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► **To cite this version:**

Nadine Bessis, Georges Bessis, Daniel Roux. Atomic fine structure calculations in space of constant negative curvature. *Physical Review A : Atomic, molecular, and optical physics [1990-2015]*, 1984, 30 (1034), 10.1103/PhysRevA.30.1094 . halshs-00905065

HAL Id: halshs-00905065

<https://shs.hal.science/halshs-00905065>

Submitted on 4 Oct 2021

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Atomic fine-structure calculations in a space of constant negative curvature

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Previous results concerning the Dirac energies and wave functions in a space of constant positive curvature are used to derive their counterparts in a space of constant negative curvature. In particular, it is shown that, when switching from a spherical closed space to a hyperbolic open space, the sign of the curvature-induced splittings and shifts in the hydrogenic fine-structure spectrum is reversed.

I. INTRODUCTION

In order to complement our previous investigation on space curvature effects in atomic structure calculations,¹⁻³ it should be instructive to comparatively examine the modifications of the hydrogenic Dirac energies and wave functions when the physical space is assumed to be a hyperbolic three-space with constant negative curvature (Milne's open universe) instead of a spherical three-space (Einstein's closed universe with constant positive curvature $1/R$). We already know, and this result has been obtained since a long time by Schrödinger⁴ and Infeld and Schild,⁵ that the hydrogenic electronic energy spectra in spherical and in hyperbolic three-spaces differ significantly since, in the first case, it is discrete everywhere, while in the last case, it consists of a finite number of (mostly negative) energy levels in addition to a continuous spectrum. Furthermore, in the nonrelativistic scheme,¹ we also know that the final expressions of the energies, in each case, can be obtained one from each other by the formal change $R \leftrightarrow iR$. This can be inferred from inspection of the wave equation. Nevertheless, one has to be cautious to take also into account an additional Z/R contribution originated from the change of the expression of the Coulombic potential

$$V(\chi) = -(Z/R) \cot \chi \rightarrow V(\chi) = -(Z/R)(\coth \chi - 1).$$

Hence, the nonrelativistic electronic energies, in the spherical three-space, are (in a.u.)

$$E_n = -\frac{Z^2}{2n^2} + \frac{n^2-1}{2R^2}, \quad (1)$$

and, in the hyperbolic three-space

$$E_n = -\frac{Z^2}{2n^2} - \frac{n^2-1}{2R^2} + \frac{Z}{R}. \quad (2)$$

In the present note, the modifications of the expressions of the hydrogenic fine-structure energies as well as the expressions of the wave functions (relativistic and nonrelativistic) are given and discussed.

II. DIRAC EQUATION IN A SPACE OF CONSTANT CURVATURE

In a space of constant curvature $1/R$, the space-time element can be conveniently written

$$ds^2 = c^2 dt^2 - R^2 d\chi^2 - R^2[\omega(\chi)]^2(d\theta^2 + \sin^2\theta d\phi^2), \quad (3)$$

where

$$\omega(\chi) = \begin{cases} \sin \chi & \text{for } R > 0 \text{ (closed space, } 0 \leq \chi \leq \pi) \\ \sinh \chi & \text{for } R < 0 \text{ (open space, } 0 \leq \chi < \infty) \end{cases}.$$

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

Starting from the generally covariant form of the Dirac equation in a curved space time, a convenient choice of the Dirac representation can be made which leads to the usual polar dependence (θ, ϕ) of the Dirac orbitals (for details, see Ref. 3). One gets the following expression of the Dirac equation for stationary states with an external electromagnetic field $(V, A_\chi, A_\theta, A_\phi)$

$$\left[\alpha_\chi \left(p_\chi + \frac{i\beta}{R\omega(\chi)} \hat{K} \right) + W + \frac{mc}{\hbar} \beta - \frac{E_T - eV}{\hbar c} \right] \psi(\chi, \theta, \phi) = 0, \quad (4)$$

where $E_T = mc^2 + E$ is the total energy:

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

$$p_\chi = -\frac{i}{R\omega(\chi)} \frac{\partial}{\partial \chi} \omega(\chi); \quad \hat{K} = \beta(1 + \vec{\sigma} \cdot \vec{\Gamma}),$$

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}; \quad \alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} \text{ for } k = \chi, \theta, \phi.$$

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

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

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

$\sigma^1, \sigma^2, \sigma^3$ are the standard (2×2) Pauli matrices; $\vec{\sigma} = (\sigma^1, \sigma^2, \sigma^3)$ and \vec{l} is the usual orbital angular momentum.

