Transformation of bound states of relativistic hydrogenlike atoms into a two-component form

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A single-step Eriksen transformation of $1S_{1/2}$, $2P_{1/2}$, and $2P_{3/2}$ states of the relativistic hydrogenlike atom is performed exactly by expressing each transformed function (TF) as a linear combination of eigenstates of the Dirac Hamiltonian. The TFs, which are four-component spinors with vanishing two lower components, are calculated numerically and have the same symmetries as the initial states. For all nuclear charges $Z \in [1 \dots 92]$ a contribution of the initial state to TFs exceeds 86% of the total probability density. Next a large contribution to TFs comes from continuum states with negative energies close to $-m_0c^2 - E_b$, where E_b is the binding energy of the initial state. The contribution of other states to TFs is less than 0.1% of the total probability density. Other components of TFs are nearly 0, which confirms both the validity of the Eriksen transformation and the accuracy of the numerical calculations. The TFs of the $1S_{1/2}$ and $2P_{1/2}$ states are close to the 1s and 2p states of the nonrelativistic hydrogenlike atom, respectively, but the TF of the $2P_{3/2}$ state differs qualitatively from the 2p state. Functions calculated with the use of a linearized Eriksen transformation, being equivalent to the second-order Foldy-Wouthuysen transformation, are compared with corresponding functions obtained by Eriksen transformation. Very good agreement between the two results is obtained.

DOI: 10.1103/PhysRevA.94.012117

I. INTRODUCTION

In their pioneering work, Foldy and Wouthuysen (FW) introduced the method of separating positive- and negativeenergy states of the Dirac Hamiltonian [1]. In the presence of external fields the odd terms of the lowest order in $1/(m_0c^2)$ are removed to the desired accuracy by a sequence of unitary transformations. As a result, the states of the Dirac Hamiltonian having positive energies are transformed to the two-component form, in which two upper components are nonzero and two lower components vanish, up to the expected accuracy. In this way one reduces the Dirac equation to two equations for two-component spinors describing states of positive and negative energies, respectively. The widely used second-order FW transformation converts the Dirac Hamiltonian into a Schrodinger Hamiltonian with relativistic corrections: the \hat{p}^4 term, the spin-orbit interaction, and the Darwin term. Works considering higher-order FW transformations are discussed in Ref. [2].

Another possibility of transforming the Dirac Hamiltonian into a two-component form was proposed by Douglas and Kroll (DK) in Ref. [3]. In this approach, used mostly in quantum chemistry, one performs a series of transformations leading to an expansion of the Dirac Hamiltonian in orders of the external potential (see [3] and [4]). In each step of the DK transformation the odd terms of the lowest order are removed up to the expected accuracy. Using this method it is possible to include many-electron effects into real atomic systems [5]. For a review of works related to this subject see Ref. [6].

Practical limitations of applying higher-order FW or DK transformations are due to complicated calculations since one has to manipulate increasing numbers of noncommuting operators. To overcome these limitations several approaches have been proposed, removing odd terms to a sufficiently high order with the use of numerical methods [7,8]. The

2469-9926/2016/94(1)/012117(11)

resulting 2×2 Schrödinger-like equations with relativistic corrections are then solved numerically for energies and wave functions. Good agreement between approximate and exact Dirac energies was reported [8–11].

One can avoid complicated calculations in special cases using transformations separating exactly the Dirac Hamiltonian into a two-component form. Such a transformation for free relativistic electrons was proposed by Foldy and Wouthuysen [1]. Case [12] found an exact form of the FW transformation for the presence of a constant magnetic field. Tsai [13] and Weaver [14] reported exact FW transformations for the presence of a magnetic field and electroweak interactions. Moss and Okninski [15] pointed out that there exist several transformations separating positive and negative states of the Dirac Hamiltonian, leading to similar but not identical results for transformed functions. Nikitin [16] reported on FW-like transformations for a constant electric field, a dipole potential, and some classes of external fields with special symmetries. The common weakness of the above methods is their inability to generalize the results to arbitrary potentials.

There exist in the literature several examples of functions transformed with the use of FW-like or DK-like transformations. Calculation of transformed functions and the transformation kernel for the FW transformations for free Dirac electrons were given by Rusin and Zawadzki in Ref. [17], and for the presence of a magnetic field in Ref. [18]. In the latter paper, the analytical expression for a transformed Gaussian wave packet was obtained. Neznamov and Silenko [19,20] analyzed the properties of functions transformed with the use of FW-like transformations and showed that the lower components of the resulting functions are of the second order of $1/(m_0c^2)$. In several works related to DK-like transformations the resulting functions were obtained numerically [6,8–11].

A transformation of the Dirac Hamiltonian for any potential converting it into a block-diagonal form was proposed by Eriksen in Refs. [21] and [22]. This transformation is performed in a single step by a unitary operator \hat{U} , which is a nonlinear function of the Dirac Hamiltonian. Because of its nonlinearity,

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 $\hat{\mathcal{U}}$ is usually approximated by a finite series in powers of $1/(m_0c^2)$ [2,21]. The validity of the Eriksen transformation and its power-series expansion was confirmed by de Vries [2] and Silenko [23]. In the lowest-order terms, the Eriksen transformation agrees with the results obtained by the FW method, but higher-order terms differ [2,19].

The subject of the present work is transformation of bound states of the Dirac Hamiltonian with a nontrivial potential by the Eriksen operator $\hat{\mathcal{U}}$ without expanding $\hat{\mathcal{U}}$ in a power series. In our approach we concentrate on the transformed functions and their properties, and not on the transformed operators. Our calculations are performed for the relativistic hydrogenlike atom whose spectrum consists of both bound and continuum states. To illustrate our method and results the transformation is performed numerically for the three lowest bound states of the relativistic hydrogenlike atom— $1S_{1/2}$, $2P_{1/2}$, and $2P_{3/2}$ —for several values of the nuclear charge Z. To our knowledge there has been no attempt to calculate functions transformed by the single-step Eriksen transformation for the Dirac Hamiltonian whose eigenfunctions are bound states.

It should be remembered that by solving the Dirac equation (analytically or numerically), one directly obtains all its eigenvalues and eigenstates that can be used for calculations of observables, and no further transformation is needed. The Dirac equation transformed to the block-diagonal form can also be used for calculation of the observables, and both approaches yield the same results because the wave functions in both representations are related to each other by the unitary transformation. Thus, the choice of representations of the Dirac equation depends on its convenience in further calculations or applications.

The paper is organized as follows. In Sec. II we describe our approach, and in Sec. III we specify wave functions of the relativistic hydrogenlike atom. In Sec. IV we show results of calculations and in Sec. V we discuss our results. The paper is concluded by a Summary (Sec. VI). In Appendixes A and B we specify details of our calculations.

II. ERIKSEN TRANSFORMATION

Let us consider the Dirac Hamiltonian describing a relativistic electron in the presence of the Coulomb potential created by the atomic nucleus,

$$\hat{\mathcal{H}} = c \sum_{i=x,y,z} \hat{\boldsymbol{\alpha}}_i \hat{\boldsymbol{p}}_i + \hat{\beta} m_0 c^2 - \frac{Z e^2}{4\pi\epsilon_0 r}, \qquad (1)$$

in which $\hat{\alpha}_i$ and $\hat{\beta}$ are Dirac matrices in the standard notation, |e| and m_0 are the electron charge and mass, respectively, and $Z \in [1 \dots 92]$ is the nuclear charge. Both eigenenergies and eigenstates of $\hat{\mathcal{H}}$ are known analytically. The latter are given by four-component spinors. The spectrum of $\hat{\mathcal{H}}$ consists of an infinite set of bound states having positive energies below $E = +m_0c^2$ and two sets of continuum states having energies above $+m_0c^2$ and below $-m_0c^2$, respectively.

The Eriksen transformation is defined by the following unitary operator [21]:

$$\hat{\mathcal{U}} = \frac{1}{\sqrt{2 + \hat{\beta}\hat{\lambda} + \hat{\lambda}\hat{\beta}}} (1 + \hat{\beta}\hat{\lambda}) \equiv \hat{\mathcal{Z}} + \hat{\mathcal{Z}}\hat{\beta}\hat{\lambda}.$$
 (2)

The above equation defines the operator $\hat{\mathcal{Z}}$,

$$\hat{\mathcal{Z}} = \frac{1}{\sqrt{2 + \hat{\beta}\hat{\lambda} + \hat{\lambda}\hat{\beta}}}.$$
(3)

The sign operator $\hat{\lambda}$ is defined as

$$\hat{\lambda} = \frac{\hat{\mathcal{H}}}{\sqrt{\hat{\mathcal{H}}^2}}.$$
(4)

It is assumed that E = 0 is not an eigenenergy of $\hat{\mathcal{H}}$, which holds for $\hat{\mathcal{H}}$ in Eq. (1)

Let $\langle \boldsymbol{r} | n \rangle = (\psi_1, \psi_2, \psi_3, \psi_4)^T$ be an arbitrary eigenfunction of $\hat{\mathcal{H}}$ corresponding to a positive energy. After the Eriksen transformation there is (see Appendix A)

$$\hat{\mathcal{U}} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = \begin{pmatrix} \hat{\mathcal{U}} \psi_1 \\ \hat{\mathcal{U}} \psi_2 \\ 0 \\ 0 \end{pmatrix}; \tag{5}$$

i.e., the transformed function has vanishing two lower components. Because $\hat{\mathcal{U}}$ in Eq. (2) is a nonlinear function of the differential operator $\hat{\nabla}$ and the position operator \hat{r} , it is not possible to express $\hat{\mathcal{U}}\psi_1$ and $\hat{\mathcal{U}}\psi_2$ in a closed form.

