Space-curvature effects in atomic fine- and hyperfine-structure calculations

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Space-curvature theoretical modifications of the fine- and hyperfine-structure energy levels have been investigated in the framework of a curved-Dirac-orbital model. Fairly accurate approximate solutions of the Dirac equation in a geometrically simple, curved space, i.e., the spherical three-space of radius R have been obtained. An efficient ladder-operator technique has been devised in order to obtain closed-form expressions of the "curved" fine- and hyperfine-structure parameters in terms of the quantum numbers. Particularly, it has been found that the degenerate one-electron fine-structure energy levels are split by an additional space-curvature contribution $\Delta_c=(-1)^{l+j+1/2}\times(j+\frac{1}{2})/(4R^2)$ which vanishes at the traditional flat-space limit ($R\to\infty$). Space-curvature modifications of both fine and hyperfine parameters, increasing with n as n^4/Z^2R^2, have been put in evidence. Besides the interest of a theoretical nature concerning specific information about the local curvature at the position of an highly excited astrophysical ion, some other practical interests of formulating quantum mechanics in a spherical three-space of parametric curvature $1/R$ are pointed out.

I. INTRODUCTION

The interest of calculating the energy levels of one-electron atoms in a curved space-time has been drawn recently in a series of papers.[1–10] In fact, the introduction of space curvature in quantum physics has been considered since a long time: Indeed, as early as the late twenties the Dirac equation was formulated in a curved space-time by Tetrode,[11] by Fock,[12] and by Fock and Ivanenko,[13] and has been reinvestigated or reviewed by several authors (see, for instance, Refs. 14—17). Among previous works, the one of Schrödinger[18] deserves a special mention. He, first, solved the nonrelativistic equation bearing his name in a space of constant curvature and put in evidence how the continuous hydrogenic spectrum is resolved into an intensely crowded line spectrum. Since the mathematical nature of the hydrogenic wave equation is not more intricate in the spherical three-space than in the flat space,[7,19,20] it is thus possible to build up a tractable "curved-orbital" model (nonrelativistic or relativistic) capable of exploring some space-curvature modifications of atomic spectrum. Without wanting to discuss immediately the critical question of the order of magnitude of the curvature induced shifts and the possibilities of their detection, this model provides within the usual framework of theoretical spectroscopy ready to use formulas of the curvature modifications of the spectrum in situations where local curvature could be important. It can also be used as a path toward flat-space calculations taking the advantage of hyperspherical parametrization.[7,12] One aspect of this last point has been illustrated by recent calculations.[21,22]

As already pointed out, our approach of the problem of finding the energy-level perturbations produced in a freely falling atom by space-time curvature differs from that of previous work:[1–6] Our calculation of curvature effects is done in the basis of already "curved" wave functions, while Tourrenc and Parker have used "flat" unperturbed wave functions (nonrelativistic and relativistic). On the other hand, Parker has obtained general expressions in terms of the Riemann tensor while we consider a "curved" space with constant positive curvature, i.e., a three-dimensional hypersphere of radius R embedded in a four-dimensional Euclidean space. The dynamical symmetries of this space have been studied by Higgs[19] and Leemon.[20] Working in that geometrically simple space allows us to keep a more direct parallelism between the "curved" and "flat" results and an easier extension to the many-electron case.

In our previous papers,[7–10] we have focused our attention on nonrelativistic atomic structure calculations in a spherical three-space. Particularly, a multipolar expansion of the Coulombic potential has been given,[7] allowing the computation of curvature-dependent two-electron matrix elements, the nonrelativistic expressions of the fine- and hyperfine-structure Hamiltonians have been derived[8,10] via a covariant formulation of the Pauli equation. For many reasons, a physically more consistent "curved-orbital" model should be relativistic, i.e., built up using the two-component "curved" Dirac orbitals. In the present paper, after briefly recalling the expression of the Dirac equation in a spherical three-space (Sec. II), approximate "curved" Dirac orbitals are derived using the Infeld-Hull[23] ladder operator technique (Sec. III). Closed-form expressions of the fine-structure energies including all the $1/R^2$ curvature contributions are given in terms of the usual relativistic quantum numbers (n,k) (Sec. IV). In order to obtain all the $1/R^2$ curvature contributions to the hyperfine-structure energies, a more elaborate solution of the "curved" Dirac equation is carried out (Sec. V). The curved form of the hyperfine-structure Hamiltonian is given and the "pseudoradial" hyperfine parameters are calculated (Sec. VI). To complement the study, in the last section the nonrelativistic expressions of the fine and hyperfine Hamiltonians are found again as a by-product of the above results. The closed form expressions of the basic integrals between "curved" generalized Kepler functions needed for both relativistic and nonrelativistic fine- and hyperfine-structure calculations are contained in Appendix B. They have been obtained by extending a novel ladder operator procedure.[9] To our knowledge, such calculations in a spherical three-space have not yet been reported.

II. DIRAC EQUATION IN SPHERICAL THREE-SPACE

The generally covariant form of the Dirac equation in a curved space-time of metric $g_{\mu\nu}(x)$ is

$$[ic\hbar\tilde{\gamma}^{\mu}(x)\hat{\nabla}_{\mu}-mc^2]\psi(x)=0\ , \tag{1}$$

where ψ is a four-component spinor, $\mu=0,1,2,3$; $\hat{\nabla}_{\mu}$ is a spin covariant derivative (for definition and details, see Appendix A). The Einstein summation convention is used, $x=(x^0,x^1,x^2,x^3)$. The $\tilde{\gamma}^{\mu}(x)$ are coordinate-dependent matrices which obey the anticommutation relations

$$\tilde{\gamma}^{\mu}(x)\tilde{\gamma}^{\nu}(x)+\tilde{\gamma}^{\nu}(x)\tilde{\gamma}^{\mu}(x)=2g^{\mu\nu}(x)\ . \tag{2}$$

In a space of constant positive curvature, the space-time line element (Einstein metric) and the volume element are

$$\begin{aligned} ds^2&=c^2dt^2-R^2d\chi^2-R^2\sin^2\chi(d\theta^2+\sin^2\theta\, d\phi^2)\ ,\\ d\tau^2&=R^3\sin^2\chi\sin\theta\, d\chi\, d\theta\, d\phi\ , \end{aligned} \tag{3}$$

where θ and ϕ lie within their traditional bounds $0\le\phi\le 2\pi$, $0\le\theta\le\pi$, and $0\le\chi\le\pi$. Setting $R\to\infty,\chi\to 0$ such that $R\chi=r$ remains finite, the spatial part of the line element (3) reduces to that of Euclidean space in which r,θ,ϕ are the usual polar coordinates.

A convenient choice of the Dirac representation, i.e., of the Dirac matrices $\tilde{\gamma}^{\mu}$, can be made which leads to the usual polar dependence (θ,ϕ) of the Dirac wave function and one gets the following expression of the Dirac equation for stationary states with an external electromagnetic field[10] ($A_0=V, A_1=A_\chi, A_2=A_\theta, A_3=A_\phi$):

$$\left[-\frac{i}{R}\alpha_\chi\left[\frac{\partial}{\partial\chi}-\frac{1-\cos\chi}{\sin\chi}-\frac{ie}{\hbar c}A_\chi\right]-\frac{i\alpha_\theta}{R\sin\chi}\left[\frac{\partial}{\partial\theta}-\frac{ie}{\hbar c}A_\theta\right]-\frac{i\alpha_\phi}{R\sin\chi\sin\theta}\left[\frac{\partial}{\partial\phi}-\frac{ie}{\hbar c}A_\phi\right]+\frac{mc}{\hbar}\beta-\frac{E_T-eV}{\hbar c}\right]\psi(\chi,\theta,\phi)=0 \tag{4}$$

or alternatively

$$\left[\alpha_\chi\left[p_\chi+\frac{i\beta\hat{K}}{R\sin\chi}\right]+W+\frac{mc}{\hbar}\beta-\frac{1}{\hbar c}(E_T-eV)\right]\psi(\chi,\theta,\phi)=0\ , \tag{5}$$

where

$$W=-\frac{e}{\hbar c}\frac{1}{R}\left[\alpha_\chi A_\chi+\frac{\alpha_\theta}{\sin\chi}A_\theta+\frac{\alpha_\phi}{\sin\chi\sin\theta}A_\phi\right]\ ,$$

$$E_T=mc^2+E$$

is the total energy,

$$\beta=\begin{bmatrix} I & 0\\ 0 & -I\end{bmatrix}\ ,$$

$$\alpha_k=\begin{bmatrix} 0 & \sigma_k\\ \sigma_k & 0\end{bmatrix}\quad\text{for } k=\chi,\theta,\phi\ ,$$

$$\sigma_\chi=(\sigma^1\cos\phi+\sigma^2\sin\phi)\sin\theta+\sigma^3\cos\theta\ ,$$

$$\sigma_\theta=(\sigma^1\cos\phi+\sigma^2\sin\phi)\cos\theta-\sigma^3\sin\theta\ ,$$

$$\sigma_\phi=-\sigma^1\sin\phi+\sigma^2\cos\phi\ ,$$

$$p_\chi=-\frac{i}{R\sin\chi}\frac{\partial}{\partial\chi}\sin\chi\ ,$$

$$\hat{K}=\beta\left[1-\alpha_\chi\left[\alpha_\theta\frac{\partial}{\partial\theta}+\frac{\alpha_\phi}{\sin\theta}\frac{\partial}{\partial\phi}\right]\right]$$

$$=\beta(1+\vec{\sigma}\cdot\vec{l}\,)\ ,$$

$\vec{\sigma}=(\sigma^1,\sigma^2,\sigma^3)$, and $\vec{l}$ is the usual orbital angular momentum. At the asymptotic flat limit ($R\to\infty$, $\chi\to 0$, $R\chi=r$), it is easily verified that

$$p_\chi\to p_r=-\frac{i}{r}\frac{\partial}{\partial r}r\ ,$$

$$W\to\overline{W}=-\frac{e}{\hbar c}\left[\alpha_r A_r+\frac{\alpha_\theta}{r}A_\theta+\frac{\alpha_\phi}{r\sin\theta}A_\phi\right]\ ,$$

