Closed-form expressions for the Dirac-Coulomb radial r^t integrals

N. Bessis,* G. Bessis,* and D. Roux
Laboratoire de Spectroscopie Théorique, Université Claude Bernard (Lyon I), F-69622 Villeurbanne, France
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A novel procedure is devised in order to obtain closed-form expressions of the Dirac-Coulomb radial r^t integrals in terms of the Dirac energy $\varepsilon=\{1+Z^2\alpha^2/[v+(k^2-Z^2\alpha^2)^{1/2}]^2\}^{-1/2}$, where $v=n-|k|$, and of the Dirac quantum number $k=(-1)^{j+l+1/2}(j+\frac{1}{2})$. In this procedure, well adapted for symbolic computation, the fundamental array of the r^t radial integrals is obtained from the r^{t-1} array.

I. INTRODUCTION

Recently,[1,2] space-curvature-induced modifications of the hydrogenic spectra have been investigated in the framework of a "curved Dirac model," and it has been shown how analytical expressions of these space-curvature modifications can be obtained in terms of the usual flat-space Dirac-Coulomb radial r^t integrals. This investigation implied the computation of many Dirac r^t integrals, with $t\geq 0$ and high values of t. If, within a nonrelativistic framework, closed-form expressions of the hydrogenic radial r^t integrals are available for any value of t, this is not the case within the Dirac framework. For special cases analytical expressions of the Dirac-Coulomb radial r^t integrals have been already given: these closed-form expressions have been obtained either using the factorization method and algebraic manipulations[3] or both the factorization method and group-theoretical considerations,[4] or also using the relativistic virial theorem.[5] In the present paper the determination of closed-form expressions of the Dirac-Coulomb r^t integrals is reinvestigated. Preliminarily, it is shown how the procedure outlined in Ref. 3 can be simplified in order to avoid the computation of off-diagonal hydrogenlike intermediate integrals (Sec. II). Nevertheless, as the values of t increase, the calculation tends to be rather cumbersome. For that reason a novel recursive procedure is proposed leading to analytical expressions of Dirac-Coulomb r^t integrals, with $t\geq 0$ in terms of the Dirac energy

$$\varepsilon=\{1+Z^2\alpha^2/[v+(k^2-Z^2\alpha^2)^{1/2}]^2\}^{-1/2},$$

where $v=0,1,2,\ldots$ and of the Dirac quantum number $k=(-1)^{j+l+1/2}(j+\frac{1}{2})$ (Sec. III).

II. THE DIRAC-COULOMB EQUATION

The Dirac hydrogenic functions are solutions of the Dirac-Coulomb equation

$$[c(\boldsymbol{\alpha}\cdot\mathbf{p})+\beta m_0c^2-(E_T-V)]\psi=0, \tag{1}$$

where $V=-Ze^2/r$ is the Coulomb potential, $E_T=m_0c^2+E_{vk}$ is the total relativistic energy of the electron, $\boldsymbol{\alpha}$ and β are the usual 4×4 Dirac matrices

$$\boldsymbol{\alpha}=\begin{bmatrix}0 & \boldsymbol{\sigma}\\ \boldsymbol{\sigma} & 0\end{bmatrix},\quad \beta=\begin{bmatrix}I & 0\\ 0 & -I\end{bmatrix}.$$

I and $\sigma_x,\sigma_y,\sigma_z$ are the 2×2 unit and Pauli matrices, respectively. The solution of Eq. (1) can be obtained in spherical coordinates when setting

$$\psi_{vkm}=\frac{1}{r}\begin{bmatrix}P_{vk}(r) & \mathscr{Y}_{ljm}\\ iQ_{vk}(r) & \mathscr{Y}_{\bar{l}jm}\end{bmatrix}, \tag{2}$$

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

$$\begin{aligned}(1+\boldsymbol{\sigma}\cdot\mathbf{l})\mathscr{Y}_{ljm}&=[j(j+1)-l(l+1)+\tfrac{1}{4}]\mathscr{Y}_{ljm}\\&=-k\mathscr{Y}_{ljm},\\(1+\boldsymbol{\sigma}\cdot\mathbf{l})\mathscr{Y}_{\bar{l}jm}&=k\mathscr{Y}_{\bar{l}jm};\quad \frac{1}{r}(\boldsymbol{\sigma}\cdot\mathbf{r})\mathscr{Y}_{ljm}=\mathscr{Y}_{\bar{l}jm}.\end{aligned} \tag{3}$$

In order that $\psi_{vkm}(r,\theta,\phi)$ be normalized, the $P_{vk}(r)$ and $Q_{vk}(r)$ functions must satisfy the integral condition

$$\int_0^\infty (P_{vk}^2+Q_{vk}^2)dr=1. \tag{4}$$

The P_{vk} and Q_{vk} functions are solutions of the coupled equations[1]

$$\begin{aligned}\left[\frac{d}{dr}+\frac{k}{r}\right]P_{vk}&=-\left[(1+\varepsilon)c+\frac{Z\alpha}{r}\right]Q_{vk},\\\left[\frac{d}{dr}-\frac{k}{r}\right]Q_{vk}&=-\left[(1-\varepsilon)c-\frac{Z\alpha}{r}\right]P_{vk},\end{aligned} \tag{5}$$

where $\varepsilon=E_T/m_0c^2$; $\alpha=1/c$ is the fine-structure constant. $v=0,1,2,\ldots$ is the Dirac radial quantum number, i.e., $v=n-j-\frac{1}{2}$.

