Position and spin in relativistic quantum mechanics

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The problem of the position and spin in relativistic quantum mechanics is analyzed in detail. It is definitively shown that the position and spin operators in the Foldy-Wouthuysen representation (but not in the Dirac one) are quantum-mechanical counterparts of the classical position and spin variables. The probabilistic interpretation is valid only for Foldy-Wouthuysen wave functions. The relativistic spin operators are discussed. The spin-orbit interaction does not exist for a free particle if the conventional operators of the orbital angular momentum and the rest-frame spin are used. Alternative definitions of the orbital angular momentum and the spin are based on noncommutative geometry, do not satisfy standard commutation relations, and can allow the spin-orbit interaction.

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I. INTRODUCTION

The position operator is very important for relativistic quantum mechanics (QM). In nonrelativistic Schrödinger QM, this operator is equal to the radius vector $\boldsymbol{r}$. However, a transition to relativistic QM leads to a dependence of this operator on a representation. It has been shown by Pryce [1] that the form of the position operator for a spin-1/2 particle is nontrivial and some possible forms have been obtained. Newton and Wigner [2] have obtained the form of the position operator having commuting components and localized eigenfunctions in the manifold of positive-energy wave functions based on the Dirac representation. Foldy and Wouthuysen have shown [3] that this operator is equal to the radius vector operator in the Foldy-Wouthuysen (FW) representation.

The spin angular momentum (or the spin for short) takes one of central places in relativistic QM. The spin of a Dirac (spin-1/2) particle is defined by the 2×2 Pauli matrices σ_i $(i = 1, 2, 3)$ which generate together with the unit matrix an irreducible representation of the SU(2) group. The Pauli matrices are Hermitian, unitary, and traceless. The classical spin is connected with the three-dimensional rotation group SO(3). Algebraically, SU(2) is the double covering group of SO(3). This relation plays an important role in the theory of rotations of spinors in nonrelativistic QM. As a result, the spin dynamics defined by the Schrödinger-Pauli equation fully corresponds to the classical picture of rotation of the spin in external fields. When quadrupole and other multipole interactions are neglected, the spin dynamics of particles with higher spins $(s > 1/2)$ is very similar to that of a spin-1/2 particle. In particular, the angular velocity of spin rotation depends on the electric and magnetic dipole moments of a particle and does not explicitly depend on the spin quantum number s. The spin operator of a nonrelativistic spin-1/2 particle, $\boldsymbol{s} = \hbar\boldsymbol{\sigma}/2$, fully corresponds to the classical spin.

A clear correspondence between quantum-mechanical operators and classical variables is a distinguishing feature of nonrelativistic QM. This correspondence takes place for all main operators including position (coordinate), momentum, and angular momentum ones.

In contrast, the connection between the quantum-mechanical operators and classical variables in relativistic QM is not so simple. It is well known that the Dirac equation distorts the connection among the energy, momentum, and velocity operators. Nevertheless, the problem of operators of relativistic QM corresponding to basic classical variables has been definitively solved in the 1960s. Moreover, the correct and definite solution of this problem is already contained in the famous paper by Foldy and Wouthuysen [3]. It has been established that quantum-mechanical counterparts of the classical variables of the radius vector (position), momentum, angular momentum, and spin of a Dirac particle are the operators $\boldsymbol{x}$, $\boldsymbol{p}$, $\boldsymbol{L} = \boldsymbol{x}\times\boldsymbol{p}$, and $\boldsymbol{s} = \hbar\boldsymbol{\Sigma}/2$ defined in the *Foldy-Wouthuysen* (FW) representation. These conclusions agree with the results obtained by Pryce [1] and Newton and Wigner [2] and have been confirmed in a lot of publications.

Unfortunately, these achievements were not reflected in textbooks and currently many researchers hold the opposite view. After more than sixty years, the scientific literature is full of incorrect (explicit or implicit) statements that the position and angular momentum of a particle are defined by the operators $\boldsymbol{r}$ and $\boldsymbol{r}\times\boldsymbol{p}$ in the *Dirac* representation. Similarly, one often uses definitions of the spin operator different from the operator obtained in the fundamental works by Foldy and Wouthuysen [3] and Fradkin and Good [4]. Such definitions may lead to a spin-orbit interaction (SOI) for a free particle. This situation is very typical, in particular, in physics of

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twisted (vortex) electrons (see the reviews [5,6]). The description of the particle position by the *Dirac* radius vector is so common that the papers containing the right description [7,8] were followed by the Comments [9,10]. A short analysis of the problem has been given in Ref. [11]. In the present work, we reproduce known (but forgotten) arguments in favor of a definite connection between classical variables and corresponding operators which shows the special role of the FW representation. We also put forward some arguments given by a contemporary development of theory of the FW transformation. These arguments relate to a description of spinning particles *in external fields*. In the present study, we focus our attention on the spin while problems connected with the operators of the position and the angular momentum are also properly addressed.

The paper is organized as follows. In the next section, we explain main distinguishing features of the relativistic FW transformation. In Sec. III, we reproduce the past (but forgotten) approach to carrying out an unambiguous determination of basic operators for a free Dirac particle and the corresponding classical variables. This approach leads to the definitions of fundamental operators of the position and spin which were generally accepted sixty years ago but have been unreasonably revised lately. Important additional arguments based on the relativistic FW transformation in external fields are presented in Sec. IV. Section V describes the relativistic operators of the position and spin. The related problems of relativistic QM (a probabilistic interpretation of a wave function, spin-orbit interaction for a free particle and *Zitterbewegung*) are expounded in Sec. VI. The results are discussed and summarized in Sec. VII.

We use the system of units $\hbar = 1$, $c = 1$. We include $\hbar$ and c explicitly when this inclusion clarifies the problem. The square and curly brackets, $[\ldots,\ldots]$ and $\{\ldots,\ldots\}$, denote commutators and Poisson brackets, respectively. The standard denotations of Dirac matrices are applied (see, e.g., Ref. [59]). In particular, $\mathbf{\Sigma} \equiv \mathrm{diag}(\boldsymbol{\sigma}, \boldsymbol{\sigma})$, $\mathbf{\Pi} = \beta\mathbf{\Sigma}$.

II. RELATIVISTIC FOLDY-WOUTHUYSEN TRANSFORMATION

The connection between fundamental classical variables and the corresponding operators is studied in the framework of relativistic QM and the FW representation happens to be very useful. Therefore, a consideration of the relativistic FW transformation is instructive.