and one finds again the usual flat-space expression of the Dirac equation in polar coordinates[24]

$$\left[\alpha_r\left[p_r+\frac{i\beta}{r}\hat{K}\right]+\overline{W}+\frac{mc}{\hbar}\beta-\frac{1}{\hbar c}(E_T-e\overline{V})\right]\overline{\psi}(r,\theta,\phi)=0\ , \tag{6}$$

$$\alpha_r=\alpha_\chi\ .$$

III. APPROXIMATE SOLUTION OF THE DIRAC EQUATION

When neglecting the magnetic interaction terms W in (5), the separation between small and large components of the "curved" Dirac spinor $\psi(\chi,\theta,\phi)$ can be achieved in the same way as in the flat space. Since, at the asymptotic flat limit, the function ψ must lead to the familiar Dirac function $\bar{\psi}(r,\theta,\phi)$, we set for ψ the following trial form

$$\psi(\chi,\theta,\phi)=\frac{1}{R\sin\chi}\begin{bmatrix}\mathscr{P}(\chi) & \mathscr{Y}_{ljm}\\ i\mathscr{Q}(\chi) & \mathscr{Y}_{\bar{l}jm}\end{bmatrix}, \tag{7}$$

where each $\mathscr{Y}_{ljm}$ spinor is a simultaneous eigenfunction of $\vec{l}^{\,2}$, $\vec{\sigma}^{\,2}$, $\vec{j}^{\,2}$, and j_z with eigenvalues $l(l+1)$, 3, $j(j+1)$, and m, respectively; $\vec{j}=\vec{l}+\frac{1}{2}\vec{\sigma}$ is the total angular momentum of the electron; $\bar{l}=l\pm1$ as $j=l\pm\frac{1}{2}$;

$$\mathscr{Y}_{ljm}=(-1)^{l-1/2+m}(2j+1)^{1/2}\times\sum_{m_s=\pm1/2}\begin{bmatrix}j & \frac{1}{2} & l\\ -m & m_s & m-m_s\end{bmatrix}\Phi^{(1/2)}_{m_s}Y_{l,m-m_s}\ , \tag{8}$$

where $Y_{l,m_l}(\theta,\phi)$ is a spherical harmonic and $\Phi^{(1/2)}$ a spinor with components $\Phi^{(1/2)}_{1/2}=\binom{1}{0}$ and $\Phi^{(1/2)}_{-1/2}=\binom{0}{1}$.

The following properties of the $\mathscr{Y}_{ljm}$ and $\mathscr{Y}_{\bar{l}jm}$ spinor hold[25]

$$(1+\vec{\sigma}\cdot\vec{l}\,)\mathscr{Y}_{ljm}=[j(j+1)-l(l+1)+\tfrac{1}{4}]\mathscr{Y}_{ljm}=-k\mathscr{Y}_{ljm}\ ,$$
$$(1+\vec{\sigma}\cdot\vec{l}\,)\mathscr{Y}_{\bar{l}jm}=k\mathscr{Y}_{\bar{l}jm},\quad\text{with } k=(-1)^{j+l+1/2}(j+\tfrac{1}{2})\ , \tag{9}$$
$$\sigma_\chi\mathscr{Y}_{ljm}=\mathscr{Y}_{\bar{l}jm}\ .$$

Finally, combining Eqs. (5), (7), and (9), and introducing the "curved" form $V=-(Ze/R)\cot\chi$ of the Coulomb potential,[14] one obtains the following coupled equations for the Dirac pseudoradial hydrogenic functions in the spherical three-space (in a.u.):

$$\frac{1}{R}\left[\frac{d}{d\chi}+\frac{k}{\sin\chi}\right]\mathscr{P}(\chi)=-\left[(1+\epsilon)c+\frac{Z\alpha}{R}\cot\chi\right]\mathscr{Q}(\chi)\ ,$$
$$\frac{1}{R}\left[\frac{d}{d\chi}-\frac{k}{\sin\chi}\right]\mathscr{Q}(\chi)=-\left[(1-\epsilon)c-\frac{Z\alpha}{R}\cot\chi\right]\mathscr{P}(\chi)\ , \tag{10}$$

where $\epsilon=E_T/mc^2$; $\alpha=1/c$ is the fine-structure constant and $\mathscr{Q}(\chi)$ can be identified with the traditional small component.

In order that $\psi(\chi,\theta,\phi)$ be normalized, the $\mathscr{P}(\chi)$ and $\mathscr{Q}(\chi)$ functions must satisfy the normalization condition

$$\int_0^\pi(\mathscr{P}^2+\mathscr{Q}^2)d\chi=1\ . \tag{11}$$

It is easily verified that, at the asymptotic flat-space limit, one finds again the usual Dirac radial hydrogenic coupled equations in flat space:[24]

$$\left[\frac{d}{dr}+\frac{k}{r}\right]\bar{P}(r)=-\left[(1+\bar{\epsilon})c+\frac{Z\alpha}{r}\right]\bar{Q}(r)\ ,$$
$$\left[\frac{d}{dr}-\frac{k}{r}\right]\bar{Q}(r)=-\left[(1-\bar{\epsilon})c-\frac{Z\alpha}{r}\right]\bar{P}(r)\ . \tag{12}$$

If analytical solutions of the "flat" coupled equations (12) are obtainable (see, for instance, Refs. 23, 26, or 27), this is not the case, to our knowledge, for the coupled equations (10) in a spherical three-space. An appropriate perturbational treatment of (10) can be undertaken after noting that

$$\frac{k}{R}\frac{1}{\sin\chi}=\frac{k}{R}\cot\chi+\frac{k}{2R^2}\left[2R\tan\frac{\chi}{2}\right]$$

and that, at the flat-space limit,

$$\frac{k}{2R^2}\left[2R\tan\frac{\chi}{2}\right]\to\frac{k}{2R^2}r\ ,$$

i.e., this last term is of an order of magnitude $1/R^2$ smaller than the remaining terms ($\simeq k/r$). Hence suitable unperturbed coupled equations to be considered are

$$\frac{1}{R}\left[\frac{d}{d\chi}+k\cot\chi\right]P(\chi)=-\left[(1+\epsilon)c+\frac{Z\alpha}{R}\cot\chi\right]Q(\chi)\ ,$$
$$\frac{1}{R}\left[\frac{d}{d\chi}-k\cot\chi\right]Q(\chi)=-\left[(1-\epsilon)c-\frac{Z\alpha}{R}\cot\chi\right]P(\chi)\ . \tag{13}$$

Following the Infeld-Hull factorization procedure[23] which has proved to be particularly elegant when solving Eqs. (12), let us set

$$P(\chi)=\mathscr{N}[(\gamma_2+\gamma_1)F(\chi)+(\gamma_2-\gamma_1)G(\chi)]\ ,$$
$$Q(\chi)=\mathscr{N}[(\gamma_2-\gamma_1)F(\chi)+(\gamma_2+\gamma_1)G(\chi)]\ , \tag{14}$$

where $\gamma_1=(k+Z\alpha)^{1/2}$, $\gamma_2=(k-Z\alpha)^{1/2}$, $\mathscr{N}$ is a normalization constant. After substituting the expression (14) for the couple P,Q into Eqs. (13), one gets

$$\frac{1}{R}\left[\gamma\cot\chi-\frac{ZR\epsilon}{\gamma}+\frac{d}{d\chi}\right]F(\chi)=-c\left[\frac{\epsilon k}{\gamma}+1\right]G(\chi)\ ,$$
$$\frac{1}{R}\left[\gamma\cot\chi-\frac{ZR\epsilon}{\gamma}-\frac{d}{d\chi}\right]G(\chi)=-c\left[\frac{\epsilon k}{\gamma}-1\right]F(\chi)\ , \tag{15}$$

where $\gamma=\gamma_1\gamma_2=(k^2-Z^2\alpha^2)^{1/2}$; since $Z<137$ and $|k|>1$, γ_1 and γ_2 are simultaneously real or pure imaginary quantities, it follows that γ is always real. After few manipulations, one obtains the separated second-order differential equations

$$\left[\frac{d^2}{d\chi^2}-\frac{\gamma(\gamma+1)}{\sin^2\chi}+2ZR\epsilon\cot\chi+R^2c^2(\epsilon^2-1)+\gamma^2\right]F(\chi)=0\;, \tag{16a}$$

$$\left[\frac{d^2}{d\chi^2}-\frac{\gamma(\gamma-1)}{\sin^2\chi}+2ZR\epsilon\cot\chi+R^2c^2(\epsilon^2-1)+\gamma^2\right]G(\chi)=0\;. \tag{16b}$$

Equations (16) are "curved" generalized Kepler wave equations and, within the Infeld and Hull classification[23] are type-E (class-I) factorizable equations (see Appendix B). From the comparison of Eqs. (16) with the Kepler equation (B1), it is easily found that the $F(\chi)$ and $G(\chi)$ functions are directly related to the Kepler $R_{SM}(\chi)$ functions [Eq. (B1)], when setting $q=ZR\epsilon$, $S=v+\gamma-1$, with $M=\gamma$ and $M=\gamma-1$ for the $F(\chi)$ and $G(\chi)$ functions, respectively. From the comparison of the coupled equations (15) with Eq. (B2), one gets

$$F(\chi)=\left[\frac{\epsilon k}{\gamma}+1\right]^{1/2}R_{v+\gamma-1,\gamma}\;,$$
$$G(\chi)=\left[\frac{\epsilon k}{\gamma}-1\right]^{1/2}R_{v+\gamma-1,\gamma-1}\;, \tag{17}$$

with the associated condition

$$R^2c^2(\epsilon^2-1)+\gamma^2=(v+\gamma)^2-Z^2R^2\epsilon^2/(v+\gamma)^2 \tag{18}$$

or

$$\epsilon^2=\left[1+\frac{Z^2\alpha^2}{(v+\gamma)^2}\right]^{-1}\left[1+\frac{\alpha^2}{R^2}v(v+2\gamma)\right]. \tag{19}$$