Owing to the bispinorial form (2) of ψ_{vkm}, the determination of the matrix elements usually needed in Dirac atomic calculations involves the computation of the following basic hydrogenic radial integrals:

$$\mathscr{I}_t=\int_0^\infty (P'P+Q'Q)r^t\,dr\ ,$$
$$\mathscr{J}_t=\frac{1}{\alpha}\int_0^\infty (P'Q+Q'P)r^t\,dr\ ,$$
$$\mathscr{K}_t=\int_0^\infty (P'P-Q'Q)r^t\,dr\ ,$$
$$\mathscr{L}_t=\frac{1}{\alpha}\int_0^\infty (P'Q-Q'P)r^t\,dr\ , \tag{6}$$

where the shortened notation $P'=P_{v'k'}(r)$, $P=P_{vk}(r),\ldots$ is used unless otherwise stated.

III. EXPRESSION OF THE DIRAC r^t INTEGRALS IN TERMS OF GENERALIZED KEPLER MATRIX ELEMENTS

Solutions of the coupled Eqs. (5) are obtainable in closed form (see, for instance, Refs. 3 and 6–9). Following the Infeld-Hull factorization procedure,[3] one gets

$$P_{vk}=\mathscr{N}\left[(\gamma_2+\gamma_1)\left|\frac{\varepsilon k}{\gamma}+1\right|^{1/2}R_S^{\gamma}-(\gamma_2-\gamma_1)\left|\frac{\varepsilon k}{\gamma}-1\right|^{1/2}R_S^{\gamma-1}\right],$$
$$Q_{vk}=\mathscr{N}\left[(\gamma_2-\gamma_1)\left|\frac{\varepsilon k}{\gamma}+1\right|^{1/2}R_S^{\gamma}-(\gamma_2+\gamma_1)\left|\frac{\varepsilon k}{\gamma}-1\right|^{1/2}R_S^{\gamma-1}\right], \tag{7}$$

where

$$\gamma_1=|k+Z\alpha|^{1/2}\ ,$$
$$\gamma_2=|k-Z\alpha|^{1/2}\ ,$$
$$\gamma=\mathrm{sgn}(k)\gamma_1\gamma_2\ ,$$
$$\varepsilon=\left[1+\frac{Z^2\alpha^2}{(v+|\gamma|)^2}\right]^{-1/2},$$

and $\mathscr{N}=(\varepsilon/8|\gamma|)^{1/2}$. P_{vk} and Q_{vk} are the large and small radial components, respectively. The $R_S^M(r)$ functions are the generalized Kepler functions that are solutions of the Infeld-Hull type F (class I) factorizable equation,

$$\left[\frac{d^2}{dr^2}-\frac{M(M+1)}{r^2}+\frac{2q}{r}+\lambda_S\right]R_S^M=0\ , \tag{8}$$

where $q=Z\varepsilon$, $\lambda_S=c^2(\varepsilon^2-1)=-Z^2\varepsilon^2/(S+1)^2$. Analytical expressions of the R_S^M functions in terms of the quantum numbers are known[10]

$$R_S^M(r)=N_{SM}r^{M+1}\exp[-qr/(S+1)]L_v^{2M+1}[2qr/(S+1)] \tag{9}$$

where $L_v^{2M+1}(\cdots)$ is a generalized Laguerre polynomial of degree $v=S+1-M$, S and M are both positive (but not necessarily integer) numbers, N_{SM} is a normalization constant. Let us note that, when setting $M=l$, $S=n-1$ $(n=1,2,\ldots)$ and $q=Z$, the expression (9) identifies with the Schrödinger hydrogenic radial functions.

The R_S^{γ} and $R_S^{\gamma-1}$ functions occurring in expression (7) involve the same values of q and S, i.e., $q=Z\varepsilon$ and $S=v+|\gamma|-1$, and the values $M=\gamma$ and $M=\gamma-1$, respectively. Since for negative values of k, γ is negative, an extended definition of the R_S^{γ} and $R_S^{\gamma-1}$ is required. Noting that the Kepler wave equation (8) depends on M via the product $M(M+1)$ and using ladder operator considerations; it is found that the following correspondence holds: $R_S^{-|\gamma|}=R_S^{|\gamma|-1}$ and $R_S^{-|\gamma|-1}=-R_S^{|\gamma|}$.