In this section, we focus our attention on such a transformation for a particle in external fields. However, a consideration of relativistic particles with different spins in external fields is not simple because of specific properties of initial equations. All these equations substantially differ from the Schrödinger equation of nonrelativistic QM. The Dirac equation in the Hamiltonian form corrupts the connection among energy, momentum, and velocity. The connection between the relativistic QM and Schrödinger QM is restored by the FW transformation [3]. In the FW representation, the relativistic QM takes the Schrödinger form. This fact has been first shown [3] for a nonrelativistic Dirac particle in electromagnetic fields and for a free relativistic Dirac particle.

The important development of QM in the FW representation has been made in Ref. [12] where the exact FW transformation operator has been derived and main properties of this operator have been determined. This operator is defined by

$$\Psi_{\mathrm{FW}} = U_{\mathrm{FW}}\Psi_D \equiv \exp\left(iS_{\mathrm{FW}}\right)\Psi_D, \tag{1}$$

where S_{FW} is the exponential FW transformation operator. The transformation is unitary ($U_{\mathrm{FW}}^{\dagger} = U_{\mathrm{FW}}^{-1}$). There is an infinite set of representations different from the FW representation whose distinctive feature is a block-diagonal form of the Hamiltonian. The FW transformation is *uniquely* defined by the condition that the exponential operator S_{FW} is *odd*,

$$\beta S_{\mathrm{FW}} = -S_{\mathrm{FW}}\beta, \tag{2}$$

and Hermitian [12,13]. This condition is equivalent to [12,13]

$$\beta U_{\mathrm{FW}} = U_{\mathrm{FW}}^{\dagger}\beta. \tag{3}$$

Eriksen [12] found the exact expression for the nonexponential FW transformation operator. It is convenient to present this expression in the form [14]

$$U_{\mathrm{FW}} = U_E = \frac{1+\beta\lambda}{\sqrt{2+\beta\lambda+\lambda\beta}}, \quad \lambda = \frac{\mathcal{H}}{(\mathcal{H}^2)^{1/2}}. \tag{4}$$

To unambiguously define the square root, these relations should be complemented by the condition that the square root of the unit matrix $\mathcal{I}$ is equal to the unit matrix [15]. The exact exponential FW transformation operator has been determined in Ref. [16]. The initial Hamiltonian operator $\mathcal{H}$ is arbitrary. It is easy to see that [12]

$$\lambda^2 = 1, \quad [\beta\lambda, \lambda\beta] = 0, \quad [\beta, (\beta\lambda+\lambda\beta)] = 0. \tag{5}$$

The equivalent form of the operator U_E [14] shows that it is properly unitary:

$$U_E = \frac{1+\beta\lambda}{\sqrt{(1+\beta\lambda)^{\dagger}(1+\beta\lambda)}}. \tag{6}$$

The additional substantiation of the Eriksen method was presented in Ref. [17].

However, Eq. (6) containing square roots of operators is not applicable for a derivation of relativistic expressions for FW Hamiltonians except for a few special cases [3,17,18]. Equation (6) can be used for a calculation of series of relativistic corrections to nonrelativistic FW Hamiltonians.

Many transformation methods allowing one to derive a block-diagonal Hamiltonian do not lead to the FW representation (see Refs. [12–14] for more details). Paradoxically, the original FW method [3] does not satisfy the Eriksen conditions and does not lead to the FW representation [13,19]. Any FW transformation method satisfying these conditions is correct. All FW Hamiltonians obtained by correct methods *coincide*. Methods which do not satisfy the Eriksen conditions can be corrected. For the original FW method [3], such corrections have been obtained in Refs. [13,16,19–21].

Contemporary QM requires relativistic methods giving compact relativistic FW Hamiltonians for any energy. The first such Hamiltonian has been derived by Blount [22]. At present, there are many different relativistic FW transformation methods (see Refs. [21,23–25] and references therein). In the present work, we use the results obtained

by the method proposed in Ref. [15] and then developed in Refs. [16,20,21,24,26]. The validity of this method has been rigorously proven in Ref. [24]. The general form of the initial Hamiltonian is given by [26]

$$\mathcal{H} = \beta\mathcal{M} + \mathcal{E} + \mathcal{O}, \quad \beta\mathcal{M} = \mathcal{M}\beta, \quad \beta\mathcal{E} = \mathcal{E}\beta, \quad \beta\mathcal{O} = -\mathcal{O}\beta. \tag{7}$$

The even operators $\mathcal{M}$ and $\mathcal{E}$ and the odd operator $\mathcal{O}$ are diagonal and off-diagonal in two spinors, respectively. Equation (7) is applicable for a particle with any spin if the number of components of a corresponding wave function is equal to $2(2s+1)$, where s is the spin quantum number. For a Dirac particle, the $\mathcal{M}$ operator is usually equal to the particle mass m:

$$\mathcal{H}_D = \beta m + \mathcal{E} + \mathcal{O}. \tag{8}$$

The approximate nonexponential FW transformation operator can be presented as follows [24]:

$$U = \frac{1+\sqrt{1+X^2}+\beta X}{\sqrt{2\sqrt{1+X^2}(1+\sqrt{1+X^2})}}, \quad X = \left\{\frac{1}{2\mathcal{M}}, \mathcal{O}\right\}. \tag{9}$$

The approximate relativistic FW Hamiltonian is given by [24]

$$\mathcal{H}_{\rm FW} = \beta\epsilon + \mathcal{E} + \frac{1}{4}\left\{\frac{1}{2\epsilon^2 + \{\epsilon, \mathcal{M}\}}, (\beta[\mathcal{O}, [\mathcal{O}, \mathcal{M}]] - [\mathcal{O}, [\mathcal{O}, \mathcal{F}]])\right\}, \quad \epsilon = \sqrt{\mathcal{M}^2 + \mathcal{O}^2}. \tag{10}$$

As an example, we can consider a spin-1/2 particle interacting with electromagnetic fields. If the particle possesses the anomalous magnetic moment (AMM) μ' and the electric dipole moment (EDM) d, its interaction is defined by the Dirac equation added by the Pauli term and the term proportional to the EDM (see Ref. [27]):

$$\left(i\gamma^\mu D_\mu - m + \frac{\mu'}{2}\sigma^{\mu\nu}F_{\mu\nu} + \frac{d}{2}\sigma^{\mu\nu}G_{\mu\nu}\right)\Psi = 0, \tag{11}$$

where $D_\mu = \partial_\mu + ieA_\mu$ is the covariant derivative, $G_{\mu\nu} = (-\boldsymbol{B}, \boldsymbol{E})$ is the tensor dual to the electromagnetic field one, and $F_{\mu\nu} = (\boldsymbol{E}, \boldsymbol{B})$.

