyperfine structure can be found in Ref. [34, 35, 36]. Other theoretical predictions for HFS including relativistic corrections can be found only for spin- $\frac{1}{2}$ nucleus [37, 38]. Contrary to these methods, our technique is not restricted to this case and it can be used for an arbitrary value of the nucleus spin including automatically the relativistic effects.

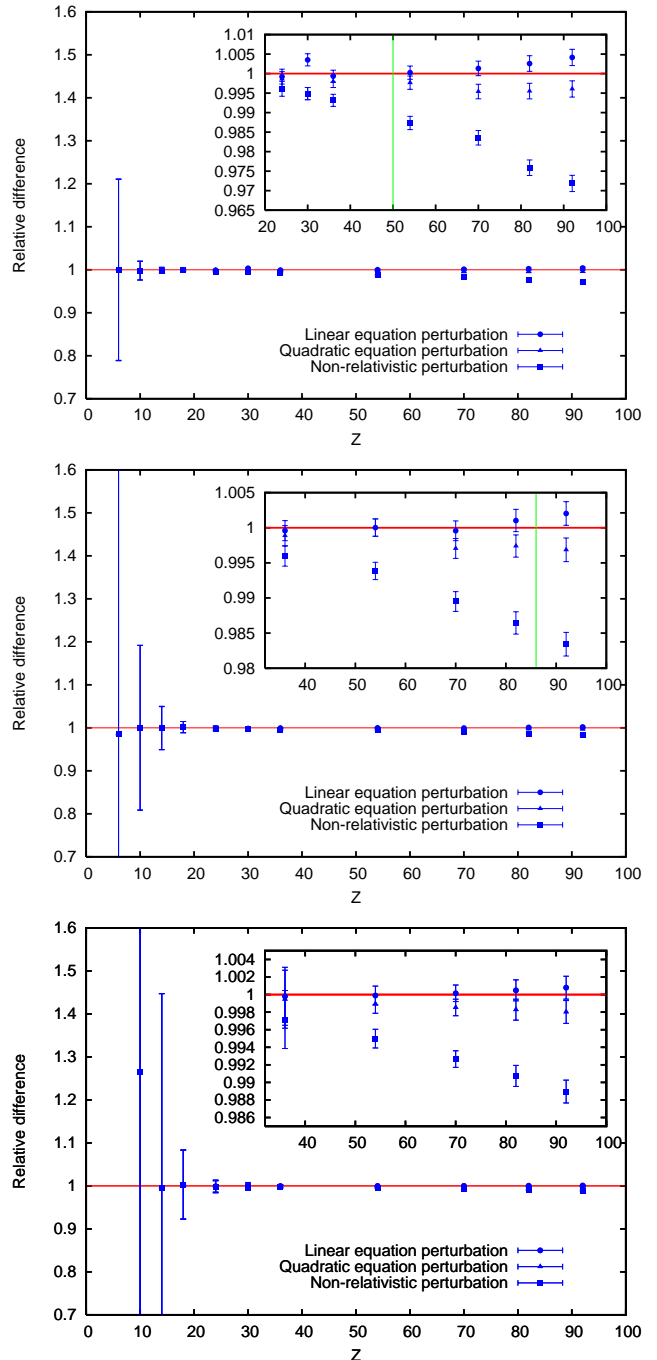


FIG. 2: Ratio between self-consistent and perturbation calculation as a function of the atomic number Z . Top: $5g$ level, middle: $7i$ level, bottom; $9h$ level. The error bars of the values are estimated considering the second order non-relativistic perturbation correction and the numerical calculation error. Values in the right of the vertical line are considerably affected from the nuclear finite size effects ($r_n / < r_N^2 >^{1/2} \geq 5\%$). For these cases, vacuum polarization and finite size mixed contribution, not considered here, could influence significantly the results.

A. Calculation of the operator

The expression for $W(\mathbf{r})$ in the HFS case is derived using the multipole development of the vector potential $\mathbf{A}(\mathbf{r})$ in the Coulomb gauge [32]. We neglect here the effect due to the the spatial distribution of the nuclear magnetic moment in the nucleus [39] (Bohr-Weisskopf effect), while effect due to the charge distribution (Bohr-Rosenthal effect) are included.