III. DIRAC ORBITALS IN AN OPEN SPACE OF CONSTANT CURVATURE

When the external electromagnetic field in (4) reduces to the Coulombic potential, i.e., when $V(\chi) = -(Z/R) \times (\coth\chi - 1)$ and $A_\chi = A_\theta = A_\phi = 0$, the perturbative procedure which has already been applied to determine the spherical three-space Dirac orbitals still holds for the case of the hyperbolic three-space. Indeed, using the same considerations as in Ref. 3, we introduce the perturbative Hamiltonian

$$\mathcal{H}_1 = -\frac{ic}{2R^2} \left(2R \tanh \frac{\chi}{2} \right) \begin{pmatrix} 0 & \sigma_\chi (1 + \vec{\sigma} \cdot \vec{l}) \\ \sigma_\chi (1 + \vec{\sigma} \cdot \vec{l}) & 0 \end{pmatrix} . \quad (5)$$

In order to be consistent when gathering all the $1/R^2$ contributions involved in the atomic structure calculations, since the perturbation \mathcal{H}_1 is of an order of magnitude $\sim 1/R^2$, it is sufficient to determine only the first order perturbed solution of the Dirac equation (4) expanded in the basis of the exact unperturbed Dirac spinors $\Phi_{\nu km}$

$$\psi_{\nu km} = \Phi_{\nu km} - \sum_{\nu', k', m'} \frac{\langle \Phi_{\nu' k' m'} | \mathcal{H}_1 | \Phi_{\nu km} \rangle}{E_{\nu' k'} - E_{\nu k}} \Phi_{\nu' k' m'} , \quad (6)$$

where

$$E_{\nu k} = -\frac{Z^2}{2(\nu + |k|)^2}$$

is the flat space electronic energy. Moreover, since, at the asymptotic flat limit ($R \rightarrow \infty, \chi \rightarrow 0, R\chi \rightarrow r$), the function $\psi_{\nu km}$ leads to the familiar Dirac functions, it is easily seen that a convenient form of the unperturbed $\Phi_{\nu km}$ functions is

$$\Phi_{\nu km}(\chi, \theta, \phi) = \frac{1}{R \sinh \chi} \begin{pmatrix} P_{\nu k}(\chi) \mathcal{Y}_{ljm} \\ iQ_{\nu k}(\chi) \mathcal{Y}_{\bar{l}jm} \end{pmatrix} , \quad (7)$$

where the \mathcal{Y}_{ljm} spinor is a simultaneous eigenfunction of l^2, σ^2, j^2 , and j_z operators with eigenvalues $l(l+1)$, 3, $j(j+1)$, and m , respectively; $\vec{j} = \vec{l} + \frac{1}{2}\vec{\sigma}$; $\bar{l} = l \pm \frac{1}{2}$ as $j = l \pm \frac{1}{2}$.

Once the above expressions of \mathcal{H}_1 and $\Phi_{\nu km}$ have been stated, the procedure which has been used to determine the unperturbed Dirac functions in a spherical three-space still holds to determine the $\Phi_{\nu km}$. We set

$$\begin{aligned} P_{\nu k} &= \mathcal{N} \left[(\gamma_2 + \gamma_1) \left(\frac{\epsilon k}{\gamma} + 1 \right)^{1/2} \mathcal{R}_1(\chi) \right. \\ &\quad \left. + (\gamma_2 - \gamma_1) \left(\frac{\epsilon k}{\gamma} - 1 \right)^{1/2} \mathcal{R}_2(\chi) \right] , \\ Q_{\nu k} &= \mathcal{N} \left[(\gamma_2 - \gamma_1) \left(\frac{\epsilon k}{\gamma} + 1 \right)^{1/2} \mathcal{R}_1(\chi) \right. \\ &\quad \left. + (\gamma_2 + \gamma_1) \left(\frac{\epsilon k}{\gamma} - 1 \right)^{1/2} \mathcal{R}_2(\chi) \right] . \end{aligned} \quad (8)$$

where

$$\gamma_1 = (k + Z\alpha)^{1/2}, \gamma_2 = (k - Z\alpha)^{1/2}, \gamma = \gamma_1 \gamma_2 ;$$

$$\epsilon = \left(E_T - \frac{Z}{R} \right) / mc^2 .$$

\mathcal{N} is a normalization constant such that

$$\int_0^\infty (P_{\nu k}^2 + Q_{\nu k}^2) d\chi = 1 . \quad (9)$$

Then, it follows that both functions $\mathcal{R}_1(\chi)$ and $\mathcal{R}_2(\chi)$ are solutions of a generalized Kepler wave equation in a space of constant negative curvature:

$$\left(\frac{d^2}{d\chi^2} - \frac{M(M+1)}{\sinh^2 \chi} + 2q \coth \chi + \lambda_S \right) \mathcal{R}_S^M(\chi) = 0 , \quad (10)$$

with $q = ZR\epsilon$; $\lambda_S = R^2 c^2 (\epsilon^2 - 1) - \gamma^2$; $\mathcal{R}_1(\chi)$ is obtained for $M = \gamma$ while $\mathcal{R}_2(\chi)$ is obtained for $M = \gamma - 1$.