The Dirac-Pauli Hamiltonian added by the EDM terms has the form (8) where $\mathcal{E}$ and $\mathcal{O}$ are defined by

$$\mathcal{E} = e\Phi - \mu'\boldsymbol{\Pi}\cdot\boldsymbol{B} - d\boldsymbol{\Pi}\cdot\boldsymbol{E}, \quad \mathcal{O} = \boldsymbol{\alpha}\cdot\boldsymbol{\pi} + i\mu'\boldsymbol{\gamma}\cdot\boldsymbol{E} - id\boldsymbol{\gamma}\cdot\boldsymbol{B}. \tag{12}$$

The calculated FW Hamiltonian is given by [27]

$$\mathcal{H}_{\rm FW} = \mathcal{H}_{\rm FW}^{\rm (MDM)} + \mathcal{H}_{\rm FW}^{\rm (EDM)}, \tag{13}$$

$$\mathcal{H}_{\rm FW}^{\rm (MDM)} = \beta\epsilon' + e\Phi + \frac{1}{4}\left\{\left(\frac{\mu_0 m}{\epsilon'+m} + \mu'\right)\frac{1}{\epsilon'}, [\boldsymbol{\Sigma}\cdot(\boldsymbol{\pi}\times\boldsymbol{E} - \boldsymbol{E}\times\boldsymbol{\pi}) - \hbar\nabla\cdot\boldsymbol{E}]\right\} - \frac{1}{2}\left\{\left(\frac{\mu_0 m}{\epsilon'} + \mu'\right), \boldsymbol{\Pi}\cdot\boldsymbol{B}\right\} + \beta\frac{\mu'}{4}\left\{\frac{1}{\epsilon'(\epsilon'+m)}, [(\boldsymbol{B}\cdot\boldsymbol{\pi})(\boldsymbol{\Sigma}\cdot\boldsymbol{\pi}) + (\boldsymbol{\Sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\pi}\cdot\boldsymbol{B}) + 2\pi\hbar(\boldsymbol{\pi}\cdot\boldsymbol{j} + \boldsymbol{j}\cdot\boldsymbol{\pi})]\right\}, \tag{14}$$

$$\mathcal{H}_{\rm FW}^{\rm (EDM)} = -d\boldsymbol{\Pi}\cdot\boldsymbol{E} + \frac{d}{4}\left\{\frac{1}{\epsilon'(\epsilon'+m)}, [(\boldsymbol{E}\cdot\boldsymbol{\pi})(\boldsymbol{\Pi}\cdot\boldsymbol{\pi}) + (\boldsymbol{\Pi}\cdot\boldsymbol{\pi})(\boldsymbol{\pi}\cdot\boldsymbol{E})]\right\} - \frac{d}{4}\left\{\frac{1}{\epsilon'}, (\boldsymbol{\Sigma}\cdot[\boldsymbol{\pi}\times\boldsymbol{B}] - \boldsymbol{\Sigma}\cdot[\boldsymbol{B}\times\boldsymbol{\pi}])\right\}. \tag{15}$$

Here $\mathcal{H}_{\rm FW}^{\rm (MDM)}$ defines the contribution from the magnetic dipole moment (MDM), $\mu_0 = e\hbar/(2m)$ is the Dirac magnetic moment, $\epsilon' = \sqrt{m^2 + \boldsymbol{\pi}^2}$, and

$$\boldsymbol{j} = \frac{1}{4\pi}\left(c\,\nabla\times\boldsymbol{B} - \frac{\partial\boldsymbol{E}}{\partial t}\right)$$

is the density of external electric current. The term in Eq. (14) proportional to $\nabla\cdot\boldsymbol{E}$ defines the Darwin (contact) interaction. While we take into account in Eq. (15) terms proportional to $\hbar^2$ and describing contact interactions with external charges and currents, such terms are zero due to the Maxwell equations

$$\nabla\cdot\boldsymbol{B} = 0, \quad \nabla\times\boldsymbol{E} = -\frac{\partial\boldsymbol{B}}{\partial t}.$$

Terms proportional to the second and higher powers of $\hbar$ and quadratic and bilinear in $\boldsymbol{E}$ and $\boldsymbol{B}$ are neglected. This Hamiltonian will be used in Sec. IV.

When $[\mathcal{E}, \mathcal{O}] = 0$, the FW transformation of the Dirac Hamiltonian (8) is exact [15]. For a free Dirac particle, the FW transformation operator is given by [3]

$$U_{\rm FW} = \frac{\epsilon + m + \boldsymbol{\gamma}\cdot\boldsymbol{p}}{\sqrt{2\epsilon(\epsilon+m)}}, \quad U_{\rm FW}^{-1} = \frac{\epsilon + m - \boldsymbol{\gamma}\cdot\boldsymbol{p}}{\sqrt{2\epsilon(\epsilon+m)}}, \quad \epsilon = \sqrt{m^2 + \boldsymbol{p}^2}. \tag{16}$$

III. POSITION AND SPIN OPERATORS FOR A FREE DIRAC PARTICLE

A definite connection among the position, angular momentum, and spin operators for a free Dirac particle and the corresponding classical variables was one of great achievements of QM in the last century. Unfortunately, this brilliant achievement was lately revised without appropriate substantiations. An incorrect interpretation of these operators is now so pervasive that it fully covers the theory of twisted (vortex) particles and is often applied in other branches of physics and also in quantum chemistry (see Refs. [28,29]).

In this section, we reproduce the previously well-known results allowing an unambiguous determination of basic op-

erators for the free Dirac particles. We follow the approach based on Refs. [1,30] and developed in Refs. [31,32].

