

Relativistic spin operators in various electromagnetic environments

Heiko Bauke,¹ Sven Ahrens,^{1,2} Christoph H. Keitel,¹ and Rainer Grobe^{1,2}

¹Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany

²Intense Laser Physics Theory Unit and Department of Physics,

Illinois State University, Normal, Illinois 61790-4560, USA

(Dated: May 6, 2014)

Different operators have been suggested in the literature to describe the electron's spin degree of freedom within the relativistic Dirac theory. We compare concrete predictions of the various proposed relativistic spin operators in different physical situations. In particular, we investigate the so-called Pauli, Foldy-Wouthuysen, Czachor, Frenkel, Chakrabarti, Pryce, and Fradkin-Good spin operators. We demonstrate that when a quantum system interacts with electromagnetic potentials the various spin operators predict different expectation values. This is explicitly illustrated for the scattering dynamics at a potential step and in a standing laser field and also for energy eigenstates of hydrogenic ions. Therefore, one may distinguish between the proposed relativistic spin operators experimentally.

PACS numbers: 03.65.Pm, 31.15.aj, 31.30.J-

1. Introduction

Elementary particles such as the electron carry some internal angular-momentum-like degree of freedom that is called spin. It is well understood that angular momentum is intrinsically tied to the group-theoretic structure of (relativistic) quantum mechanics [1]. The understanding of the physical nature of the spin, however, is still incomplete [2–4]. Historically, the concept of spin was introduced in order to explain some experimental findings such as the emission spectra of alkali metals and the Stern-Gerlach experiment. A direct measuring of the spin (or more precisely the electron's magnetic moment), however, was missing until the pioneering work by Dehmelt [5]. Pauli and Bohr even claimed that the spin of free electrons was impossible to measure for fundamental reasons [6]. Recent renewed interest in fundamental aspects of the spin [7] arose, for example, from high-precision measurement experiments for the electron's magnetic moment [8–13], the growing field of (relativistic) quantum information theory [14–21], quantum spintronics [22], spin effects in graphene [23–25], and light-matter interactions at relativistic intensities [26–30].

Although the spin is regarded as a fundamental property of the electron, there is no universally accepted spin operator. In fact, one can find in the literature several proposals of different spin operators for the Dirac theory [7]. These operators are often motivated by abstract group-theoretic considerations rather than by experimental evidence. In our view, there are very few works that consider specific experimental schemes and predict concrete expectation values for spin observables in a relativistic setting. Such predictions, however, are required to judge which of the proposed relativistic generalizations of the spin or (equivalently) of the position operators are best suited to describe experimental observations. For example, a paper by Czachor [14] proposed to use an Einstein-Podolsky-Rosen type of experiment and the associated degree of violation of the Bell inequality to test various relativistic concepts, such as the relativistic position operator. This work also predicts that the center of mass and the center of charge might not necessarily agree for a relativistic electron leading to possible implications

for quantum cryptography. Another example is the work [31] by Choi *et al.*, who studied spin entanglement of massive Dirac particles.

In this work we examine seven proposals for the relativistic spin operator, which we tentatively call here the Pauli, the Foldy-Wouthuysen, the Czachor, the Frenkel, the Chakrabarti, the Fradkin-Good, and the Pryce spin operators. Our aim is to investigate and to compare their mathematical properties and to analyze how different definitions of relativistic spin operators may lead to different predictions for spin expectation values in various experimental setups. The seven spin operators discussed in this work share the same nonrelativistic limit, obtained by assuming that the particle's kinematic momentum is small compared to m_0c , with m_0 denoting the particle's rest mass and c the speed of light. Thus, any differences in the spin's properties are purely relativistic effects and require most likely accelerated particles. While several works have tried to relate the different functional forms of these operators to each other, a study that shows how the predictions depend on the choice of the relativistic spin operator for an electron whose dynamical evolution is governed by external electromagnetic fields is lacking. This requires a concrete computational analysis yielding concrete predictions about expectation values that can be directly compared with experimental results. Using numerical wave function solutions to the time-dependent Dirac equation, we evaluate and compare the various predictions that result from different relativistic spin operators. In this way we aim to build a bridge between theoretical considerations and experiment.

A relativistic spin operator may be introduced by splitting the undisputed total angular momentum operator $\hat{\mathbf{J}}$ into an external part $\hat{\mathbf{L}}$ and an internal part $\hat{\mathbf{S}}$ commonly referred to as the orbital angular momentum and the spin, viz. $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$. Because the orbital angular momentum is related to the position operator $\hat{\mathbf{r}}$ and the momentum operator $\hat{\mathbf{p}} = -i\nabla$ (units are used in this paper for which $\hbar = 1$) via $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$, different definitions of the spin operator $\hat{\mathbf{S}}$ imply different relativistic position operators $\hat{\mathbf{r}}$. The latter would be difficult to discriminate experimentally as it couples only to a gravitational field, while the

spin couples also to the more easily controllable magnetic field. The rather fundamental question which mathematical operators actually correspond to experimentally measured observables has become more relevant as laser-particle experiments have entered the regime in which the particle must be described in a fully relativistic framework [27, 32].

This paper is organized as follows. In Sec. 2 we briefly review the Dirac equation and introduce some notation that will be utilized in Sec. 3, where the seven spin operators are defined and their mathematical properties are analyzed. The expectation values of the spin operators are evaluated for relativistic scattering dynamics in Sec. 4 and for the bound states of hydrogenic ions in Sec. 5. We formulate our conclusions in Sec. 6.

2. The Dirac equation

A Lorentz invariant quantum mechanical description of the motion of an electron is given by the time-dependent Dirac equation. For a particle of rest mass m_0 and charge q moving in the electromagnetic potentials $\phi(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ it is given by

$$i \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \hat{H} \Psi(\mathbf{r}, t) = (c\boldsymbol{\alpha} \cdot (\hat{\mathbf{p}} - q\mathbf{A}(\mathbf{r}, t)) + q\phi(\mathbf{r}, t) + m_0 c^2 \beta) \Psi(\mathbf{r}, t), \quad (1)$$

with the matrices $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)^\top$ and β . These 4×4 matrices obey the algebra

$$\alpha_i^2 = \beta^2 = 1, \quad \alpha_i \alpha_k + \alpha_k \alpha_i = 2\delta_{i,k}, \quad \alpha_i \beta + \beta \alpha_i = 0. \quad (2)$$

To briefly discuss our notation and abbreviations, we use the Dirac representation for the matrices α_i and β such that

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{pmatrix}, \quad (3)$$

where the three 2×2 Pauli matrices $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)^\top$ are given by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (4)$$

and \mathbb{I}_2 denotes the 2×2 identity matrix. The free-particle Dirac Hamiltonian with $\mathbf{A}(\mathbf{r}, t) = 0$ and $\phi(\mathbf{r}, t) = 0$ will be denoted by \hat{H}_0 . The doubly degenerate spectrum of the free Dirac Hamiltonian is given by $\text{spec}(\hat{H}_0) = \pm c p_0(\mathbf{p})$, where $p_0(\mathbf{p})$ is the scaled positive energy $p_0(\mathbf{p}) = (m_0^2 c^2 + \mathbf{p}^2)^{1/2}$ for the momentum vector \mathbf{p} . We will also use the operator \hat{p}_0 to denote

$$\hat{p}_0 = \sqrt{m_0^2 c^2 + \hat{\mathbf{p}}^2}. \quad (5)$$

For a given momentum eigenvalue \mathbf{p} , the associated eigenvectors for the positive and negative energies $\pm p_0(\mathbf{p})c$ can be chosen as

$$\phi_{\chi, \mathbf{p}}^+(\mathbf{r}, t) = \mathbf{u}_{\chi, \mathbf{p}} e^{i(\mathbf{p} \cdot \mathbf{r} - c p_0(\mathbf{p})t)}, \quad (6a)$$

$$\phi_{\chi, \mathbf{p}}^-(\mathbf{r}, t) = \mathbf{v}_{\chi, \mathbf{p}} e^{i(\mathbf{p} \cdot \mathbf{r} + c p_0(\mathbf{p})t)}, \quad (6b)$$

where we have introduced the vectors

$$\mathbf{u}_{\chi, \mathbf{p}} = \sqrt{\frac{m_0 c + p_0(\mathbf{p})}{2 p_0(\mathbf{p})}} \begin{pmatrix} \chi \\ \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{m_0 c + p_0(\mathbf{p})} \chi \end{pmatrix}, \quad (7a)$$

$$\mathbf{v}_{\chi, \mathbf{p}} = \sqrt{\frac{m_0 c + p_0(\mathbf{p})}{2 p_0(\mathbf{p})}} \begin{pmatrix} -\frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{m_0 c + p_0(\mathbf{p})} \chi \\ \chi \end{pmatrix}. \quad (7b)$$

The quantity χ denotes an arbitrary complex two-component vector with $\chi^\dagger \cdot \chi = 1$. Note that while (6a) corresponds to states that travel in the direction given by the vector \mathbf{p} , the states given by (6b) travel in the opposite direction of \mathbf{p} . The two fold degenerate eigenspace of \hat{H}_0 for each eigenvalue $c p_0$ can be spanned by the two (mutually orthogonal) eigenfunctions $\phi_{\chi, \mathbf{p}}^+(\mathbf{r}, t)$ and $\phi_{\chi_\perp, \mathbf{p}}^+(\mathbf{r}, t)$, where the normalized vector χ_\perp is orthogonal to χ .

Obviously, any superposition of the two functions $\phi_{\chi, \mathbf{p}}^+(\mathbf{r}, t)$ and $\phi_{\chi_\perp, \mathbf{p}}^+(\mathbf{r}, t)$ is also an energy eigenstate. Analogous statements hold for the negative-energy eigenstates. The functions $\phi_{\chi, \mathbf{p}}^-(\mathbf{r}, t)$ and $\phi_{\chi_\perp, \mathbf{p}}^-(\mathbf{r}, t)$ form a basis, thus each wave packet can be written as a superposition of $\phi_{\chi, \mathbf{p}}^\pm(\mathbf{r}, t)$ and $\phi_{\chi_\perp, \mathbf{p}}^\pm(\mathbf{r}, t)$. In the course of our presentation, it will be useful to introduce the energy subspace operators

$$\hat{\Lambda}^\pm = \frac{1}{2} \left(1 \pm \frac{\hat{H}_0}{c \hat{p}_0} \right) \quad (8)$$

that single out positive- and negative-energy contributions, respectively, from an arbitrary superposition.

3. Seven variations on spin

In this section we will define seven different spin operators referred to as Pauli, Foldy-Wouthuysen, Czachor, Frenkel, Chakrabarti, Pryce, and Fradkin-Good spin operators. Each of these operators is characterized by a triplet $\hat{\mathbf{S}} = (\hat{S}_1, \hat{S}_2, \hat{S}_3)^\top$. For simplicity, we will also denote the spin component in a given \mathbf{n} direction by $\hat{S}_\mathbf{n}$ defined as $\hat{S}_\mathbf{n} = \mathbf{n} \cdot \hat{\mathbf{S}}$. For some calculations it will be beneficial to parametrize the vector \mathbf{n} as $\mathbf{n} = (\sin \vartheta \cos \varphi, \sin \vartheta \sin \varphi, \cos \vartheta)^\top$ and to define the two orthogonal vectors

$$\chi_\uparrow = \begin{pmatrix} \cos(\vartheta/2) \\ \sin(\vartheta/2) e^{i\varphi} \end{pmatrix}, \quad \chi_\downarrow = \begin{pmatrix} -\sin(\vartheta/2) e^{-i\varphi} \\ \cos(\vartheta/2) \end{pmatrix}, \quad (9)$$

which are the eigenvectors of $\mathbf{n} \cdot \boldsymbol{\sigma}$. Furthermore, we define the triplet of operators $\hat{\boldsymbol{\Sigma}} = (\hat{\Sigma}_1, \hat{\Sigma}_2, \hat{\Sigma}_3)^\top$ via

$$\hat{\Sigma}_i = -i\alpha_j \alpha_k \quad (10)$$

with (i, j, k) being a cyclic permutation of $(1, 2, 3)$. Its individual components fulfill the usual angular momentum commutator relationship $[\hat{\Sigma}_i, \hat{\Sigma}_j] = 2i\epsilon_{i,j,k} \hat{\Sigma}_k$ with the Levi-Civita symbol $\epsilon_{i,j,k}$. This operator is normalized to $\hat{\boldsymbol{\Sigma}}^\dagger \cdot \hat{\boldsymbol{\Sigma}} = 3$ and its components have the doubly degenerate eigenvalues ± 1 . The standard representation of $\hat{\boldsymbol{\Sigma}}$ is given by

$$\hat{\Sigma}_i = \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix}. \quad (11)$$

TABLE 1: Brief summary of the proposed spin operators' definitions and their mathematical properties. The table indicates from left to right the definition of the various spin operators, if they commute with the free Dirac Hamiltonian, if they obey the angular momentum algebra, if eigenvalues are $\pm 1/2$, and if the operators are related to the Pauli spin operator via an orthogonal transformation.