Let us now consider the determination of the integrals (6) for the special cases $v'=v$ with $k'=k$ or $k'=-k$. Both cases correspond to the same values of $|\gamma|$, S, and ε, i.e., $|\gamma'|=|\gamma|$, $S'=S$, and $\varepsilon'=\varepsilon$. From Eq. (7), one gets the following expressions in terms of the diagonal $(S'=S)$ Kepler matrix elements $\langle S\gamma|r^t|S\gamma'\rangle$, hereafter noted $\langle\gamma||\gamma'\rangle$:

$$I_t(k'=k)=\frac{\varepsilon^2k^2}{2\gamma^2}(\langle\gamma||\gamma\rangle+\langle\gamma-1||\gamma-1\rangle)+\frac{\varepsilon k}{2\gamma}(\langle\gamma||\gamma\rangle-\langle\gamma-1||\gamma-1\rangle)+\frac{Z\alpha\varepsilon}{\gamma}\left[\frac{\varepsilon^2k^2}{\gamma^2}-1\right]^{1/2}\langle\gamma||\gamma-1\rangle\ ,$$
$$J_t(k'=k)=-\frac{Z\alpha\varepsilon^2k}{2\gamma^2}(\langle\gamma||\gamma\rangle+\langle\gamma-1||\gamma-1\rangle)-\frac{Z\alpha\varepsilon}{2\gamma}(\langle\gamma||\gamma\rangle-\langle\gamma-1||\gamma-1\rangle)-\frac{\varepsilon k}{\gamma}\left[\frac{\varepsilon^2k^2}{\gamma^2}-1\right]^{1/2}\langle\gamma||\gamma-1\rangle\ ,$$
$$K_t(k'=k)=\frac{\varepsilon^2k}{2\gamma}(\langle\gamma||\gamma\rangle-\langle\gamma-1||\gamma-1\rangle)+\tfrac{1}{2}\varepsilon(\langle\gamma||\gamma\rangle+\langle\gamma-1||\gamma-1\rangle)\ ,$$
$$L_t(k'=k)=0\ ,$$
$$I_t(k'=-k)=\varepsilon\langle\gamma||\gamma-1\rangle\ ,$$
$$J_t(k'=-k)=\frac{\varepsilon}{2\alpha}\left[\frac{\varepsilon^2k^2}{\gamma^2}-1\right]^{1/2}(\langle\gamma||\gamma\rangle-\langle\gamma-1||\gamma-1\rangle)\ ,$$
$$K_t(k'=-k)=\frac{Z\alpha\varepsilon}{2\gamma}\left[\frac{\varepsilon^2k^2}{\gamma^2}-1\right]^{1/2}(\langle\gamma||\gamma\rangle+\langle\gamma-1||\gamma-1\rangle)+\frac{\varepsilon^2k^2}{\gamma^2}\langle\gamma||\gamma-1\rangle\ ,$$
$$L_t(k'=-k)=-\frac{\varepsilon k}{2\gamma}\left[\frac{\varepsilon^2k^2}{\gamma^2}-1\right]^{1/2}(\langle\gamma||\gamma\rangle+\langle\gamma-1||\gamma-1\rangle)-\frac{Z\alpha\varepsilon^2k}{\gamma^2}\langle\gamma||\gamma-1\rangle\ . \tag{10}$$

TABLE I. Expressions of the ($v'=v$) Dirac radial r^t integrals.

	$k'=k$	$k'=-k$
I_0	1	$-\frac{\gamma}{Z\alpha}\left[\frac{\varepsilon^2k^2}{\gamma^2}-1\right]^{1/2}$
I_1	$\frac{1}{2Z}\left[\frac{3Z^2\alpha^2\varepsilon}{1-\varepsilon^2}-k(1+\varepsilon k)\right]$	$\frac{3Z\alpha^2\varepsilon}{2(1-\varepsilon^2)}I_0$
I_2	$\frac{Z^2\alpha^4(1+4\varepsilon^2)}{2(1-\varepsilon^2)^2}-\frac{k^2(1+2\varepsilon^2)+3\varepsilon k-1}{2(1-\varepsilon^2)}$	$\left[\frac{Z^2\alpha^4(1+4\varepsilon^2)}{2(1-\varepsilon^2)^2}+\frac{\alpha^2(1-k^2)}{2(1-\varepsilon^2)}\right]I_0$
J_0	$\frac{k(\varepsilon^2-1)}{Z\alpha^2}$	0
J_1	$\frac{1}{2}(1-2\varepsilon k)$	$\frac{1}{2}I_0$
J_2	$\frac{1}{2Z}\left[\frac{Z^2\alpha^2[3\varepsilon-k(1+2\varepsilon^2)]}{1-\varepsilon^2}-k(1-k^2)\right]$	$\frac{3Z\alpha^2\varepsilon}{2(1-\varepsilon^2)}I_0$
K_0	ε	εI_0
K_1	$\frac{1}{2Z}\left[\frac{Z^2\alpha^2(1+2\varepsilon^2)}{1-\varepsilon^2}-k(k+\varepsilon)\right]$	$\frac{Z\alpha^2(1+2\varepsilon^2)}{2(1-\varepsilon^2)}I_0$
K_2	$\frac{Z^2\alpha^4\varepsilon(3+2\varepsilon^2)}{2(1-\varepsilon^2)^2}-\frac{\alpha^2\varepsilon(3k^2+3\varepsilon k-1)}{2(1-\varepsilon^2)}$	$\left[\frac{Z^2\alpha^4\varepsilon(3+2\varepsilon^2)}{2(1-\varepsilon^2)}+\frac{\alpha^2\varepsilon(1-k^2)}{2(1-\varepsilon^2)}\right]I_0$
L_t	0	$-\frac{2k}{t+1}J_t$