The normalization constant $\mathscr{N}$ in the expression (14) of P and Q is readily obtained by generalizing a procedure outlined in Ref. 9. One gets (see Appendix C)

$$\mathscr{N}=\left[\frac{\epsilon}{8\gamma}\right]^{1/2}\left[1+\frac{\alpha^2}{R^2}v(v+2\gamma)\right]^{-1/2}. \tag{20}$$

Finally, an approximate solution of the Dirac equation in a spherical three-space has been obtained in terms of the "curved" generalized Kepler functions R_{SM} and of the spherical spinors $\mathscr{Y}_{ljm}$ [see Eqs. (B4) and (8)]

$$\Phi_{vkm}=\frac{1}{R\sin\chi}\begin{bmatrix}P_{vk}\;\mathscr{Y}_{ljm}\\ iQ_{vk}\;\mathscr{Y}_{\bar{l}jm}\end{bmatrix}, \tag{21}$$

where

$$P_{vk}=\mathscr{N}\left[(\gamma_2+\gamma_1)\left[\frac{\epsilon k}{\gamma}+1\right]^{1/2}R_{v+\gamma-1,\gamma}+(\gamma_2-\gamma_1)\left[\frac{\epsilon k}{\gamma}-1\right]^{1/2}R_{v+\gamma-1,\gamma-1}\right],$$

$$Q_{vk}=\mathscr{N}\left[(\gamma_2-\gamma_1)\left[\frac{\epsilon k}{\gamma}+1\right]^{1/2}R_{v+\gamma-1,\gamma}+(\gamma_2+\gamma_1)\left[\frac{\epsilon k}{\gamma}-1\right]^{1/2}R_{v+\gamma-1,\gamma-1}\right].$$

It should be noted that, at the asymptotic flat limit, the $R_{SM}(\chi)$ functions reduce to the generalized Kepler function $\bar{R}_{SM}(r)$ [see Eq. (B7)] with $q=Z\bar{\epsilon}$,

$$\bar{\epsilon}=\left[1+\frac{Z^2\alpha^2}{(v+\gamma)^2}\right]^{-1/2}$$

and the expression (21) gives again the flat Dirac hydrogenic functions.

IV. FINE-STRUCTURE ENERGIES

The zeroth-order energy in our perturbational treatment of the Dirac equation, directly follows from the expression (19) of ϵ^2. Since $\epsilon=1+\alpha^2E^{(0)}$, one gets

$$E_{vk}^{(0)}=\frac{1}{\alpha^2}\left[\left[1+\frac{Z^2\alpha^2}{(v+\gamma)^2}\right]^{-1/2}\times\left[1+\frac{\alpha^2}{R^2}v(v+2\gamma)\right]^{1/2}-1\right]. \tag{22}$$

In order to include all the $1/R^2$ curvature contributions to the fine-structure energy levels, it is sufficient to calculate the first-order perturbation energy $E_{vk}^{(1)}$. Indeed, the Dirac equation can be written again

$$(\mathscr{H}_0+\mathscr{H}_1)\Psi_{vkm}=E_T\Psi_{vkm}\;, \tag{23}$$

where $\mathscr{H}_0$ is the zeroth-order Hamiltonian with eigenfunction Φ_{vkm} and eigenvalue $E_T^{(0)}=mc^2+E_{vk}^{(0)}$ and

$$\mathscr{H}_1=\frac{ic}{R}\left[\frac{1}{\sin\chi}-\cot\chi\right]\alpha_\chi\beta\hat{K}$$

or

$$\mathscr{H}_1=\frac{ic}{2R^2}\left[2R\tan\frac{\chi}{2}\right]\begin{bmatrix}0 & \sigma_\chi(1+\vec{\sigma}\cdot\vec{l}\,)\\ \sigma_\chi(1+\vec{\sigma}\cdot\vec{l}\,) & 0\end{bmatrix}.$$

As pointed out before, at the asymptotic flat-space limit $2R\tan(\chi/2)\to r$ and it is easily seen that $\mathscr{H}_1$ is of an order of magnitude $\sim 1/R^2$. The first-order perturbation energy is

$$E_{vk}^{(1)}=\langle\Phi_{vkm}\,|\,\mathscr{H}_1\,|\,\Phi_{vkm}\rangle\;. \tag{24}$$

Using the expression (21) of the Dirac spinor Φ_{vkm} together with the properties (9) of the $\mathscr{Y}_{ljm}$ and $\mathscr{Y}_{\bar{l}jm}$ spinors, one gets

$$E_{vk}^{(1)}=-\frac{kc}{R^2}\int_0^\pi\left[2R\tan\frac{\chi}{2}\right]P_{vk}Q_{vk}\,d\chi\;, \tag{25}$$

where the P_{vk} and Q_{vk} are linear combinations of the "curved" generalized Kepler $R_{v+\gamma-1,\gamma}$ and $R_{v+\gamma-1,\gamma-1}$ functions. The calculation of $E_{vk}^{(1)}$ is detailed in the Appendix C, one obtains

$$E_{vk}^{(1)}=-\frac{k}{4R^2}\left[1-2k\left[1+\frac{Z^2\alpha^2}{(v+\gamma)^2}\right]^{-1/2}\right]+O\left[\frac{1}{R^4}\right]. \tag{26}$$

Finally, including the curvature effects (up to $1/R^2$), the Dirac energy $E_{vk}=E_{vk}^{(0)}+E_{vk}^{(1)}$ is

$$E_{vk}=\frac{1}{\alpha^2}\left[\left[1+\frac{Z^2\alpha^2}{(v+\gamma)^2}\right]^{-1/2}-1\right]-\frac{k}{4R^2}+\frac{(v+\gamma)^2+Z^2\alpha^2}{2R^2}\left[1+\frac{Z^2\alpha^2}{(v+\gamma)^2}\right]^{-1/2}. \tag{27}$$

When retaining in E_{vk} the terms up to α^2 and introducing the usual radial quantum number $n=v+|k|$, one obtains

$$E_{nk}=-\frac{Z^2}{2n^2}+\frac{Z^4\alpha^2}{2n^3}\left[\frac{3}{4n}-\frac{1}{|k|}\right]+\frac{n^2}{2R^2}-\frac{k}{4R^2}+\frac{Z^2\alpha^2}{4R^2}\left[1-\frac{2n}{|k|}\right] \tag{28}$$

or alternatively

$$E_{nk}=-\frac{Z^2}{2n^2}\left[1-\frac{n^4}{Z^2R^2}\right]+\frac{3Z^4\alpha^2}{8n^4}\left[1+\frac{2n^4}{3Z^2R^2}\right]-\frac{Z^4\alpha^2}{2n^3|k|}\left[1+\frac{n^4}{Z^2R^2}\right]-\frac{k}{4R^2}. \tag{29}$$

The two first terms in (28) are just the electronic and fine-structure hydrogenic flat-space energies and the remaining terms correspond to additional curvature contributions which vanish at the asymptotic flat-space limit. From (29), it appears that the curvature modifications of the energies increase with n as n^4/Z^2R^2. The last term, $-k/4R^2$, will induce splittings in the hydrogenic spectrum which, qualitatively in some respects, are comparable to the Lamb effect. In Table I, these curvature modifications of the theoretical spectra are compared with the Lamb-shift contributions,[28]

$$w_{nlj}=\frac{Z^4\alpha^2}{n^3}\frac{\kappa}{k(2l+1)},$$

where $\kappa=1.159\,644\times10^{-3}$. Obviously, the curvature-induced splitting should be detectable and comparable to the Lamb shift, only in regions where the local curvature is really important. As pointed out by Parker,[4] the curvature contributions to the energy levels should be comparable to the Lamb shift for $R\simeq2\times10^{-3}$ cm.

V. "CURVED" DIRAC ORBITALS

In order to be somewhat consistent when gathering all the $1/R^2$ curvature contributions to the hyperfine-structure energies, it is necessary to determine, first, a solution of the Dirac equation containing all the $1/R^2$ terms of the exact eigenfunction. Since the perturbation $\mathscr{H}_1$ is of an order of magnitude $\sim 1/R^2$ [see Eq. (23)], one has to calculate the first-order perturbed function

$$\Psi_{vkm}=\Phi_{vkm}-\sum_{v',k',m'}\frac{\langle\Phi_{v'k'm'}|\mathscr{H}_1|\Phi_{vkm}\rangle}{E_{v'k'}-E_{vk}}\Phi_{v'k'm'}. \tag{30}$$

From (9), it follows that $\sigma_\chi(1+\vec{\sigma}\cdot\vec{l}\,)\mathscr{Y}_{\bar{l}jm}=k\mathscr{Y}_{ljm}$ and $\sigma_\chi(1+\vec{\sigma}\cdot\vec{l}\,)\mathscr{Y}_{ljm}=-k\mathscr{Y}_{\bar{l}jm}$, and therefore, since $\mathscr{H}_1$ is contradiagonal, one gets

$$\langle\Phi_{v'k'm'}|\mathscr{H}_1|\Phi_{vkm}\rangle=-\frac{k}{2R^2}\delta_{m'm}\delta_{k'k}T_{v'v}, \tag{31}$$

where

$$T_{v'v}=\frac{1}{\alpha}\int_o^\pi(P_{v'k}Q_{vk}+Q_{v'k}P_{vk})\left[2R\tan\frac{\chi}{2}\right]d\chi.$$

As long as we are concerned just by the evaluation of the $1/R^2$ contributions to ψ_{vkm}, it is easily inferred that $T_{v'v}$ can be replaced by its effective value, i.e., its asymptotic flat-space limit

$$\bar{T}_{v'v}=\frac{1}{\alpha}\int_0^\infty(\bar{P}_{v'k}\bar{Q}_{vk}+\bar{Q}_{v'k}\bar{P}_{vk})r\,dr. \tag{32}$$

TABLE I. Fine structure of the hydrogenic energy levels (in a.u.)