Definition	$\hat{S} = \hat{S}^\dagger$	$[\hat{H}_0, \hat{S}] = 0$	$[\hat{S}_i, \hat{S}_j] = i\varepsilon_{i,j,k}\hat{S}_k$	Eigenvalues equal to $\pm 1/2$	$\hat{S} = \hat{T}\hat{S}_P\hat{T}^{-1}$
$\hat{S}_P = \frac{1}{2}\hat{\Sigma}$	yes	no	yes	yes	—
$\hat{S}_{FW} = \frac{1}{2}\hat{\Sigma} + \frac{i\beta}{2\hat{p}_0}\hat{p} \times \alpha - \frac{\hat{p} \times (\hat{\Sigma} \times \hat{p})}{2\hat{p}_0(\hat{p}_0 + m_0c)}$	yes	yes	yes	yes	yes
$\hat{S}_{Cz} = \frac{m_0^2c^2}{2\hat{p}_0^2}\hat{\Sigma} + \frac{im_0c\beta}{2\hat{p}_0^2}\hat{p} \times \alpha + \frac{\hat{p} \cdot \hat{\Sigma}}{2\hat{p}_0^2}\hat{p}$	yes	yes	no	no	no
$\hat{S}_F = \frac{1}{2}\hat{\Sigma} + \frac{i\beta}{2m_0c}\hat{p} \times \alpha$	yes	yes	no	no	no
$\hat{S}_{Ch} = \frac{1}{2}\hat{\Sigma} + \frac{i}{2m_0c}\alpha \times \hat{p} + \frac{\hat{p} \times (\hat{\Sigma} \times \hat{p})}{2m_0c(m_0c + \hat{p}_0)}$	no	no	yes	yes	yes
$\hat{S}_{Pr} = \frac{1}{2}\beta\hat{\Sigma} + \frac{1}{2}\hat{\Sigma} \cdot \hat{p}(1 - \beta)\frac{\hat{p}}{\hat{p}^2}$	yes	yes	yes	yes	yes
$\hat{S}_{FG} = \frac{1}{2}\beta\hat{\Sigma} + \frac{1}{2}\hat{\Sigma} \cdot \hat{p}\left(\frac{\hat{H}_0}{c\hat{p}_0} - \beta\right)\frac{\hat{p}}{\hat{p}^2}$	yes	yes	no	yes	no

Various spin operators can be defined in terms of the Pauli-Lubanski vector \hat{W} and the related scalar operator \hat{W}_0 . Introducing the generator of the Lorentz boosts

$$\hat{N} = \frac{1}{2c^2}(\mathbf{r}\hat{H}_0 + \hat{H}_0\mathbf{r}), \quad (12)$$

\hat{W} and \hat{W}_0 are defined as

$$\hat{W} = \frac{1}{c}\hat{H}_0\hat{\mathbf{J}} + c\hat{p} \times \hat{N} = \frac{1}{4c}(\hat{H}_0\hat{\Sigma} + \hat{\Sigma}\hat{H}_0), \quad (13)$$

$$\hat{W}_0 = \hat{p} \cdot \hat{\mathbf{J}} = \frac{1}{2}\hat{p} \cdot \hat{\Sigma}. \quad (14)$$

With these definitions we are prepared now to summarize briefly the proposed spin operators, to give their explicit expressions, and to discuss some of their properties. An overview of the proposed spin operators is also given in Table 1.

3.1. Pauli spin operator

The Pauli spin operator [33–38] is a direct generalization of the spin operator of nonrelativistic quantum mechanics. Expressing the total angular momentum operator $\hat{\mathbf{J}}$ as $\hat{\mathbf{J}} = \mathbf{r} \times \hat{\mathbf{p}} + \hat{\Sigma}/2$, it appears quite natural to identify $\mathbf{r} \times \hat{\mathbf{p}}$ as the orbital angular momentum and to define

$$\hat{S}_P = \frac{1}{2}\hat{\Sigma} \quad (15)$$

as the relativistic Pauli spin operator. In many standard textbooks on relativistic quantum dynamics [34, 37, 38] this operator is considered as the relativistic spin operator. The energy shift for a hydrogenic ground state ψ_\uparrow (see Sec. 5) that is exposed to a weak homogeneous magnetic field $\mathbf{B} = (0, 0, B)^\top$ (anomalous Zeeman effect) relative to the field-free case is, with the atomic number Z [39, 40],

$$\frac{Bq}{m_0} \frac{1}{6} \left(1 + 2\sqrt{1 - Z^2\alpha_{el}^2}\right) = \frac{Bq}{m_0} \langle \psi_\uparrow | \hat{S}_{P,3} | \psi_\uparrow \rangle \quad (16)$$

(with α_{el} denoting the fine-structure constant), which is often brought up as an argument for \hat{S}_P representing the relativistic spin [34].

The components of the Pauli spin operator are generators of the SU(2) algebra and fulfill the angular momentum algebra

$$[\hat{S}_{P,i}, \hat{S}_{P,j}] = i\varepsilon_{i,j,k}\hat{S}_{P,k}; \quad (17)$$

the total squared length is $\hat{S}_P^2 = 3/4$. The degenerate eigenvalues s_P and the normalized orthogonal eigenvectors s_P of $\hat{S}_{P,n}$ are given by

$$\begin{aligned} s_{P\uparrow} = \frac{1}{2} : \quad & s_{P\uparrow,1} = \mathbf{u}_{\chi_\uparrow,0} e^{i\mathbf{p}\cdot\mathbf{r}}, \quad s_{P\uparrow,2} = \mathbf{v}_{\chi_\uparrow,0} e^{i\mathbf{p}\cdot\mathbf{r}} \\ s_{P\downarrow} = -\frac{1}{2} : \quad & s_{P\downarrow,1} = \mathbf{u}_{\chi_\downarrow,0} e^{i\mathbf{p}\cdot\mathbf{r}}, \quad s_{P\downarrow,2} = \mathbf{v}_{\chi_\downarrow,0} e^{i\mathbf{p}\cdot\mathbf{r}}, \end{aligned} \quad (18)$$

with χ_\uparrow and χ_\downarrow as defined in (9), which are also the eigenvectors of the nonrelativistic Pauli spin operator $\hat{S}_{P,nr} = \hat{\sigma}/2$. The relativistic Pauli spin operator does not commute with the free Hamiltonian,

$$[\hat{H}_0, \hat{S}_{P,n}] = icn(\hat{p} \times \alpha). \quad (19)$$

As a consequence of this nonvanishing commutator, even for a free particle the expectation value of $\hat{S}_{P,n}$ can evolve nontrivially in time, leading, for example, to the zitterbewegung [41–43] of the Pauli spin, if the quantum state is a superposition of states of positive- and negative-energy solutions of the free Dirac Hamiltonian. This is often considered an undesirable feature for a relativistic spin operator because an intrinsic observable should be constant when no forces act.

3.2. Foldy-Wouthuysen spin operator

A second definition of the spin is based on the Foldy-Wouthuysen transformation [44–48], which is a unitary trans-

formation \hat{T}_{FW} that turns the Dirac equation (1) into block-diagonal form, reducing positive- and negative-energy states to two-component wave functions. For the free-particle Hamiltonian \hat{H}_0 Foldy and Wouthuysen showed that

$$\hat{T}_{\text{FW}}^{-1} \hat{H}_0 \hat{T}_{\text{FW}} = c\beta \hat{p}_0, \quad (20)$$

with

$$\hat{T}_{\text{FW}} = \frac{\hat{p}_0 + m_0c - \beta \boldsymbol{\alpha} \cdot \hat{\mathbf{p}}}{\sqrt{2\hat{p}_0(\hat{p}_0 + m_0c)}}. \quad (21)$$

Furthermore, Foldy and Wouthuysen postulated that the spin operator in the transformed representation is \hat{S}_{P} indeed, leading to the Foldy-Wouthuysen spin operator

$$\hat{S}_{\text{FW}} = \hat{T}_{\text{FW}} \hat{S}_{\text{P}} \hat{T}_{\text{FW}}^{-1} \quad (22)$$

or more explicitly

$$\hat{S}_{\text{FW}} = \frac{1}{2} \hat{\boldsymbol{\Sigma}} + \frac{i\beta}{2\hat{p}_0} \hat{\mathbf{p}} \times \boldsymbol{\alpha} - \frac{\hat{\mathbf{p}} \times (\hat{\boldsymbol{\Sigma}} \times \hat{\mathbf{p}})}{2\hat{p}_0(\hat{p}_0 + m_0c)}. \quad (23)$$

Two years before the celebrated Foldy-Wouthuysen paper [44] the equivalent expression

$$\hat{S}_{\text{FW}} = \frac{1}{2c\hat{p}_0} \left(m_0c^2 \hat{\boldsymbol{\Sigma}} - ic\beta \boldsymbol{\alpha} \times \hat{\mathbf{p}} + \frac{c^2 \hat{\mathbf{p}} \cdot \hat{\boldsymbol{\Sigma}}}{c\hat{p}_0 + m_0c^2} \hat{\mathbf{p}} \right) \quad (24)$$

for the Foldy-Wouthuysen spin operator was given by Pryce in [49]. In this publication it was also shown that this spin operator is closely related to the Czachor and the Frenkel spin operators via the associated position operators. A further representation of the Foldy-Wouthuysen spin operator (21) can be written in terms of the Pauli-Lubanski vector [48]

$$\hat{S}_{\text{FW}} = \frac{1}{m_0c} \left(\frac{c\hat{p}_0}{\hat{H}_0} \hat{\mathbf{W}} - \frac{\hat{W}_0}{\hat{p}_0 + m_0c} \hat{\mathbf{p}} \right). \quad (25)$$

A further equivalent expression that is sometimes given in the literature is given by [7]

$$\hat{S}_{\text{FW}} = \frac{\hat{p}_0}{2m_0c} \hat{\boldsymbol{\Sigma}} - \frac{\hat{\mathbf{p}} \cdot \hat{\boldsymbol{\Sigma}}}{2m_0c(m_0c + \hat{p}_0)} \hat{\mathbf{p}} - \hat{\mathbf{p}} \times \boldsymbol{\alpha} \frac{i\hat{H}_0}{2m_0c^2\hat{p}_0}. \quad (26)$$

As \hat{S}_{FW} is unitarily equivalent to \hat{S}_{P} , its components fulfill the same commutator relationships. From $[c\beta \hat{p}_0, \hat{S}_{\text{P}}] = 0$ it follows $[\hat{H}_0, \hat{S}_{\text{FW}}] = 0$. Thus, the Foldy-Wouthuysen spin operator is conserved for free particles and $\hat{S}_{\text{FW},n}$ and \hat{H}_0 have a common set of eigenvectors. The degenerate eigenvalues s_{FW} and the normalized orthogonal eigenvectors s_{FW} of $\hat{S}_{\text{FW},n}$ and \hat{H}_0 are given by

$$\begin{aligned} s_{\text{FW}\uparrow} &= \frac{1}{2} : & s_{\text{FW}\uparrow,1} &= \mathbf{u}_{\chi_1, \mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}}, & s_{\text{FW}\uparrow,2} &= \mathbf{v}_{\chi_1, \mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}}, \\ s_{\text{FW}\downarrow} &= -\frac{1}{2} : & s_{\text{FW}\downarrow,1} &= \mathbf{u}_{\chi_1, \mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}}, & s_{\text{FW}\downarrow,2} &= \mathbf{v}_{\chi_1, \mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}}. \end{aligned} \quad (27)$$

The eigenvectors $s_{\text{FW}\uparrow,1}$ and $s_{\text{FW}\downarrow,1}$ have the positive-energy eigenvalue $c p_0(\mathbf{p})$, whereas $s_{\text{FW}\uparrow,2}$ and $s_{\text{FW}\downarrow,2}$ have the negative-energy eigenvalue $-c p_0(\mathbf{p})$.