As it has been shown previously,[1] since the R_S^M functions are solutions of a (type F) factorizable equation, the following relation holds for Kepler matrix elements of any derivable function $f(r)$, and still holds for negative values of γ when introducing the above extended definition of the Kepler function:

$$\frac{1}{\alpha}\left[\frac{\varepsilon^2k^2}{\gamma^2}-1\right]^{1/2}\langle S\gamma\,|f\,|S\gamma-1\rangle$$
$$=\langle S\gamma\,|\left[\frac{\gamma}{r}-\frac{Z\varepsilon}{\gamma}-\frac{1}{2}\frac{d}{dr}\right]f\,|S\gamma\rangle$$
$$=\langle S\gamma-1\,|\left[\frac{\gamma}{r}-\frac{Z\varepsilon}{\gamma}+\frac{1}{2}\frac{d}{dr}\right]f\,|S\gamma-1\rangle\,. \quad (11)$$

Hence the use of this expression for the off-diagonal $\langle S\gamma\,|\,r^t\,|\,S\gamma-1\rangle$ matrix elements allows the computation of the Dirac integrals (10) only in terms of diagonal Kepler matrix elements $\langle S\gamma\,|\,r^t\,|\,S\gamma\rangle$ and $\langle S\gamma-1\,|\,r^t\,|\,S\gamma-1\rangle$, which are easily obtainable when substituting $S+1=Z\alpha\varepsilon(1-\varepsilon^2)^{-1/2}$ for n and γ for l into the well-known expressions of the $\langle nl\,|\,r^t\,|\,nl\rangle$ hydrogenic integrals.

Particularly let us consider the determination of the integrals I_0, J_0, K_0, and L_0. Setting $f(r)\equiv 1$, $\langle\gamma\,|\,\gamma\rangle=1$, $\langle\gamma\,|\,1/r\,|\,\gamma\rangle=Z\varepsilon/(S+1)^2=(1-\varepsilon^2)/Z\varepsilon\alpha^2$ in Eq. (11) and keeping in mind that $\gamma^2=k^2-Z^2\alpha^2$, one gets

$$\langle\gamma\,|\,\gamma-1\rangle=-\frac{\gamma}{Z\alpha\varepsilon}\left[\frac{\varepsilon^2k^2}{\gamma^2}-1\right]^{1/2}.$$

Then, using Eq. (10), after some algebraic manipulations, one obtains the expressions of the integrals I_0, J_0, K_0, and L_0, which are reported in Table I.

Finally, it is noteworthy that the use of Eqs. (10) and (11) allows the determination of analytical expressions of the r^t integrals (10), for any value of t since the recurrence formula[11] relating the hydrogenic integrals $\langle nl\,|\,r^t\,|\,nl\rangle$ can be used in order to determine recursively any diagonal Kepler matrix element. In terms of ε and k, one gets

$$\frac{(t+1)(1-\varepsilon^2)}{Z^2\alpha^2\varepsilon^2}\langle\gamma\,|\,r^t\,|\,\gamma\rangle$$
$$=\frac{2t+1}{Z\varepsilon}\langle\gamma\,|\,r^{t-1}\,|\,\gamma\rangle-\frac{t[(2\gamma+1)^2-t^2]}{4Z^2\varepsilon^2}\langle\gamma\,|\,r^{t-2}\,|\,\gamma\rangle\,. \quad (12)$$

Nevertheless, as the values of t increase, despite the proposed simplifications avoiding the computation of the off-diagonal Kepler matrix elements $\langle\gamma\,|\,r^t\,|\,\gamma-1\rangle$ and the easy use of Eq. (12), the overall determination of analytical expressions of the Dirac r^t integrals becomes rather intricated and cumbersome. As will be shown hereafter, a direct procedure, merely using the properties of the coupled radial Dirac equations (5), leads to a much more efficient recursive determination of these r^t Dirac integrals.