	Electronic energy	Flat fine structure	Curvature fine-structure contributions	Lamb shift
$E_{nd_{5/2}}$		$\frac{Z^4\alpha^2}{2n^3}\left[\frac{3}{4n}-\frac{1}{3}\right]$	$\frac{3}{4R^2}+\frac{Z^2\alpha^2}{4R^2}\left[1-\frac{2n}{3}\right]$	$\frac{Z^4\alpha^2}{n^3}\frac{\kappa}{15}$
$E_{nd_{3/2}}$		$\frac{Z^4\alpha^2}{2n^3}\left[\frac{3}{4n}-\frac{1}{2}\right]$	$-\frac{1}{2R^2}$; $+\frac{Z^2\alpha^2}{4R^2}(1-n)$	$-\frac{Z^4\alpha^2}{n^3}\frac{\kappa}{10}$
$E_{np_{3/2}}$	$\frac{-Z^2}{2n^2}+\frac{n^2}{2R^2}$		$\frac{1}{2R^2}$	$\frac{Z^4\alpha^2}{n^3}\frac{\kappa}{6}$
$E_{np_{1/2}}$		$\frac{Z^4\alpha^2}{2n^3}\left[\frac{3}{4n}-1\right]$	$-\frac{1}{4R^2}$; $+\frac{Z^2\alpha^2}{4R^2}(1-2n)$	$-\frac{Z^4\alpha^2}{n^3}\frac{\kappa}{3}$
$E_{ns_{1/2}}$			$\frac{1}{4R^2}$	$\frac{Z^4\alpha^2}{n^3}\kappa$

The $\bar{P}_{vk}$ and $\bar{Q}_{vk}$ functions are given by (21) where the curved generalized Kepler $R_{SM}(\chi)$ functions are replaced by the flat ones $\bar{R}_{SM}(r)$. The calculations of $\bar{T}_{v'v}$ in terms of the flat radial integrals $\langle S',M \mid r \mid S,M \rangle$ and $\langle S',M-1 \mid r \mid S,M-1 \rangle$ is detailed in the Appendix C and, finally, the "curved" Dirac orbitals can be written

$$\psi_{vkm}=\Phi_{vkm}-\frac{1}{R^2}\sum_{v'(\neq v)} c_{v'v}\Phi_{v'km} , \tag{33}$$

where

$$c_{v'v}=\frac{k}{Z^2}\frac{[(v+|k|)(v'+|k|)]^2}{(v-v')(v+v'+2|k|)}\bar{T}_{v'v} .$$

Let us remark that, owing to the $1/R^2$ factor in (33), in the practical computation of a matrix element $\langle \psi_{vkm} \mid W \mid \psi_{vkm} \rangle$ (up to $1/R^2$) the off-diagonal $v'\neq v$ generated matrix elements between the Φ_{vkm} functions can be replaced by their flat evaluation.

VI. DIRAC HYPERFINE-STRUCTURE ENERGIES

As usually done, we shall limit ourselves to the consideration of the dipolar magnetic and quadrupolar electric hyperfine-structure interactions.

A. Dipolar magnetic hyperfine interaction

Infeld and Schild[29] have already examined the solutions of Maxwell equations with a singularity at the spatial origin. Particularly, for the case of a spherical three-space, they have given the expressions of the vector potential components A_k in terms of the eigenfunctions of a differential equation. Starting from their results, we have obtained the following expression of the vector potential components associated with a static magnetic dipole moment $\vec{\mu}_N=\mu_N\vec{k}$ lying along the z axis:[10]

$$A_1=A_2=0,\ \ A_3=(\mu_N/R)\cot\chi\,\sin^2\theta . \tag{34}$$

Consequently, one gets the following expression of the dipolar magnetic hyperfine interaction [see Eq. (5)]:

$$W_D=-\frac{e}{\hbar c}\frac{\mu_N}{R^2}\frac{\cos\chi}{\sin^2\chi}\sin\theta\begin{bmatrix}0 & \sigma_\phi\\ \sigma_\phi & 0\end{bmatrix} . \tag{35}$$

In order to derive the dipolar magnetic hyperfine Hamiltonian in a spherical three-space, let us introduce the local Cartesian unit vector $(\vec{i},\vec{j},\vec{k})$ with origin 0 ($\chi=0$) and the unit vectors $(\vec{u}_\chi,\vec{u}_\theta,\vec{u}_\phi)$ associated with the spherical coordinates,

$$\begin{aligned}\vec{u}_\chi&=\sin\theta(\cos\phi\,\vec{i}+\sin\phi\,\vec{j})+\cos\theta\,\vec{k} ,\\ \vec{u}_\theta&=\cos\theta(\cos\phi\,\vec{i}+\sin\phi\,\vec{j})-\sin\theta\,\vec{k} ,\\ \vec{u}_\phi&=-\sin\phi\,\vec{i}+\cos\phi\,\vec{j} .\end{aligned} \tag{36}$$

Introducing the tensorial notation $C^{(1)}$ of $\vec{u}$ and $\sigma^{(1)}$ of $\vec{\sigma}$, it is easily verified that

$$\sin\theta\,\sigma_\phi=-i\sqrt{2}(C^{(1)}\sigma^{(1)})^{(1)}_0 . \tag{37}$$

Hence the dipolar magnetic hyperfine Hamiltonian in a spherical three-space is

$$W_D=\begin{bmatrix}0 & \mathscr{H}_D\\ \mathscr{H}_D & 0\end{bmatrix}$$

where

$$\mathscr{H}_D=2i\sqrt{2}\mu_\beta\beta_N\left[\frac{\mu_N}{I}\right]\frac{\cos\chi}{R^2\sin^2\chi}\vec{I}\cdot(C^{(1)}\sigma^{(1)})^{(1)} , \tag{38}$$

where μ_β and β_N are the Bohr and nuclear magneton and μ_N and I, the values of the dipolar magnetic moment and spin of the nucleus.

At the asymptotic flat-space limit, the expression (38) reduces to the well known flat-space expression (39)

$$\bar{\mathscr{H}}_D=2i\sqrt{2}\mu_\beta\beta_N\left[\frac{\mu_N}{I}\right]\frac{1}{r^2}\vec{I}\cdot(C^{(1)}\sigma^{(1)})^{(1)} . \tag{39}$$

The determination of the dipolar magnetic hyperfine energies $\langle \psi_{vkm} \mid W_D \mid \psi_{vkm} \rangle$ in a spherical three-space amounts to calculate two types of integrals: one involving the spin and angular (θ,ϕ) variables which, as expected, is the same as in flat space[25]

$$\langle \mathscr{Y}_{ljm} \mid (C^{(1)}\sigma^{(1)})^{(1)}_q \mid \mathscr{Y}_{l'j'm'} \rangle=(-1)^{j+l'-m+1}\delta_{l',l\pm1}[(2j+1)(2j'+1)]^{1/2}\begin{bmatrix}j & 1 & j'\\ -m & q & m'\end{bmatrix}\begin{bmatrix}j' & 1 & j\\ -\frac{1}{2} & 1 & \frac{1}{2}\end{bmatrix} \tag{40}$$

and the other, i.e., the pseudoradial integral involving the hyperspherical variable χ is

$$f_D(v',v)=\int_0^\pi (P_{v'k}Q_{vk}+Q_{v'k}P_{vk})\frac{\cos\chi}{R^2\sin^2\chi}d\chi . \tag{41}$$

When computing off-diagonal $f_D(v\neq v')$ this integral can be replaced by its asymptotic flat limit owing to the remarks on the order of magnitudes (in $1/R^2$) (see Sec. V)

$$\bar{f}_D(v',v)=\int_0^\infty (\bar{P}_{v'k}\bar{Q}_{vk}+\bar{Q}_{v'k}\bar{P}_{vk})r^{-2}dr . \tag{42}$$

The computation of f_D for $v'=v$ is detailed in the Appendix C.

B. Quadrupolar electric hyperfine interaction

The expression of the quadrupolar electric interaction directly follows from the multipolar expansion of the Coulombic interaction between two particules i and j, which has been derived in Ref. 7

$$\frac{1}{R}\cot\omega_{ij}=\frac{1}{R}\cot\chi_>+\sum_{l=1}^{\infty}C_i^{(l)}C_j^{(l)}\mathscr{F}_l(\chi_>)\mathscr{G}_l(\chi_<) , \tag{43}$$

where

$$\mathscr{F}_l(\chi)=\frac{1}{(2l-1)!!}(\sin\chi)^l\left[\frac{d}{d(\cos\chi)}\right]^l(\cot\chi)\ ,$$

$$\mathscr{G}_l(\chi)=\frac{(-1)^{l+1}(2l+1)!!}{(l-1)!(l+1)!}(\sin\chi)^l\left[\frac{d}{d(\cos\chi)}\right]^l(\chi\cot\chi)\ ,$$

$\chi_<$ and $\chi_>$ have the usual meaning. As it has been verified,[7] at the asymptotic flat limit, the $\mathscr{F}_l(\chi)$ and $\mathscr{G}_l(\chi)$ functions converge to the flat radial harmonic functions $(1/r)^{l+1}$ and r^l, respectively.