To overcome this problem one notes that for an arbitrary eigenstate $|n\rangle$ of $\hat{\mathcal{H}}$ having energy $E_n \neq 0$ there is

$$\hat{\lambda}|n\rangle = \frac{E_n}{|E_n|}|n\rangle \equiv \epsilon_n|n\rangle, \tag{6}$$

where $\epsilon_n = \pm 1$ is the sign of E_n . Thus, using Eq. (6) one can calculate the matrix elements of the numerator of $\hat{\mathcal{U}}$ in Eq. (2) between the eigenstates of $\hat{\mathcal{H}}$ in Eq. (1). Similarly, expanding $\hat{\mathcal{Z}}$ in Eq. (3) in a power series of $(\hat{\beta}\hat{\lambda} + \hat{\lambda}\hat{\beta})$ one can calculate matrix elements of $\hat{\mathcal{Z}}$ between the eigenstates of $\hat{\mathcal{H}}$. Thus, in spite of the fact that we do not know the explicit form of $\hat{\mathcal{U}}$ in Eq. (2), we have a way to calculate its *matrix elements* between all eigenstates of $\hat{\mathcal{H}}$. This observation indicates the method of calculating the transformed functions in Eq. (5).

Let $|n_0\rangle$ and $|\chi\rangle = \hat{\mathcal{U}}|n_0\rangle$ be an eigenstate of $\hat{\mathcal{H}}$ and its Eriksen-transformed counterpart, respectively. Since $|n\rangle$ form a complete set of states in the space of four-component spinors, we may express $|\chi\rangle$ as a linear combination of $|n\rangle$:

$$|\chi\rangle = \sum_{n} a_{n} |n\rangle, \quad a_{n} = \langle n | \hat{\mathcal{U}} | n_{0} \rangle.$$
 (7)

Equation (7) indicates the way to calculate the function $|\chi\rangle$. First, one selects a large but finite set of eigenstates of $\hat{\mathcal{H}}$ in Eq. (1), including both bound and continuum states having positive or negative energies. Then we calculate (analytically or numerically) the matrix elements $\langle n|\hat{\mathcal{U}}|n_0\rangle$ between all states in the selected set. Finally, we calculate $\langle r|\chi\rangle$ as a sum over all eigenfunctions $\langle r|n\rangle$ of $\hat{\mathcal{H}}$, as given in Eq. (7). In our approach we make only one approximation, namely, we truncate the infinite set of eigenstates of $\hat{\mathcal{H}}$ into a finite one.

Below we describe the consecutive steps necessary to calculate the transformed functions $|\chi\rangle$. Our derivation is restricted to the transformation of the $1S_{1/2}$ state of the relativistic hydrogenlike atom; its generalization to other states is straightforward.

A. Discretization of continuum states

Consider an arbitrary state $|n\rangle$ of $\hat{\mathcal{H}}$. The bound states $|n\rangle$ depend on the integer quantum number n, while the continuum states depend on the absolute value of the electron's momentum $p = \sqrt{(E/c)^2 - (m_0 c)^2}$ and the sign of the energy branch $\epsilon = \pm 1$. Three other quantum numbers describing $|n\rangle$, namely, the total angular momentum j, the orbital number l, and $m = j_z$, are omitted in the present section. We assume that the bound states are normalized to the Kronecker delta, $\langle n_1|n_2 \rangle = \delta_{n_1,n_2}$, while the continuum states are normalized to the Dirac delta, $\langle p_1^{\epsilon_i} | p_2^{\epsilon_j} \rangle = \delta(p_1 - p_2) \delta_{\epsilon_i, \epsilon_j}$.

Let $\psi_{1S}(\mathbf{r}) = \langle \mathbf{r} | 1S \rangle$ denote the $1S_{1/2}$ state of the relativistic hydrogenlike atom with spin up. Then writing $|n_0\rangle = |1S\rangle$ in Eq. (7) one obtains

$$\chi_{1S}(\boldsymbol{r}) \equiv \langle \boldsymbol{r} | \hat{\mathcal{U}} | 1S \rangle = \sum_{n} a_{n} \psi_{n}(\boldsymbol{r}) + \sum_{\epsilon = \pm} \int_{0}^{\infty} a_{p}^{\epsilon} \psi_{p}^{\epsilon}(\boldsymbol{r}), \quad (8)$$

where $a_n = \langle \psi_n | \chi_{1S} \rangle$ and $a_p^{\epsilon} = \langle \psi_p^{\epsilon} | \chi_{1S} \rangle$. The difficulty is caused by the different normalization of bound and continuum states. To surmount this problem we follow Refs. [24] and [25] by replacing the continuum functions $\psi_p^{\epsilon}(\mathbf{r})$ in Eq. (8) with the so-called discretized functions $\Psi_{p_i}^{\epsilon}(\mathbf{r})$,

$$\chi_{1S}(\mathbf{r}) \simeq \sum_{n} a_{n} \psi_{n}(\mathbf{r}) + \sum_{\epsilon = \pm} \sum_{p_{i}} \left(a_{p_{i}}^{\epsilon} \sqrt{\Delta p} \right) \\ \times \left(\frac{1}{\sqrt{\Delta p}} \int_{p_{i} - \frac{\Delta p}{2}}^{p_{i} + \frac{\Delta p}{2}} \psi_{p}^{\epsilon}(\mathbf{r}) dp \right)$$
(9)

$$=\sum_{n}a_{n}\psi_{n}(\boldsymbol{r})+\sum_{\epsilon=\pm}\sum_{p_{i}}A_{p_{i}}^{\epsilon}\Psi_{p_{i}}^{\epsilon}(\boldsymbol{r}),\qquad(10)$$

where $A_{p_i}^{\epsilon}$ and $\Psi_{p_i}^{\epsilon}(\mathbf{r})$ are defined within the first and second sets of large parentheses in Eq. (9), respectively. As shown in Refs. [24–26], for $\Delta p \rightarrow 0$ the summation over p_i in Eq. (10) reduces to the integration over dp, as given in Eq. (8). The essential features of functions $\Psi_{p_i}^{\epsilon}(\mathbf{r})$ are that (a) they are localized and integrable in the real space [26]; (b) they are normalized to the Kronecker delta, $\langle \Psi_{p_i}^{\epsilon_i} | \Psi_{p_j}^{\epsilon_j} \rangle = \delta_{p_i, p_j} \delta_{\epsilon_i, \epsilon_j}$; (c) they are orthogonal to all functions ψ_n of bound states; and (d) $\Psi_{p_i}^{\epsilon_i}$ and ψ_n form a complete basis for four-component spinors. Therefore, the bound states $\psi_n(\mathbf{r})$ and discretized functions $\Psi_{p_i}^{\epsilon}(\mathbf{r})$ can be treated similarly, i.e., all integrals including continuum functions $\psi_p(\mathbf{r})$ may be replaced by sums over discretized functions $\Psi_{p_i}^{\epsilon}(\mathbf{r})$. The discretized functions in Eq. (10) are also called eigendifferentials in the literature [27].

B. Probability amplitudes

To find the probability amplitudes a_n and $A_{p_i}^{\epsilon}$ in Eq. (10) we calculate the matrix elements of $\hat{\mathcal{U}}$ between eigenstate $1S_{1/2}$ and eigenstate $|n\rangle$,

$$a_n = \langle n | \hat{\mathcal{U}} | 1S \rangle = \langle n | \hat{\mathcal{Z}} | 1S \rangle + \langle n | \hat{\mathcal{Z}} \hat{\beta} \hat{\lambda} | 1S \rangle, \qquad (11)$$

$$A_{p_i}^{\epsilon} = \left\langle \Psi_{p_i}^{\epsilon} \middle| \hat{\mathcal{U}} | 1S \right\rangle = \left\langle \Psi_{p_i}^{\epsilon} \middle| \hat{\mathcal{Z}} | 1S \right\rangle + \left\langle \Psi_{p_i}^{\epsilon} \middle| \hat{\mathcal{Z}} \hat{\beta} \hat{\lambda} | 1S \right\rangle, \quad (12)$$

with the normalization condition

$$\sum_{n} |a_{n}|^{2} + \sum_{\epsilon=\pm} \sum_{p_{i}} |A_{p_{i}}^{\epsilon}|^{2} = 1.$$
 (13)