Within the Infeld-Hull classification,⁶ this eigenequation (10) is a type E factorizable equation with associated ladder operators $H_M^\pm = M \coth \chi - q/M \mp (d/d\chi)$ and factorization function $L(M) = -M^2 - q^2/M^2$. As long as $M^2 < q$, the factorization function $L(M)$ is an increasing function of M and, therefore, (class I) quadratically integrable solutions of (10) exist, with associated eigenvalue $\lambda_S = L(S+1)$, when the following condition is fulfilled:

$$(S+1)^2 < q . \quad (11)$$

The associated quantization condition is $S - M = \nu$, where ν is a non-negative integer ($\nu = 0, 1, 2, \dots$) and, as a consequence of condition (11), the eigenequation (10) has a finite number of discrete eigenvalues λ_S .

It should be noted that, for $M = l$, $S = n - 1$, $n - 1 - 1 = \nu$, and $q = ZR$, the generalized Kepler eigenequation (10) reduces to the hydrogenic pseudoradial wave equation in a space of constant negative curvature and one finds again the results of Infeld and Schild concerning the discrete energy levels.

Using previous results,⁷ one obtains the following expression of the $\mathcal{R}_S^M(\chi)$ functions:

$$\mathcal{R}_S^M(\chi) = N_{SM} (\sinh \chi)^{S+1} \exp \left(-\frac{q\chi}{S+1} \right) P_\nu^{(a,b)}(\coth \chi) , \quad (12)$$

where $P_\nu^{(a,b)}$ is a Jacobi polynomial with $a = -(S+1) - q/(S+1)$ and $b = -(S+1) + q/(S+1)$; N_{SM} is the normalization constant.

In the same way as in the spherical three-space the $\mathcal{R}_1(\chi)$ and $\mathcal{R}_2(\chi)$ functions in (8) are both generalized Kepler functions (12) with the same value $S = \nu + \gamma - 1$; i.e., $\mathcal{R}_1(\chi) = R \mathcal{Y}_{\nu+\gamma-1}$ and $\mathcal{R}_2(\chi) = R \mathcal{Y}_{\nu-\gamma-1}$ and moreover the $P_{\nu k}$ and $Q_{\nu k}$ exhibit the same dependence in terms of \mathcal{R}_1 and \mathcal{R}_2 in the two spaces. At this level, it is worthwhile to note that all the above results concerning the Kepler functions $\mathcal{R}_S^M(\chi)$ in a hyperbolic three-space can formally be derived from the analogous previous results concerning the Kepler functions in a spherical three-space (see Appendix B of Ref. 3) when making the changes $\chi \rightarrow -i\chi$ and $R \rightarrow iR$. In particular, the procedure lying on ladder operator considerations,⁸ which has been used to determine the expressions of matrix elements between the Kepler functions in the terms of the quantum numbers in a spherical three-space still holds for the case of the hyperbolic three-space and, therefore, all the required results can be readily ob-

tained by making the above changes in the analogous expressions of Ref. 3. One gets

$$\epsilon^2 = \left[1 + \frac{Z^2 \alpha^2}{(v + \gamma)^2} \right]^{-1} \left[1 - \frac{\alpha^2}{R^2} v(v + 2\gamma) \right], \quad (13)$$

$$\mathcal{N} = \left(\frac{\epsilon}{8\gamma} \right)^{1/2} \left[1 - \frac{\alpha^2}{R^2} v(v + 2\gamma) \right]. \quad (14)$$

Then, the unperturbed spinors $\Phi_{\nu km}$ are completely defined [see Eqs. (7), (8), and (12)]. Finally, the Dirac spinor $\psi_{\nu km}$ can be written [see Eq. (33) of Ref. 3]

$$\psi_{\nu km} = \Phi_{\nu km} + \frac{1}{R^2} \sum_{\nu' \neq \nu} c_{\nu' \nu} \Phi_{\nu' km}, \quad (15)$$

$$\psi_{nlm_l}(\chi, \theta, \phi) = N_{nl} (\sinh \chi)^{n-1} \exp \left[-\frac{ZR\chi}{n} \right] P_{\nu}^{[-n - (ZR/n), -n + (ZR/n)]} (\coth \chi) Y_l^{m_l}(\theta, \phi). \quad (17)$$

IV. FINE-STRUCTURE ENERGIES IN AN OPEN SPACE OF CONSTANT CURVATURE

As pointed out in the preceding section, the expressions of the fine-structure energies in the open space of constant curvature can be directly derived from their analogous expressions in the closed space by merely transposing R into iR . Nevertheless, it must be kept in mind that, in the open space, $\epsilon = \alpha^2 [1 + E_{\nu k}^{(0)} - Z/R]$ while it is $\epsilon = \alpha^2 [1 + E_{\nu k}^{(0)}]$ in the closed space.