If one introduces the curved expression of the quadrupole moment of the nucleus

$$Q_N^{(2)}=\sum_n e_n g_e C^{(2)}(\theta_n,\phi_n)\mathscr{G}_2(\chi_n)\ , \tag{44}$$

where e_n, g_e, and $(\chi_n\theta_n\phi_n)$ are, respectively, the charge, the orbital gyromagnetic factor, and the coordinates of nucleon n, one gets the following expression for the quadrupolar electric hyperfine interaction:

$$W_Q=-e(\cos\chi/R^3\sin^3\chi)C^{(2)}\cdot Q_N^{(2)}\ . \tag{45}$$

At the asymptotic flat limit, one finds again the classical expression

$$\overline{W}_Q=-(e/r^3)C^{(2)}\cdot Q_N^{(2)}\ . \tag{46}$$

The determination of the quadrupolar electric hyperfine energies $\langle\psi_{vkm}\mid W_Q\mid\psi_{vkm}\rangle$ in a spherical three-space leads to the calculation of the following integrals:

$$\langle\mathscr{Y}_{ljm}\mid C_q^{(2)}\mid\mathscr{Y}_{l'j'm'}\rangle=(-1)^{2j-m+1/2}[(2j+1)(2j'+1)]^{1/2}\begin{bmatrix} j & 2 & j' \\ -m & q & m'\end{bmatrix}\begin{bmatrix} j & 2 & j' \\ \frac{1}{2} & 0 & -\frac{1}{2}\end{bmatrix} \tag{47}$$

and

$$f_Q(v',v)=\int_0^{\pi}(P_{v'k}P_{vk}+Q_{v'k}Q_{vk})\frac{\cos\chi}{R^3\sin^3\chi}d\chi\ . \tag{48}$$

When calculating f_Q the same arguments as before when calculating f_D hold and one can replace the off-diagonal $v'\neq v$ integrals f_Q by their flat definition

$$\bar{f}_Q(v',v)=\int_0^{\infty}(\bar{P}_{v'k}\bar{P}_{vk}+\bar{Q}_{v'k}\bar{Q}_{vk})r^{-3}dr\ . \tag{49}$$

VII. NONRELATIVISTIC FINE- AND HYPERFINE-STRUCTURE HAMILTONIANS

One could obtain the nonrelativistic expressions of the fine and hyperfine Hamiltonians after separating the small and large component of the Dirac spinor. Indeed, setting

$$\psi=\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}$$

and $W=W_D$ in the Dirac equation (5), one gets

$$\psi_2=\frac{\hbar}{2mc}\omega(\chi)\left[\sigma_\chi\hat{\Pi}-\frac{e\mu}{\hbar c}\frac{\cos\chi}{R^2\sin^2\chi}\sigma_\phi\sin\theta\right]\psi_1\ ,$$
$$(H_0+H_1+H_D-E)\psi_1=0\ , \tag{50}$$

where

$$\omega(\chi)=\left[1+\frac{E-eV}{2mc^2}\right]^{-1}\ ,$$

$$\hat{\Pi}=p_\chi+\frac{i(1+\vec{\sigma}\cdot\vec{l}\,)}{R\sin\chi}\ ,$$

$$H_0+H_1=V+\frac{\hbar^2}{2m}\sigma_\chi\hat{\Pi}\omega(\chi)\sigma_\chi\hat{\Pi}\ ,$$

$$H_D=-2\mu_\beta\mu_N\omega(\chi)\frac{\cos\chi}{R^2\sin^2\chi}\sin\theta(\sigma_\chi\hat{\Pi}\sigma_\phi+\sigma_\phi\sigma_\chi\hat{\Pi})\ .$$

In this last expression, the μ_N^2 term has been disregarded owing to its relative order of magnitude. Using the expression

$$(\vec{\sigma}\cdot\vec{l}\,)=-i\sigma_\phi\frac{\partial}{\partial\theta}+i\sigma_\theta\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}$$

and since the Pauli matrices satisfy $\sigma_\chi\sigma_\theta=i\sigma_\phi$ (cyclic), one obtains the anticommutation property $(1+\vec{\sigma}\cdot\vec{l}\,)\sigma_\chi=-\sigma_\chi(1+\vec{\sigma}\cdot\vec{l}\,)$. After a little rearrangement using this last property and the expression (5) of p_χ, one finds

$$H_0=-\frac{1}{2R^2\sin^2\chi}\left[\frac{\partial}{\partial\chi}\left[\sin^2\chi\frac{\partial}{\partial\chi}\right]-l^2\right]+V\ ,$$
$$H_1=\frac{\alpha^2}{2}\vec{l}\cdot\vec{s}\frac{1}{R^2\sin\chi}\frac{dV}{d\chi}-\frac{\alpha^2}{2}(E-V)^2+\frac{\alpha^2}{8}\Delta V$$
$$+\left[\frac{1}{2}+\vec{l}\cdot\vec{s}\right]\frac{1-\cos\chi}{R^2\sin^2\chi}+\frac{1}{2R^2}+\frac{Z\alpha^2(1-\cos\chi)}{4R^3\sin^3\chi}\ , \tag{51}$$

where $\vec{s}=\frac{1}{2}\vec{\sigma}$ and $\omega(\chi)\simeq1-(\alpha^2/2)(E-V)$.

Since one can write

$$\mu_N\sin\theta\,\sigma_\theta=2[(\vec{\mu}_N\cdot\vec{u})(\vec{s}\cdot\vec{u})-(\vec{\mu}_N\cdot\vec{s}\,)]\ ,$$
$$\mu_N\cos\theta\,\sigma_\chi=2(\vec{\mu}_N\cdot\vec{u})(\vec{s}\cdot\vec{u})\ ,$$

where $\vec{u}$ is the unit vector defined by (36), one finds

$$H_D=-2\mu_\beta(\vec{\mu}_N\cdot\vec{l}\,)\frac{\cos\chi}{R^3\sin^3\chi}$$
$$+2\mu_\beta\vec{\mu}_N\cdot\frac{\vec{s}-(1+2\cos\chi)(\vec{u}\cdot\vec{s}\,)\vec{u}}{R^3\sin^3\chi}$$
$$-\mu_\beta\vec{\mu}_N\cdot[\vec{s}-(\vec{u}\cdot\vec{s}\,)\vec{u}]\frac{1}{R^3\sin^2\chi}\frac{d\omega}{d\chi}$$
$$-2\mu_\beta\vec{\mu}_N\cdot[\vec{s}-(\vec{u}\cdot\vec{s}\,)\vec{u}]\frac{(1-\cos\chi)\cos\chi}{R^3\sin^3\chi}\ , \tag{52}$$

where $\mu_\beta=e\hbar/2mc$ is the Bohr magneton.

These expressions (51) and (52) can be compared with the flat expressions

$$\bar{H}_0=-\frac{1}{2r^2}\left[\frac{\partial}{\partial r}\left[r^2\frac{\partial}{\partial r}\right]-l^2\right]+V\,,$$
$$\bar{H}_1=\frac{\alpha^2}{2}\vec{l}\cdot\vec{s}\,\frac{1}{r^2}\frac{dV}{dr}-\frac{\alpha^2}{2}(E-V)^2+\frac{\alpha^2}{8}\Delta V\,, \qquad (53)$$
$$\bar{H}_D=-2\mu_\beta(\vec{\mu}_N\cdot\vec{l}\,)\frac{1}{r^3}+2\mu_\beta\vec{\mu}_N\cdot\left[\vec{s}-\frac{3(\vec{s}\cdot\vec{r})\vec{r}}{r^2}\right]\frac{1}{r^3}$$
$$-\mu_\beta\vec{\mu}_N\cdot\left[\vec{s}-\frac{(\vec{s}\cdot\vec{r})\vec{r}}{r^2}\right]\frac{1}{r^2}\frac{d\bar{\omega}}{dr}\,.$$

One recognizes in (51), the curved form of the Schrödinger Hamiltonian H_0, of the one-electron fine-structure Hamiltonian H_1 completed by an additional term which vanishes at the flat limit, and in (52), the curved form of the dipolar magnetic hyperfine-structure Hamiltonian where the third term, after averaging considerations, leads to the Fermi contact term[30] and the last term vanishes, at the asymptotic flat limit. These expressions had been recently obtained via the covariant form of the Pauli equation.[8,10] Finally, the pseudoradial fine-structure and hyperfine-structure integrals originating from the "curved" expressions (51) and (52) of the Hamiltonians can be calculated when using the results of Appendix B with $S=n-1$ and $M=l$.

VIII. CONCLUSION

Finally, we have proposed a geometrically simple heuristic model in order to roughly investigate the space-curvature effects in atomic structure calculations. Since space-curvature concept is deeply rooted in the relativity theory, it seems theoretically more consistent to build up the model with Dirac orbitals rather than with nonrelativistic orbitals. Indeed, spin-curvature interaction terms have been more naturally introduced than in our preliminary nonrelativistic studies.[7–10] Two specific close approximations of the Dirac functions in a spherical three-space have been obtained which both are expressed in terms of the curved generalized Kepler functions.

Although the approximate curved Dirac functions (Sec. III) do not carry the correct $1/R^2$ dependence, they are of interest owing to their closed expression for constructing orbital basis for many-electron calculations. Nevertheless, the more elaborate ones (Sec. V) are more suitable for hydrogenic atoms.

The calculation of Dirac matrix elements of Hermitian operators has been rendered as tractable in the spherical three-space as in the flat space. An efficient ladder operator procedure has been devised for obtaining closed-form expressions of the Kepler integrals in terms of the quantum numbers. This technique has avoided a problematical termwise integration (noninteger quantum numbers).

Physically, we have put in evidence the curvature modifications of the flat fine-structure hydrogenic energy levels: curvature-induced shifts of the nondegenerate levels and splitting of the degenerate levels. These results generalize the nonrelativistic ones obtained in a restricted case[8] ($l=n-1$ and $l=n-2$ levels[31]). It should be noted that this space-curvature splitting of degenerate levels which, in some respects, compare with the Lamb shift, is independent of n. Obviously, this curvature induced splitting $\Delta_c \simeq k/4R^2$ of the degenerate levels should be detectable only if R is extremely small. Nevertheless, such a tractable model, putting in evidence the quantum number (n,k) dependence of the space-curvature modifications of the spectra could contribute to distinguish between the space-curvature effects and the other small perturbations of the spectra such as radiative corrections, nuclear effects, etc., and to extract from atomic spectra some specific information about the local curvature at the position of a highly excited astrophysical ion.

On the other hand, as pointed out by Teague and Thomas,[32] there could be some practical interest of casting quantum-mechanical problems in a spherical three-space since the complete set of basis functions involves only discrete functions. Moreover, the use of the curved model may also present some advantages in many-center molecular problems when changing of center. These points need a more elaborate investigation and will be discussed elsewhere.

APPENDIX A: DETERMINATION OF DIRAC EQUATION IN A SPHERICAL THREE-SPACE

The spin covariant derivatives of a spinor and of a matrix are, respectively,

$$\hat{\nabla}_\mu\psi=\frac{\partial\psi}{\partial\chi^\mu}+i\left[\frac{e}{\hbar c}A_\mu+\Gamma_\mu\right]\psi\,,$$
$$\hat{\nabla}_\mu B_{\nu\rho\cdots}=B_{\nu\rho\cdots;\mu}+i[\Gamma_\mu,B_{\nu\rho\cdots}]\,, \qquad (A1)$$

where the subscripts $;\mu$ stand for the covariant derivative, the Γ_μ are the Fock-Ivanenko matrices and the A_μ are the electromagnetic four-vector components.