IV. RECURSIVE DETERMINATION OF THE DIRAC r^t INTEGRALS

Combining together Eq. (5) for $P=P_{vk}$, $Q=Q_{vk}$ with their companions for $P'=P_{v'k'}$ and $Q'=Q_{v'k'}$, one can write

$$\frac{d}{dr}(P'P+Q'Q)+\frac{k'+k}{r}(P'P-Q'Q) = -\frac{2}{\alpha}(P'Q+Q'P)+\frac{\varepsilon'-\varepsilon}{\alpha}(P'Q-Q'P) ,$$

$$\frac{d}{dr}(P'P-Q'Q)+\frac{k'+k}{r}(P'P+Q'Q) = -\frac{1}{\alpha}(\varepsilon'+\varepsilon+2Z\alpha^2/r)(P'Q+Q'P) ,$$

$$\frac{d}{dr}(P'Q+Q'P)+\frac{k'-k}{r}(P'Q-Q'P) = -\frac{2}{\alpha}(P'P+Q'Q) + \frac{1}{\alpha}(\varepsilon'+\varepsilon+2Z\alpha^2/r)(P'P-Q'Q) ,$$

$$\frac{d}{dr}(P'Q-Q'P)+\frac{k'-k}{r}(P'Q+Q'P) = -\frac{1}{\alpha}(\varepsilon'-\varepsilon)(P'P+Q'Q) . \quad (13)$$

Multiplying both sides of Eq. (13) by r^t, one gets, after integrating by parts and taking into account the vanishing conditions at the bounds of the Dirac radial functions

$$t\mathscr{I}_{t-1}-2\mathscr{J}_t-(k'+k)\mathscr{K}_{t-1}+(\varepsilon'-\varepsilon)\mathscr{L}_t=0 ,$$

$$(k'+k)\mathscr{I}_{t-1}+(\varepsilon'+\varepsilon)\mathscr{J}_t+2Z\alpha^2\mathscr{J}_{t-1}-t\mathscr{K}_{t-1}=0 ,$$

$$2\mathscr{I}_t-t\alpha^2\mathscr{J}_{t-1}-(\varepsilon'+\varepsilon)\mathscr{K}_t -2Z\alpha^2\mathscr{K}_{t-1}+(k'-k)\alpha^2\mathscr{L}_{t-1}=0 , \quad (14)$$

$$(\varepsilon'-\varepsilon)\mathscr{I}_t+(k'-k)\alpha^2\mathscr{J}_{t-1}-t\alpha^2\mathscr{L}_{t-1}=0 .$$

Let us now focus our attention on the previous special cases $v'=v, k'=\pm k$. Hereafter, the shortened notation $I_t=\mathscr{I}_t(v'=v),\ldots$ will be used.

A. Recurrence relations for the ($k'=k$) r^t integrals

For $k'=k$, the Eqs. (14) reduce to

$$tI_{t-1}-2J_t-2kK_{t-1}=0 ,$$
$$2kI_{t-1}+2\varepsilon J_t+2Z\alpha^2J_{t-1}-tK_{t-1}=0 , \quad (15)$$
$$2I_t-t\alpha^2J_{t-1}-2\varepsilon K_t-2Z\alpha^2K_{t-1}=0 .$$

Setting successively $t=0$ in the first and third Eqs. (15) and $t=1$ in the two first Eqs. (15), one gets the following system of linear equations allowing the determination of the integrals J_0, J_1, K_0, and K_{-1} in terms of I_0

$$J_0+kK_{-1}=0 ,$$
$$\varepsilon K_0+Z\alpha^2K_{-1}=I_0 ,$$
$$J_1+kK_0=\tfrac{1}{2}I_0 , \quad (16)$$
$$\varepsilon J_1+Z\alpha^2J_0-\tfrac{1}{2}K_0=-kI_0 .$$

Since $I_0=1$ (normalization condition), one easily finds the expressions of the $k'=k$ Dirac radial integral K_{-1}, K_0, J_0, and J_1 in terms of ε and k, i.e., $K_{-1}=(1-\varepsilon^2)/Z\alpha^2$, $K_0=\varepsilon$, $J_0=k(\varepsilon^2-1)/Z\alpha^2$, and $J_1=\frac{1}{2}(1-2\varepsilon k)$.

It should be noted that the above result $K_0=\varepsilon$ together with the normalization condition $I_0=1$ leads, in a straightforward way to the previous result of Crubellier and Feneuille[4] obtained by simultaneously using the factorization method and group theoretical [0(2,1)] considerations, i.e.,

$$\int_0^\infty Q_{vk}^2 dr=\tfrac{1}{2}(1-\varepsilon) . \quad (17)$$

More recently, the expressions of (I_0+K_0), (I_0-K_0), J_0, J_1, and K_{-1} have been derived by Goldman and Drake,[5] by means of the relativistic virial theorem.