3.3. Czachor spin operator

The third spin vector has been discussed by Czachor [14], but already appeared in an earlier work by Pryce [49]. It can be defined on the basis of the spatial components of the Pauli-Lubanski vector $\hat{\mathbf{W}}$. If we multiply the vector $\hat{\mathbf{W}}$ with the inverse of the free Dirac Hamiltonian, we can define the Pauli-Lubanski-based spin operator

$$\hat{S}_{\text{Cz}} = \hat{\mathbf{W}} c \hat{H}_0^{-1}. \quad (28)$$

Using energy subspace projection operators (8), we can rewrite this particular spin operator in the form

$$\hat{S}_{\text{Cz}} = \frac{1}{2} (\hat{\Lambda}^+ \hat{\boldsymbol{\Sigma}} \hat{\Lambda}^+ + \hat{\Lambda}^- \hat{\boldsymbol{\Sigma}} \hat{\Lambda}^-). \quad (29)$$

Using the projector-based representation (29), one can easily see that the individual spin components cannot satisfy the usual angular momentum commutator relationships. For a comparison with the other spin vectors, we rewrite \hat{S}_{Cz} also in the more explicit form

$$\hat{S}_{\text{Cz}} = \frac{m_0^2 c^2}{2\hat{p}_0^2} \hat{\boldsymbol{\Sigma}} + \frac{im_0c\beta}{2\hat{p}_0^2} \hat{\mathbf{p}} \times \boldsymbol{\alpha} + \frac{\hat{\mathbf{p}} \cdot \hat{\boldsymbol{\Sigma}}}{2\hat{p}_0^2} \hat{\mathbf{p}}. \quad (30)$$

While the Czachor spin operator has the nice feature that it commutes with the free Dirac Hamiltonian

$$[\hat{H}_0, \hat{S}_{\text{Cz},n}] = 0, \quad (31)$$

its components do not fulfill the angular momentum algebra. In fact, the commutator relation

$$[\hat{S}_{\text{Cz},i}, \hat{S}_{\text{Cz},j}] = i\epsilon_{i,j,k} \left(\hat{S}_{\text{Cz},k} - \frac{\hat{\boldsymbol{\Sigma}} \cdot \hat{\mathbf{p}}}{2\hat{p}_0^2} \hat{p}_k \right) \quad (32)$$

holds. Consequently, the absolute values of the Czachor spin operator's eigenvalues are not equal to 1/2. The degenerate eigenvalues s_{Cz} and the nonnormalized orthogonal eigenvectors s_{Cz} of $\hat{S}_{\text{Cz},(0,0,1)^T}$ are given by

$$\begin{aligned} s_{\text{Cz}\uparrow} &= \frac{p_0(\mathbf{p}_{\parallel})}{2p_0(\mathbf{p})} : & s_{\text{Cz}\uparrow,1} &= \begin{pmatrix} p_0(\mathbf{p}_{\perp})^2 + p_0(\mathbf{p}_{\perp})p_0(\mathbf{p}) \\ p_z(p_x + ip_y) \\ 0 \\ m_0c(p_x + ip_y) \end{pmatrix} e^{i\mathbf{p}\cdot\mathbf{r}}, \\ s_{\text{Cz}\uparrow,2} &= \begin{pmatrix} -p_z(p_x - ip_y) \\ p_0(\mathbf{p}_{\perp})^2 - p_0(\mathbf{p}_{\perp})p_0(\mathbf{p}) \\ m_0c(p_x - ip_y) \\ 0 \end{pmatrix} e^{i\mathbf{p}\cdot\mathbf{r}}, \\ s_{\text{Cz}\downarrow} &= -\frac{p_0(\mathbf{p}_{\parallel})}{2p_0(\mathbf{p})} : & s_{\text{Cz}\downarrow,1} &= \begin{pmatrix} -p_z(p_x - ip_y) \\ p_0(\mathbf{p}_{\perp})^2 + p_0(\mathbf{p}_{\perp})p_0(\mathbf{p}) \\ m_0c(p_x - ip_y) \\ 0 \end{pmatrix} e^{i\mathbf{p}\cdot\mathbf{r}}, \\ s_{\text{Cz}\downarrow,2} &= \begin{pmatrix} p_0(\mathbf{p}_{\perp})^2 - p_0(\mathbf{p}_{\perp})p_0(\mathbf{p}) \\ +p_z(p_x + ip_y) \\ 0 \\ m_0c(p_x + ip_y) \end{pmatrix} e^{i\mathbf{p}\cdot\mathbf{r}}, \end{aligned} \quad (33)$$

where \mathbf{p}_\perp and \mathbf{p}_\parallel denote the momentum components perpendicular and parallel to the spin orientation $\mathbf{n} = (0, 0, 1)^\top$. Eigenfunctions for other spin orientations may be found by an appropriate Lorentz rotation. The eigenvalues are functions of the momenta that are parallel to the polarization direction of the eigenstate. In particular, the absolute values of the Czachor spin operator's eigenvalues are less than 1/2.

As the Czachor spin operator and the Pauli spin operator have different eigenvalues, the Czachor spin operator cannot be related to the Pauli spin operator via a similarity transformation. This means that there is no operator \hat{T}_{Cz} such that \hat{S}_{Cz} equals $\hat{T}_{Cz}\hat{S}_P\hat{T}_{Cz}^{-1}$. As a consequence of the definition (29), the operator identities

$$\hat{\Lambda}^+\hat{S}_{P,n}\hat{\Lambda}^+ = \hat{\Lambda}^+\hat{S}_{Cz,n}\hat{\Lambda}^+, \quad (34a)$$

$$\hat{\Lambda}^-\hat{S}_{P,n}\hat{\Lambda}^- = \hat{\Lambda}^-\hat{S}_{Cz,n}\hat{\Lambda}^- \quad (34b)$$

hold. Consequently, the Pauli and the Czachor spin operators yield the same expectation values when applied to the subspaces of the eigenstates (6) of the free-particle Dirac Hamiltonian \hat{H}_0 with positive energy or negative energy, respectively.

We also note that the eigenfunctions of the Foldy-Wouthuysen spin operator with momentum strictly perpendicular or strictly parallel to the spin orientation \mathbf{n} are eigenfunctions of the Czachor spin operator, too. Furthermore, the total squared length of the spin operator \hat{S}_{Cz} is $\hat{S}_{Cz}^2 = (3m_0^2c^2 + \hat{\mathbf{p}}^2)/(4m_0^2c^2 + 4\hat{\mathbf{p}}^2)$. The fact that it is shorter than the squared length of the Pauli operator $\hat{S}_P^2 = 3/4$ was associated with the Lorentz contraction in [14]. In particular, for an ultrarelativistic particle, that is, $|\mathbf{p}| \rightarrow \infty$, we have $\hat{S}_{Cz}^2 \rightarrow 1/4$. In this limit, the spin components in the two directions perpendicular to \mathbf{p} vanish.

3.4. Frenkel spin operator

A fourth definition of the spin is the quantum mechanical analog of a classical spin vector as studied originally by Frenkel [49–53]

$$\hat{S}_F = \frac{1}{2}\hat{\Sigma} + \frac{i\beta}{2m_0c}\hat{\mathbf{p}} \times \boldsymbol{\alpha}. \quad (35)$$

It also commutes with the free Dirac Hamiltonian

$$[\hat{H}_0, \hat{S}_{F,n}] = 0, \quad (36)$$

but similarly to the Czachor operator it does not obey the angular momentum algebra, viz.,

$$[\hat{S}_{F,i}, \hat{S}_{F,j}] = i\epsilon_{i,j,k}\left(\hat{S}_{F,k} + \frac{\hat{\Sigma} \cdot \hat{\mathbf{p}}}{2m_0^2c^2}\hat{p}_k\right). \quad (37)$$

The degenerate eigenvalues s_F and the normalized orthogonal eigenvectors s_F of $\hat{S}_{F,n}$ are given by

$$\begin{aligned} s_{F\uparrow} &= \frac{p_0(\mathbf{p}_\perp)}{2m_0c} : & s_{F\uparrow,1} &= \mathbf{u}_{\chi_{\uparrow,p_\perp}} e^{i\mathbf{p}\cdot\mathbf{r}}, & s_{F\uparrow,2} &= \mathbf{v}_{\chi_{\uparrow,p_\perp}} e^{i\mathbf{p}\cdot\mathbf{r}}, \\ s_{F\downarrow} &= -\frac{p_0(\mathbf{p}_\perp)}{2m_0c} : & s_{F\downarrow,1} &= \mathbf{u}_{\chi_{\downarrow,p_\perp}} e^{i\mathbf{p}\cdot\mathbf{r}}, & s_{F\downarrow,2} &= \mathbf{v}_{\chi_{\downarrow,p_\perp}} e^{i\mathbf{p}\cdot\mathbf{r}}, \end{aligned} \quad (38)$$

where \mathbf{p}_\perp is the component of the momentum vector \mathbf{p} that is perpendicular to \mathbf{n} . Because the Frenkel spin operator and the Pauli spin operator have different eigenvalues, the Frenkel spin operator cannot be related to the Pauli spin operator via a similarity transform. This means that there is no operator \hat{T}_F such that \hat{S}_F equals $\hat{T}_F\hat{S}_P\hat{T}_F^{-1}$. We also note that the total squared length of the Frenkel spin operator is $\hat{S}_F^2 = (3m_0^2c^2 + 2\hat{\mathbf{p}}^2)/(4m_0^2c^2)$. The magnitude of the eigenvalues and the total squared length \hat{S}_F^2 increase to infinity as the momentum grows.

3.5. Chakrabarti spin operator

A fifth proposal for the spin operator has been introduced by Chakrabarti [54–57]. It is defined via the similarity transformation

$$\hat{S}_{Ch} = \hat{T}_{Ch}\hat{S}_P\hat{T}_{Ch}^{-1} \quad (39)$$

that is induced by the antiunitary Lorentz boost operator

$$\hat{T}_{Ch} = \frac{\hat{p}_0 + m_0c + \boldsymbol{\alpha} \cdot \hat{\mathbf{p}}}{[2m_0c(\hat{p}_0 + m_0c)]^{1/2}} \quad (40a)$$

and its inverse, which is explicitly given by

$$\hat{T}_{Ch}^{-1} = \frac{\hat{p}_0 + m_0c - \boldsymbol{\alpha} \cdot \hat{\mathbf{p}}}{[2m_0c(\hat{p}_0 + m_0c)]^{1/2}}. \quad (40b)$$

The explicit form of the (non-Hermitian) Chakrabarti spin operator follows as

$$\hat{S}_{Ch} = \frac{1}{2}\hat{\Sigma} + \frac{i}{2m_0c}\boldsymbol{\alpha} \times \hat{\mathbf{p}} + \frac{1}{2m_0c(m_0c + \hat{p}_0)}\hat{\mathbf{p}} \times (\hat{\Sigma} \times \hat{\mathbf{p}}). \quad (41)$$

In [58, 59] the so-called Gürsey-Ryder operator

$$\hat{S}_{Ch} = \frac{\hat{p}_0}{2m_0c}\hat{\Sigma} - \frac{\hat{\mathbf{p}} \cdot \hat{\Sigma}}{2m_0c(m_0c + \hat{p}_0)}\hat{\mathbf{p}} - \frac{i}{2m_0c}\hat{\mathbf{p}} \times \boldsymbol{\alpha} \quad (42)$$

was considered, which is just another algebraic expression for the Chakrabarti spin operator.

The antiunitary similarity transformation operator \hat{T}_{Ch} is also Hermitian and β -pseudo-unitary, that is, $\hat{T}_{Ch}^\dagger = \beta\hat{T}_{Ch}^{-1}\beta^{-1}$, which may be simplified to $\hat{T}_{Ch} = \beta\hat{T}_{Ch}^{-1}\beta$. The operator \hat{T}_{Ch} transforms the operator $\beta(\hat{p}_0 + \boldsymbol{\alpha} \cdot \hat{\mathbf{p}})$ into a diagonal momentum-independent form, viz.,

$$\hat{T}_{Ch}\beta(\hat{p}_0 + \boldsymbol{\alpha} \cdot \hat{\mathbf{p}})\hat{T}_{Ch}^{-1} = m_0c\beta. \quad (43)$$

Similarly, when applied to the free Dirac Hamiltonian \hat{H}_0 the operator \hat{T}_{Ch} makes it almost diagonal, viz.,

$$\hat{T}_{Ch}\hat{H}_0\hat{T}_{Ch}^{-1} = c\beta\hat{p}_0 + \hat{h}, \quad (44)$$

where \hat{h} is in the Dirac representation the matrix

$$\hat{h} = 2c \begin{pmatrix} 0 & 0 \\ \boldsymbol{\sigma} \cdot \hat{\mathbf{p}} & 0 \end{pmatrix}. \quad (45)$$

Here 0 denotes a 2×2 zero matrix. Note that the transformed Hamiltonian (44) is not Hermitian as a consequence of \hat{T}_{Ch} not being unitary.