The theory of a dynamical system is built up in terms of a number of algebraic quantities, called dynamical variables, each of which is defined with respect to a system of spacetime coordinates. There are ten independent *fundamental quantities* $P_\mu = (H, \boldsymbol{P})$, $J_{\mu\nu}$ $(\mu, \nu = 0, 1, 2, 3)$ describing the momentum and total angular momentum and characteristic for the dynamical system [1,30–32]. The antisymmetric tensor $J_{\mu\nu}$ is defined by the two vectors, $\boldsymbol{J}$ and $\boldsymbol{K}$. As a result, there are the ten infinitesimal generators of the Poincaré group (inhomogeneous Lorentz group [1]), namely, the generators of the infinitesimal space translations $\boldsymbol{P} = (P_i)$, the generator of the infinitesimal time translation H, the generators of infinitesimal rotations $\boldsymbol{J} = (J_i)$, and the generators of infinitesimal Lorentz transformations (boosts) $\boldsymbol{K} = (K_i)$ $(i = 1, 2, 3)$ [1,30–36]. These ten generators satisfy the following Poisson brackets [1,30–35]:

$$\{P_i, P_j\} = 0, \quad \{P_i, H\} = 0, \quad \{J_i, H\} = 0,$$
$$\{J_i, J_j\} = e_{ijk}J_k, \quad \{J_i, P_j\} = e_{ijk}P_k, \quad \{J_i, K_j\} = e_{ijk}K_k,$$
$$\{K_i, H\} = P_i, \quad \{K_i, K_j\} = -e_{ijk}J_k, \quad \{K_i, P_j\} = \delta_{ij}H. \quad (17)$$

In the multiparticle case, the momenta and energies of particles are additive, $\boldsymbol{P} = \sum_k \boldsymbol{P}^{(k)}$, $H = \sum_k H^{(k)}$. Counterparts of these generators in QM are ten corresponding operators. A connection between the classical and quantum mechanics manifests itself in the fact that the commutators of these operators are equal to the corresponding Poisson brackets multiplied by the imaginary unit i. Equation (17) describes the Lie algebra of classical motion for a free particle which leads to the ten-dimensional Poincaré algebra. The *only* additional equation which should be satisfied defines the orbital and spin parts of the total angular momentum:

$$\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}, \quad \boldsymbol{L} \equiv \boldsymbol{Q} \times \boldsymbol{P}. \quad (18)$$

There is a latitude in the definition of the position, orbital angular momentum (OAM), and spin. An exhaustive list of appropriate definitions has been presented in Ref. [1].

A consideration of the particle position variables Q_i brings the following Poisson brackets [1,31,32]:

$$\{Q_i, P_j\} = \delta_{ij}, \quad \{Q_i, J_j\} = e_{ijk}Q_k,$$
$$\{Q_i, K_j\} = \tfrac{1}{2}(Q_j\{Q_i, H\} + \{Q_i, H\}Q_j) - t\delta_{ij}. \quad (19)$$

The last term in the relation for $\{Q_i, K_j\}$ has been missed in Refs. [31,32]. It follows from Eqs. (17)–(19) that

$$\{L_i, P_j\} = e_{ijk}P_k, \quad \{S_i, P_j\} = 0. \quad (20)$$

Equations (17)–(20) should be satisfied for any correct definition of fundamental variables. However, these equations do not uniquely define the fundamental variables and different sets of the variables $\boldsymbol{Q}, \boldsymbol{L}, \boldsymbol{S}$ can be used [1].

The *conventional* particle position defines the *center of charge* of a charged particle if the particle EDM is negligible. The term "mass point" is also useful. For a single particle, the *mass point* always coincides with the conventional particle position. It also coincides with the center of charge of a charged particle when the particle EDM is neglected. Under this assumption, the mass point is the center of both positive and negative charges of an uncharged particle like a neutron. The Poisson brackets for the conventional particle position are equal to zero:

$$\{Q_i, Q_j\} = 0. \quad (21)$$

The property (21) is equivalent to the commutativity of the particle position operators [cf. Eq. (29)] and is nontrivial (see Refs. [1,32]). Other sets of fundamental variables violating Eq. (21) can also be used [1]. We will consider this problem in Secs. V and VI. Equations (17)–(21) describe a classical Hamiltonian system.

The well-known deep connection between the Poisson brackets in classical mechanics (CM) and the commutators in QM also takes place in this case. It is important that this connection remains valid *in any representation*. We need only to present the corresponding commutation relations for free spinning Dirac fermions. These relations allow one to establish definite forms of operators corresponding to basic classical variables in the Dirac and FW representations.

In the framework of CM, Eqs. (17)–(21) allow one to obtain the following Poisson brackets [1,32,37]

$$\{Q_i, L_j\} = e_{ijk}Q_k, \quad \{Q_i, S_j\} = 0, \quad \{P_i, S_j\} = 0,$$
$$\{L_i, L_j\} = e_{ijk}L_k, \quad \{S_i, S_j\} = e_{ijk}S_k. \quad (22)$$

Evidently,

$$\{L_i, S_j\} = 0. \quad (23)$$

The main variables of a free spinning particle in CM are specified by Eqs. (18) and

$$H = \sqrt{m^2 + \boldsymbol{P}^2}, \quad \boldsymbol{K} = \boldsymbol{Q}H - \frac{\boldsymbol{S} \times \boldsymbol{P}}{m + H} - t\boldsymbol{P} \quad (24)$$

(see also Refs. [34,35] and Eq. (A.23) in Ref. [38]). In Refs. [32,33,36,38], the last term in the relation for $\boldsymbol{P}$ has been missed.

The Poisson brackets (22) and (23) show that the variable $\boldsymbol{Q}$ defined by Eq. (21) does not depend on the spin and is the same for spinning and spinless particles with equal $\boldsymbol{Q}, \boldsymbol{P}$, and H. For a particle ensemble, the variable $\boldsymbol{Q}$ defines the position of the center of charge. Otherwise, a violation of the condition (21) leads to a dependence of $\boldsymbol{Q}$ on the spin.