From Eqs. (15), after some algebraic manipulations, one obtains the following relations:

$$2J_t=tI_{t-1}-2kK_{t-1} ,$$

$$4Z(1-\varepsilon^2)(t+1)I_t =[4Z^2\alpha^2\varepsilon-(2k+\varepsilon t)(2\varepsilon k+t+1)t]I_{t-1} +[4Z^2\alpha^2(t+1)+t(2\varepsilon k+t)(2\varepsilon k+t+1)]K_{t-1} ,$$

$$(2\varepsilon k+t+1)K_t=[2k+\varepsilon(t+1)]I_t+2Z\alpha^2J_t . \quad (18)$$

Hence starting from $t=1$ and using the particular values $I_0=1$ and $K_0=\varepsilon$, these recurrence relations allow the determination of any ($v'=v$, $k'=k$) integral in terms of ε and k. Particularly, one obtains the closed-form expressions that have been reported in Table I.

At the nonrelativistic limit, i.e., when retaining the terms up to $Z^2\alpha^2$, introducing the usual radial quantum number $n\simeq v+|\gamma|$ and keeping in mind that $k(k+1)=l(l+1)$, the integrals of Table I reduce to the closed-form expressions that are given in Table II. As expected, one recognizes in the expressions of the I_t and K_t integrals of this last table the well-known expressions of the hydrogenic radial $\langle nl\,|\,r^t\,|\,nl\rangle$ integrals.

B. Recurrence relations for the ($k'=-k$)r^t integrals

For $k'=-k$, the Eqs. (14) reduce to

$$tI_{t-1}-2J_t=0 ,$$
$$2\varepsilon J_t+2Z\alpha^2J_{t-1}-tK_{t-1}=0 ,$$
$$2I_t-\alpha^2tJ_{t-1}-2\varepsilon K_t-2Z\alpha^2K_{t-1}-2k\alpha^2L_{t-1}=0 , \quad (19)$$
$$2kJ_{t-1}+tL_{t-1}=0 .$$

After some algebraic manipulations, one gets the following recurrence relations:

$$4(1-\varepsilon^2)tJ_{t+1}-4Z\alpha^2\varepsilon(2t+1)J_t +\alpha^2(4k^2-4Z^2\alpha^2-t^2)(t+1)J_{t-1}=0 ,$$

$$I_t=\frac{2}{t+1}J_{t+1} ,$$

$$K_t=\frac{2}{t+1}(\varepsilon J_{t+1}+Z\alpha^2J_t) , \quad (20)$$

$$L_t=-\frac{2k}{t+1}J_t .$$

TABLE II. Nonrelativistic limit of the $(v'=v)$ Dirac r^t integrals.

	$k'=k$	$k'=-k$
I_0	1	$w\left[1-\frac{Z^2\alpha^2}{2n^2}\frac{\lvert k\rvert}{(n+\lvert k\rvert)}\right];w=-\mathrm{sgn}(k)\left[1-\frac{k^2}{n^2}\right]^{1/2}$
I_1	$\frac{1}{2Z}\left[3n^2-l(l+1)+Z^2\alpha^2\left[\frac{3}{2}-\frac{3n}{\lvert k\rvert}+\frac{k^2}{2n^2}\right]\right]$	$\frac{w}{2Z}\left[3n^2+Z^2\alpha^2\left[\frac{3}{2}-\frac{3n}{\lvert k\rvert}-\frac{3\lvert k\rvert}{(n+\lvert k\rvert)}\right]\right]$
I_2	$\frac{1}{2Z^2}\left[5n^4+n^2-3n^2l(l+1)\right.$ $\left.+Z^2\alpha^2\left[6n^2+1-l(l+1)-\frac{1}{2}k-\frac{n}{\lvert k\rvert}[10n^2+1-3l(l+1)]\right]\right]$	$\frac{w}{2Z^2}\left[5n^4+n^2-n^2k^2+Z^2\alpha^2\left[6n^2+1-k^2-\frac{n}{\lvert k\rvert}(10n^2+1-k^2)\right.\right.$ $\left.\left.-\frac{\lvert k\rvert(5n^2+1-k^2)}{2(n+\lvert k\rvert)}\right]\right]$
J_0	$-\frac{Zk}{n^2}\left[1+\frac{Z^2\alpha^2}{n}\left[\frac{1}{n}-\frac{1}{\lvert k\rvert}\right]\right]$	0
J_1	$\frac{1}{2}-k+\frac{Z^2\alpha^2k}{2n^2}$	$\frac{w}{2}\left[1-\frac{Z^2\alpha^2}{2n^2}\frac{\lvert k\rvert}{(n+\lvert k\rvert)}\right]$
J_2	$\frac{(1-k)}{2Z}\left[3n^2-l(l+1)+Z^2\alpha^2\left[\frac{3}{2}-\frac{3n}{\lvert k\rvert}+\frac{k}{2(1-k)}\right]\right]$	$\frac{w}{2Z}\left[3n^2+Z^2\alpha^2\left[\frac{3}{2}-\frac{3n}{k}-\frac{3\lvert k\rvert}{2(n+\lvert k\rvert)}\right]\right]$
K_0	$1-\frac{Z^2\alpha^2}{2n^2}$	$w\left[1-\frac{Z^2\alpha^2}{2n^2}\left[1+\frac{\lvert k\rvert}{(n+\lvert k\rvert)}\right]\right]$
K_1	$\frac{1}{2Z}\left[3n^2-l(l+1)+Z^2\alpha^2\left[1-\frac{3n}{\lvert k\rvert}+\frac{k}{2n^2}\right]\right]$	$\frac{w}{2Z}\left[3n^2+Z^2\alpha^2\left[1-\frac{3n}{\lvert k\rvert}-\frac{3\lvert k\rvert}{2(n+\lvert k\rvert)}\right]\right]$
K_2	$\frac{1}{2Z^2}\left[5n^4+n^2-3n^2l(l+1)\right.$ $\left.+Z^2\alpha^2\left[\frac{11}{2}n^2-\frac{3}{2}k^2+\frac{1}{2}-\frac{n}{\lvert k\rvert}[10n^2+1-3l(l+1)]\right]\right]$	$\frac{w}{2Z^2}\left[5n^4+n^2-n^2k^2+Z^2\alpha^2\left[\frac{11}{2}n^2+\frac{1}{2}(1-k^2)-\frac{n}{\lvert k\rvert}(10n^2+1-k^2)\right.\right.$ $\left.\left.+\frac{\lvert k\rvert(5n^2+1-k^2)}{2(n+\lvert k\rvert)}\right]\right]$