We also note that the operator $\beta\hat{S}_{\text{Ch}}$ is Hermitian with respect to the usual scalar product, thus \hat{S}_{Ch} is β -pseudo-Hermitian. Because \hat{S}_{Ch} originates from a similarity transformation of \hat{S}_{P} it satisfies

$$[\hat{S}_{\text{Ch},i}, \hat{S}_{\text{Ch},j}] = i\varepsilon_{i,j,k}\hat{S}_{\text{Ch},k}; \quad (46)$$

its squared length is $\hat{S}_{\text{Ch}}^2 = 3/4$, but its time evolution is non-trivial because of the nonvanishing commutator

$$[\hat{H}_0, \hat{S}_{\text{Ch},n}] = \mathbf{n} \cdot \left(i\boldsymbol{\alpha} \times \hat{\mathbf{p}} \left(\frac{\hat{p}_0}{m_0} + c\beta \right) + \frac{\hat{\mathbf{p}} \times (\hat{\boldsymbol{\Sigma}} \times \hat{\mathbf{p}})}{m_0} \right). \quad (47)$$

The degenerate eigenvalues s_{Ch} and the normalized eigenvectors s_{Ch} of $\hat{S}_{\text{Cz},n}$ follow directly via $s_{\text{Ch}} = \hat{T}_{\text{Ch}}s_{\text{P}}$ (see (18)) and are given by

$$\begin{aligned} s_{\text{Ch}\uparrow} = \frac{1}{2} : \quad & s_{\text{Ch}\uparrow,1} = \mathbf{u}_{\chi_{\uparrow},\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}}, \quad s_{\text{Ch}\uparrow,2} = \mathbf{v}_{\chi_{\uparrow},-\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}}, \\ s_{\text{Ch}\downarrow} = -\frac{1}{2} : \quad & s_{\text{Ch}\downarrow,1} = \mathbf{u}_{\chi_{\downarrow},\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}}, \quad s_{\text{Ch}\downarrow,2} = \mathbf{v}_{\chi_{\downarrow},-\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}}. \end{aligned} \quad (48)$$

Note that the Chakrabarti spin operator shares two of its eigenvectors with the Foldy-Wouthuysen spin operator, viz., $s_{\text{Ch}\uparrow,1} = s_{\text{FW}\uparrow,1}$ and $s_{\text{Ch}\downarrow,1} = s_{\text{FW}\downarrow,1}$. Therefore, the Foldy-Wouthuysen spin operator and the Chakrabarti spin operator are equivalent when applied to the subspace of the eigenstates (6a) of the free-particle Dirac Hamiltonian with positive energy. In other words, the operator identity

$$\hat{S}_{\text{FW},n}\hat{\Lambda}^+ = \hat{S}_{\text{Ch},n}\hat{\Lambda}^+ \quad (49)$$

holds, which also follows by comparing the expressions (26) and (42) for the Foldy-Wouthuysen and the spin operators. In contrast, the operators $\hat{S}_{\text{FW},n}\hat{\Lambda}^-$ and $\hat{S}_{\text{Ch},n}\hat{\Lambda}^-$ are *not* equivalent, however, the following operator equality holds

$$\hat{\Lambda}^- \hat{S}_{\text{FW},n} \hat{\Lambda}^- = \hat{\Lambda}^- \hat{S}_{\text{Ch},n} \hat{\Lambda}^-. \quad (50)$$

As a consequence of the non-Hermiticity, the eigenvectors of the Chakrabarti spin operator are not all pairwise orthogonal to each other, in particular not the states $s_{\text{Ch}\uparrow,2}$ and $s_{\text{Ch}\downarrow,2}$, which have *different* spin orientations. Furthermore, expectation values of the Chakrabarti spin operator can lie outside the spectral range between $-1/2$ and $1/2$. For example, for the Gaussian wave packet of momentum width σ and mean momentum $\bar{\mathbf{p}} = (\bar{p}_x, 0, 0)^\top$,

$$\Psi(\mathbf{r}) = \int \frac{1}{(2\pi)^{3/2} \sqrt{2\pi\sigma}} \exp\left(i\mathbf{p} \cdot \mathbf{r} - \frac{(\mathbf{p} - \bar{\mathbf{p}})^2}{4\sigma^2}\right) \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} d^3p \quad (51)$$

we obtain for the expectation value of the Chakrabarti spin in the z direction

$$\begin{aligned} \langle \Psi | \hat{S}_{\text{Ch},3} | \Psi \rangle = \\ \frac{1}{2} + \frac{1}{\sqrt{2\pi}\sigma} \int \exp\left(-\frac{(p_x - \bar{p}_x)^2}{2\sigma^2}\right) \frac{p_x^2/(m_0c)^2}{2\sqrt{p_x^2/(m_0c)^2 + 1}} dp_x. \end{aligned} \quad (52)$$

In the limit $\sigma \rightarrow 0$ we find

$$\langle \Psi | \hat{S}_{\text{Ch},3} | \Psi \rangle = \frac{1}{2} + \frac{\bar{p}_x^2/(m_0c)^2}{2\sqrt{\bar{p}_x^2/(m_0c)^2 + 1}}, \quad (53)$$

which is strictly larger than $1/2$ and grows in leading order linearly as $|\bar{p}_x| \rightarrow \infty$. This example also illustrates that the expectation values $\langle \Psi | \hat{S}_{\text{FW},n} | \Psi \rangle$ and $\langle \Psi | \hat{S}_{\text{Ch},n} | \Psi \rangle$ are *not* equal for general states, as it was claimed recently in [57].

3.6. Pryce spin operator

A sixth proposal for a relativistic spin operator goes back to Pryce [49, 58, 60, 61], who introduced the operator

$$\hat{S}_{\text{Pr}} = \frac{1}{m_0c} \left(\hat{\mathbf{W}} - \frac{\hat{W}_0}{\hat{H}_0/c + m_0c} \hat{\mathbf{p}} \right), \quad (54)$$

which was applied in the context of quantum field theory [62] and relativistic quantum information [63]. Utilizing the definitions (13) and (14) the Pryce spin operator's form is given by

$$\hat{S}_{\text{Pr}} = \frac{1}{2}\beta\hat{\boldsymbol{\Sigma}} + \frac{c\gamma^5(\beta+1)}{2(\hat{H}_0 + m_0c^2)}\hat{\mathbf{p}}, \quad (55)$$

where the 4×4 matrix $\gamma^5 = i\alpha_3\alpha_2\alpha_1$ is in the Dirac representation defined as

$$\gamma^5 = \begin{pmatrix} 0 & \mathbb{I}_2 \\ \mathbb{I}_2 & 0 \end{pmatrix}. \quad (56)$$

The equivalent expression for the Pryce spin operator

$$\hat{S}_{\text{Pr}} = \frac{1}{2\hat{H}_0} \left(m_0c^2\hat{\boldsymbol{\Sigma}} - ic\beta\boldsymbol{\alpha} \times \hat{\mathbf{p}} + \frac{c^2\hat{\mathbf{p}} \cdot \hat{\boldsymbol{\Sigma}}}{\hat{H}_0 + m_0c^2} \hat{\mathbf{p}} \right) \quad (57)$$

was given in [49], which is almost identical to the definition (24) of the Foldy-Wouthuysen spin operator except that $c\hat{p}_0$ has been replaced by \hat{H}_0 . Using the operator identities

$$\hat{H}_0^{-1} = \frac{\boldsymbol{\alpha} \cdot \hat{\mathbf{p}} + m_0c\beta}{c\hat{\mathbf{p}}^2} \quad (58)$$

and

$$(\hat{H}_0 + m_0c^2)^{-1} = \frac{\boldsymbol{\alpha} \cdot \hat{\mathbf{p}} + m_0c(\beta-1)}{c\hat{\mathbf{p}}^2}, \quad (59)$$

we may turn (55) and (57) into a form that is more convenient for actual calculations, yielding

$$\hat{S}_{\text{Pr}} = \frac{1}{2}\beta\hat{\boldsymbol{\Sigma}} + \frac{\gamma^5(\beta+1)\boldsymbol{\alpha} \cdot \hat{\mathbf{p}}}{2\hat{\mathbf{p}}^2} \hat{\mathbf{p}} \quad (60)$$

or equivalently

$$\hat{S}_{\text{Pr}} = \frac{1}{2}\beta\hat{\boldsymbol{\Sigma}} + \frac{1}{2}\hat{\boldsymbol{\Sigma}} \cdot \hat{\mathbf{p}}(1-\beta) \frac{\hat{\mathbf{p}}}{\hat{\mathbf{p}}^2}. \quad (61)$$

This form is unexpectedly simple and was suggested independently from Pryce by Stech in [64]. This form suggests that the relativistic Pryce spin operator is a function of the momentum operator's direction only, not depending on the mass m_0 , the speed of light c , or the amount of the momentum. In the Dirac representation, the operator is block diagonal, viz.,

$$\hat{S}_{\text{Pr}} = \frac{1}{2}\beta\hat{\Sigma} + \frac{1}{\hat{p}^2} \begin{pmatrix} 0 & 0 \\ 0 & \boldsymbol{\sigma} \cdot \hat{\mathbf{p}} \end{pmatrix} \hat{\mathbf{p}}. \quad (62)$$

The spin operator \hat{S}_{Pr} fulfills the angular momentum algebra

$$[\hat{S}_{\text{Pr},i}, \hat{S}_{\text{Pr},j}] = i\epsilon_{i,j,k}\hat{S}_{\text{Pr},k}, \quad (63)$$

its squared length is $\hat{S}_{\text{Pr}}^2 = 3/4$, and it commutes with the free Dirac Hamiltonian $[\hat{H}_0, \hat{S}_{\text{Pr}}] = 0$. The degenerate eigenvalues s_{Pr} and the orthogonal normalized eigenvectors of $\hat{S}_{\text{Pr},n}$ are given by

$$\begin{aligned} s_{\text{Pr}\uparrow} = \frac{1}{2} : \quad s'_{\text{Pr}\uparrow,1} &= \begin{pmatrix} \chi_{\uparrow} \\ 0 \end{pmatrix} e^{ip\cdot r}, \quad s'_{\text{Pr}\uparrow,2} = \begin{pmatrix} 0 \\ \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{|\mathbf{p}|} \chi_{\uparrow} \end{pmatrix} e^{ip\cdot r}, \\ s_{\text{Pr}\downarrow} = -\frac{1}{2} : \quad s'_{\text{Pr}\downarrow,1} &= \begin{pmatrix} \chi_{\downarrow} \\ 0 \end{pmatrix} e^{ip\cdot r}, \quad s'_{\text{Pr}\downarrow,2} = \begin{pmatrix} 0 \\ \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{|\mathbf{p}|} \chi_{\downarrow} \end{pmatrix} e^{ip\cdot r}. \end{aligned} \quad (64)$$

The eigenvectors in (64) have a particular simple form; however, they are not simultaneously eigenvectors of the free Dirac Hamiltonian \hat{H}_0 and $\hat{S}_{\text{Pr},n}$. The simultaneous eigenvectors of both operators can be written in the matrix form

$$\begin{pmatrix} s_{\text{Pr}\uparrow,1} & s_{\text{Pr}\downarrow,1} & s_{\text{Pr}\uparrow,2} & s_{\text{Pr}\downarrow,2} \end{pmatrix} = \begin{pmatrix} \mathbf{u}_{\mathbf{v}_{\uparrow},\mathbf{p}} & \mathbf{u}_{\mathbf{v}_{\downarrow},\mathbf{p}} & \mathbf{v}_{\mathbf{v}_{\uparrow},\mathbf{p}} & \mathbf{v}_{\mathbf{v}_{\downarrow},\mathbf{p}} \end{pmatrix} \begin{pmatrix} (\chi_{\uparrow} \ \chi_{\downarrow}) & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{|\mathbf{p}|} (\chi_{\uparrow} \ \chi_{\downarrow}) \end{pmatrix} e^{ip\cdot r} \quad (65)$$

with $\mathbf{v}_{\uparrow} = (1, 0)^{\text{T}}$ and $\mathbf{v}_{\downarrow} = (0, 1)^{\text{T}}$. The eigenvectors $s_{\text{Pr}\uparrow,1}$ and $s_{\text{Pr}\downarrow,1}$ have the positive energy-eigenvalue $cp_0(\mathbf{p})$, whereas $s_{\text{Pr}\uparrow,2}$ and $s_{\text{Pr}\downarrow,2}$ have the negative energy-eigenvalue $-cp_0(\mathbf{p})$. Note that $s'_{\text{Pr}\uparrow,1}$ and $s'_{\text{Pr}\downarrow,1}$ are also eigenvectors of the Pauli spin operator, while $s_{\text{Pr}\uparrow,1}$ and $s_{\text{Pr}\downarrow,1}$ are also eigenvectors of the Foldy-Wouthuysen spin operator.