The operator \hat{Z} has vanishing matrix elements between the eigenstates of $\hat{\mathcal{H}}$ having positive and negative energies (see Appendix A). Since $|1S\rangle$ state has positive energy there is $\hat{\lambda}|1S\rangle = |1S\rangle$ [see Eq. (6)]. The use of Eq. (6) leads to the exact treatment of the sign operator $\hat{\lambda}$ in the calculation of the matrix elements of $\hat{\mathcal{U}}$. Inserting the unity operator

$$\hat{\mathbf{l}} = \sum_{n} |n\rangle \langle n| + \sum_{\epsilon = \pm 1} \sum_{p_i} |\Psi_{p_i}^{\epsilon}\rangle \langle \Psi_{p_i}^{\epsilon}|$$
(14)

into expressions for a_n and $A_{p_i}^{\epsilon}$ in Eqs. (11) and (12), we obtain

$$a_{n} = \langle n|\hat{\mathcal{Z}}|1S\rangle + \sum_{n'} \langle n|\hat{\mathcal{Z}}|n'\rangle \langle n'|\hat{\beta}|1S\rangle + \sum_{p_{j}} \langle n|\hat{\mathcal{Z}}|\Psi_{p_{j}}^{+}\rangle \langle \Psi_{p_{j}}^{+}|\hat{\beta}|1S\rangle, \qquad (15)$$

$$A_{p_{i}}^{+} = \langle \Psi_{p_{i}}^{+} | \hat{\mathcal{Z}} | 1S \rangle + \sum_{n'} \langle \Psi_{p_{i}}^{+} | \hat{\mathcal{Z}} | n' \rangle \langle n' | \hat{\beta} | 1S \rangle + \sum_{n'} \langle \Psi_{p_{i}}^{+} | \hat{\mathcal{Z}} | \Psi_{p_{j}}^{+} \rangle \langle \Psi_{p_{j}}^{+} | \hat{\beta} | 1S \rangle, \qquad (16)$$

$$A_{p_i}^- = \sum_{p_j} \langle \Psi_{p_i}^- | \hat{\mathcal{Z}} | \Psi_{p_j}^- \rangle \langle \Psi_{p_j}^- | \hat{\beta} | 1S \rangle.$$
(17)

Thus, to find the probability amplitudes a_n and $A_{p_i}^{\epsilon}$ one needs to calculate seven types of matrix elements:

D;

The matrix elements of $\hat{\beta}$ between two eigenstates of $\hat{\mathcal{H}}$ are obtained in a standard way by computing four integrals between the components of these states (see below). Calculation of the matrix elements of $\hat{\mathcal{Z}}$ is more complicated since this operator cannot be represented in a closed form [see Eq. (3)]. To find $\hat{\mathcal{Z}}$ in Eq. (3) we introduce an auxiliary operator,

$$\hat{S} = \hat{\lambda}\hat{\beta} + \hat{\beta}\hat{\lambda} = \sum_{s} \xi_{s} |s\rangle \langle s|, \qquad (19)$$

where ξ_s and $|s\rangle$ are the eigenvalues and eigenvectors of \hat{S} , respectively. Then, assuming that the square root exists, one has

$$\hat{\mathcal{Z}} = \sum_{s} \frac{1}{\sqrt{2 + \xi_s}} |s\rangle \langle s|.$$
(20)

Equations (19) and (20) give us a practical way to calculate \hat{z} in four steps. We first select the basis, consisting of three sets of eigenstates of $\hat{\mathcal{H}}$: bound states $\{\psi_n\}$, discretized states having positive energies $\{\Psi_{p_i}^+\}$, and discretized states having negative energies $\{\Psi_{p_i}^-\}$. Then we calculate the matrix elements of \hat{S} in Eq. (19) between these states. The resulting matrix has a block-diagonal form plotted schematically in Fig. 1. The three sets of states composing the basis of matrix \hat{S}_{n_1,n_2} are infinite and the matrix in Fig. 1 is of infinite order. In our calculations we truncate the infinite sets to finite ones (see Table I). In the third step one calculates all eigenvalues and eigenstates of \hat{S} , as given in Eq. (20). After this process \hat{z} is approximated by a finite matrix of size = 1576 × 1576 (see Table I).

	ψ_{1s}	$\psi_{2\text{s}}$		ψ_{Ns}	$\Psi^{+}_{\ p1}$	$\Psi^{\!+}_{\ \rm p2}$		$\Psi^{+}_{\ pN}$	$\Psi^{-}_{\rm p1}$	$\Psi^{-}_{\rm p2}$		$\Psi^{-}{}_{\rm pN}$
ψ_{1s}	$2\beta_{1s1s}$	x	x	х	у	у	у	у				
$\psi_{2\text{s}}$	x	$2\beta_{2s2s}$	x	х	у	у	у	у	0			
	x	х	$2\beta_{nsns}$	x	у	у	у	у			0	
ψ_{ns}	x	х	х	$2\beta_{NsNs}$	у	у	у	у				
$\Psi^{+}_{\ p1}$	у	у	у	у	2β ⁺ _{p1p1}	0	0	0				
$\Psi^{+}_{\ p2}$	у	у	у	у	0	2β ⁺ _{p2p2}	0	0	0			
	у	у	у	у	0	0	2β ⁺ _{pnpn}	0				
$\Psi^{+}_{\ pN}$	у	у	у	у	0	0	0	2β [*] _{pN pN}				
$\Psi^{\rm p1}$									-2β ⁻ _{p1p1}	0	0	0
$\Psi^{\rm p2}$	0			0			0	-2β ⁻ _{p2p2}	0	0		
							0	0	-2β ⁻ _{pnpn}	0		
Ψ_{pN}^{-}									0	0	0	-2β ⁻ _{pN pN}

FIG. 1. Schematic matrix $\hat{S} = \hat{\beta}\hat{\lambda} + \hat{\lambda}\hat{\beta}$ in the basis of states ψ_{nS} and discretized functions $\Psi_{p_i}^{\pm}$ in Eq. (10). Diagonal matrix elements, which dominate over nondiagonal ones, are shown explicitly. Nondiagonal elements between bound states are indicated by *x*, while nondiagonal elements between bound and continuum states are indicated by *y*. Note the block-diagonal form of matrix \hat{S} and vanishing matrix elements between states of positive and states of negative energies.

C. Foldy-Wouthuysen-like approximation for $\hat{\mathcal{U}}$

Following Eriksen, one can formally expand the square root in Eq. (3), treating $\hat{q} = \hat{\beta}\hat{\lambda} - 1$ as an expansion parameter. In the second order in \hat{q} , one obtains [21]

$$\hat{\mathcal{U}} \simeq 1 + \frac{1}{2}\hat{q} - \frac{1}{8}(\hat{q} + \hat{q}^*) + \dots$$
 (21)

Eriksen showed that this expansion is equivalent to the FW transformation in the second order of $1/(m_0c^2)$. Functions transformed with the use of Eriksen and FW transformations have similar upper components. For this reason we refer to the transformation defined in Eq. (21) as the FW-like expansion of the Eriksen operator. After simple algebra one obtains

$$\hat{\mathcal{U}}^{\text{FW}} = \frac{3}{4} + \frac{1}{2}\hat{\beta}\hat{\lambda} - \frac{1}{8}(\hat{\beta}\hat{\lambda} + \hat{\lambda}\hat{\beta}).$$
(22)

The operator $\hat{\mathcal{U}}^{\text{FW}}$ in Eq. (22) is a linear function of $\hat{\mathcal{S}} = \hat{\beta}\hat{\lambda} + \hat{\lambda}\hat{\beta}$, and it is not necessary to calculate its inverted square

TABLE I. Model parameters used in calculations.

Quantity	Value
Number of bound states	40
Number of continuum states	
For $E > 0$	512
For $E < 0$	1024
Summation over discretized states in Eqs.	(9) and (10)
Δp	$0.1 \ \hbar (r_B/Z)^{-1}$
Lower limit of p_i	$0.1 \ \hbar (r_B/Z)^{-1}$
Upper limit of p_i	
For $E > 0$	$51.2 \hbar (r_B/Z)^{-1}$
For $E < 0$	$102.4 \ \hbar (r_B/Z)^{-1}$

root $\hat{\mathcal{Z}}$ [see Eqs. (3) and (20)]. This simplifies calculations of transformed functions $\hat{\mathcal{U}}^{\text{FW}} |\psi\rangle$.

Let $|n_1\rangle$ and $|n_2\rangle$ be two eigenstates of $\hat{\mathcal{H}}$, whose signs are ϵ_1 and ϵ_2 , respectively. For $\epsilon_1 = \epsilon_2$ we have

$$\langle n_1 | \hat{\mathcal{U}}^{\rm FW} | n_2 \rangle = \frac{3}{4} \delta_{n_1, n_2} + \frac{1}{4} \epsilon_2 \hat{\beta}_{n_1, n_2},$$
 (23)

while for $\epsilon_1 = -\epsilon_2$ there is

$$\langle n_1 | \hat{\mathcal{U}}^{\text{FW}} | n_2 \rangle = \frac{1}{2} \epsilon_2 \hat{\beta}_{n_1, n_2}.$$
(24)

Comparing Eqs. (15)–(17) and Eqs. (23) and (24) we see that in both cases one has to calculate the same matrix elements of $\hat{\beta}$, as listed in Eq. (18).

III. EIGENSTATES OF $\hat{\mathcal{H}}$ AND SELECTION RULES FOR $\hat{\beta}_{n_1,n_2}$

In this section we find selection rules for the matrix elements of $\hat{\beta}$ between eigenstates of $\hat{\mathcal{H}}$. Next we introduce the radial wave functions of bound and continuum states of $\hat{\mathcal{H}}$. We also qualitatively estimate magnitudes of radial integrals used in the matrix elements of $\hat{\beta}$.