The hyperfine structure due to the magnetic dipole interaction is obtained by taking into account the first magnetic multipole term. Using the Coulomb gauge [31, 32] we have:

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

where the symbol “ \circ ” indicates here the general scalar product between tensor operators. \mathbf{M}^1 operates only on the nuclear part $|Im_I\rangle$ and \mathbf{C}^{11} on the pion part $|nlm\rangle$ of the wave function. Using this expression, we can decompose the perturbation term $W(\mathbf{r})$ as:

$$W(\mathbf{r}) = W_1(\mathbf{r}) + W_2(\mathbf{r}), \quad (26)$$

where

$$W_1(\mathbf{r}) = +i\hbar e [2A_i(\mathbf{r})\partial^i + [\partial_i, A^i(\mathbf{r})]], \quad (27)$$

is the linear part and

$$W_2(\mathbf{r}) = -e^2 A^i(\mathbf{r})A_i(\mathbf{r}), \quad (28)$$

is the quadratic part.

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

$$W_1(\mathbf{r}) = +2i\hbar e A_i(\mathbf{r})\partial^i = -2i\hbar e \mathbf{A}(\mathbf{r}) \cdot \vec{\nabla} = -e\mu_0\hbar \frac{\sqrt{2}}{2\pi} r^{-2} (\mathbf{C}^{11} \cdot \vec{\nabla}) \circ \mathbf{M}^1. \quad (29)$$

Using the properties of the spherical tensor [32, 40], we can show that:

$$\mathbf{C}_q^{11} \cdot \vec{\nabla} = -\frac{r^{-1}}{\sqrt{2}} L_q, \quad (30)$$

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 wavefunction, and the nuclear operator \mathbf{M}^1 :

$$W_1(\mathbf{r}) = \frac{e\mu_0\hbar}{2\pi} r^{-3} (\mathbf{L} \circ \mathbf{M}^1) = \mathbf{T}^1 \circ \mathbf{M}^1 \quad (31)$$

with

$$T_q^1 = \frac{e\mu_0\hbar}{2\pi} r^{-3} L_q. \quad (32)$$

The expected value of the operator W_1 can be evaluated applying the scalar product properties in spherical coordinates [40, 41]:

$$\langle n'l'IF'm'_F | W_1 | nlIFm_F \rangle = (-1)^{l'+I+F} \delta_{FF'} \delta_{m_F m'_F} \delta_{II'} \times \left\{ \begin{matrix} F & I & l' \\ 1 & l & I \end{matrix} \right\} \langle n'l' || T^1 || nl \rangle \langle I || M^1 || I \rangle, \quad (33)$$

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

$$\begin{aligned} \langle n'l' || T^1 || nl \rangle &= \delta_{l0} \frac{(-1)^{l-1}}{\begin{pmatrix} l & 1 & l \\ -1 & 0 & 1 \end{pmatrix}} \langle n'l'1 | T_0^1 | nl1 \rangle = \\ &= \delta_{l0} \sqrt{l} \sqrt{l+1} \sqrt{2l+1} \frac{e\mu_0\hbar}{2\pi} \langle n'l'1 | r^{-3} L_z | nl1 \rangle = \\ &= \delta_{l0} \delta_{l1} \sqrt{l} \sqrt{l+1} \sqrt{2l+1} \frac{e\mu_0\hbar}{2\pi} \langle n'l | r^{-3} | nl \rangle, \end{aligned} \quad (34)$$

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 on the nucleus by $\langle II | M_0^1 | II \rangle = \mu_I \mu_N$ [32, 33] where μ_I is the nuclear dipole momentum in units of the nuclear magneton $\mu_N = e\hbar/2m_p c$:

$$\langle I || M^1 || I \rangle = \frac{\mu_I \mu_N}{\begin{pmatrix} I & 1 & I \\ -I & 0 & I \end{pmatrix}}. \quad (35)$$

Considering Eq. (32), the total expression for $W_1(\mathbf{r})$ becomes:

$$\begin{aligned} \langle n'l'IF'm'_F | W_1 | nlIFm_F \rangle &= \\ &= \delta_{FF'} \delta_{m_F m'_F} \delta_{l1} \mu_I \mu_N \times \\ &\frac{e\mu_0\hbar}{2\pi} \frac{F(F+1) - I(I+1) - l(l+1)}{2I} \langle n'l | r^{-3} | nl \rangle. \end{aligned} \quad (36)$$