Because $s_{\text{Pr}\uparrow,1}$ and $s_{\text{Pr}\downarrow,1}$ are positive-energy eigenfunctions of the free Dirac Hamiltonian too, the operator identity

$$\hat{S}_{\text{FW},n}\hat{\Lambda}^+ = \hat{S}_{\text{Pr},n}\hat{\Lambda}^+ \quad (66)$$

holds. Note, however, that the operators $\hat{\Lambda}^-\hat{S}_{\text{FW},n}\hat{\Lambda}^-$ and $\hat{\Lambda}^-\hat{S}_{\text{Pr},n}\hat{\Lambda}^-$ are *not* equivalent but states from different energy subspaces are coupled identically, viz.,

$$\Lambda^+\hat{S}_{\text{FW}}\Lambda^- = \Lambda^+\hat{S}_{\text{Pr}}\Lambda^- = \Lambda^-\hat{S}_{\text{FW}}\Lambda^+ = \Lambda^-\hat{S}_{\text{Pr}}\Lambda^+. \quad (67)$$

As $\hat{S}_{\text{Pr},n}$ and $\hat{S}_{\text{FW},n}$ share the same eigenvalues, it is possible to express the Pryce operator as a similarity transformation based

on \hat{S}_{Pr} , similar to the corresponding transformations for \hat{S}_{FW} and \hat{S}_{Ch} . In fact, one can show that $\hat{S}_{\text{Pr}} = \hat{T}_{\text{Pr}}\hat{S}_{\text{Pr}}\hat{T}_{\text{Pr}}^{-1}$ with the unitary operator

$$\hat{T}_{\text{Pr}} = \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & i\frac{\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}}{|\hat{\mathbf{p}}|} \end{pmatrix}. \quad (68)$$

Utilizing this transformation, it is possible to formulate relativistic quantum mechanics in a representation where the free Hamiltonian takes the form

$$\hat{T}_{\text{Pr}}^{-1}\hat{H}_0\hat{T}_{\text{Pr}} = (mc^2 - i\gamma^5 c|\hat{\mathbf{p}}|)\beta \quad (69)$$

similar to the Foldy-Wouthuysen picture.

3.7. Fradkin-Good operator

An operator that has a definition similar to the Pryce operator was considered by Fradkin and Good in [65], the so-called polarization vector, which is defined as

$$\hat{S}_{\text{FG}} = \frac{1}{2}\beta\hat{\Sigma} + \frac{1}{2}\hat{\Sigma} \cdot \hat{\mathbf{p}} \left(\frac{\hat{H}_0}{c\hat{p}_0} - \beta \right) \frac{\hat{\mathbf{p}}}{\hat{p}^2}. \quad (70)$$

It has been studied extensively in [59, 65]. The squared length of \hat{S}_{FG} is $\hat{S}_{\text{FG}}^2 = 3/4$ and it commutes with the free Dirac Hamiltonian $[\hat{H}_0, \hat{S}_{\text{FG}}] = 0$, but it does not fulfill the angular momentum algebra; rather

$$[\hat{S}_{\text{FG},i}, \hat{S}_{\text{FG},j}] = i\epsilon_{i,j,k}\hat{S}_{\text{FG},k} \frac{\hat{H}_0}{c\hat{p}_0}. \quad (71)$$

The degenerate eigenvalues s_{FG} and the normalized orthogonal eigenvectors s_{FG} of $\hat{S}_{\text{FG},n}$ and \hat{H}_0 are given by

$$\begin{aligned} s_{\text{FG}\uparrow} = \frac{1}{2} : \quad s_{\text{FG}\uparrow,1} &= \mathbf{u}_{\chi_{\uparrow},\mathbf{p}} e^{ip\cdot r}, \quad s_{\text{FG}\uparrow,2} = \mathbf{v}_{\chi_{\downarrow},\mathbf{p}} e^{ip\cdot r}, \\ s_{\text{FG}\downarrow} = -\frac{1}{2} : \quad s_{\text{FG}\downarrow,1} &= \mathbf{u}_{\chi_{\downarrow},\mathbf{p}} e^{ip\cdot r}, \quad s_{\text{FG}\downarrow,2} = \mathbf{v}_{\chi_{\uparrow},\mathbf{p}} e^{ip\cdot r}. \end{aligned} \quad (72)$$

The eigenfunctions of $\hat{S}_{\text{FG},n}$ are also eigenfunctions of $\hat{S}_{\text{FW},n}$ but in the case of negative-energy states with opposite eigenvalues. Thus

$$\hat{S}_{\text{FW},n}\hat{\Lambda}^+ = \hat{S}_{\text{FG},n}\hat{\Lambda}^+, \quad (73)$$

$$\hat{S}_{\text{FW},n}\hat{\Lambda}^- = -\hat{S}_{\text{FG},n}\hat{\Lambda}^-. \quad (74)$$

Comparing the definitions (61) and (70) immediately reveals the operator identity

$$\hat{S}_{\text{Pr},n}\hat{\Lambda}^+ = \hat{S}_{\text{FG},n}\hat{\Lambda}^+. \quad (75)$$

The Fradkin-Good operator \hat{S}_{FG} is not related to the Pauli operator \hat{S}_{P} via a similarity transformation; instead

$$\hat{S}_{\text{FG}} = \hat{T}_{\text{FW}}\beta\hat{S}_{\text{P}}\hat{T}_{\text{FW}}^{-1} \quad (76)$$

with \hat{T}_{FW} as defined in (21).

3.8. Applying spin operators to wave functions

The spin operators in Table 1 are defined as functions of the canonical momentum operator $\hat{\mathbf{p}}$, which has in position space representation the form $\hat{\mathbf{p}} = -i\nabla$. Consequently, the spin operators in Table 1 are rather complicated differential operators and their application to position space wave functions $\Psi(\mathbf{r})$ is not straightforward. Furthermore, the spin operators are not gauge independent as expectation values of the canonical momentum operator depend on the choice of the gauge. One can deal with both issues in the following way.

Noting that in canonical momentum space the canonical momentum operator $\hat{\mathbf{p}}$ is just a real-valued vector and that none of the proposed spin operators depends on position, one can apply the spin operators easily to wave functions given in canonical momentum space

$$\tilde{\Psi}(\mathbf{p}, t) = \frac{1}{(2\pi)^{3/2}} \int \Psi(\mathbf{r}, t) \exp(-i\mathbf{r} \cdot \mathbf{p}) d^3r, \quad (77)$$

where the operators in Table 1 become plain matrices. The spin operators as proposed in Table 1 can represent operators that correspond to measurable observables only in gauges with $\mathbf{A}(\mathbf{r}, t) = 0$ where the canonical momentum operator equals the physical kinematic momentum operator. Physical spin operators for general gauges with $\mathbf{A}(\mathbf{r}, t) \neq 0$, however, can be obtained by replacing $\hat{\mathbf{p}}$ by $\hat{\mathbf{p}} - q\mathbf{A}(\mathbf{r}, t)$ in the definitions in Table 1. In this way the spin operators become position dependent and consequently the canonical momentum representation (Fourier representation) of the spin operators are no longer plain matrices and therefore difficult to apply whether the wave function is given in position space or Fourier space. For this reason we will concentrate below on physical setups with vanishing vector potential.

4. Time dependence of the spin in scattering dynamics

Summarizing the results of Sec. 3, the following operator identities hold:

$$\Lambda^+ \hat{\mathbf{S}}_P \Lambda^+ = \Lambda^+ \hat{\mathbf{S}}_{Cz} \Lambda^+, \quad (78)$$

$$\hat{\mathbf{S}}_{FW} \Lambda^+ = \hat{\mathbf{S}}_{Ch} \Lambda^+ = \hat{\mathbf{S}}_{Pr} \Lambda^+ = \hat{\mathbf{S}}_{FG} \Lambda^+. \quad (79)$$

Thus, the Pauli and the Czachor spin operators yield the same expectation values in the subspace free-particle states with positive energy and also the Foldy-Wouthuysen, the Chakrabarti, the Pryce, and the Fradkin-Good spin operators are equivalent in the positive-energy subspace of free-particle states. If an interaction with some external fields is introduced a superposition of positive-energy free-particle solutions may evolve such that negative-energy free-particle states become populated and therefore it is possible to distinguish between the various spin operators by determining their expectation values. For a detailed discussion of the quantum field-theoretic interpretation of transitions to negative-energy states see [66].

4.1. Reflection of a wave packet at a step potential

As a first example let us consider the relativistic spin dynamics in scattering at a smooth two-dimensional step potential

$$q\phi(x, y) = \frac{V_0}{2} \left(1 + \tanh \frac{x}{w} \right) \quad (80)$$

with $V_0 = 1.95m_0c^2$ and $w = 1/(4c)$ (in atomic units) such that the barrier is high but still below the critical value $2m_0c^2$ that would permit Klein tunneling [67]. The initial state is a Gaussian superposition of common eigenstates of $\hat{\mathbf{p}}$, \hat{H}_0 , and $\hat{\mathbf{S}}_{FW,2}$ having positive energy and positive spin in the y direction

$$\Psi(\mathbf{r}, 0) = \frac{1}{2\pi} \int g(\mathbf{p}') \mathbf{u}_{\chi_\uparrow, \mathbf{p}'} e^{i\mathbf{p}' \cdot \mathbf{r}} d^2p', \quad (81)$$

with $\mathbf{r} = (x, y)^T$, $\mathbf{p}' = (p'_x, p'_y)^T$, and $\chi_\uparrow = (1, i)^T / \sqrt{2}$ here and $g(\mathbf{p}')$ denoting a Gaussian weight function corresponding to a spatial width of 0.025 a.u. in the x and y directions. The wave packet's initial center of mass is at $(-0.175 \text{ a.u.}, 0 \text{ a.u.})^T$ and its initial mean momentum is $(m_0c, 0)^T$ such that the two-dimensional wave packet approaches the barrier from the left. The quantum dynamics is simulated by solving the time-dependent Dirac equation numerically by a Fourier split operator method [42, 68]. When the wave packet interacts with the barrier negative-energy states become occupied as indicated by the quantity $\langle \Psi(t) | \Lambda^- | \Psi(t) \rangle$ in Fig. 1(a). After reflection when the wave packet has left the interaction zone, however, negative-energy states are no longer occupied.

We determine spin expectation values in the y direction. All spin expectation values change during the interaction with the potential step. Initially, the Pauli and the Czachor spin operators yield the same expectation values as a result of the initial condition and the Foldy-Wouthuysen, the Chakrabarti, the Pryce, and the Fradkin-Good spin operators all give an expectation value of 1/2, see Fig. 1(b). When the wave packet interacts with the step potential and a substantial fraction of free-particle negative-energy states is occupied the spin expectation values change in a specific way such that they differ for all proposed spin operators. In particular, the spin expectation values for the Foldy-Wouthuysen, the Chakrabarti, the Pryce, and the Fradkin-Good spin operators are reduced. In the cases of the Pryce and the Fradkin-Good spin operators the change of the expectation value is so small (about 1 %) that it is not visible on the scale of Fig. 1(b) and therefore Fig. 1(c) shows a magnification of Fig. 1(b).

The net effect of the scattering dynamics on the expectation value of the spin depends on the spin operator as shown in Table 2. While the Foldy-Wouthuysen, the Chakrabarti, the Pryce, and the Frenkel spin operators predict a small change of the spin's expectation value as a net effect of the step potential, the Pauli and the Czachor spin operators predict that the spin expectation value after interaction with the barrier is the same as before.

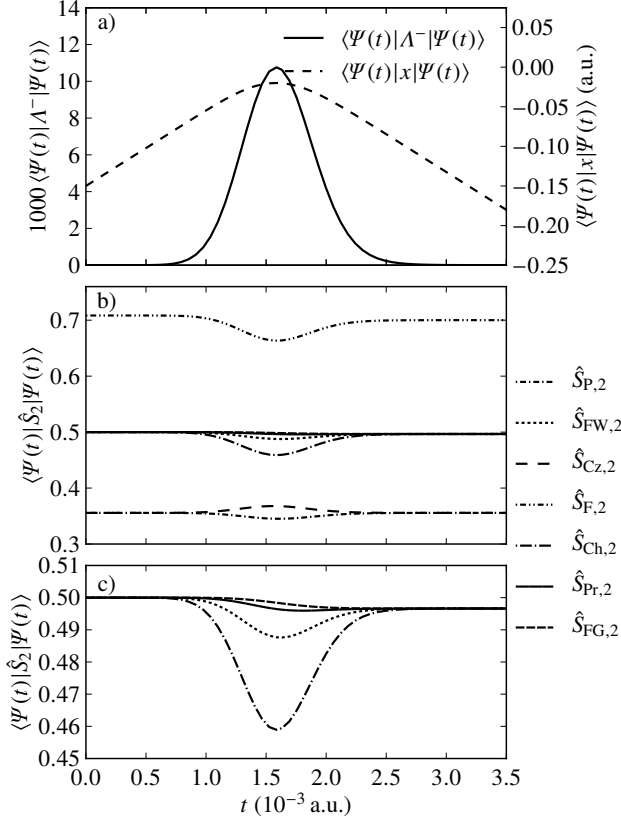


FIG. 1: Relativistic spin dynamics in scattering at a step potential (80). Sub-figure (a) shows the occupation probability $\langle \Psi | \Lambda^- | \Psi \rangle$ of negative-energy free-particles and the x -coordinate of the center of mass $\langle \Psi | x | \Psi \rangle$. Sub-figure (b) presents the expectation values of various spin operators as a function of time t and sub-figure (c) shows a magnification of sub-figure (b). All results given in atomic units, particle's mass equals $m_0 = 1$ a.u.