A. Selection rules for $\hat{\beta}_{n_1,n_2}$

Because of the spherical symmetry of the problem, the eigenstates $\langle \boldsymbol{r} | n \rangle$ are products of the radial functions g(r) and f(r), and the function $\Omega(\theta, \varphi)$, depending on angular variables. The latter is characterized by three quantum numbers: the orbital angular momentum l, the total angular momentum j, and $m = j_z$. The auxiliary quantum number κ is defined as

$$\kappa = \begin{cases} -j - \frac{1}{2} & \text{for } j = l + \frac{1}{2}, \\ j + \frac{1}{2} & \text{for } j = l - \frac{1}{2}. \end{cases}$$
(25)

It is either a positive or a negative integer, but not 0. The eigenstates of $\hat{\mathcal{H}}$ are [28,29]

$$\psi_n(r,\theta,\varphi) = \begin{pmatrix} g(r) \ \Omega_{\kappa,m}(\theta,\varphi) \\ if(r) \ \Omega_{\kappa,-m}(\theta,\varphi) \end{pmatrix},$$
(26)

where $\Omega_{\kappa,m}(\theta,\varphi)$ are two-component spinors,

$$\Omega_{\kappa,m}(\theta,\varphi) = \begin{pmatrix} \sqrt{\frac{\kappa + \frac{1}{2} - m}{2\kappa + 1}} Y_{\kappa,m-1/2}(\theta,\varphi) \\ -\frac{\kappa}{|\kappa|} \sqrt{\frac{\kappa + \frac{1}{2} + m}{2\kappa + 1}} Y_{\kappa,m+1/2}(\theta,\varphi) \end{pmatrix}, \qquad (27)$$

and $Y_{a,b}(\theta,\varphi)$ are the spherical harmonics. For a > 0 the latter are defined as

$$Y_{a,b}(\theta,\varphi) = (-1)^b \sqrt{\frac{2a+1}{4\pi} \frac{(a-b)!}{(a+b)!}} P_a^b(\cos(\theta)) e^{ib\varphi}, \quad (28)$$

where $P_a^b(\cos(\theta))$ are the associated Legendre polynomials in the usual notation [31]. For a < 0 there is $Y_{a,b}(\theta,\varphi) = Y_{-a,-b}(\theta,\varphi)$, and for |a| < |b| there is $Y_{a,b}(\theta,\varphi) \equiv 0$. The functions $\Omega_{\kappa,m}(\theta,\varphi)$ fulfill the orthogonality relation [29]

$$\int_0^{\pi} \int_0^{2\pi} \Omega_{\kappa_1, m_1}(\theta, \varphi) \Omega_{\kappa_2, m_2}(\theta, \varphi) \sin(\theta) d\theta d\varphi = \delta_{\kappa_1 \kappa_2} \delta_{m_1 m_2}.$$
(29)

TABLE II. Quantum numbers characterizing eigenstates of the relativistic hydrogenlike atom used for calculations in Figs. 2 to 6.

Eigenstate	κ	т	n_r	Examples of intermediate states
$1S_{1/2}$	-1	1/2	0	$1S_{1/2}, 2S_{1/2}, 3S_{1/2}, \ldots$
$2P_{1/2}$	1	1/2	1	$2P_{1/2}, 3P_{1/2}, 4P_{1/2}, \ldots$
$2P_{3/2}$	-2	3/2	1	$2P_{3/2}, 3P_{3/2}, 4P_{3/2}, \ldots$

The matrix element of $\hat{\beta}$ between two eigenstates $|n_1\rangle$ and $|n_2\rangle$ is

$$\hat{\beta}_{n_1,n_2} = \int d^3 \boldsymbol{r} \begin{pmatrix} g_1 \Omega_{\kappa_1,m_1} \\ if_1 \Omega_{\kappa_1,-m_1} \end{pmatrix}^{\dagger} \begin{pmatrix} \hat{1} & 0 \\ 0 & -\hat{1} \end{pmatrix} \begin{pmatrix} g_2 \Omega_{\kappa_2,m_2} \\ if_2 \Omega_{\kappa_2,-m_2} \end{pmatrix}$$
$$= \delta_{\kappa_1 \kappa_2} \delta_{m_1 m_2} \int_0^\infty (g_1 g_2 - f_1 f_2) r^2 dr.$$
(30)

Equation (30) gives selection rules for the matrix elements of $\hat{\beta}$ between eigenstates of $\hat{\mathcal{H}}$. The matrix element $\hat{\beta}_{n_1,n_2}$ is nonzero only for states having the same quantum numbers κ and m. Returning to Eqs. (15)–(17) we see that all intermediate states $|n'\rangle$ and $|\Psi_{p_j}^{\pm}\rangle$ must be described by the same quantum numbers $\kappa = -1$ and m = 1/2 as the initial state $|1S\rangle$. This holds for both the bound and the continuum eigenstates of $\hat{\mathcal{H}}$. Below we analyze three groups of states characterized by the quantum numbers listed in Table II. Extension of the results to states described by other quantum numbers is straightforward.

B. Radial wave functions

To complete determination of the matrix elements $\hat{\beta}_{n_1,n_2}$ in Eq. (30) we need to calculate the integrals over the radial functions g(r) and f(r). These functions are known explicitly for both bound and continuum states. The integrals in Eq. (30) can be computed either numerically or analytically; see below. In this work we use analytical expressions for the integrals, which is more accurate for large quantum numbers *n* or large values of electron momentum.

For bound eigenstates the functions g(r) and f(r) are [29,30]

$$rg(r) = -\mathcal{A}\sqrt{1+W_{n_r}} \mathcal{B}\{n_r\mathcal{F}_1 - (N-\kappa)\mathcal{F}_0\}, \quad (31)$$

$$rf(r) = -\mathcal{A}\sqrt{1 - W_{n_r}} \mathcal{B}\{n_r \mathcal{F}_1 + (N - \kappa)\mathcal{F}_0\}, \quad (32)$$

where

$$\mathcal{A} = \frac{\sqrt{\Gamma(2\gamma + 1 + n_r)}}{\Gamma(2\gamma + 1)\sqrt{4N(N - \kappa)n_r!}} \left(\frac{2Z}{Nr_B}\right)^{1/2}, \quad (33)$$

$$\mathcal{B} = \exp\left(-\frac{Zr}{Nr_B}\right) \left(\frac{2Zr}{Nr_B}\right)^{\gamma},\tag{34}$$

$$\mathcal{F}_{\nu} = {}_{1}F_{1}\left(-n_{r}+\nu,2\gamma+1,\frac{2Zr}{Nr_{B}}\right), \qquad (35)$$

where $\nu = 0, 1$. The discrete energy is

$$E_{n_r} = m_0 c^2 \left\{ 1 + \left(\frac{\alpha Z}{n_r + \gamma}\right)^2 \right\}^{-1/2},$$
 (36)

in which $\gamma = \sqrt{\kappa^2 - (\alpha Z)^2}$, $\alpha = e^2/(4\pi \epsilon_0 \hbar c) \simeq 1/137$ is the fine-structure constant, $W_{n_r} = E_{n_r}/m_0 c^2 < 1$, $N = \sqrt{n_\kappa^2 - 2n_r(|\kappa| - \gamma)}$, $n_\kappa = n_r + |\kappa|$, $r_B \simeq 0.51$ Å is the Bohr radius, and the function $_1F_1(a,c,z)$ is the confluent hypergeometric function in the standard notation [31]. Since the first argument of the confluent hypergeometric function in Eq. (35) is a negative integer, this function reduces to a polynomial of the order $n_r - \nu$ of $z = 2Zr/(Nr_B)$. Expanding E_{n_r} in Eq. (36) in the vicinity of $m_0 c^2$ one obtains

$$W_{n_r} = \frac{E_{n_r}}{m_0 c^2} \simeq 1 - \frac{(\alpha Z)^2}{2(n_r + |\kappa|)^2} + \cdots .$$
(37)

Thus the functions g(r) in Eq. (31) are of the order of unity, while the functions f(r) in Eq. (31) are of the order of $\alpha Z < 1$.

Let $|1\rangle$ and $|2\rangle$ be two eigenstates of $\hat{\mathcal{H}}$ with the same quantum numbers κ and *m*. Then

$$\langle 1|2 \rangle = \int_0^\infty [g_1(r)g_2(r) + f_1(r)f_2(r)]r^2 dr = \delta_{1,2}, \quad (38)$$

$$\langle 1|\hat{\beta}|2 \rangle = \int_0^\infty [g_1(r)g_2(r) - f_1(r)f_2(r)]dr = \hat{\beta}_{12}. \quad (39)$$

Subtracting the above equations one finds

$$\hat{\beta}_{12} = \delta_{1,2} - 2 \int_0^\infty f_1(r) f_2(r) r^2 dr.$$
(40)

Since in Eq. (40) the functions $f_1(r)$ and $f_2(r)$ are of the order of αZ , the diagonal matrix elements of $\hat{\beta}$ are of the order of unity, while the nondiagonal ones are of the order of $(\alpha Z)^2 \ll 1$.