In CM, the position vector satisfying Eq. (21) is the radius vector $\boldsymbol{R}$. For a free Dirac particle, the most straightforward way for a determination of the position and spin operators in any representation is the use of the FW representation as a starting point. The reason is a deep similarity between the classical Hamiltonian (24) (which is spin independent for a free particle) and the corresponding FW Hamiltonian [3]

$$\mathcal{H}_{\rm FW} = \beta\sqrt{m^2 + \boldsymbol{p}^2}, \quad \boldsymbol{p} \equiv -i\hbar\frac{\partial}{\partial \boldsymbol{r}}. \quad (25)$$

In addition, the lower spinor of the FW wave function $\Psi_{\rm FW}$ is equal to zero if the total particle energy is positive. The Hamiltonian (25) results from the FW transformation of the Dirac Hamiltonian

$$\mathcal{H}_D = \beta m + \boldsymbol{\alpha} \cdot \boldsymbol{p}. \quad (26)$$

The remaining operators read [32]

$$\boldsymbol{j}=\boldsymbol{l}+\boldsymbol{s},\quad \boldsymbol{l}\equiv\boldsymbol{q}\times\boldsymbol{p},\quad \boldsymbol{K}=\frac{1}{2}(\boldsymbol{q}\mathcal{H}+\mathcal{H}\boldsymbol{q})-\frac{\boldsymbol{s}\times\boldsymbol{p}}{\beta m+\mathcal{H}}-t\boldsymbol{p}, \tag{27}$$

where $\boldsymbol{q}$ is the position operator.

The operators being counterparts of fundamental classical variables should satisfy the relations [cf. Eqs. (17)–(23)]

$$\begin{aligned}
&[p_i,p_j]=0,\quad [p_i,\mathcal{H}]=0,\quad [j_i,\mathcal{H}]=0,\quad [j_i,j_j]=ie_{ijk}j_k,\quad [j_i,p_j]=ie_{ijk}p_k,\\
&[j_i,K_j]=ie_{ijk}K_k,\quad [K_i,\mathcal{H}]=ip_i,\quad [K_i,K_j]=-ie_{ijk}j_k,\quad [K_i,p_j]=i\delta_{ij}\mathcal{H},\\
&[q_i,K_j]=\tfrac{1}{2}(q_j[q_i,\mathcal{H}]+[q_i,\mathcal{H}]q_j)-it\delta_{ij},\quad [q_i,p_j]=i\delta_{ij},\quad [q_i,j_j]=ie_{ijk}q_k,\\
&[q_i,s_j]=0,\quad [s_i,p_j]=0,\quad [l_i,s_j]=0,\quad [l_i,l_j]=ie_{ijk}l_k,\quad [s_i,s_j]=ie_{ijk}s_k,
\end{aligned} \tag{28}$$

$$[q_i,q_j]=0. \tag{29}$$

Let us first consider the set of operators $\boldsymbol{p}$, $\mathcal{H}_D$, $\boldsymbol{j}$, $\boldsymbol{K}$, $\boldsymbol{q}$, $\boldsymbol{s}_D$, where $\boldsymbol{s}_D=\hbar\boldsymbol{\Sigma}/2$ and all these operators are defined in the Dirac representation (in particular, the position operator is the Dirac radius vector $\boldsymbol{r}$). Some of commutators in Eq. (28) which contain $\boldsymbol{K}$ are not satisfied by these operators. This fact follows from a noncoincidence of the position operator in the Dirac representation with $\boldsymbol{r}$ which has been shown for the first time in Ref. [1].

A consideration of the set of operators $\boldsymbol{p}$, $\mathcal{H}_{\rm FW}$, $\boldsymbol{j}$, $\boldsymbol{K}$, $\boldsymbol{q}$, $\boldsymbol{s}$ defined in the FW representation leads to an opposite conclusion. In this representation, the definition of $\boldsymbol{s}$ is the same ($\boldsymbol{s}=\hbar\boldsymbol{\Sigma}/2$) and the position operator $\boldsymbol{q}$ is equal to the FW radius vector $\boldsymbol{x}$. We can check that Eqs. (28) and (29) are now satisfied. Thus, the counterparts of the classical Hamiltonian, the position vector, the orbital angular momentum (OAM), and the spin are the operators $\mathcal{H}_{\rm FW}$, $\boldsymbol{x}$, $\boldsymbol{x}\times\boldsymbol{p}$, and $\hbar\boldsymbol{\Sigma}/2$ *defined in the FW representation*. The operators $\boldsymbol{p}$ and $\boldsymbol{J}$ are not changed by the transformation from the Dirac representation to the FW one and the counterpart of the classical variable $\boldsymbol{K}$ is the FW operator (27) with $\boldsymbol{q}=\boldsymbol{x}$.

Evidently, the Hamiltonian (25) commutes with the OAM and spin operators.

The choice between the definitions of fundamental operators in the Dirac and FW representations becomes evident when the commutators of the Hamiltonian with the position operator are considered. The corresponding Poisson bracket following from Eq. (24) is equal to

$$\{H,\boldsymbol{Q}\}=-\frac{\boldsymbol{p}}{H}.$$

Since the center-of-charge velocity is defined by

$$\boldsymbol{V}\equiv\frac{d\boldsymbol{Q}}{dt}=\frac{\partial H}{\partial\boldsymbol{p}}=\frac{\boldsymbol{p}}{H},$$

we obtain the relation

$$\boldsymbol{V}=\frac{\boldsymbol{p}}{H}. \tag{30}$$

The commutators are given by

$$\begin{aligned}
[\mathcal{H}_D,\boldsymbol{r}]&=-i\frac{d\boldsymbol{r}}{dt}\equiv-i\boldsymbol{v}_D=-i\boldsymbol{\alpha},\\
[\mathcal{H}_{\rm FW},\boldsymbol{x}]&=-i\frac{d\boldsymbol{x}}{dt}\equiv-i\boldsymbol{v}_{\rm FW}=-i\frac{\boldsymbol{p}}{\mathcal{H}_{\rm FW}}.
\end{aligned} \tag{31}$$

Equations (30) and (31) show that only the FW operators are the quantum-mechanical counterparts of the corresponding classical variables. The connection between the velocity and momentum operators is closely related to the problem of *Zitterbewegung* considered in Sec. VI C. An importance of the proportionality between the velocity and momentum operators has been noted in Refs. [49–51].