Starting from the value $t=1$ and noting that $J_0=0$ [see the first Eq. (19) for $t=0$], the use of these recurrence relations (20) allows a straightforward determination of any $(k'=-k)$ integral I_t, J_t, K_t, or L_t in terms of I_0. A closed-form expression of I_0 has been already obtained (see Sec. III) and one gets the $v'=v$, $k'=-k$ Dirac radial integrals which, as an illustrative example, are reported in Table I. Their nonrelativistic limits are given in Table II.

C. Relativistic Zeeman effect

Although this work was originally undertaken for the purpose of calculating space-curvature-induced modifications of the hydrogenic spectra, the present results remain quite useful when dealing with the traditional Dirac atomic-structure calculations. For instance, let us show how the relativistic expression of the Landé g factor can be obtained nicely in terms of ε and k.

The relativistic[12] Landé g factor is defined by the relation

$$\langle \psi_{vkm} \,|\, e\boldsymbol{\alpha}\cdot\mathbf{A} \,|\, \psi_{vkm} \rangle = \beta_e g \langle \psi_{vkm} \,|\, \mathbf{H}\cdot\mathbf{J} \,|\, \psi_{vkm} \rangle \;, \quad (21)$$

where $\mathbf{H}$ is the external uniform magnetic field and $\mathbf{A}=-\frac{1}{2}(\mathbf{r}\times\mathbf{H})$, β_e is the Bohr magneton. Noting that $\boldsymbol{\sigma}\cdot\mathbf{A}=-\frac{1}{2}(\boldsymbol{\sigma}\times\mathbf{r})\cdot\mathbf{H}$ and using the following expressions of the reduced matrix elements involved in Eq. (21)

$$\langle \tfrac{1}{2}\bar{l}j \,||\boldsymbol{\sigma}\times\mathbf{r}||\, \tfrac{1}{2}lj\rangle = \tfrac{1}{2}r(-1)^{j+l-1/2}(2j+1)^{3/2}[j(j+1)]^{-1/2}$$

and

$$\langle j||\mathbf{j}||j\rangle = [j(j+1)(2j+1)]^{1/2} \;,$$

one gets (in a.u.)

$$g=(-1)^{l+j+1/2}\frac{(2j+1)}{j(j+1)}\int_0^\infty P_{vk}Q_{vk}r\,dr \;. \quad (22)$$

Picking up from Table I the expression of $J_1(k'=k)$, one finds the relativistic expression of g in terms of ε and k, i.e.,

$$g=-\frac{k}{2j(j+1)}(1-2\varepsilon k) \;. \quad (23)$$

From Table II, after noting that $\frac{1}{2}-k=j(j+1)-l(l+1)+\frac{3}{4}$ [see Eq. (3)], one obtains

$$g=1+\frac{j(j+1)-l(l+1)+\frac{3}{4}}{2j(j+1)}-\frac{Z^2\alpha^2k^2}{2n^2j(j+1)} \;. \quad (24)$$

As expected, the two first terms in Eq. (24) correspond to the well-known nonrelativistic expression of the Landé g factor and the last term to the Breit-Margenau correction.