The covariant derivative of a vector ϕ^ν is defined in terms of the Christoffel symbols

$$\phi^\nu{}_{;\mu}=\frac{\partial\phi^\nu}{\partial\chi^\mu}+\Gamma^\nu{}_{\alpha\mu}\phi^\alpha\,,$$
$$\phi_{\nu;\mu}=\frac{\partial\phi_\nu}{\partial\chi^\mu}-\Gamma^\alpha{}_{\nu\mu}\phi_\alpha\,, \qquad (A2)$$

where, following from the vanishing condition $g_{\nu\mu;\alpha}=0$, the Christoffel symbols are

$$\Gamma^\nu{}_{\alpha\mu}=\frac{1}{2}g^{\nu\rho}\left[\frac{\partial g_{\alpha\rho}}{\partial\chi^\mu}+\frac{\partial g_{\mu\rho}}{\partial\chi^\alpha}-\frac{\partial g_{\alpha\mu}}{\partial\chi^\rho}\right],$$
$$\Gamma^\nu{}_{\alpha\mu}=\Gamma^\nu{}_{\mu\alpha}\,. \qquad (A3)$$

The Fock-Ivanenko matrices Γ_μ are obtained from the vanishing condition

$$\hat{\nabla}_\mu\tilde{\gamma}_\nu=\gamma_{\nu;\mu}+i[\Gamma_\mu,\tilde{\gamma}_\nu]=0 \qquad (A4)$$

and are given by the expression

$$\Gamma_\mu=-\tfrac{1}{4}i\tilde{\gamma}^\nu\tilde{\gamma}_{\nu;\mu}\,. \qquad (A5)$$

It is easily found that a convenient choice of the Dirac matrices $\tilde{\gamma}^{\mu}(\chi)$ which obey the anticommutation relations (2) and lead to the usual polar dependence (θ,ϕ) of the Dirac wave function is

$$\begin{aligned}
&\tilde{\gamma}^0=\gamma^0 ,\\
&\tilde{\gamma}^1=(1/R)(\gamma^1\sin\theta\cos\phi+\gamma^2\sin\theta\sin\phi+\gamma^3\cos\theta) ,\\
&\tilde{\gamma}^2=(R\sin\chi)^{-1}(\gamma^1\cos\theta\cos\phi+\gamma^2\cos\theta\sin\phi-\gamma^3\sin\theta) ,\\
&\tilde{\gamma}^3=(R\sin\chi\sin\theta)^{-1}(-\gamma^1\sin\phi+\gamma^2\cos\phi) ,
\end{aligned} \tag{A6}$$

where the γ^{μ} are the constant Dirac matrices

$$\begin{aligned}
&\gamma^0=\beta=\begin{bmatrix} I & 0\\ 0 & -I\end{bmatrix},\quad \gamma^k=\begin{bmatrix} 0 & \sigma^k\\ -\sigma^k & 0\end{bmatrix},\quad k=1,2,3\\
&I=\begin{bmatrix} 1 & 0\\ 0 & 1\end{bmatrix},\quad \sigma^1=\begin{bmatrix} 0 & 1\\ 1 & 0\end{bmatrix},\\
&\sigma^2=\begin{bmatrix} 0 & -i\\ i & 0\end{bmatrix},\quad \sigma^3=\begin{bmatrix} 1 & 0\\ 0 & -1\end{bmatrix}.
\end{aligned} \tag{A7}$$

These constant Dirac matrices γ^{μ} obey the anticommutation relations (2) where $g^{\mu\nu}$ is the Lorentz diagonal constant metric $(1,-1,-1,-1)$.

From the above definitions, the nonvanishing Christoffel symbols and the Fock-Ivanenko matrices in a curved space-time with line element (3) are found to be

$$\begin{aligned}
&\Gamma^1_{22}=-\sin\chi\cos\chi,\quad \Gamma^1_{33}=-\sin\chi\cos\chi\sin^2\theta ,\\
&\Gamma^2_{33}=-\sin\theta\cos\theta,\quad \Gamma^2_{12}=\Gamma^2_{21}=\Gamma^3_{13}=\Gamma^3_{31}=\cot\chi ,\\
&\Gamma^3_{23}=\Gamma^3_{32}=\cot\theta,\quad \Gamma_0=\Gamma_1=0 ,\\
&\Gamma_k=\frac{i}{2}\frac{1-\cos\chi}{\sin\chi}\tilde{\gamma}_k\tilde{\gamma}^1 \quad \text{for } k=2,3 .
\end{aligned} \tag{A8}$$

One obtains for stationary states, expression (4) of the Dirac equation.

APPENDIX B: GENERALIZED KEPLER FUNCTIONS AND MATRIX ELEMENTS

1. Solution of the Kepler eigenequation

The "curved" generalized Kepler functions $R_{SM}(\chi)$ are solutions of the Infeld-Hull type-E (class-I) factorizable equation of the standard form[23]

$$\left[\frac{d^2}{d\chi^2}-\frac{M(M+1)}{\sin^2\chi}+2q\cot\chi+\lambda_S\right]R_{SM}(\chi)=0 \tag{B1}$$

with $0\le\chi\le\pi$. The associated quantization condition is $S-M=v$, where v is a non-negative integer ($v=0,1,2,\ldots$). Hence the normalized eigenfunctions $R_{SM}(\chi)$ are solutions of the following pair of difference differential equations:

$$\begin{aligned}
&H_M^-R_{SM}=\Lambda_S(M)R_{S,M-1} ,\\
&H_M^+R_{S,M-1}=\Lambda_S(M)R_{SM} ,\\
&\Lambda_S(M)=[\lambda_S-L(M)]^{1/2},\quad \lambda_S=L(S+1) ,
\end{aligned} \tag{B2}$$

where the ladder operators $H_M^{\pm}$ and associated factorization function are

$$\begin{aligned}
&H_M^{\pm}=M\cot\chi-\frac{q}{M}\mp\frac{d}{d\chi} ,\\
&L(M)=M^2-q^2/M^2 .
\end{aligned} \tag{B3}$$

Analytical expressions of the R_{SM} functions in terms of the quantum numbers are known[33]

$$R_{SM}(\chi)=N_v(\sin\chi)^{S+1}\exp[-q\chi/(S+1)]P_v^{a,a^*}(-i\cot\chi) , \tag{B4}$$

where $a=-(S+1)+iq/(S+1)$ and, in spite of the presence of the imaginary quantities, the Jacobi polynomials P_v^{a,a^*} in (16) are real polynomials in $\cot\chi$; N_v is a normalization constant.

In flat space, the generalized Kepler functions $\bar{R}_{SM}(r)$ are solutions of the Infeld-Hull type-F (class-I) factorizable equation of the standard form[23]

$$\left[\frac{d^2}{dr^2}-\frac{M(M+1)}{r^2}+\frac{2\bar{q}}{r}+\bar{\lambda}_S\right]\bar{R}_{SM}(r)=0 \tag{B5}$$

with $0\le r<\infty$.

The normalized eigenfunctions $\bar{R}_{SM}(r)$ are solutions of (B2) where the ladder operators $\bar{H}_M^{\pm}$ and associated factorization function are

$$\begin{aligned}
&\bar{H}_M^{\pm}=\frac{M}{r}-\frac{\bar{q}}{M}\mp\frac{d}{dr} ,\\
&\bar{L}(M)=-\bar{q}^2/M^2 .
\end{aligned} \tag{B6}$$

The analytical expression of the $\bar{R}_{SM}(r)$ function is[33]

$$\bar{R}_{SM}(r)=\bar{N}_v r^{M+1}\exp[-\bar{q}r/(S+1)]L_v^{2M+1}(2\bar{q}r/S+1) . \tag{B7}$$

Let us note that when setting $M=\gamma$, $S=v+\gamma-1$ $(v=0,1,\ldots)$, the expression (B4) with $q=ZR\epsilon$ in the spherical three-space [or the expression (B7) with $\bar{q}=Z\epsilon$ in the flat space] identifies to the generalized Kepler functions. When setting $M=l$, $S=n-1$ $(n=1,2,\ldots)$, and $q=ZR$ in the spherical three-space (or $\bar{q}=Z$ in the flat space), the expression (B4) [or (B7)] identifies to the "curved" (or "flat") hydrogenic radial functions.

2. Relations between matrix elements

As pointed out in Ref. 9, since the $R_{SM}(\chi)$ [and the $\bar{R}_{SM}(r)$] are eigenfunctions of factorizable equations, there exist particular relations between matrix elements of any derivable function. Full advantage of these relations is taken in order to obtain closed-form expressions of the radial Dirac integrals in terms of the quantum numbers. Using the expression (B3) of the ladder operators, one can write

$$\cot\chi=\frac{q}{M^2}+\frac{1}{2M}(H_M^++H_M^-) \tag{B8a}$$

and/or

$$\cot\chi=\frac{q}{(M-1)^2}+\frac{1}{2(M-1)}(H_{M-1}^{+}+H_{M-1}^{-})\ . \tag{B8b}$$

Then, using the Eqs. (B2) together with the mutual adjointness property of H_M^+ and H_M^-, one gets alternative expressions for a same matrix element involving any derivable function $f(\chi)$

$$\begin{aligned}\langle S',M-1\,|\,f\cot\chi\,|\,S,M-1\rangle&=\frac{q}{M^2}\langle S',M-1\,|\,f\,|\,S,M-1\rangle-\frac{1}{2M}\left\langle S',M-1\left|\frac{df}{d\chi}\right|S,M-1\right\rangle\\&\quad+\frac{1}{2M}[\Lambda_S(M)\langle S',M-1\,|\,f\,|\,S,M\rangle+\Lambda_{S'}(M)\langle S',M\,|\,f\,|\,S,M-1\rangle]\end{aligned} \tag{B9a}$$

$$\begin{aligned}&=\frac{q}{(M-1)^2}\langle S',M-1\,|\,f\,|\,S,M-1\rangle+\frac{1}{2(M-1)}\left\langle S',M-1\left|\frac{df}{d\chi}\right|S,M-1\right\rangle\\&\quad+\frac{1}{2(M-1)}[\Lambda_S(M-1)\langle S',M-1\,|\,f\,|\,S,M-2\rangle\\&\quad+\Lambda_{S'}(M-1)\langle S',M-2\,|\,f\,|\,S,M-1\rangle]\ .\end{aligned} \tag{B9b}$$

It is easily verified that relations analogous to (B9) hold in flat space with r^{-1} and df/dr in the place of $\cot\chi$ and $df/d\chi$.