TABLE 2: Initial and final spin expectation values for the scattering dynamics in Fig. 1. In contrast to other operators, the Pauli and the Czachor spin operators predict that the spin expectation value after interaction with the barrier is the same as before.

Operator	$\langle \psi_\uparrow \hat{S}_i \psi_\uparrow \rangle$ at $t = 0$ a.u.	$\langle \psi_\uparrow \hat{S}_i \psi_\uparrow \rangle$ at $t = 0.0035$ a.u.
\hat{S}_P	0.3556	0.3556
\hat{S}_{FW}	0.5000	0.4966
\hat{S}_{Cz}	0.3556	0.3556
\hat{S}_F	0.7084	0.7001
\hat{S}_{Ch}	0.5000	0.4966
\hat{S}_{Pr}	0.5000	0.4966
\hat{S}_{FG}	0.5000	0.4966

4.2. Spin dynamics in standing laser fields

A similar distinction among the spin operators can be observed in a rather different scattering dynamics of an electron in a standing wave formed by two monochromatic laser fields. In contrast to the prior example in Sec. 4.1, the electron has sharp

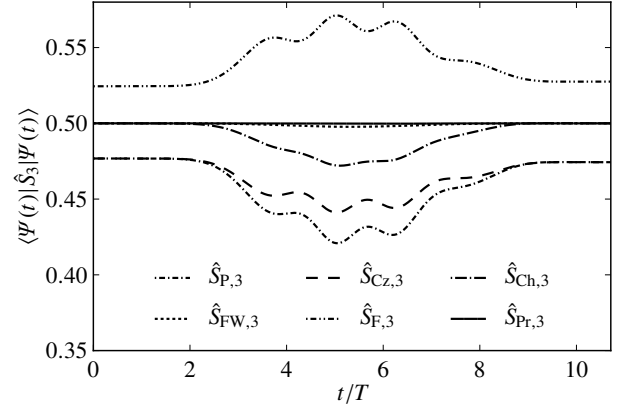


FIG. 2: Spin expectation values for Kapitza-Dirac scattering in a standing laser field as a function of time (in units of the laser period T) for parameters given in the text.

momentum and is therefore spatially delocalized and also the interaction region is infinitely extended. Such a dynamic can lead to the so-called Kapitza-Dirac effect [28, 69, 70].

The system is described by the Dirac equation (1), where the effect of the time-averaged laser field can be modeled by the ponderomotive potential [71]

$$q\phi(\mathbf{r}, t) = V_0 \cos^2(\mathbf{k} \cdot \mathbf{r})w(t). \quad (82)$$

Here V_0 is the potential amplitude, \mathbf{k} is the laser's wave vector, and $w(t)$ denotes the temporal envelope of the standing light wave. As a consequence of the infinite extension of the periodic laser field, only discrete subsets of momenta are coupled. This allows us to expand the quantum wave function in a basis of Foldy-Wouthuysen spin operator eigenfunctions

$$\begin{aligned} \psi(\mathbf{r}, t) = \sum_n & \left(c_n^{+\chi_\uparrow}(t) \mathbf{u}_{\chi_\uparrow, \mathbf{p}} + c_n^{+\chi_\downarrow}(t) \mathbf{u}_{\chi_\downarrow, \mathbf{p}} \right. \\ & \left. + c_n^{-\chi_\uparrow}(t) \mathbf{v}_{\chi_\uparrow, \mathbf{p}} + c_n^{-\chi_\downarrow}(t) \mathbf{v}_{\chi_\downarrow, \mathbf{p}} \right) e^{i(\mathbf{p} + n\mathbf{k}) \cdot \mathbf{r}}. \quad (83) \end{aligned}$$

Inserting this ansatz into the time-dependent Dirac equation, we find a coupled set of ordinary differential equations for the amplitudes of each mode. These differential equations are solved numerically with the initial condition that all amplitudes are zero except $c_0^{+\chi_\uparrow}(0) = 1$. (See [70] for technical details.)

In Fig. 2 we give a specific realization of a spin dynamics in a standing laser field, where the corresponding electric field vector points in the z direction, $V_0 = 0.88m_0c^2$, and the wave vector points in the x direction, $\mathbf{k} = (0.5, 0, 0)^T m_0c$. The temporal envelope function was given by $w(t) = \sin^2(\pi t/t_{\text{end}})$ with $0 < t < t_{\text{end}} = 10.7T$ and T denoting the laser period. The electron's initial momentum is $\mathbf{p} = (-0.3169, 0, 0.1)^T m_0c$ and the spin is initially oriented in the z direction, i. e., $\chi_\uparrow = (1, 0)^T$. When the full time dependence of the laser field is taken into account (instead of just the ponderomotive model potential (82)) these parameters lead to the relativistic three-photon Kapitza-Dirac effect as investigated in [28].

In close analogy to the dynamics in Sec. 4.1 we find again three different values for the expectation value of the initial spin for time $t = 0$ (where the ponderomotive potential (82) is

zero) depending on the choice of the spin operator (see Fig. 2). The deviation from $1/2$ is smaller than in Fig. 1 due to the less relativistic electron momentum here. For times where the ponderomotive potential (82) is nonzero we observe a time evolution of the spin expectation values qualitatively similar to that in Fig. 1. During the interaction with the laser field these values vary in an oscillatory fashion over time and all differ significantly from each other except those associated with the Foldy-Wouthuysen and the Pryce operators, which remain almost constant over time. Again the discrepancy in the expectation values can be traced back to significant transient excitations of negative-energy free-particle states as represented by the amplitudes $c_n^{-X\uparrow}(t)$ and $c_n^{-X\downarrow}(t)$.

5. Relativistic spin of the electron in the hydrogenic bound states

5.1. Hydrogenic bound states

In this section we are going to investigate the spin of hydrogenic bound states for a highly charged ion at rest with respect to different definitions of the relativistic spin operator. The degenerate bound states of the Dirac Hamiltonian for the Coulomb potential $q\phi(\mathbf{r}, t) = -Z/|\mathbf{r}|$ with atomic number Z ,

$$\hat{H}_C = \hat{H}_0 - \frac{Z}{|\mathbf{r}|} \quad (84)$$

are commonly expressed as simultaneous eigenstates $\psi_{n,\kappa,j,m}$ of \hat{H}_C , $\hat{\mathbf{J}}^2$, \hat{J}_3 , and the so-called spin-orbit operator $\hat{K} = \beta\{\hat{\Sigma} \cdot [\mathbf{r} \times (-i\nabla) + 1]\}$ fulfilling the eigenequations [72, 73]

$$\hat{H}_C \psi_{n,\kappa,j,m} = \mathcal{E}(n, \kappa) \psi_{n,\kappa,j,m}, \quad n = 1, 2, \dots, \quad (85a)$$

$$\hat{K} \psi_{n,\kappa,j,m} = \kappa \psi_{n,\kappa,j,m}, \quad |\kappa| = 1, 2, \dots, n, \kappa \neq -n, \quad (85b)$$

$$\hat{\mathbf{J}}^2 \psi_{n,\kappa,j,m} = j(j+1) \psi_{n,\kappa,j,m}, \quad j = |\kappa| - \frac{1}{2}, \quad (85c)$$

$$\hat{J}_3 \psi_{n,\kappa,j,m} = m \psi_{n,\kappa,j,m}, \quad m = -j, (j-1), \dots, j. \quad (85d)$$

The eigenenergies $\mathcal{E}(n, \kappa)$ are given with α_{el} denoting the fine-structure constant by

$$\mathcal{E}(n, \kappa) = m_0 c^2 \left[1 + \left(\frac{\alpha_{\text{el}}^2 Z^2}{n-|\kappa| + \sqrt{k^2 - \alpha_{\text{el}}^2 Z^2}} \right)^2 \right]^{-1/2}. \quad (86)$$

Each eigenfunction $\psi_{n,\kappa,j,m}$ belongs to one of two manifolds: For $\kappa = j + 1/2 \in \{1, 2, \dots, n\}$,

$$\psi_{n,\kappa,j,m}(r, \theta, \phi) = \begin{pmatrix} g_{n,\kappa,j}(r) \sqrt{\frac{j+m}{2j}} Y_{j-1/2, m-1/2}(\theta, \phi) \\ g_{n,\kappa,j}(r) \sqrt{\frac{j-m}{2j}} Y_{j-1/2, m+1/2}(\theta, \phi) \\ -f_{n,\kappa,j}(r) i \sqrt{\frac{j-m+1}{2j+2}} Y_{j+1/2, m-1/2}(\theta, \phi) \\ f_{n,\kappa,j}(r) i \sqrt{\frac{j+m+1/2}{2j+2}} Y_{j+1/2, m+1/2}(\theta, \phi) \end{pmatrix} \quad (87a)$$

and for $\kappa = -j - 1/2 \in \{-1, -2, \dots, -(n-1)\}$,

$$\psi_{n,\kappa,j,m}(r, \theta, \phi) = \begin{pmatrix} -g_{n,\kappa,j}(r) \sqrt{\frac{j-m+1}{2j+2}} Y_{j+1/2, m-1/2}(\theta, \phi) \\ g_{n,\kappa,j}(r) \sqrt{\frac{j+m+1}{2j+2}} Y_{j+1/2, m+1/2}(\theta, \phi) \\ f_{n,\kappa,j}(r) i \sqrt{\frac{j+m}{2j}} Y_{j-1/2, m-1/2}(\theta, \phi) \\ f_{n,\kappa,j}(r) i \sqrt{\frac{j-m}{2j}} Y_{j-1/2, m+1/2}(\theta, \phi) \end{pmatrix}. \quad (87b)$$

The radial functions $g_{n,\kappa,j}(r)$ and $f_{n,\kappa,j}(r)$ can be expressed in terms of confluent hypergeometric functions [74, 75] and $Y_{l,m}(\theta, \phi)$ denote the complex-valued orthonormal spherical harmonics as defined in [76].

Explicitly, the degenerate hydrogenic ground state is [75]

$$\psi_{1,1,\frac{1}{2},\frac{1}{2}}(r, \theta, \phi) = \mathcal{N} \psi(r) \begin{pmatrix} Y_{0,0}(\theta, \phi) \\ 0 \\ i \frac{1-\gamma}{Z\alpha_{\text{el}}} \sqrt{\frac{1}{3}} Y_{1,0}(\theta, \phi) \\ -i \frac{1-\gamma}{Z\alpha_{\text{el}}} \sqrt{\frac{2}{3}} Y_{1,1}(\theta, \phi) \end{pmatrix} \quad (88a)$$

$$\psi_{1,1,\frac{1}{2},-\frac{1}{2}}(r, \theta, \phi) = \mathcal{N} \psi(r) \begin{pmatrix} 0 \\ Y_{0,0}(\theta, \phi) \\ i \frac{1-\gamma}{Z\alpha_{\text{el}}} \sqrt{\frac{2}{3}} Y_{1,-1}(\theta, \phi) \\ -i \frac{1-\gamma}{Z\alpha_{\text{el}}} \sqrt{\frac{1}{3}} Y_{1,0}(\theta, \phi) \end{pmatrix} \quad (88b)$$

with $\gamma = \sqrt{1 - Z^2 \alpha_{\text{el}}^2}$, the radial function

$$\psi(r) = \frac{e^{-m_0 Z r}}{(2m_0 Z r)^{1-\gamma}}, \quad (89)$$

the normalizing factor

$$\mathcal{N} = (2m_0 Z)^{3/2} \sqrt{\frac{1+\gamma}{2\tilde{\Delta}(1+2\gamma)}}, \quad (90)$$

and the electron rest mass m_0 . In momentum space, the degenerate bound states (88) may be expressed as [77]

$$\tilde{\psi}_{1,1,\frac{1}{2},\frac{1}{2}}(p, \theta', \phi') = \mathcal{N} \begin{pmatrix} \mathcal{J}_0(m_0 Z, \gamma, p) Y_{0,0}(\theta', \phi') \\ 0 \\ \frac{1-\gamma}{Z\alpha} \mathcal{J}_1(m_0 Z, \gamma, p) \sqrt{\frac{1}{3}} Y_{1,0}(\theta', \phi') \\ -\frac{1-\gamma}{Z\alpha} \mathcal{J}_1(m_0 Z, \gamma, p) \sqrt{\frac{2}{3}} Y_{1,1}(\theta', \phi') \end{pmatrix} \quad (91a)$$

$$\tilde{\psi}_{1,1,\frac{1}{2},-\frac{1}{2}}(p, \theta', \phi') = \mathcal{N} \begin{pmatrix} 0 \\ \mathcal{J}_0(m_0 Z, \gamma, p) Y_{0,0}(\theta', \phi') \\ \frac{1-\gamma}{Z\alpha} \mathcal{J}_1(m_0 Z, \gamma, p) \sqrt{\frac{2}{3}} Y_{1,-1}(\theta', \phi') \\ -\frac{1-\gamma}{Z\alpha} \mathcal{J}_1(m_0 Z, \gamma, p) \sqrt{\frac{1}{3}} Y_{1,0}(\theta', \phi') \end{pmatrix} \quad (91b)$$

by using the functions $\mathcal{J}_0(z, \gamma, p)$ and $\mathcal{J}_1(z, \gamma, p)$ as defined in (A.6) and (A.7), respectively.