D. General off-diagonal ($v'\neq v$; $k'\neq k$) Dirac r^t integrals

It is noteworthy that the use of the recursive relations (11) provides the possibility to express the integrals $\mathscr{I}_t$, $\mathscr{J}_t$, $\mathscr{K}_t$, and $\mathscr{L}_t$ as linear combinations of $\mathscr{I}_{t-1}$, $\mathscr{J}_{t-1}$, $\mathscr{K}_{t-1}$, and $\mathscr{L}_{t-1}$. Indeed, after few algebraic manipulations Eq. (11) can be written in the following form:

$$\begin{aligned}
&(\varepsilon'-\varepsilon)\mathscr{I}_t=-(k'-k)\alpha^2\mathscr{J}_{t-1}+t\alpha^2\mathscr{L}_{t-1} \;,\\
&(\varepsilon'+\varepsilon)\mathscr{J}_t=-(k'+k)\mathscr{I}_{t-1}-2Z\alpha^2\mathscr{J}_{t-1}+t\mathscr{K}_{t-1} \;,\\
&(\varepsilon'+\varepsilon)(\varepsilon'-\varepsilon)\mathscr{K}_t=-[2(k'-k)+t(\varepsilon'-\varepsilon)]\alpha^2\mathscr{J}_{t-1}-2Z(\varepsilon'-\varepsilon)\alpha^2\mathscr{K}_{t-1}+[2t+(k'-k)(\varepsilon'-\varepsilon)]\alpha^2\mathscr{L}_{t-1} \;,\\
&(\varepsilon'+\varepsilon)(\varepsilon'-\varepsilon)\mathscr{L}_t=-[2(k'+k)+t(\varepsilon'+\varepsilon)]\mathscr{I}_{t-1}-4Z\alpha^2\mathscr{J}_{t-1}+[2t+(k'+k)(\varepsilon'+\varepsilon)]\mathscr{K}_{t-1} \;.
\end{aligned} \quad (25)$$

Hence the calculation of any off-diagonal $(v'\neq v, k'\neq k)$ r^t integral ultimately amounts to calculate the key integrals $\mathscr{I}_0$, $\mathscr{J}_0$, $\mathscr{K}_0$, and $\mathscr{L}_0$. Since $|\gamma'|\neq|\gamma|$ and $\varepsilon'\neq\varepsilon$, their determination via the explicit expressions (7) of P_{vk} and Q_{vk} implies the computation of the off-diagonal matrix elements between Kepler functions with $S'\neq S$, $M'\neq M$, and $q'\neq q$, i.e., to have at disposal closed-form expressions for the $n'\neq n$, $l'\neq l$, and $Z'\neq Z$ hydrogenic r^t integrals. If, for $Z'=Z$, such expressions are available (see, for instance, Refs. 9, 10, 13, and 14), this is not the case for $Z'\neq Z$. Nevertheless, the procedure outlined in Ref. 10 still holds for the determination of a closed-form expression of the $(n'\neq n$, $l'\neq l$, and $Z'\neq Z)$ hydrogenic r^t integrals. In terms of ε and k, one obtains the following expression of the required Kepler $(\varepsilon'\neq\varepsilon)$ matrix elements:

$$\langle S'\gamma' \,|\, r^t \,|\, S\gamma\rangle = CC'\sum_{u=0}^{v}\begin{bmatrix} v \\ u\end{bmatrix}\frac{(-2\mu)^u}{\Gamma(2\gamma+u+2)}\sum_{u'=0}^{v'}\begin{bmatrix} v' \\ u'\end{bmatrix}\frac{(-2\mu')^{u'}}{\Gamma(2\gamma'+u'+2)}\frac{\Gamma(\gamma+\gamma'+t+u+u'+3)}{(\mu+\mu')^{\gamma+\gamma'+t+u+u'+3}} \;, \quad (26)$$

where

$$\mu=\frac{1}{\alpha}(1-\varepsilon^2)^{1/2} \;,$$

$$C=(-)^l(2)^{\gamma+3/2}\frac{\Gamma(\gamma+1+Z\varepsilon/\mu)^{1/2}}{v!(2Z\varepsilon/\mu)} \;.$$

This expression holds for $\gamma>0$ and $\gamma'>0$; when γ or γ' are negative, one has first to introduce the correspondence $R_S^{-|\gamma|}=R_S^{|\gamma|-1}$ and $R_S^{-|\gamma|-1}=-R_S^{|\gamma|}$.

As a concluding remark, let us mention that the recursive procedure outlined in the present paper is particularly well adapted for the use of symbolic computation programs such as REDUCE[15] or MACSYMA[16]. Thus one could obtain compact closed-formed expressions of Dirac-Coulomb radial integrals of any function $f(r)$ that can be expanded in a series of r^t.

*Present address: Laboratoire de Physique des Lasers, Université Paris 13, F-93430 Villetaneuse, France.

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