The continuum radial functions g(r) and f(r) are [28,29,32]

$$rg(r) = +\sqrt{(|W_p| + \epsilon)}(\mathcal{DF} + \mathcal{D}^*\mathcal{F}^*), \qquad (41)$$

$$rf(r) = i\epsilon\sqrt{(|W_p| - \epsilon)}(\mathcal{DF} - \mathcal{D}^*\mathcal{F}^*).$$
(42)

The electron energy is

$$E_p = \epsilon \sqrt{(m_0 c^2)^2 + (cp)^2}.$$
 (43)

Here $\epsilon = \pm 1$ is the energy sign, $W_p = E_p/(m_0c^2)$, and $|W_p| > 1$. Then

$$\mathcal{D} = \frac{e^{\pi y/2} |\Gamma(\gamma + iy)|}{2(\pi |W_p|)^{1/2} \Gamma(2\gamma + 1)} [e^{i\eta}(\gamma + iy)], \qquad (44)$$

$$\mathcal{F} = (2kr)^{\gamma} e^{-ikr} {}_{1}F_{1}(\gamma + 1 + iy, 2\gamma + 1, 2ikr).$$
(45)

The momentum of the relativistic electron is $\hbar k = (\hbar/\lambda_c)\sqrt{W_p^2 - 1} > 0$, where $\lambda_c = \hbar/(m_0c)$ is the Compton wavelength. Finally, $y = \alpha Z W_p / \sqrt{W_p^2 - 1}$ and

$$e^{i\eta} = \left(-\frac{\kappa - iy/W_p}{\gamma + iy}\right)^{1/2}.$$
(46)

The function $\psi_p^{\epsilon}(r) = \binom{g(r)}{f(r)}$ is normalized to $\delta(p_1 - p_2)\delta_{\epsilon_1\epsilon_2}$. The asymptotic forms of g(r) and f(r) are

$$rg(r) \simeq + \sqrt{\frac{|W_p| + \epsilon}{\pi |W_p|}} \cos(kr + \delta),$$
 (47)

$$rf(r) \simeq -\epsilon \sqrt{\frac{|W_p| - \epsilon}{\pi |W_p|}} \sin(kr + \delta),$$
 (48)

where

$$\delta = y \ln(2kr) - \arg[\Gamma(\gamma + iy)] - \frac{\pi\gamma}{2} + \eta.$$
 (49)

Thus, for large arguments, g(r) and f(r) reduce to trigonometric functions with slowly varying phases. For small electron momenta there is $|W_p| \simeq 1 + p^2/(2m_0^2c^2)$. Then, for $\epsilon = +1$, the function g(r) in Eq. (41) is of the order of unity, while f(r) in Eq. (42) is of the order of $p/(m_0c) \ll 1$. For $\epsilon = -1$ the magnitudes of g(r) and f(r) reverse: f(r) is of the order of unity, while g(r) is of the order of $p/(m_0c) \ll 1$. For large electron momenta, $p \ge m_0c$, the magnitudes of g(r) and f(r) are similar.

Let us qualitatively estimate the magnitudes of the matrix elements $\hat{\beta}_{nS,p\epsilon}$ between the bound state $|nS\rangle$ and the continuum state $|p \epsilon\rangle$ of small momentum, described by the same values of κ and m. Combining the above estimations with those for the functions of bound states [see Eq. (37)] we have

$$\hat{\beta}_{nS,p\epsilon} \propto \begin{cases} \alpha Zp/(m_0c) & \text{for } \epsilon = +1, \\ \alpha Z & \text{for } \epsilon = -1. \end{cases}$$
(50)

Since $p/(m_0 c) \ll 1$, the continuum states having negative energies are expected to make much larger contributions to the transformed functions than the continuum states having positive energies. This conclusion is confirmed numerically below.

The matrix elements of $\hat{\beta}$ between radial wave functions can be calculated analytically or numerically. There are several works related to this subject; see, e.g., Refs. [33–36]. For the analytical results for the diagonal matrix elements, we refer the reader to Appendix B.

IV. RESULTS

Our calculations were performed numerically for spin-up states $1S_{1/2}$, $2P_{1/2}$, and $2P_{3/2}$ for $Z \in \{1 \dots 92\}$, but for brevity we quote results for five representative values of Z. In Table I we list numerical and model parameters used in the calculations.

We begin with the analysis of matrix elements of $\hat{\beta}$ between bound states. In Table III we list the values of $\hat{\beta}_{1S,ns}$ for several Z and n. For all Z the diagonal elements $\hat{\beta}_{1S,1S}$ dominate over the nondiagonal ones, which agrees with qualitative estimations in Eq. (40). The nondiagonal elements of $\hat{\beta}$ gradually decay with n, and the analysis indicates that they vanish as $1/n^{3/2}$. For small Z the diagonal elements are nearly equal to unity, while the nondiagonal ones are negligible. With

TABLE III. Matrix elements of $\hat{\beta}$ between bound states of the relativistic hydrogenlike atom for several values of the nuclear charge Z.

Ζ	Element	$\hat{eta}_{1S,1S}$	$\hat{eta}_{1S,3S}$	$\hat{eta}_{1S,5S}$	$\hat{eta}_{1S,10S}$
1	Н	0.99	-3.7×10^{-6}	-2.0×10^{-6}	-7.9×10^{-7}
24	Cr	0.98	-2.1×10^{-3}	-1.1×10^{-3}	-4.6×10^{-4}
47	Ag	0.94	-8.2×10^{-3}	-4.4×10^{-3}	-1.7×10^{-3}
74	W	0.84	-2.0×10^{-2}	-1.1×10^{-2}	-4.2×10^{-3}
92	U	0.74	-3.2×10^{-2}	-1.6×10^{-2}	-6.4×10^{-3}



FIG. 2. Matrix elements $\hat{\beta}_{nS,p\pm}$ versus effective wave vector $K = (p/\hbar)(\alpha Z)$ for several values of *n*. Results for n = 1 are obtained analytically from Eq. (B8).

increasing Z the diagonal elements gradually decrease and other bound states begin to be relevant.

Next we calculate the matrix elements of $\hat{\beta}_{nS,p\epsilon}$ between bound states $|nS\rangle$ and continuum states $|p \epsilon\rangle$ as functions of the effective wave vector $K = (p/\hbar)(\alpha Z)$. In Fig. 2 we plot the matrix elements $\hat{\beta}_{1S,p-}$ and $\hat{\beta}_{nS,p+}$ for Z = 92 and several values of *n*. The elements $\hat{\beta}_{1S,p\pm}$ are calculated analytically from Eq. (B8).

Each curve in Fig. 2 has an asymmetric bell-like shape; it vanishes at K = 0, has a maximum or minimum in the vicinity of $K \simeq \alpha Z/(r_B n_\kappa)$, and decreases to 0 for large K. The magnitudes of $\hat{\beta}_{1S,p-}$ are much larger than those of $\hat{\beta}_{nS,p+}$, which emphasizes the greater contribution of negative-energy states to $\hat{\mathcal{U}}|1S\rangle$. Finally, the magnitude of $\hat{\beta}_{nS,p+}$ decreases with n, so that only the first few states make significant contributions to $\hat{\mathcal{U}}|1S\rangle$.

Having calculated the matrix elements $\hat{\beta}_{nS,mS}$ and $\hat{\beta}_{nS,p\pm}$ we compute the probability amplitudes a_n and $A_{p_i}^{\epsilon}$ and the resulting probability densities $|a_n|^2$ and $|A_{p_i}^{\epsilon}|^2$, as given in Eqs. (11) and (12). The results for Z = 92 are shown in Fig. 3. The state $1S_{1/2}$ makes the largest contribution to χ_{1S} and dominates over contributions of all other states. But, surprisingly, the next significant contributions to χ_{1S} originate from the continuum states of negative energies around $E_p^- \simeq$ $-1.5m_0c^2$. The contributions for other states are negligible. For the relativistic hydrogen atom (Z = 1) the corresponding probability densities are similar to those in Fig. 3, but with a much larger contribution of the $1S_{1/2}$ state (see below).

Let $P_{1S} = |a_{1S}|^2$ denote the probability density for the $1S_{1/2}$ state of $\hat{\mathcal{H}}$. Let $P^{\pm} = \sum_i |A_{p_i}^{\pm}|^2$ be the integrated probability density for continuum states of $\hat{\mathcal{H}}$ and $P_{nS} = \sum_{n>1} |a_n|^2$ be the integrated probability density for bound states of $\hat{\mathcal{H}}$ except the



FIG. 3. Probability densities $|a_n|^2$ and $|A_{p_i}^{\pm}|^2$ calculated from Eqs. (15)–(17) for Z = 92 versus the electron energy. The probability densities $|a_n|^2$ for the three lowest *n*'s are shown explicitly. Shaded areas indicate integrated probability densities P^{\pm} for continuum states of positive and negative energies; see Fig. 4 for Z = 92.

 $1S_{1/2}$ state. We plot these four quantities in Fig. 4 as functions of the nuclear charge $Z \in [1 \dots 92]$.