Finally, including the curvature effects (up to $1/R^2$), the

where

$$c_{\nu' \nu} = \frac{k}{Z^2} \frac{[(v + |k|)(v' + |k|)]^2}{(v - v')(v + v' + 2|k|)} \times \int_0^\infty (\bar{P}_{\nu' k} \bar{Q}_{\nu k} + \bar{Q}_{\nu' k} \bar{P}_{\nu k}) r dr.$$

The (flat) $\bar{P}_{\nu k}(r)$ and $\bar{Q}_{\nu k}(r)$ functions are given by (8) where the curved generalized Kepler $R_S^M(\chi)$ are replaced by the traditional radial functions $\bar{R}_S^M(r)$ involving the Laguerre polynomials.

$$\bar{R}_S^M(r) = \bar{N}_{SM} r^{M+1} \exp \left[-\frac{Zr}{(S+1)} \right] L_{\nu}^{2M+1} [2Zr/(S+1)]. \quad (16)$$

Let us remark that, following from the expression (12) of the radial Kepler function, one gets the expression of the nonrelativistic hydrogenic wave function in a space of constant negative curvature

Dirac energy is $E_{\nu k} = E_{\nu k}^{(0)} + \langle \Phi_{\nu km} | \mathcal{H}' | \Phi_{\nu km} \rangle$ and one gets

$$E_{\nu k} = \frac{1}{\alpha^2} \left[\left(1 + \frac{Z^2 \alpha^2}{(v + \gamma)^2} \right)^{-1/2} - 1 \right] + \frac{Z}{R} + \frac{k}{4R^2} - \frac{(v + \gamma)^2 + Z^2 \alpha^2}{2R^2} \left(1 + \frac{Z^2 \alpha^2}{(v + \gamma)^2} \right)^{-1/2} \quad (18)$$

The first term is just the usual flat fine-structure hydrogenic energy and the remaining terms correspond to curvature

TABLE I. Hydrogenic fine-structure energies in a space of constant curvature (in a.u.). The upper (or lower) sign corresponds to positive (or negative) curvature.

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

^aThe electronic energy contains the additional term (Z/R) but only for the case of negative curvature.

contributions which vanish at the asymptotic flat limit.

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

$$E_{nk} = -\frac{Z^2}{2n^2} + \frac{Z^4\alpha^2}{2n^3} \left(\frac{3}{4n} - \frac{1}{|k|} \right) + \frac{Z}{R} - \frac{n^2}{2R^2} + \frac{k}{4R^2} - \frac{Z^2\alpha^2}{4R^2} \left(1 - \frac{2n}{|k|} \right). \quad (19)$$

The space-curvature (positive or negative) theoretical modifications of the hydrogenic energies are shown in Table I in comparison with the Lamb shift contributions. From the table it can be shown that, following the geometrical structure, i.e., closed (or open) of the space, the degenerate states are split by a Z -independent curvature induced contribution $\Delta E_c = k/4R^2$ having the same (or the opposite) sign as the Lamb contribution

$$\Delta E_{\text{Lamb}} = \frac{Z^4\alpha^2}{n^3} \frac{\varkappa}{k(2l+1)}$$

where $\varkappa = 1.159\,644 \times 10^{-3}$. Nevertheless, the curvature effects should be, of course, quantitatively comparable to the Lamb effects, but only in regions with really large cur-

vature, i.e., for $R \approx 2 \times 10^{-3}$ cm (see, for instance, Ref. 9). It is interesting to note that, even for such a large value of R , as a consequence of the condition (11), i.e., $n^2 < ZR$, the number of discrete energy levels of the hydrogenic atom is rather a large number ($\approx 614\sqrt{Z}$).

V. CONCLUSION

In this note, we have summarized some results concerning atomic structure calculations in a space of constant negative curvature. Particularly, it has been shown how the change of the sign of the space curvature amounts to make the changes $R \rightarrow iR$, $\chi \rightarrow -i\chi$, and $\epsilon \rightarrow \epsilon - (Z\alpha^2/R)$ in the expressions of the Dirac energies and wave functions. As a consequence, the sign of the curvature induced splittings and shifts in the hydrogenic fine-structure spectrum is reversed when switching from a closed space to an open space. The same conclusions can be drawn for the curvature contributions to the hyperfine structure energy levels. Since their expressions are easily derivable from previous results,³ they have not been reproduced. If these curvature modifications of the hydrogenic spectrum were detectable, idealistically they could help obtain some indication about the sign of the space curvature.

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