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

To find the final expression of the HFS energy shift, we have to evaluate the contribution of the operator $W_2(\mathbf{r}) = -e^2 A^i(\mathbf{r})A_i(\mathbf{r})$ in the $\langle W \rangle$ diagonal terms. Using Eq. (25), we have:

$$\begin{aligned} \langle nlIFm_F | W_2 | nlIFm_F \rangle &= +2 \left(\frac{e\mu_0}{4\pi} \right)^2 \times \\ &\langle nlIFm_F | (r^{-2} \mathbf{C}^{11} \circ \mathbf{M}^1) \cdot (r^{-2} \mathbf{C}^{11} \circ \mathbf{M}^1) | nlIFm_F \rangle. \end{aligned} \quad (37)$$

We are in presence of three independent scalar products: two scalar products between the tensor \mathbf{C}^{11} and the vector \mathbf{M}^1 , and the scalar product between the vectorial operators $\mathbf{C}^{11} \circ \mathbf{M}^1$. The “ \cdot ” scalar product in W_2 can be

decomposed using the properties of the reduced matrix elements of a generic operator product X^K , of rank K , between non-commuting tensor operators U^k and V^k of rank k . For our case, this scalar product corresponds to a tensor product with $K = 0$, and $k = 1$:

$$X^0 = U^1 \cdot V^1 = (r^{-2}\mathbf{C}^{11} \circ \mathbf{M}^1) \cdot (r^{-2}\mathbf{C}^{11} \circ \mathbf{M}^1), \quad (38)$$

$$U^1 = V^1 = (r^{-2}\mathbf{C}^{11} \circ \mathbf{M}^1). \quad (39)$$

We have [40]:

$$\langle nlIF || X^0 || nlIF \rangle = \sum_{F'} \left\{ \begin{array}{ccc} 1 & 1 & 0 \\ F & F & F' \end{array} \right\} \times \langle nlIF || U^1 || nlIF' \rangle \langle nlIF' || V^1 || nlIF \rangle. \quad (40)$$

V^1 and U^1 are scalar products between commutative tensor operators, and their reduced matrix element $\langle F' || V || F \rangle$ can be calculated applying again the Wigner-Eckart theorem for the component $q = 0$:

$$\langle nlIF' || V^1 || nlIF \rangle = \frac{\langle nlIF'F' || V_0^1 || nlIFF \rangle}{\begin{pmatrix} F' & 1 & F \\ -F' & 0 & F \end{pmatrix}}. \quad (41)$$

where [42]:

$$V_0^1 = U_0^1 = r^{-2}(\mathbf{C}^{11} \circ \mathbf{M}^1)_0 = r^{-2} \sum_q (-1)^q \frac{q}{\sqrt{2}} C_q^1 M_{-q}^1, \quad (42)$$

which can be written as:

$$V_0^1 = U_0^1 = G^1 \cdot M^1 = \sum_q (-1)^q G_q^1 M_{-q}^1, \quad (43)$$

where

$$G_q^1 = \frac{q}{\sqrt{2}} C_q^1. \quad (44)$$

Using again the tensor operator properties, it is possible to decompose the V_0 and U_0 matrix elements:

$$\langle nlIF'F' || V_0 || nlIFF \rangle = r^{-2} (-1)^{l+I+F} \delta_{FF'} \delta_{m_F m'_F} \times \left\{ \begin{array}{ccc} F & I & l \\ 1 & l & I \end{array} \right\} \langle nl || r^{-2} G^1 || nl \rangle \langle I || M^1 || I \rangle. \quad (45)$$

The reduced matrix element $\langle || r^{-2} G^1 || \rangle$ is the same for any choice of q and in particular $q = 0$. It is thus equal to zero due to its expression and to the properties of the spherical harmonics and of the 3j-symbols. This result implies that the reduced matrix elements of U^1 and V^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 wavefunction, i.e., W_2 does not contribute to the HFS energy shift.

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

$$E_{(1)}^{nlF} = \frac{\mu_I \mu_N e \mu_0 \hbar}{2\pi\mu \left(1 + \frac{\mathcal{E}_0^{nl}}{\mu c^2}\right) \left[1 + \left(1 + \frac{\mathcal{E}_0}{\mu c^2}\right)^{-2}\right]^\times} \left[\frac{F(F+1) - I(I+1) - l(l+1)}{2I} \right] \langle nl | r^{-3} | nl \rangle. \quad (46)$$

This formula is obtained by a perturbation approach of the KG equation. For this reason, all the relativistic effects are automatically included in Eq. (46). In the non-relativistic limit $c \rightarrow \infty$ we find the usual expression of the HFS for the Schrödinger equation [43]

B. Numerical results and behaviors

We present here some calculations for a selection of pionic and kaonic atom transitions. The first part is dedicated to the $5 \rightarrow 4$ transitions in pionic nitrogen, essential to deduce a pion mass value from a recent measurement of the $5g \rightarrow 4f$ transition in pionic nitrogen [10, 11, 12, 13, 18] and for the proposed kaon mass measurement [2]. In the second part we will study the dependence of the HFS splitting against Z to observe the role of the relativistic corrections.