For small Z the probability density P_{1S} is close to unity, which means that, for light atoms, χ_{1S} is almost entirely composed of state $1S_{1/2}$. For larger Z this probability density



FIG. 4. Contribution of various eigenstates in transformed function χ_{1S} versus nuclear charge Z. Solid line: probability density $|a_1|^2$ for the $1S_{1/2}$ state. Dot-dashed line: integrated density P^- for continuum states of negative energies. Dashed line: integrated density P^+ for continuum states of positive energies. Dotted line: integrated densities P_{nS} for bound states of $\hat{\mathcal{H}}$ except the $1S_{1/2}$ state.



FIG. 5. Electron wave functions prior to and after Eriksen and FW-like transformations for the $1S_{1/2}$ state of a relativistic hydrogenlike atom with nuclear charge Z = 92. Negative values: functions rf_{1S} , $r\hat{\mathcal{U}}f_{1S}$, and $r\hat{\mathcal{U}}^{FW}f_{1S}$. According to the Eriksen theory the function $r\hat{\mathcal{U}}f_{1S}$ should be identically 0. The FW-like transformed function $r\hat{\mathcal{U}}^{FW}f_{1S}$ is also close to 0, but its magnitude is larger than the magnitude of $r\hat{\mathcal{U}}f_{1S}$. Positive values: functions rg_{1S} , $r\hat{\mathcal{U}}g_{1S}$, $r\hat{\mathcal{U}}^{FW}g_{1S}$, and rg_{1S}^{NR} . Note the small difference between exact $r\hat{\mathcal{U}}g_{1S}$ and approximate $r\hat{\mathcal{U}}^{FW}g_{1S}$ functions.

gradually decreases, but for Z = 92, it is still $P_{1S} \simeq 86\%$. Thus, even for very heavy atoms the transformed function is composed mostly of the $1S_{1/2}$ state. For small Z all three integrated probability densities P^{\pm} and P_{nS} are negligible, but for larger Z the P^{-} becomes about 14%. However, neither P^{+} nor P_{nS} exceeds 0.1% in the whole range of Z, so that their contributions to χ_{1S} may be neglected.

Having determined the expansion probability amplitudes a_n and $A_{p_i}^{\pm}$ we calculate the transformed function $\hat{\mathcal{U}}\psi_{1S}$ in Eq. (5). In Fig. 5 we plot the results for Z = 92. Functions rg_{1S} and rf_{1S} of the $1S_{1/2}$ state are represented by dashed lines, while $r\hat{\mathcal{U}}g_{1S}$ and $r\hat{\mathcal{U}}f_{1S}$ of Eq. (2) are indicated by solid lines. Dash-dotted lines are functions transformed with the use of $\hat{\mathcal{U}}^{FW}$ given in Eq. (22). Finally, the dotted line shows the 1s function of the nonrelativistic hydrogenlike atom,

$$rg_{1s}^{\rm NR}(r) = 2r \left(\frac{Z}{r_B}\right)^{3/2} e^{-rZ/r_B}.$$
 (51)

The transformed function $r\hat{\mathcal{U}}f_{1S}$, which is the lower component of χ_{1S} , should be identically 0 for all *r*. As shown in Fig. 5, this property is satisfied to a high accuracy, except in the the vicinity of r = 0. To estimate the accuracy of calculations for $r\hat{\mathcal{U}}f_{1S}$ we compute the norm of this function:

$$\mathcal{N}_{rf_{1S}} = \int_0^\infty |f_{1S}(r)| r^2 dr.$$
 (52)

TABLE IV. Norms of the rg(r) and rf(r) functions prior to and after Eriksen and FW-like transformations, calculated using Eq. (52) for different nuclear charges Z.

Ζ	Element	\mathcal{N}_{rg}	\mathcal{N}_{rf}	$\mathcal{N}_{r\hat{\mathcal{U}}f}$	$\mathcal{N}_{r\hat{\mathcal{U}}^{\mathrm{FW}_f}}$
1	Н	1.000	1.3×10^{-5}	1.01×10^{-10}	1.02×10^{-10}
24	Cr	0.992	0.008	3.57×10^{-7}	$4.28 imes 10^{-6}$
47	Ag	0.970	0.030	7.62×10^{-6}	9.51×10^{-5}
74	Ŵ	0.921	0.079	5.27×10^{-5}	$7.86 imes 10^{-4}$
92	U	0.871	0.129	1.33×10^{-4}	2.29×10^{-3}

Similarly, we calculate the norms of rg_{1S} , rf_{1S} , $r\hat{\mathcal{U}}f_{1S}$, and $r\hat{\mathcal{U}}^{\text{FW}}f_{1S}$ for several values of the nuclear charge Z. The results are listed in Table IV. Since the function $r\hat{\mathcal{U}}f_{1S}$ should be identically 0, its norm in Eq. (52) should vanish. In practice, the norm of $r\hat{\mathcal{U}}f_{1S}$ is slightly different from 0 but negligibly small compared with the norm of rf_{1S} . This occurs both for Z = 1 and for Z = 92.

It is shown in Table IV that the norm of $r\hat{U}f_{1S}$ is always smaller than the norm of $r\hat{U}^{FW}f_{1S}$, which means that, as expected, the exact transformation is more accurate than the approximate one. On the other hand, for small Z the FW-like transformation is almost as accurate as the Eriksen transformation. However, as reported in Table IV, irrespective of its poorer accuracy, the FW-like transformation for the $1S_{1/2}$ state is quite accurate for all $Z \in [1...92]$.

Returning to Fig. 5, it is shown that the functions $r\hat{\mathcal{U}}g_{1S}$ and $r\hat{\mathcal{U}}^{FW}g_{1S}$ are almost identical, i.e., both transformations lead to similar results. Next, the transformed functions are closer to the rg_{1S} function of the $1S_{1/2}$ state of the relativistic hydrogenlike atom than to the 1s state of the Schrodinger hydrogenlike atom. Since the latter function is close to the rg_{1S} state of the Dirac hydrogenlike atom, it is expected that also the Eriksen and FW-like transformations of the nonrelativistic function would be close to the $r\hat{\mathcal{U}}g_{1S}$ function.

Finally, with a high accuracy, $r\hat{\mathcal{U}}g_{1S}$ and $r\hat{\mathcal{U}}^{FW}g_{1S}$ are normalized to unity. Using Fig. 5 and Table IV, one can compare the results of the FW-like transformation with the results of the exact transformation separating positive- and negative-energy states for the Dirac Hamiltonian with nontrivial potential. Figure 5 and Table IV prove the high accuracy of the FW-like transformation often used in nonrelativistic quantum mechanics.

We also performed calculations of transformed functions of the $2P_{1/2}$ and $2P_{3/2}$ states of the relativistic hydrogenlike atom. The results for matrix elements and contributions of various states to the resulting functions are similar to those presented in Figs. 2–4 and Tables III and IV. In Fig. 6 we plot the upper components of the $2P_{1/2}$ and $2P_{3/2}$ functions prior to and after the Eriksen and FW-like transformations. For both values of *j* the functions after Eriksen and FWlike transformations are practically indistinguishable. For j =1/2 and j = 3/2 the functions $r\hat{\mathcal{U}}g$ are close to the original (nontransformed) functions of the $2P_{1/2}$ and $2P_{3/2}$ states of the relativistic hydrogenlike atom. For j = 1/2 the function $r\hat{\mathcal{U}}g$ is close to the radial function 2p of the nonrelativistic hydrogenlike atom, while the transformed function of the $2P_{3/2}$ state is qualitatively different from the 2p state.



FIG. 6. Upper components of the $2P_{1/2}$ and $2P_{3/2}$ states of a relativistic hydrogenlike atom for Z = 92 prior to and after Eriksen and FW-like transformations. Note the small differences in functions resulting from Eriksen vs FW-like transformations. The functions rg, $r\hat{\mathcal{U}}g$, and $r\hat{\mathcal{U}}^{FW}g$ for j = 1/2 are close to the 2p function of the nonrelativistic hydrogenlike atom, but for j = 3/2 they differ qualitatively from the 2p function.

V. DISCUSSION

The results presented in Sec. IV are obtained for the nuclear charge $Z \in [1...92]$. Strictly speaking, they are valid only for the hydrogen atom, since in real atoms the presence of many electrons and interactions between them modify the forms of atomic orbitals and continuum states, so that they cease to be the eigenstates of $\hat{\mathcal{H}}$ in Eq. (1). To overcome this problem we may, to some extent, approximate the presence of other electrons by introducing an additional phenomenological potential acting on electrons in atomic orbitals. Following Ref. [37], for the 1*s* state the Coulomb potential in Eq. (1) should be replaced with

$$V_{\rm eff}(r) = -\frac{1}{4\pi\epsilon_0} \frac{e^2(Z-0.3)}{r} + V_0(Z),$$
 (53)

in which $V_0(Z)$ does not depend on r. After this modification, the new potential is still Coulomb-like but with the effective value of $Z^* = Z - 0.3$. As shown in Fig. 4, differences between the four probability densities calculated for Z and Z^* are small. Therefore, the results shown in Figs. 2 to 5 for Z = 92 are very close to those computed for $Z^* = 91.7$. For 2p or 2s states, the potential in Eq. (53) should have a different value of the effective charge $Z^* < Z$ [37] and the transformed p-like functions in the effective potential in Eq. (53) should be close to the corresponding functions in Fig. 6. We conclude that the results shown in Figs. 2 to 6 and Tables III and IV remain valid for all $Z \in [1 \dots 92]$ in the range of applicability of the approximation given in Eq. (53).