Of course, the counterparts of the fundamental classical variables can be determined in any representation. In the Dirac representation, they are defined by the transformation of the corresponding FW operators [3,32,34–37]. This transformation is inverse with respect to the FW one and is performed by the operator $U_{\rm FW}^{-1}$. If we denote by A any fundamental operator in the FW representation, the same operator in the Dirac representation is equal to $U_{\rm FW}^{-1}AU_{\rm FW}$. Thus, the counterparts of the fundamental classical variables in the Dirac representation read

$$\begin{aligned}
&\boldsymbol{P}\to\boldsymbol{p}=\boldsymbol{p}_D=\boldsymbol{p}_{\rm FW},\quad H\to\mathcal{H}_D=U_{\rm FW}^{-1}\mathcal{H}_{\rm FW}U_{\rm FW},\\
&\boldsymbol{J}\to\boldsymbol{j}=\boldsymbol{j}_D=\boldsymbol{j}_{\rm FW},\quad \boldsymbol{Q}\to\boldsymbol{q}=\boldsymbol{X}=U_{\rm FW}^{-1}\boldsymbol{x}U_{\rm FW},\\
&\boldsymbol{L}\to\boldsymbol{l}=\boldsymbol{l}_D=U_{\rm FW}^{-1}\boldsymbol{x}\times\boldsymbol{p}U_{\rm FW}=\boldsymbol{X}\times\boldsymbol{p},\quad \boldsymbol{S}\to\boldsymbol{s}=\boldsymbol{\mathcal{S}}=\frac{\hbar}{2}U_{\rm FW}^{-1}\boldsymbol{\Sigma}U_{\rm FW},
\end{aligned}$$

$$\boldsymbol{K} \to \boldsymbol{K}_D = U_{\rm FW}^{-1}\left[\frac{1}{2}(\boldsymbol{x}\mathcal{H}_{\rm FW} + \mathcal{H}_{\rm FW}\boldsymbol{x}) - \frac{\boldsymbol{s}\times\boldsymbol{p}}{m+\mathcal{H}_{\rm FW}} - t\boldsymbol{p}\right]U_{\rm FW}$$
$$= \frac{1}{2}(\boldsymbol{X}\mathcal{H}_D + \mathcal{H}_D\boldsymbol{X}) - \frac{\boldsymbol{\mathcal{S}}\times\boldsymbol{p}}{m+\mathcal{H}_D} - t\boldsymbol{p}. \tag{32}$$

Here the operators of the position ("mean position" [3]) and the spin ("mean spin angular momentum" [3]) in the Dirac representation are equal to [1,3,19]

$$\boldsymbol{q} = \boldsymbol{X} = \boldsymbol{r} - \frac{\boldsymbol{\Sigma}\times\boldsymbol{p}}{2\epsilon(\epsilon+m)} + \frac{i\boldsymbol{\gamma}}{2\epsilon} - \frac{i(\boldsymbol{\gamma}\cdot\boldsymbol{p})\boldsymbol{p}}{2\epsilon^2(\epsilon+m)}, \tag{33}$$

$$\boldsymbol{\mathcal{S}} = \frac{m}{2\epsilon}\boldsymbol{\Sigma} - i\frac{\boldsymbol{\gamma}\times\boldsymbol{p}}{2\epsilon} + \frac{\boldsymbol{p}(\boldsymbol{\Sigma}\cdot\boldsymbol{p})}{2\epsilon(\epsilon+m)}, \quad \epsilon = \sqrt{m^2+\boldsymbol{p}^2}. \tag{34}$$

We underline that the conventional spin operator corresponding to the classical rest-frame spin commutes with the OAM operator, the Hamiltonian, and the position and momentum operators *in any representation*. For any operators satisfying the relation $C_{\rm FW} = [A_{\rm FW}, B_{\rm FW}]$,

$$C_D = U_{\rm FW}^{-1}C_{\rm FW}U_{\rm FW} = U_{\rm FW}^{-1}(A_{\rm FW}B_{\rm FW} - B_{\rm FW}A_{\rm FW})U_{\rm FW} = U_{\rm FW}^{-1}A_{\rm FW}U_{\rm FW}U_{\rm FW}^{-1}B_{\rm FW}U_{\rm FW} - U_{\rm FW}^{-1}B_{\rm FW}U_{\rm FW}U_{\rm FW}^{-1}A_{\rm FW}U_{\rm FW} = [A_D, B_D].$$

The validity of the above-mentioned results on the position, spin, and other fundamental operators in the Dirac and FW representations has been demonstrated by *numerous* methods. Newton and Wigner [2] (see also Ref. [39]) have investigated localized states for elementary systems. They have shown that the operator (33) is the only position operator (with commuting components) in the Dirac theory which has localized eigenfunctions in the manifold of wave functions describing positive-energy states [2]. Therefore, the operator (33) is called the Newton-Wigner (NW) position operator.

It is important that the deep similarity between the fundamental classical variables and the corresponding FW operators does not disappear for different definitions of the position operator. It has been shown still in Ref. [1] that definitions of this operator violating the relation $[q_i, q_j] = 0$ are possible for spinning particles. The subsequent investigations [38,40–45] have confirmed the possibility of position operators with noncommutative components for spinning particles. However, the position operator with commutative components should satisfy Eqs. (27)–(33).

The fundamental conclusion that the NW position operator $\boldsymbol{q}$ and the radius vector in the FW representation $\boldsymbol{x}$ are identical has been confirmed in many papers [46–54]. Some of them have been fulfilled by different methods. In particular, the extended-type position operator has been proposed in Ref. [52] and definite relations between the velocity ($\dot{\boldsymbol{q}}$) and momentum operators have been introduced in Refs. [49,50].

The equivalence of the classical spin $\boldsymbol{S}$ and the FW mean-spin operator has also been shown in Refs. [4,46,50,51,54–58]. A rather important result has been obtained by Fradkin and Good [4]. They not only have confirmed Eq. (34) for the spin operator in the Dirac representation but also have demonstrated that the result obtained by Foldy and Wouthuysen remains valid for a Dirac particle in electric and magnetic fields. The FW mean-spin operator defines the rest-frame spin [4], while the use of the four-component spin operator a^μ is also admissible [4,59]. This operator is orthogonal to the four-momentum one ($a^\mu p_\mu = 0$) and is defined by

$$a^\mu = \frac{1}{2m}e^{\alpha\beta\nu\mu}p_\alpha S_{\beta\nu}, \tag{35}$$

where $S_{\beta\nu}$ is the antisymmetric spin tensor. Evidently, the four-component spin operator

$$a^\mu = (a^0, \boldsymbol{a}) = \left[\frac{\boldsymbol{p}\cdot\boldsymbol{s}}{m},\ \boldsymbol{s} + \frac{\boldsymbol{p}(\boldsymbol{s}\cdot\boldsymbol{p})}{m(\epsilon+m)}\right] \tag{36}$$

also commutes with the Hamiltonian. However, $\boldsymbol{a}$ cannot be the conventional spin operator because it does not commute with the operators $\boldsymbol{q}, \boldsymbol{l}$ and does not satisfy other commutative relations [see Eq. (28)]. Certainly, the rest-frame spin $\boldsymbol{s}$ is invariant relative to Lorentz boosts.