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

The precise measurement of $5g \rightarrow 4f$ transition in pionic nitrogen and the related QED predictions allow for the precise measurement of the pion mass. In the same way, the transition $8k \rightarrow 7i$ in kaonic nitrogen can be used for a precise mass measurement of the kaon [2]. For this transitions, strong interaction effects between meson and nucleus are negligible, and the level energies are directly dependent to the reduced mass of the atom. The nuclear spin of the nitrogen isotope ^{14}N is equal to one leading to the presence 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 non-relativistic formula [27, 43] (the role of the relativistic effects is here negligible), if one neglect the HFS contribution to the transition energy:

$$A_{nlIF \rightarrow n' l' IF'} = \frac{(2F+1)(2F'+1)}{2I+1} \left\{ \begin{array}{ccc} l' & F' & I \\ F & l & 1 \end{array} \right\}^2 A_{nl \rightarrow n' l'}, \quad (47)$$

TABLE IV: Energy (in eV) contribution for the selected levels in pionic nitrogen. The first error take into account neglected next 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
Vac. Pol. (Uehling)	1.2485	2.9470
Vac. Pol. Wichman-Kroll	-0.0007	-0.0010
Vac. Pol. Loop after Loop	0.0008	0.0038
Vac. Pol. 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

TABLE V: Hyperfine transition energies and transition rate in pionic nitrogen.

Transition	F-F'	Trans. rate (s^{-1})	Trans. E (eV)	Shift (eV)
$5f \rightarrow 4d$	4-3	4.57×10^{13}	4057.68762	-0.00605
	3-2	3.16×10^{13}	4057.69708	0.00341
	3-3	2.98×10^{13}	4057.68457	-0.00910
	2-1	2.13×10^{13}	4057.70313	0.00946
	2-2	2.25×10^{13}	4057.69479	0.00112
	2-3	0.01×10^{13}	4057.68229	-0.01138
$5g \rightarrow 4f$	5-4	7.13×10^{13}	4055.37793	-0.00304
	4-3	5.47×10^{13}	4055.38210	0.00113
	4-4	5.27×10^{13}	4055.37616	-0.00481
	3-2	4.17×10^{13}	4055.38514	0.00417
	3-3	0.36×10^{13}	4055.38068	-0.00029
	3-4	0.01×10^{13}	4055.37474	-0.00623

where

$$A_{nl \rightarrow n'l'} = \frac{4(E_{nl} - E_{n'l'})^3}{3m^2 c^4 \hbar} \frac{\alpha}{(Z\alpha)^2} \frac{l}{2l+1} (R_{nl}^{n'l'})^2, \quad (48)$$

with

$$R_{nl}^{n'l'} = \frac{1}{a_0^2} \int_0^\infty \varphi_{nl}^*(r) \varphi_{n'l'}(r) r^3 dr, \quad (49)$$

where $a_0 = \hbar/(\mu c Z \alpha)$ is the Bohr radius.

For these calculations, presented in Tables IV and IV B 1 we used the nitrogen nuclear mass value from Ref. [28]. The *Coulomb* term in the Table includes the non-relativistic recoil correction using the reduced mass on the KG equation. The pion and nucleus charge distribution contribution are also included. The pion charge distribution radius contribution is included following [25, 44]. For the pion charge distribution radius we take $r_{\text{pion}} = 0.672 \pm 0.08$ [30]. For the nuclei we take values from Ref. [29]. The leading QED corrections, vacuum polarization, contribution is calculated