3. Analytical expressions of the diagonal ($S'=S$) matrix elements

Let us set $S'=S$ in (B9) and introduce the shortened notation $\langle S,M\,|\,f\,|\,S,M'\rangle=\langle M\,|\,f\,|\,M'\rangle$ and $\Lambda_S(M)=\Lambda(M)$. First, setting $f=1$ in (B9), one gets

$$\begin{aligned}\langle M-1\,|\cot\chi\,|\,M-1\rangle&=\frac{q}{M^2}+\frac{\Lambda(M)}{M}\langle M-1\,|\,M\rangle\\&=\frac{q}{(M-1)^2}+\frac{\Lambda(M-1)}{M-1}\langle M-2\,|\,M-1\rangle\ .\end{aligned} \tag{B10}$$

Therefore, this matrix element (B10) must be independent of M and, since $\Lambda(S+1)=0$, it is equal to $q/(S+1)^2$. One gets for any value of M

$$\langle S,M\,|\cot\chi\,|\,S,M\rangle=q/(S+1)^2\ . \tag{B11}$$

Setting in (B9) $f=\cot\chi$, $f\cot\chi=(1/\sin^2\chi)-1$ and using (B11), one gets, after some rearrangements

$$\begin{aligned}(M-\tfrac{1}{2})\left\langle M-1\left|\frac{1}{\sin^2\chi}\right|M-1\right\rangle&=M+\frac{q^2}{M(S+1)^2}+\Lambda(M)\langle M-1\,|\cot\chi\,|\,M\rangle\\&=(M-1)+\frac{q^2}{(M-1)(S+1)^2}+\Lambda(M-1)\langle M-2\,|\cot\chi\,|\,M-1\rangle\ .\end{aligned} \tag{B12}$$

Using the same arguments as above, it follows that both right sides of (B12) are equal to $(S+1)+q^2/(S+1)^3$ and one gets

$$\left\langle S,M\left|\frac{1}{\sin^2\chi}\right|S,M\right\rangle=\frac{q^2}{(M+\frac{1}{2})(S+1)^3}\left[1+\frac{(S+1)^4}{q^2}\right]\ . \tag{B13}$$

Setting in (B9), $f=1/\sin^2\chi$, one gets

$$\begin{aligned}M(M-1)\left\langle M-1\left|\frac{\cos\chi}{\sin^3\chi}\right|M-1\right\rangle-q\left\langle M-1\left|\frac{1}{\sin^2\chi}\right|M-1\right\rangle&=M\Lambda(M)\left\langle M-1\left|\frac{1}{\sin^2\chi}\right|M\right\rangle\\&=(M-1)\Lambda(M-1)\left\langle M-2\left|\frac{1}{\sin^2\chi}\right|M-1\right\rangle\ .\end{aligned} \tag{B14}$$

Therefore, the left side of (B14) is independent of M and equal to zero. Using (B13), one gets

$$\left\langle S,M\left|\frac{\cos\chi}{\sin^3\chi}\right|S,M\right\rangle=\frac{q^3}{(S+1)^3M(M+1)(M+\frac{1}{2})}\left[1+\frac{(S+1)^4}{q^2}\right]\ . \tag{B15}$$

Setting in (B9)

$$f=\frac{\cos\chi}{\sin^3\chi},\quad \frac{df}{d\chi}=-\frac{3\cos^2\chi}{\sin^4\chi}-\frac{1}{\sin^2\chi}\ ,$$

using both (B13) and (B14) and noting that $-M=-2M^2+M(2M-1)$, $M-1=-2(M-1)^2+(M-1)(2M-1)$, one gets, after a little manipulation

$$\begin{aligned}
&(2M-3)(2M-1)(2M+1)M(M-1)\left\langle M-1\left|\frac{\cos^2\chi}{\sin^4\chi}\right|M-1\right\rangle\\
&\quad=\frac{4q^2}{(S+1)^3}\left[1+\frac{(S+1)^4}{q^2}\right]\left[\frac{2M+1}{M}q^2+(2M+1)M^2(M-1)-\tfrac{1}{2}M(M-1)(2M-1)(2M+1)\right]\\
&\qquad+2M(M-1)(2M-1)(2M+1)\Lambda(M)\left\langle M-1\left|\frac{\cos\chi}{\sin^3\chi}\right|M\right\rangle\\
&\quad=\frac{4q^2}{(S+1)^3}\left[1+\frac{(S+1)^4}{q^2}\right]\left[\frac{2M-3}{M-1}q^2+(2M-3)M(M-1)^2-\tfrac{1}{2}M(M-1)(2M-3)(2M-1)\right]\\
&\qquad+2M(M-1)(2M-3)(2M-1)\Lambda(M-1)\left\langle M-2\left|\frac{\cos\chi}{\sin^3\chi}\right|M-1\right\rangle . \qquad\text{(B16)}
\end{aligned}$$

After noting that

$$\frac{2M+1}{M}=3-\frac{M(M-1)}{M^2},\quad \frac{2M-3}{M-1}=3-\frac{M(M-1)}{(M-1)^2}$$

and that

$$(2M+1)M^2(M-1)=3M^3(M-1)-M^2(M-1)^2\ ,$$

$$(2M-3)M(M-1)^2=3M(M-1)^3-M^2(M-1)^2\ ,$$

one finds

$$\begin{aligned}
&\frac{1}{M(M-1)}\left[(2M-3)(2M-1)(2M+1)M(M-1)\left\langle M-1\left|\frac{\cos^2\chi}{\sin^4\chi}\right|M-1\right\rangle\right.\\
&\qquad\left.-\frac{4q^2}{(S+1)^3}\left[1+\frac{(S+1)^4}{q^2}\right][3q^2-M^2(M-1)^2]\right]\\
&=\frac{4q^2}{(S+1)^3}\left[1+\frac{(S+1)^4}{q^2}\right]\left[-\frac{q^2}{M^2}+3M^2-\tfrac{1}{2}(2M-1)(2M+1)\right]+2(2M-1)(2M+1)\Lambda(M)\left\langle M-1\left|\frac{\cos\chi}{\sin^3\chi}\right|M\right\rangle\\
&=\frac{4q^2}{(S+1)^3}\left[1+\frac{(S+1)^4}{q^2}\right]\left[-\frac{q^2}{(M-1)^2}+3(M-1)^2-\tfrac{1}{2}(2M-3)(2M-1)\right]\\
&\qquad+2(2M-3)(2M-1)\Lambda(M-1)\left\langle M-2\left|\frac{\cos\chi}{\sin^3\chi}\right|M-1\right\rangle . \qquad\text{(B17)}
\end{aligned}$$

Therefore, the left side of (B17) is independent of M, and, finally, one obtains

$$\begin{aligned}
\left\langle S,M\left|\frac{\cos^2\chi}{\sin^4\chi}\right|S,M\right\rangle&=\frac{4q^4[3(S+1)^2-M(M+1)]}{(S+1)^5(2M-1)(2M+1)(2M+3)M(M+1)}\left[1+\frac{(S+1)^4}{q^2}\right]\\
&\quad\times\left[1+\frac{1}{q^2}(S+1)^2M(M+1)\left[1-\frac{1}{2}\frac{(2S+1)(2S+3)}{3(S+1)^2-M(M+1)}\right]\right] . \qquad\text{(B18)}
\end{aligned}$$

This procedure can be continued in chain yielding the analytical expressions of matrix elements of the successive derivatives of $\cot\chi$. It should be noted that, at the asymptotic flat limit, for $S=n-1$ and $M=l$, the expressions (B11), (B13), (B15), and (B18) reduce to the well-known analytical expressions of the $\langle n,l\,|\,r^{-k}\,|\,n,l\rangle$ integrals with $k=1$, 2, 3, and 4, respectively.

Since, one is mainly interested with the predominant $1/R^2$ contributions, the asymptotic procedure described in Ref. 9

is sufficient to yield the exact contribution required for the calculation of the dipolar magnetic hyperfine parameter f_D. One can write

$$\left\langle S,M \left| \frac{1}{\sin\chi} \right| S,M \right\rangle = \langle S,M \mid \cot\chi \mid S,M \rangle + \frac{1}{2R^2} \left\langle S,M \left| 2R \tan\frac{\chi}{2} \right| S,M \right\rangle ,$$
$$\left\langle S,M \left| \frac{\cos\chi}{\sin^2\chi} \right| S,M \right\rangle = \left\langle S,M \left| \frac{1}{\sin^2\chi} \right| S,M \right\rangle - \frac{1}{2} - \frac{1}{8R^2} \left\langle S,M \left| \left[2R \tan\frac{\chi}{2} \right]^2 \right| S,M \right\rangle , \tag{B19}$$
$$\left\langle S,M \left| \frac{1}{R^3\sin^3\chi} \right| S,M \right\rangle = \left\langle S,M \left| \frac{\cos\chi}{R^3\sin^3\chi} \right| S,M \right\rangle + \frac{1}{R^2} \left\langle S,M \left| \left[2R \tan\frac{\chi}{2} \right]^{-1} \right| S,M \right\rangle .$$

Then, one replaces the $\langle S,M \mid (2R \tan\chi/2)^k \mid S,M \rangle$ integrals by the flat evaluation (see, for instance, Ref. 9 when setting $Z=q$, $n=S+1$, $l=M$)

$$\langle S,M \mid r \mid S,M \rangle = \frac{1}{2q}[3(S+1)^2 - M(M+1)] ,$$
$$\langle S,M \mid r^2 \mid S,M \rangle = \frac{(S+1)^2}{2q^2}[5(S+1)^2 + 1 - 3M(M+1)] , \tag{B20}$$
$$\langle S,M \mid r^{-1} \mid S,M \rangle = q/(S+1)^2 .$$