It is not meaningful to analyze higher terms of the expansion of $\hat{\mathcal{U}}$ in power series of αZ , since one neglects the presence

of radiative corrections to the Coulomb potential which may be of comparable magnitude. In our work we do not expand $\hat{\mathcal{U}}$ in a series, but calculate $\hat{\mathcal{U}}\psi$ exactly in a finite but large basis. Within our approach we may incorporate QED effects by adding to the Coulomb potential an additional potential, $V_{\text{rad}}(r)$. This potential is short-range, has spherical symmetry, and vanishes for $r \gg \lambda_c$ [30,38,39].

As pointed out by Eriksen, a transformation analogous to that in Eq. (2) can be applied to two-body interactions [21]. Similarly, within the Hartree-Fock approximation, the Coulomb potential in Eq. (1) can be replaced by a selfconsistent potential with spherical symmetry [5] and our approach can be generalized to many-electron systems. In Sec. IV we limit the analysis to the lowest bound states of the relativistic hydrogenlike atom. Our method could be easily generalized to computations of the Eriksen transformation of other bound eigenstates of $\hat{\mathcal{H}}$, as described by other quantum numbers, κ , m, and n_r . A convenient feature of the relativistic Coulomb problem is its radial symmetry, which limits the number of states entering into summations in Eqs. (11) and (12) to those having the same quantum numbers κ and m. This simplifies the computation of matrix elements in Eq. (18) by reducing them to one-dimensional integrals [see Eq. (30)]. This simplification is not essential to our problem but, in practice, reduces the sizes of matrices \hat{S} and \hat{Z} [see Eqs. (19) and (20)].

The advantage of the present approach, compared to the series of FW- or DK-like transformations, is a clear physical interpretation of states entering into the transformed functions $\hat{\mathcal{U}}\psi$. As shown in Figs. 3 and 4, the state $\hat{\mathcal{U}}\psi$ consists mostly of the initial state ψ and continuum states having negative energies in the vicinity of $E \simeq -m_0c^2 - E_b$. Our figures show marginal contributions of other bound or continuum states to $\hat{\mathcal{U}}\psi$. The selection rules in Eq. (30) automatically choose the proper angular symmetry of the transformed function $\hat{\mathcal{U}}\psi$. Radial functions forming $\chi_{1S}(\mathbf{r})$ have the same quantum numbers κ and m as the initial state ψ . In contrast, the Gaussian or exponential orbitals, frequently used in numerical calculations in quantum chemistry, are somewhat artificial.

Our results shown in Figs. 3 and 4 possibly explain the accuracy of eliminating negative-energy components in FW-like and DK-like methods, as reported in Refs. [5] and [8–11]. It is shown that the contribution of negative-energy states to the transformed functions $\hat{\mathcal{U}}\psi$ varies from parts of single percent to the total probability density for light atoms to 14% of the total probability density for heavy atoms. Therefore, for all nuclear charges $Z \in [1 \dots 92]$, the presence of negative-energy states in the function $\hat{\mathcal{U}}\psi$ can always be treated as a perturbation to states of $\hat{\mathcal{H}}$ having positive energies and it can be effectively removed by series of FW-like or DK-like transformations.

The Moss-Okninski transformation [15] was used by Rusin and Zawadzki to transform a Gaussian wave packet in the presence of an external magnetic field [18]. After the transformation the packet retained the bell-like shape but its width had changed [18]. As shown in Figs. 5 and 6, the shape of wave functions of the relativistic hydrogenlike atom is also retained after transformations. The results in Fig. 5 and Table IV for the FW-transformed functions agree with those of Silenko [23], who found that the lower components of any function transformed by the FW-like transformation are of second order in $1/(m_0c^2)$.

The precision of the results in Sec. IV depends on the accuracy of special functions in Eqs. (31) and (32) and Eqs. (41) and (42), namely, the confluent hypergeometric functions, gamma functions, and hypergeometric functions. These functions have been calculated using methods described in detail in Ref. [40] and tested with the results obtained on a Web-page calculator for special functions [41]. Functions g(r) and f(r) calculated numerically were checked for their orthogonality to other functions. The exact results for diagonal and nondiagonal matrix elements of $\hat{\beta}$ and \hat{S} served as additional tests of the employed procedures. Asymptotic forms of g(r) and f(r) were used for testing the exact functions g(r) and f(r) in Eqs. (41) and (42) and their normalization. A convenient feature of our problem is the possibility of analytical calculations for all matrix elements of $\hat{\beta}$ in Eq. (18). There are two tests of accuracy of the numerical procedures: the sum rule for the probability amplitudes a_n and $A_{n_i}^{\epsilon}$ in Eq. (13) and the requirement that function $\hat{\mathcal{U}}\psi$ has vanishing lower components. As shown in Fig. 5 and Table IV, a high accuracy of numerical calculations is achieved.

VI. SUMMARY

We calculated the single-step Eriksen transformation of the wave functions for the $1S_{1/2}$, $2P_{1/2}$, and $2P_{3/2}$ states of the relativistic hydrogenlike atom. In the new representation the functions have two nonzero components. The proposed method does not require an expansion of the Eriksen operator $\hat{\mathcal{U}}$ in the power series of $1/(m_0c^2)$ or the potential. Our approach is based on the observation that, although the operator $\hat{\mathcal{U}}$ defining the transformation is not given in an explicit form, it is possible to calculate analytically or numerically its matrix elements between eigenstates of $\hat{\mathcal{H}}$. To exploit this observation, we expressed the transformed wave functions in the form of linear combinations of eigenstates of $\hat{\mathcal{H}}$ for a sufficiently large set of states. The continuum states of $\hat{\mathcal{H}}$ are replaced with the so-called discretized functions (eigendifferentials), which allow one to treat bound and continuum states in a similar way. Our results may possibly explain the accuracy of FW-like and DK-like transformations reported in the literature, since the contribution from states of negative energies to the total probability density can be safely treated as a perturbation to the contribution of states with positive energies. As expected, lower components of $\hat{\mathcal{U}}\psi$ are nearly 0 except in the vicinity of r = 0. This result confirms the accuracy of the Eriksen transformation and numerical calculations. The upper components of $\hat{\mathcal{U}}\psi$ are well-localized functions, similar to their counterparts in the Dirac representation. The nonvanishing components of $\hat{\mathcal{U}}\psi$ and $\hat{\mathcal{U}}^{FW}\psi$ are close to each other, which confirms the accuracy of the FW-like transformation. In conclusion, it is believed that the reported results contribute to a better understanding of the Eriksen and Foldy-Wouthuysen transformations.

ACKNOWLEDGMENTS

I acknowledge Mrs. Aneta Osowska and Prof. Wlodek Zawadzki for help and discussions during the preparation and reading of the manuscript. I acknowledge Casio Company for designing and operating the Free On-Line calculator for special functions (see Ref. [41]), which was used for validation of the numerical procedures calculating the radial functions of the relativistic hydrogenlike atom.

APPENDIX A: PROPERTIES OF $\hat{\mathcal{Z}}$ AND $\hat{\mathcal{U}}$ OPERATORS

Here we show that the operator $\hat{\mathcal{Z}}$ in Eq. (3) has vanishing matrix elements between eigenstates of $\hat{\mathcal{H}}$ for positive and negative energies. Consider matrix $\hat{\mathcal{S}}$ in Fig. 1, which is block-diagonal with vanishing matrix elements between eigenstates of $\hat{\mathcal{H}}$ having positive and negative energies. Schematically, in the basis used in Fig. 1, its form is $\hat{\mathcal{S}} = \begin{pmatrix} \hat{\mathcal{S}}^+ & 0 \\ 0 & \hat{\mathcal{S}}^- \end{pmatrix}$, where the operators $\hat{\mathcal{S}}^{\pm}$ are constructed from matrix elements of $\hat{\beta}$ between states having the same energy signs. Then any integer power of $\hat{\mathcal{S}}$ is also block-diagonal: $(\hat{\mathcal{S}})^m = \begin{pmatrix} (\hat{\mathcal{S}}^+)^m & 0 \\ 0 & (\hat{\mathcal{S}}^-)^m \end{pmatrix}$. The operator $\hat{\mathcal{Z}}$ can be expanded in power series, $\hat{\mathcal{Z}} = \sum_{m=0}^{\infty} z_m (\hat{\mathcal{S}})^m$, with suitably chosen coefficients z_m (see Ref. [21]). Since each term in this series is block-diagonal, the operator $\hat{\mathcal{Z}}$ is block-diagonal as well, and its matrix elements between eigenstates of $\hat{\mathcal{H}}$ for different energy signs vanish. This completes the proof.