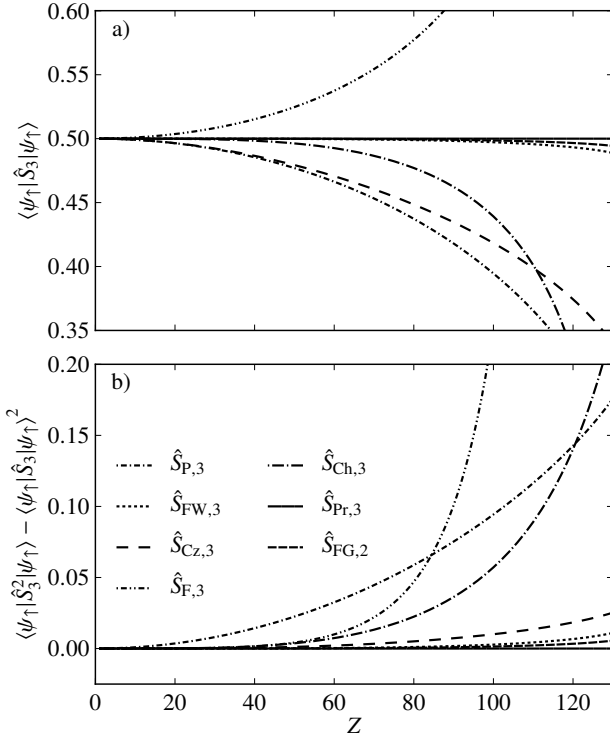


FIG. 3: (a) Spin expectation values, adopted from [78]) and (b) spin variance of various relativistic spin operators for the hydrogenic ground state (88a) as a function of the atomic number Z . For the ground state (88b) we find the same spin variance and the same spin expectation values but with opposite sign (not displayed in the plots).

5.2. Spin expectation values and spin variance

In momentum space representation, the relativistic spin operators introduced in Sec. 3 are simple matrices, thus, with the momentum space representation (91) spin expectation values as well as the spin variance of the degenerate hydrogenic ground states can be calculated. For simplicity, we calculate spin expectation values in the z direction, that is, $\mathbf{n} = (0, 0, 1)^T$, for the remainder of this section. The spin expectation values $\langle \psi_\uparrow | \hat{S}_3 | \psi_\uparrow \rangle$ and the spin variance $\langle \psi_\uparrow | \hat{S}_3^2 | \psi_\uparrow \rangle - \langle \psi_\uparrow | \hat{S}_3 | \psi_\uparrow \rangle^2$ are displayed in Fig. 3(a) for the state $\psi_\uparrow = \psi_{1,1,\frac{1}{2},\frac{1}{2}}$ as a function of the atomic number Z . In general, the spin expectation values and the spin variance are complicated functions of the nuclear charge Z . For the Pauli and the Pryce spin operators, however, the spin expectation values and the spin variance are given explicitly by

$$\langle \psi_\uparrow | \hat{S}_{P,3} | \psi_\uparrow \rangle = \frac{1}{6} \left(1 + 2 \sqrt{1 - Z^2 \alpha_{\text{el}}^2} \right), \quad (92a)$$

$$\langle \psi_\uparrow | \hat{S}_{P,3}^2 | \psi_\uparrow \rangle - \langle \psi_\uparrow | \hat{S}_{P,3} | \psi_\uparrow \rangle^2 = \frac{1}{4} - \left(\frac{1}{6} \left(1 + 2 \sqrt{1 - Z^2 \alpha_{\text{el}}^2} \right) \right)^2 \quad (92b)$$

and

$$\langle \psi_\uparrow | \hat{S}_{Pr,3} | \psi_\uparrow \rangle = \frac{1}{2}, \quad (93a)$$

$$\langle \psi_\uparrow | \hat{S}_{Pr,3}^2 | \psi_\uparrow \rangle - \langle \psi_\uparrow | \hat{S}_{Pr,3} | \psi_\uparrow \rangle^2 = 0, \quad (93b)$$

respectively.

For small atomic numbers ($Z \lesssim 20$), all spin operators yield about $1/2$; for larger Z when relativistic effects set in, however, expectation values differ significantly from each other. While for Pauli, Fouldy-Wouthuysen, Czachor, Chakrabarti, and Fradkin-Good spin operators the spin expectation value is reduced, the expectation value of the Frenkel spin operator exceeds $1/2$. Only for the Pryce operator do we find that the spin expectation values is $1/2$ for all values of Z , implying zero spin variance as shown in Fig. 3(b). Spin expectation values and spin variances for the state $\psi_\downarrow = \psi_{1,1,\frac{1}{2},-\frac{1}{2}}$ follow by symmetry via

$$\langle \psi_\uparrow | \hat{S}_3 | \psi_\uparrow \rangle = - \langle \psi_\downarrow | \hat{S}_3 | \psi_\downarrow \rangle \quad (94)$$

and

$$\langle \psi_\uparrow | \hat{S}_3^2 | \psi_\uparrow \rangle - \langle \psi_\uparrow | \hat{S}_3 | \psi_\uparrow \rangle^2 = \langle \psi_\downarrow | \hat{S}_3^2 | \psi_\downarrow \rangle - \langle \psi_\downarrow | \hat{S}_3 | \psi_\downarrow \rangle^2. \quad (95)$$

The different predictions for spin expectation values and spin variances that follow from different definitions of the relativistic spin operator may serve as a basis for an experimental test for a relativistic spin operator [78] that is implemented by a particular spin measurement experiment. We assume that the electron of a highly charged hydrogenlike ion was prepared in its ground state ψ_\uparrow , e. g., by exposing the ion to a strong magnetic field in the z direction and turning it off adiabatically. A spin measurement experiment for such a state will yield spin $1/2$ with probability $P_\uparrow = 1/2 + \langle \psi_\uparrow | \hat{S}_3 | \psi_\uparrow \rangle$ where \hat{S}_3 is the spin operator that is realized by the particular measurement procedure. For hydrogenlike uranium, $Z = 92$, our theoretical predictions yield, for example, for the Pauli operator $P_\uparrow = 91.4\%$, for the Fouldy-Wouthuysen operator $P_\uparrow = 99.8\%$, and $P_\uparrow = 100\%$ in the case of the Pryce operator. Note that it is a completely open question how experimental procedures that aim to measure the electron spin state map to mathematical spin operators.

5.3. Pryce spin operator in systems with spherical symmetry

We demonstrated that only the Pryce spin operator yields spin expectation values of $\pm 1/2$ for the ground states of hydrogenlike ions. In the following we will show that this is a consequence of the spherical symmetry of the Coulomb potential and that each system with spherical symmetry has some energy eigenstates that are eigenstates of the Pryce spin operator, too. One can show [74, 75] that every bound eigenstate of any system with spherically symmetric potential $\phi(\mathbf{r}|)$,

$$\hat{H}_s = \hat{H}_0 + q\phi(\mathbf{r}|), \quad (96)$$

has the form (87a) or (87b), respectively. Only the radial functions $g_{n,\kappa,j}(r)$ and $f_{n,\kappa,j}(r)$ depend on the specific potential. Consequently, the momentum space representations of (87) have for $\kappa = j + 1/2$ the form

$$\tilde{\psi}_{n,\kappa,j,m}(p, \theta', \phi') = \begin{pmatrix} \tilde{g}_{n,\kappa,j}(p) \sqrt{\frac{j+m}{2j}} Y_{j-1/2,m-1/2}(\theta', \phi') \\ \tilde{g}_{n,\kappa,j}(p) \sqrt{\frac{j-m}{2j}} Y_{j-1/2,m+1/2}(\theta', \phi') \\ -\tilde{f}_{n,\kappa,j}(p) i \sqrt{\frac{j-m+1}{2j+2}} Y_{j+1/2,m-1/2}(\theta', \phi') \\ \tilde{f}_{n,\kappa,j}(p) i \sqrt{\frac{j+m+1/2}{2j+2}} Y_{j+1/2,m+1/2}(\theta', \phi') \end{pmatrix} \quad (97a)$$

and for $\kappa = -j - 1/2$

$$\tilde{\psi}_{n,\kappa,j,m}(p, \theta', \phi') = \begin{pmatrix} -\tilde{g}_{n,\kappa,j}(p) \sqrt{\frac{j-m+1}{2j+2}} Y_{j+1/2,m-1/2}(\theta', \phi') \\ \tilde{g}_{n,\kappa,j}(p) \sqrt{\frac{j+m+1}{2j+2}} Y_{j+1/2,m+1/2}(\theta', \phi') \\ \tilde{f}_{n,\kappa,j}(p) i \sqrt{\frac{j+m}{2j}} Y_{j-1/2,m-1/2}(\theta', \phi') \\ \tilde{f}_{n,\kappa,j}(p) i \sqrt{\frac{j-m}{2j}} Y_{j-1/2,m+1/2}(\theta', \phi') \end{pmatrix}, \quad (97b)$$

respectively, with

$$\tilde{g}_{n,\kappa,j}(p) = \sqrt{\frac{2}{\pi}} (-i)^{j-1/2} \int_0^\infty g_{n,\kappa,j}(r) j_{j-1/2}(rp) r^2 dr, \quad (98a)$$

$$\tilde{f}_{n,\kappa,j}(p) = \sqrt{\frac{2}{\pi}} (-i)^{j+1/2} \int_0^\infty f_{n,\kappa,j}(r) j_{j+1/2}(rp) r^2 dr \quad (98b)$$

for (97a) and

$$\tilde{g}_{n,\kappa,j}(p) = \sqrt{\frac{2}{\pi}} (-i)^{j+1/2} \int_0^\infty g_{n,\kappa,j}(r) j_{j+1/2}(rp) r^2 dr, \quad (98c)$$

$$\tilde{f}_{n,\kappa,j}(p) = \sqrt{\frac{2}{\pi}} (-i)^{j-1/2} \int_0^\infty f_{n,\kappa,j}(r) j_{j-1/2}(rp) r^2 dr \quad (98d)$$

for (97b) (see also the appendix). The momentum space representation of the Pryce spin operator in the z direction is

$$\hat{S}_{\text{Pr},3} = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} + \cos^2(\theta') & \cos(\theta') \sin(\theta') e^{-i\phi'} \\ 0 & 0 & \cos(\theta') \sin(\theta') e^{i\phi'} & \frac{1}{2} - \cos^2(\theta') \end{pmatrix}. \quad (99)$$

With this result one can show that

$$\hat{S}_{\text{Pr},3} \psi_{n,\kappa,j,j} = +\frac{1}{2} \psi_{n,\kappa,j,j}, \quad (100a)$$

$$\hat{S}_{\text{Pr},3} \psi_{n,\kappa,j,-j} = -\frac{1}{2} \psi_{n,\kappa,j,-j} \quad (100b)$$

by employing (97a) and (99) and expressing the spherical harmonics in terms of trigonometric functions. Thus, eigenstates of central potentials with extremal quantum number $m = \pm j$ are eigenstates of the Pryce spin operator with eigenvalue $\pm 1/2$.