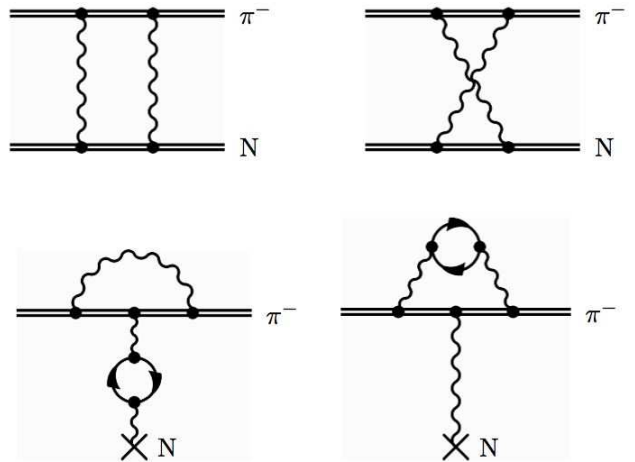


FIG. 3: Diagrams relative to the unevaluated QED contributions: second order recoil correction (top), and vacuum polarization and self-energy mixed diagrams (bottom). Their effects are estimated using the available formulas for spin- $\frac{1}{2}$ particles.

self-consistently, thus taking into account the loop-after-loop contribution to all orders, at the Uehling approximation. This is obtained by including the Uehling potential into the KG equation [23]. Other Higher-order vacuum polarization contribution are calculated as perturbation to the KG equations: *Wichman-Kroll* and *Källén-Sabry* [45, 46]. The self-energy is calculated using the expression in Ref. [47] and it includes the recoil correction. The *Relativistic recoil* term has been evaluated adapting the formulas from Refs. [38, 48] (more details can be found in Ref. [13]). The calculations presented here do not take into account second order recoil effects (Fig. 3 top), or higher QED corrections as vacuum polarization and self-energy mixed diagrams (Fig. 3 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's. For the $5 \rightarrow 4$ 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 [49] (Fig. 3 bottom-left), and 0.0006 meV for the diagram with the vacuum polarization loop inside the self-energy loop [50] (Fig. 3 bottom-right). The second order recoil contributions are in the order of 0.04 meV [51] (Fig. 3 top). The largest contribution comes from the unevaluated diagram with the vacuum polarization loop in the nuclear photon line [49].

Assuming a statistical population distribution of the HFS sublevels, we can use Eq. (47) to calculate the mean value of the transitions using the results in Table IV B 1. Comparing this calculation with the one without the HFS, we obtain a value for the HFS shift. For transitions $5g \rightarrow 4f$ and $5f \rightarrow 4d$ we obtain shifts of 0.8 and 2.2 meV, respectively. These values correspond to a cor-

TABLE VI: Energy (in eV) contribution for the selected levels in kaonic nitrogen. The first error take into account neglected next 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
Vac. Pol. (Uehling)	1.1678	1.8769
Vac. Pol. Wichman-Kroll	-0.0007	-0.0008
Vac. Pol.two-loop Uehling	0.0007	0.0016
Vac. Pol. 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

TABLE VII: Hyperfine transition energies and transition rate in kaonic nitrogen.

Transition	F-F'	Trans. rate (s^{-1})	Trans. E (eV)	Shift (eV)
$8i \rightarrow 7h$	7-6	1.19×10^{13}	2970.41691	-0.00216
	6-5	1.00×10^{13}	2970.41956	0.00050
	6-6	0.98×10^{13}	2970.41453	-0.00453
	5-4	0.84×10^{13}	2970.42172	0.00265
	5-5	0.03×10^{13}	2970.41753	-0.00154
	5-6	0.00×10^{13}	2970.41250	-0.00656
$8k \rightarrow 7i$	8-7	1.54×10^{13}	2969.63649	-0.00149
	7-6	1.33×10^{13}	2969.63827	0.00029
	7-7	1.31×10^{13}	2969.63472	-0.00326
	6-5	1.15×10^{13}	2969.63976	0.00178
	6-6	0.03×10^{13}	2969.63673	-0.00126
	6-7	0.00×10^{13}	2969.63318	-0.00480

rection to the pion mass between 0.2 and 0.6 ppm.

The transition energies for the $8 \rightarrow 7$ transitions in kaonic nitrogen are presented in Tables VI and IV B 1. As for the pionic nitrogen, the error contribution due to the QED correction not considered is dominated by the unevaluated diagram with the vacuum polarization loop in the nuclear photon line [49], the associated correction is estimated in the order of 0.5 meV. For $8k \rightarrow 7i$ and $8i \rightarrow 7h$ transitions we have a HFS shift of 0.6 and 0.8 meV, respectively, which correspond to a correction of the kaon mass between 0.2 and 0.3 ppm.