We also note important analyzes presented in Refs. [56,57,60]. It has been shown in Refs. [56,57] that the operator defining the conventional spin in the Dirac representation is the mean-spin operator (34) introduced by Foldy and Wouthuysen. It has been concluded in Ref. [60] that the Gordon decomposition of the energy momentum and spin currents of the Dirac electron corresponds to the FW transformation of its wave function.

Dirac particles in (1+1) dimensions have been considered in Refs. [61,62]. In the FW representation, wave packets described by the (1+1)-dimensional Dirac equation also behave much more like a classical particle than in the Dirac representation [61,62].

Thus, the correct forms of conventional operators of the position and spin of a free Dirac particle are defined by Eqs. (33) and (34) in the Dirac representation. These operators are equal to the radius vector $\boldsymbol{x}$ and to the spin operator $\hbar\boldsymbol{\Sigma}/2$ in the FW representation.

IV. CLASSICAL LIMIT FOR A DIRAC FERMION AND SPIN-0 AND SPIN-1 BOSONS IN EXTERNAL FIELDS

In the precedent section, we have analyzed free particles and this analysis is fully based on the results obtained many years ago. However, the contemporary development of theory of the FW transformation allows us to put forward important arguments in favor of the similarity between the classical position and spin and the corresponding operators in the FW representation. This section, unlike the precedent one, is devoted to a consideration of particles *in external fields*.

Relativistic methods giving compact relativistic FW Hamiltonians for any energy allow one to establish a direct connection between classical and quantum-mechanical Hamiltonians. To find this connection, it is convenient to pass to the classical limit of relativistic quantum-mechanical equations. Importantly, this procedure is very simple in the FW representation. When the conditions of the Wentzel-Kramers-Brillouin approximation are satisfied, the classical limit can be obtained by replacing the FW operators with the respective classical variables [63]. This property leads to the conclusion that the quantum-mechanical counterparts of the classical variables are the corresponding operators *in the FW representation*.

Let us begin the analysis of Dirac particle interactions with external fields from the result obtained in Ref. [4]. In this paper, the equation of spin motion has been derived *in the Dirac representation* and its classical limit has been obtained. A particle with an AMM has been considered and the initial Dirac-Pauli equation [Eq. (11) with $d = 0$] has been used. In the classical limit, Fradkin and Good have obtained the equation [4] coinciding with the famous classical Thomas-Bargmann-Michel-Telegdi (T-BMT) one [64,65]. The presence of the Thomas term shows that the both equations are derived for the rest-frame spin $\boldsymbol{\mathcal{S}}$ but not for the spin in the laboratory frame or in the instantaneously accompanying one. The distinction between the rest frame and the instantaneously accompanying one can be made only for an accelerated particle.

The use of the FW representation leads to the same conclusion. The relativistic FW Hamiltonian for the Dirac particle with the AMM and EDM obtained in Ref. [27] is given by Eqs. (13)–(15). To compare the position and spin operators with their classical counterparts, we can use the weak-field approximation and can disregard terms proportional to $\hbar^2$ and describing contact interactions. When the fields are uniform, the gauge $\Phi = -\boldsymbol{E}\cdot\boldsymbol{x}$, $\boldsymbol{A} = (\boldsymbol{B}\times\boldsymbol{x})/2$ can be used. In this case, the Hamiltonian (13) takes the form

$$\begin{aligned}
\mathcal{H}_{\rm FW} &= \beta\sqrt{m^2+\left(\boldsymbol{p}-\frac{e}{2}\boldsymbol{B}\times\boldsymbol{x}\right)^2} - e\boldsymbol{E}\cdot\boldsymbol{x} + \boldsymbol{\Omega}\cdot\boldsymbol{s}, \quad \boldsymbol{\Omega} = \boldsymbol{\Omega}_{\rm MDM}+\boldsymbol{\Omega}_{\rm EDM},\\
\boldsymbol{\Omega}_{\rm MDM} &= \frac{e}{m}\left[-\beta\left(\frac{m}{\epsilon}+a\right)\boldsymbol{B} + \beta\frac{a}{\epsilon(\epsilon+m)}(\boldsymbol{p}\cdot\boldsymbol{B})\boldsymbol{p} + \frac{1}{\epsilon}\left(\frac{m}{\epsilon+m}+a\right)\boldsymbol{p}\times\boldsymbol{E}\right],\\
\boldsymbol{\Omega}_{\rm EDM} &= -\frac{e\eta}{2m}\left[\beta\boldsymbol{E} - \beta\frac{(\boldsymbol{p}\cdot\boldsymbol{E})\boldsymbol{p}}{\epsilon(\epsilon+m)} + \frac{\boldsymbol{p}\times\boldsymbol{B}}{\epsilon}\right], \quad \boldsymbol{s} = \frac{\boldsymbol{\Sigma}}{2}, \quad \epsilon = \sqrt{m^2+\boldsymbol{p}^2},
\end{aligned} \tag{37}$$

where $a = (g-2)/2$, $g = 4mc(\mu_0+\mu')/(e\hbar)$, and $\eta = 4mcd/(e\hbar)$ is the "gyroelectric" factor corresponding to g. The matrix β may be removed if one considers positive-energy states and disregards the zero lower spinor. The equation of spin motion is given by

$$2\frac{d\boldsymbol{s}}{dt} = \frac{d\boldsymbol{\Sigma}}{dt} = \boldsymbol{\Omega}\times\boldsymbol{\Sigma}. \tag{38}$$

The operator of the angular velocity of spin rotation $\boldsymbol{\Omega}$ has the two parts, $\boldsymbol{\Omega}_{\rm MDM}$ and $\boldsymbol{\Omega}_{\rm EDM}$, defining the contributions of the magnetic dipole moment and the EDM, respectively.

The related relativistic FW Hamiltonians derived in Refs. [15,23,25,26] agree with the Hamiltonian (37). We underline that the method of the relativistic FW transformation used in Ref. [25] substantially differs from that applied in other above-mentioned works. The operator $\boldsymbol{\Omega}_{\rm MDM}$ is in compliance with the operator of the angular velocity of spin motion in the Dirac representation obtained in Ref. [4].