This has an interesting consequence for the spin of superpositions of states with $m = \pm j$ as, for example, $\Psi(\mathbf{r}, t) = c_1 \psi_1(\mathbf{r}, t) + c_2 \psi_2(\mathbf{r}, t)$ with $\psi_i(\mathbf{r}, t) = \psi_{n,j_i+1/2,j_i,j_i}(\mathbf{r}) e^{-\mathcal{E}(n,j_i+1/2)t}$. The spin expectation value of this state is given by

$$\langle \Psi | \hat{S}_3 | \Psi \rangle = |c_1|^2 \langle \psi_1 | \hat{S}_3 | \psi_1 \rangle + |c_2|^2 \langle \psi_2 | \hat{S}_3 | \psi_2 \rangle + 2 \text{Re} \langle c_1 \psi_1 | \hat{S}_3 | c_2 \psi_2 \rangle. \quad (101)$$

As the states ψ_1 and ψ_2 have different energies the mixing term $\langle c_1 \psi_1 | \hat{S}_3 | c_2 \psi_2 \rangle$ and therefore the spin expectation value oscillates in time with the frequency $|\mathcal{E}(n, j_1 + 1/2) - \mathcal{E}(n, j_2 + 1/2)|$ unless $\psi_1(\mathbf{r}, t)$ and $\psi_2(\mathbf{r}, t)$ are eigenfunctions of the spin operator \hat{S}_3 , as is the case for the Pryce spin operator. The $|\mathcal{E}(n, j_1 + 1/2) - \mathcal{E}(n, j_2 + 1/2)|$ varies over several orders of magnitude depending on the parameters n, j_1, j_2 , and Z and can be made small by increasing the quantum number n .

The Pryce spin operator allows us to establish a notable correspondence between the relativistic Dirac theory and the nonrelativistic Pauli theory of systems with spherical symmetry. In the nonrelativistic case, the Pauli Hamiltonian for some spherically symmetric potential $\phi(|\mathbf{r}|)$ and the operator of total angular momentum are defined as

$$\hat{H}_{s,\text{nr}} = \frac{\hat{\mathbf{p}}^2}{2m_0} + q\phi(|\mathbf{r}|) \quad (102)$$

and $\hat{\mathbf{J}}_{\text{nr}} = \mathbf{r} \times \hat{\mathbf{p}} + \boldsymbol{\sigma}/2$, respectively. The second term in the nonrelativistic total angular momentum equals the nonrelativistic Pauli spin operator

$$\hat{S}_{\text{P,nr}} = \frac{1}{2} \boldsymbol{\sigma}. \quad (103)$$

In analogy to the Dirac theory, the two-component eigenfunctions of the Pauli Hamiltonian (102) can be expressed as simultaneous eigenstates $\psi_{n,\kappa,j,m}^{\text{nr}}$ of $\hat{H}_{s,\text{nr}}$, $\hat{\mathbf{J}}_{\text{nr}}^2$, $\hat{J}_{\text{nr},3}$, and the nonrelativistic spin-orbit operator $\hat{K}_{\text{nr}} = \boldsymbol{\sigma} \cdot [\mathbf{r} \times (-i\nabla) + \mathbb{I}_2]$ fulfilling the eigenequations [72, 73]

$$\hat{H}_{s,\text{nr}} \psi_{n,\kappa,j,m}^{\text{nr}} = \mathcal{E}_{\text{nr}}(n) \psi_{n,\kappa,j,m}^{\text{nr}}, \quad n = 1, 2, \dots, \quad (104a)$$

$$\hat{K}_{\text{nr}} \psi_{n,\kappa,j,m}^{\text{nr}} = \kappa \psi_{n,\kappa,j,m}^{\text{nr}}, \quad |\kappa| = 1, 2, \dots, n, \kappa \neq -n, \quad (104b)$$

$$\hat{\mathbf{J}}_{\text{nr}}^2 \psi_{n,\kappa,j,m}^{\text{nr}} = j(j+1) \psi_{n,\kappa,j,m}^{\text{nr}}, \quad j = |\kappa| - \frac{1}{2}, \quad (104c)$$

$$\hat{J}_{\text{nr},3} \psi_{n,\kappa,j,m}^{\text{nr}} = m \psi_{n,\kappa,j,m}^{\text{nr}}, \quad m = -j, (j-1), \dots, j, \quad (104d)$$

where $\mathcal{E}_{\text{nr}}(n)$ denotes the eigenenergies. The $\psi_{n,\kappa,j,m}^{\text{nr}}$ are in general not eigenfunctions of $\hat{S}_{\text{P,nr}}$. One can show [72], however, that

$$\hat{S}_{\text{P,nr},3} \psi_{n,\kappa,j,j}^{\text{nr}} = +\frac{1}{2} \psi_{n,\kappa,j,j}^{\text{nr}}, \quad (105a)$$

$$\hat{S}_{\text{P,nr},3} \psi_{n,\kappa,j,-j}^{\text{nr}} = -\frac{1}{2} \psi_{n,\kappa,j,-j}^{\text{nr}} \quad (105b)$$

hold. A comparison of (100) and (105) shows that the nonrelativistic Pauli spin operator $\hat{S}_{\text{P,nr}}$ and the relativistic Pryce spin operator \hat{S}_{Pr} play an analogous role within the theories they belong to.

6. Discussion and conclusions

We have reconsidered the electron's spin degree of freedom within relativistic quantum mechanics. The motivation of our investigation was the observation that there is no universally accepted spin operator in the Dirac theory. In fact, several relativistic spin operators have been proposed in the literature. We investigated the properties of some popular proposed spin operators and analyzed how the different spin operators can lead to different theoretical predictions for expectation values of the spin in different physical setups.

The two pairs given by the Pauli and the Czachor spins and by the Foldy-Wouthuysen and the Chakrabarti spins, respectively, act as identical operators in each of two the subspaces of free-particle states with positive and negative energy. On the basis of the spin operators' mathematical properties, the Foldy-Wouthuysen and the Pryce spin operators seem to be the most promising candidates for a proper relativistic spin operator. Both operators commute with the free Dirac Hamiltonian as well as with the total angular momentum operator and the linear momentum operator. Furthermore, they obey the angular momentum algebra and have eigenvalues $\pm 1/2$. The Foldy-Wouthuysen and the Pryce spin operators are equivalent on the subspace of wave functions that are superpositions of free-particle eigenstates with positive energy. However, we demonstrated in three different physical setups that if interaction potentials are present one can distinguish between both operators because they may lead to different expectation values for the same quantum state. The three setups reveal a rather consistent behavior.

The various proposed spin operators are usually motivated by abstract theoretical considerations rather than experimental evidence. The fact that these spin operators yield different pre-

dictions about the expectation value of the spin in several setups as, for example, for electrons in scattering at a step potential, electrons in standing laser fields, or hydrogenic eigenstates as considered here, offers the opportunity to discriminate between the various proposed spin operators. In this way one may rule out some operators for which the theoretical predictions are incompatible with experimental results. The identification of the correct relativistic spin operator would immediately induce relativistic operators for the orbital angular momentum and the position. Thus, the identification of the right description of the spin within the Dirac theory has broad implications beyond the spin itself.

We provided precise predictions about what could be measured if a spin measurement procedure implements a physical realization of a particular spin operator. However, we did not dwell on how to measure the spin. In fact, experiments that measure the spin (and not mere spin effects) are challenging from a technological point of view as well as conceptually even today. As pointed out earlier, it is a completely open question how experimental measuring procedures map to mathematical spin operators. See [2] for an in-depth discussion. There is an ongoing effort to advance spin measurement techniques. A Stern-Gerlach experiment for electrons may be feasible [79–81]. The spin may be measured indirectly via transferring it to orbital angular momentum [82].

Acknowledgments

We enjoyed several helpful discussions with C. C. Gerry, K. Z. Hatsagortsyan, S. Meuren, C. Müller, O. Skoromnik, Q. Su, and E. Yakaboylu. R. G. acknowledges the kind hospitality of the Max Planck Institute for Nuclear Physics in Heidelberg. This work was supported by the NSF.

A. Fourier transform in spherical coordinates

Using the vectors \mathbf{r} and \mathbf{p} and their representation in spherical coordinates $\mathbf{r} = (r \sin \theta \cos \phi, r \sin \theta \sin \phi, r \cos \theta)^\top$ and $\mathbf{p} = (p \sin \theta' \cos \phi', p \sin \theta' \sin \phi', p \cos \theta')^\top$ the (inverse) Fourier transform of some function $f(\mathbf{r})$ is defined as

$$\begin{aligned} \mathcal{F}^\pm[f(\mathbf{r})] &= \frac{1}{(2\pi)^{3/2}} \int f(\mathbf{r}) \exp(\pm i \mathbf{r} \cdot \mathbf{p}) d^3 r \\ &= \frac{1}{(2\pi)^{3/2}} \int_0^\infty \int_0^\pi \int_0^{2\pi} f(r, \theta, \phi) \exp(\pm i r p (\sin \theta \sin \theta' \cos(\phi - \phi') + \cos \theta \cos \theta')) r^2 \sin \theta d\phi d\theta dr. \end{aligned} \quad (\text{A.1})$$

For functions not depending on the azimuthal angle $f(r, \theta, \phi) = f(r, \theta)$ the (inverse) Fourier transform simplifies to

$$\mathcal{F}^\pm[f(\mathbf{r})] = \frac{1}{\sqrt{2\pi}} \int_0^\infty \int_0^\pi f(r, \theta) J_0(rp \sin \theta \sin \theta') \exp(\pm i r p \cos \theta \cos \theta') r^2 \sin \theta d\theta dr \quad (\text{A.2})$$

with $J_0(x)$ denoting the zeroth-order Bessel function of the first kind. For spherically symmetric functions $f(r, \theta, \phi) = f(r)$ we finally get

$$\mathcal{F}^\pm[f(\mathbf{r})] = \sqrt{\frac{2}{\pi}} \int_0^\infty f(r) r^2 j_0(rp) dr. \quad (\text{A.3})$$

Note that for spherically symmetric functions the Fourier transform and its inverse have the same form.

If the radial and angular dependences separate, e. g., $f(r, \theta, \phi) = R(r)Y_{l,m}(\theta, \phi)$ with $Y_{l,m}(\theta, \phi)$ denoting the complex-valued orthonormal spherical harmonics, it is beneficial to utilize the generalized Jacobi-Anger identities

$$\frac{1}{(2\pi)^{3/2}} \exp(\pm i \mathbf{r} \cdot \mathbf{p}) = \sqrt{\frac{2}{\pi}} \sum_{l=0}^{\infty} (\pm i)^l j_l(rp) \sum_{m=-l}^l Y_{l,m}(\theta, \phi) Y_{l,m}^*(\theta', \phi') = \sqrt{\frac{2}{\pi}} \sum_{l=0}^{\infty} (\pm i)^l j_l(rp) \sum_{m=-l}^l Y_{l,m}^*(\theta, \phi) Y_{l,m}(\theta', \phi') \quad (\text{A.4})$$

with the spherical Bessel functions of the first kind $j_l(x)$ as defined in [76]. By using (A.4) and the orthonormalization of the spherical harmonics, we find

$$\mathcal{F}^{\pm}[R(r)Y_{l,m}(\theta, \phi)] = (\pm i)^l Y_{l,m}(\theta', \phi') \sqrt{\frac{2}{\pi}} \int_0^{\infty} R(r) j_l(rp) r^2 dr. \quad (\text{A.5})$$

Specifying $R(r)$ as $R(r) = e^{-\gamma r}/(2\gamma r)^{1-\gamma}$, we may define the two functions $\mathcal{J}_0(z, \gamma, p)$ and $\mathcal{J}_1(z, \gamma, p)$ as

$$\mathcal{J}_0(z, \gamma, p) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} \frac{e^{-\gamma r}}{(2\gamma r)^{1-\gamma}} r^2 j_0(rp) dr = \sqrt{\frac{2}{\pi}} \frac{2^{\gamma-1} \check{\Delta}(\gamma+1)}{z^2 p (1 + p^2/z^2)^{(\gamma+1)/2}} \sin((1+\gamma) \arctan(p/z)), \quad (\text{A.6})$$

$$\begin{aligned} \mathcal{J}_1(z, \gamma, p) &= \sqrt{\frac{2}{\pi}} \int_0^{\infty} \frac{e^{-\gamma r}}{(2\gamma r)^{1-\gamma}} r^2 j_1(rp) dr \\ &= \sqrt{\frac{2}{\pi}} \frac{2^{\gamma-1} \check{\Delta}(\gamma)}{z^2 p (1 + p^2/z^2)^{(\gamma+1)/2}} \left(-(1+\gamma) \cos((1+\gamma) \arctan(p/z)) + \frac{z}{p} \sin((1+\gamma) \arctan(p/z)) \right) \end{aligned} \quad (\text{A.7})$$

for $0 < \gamma < 1$. The Eqs. (A.6) and (A.7) are two special cases of a more general formula that may be useful in investigating excited states of the hydrogen atom (see Eq. (32.7) in [83]).

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