As a general note, we remark that if we assume a statistical distribution of the initial state sublevels populations, transitions $nl \rightarrow n's$ with a s orbital as final state have an average HFS shift equal to zero due to an exact cancellation between the weighted excited sublevels energy shifts as seen from Eq. (47).

TABLE VIII: HFS separation of the $F=1/2$ and $F=3/2$ levels for the $9p$ orbital for pionic atoms with spin $\frac{1}{2}$ nucleus

Element	Z	$9p$ energy (eV)	HFS splitting (eV)
H	1	0.0000	0.0001
3He	2	-174.8370	-0.0009
${}^{13}C$	6	-1633.4017	0.0060
${}^{15}N$	7	-2226.8125	-0.0039
${}^{19}F$	9	-3689.4351	0.0767
${}^{31}P$	15	-10286.6344	0.1544
${}^{57}Fe$	26	-31023.6282	0.0642
${}^{77}Se$	34	-53146.2137	0.8284
${}^{89}Y$	39	-69987.0032	-0.3139
${}^{107}Ag$	47	-101681.1985	-0.4257
${}^{129}Xe$	54	-134178.0092	-4.1177
${}^{183}W$	74	-250634.4239	1.2562
${}^{202}Pb$	82	-306731.5682	7.8151

2. General behavior of the hyperfine structure correction over Z

For the non-relativistic 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 $(E_{F=3/2}^{9p} - E_{F=1/2}^{9p})/(\mathcal{E}_0\mu I)$ 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 interaction shifts, particularly for high values of Z . The results are summarized in Table IV B 2. For these calculations we used the nuclear mass values from Ref. [28], the nuclear radii from Refs. [29, 52] and the nuclear magnetic moments from Ref. [53].

For higher Z values a non-linear dependence on $Z\alpha$ appears as we can see in Fig. IV B 2. This non-linearity originates in the two different parts of Eq. (46): the non-trivial dependency on \mathcal{E}_0 in the denominator and the expectation value $\langle nl|r^{-3}|nl\rangle$.

V. CONCLUSIONS

We have presented here a new perturbation method for the Klein-Gordon equation in bound systems, that is very easy to implement in computer codes. We apply this new method to calculate the HFS of pionic and kaonic atoms using the formalism presented in this paper. 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 on the theoretical predictions, of the order of 1 meV for the $5 \rightarrow 4$ transition, corresponds to a systematic error of ≈ 0.34 ppm for the pion mass evaluation, considerably smaller than the error of previous theoretical predictions

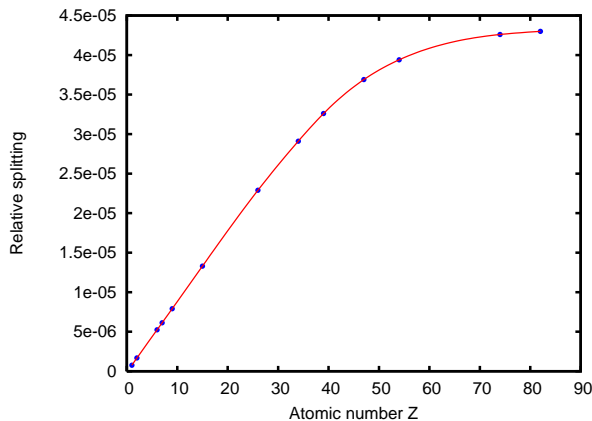


FIG. 4: Value of relative splitting $(E_{F=3/2}^{9p} - E_{F=3/2}^{9p})/(\mathcal{E}_0\mu_I)$ for pionic atoms with different values of Z . Nuclear masses, radii and magnetic moments values have been obtained from Refs. [28, 29, 52, 53].

[54].

The perturbation method for the Klein-Gordon equation has been used for the calculation of the HFS of pionic atoms, but it can be applied to different types of

perturbation. For mesonic atoms with high Z , the nuclear quadrupole moment may not be negligible. The effect of such moments can be easily evaluated using the same perturbation method. In this case, HFS due to the quadrupole moment can be predicted using the next multipole in the development of the electric potential of the nucleus to evaluate the correspondent perturbation operator. In the same way, strong interaction effects can be taken into account introducing the optical potential [36, 55] as perturbation. These two applications are very important for the calculation of the atomic levels in heavy pionic ions, where the relativistic effects, automatically taken into account by the KG equation, are not negligible.

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