The operator $\hat{\mathcal{Z}}$ has block-diagonal form in the representation of the Dirac spinors. To show this we first note that $\hat{\mathcal{S}}$ is block-diagonal in this representation. Expressing $\hat{\lambda}$ in the form of 2×2 blocks, $\hat{\lambda} = \begin{pmatrix} \hat{\lambda}_{11} & \hat{\lambda}_{12} \\ \hat{\lambda}_{21} & \hat{\lambda}_{22} \end{pmatrix}$, there is $\hat{\mathcal{S}} = \hat{\beta}\hat{\lambda} + \hat{\lambda}\hat{\beta} = \begin{pmatrix} 2\hat{\lambda}_{11} & 0 \\ 0 & -2\hat{\lambda}_{22} \end{pmatrix}$. Repeating the arguments presented above we find $\hat{\mathcal{Z}} = \begin{pmatrix} \hat{z}_{11} & 0 \\ 0 & \hat{z}_{22} \end{pmatrix}$.

Next we show that $\hat{\mathcal{U}}$ in Eq. (2) transforms any eigenstate of the Dirac Hamiltonian to the two-component form. Let $\psi^{\pm} = \binom{g^{\pm}}{f^{\pm}}$ be eigenstates of $\hat{\mathcal{H}}$ of positive or negative energies, respectively, and g^{\pm} and f^{\pm} be the two-component vectors. Then $\hat{\lambda}\psi^{\pm} = \pm\psi^{\pm}$ and

$$\hat{\mathcal{U}}\psi^{+} = \hat{\mathcal{Z}}(1+\hat{\beta}\hat{\lambda})\psi^{+} = \begin{pmatrix} \hat{\mathcal{Z}}_{11}g^{+}\\ 0 \end{pmatrix}, \qquad (A1)$$

$$\hat{\mathcal{U}}\psi^{-} = \hat{\mathcal{Z}}(1+\hat{\beta}\hat{\lambda})\psi^{-} = \begin{pmatrix} 0\\ \hat{\mathcal{Z}}_{22}f^{-} \end{pmatrix}.$$
 (A2)

This completes the proof.

The operators $\hat{\beta}\hat{\lambda}$ and $\hat{\lambda}\hat{\beta}$ commute, which can be shown directly. Expanding \hat{Z} in a power series of $(\hat{S} - 2)$ we find that each term in the series commutes with $\hat{\beta}\hat{\lambda}$ and $\hat{\lambda}\hat{\beta}$. Therefore \hat{Z} commutes with $\hat{\beta}\hat{\lambda}$ and $\hat{\lambda}\hat{\beta}$, which allows one to interchange the orders of \hat{Z} and $\hat{\beta}\hat{\lambda}$ in the definition of \hat{U} in Eq. (2).

APPENDIX B: MATRIX ELEMENTS OF $\hat{\beta}$

The diagonal matrix elements of $\hat{\beta}$ can be obtained without direct specification of the wave functions $\langle \boldsymbol{r} | n \rangle$ (see, e.g., Ref. [33]). Here we calculate these elements with the use of the Hellmann-Feynman theorem. Let us treat the electron mass m_0 in Eq. (1) as a variable parameter. Then

$$\langle n(m_0) | \hat{\mathcal{H}}(m_0) | n(m_0) \rangle = E(m_0). \tag{B1}$$

Differentiating both sides of Eq. (B1) with respect to m_0 one obtains

$$\langle n|\hat{\beta}|n\rangle = \frac{1}{c^2} \frac{\partial E(m_0)}{\partial m_0},$$
 (B2)

and the diagonal matrix elements of $\hat{\beta}$ can be obtained by straightforward differentiations of both sides of Eqs. (36) and (43) with respect to m_0 . The results of Eq. (36) are known [33], but to our knowledge, their extension to the continuum states in Eq. (43) has not been published yet.

Next, we consider the diagonal matrix elements between discretized functions defined in Eq. (9). Combining Eqs. (9), (43), and (B2) one has

$$\begin{split} \left\langle \Psi_{p_{i}}^{\epsilon_{i}} \left| \hat{\beta} \right| \Psi_{p_{j}}^{\epsilon_{j}} \right\rangle \\ &= \frac{1}{\Delta p} \int_{p_{i} - \Delta p/2}^{p_{i} + \Delta p/2} \int_{p_{j} - \Delta p/2}^{p_{j} + \Delta p/2} \left\langle \psi_{p_{1}}^{\epsilon_{i}} \left| \hat{\beta} \right| \psi_{p_{1}}^{\epsilon_{j}} \right\rangle dp_{1} dp_{2} \\ &= \frac{\delta_{\epsilon_{i},\epsilon_{j}}}{\Delta p} \int_{p_{i} - \Delta p/2}^{p_{i} + \Delta p/2} \int_{p_{j} - \Delta p/2}^{p_{j} + \Delta p/2} \frac{\partial E_{p_{1}}}{c^{2} \partial m_{0}} \delta(p_{1} - p_{2}) dp_{1} dp_{2} \\ &= \frac{\delta_{\epsilon_{i},\epsilon_{j}} \delta_{p_{i},p_{j}}}{\Delta p} \int_{p_{i} - \Delta p/2}^{p_{i} + \Delta p/2} \frac{m_{0}c^{2}}{E_{p}} dp \end{split}$$
(B3)

$$\xrightarrow{\Delta p \to 0} \delta_{\epsilon_i, \epsilon_j} \delta_{p_i, p_j} \frac{m_0 c^2}{E_{p_i}}.$$
 (B4)

The energy E_p in Eq. (B3) is given in Eq. (43). Using the same approach to the diagonal matrix elements of \hat{Z} between discretized states we find

$$\begin{split} \langle \Psi_{p_i}^- | \hat{\mathcal{Z}} | \Psi_{p_j}^- \rangle &= \frac{\delta_{p_i, p_j}}{\Delta p} \int_{p_i - \Delta p/2}^{p_i + \Delta p/2} \frac{dp}{\sqrt{2 + 2m_0 c^2/E_p}} \\ &\simeq \frac{\delta_{p_i, p_j}}{\sqrt{2 + 2m_0 c^2/E_{p_i}}}. \end{split} \tag{B5}$$

Since functions ψ_p^{ϵ} are normalized to $\delta(p_1 - p_2)\delta_{\epsilon_1\epsilon_2}$, the nondiagonal matrix elements of $\hat{\beta}$ and \hat{Z} between continuum functions vanish.

Calculation of the matrix elements of $\hat{\beta}$ between discretized states in Eq. (10) and bound states requires computation of the integral

$$\langle \Psi_{p_i}^{\epsilon} | \hat{\beta} | 1S \rangle = \frac{1}{\sqrt{\Delta p}} \int_{p_i - \Delta/2}^{p_i + \Delta/2} \langle \psi_p^{\epsilon} | \hat{\beta} | 1S \rangle dp$$

$$\xrightarrow{\Delta p \to 0} \sqrt{\Delta p} \langle \psi_{p_i}^{\epsilon} | \hat{\beta} | 1S \rangle.$$
(B6)

The element $\hat{\beta}_{1S,p-}$ is a combination of two integrals of the form

$$Q^{\epsilon} = T_0 \int_0^\infty e^{-(C_0 + i\epsilon K)r} (2rC_0)^{\gamma} (2Kr)^{\gamma} {}_1F_1(a,\mu,2iKr)dr,$$
(B7)

in which T_0 is an *r*-independent constant [see Eqs. (31) and (32) and Eqs. (41) and (42)], $a = \gamma + 1 + iy$, $\mu = 2\gamma + 1$, $C_0 = Z/r_B$, and $K = (p/\hbar)(\alpha Z)$. The integral in Eq. (B7) can be calculated analytically and we obtain

$$Q^{\epsilon} = T_0 \Gamma(\mu) (4C_0)^{\gamma} \frac{K^{\gamma}}{(C_0 + i\epsilon K)^{\mu}} \left(\frac{C_0 - i\epsilon K}{C_0 + i\epsilon K}\right)^a.$$
(B8)

The remaining matrix elements $\hat{\beta}_{nS,p\epsilon}$ can be expressed in terms of special functions and below we list formulas necessary for the calculations. For bound states the confluent hypergeometric function is the polynomial defined recurrently,

$$_{1}F_{1}(-n,c,z) = \sum_{i=0}^{n} t_{n,j} z^{j},$$
 (B9)

$$t_{n,j+1} = t_{n,j} \frac{-n+j-1}{j(c+j-1)},$$
 (B10)

with $t_{n,0} = 1$. The matrix elements $\hat{\beta}_{nS,mS}$ between bound functions can be calculated with the use of the Euler integral:

$$\int_0^\infty x^{b-1} e^{-sx} dx = \frac{1}{s^b} \Gamma(b).$$
 (B11)

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For calculations of the matrix elements $\hat{\beta}_{nS,p\epsilon}$ between bound and continuum states we use the formula [42]

$$\int_{0}^{\infty} e^{-st} t^{b-1} {}_{1}F_{1}(a,c,kt)dt = \frac{\Gamma(s)}{z^{b}} {}_{2}F_{1}(a,b,c,k/s), \quad (B12)$$

assuming that $\operatorname{Re}(b) > 0$ and $\operatorname{Re}(s) > \max[\operatorname{Re}(k),0]$, where $_2F_1(a,b,c,z)$ is the hypergeometric function in the standard notation [31]. We use also the identities $_2F_1(a,b,c,z) = _2F_1(b,a,c,z)$ and $_2F_1(a,b,c,z) = (1 - z)^{-a} _2F_1(a,c-b,c,z/(z-1))$. More general expressions for the matrix elements of $\hat{\beta}$ are given in Refs. [34–36].

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