Finally, using previous results (B11), (B13), and (B15) one obtains

$$\left\langle S,M \left| \frac{1}{\sin\chi} \right| S,M \right\rangle = \frac{q}{(S+1)^2} \left[1 + \frac{(S+1)^2[3(S+1)^2 - M(M+1)]}{4q^2} \right] ,$$
$$\left\langle S,M \left| \frac{\cos\chi}{\sin^2\chi} \right| S,M \right\rangle = \frac{q^2}{(M+\frac{1}{2})(S+1)^3} \left[1 + \frac{(S+1)^4}{q^2} \right] - \frac{1}{2} , \tag{B21}$$
$$\left\langle S,M \left| \frac{1}{\sin^3\chi} \right| S,M \right\rangle = \frac{q^3}{(S+1)^3 M(M+1)(M+\frac{1}{2})} \left[1 + \frac{(S+1)[4(S+1)^3 + M(M+1)(2M+1)]}{4q^2} \right] .$$

APPENDIX C: CALCULATION OF THE DIRAC PSEUDORADIAL INTEGRALS

The determination of matrix elements of an Hermitian operator between the Dirac spinors (21) involves the calculation of pseudoradial integrals which are of the general form

$$I_{v'v}(f) = \int_0^\pi (P_{v'k}P_{vk} + Q_{v'k}Q_{vk}) f(\chi) d\chi$$

or (C1)

$$J_{v'v}(f) = \int_0^\pi (P_{v'k}Q_{vk} + Q_{v'k}P_{vk}) f(\chi) d\chi .$$

Using the expression (21) of the $P_{vk}(\chi)$ and $Q_{vk}(\chi)$ functions in terms of the generalized Kepler functions $R_{SM}(\chi)$ one gets the following expressions:

$$I_{v'v}(f) = 4\mathcal{N}'\mathcal{N}[k\mathcal{K}_{v'v}(f) - Z\alpha\mathcal{L}_{v'v}(f)] ,$$
$$J_{v'v}(f) = 4\mathcal{N}'\mathcal{N}[-Z\alpha\mathcal{K}_{v'v}(f) + k\mathcal{L}_{v'v}(f)] , \tag{C2}$$

where

$$\mathcal{K}_{v'v}(f) = d_1\langle S',M|f|S,M\rangle + d_2\langle S',M-1|f|S,M-1\rangle ,$$
$$\mathcal{L}_{v'v}(f) = d_3\langle S',M-1|f|S,M\rangle + d_4\langle S',M|f|S,M-1\rangle ,$$
$$d_1 = \left[\left[\frac{\epsilon' k}{\gamma} + 1 \right] \left[\frac{\epsilon k}{\gamma} + 1 \right] \right]^{1/2} ,$$
$$d_2 = \left[\left[\frac{\epsilon' k}{\gamma} - 1 \right] \left[\frac{\epsilon k}{\gamma} - 1 \right] \right]^{1/2} ,$$
$$d_3 = \left[\left[\frac{\epsilon' k}{\gamma} + 1 \right] \left[\frac{\epsilon k}{\gamma} - 1 \right] \right]^{1/2} ,$$
$$d_4 = \left[\left[\frac{\epsilon' k}{\gamma} - 1 \right] \left[\frac{\epsilon k}{\gamma} + 1 \right] \right]^{1/2} .$$

1. Diagonal ($v'=v$) pseudoradial integrals

For $v'=v$, i.e., $S'=S$, $\mathcal{K}_{v'v}$ reduces to

$$\mathcal{K}_{vv} = \left[\frac{\epsilon k}{\gamma} + 1 \right] \langle S,M \mid f \mid S,M \rangle + \left[\frac{\epsilon k}{\gamma} - 1 \right] \langle S,M-1 \mid f \mid S,M-1 \rangle \tag{C3}$$

Since

$$\lambda_S = R^2c^2(\epsilon^2 - 1) + \gamma^2 ,$$
$$L(\gamma) = -\frac{Z^2R^2\epsilon^2}{\gamma^2} + \gamma^2$$

[see Eqs. (16) and (B1), (B2), and (B3)], it can be shown that $d_3 = d_4 = -(\alpha/R)\Lambda_S(\gamma)$. Then, using the relations (B9), one gets

$$\mathscr{L}_{vv} = -\frac{2\alpha}{R}\left\langle S,M-1\left|\left[\left[M\cot\chi - \frac{q}{M}\right]f + \frac{1}{2}\frac{df}{d\chi}\right]\right|S,M-1\right\rangle$$

and/or (C4)

$$\mathscr{L}_{vv} = -\frac{2\alpha}{R}\left\langle S,M\left|\left[\left[M\cot\chi - \frac{q}{M}\right]f - \frac{1}{2}\frac{df}{d\chi}\right]\right|S,M\right\rangle$$

Finally, the calculation of the pseudoradial Dirac integrals amounts to the calculation of integrals between Kepler functions of same M ($M=\gamma$ or $M=\gamma-1$) with $S+1=v+\gamma$ and $q=ZR\epsilon$. Finally, one gets

$$I_{vv}(f) = 4\mathscr{N}^2\left[(\epsilon\gamma+k)\langle\gamma\,|\,f\,|\,\gamma\rangle + (\epsilon\gamma-k)\langle\gamma-1\,|\,f\,|\,\gamma-1\rangle + \frac{2Z\alpha^2}{R}\left\langle\gamma\left|\left[\gamma\cot\chi f - \frac{1}{2}\frac{df}{d\chi}\right]\right|\gamma\right\rangle\right], \tag{C5}$$

$$J_{vv}(f) = -4\mathscr{N}^2\left[Z\alpha(\langle\gamma\,|\,f\,|\,\gamma\rangle - \langle\gamma-1\,|\,f\,|\,\gamma-1\rangle) + \frac{2k}{ZR}\left\langle\gamma\left|\left[\gamma\cot\chi f - \frac{1}{2}\frac{df}{d\chi}\right]\right|\gamma\right\rangle\right], \tag{C6}$$

where the shortened notation $\langle\gamma\,|\,f\,|\,\gamma\rangle$ stands for diagonal matrix elements between the generalized Kepler functions $R_{v+\gamma-1,\gamma}(\chi)$.

a. Normalization of the curved Dirac orbitals

In order that the Dirac spinor Φ_{vkm} be normalized the $P_{vk}(\chi)$ and $Q_{vk}(\chi)$ functions (14) must satisfy the integral condition $I_{vv}(f=1)=1$, i.e.,

$$4\mathscr{N}^2\left[2\epsilon\gamma + \frac{2Z\alpha^2}{R}\gamma\langle\gamma\,|\cot\chi\,|\,\gamma\rangle\right] = 1\ . \tag{C7}$$

Using (B11), the expression (19) of ϵ^2 and keeping in mind that $\gamma^2=k^2-Z^2\alpha^2$, one gets the expression (20) of $\mathscr{N}$.

b. Diagonal ($v'=v$) dipolar magnetic hyperfine integral f_D

From (41) and (C1), it is easily seen that $f_D(v,v)=J_{vv}(f=\cos\chi/R^2\sin^2\chi)$. Using (C6) together with the required integrals (B21), one obtains

$$f_D = \frac{4\mathscr{N}^2 Z\alpha}{R^2}\left[\frac{\epsilon k}{\gamma} + \frac{Z^2R^2\epsilon^2(1-2\epsilon k)}{(v+\gamma)^3(\gamma^2-\frac{1}{4})}\left[1+\frac{(v+\gamma)^4}{Z^2R^2\epsilon^2}\right]\right]. \tag{C8}$$

c. Diagonal ($v'=v$) quadrupolar electric hyperfine integral f_Q

From (48) and (C1), it is easily seen that $f_Q(v,v)=I_{vv}(f=\cos\chi/R^3\sin^3\chi)$ or, using (C5)

$$f_Q = 4\mathscr{N}^2\left[(\epsilon\gamma+k)\left\langle\gamma\left|\frac{\cos\chi}{R^3\sin^3\chi}\right|\gamma\right\rangle + (\epsilon\gamma-k)\left\langle\gamma-1\left|\frac{\cos\chi}{R^3\sin^3\chi}\right|\gamma-1\right\rangle + \frac{2Z\alpha^2}{R^4}\left\langle\gamma\left|\left[\gamma+\frac{3}{2}\right]\frac{\cos^2\chi}{\sin^4\chi} + \frac{1}{2}\frac{1}{\sin^2\chi}\right|\gamma\right\rangle\right]. \tag{C9}$$

This hyperfine parameter can be exactly calculated from formulas (B13), (B15), and (B18). However, since its final expression in terms of the quantum numbers is cumbersome, it has not been reported hereafter.

2. Calculation of the first-order perturbed energy $E_{vk}^{(1)}$

From (25) and (C1), it is easily seen that

$$E_{vk}^{(1)} = -\frac{kc}{2R^2}J_{vv}\left[f=2R\tan\frac{\chi}{2}\right]$$

and one gets

$$E_{vk}^{(1)} = -\frac{2kc}{R^2}\mathcal{N}^2\left[-Z\alpha\left[\frac{\epsilon k}{\gamma}+1\right]\left\langle\gamma\left|2R\tan\frac{\chi}{2}\right|\gamma\right\rangle - Z\alpha\left[\frac{\epsilon k}{\gamma}-1\right]\left\langle\gamma-1\left|2R\tan\frac{\chi}{2}\right|\gamma-1\right\rangle\right.$$
$$\left. + 2k\left[\frac{\epsilon^2k^2}{\gamma^2}-1\right]^{1/2}\left\langle\gamma\left|2R\tan\frac{\chi}{2}\right|\gamma-1\right\rangle\right]. \qquad \text{(C10)}$$

As has been justified in the main text, the integrals $\langle\gamma\,|\,2R\tan\chi/2\,|\,\gamma'\rangle$ will be replaced by their well-known flat expressions

$$\langle\gamma\,|\,r\,|\,\gamma\rangle = [3(v+\gamma)^2-\gamma(\gamma+1)]/2Z\epsilon\ ,$$
$$\langle\gamma\,|\,r\,|\,\gamma-1\rangle = -3(v+\gamma)[(v+\gamma)^2-\gamma^2]^{1/2}/2Z\epsilon\ .$$

Thus one obtains the expression (26) of $E_{vk}^{(1)}$.

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