We can now compare the Hamiltonian (37) and the equation of spin motion (38) with their classical counterparts. In the same approximation, the classical Hamiltonian of a spinning particle in uniform electric and magnetic fields has the form

$$H = \sqrt{m^2+\left(\boldsymbol{P}-\frac{e}{2}\boldsymbol{B}\times\boldsymbol{R}\right)^2} - e\boldsymbol{E}\cdot\boldsymbol{R} + \boldsymbol{\Omega}\cdot\boldsymbol{S}, \tag{39}$$

where the angular velocity of spin rotation $\boldsymbol{\Omega} = \boldsymbol{\Omega}_{\rm MDM}+\boldsymbol{\Omega}_{\rm EDM}$ is defined by (see Refs. [66–68] and references therein)

$$\begin{aligned}
\boldsymbol{\Omega}_{\rm MDM} &= \frac{e}{m}\left[-\left(\frac{m}{\varepsilon}+a\right)\boldsymbol{B} + \frac{a}{\varepsilon(\varepsilon+m)}(\boldsymbol{P}\cdot\boldsymbol{B})\boldsymbol{P} + \frac{1}{\varepsilon}\left(\frac{m}{\varepsilon+m}+a\right)\boldsymbol{P}\times\boldsymbol{E}\right],\\
\boldsymbol{\Omega}_{\rm EDM} &= -\frac{e\eta}{2m}\left[\boldsymbol{E} - \frac{(\boldsymbol{P}\cdot\boldsymbol{E})\boldsymbol{P}}{\varepsilon(\varepsilon+m)} + \frac{\boldsymbol{P}\times\boldsymbol{B}}{\varepsilon}\right], \quad \varepsilon = \sqrt{m^2+\boldsymbol{P}^2}.
\end{aligned} \tag{40}$$

The comparison of Eqs. (37) and (38) with Eqs. (39) and (40) unambiguously shows that the classical counterparts of the FW position operator $\boldsymbol{x}$ and the FW spin operator $\boldsymbol{s} = \hbar\boldsymbol{\Sigma}/2$ are the radius vector $\boldsymbol{R}$ and the rest-frame spin $\boldsymbol{S}$, respectively. This is a strong argument in favor of the statements that the position operators are the FW radius vector $\boldsymbol{x}$ and the Dirac operator (33) and that the conventional spin operators are the FW operator $\hbar\boldsymbol{\Sigma}/2$ and the Dirac operator (34). In this section, Eqs. (33) and (34) define the Dirac position and spin operators only approximately because the FW transformation operator depends on external fields.

One can confirm these statements for a Dirac particle in gravitational fields and noninertial frames. It has been definitely shown in many papers devoted to this problem [69–78] that the relativistic quantum-mechanical Hamiltonians and equations of motion in the FW representation are similar to the corresponding classical ones. As an example, let us consider the Dirac particle in the general noninertial frame. This frame is characterized by the acceleration $\mathfrak{a}$ and the rotation with the angular velocity $\boldsymbol{\omega}$. The relativistic FW Hamiltonian reads [73]

$$\mathcal{H}_{\rm FW}=\frac{\beta}{2}\left[\left(1+\frac{\mathfrak{a}\cdot\boldsymbol{x}}{c^2}\right)\epsilon+\epsilon\left(1+\frac{\mathfrak{a}\cdot\boldsymbol{x}}{c^2}\right)\right]-\boldsymbol{\omega}\cdot\boldsymbol{l}+\frac{\hbar}{2}\boldsymbol{\Omega}\cdot\boldsymbol{\Sigma},$$

$$\boldsymbol{\Omega}=\beta\frac{\mathfrak{a}\times\boldsymbol{p}}{\epsilon+mc^2}-\boldsymbol{\omega},\quad \epsilon=\sqrt{m^2c^4+c^2\boldsymbol{p}^2},\quad \boldsymbol{l}=\boldsymbol{x}\times\boldsymbol{p}. \tag{41}$$

Let us stress that Eq. (41) has been derived for the strong kinematical effects when the ratios $|\mathfrak{a}\cdot\boldsymbol{x}|/c^2$ and $|\boldsymbol{\omega}\times\boldsymbol{x}|/c$ are not small.

The corresponding classical Hamiltonian can be obtained with a substitution of the metric of the general noninertial frame into Eq. (3.18) from Ref. [73]:

$$H=\left(1+\frac{\mathfrak{a}\cdot\boldsymbol{R}}{c^2}\right)\varepsilon-\boldsymbol{\omega}\cdot\boldsymbol{L}+\boldsymbol{\Omega}\cdot\boldsymbol{S},$$

$$\boldsymbol{\Omega}=\frac{\mathfrak{a}\times\boldsymbol{P}}{\varepsilon+mc^2}-\boldsymbol{\omega},\quad \varepsilon=\sqrt{m^2c^4+c^2\boldsymbol{P}^2}. \tag{42}$$

It follows from Eqs. (41) and (42) that the position and spin operators are the FW operators $\boldsymbol{x}$ and $\boldsymbol{s}=\hbar\boldsymbol{\Sigma}/2$ and the Dirac operators (33) and (34), respectively.

Because of the unification of relativistic QM in the FW representation [79], similar statements can be made for spin-0 and spin-1 particles. In connection with this unification, we can mention the existence of bosonic symmetries of the standard Dirac equation [80–86]. When terms proportional to $\hbar^2$ are disregarded and the weak-field approximation is used, the relativistic Hamiltonian for a spin-0 particle in the uniform electric and magnetic fields has the form [87]

$$\mathcal{H}_{\rm FW}=\rho_3\sqrt{m^2+\left(\boldsymbol{p}-\frac{e}{2}\boldsymbol{B}\times\boldsymbol{x}\right)^2}-e\boldsymbol{E}\cdot\boldsymbol{x}, \tag{43}$$

where ρ_3 is the corresponding Pauli matrix acting on a two-component wave function. On the same conditions, the relativistic Hamiltonian for a spin-1 particle with the AMM and EDM in the uniform electric and magnetic fields is given by [88]

$$\begin{aligned}
\mathcal{H}_{\rm FW}&=\beta\sqrt{m^2+\left(\boldsymbol{p}-\frac{e}{2}\boldsymbol{B}\times\boldsymbol{x}\right)^2}-e\boldsymbol{E}\cdot\boldsymbol{x}+\boldsymbol{\Omega}\cdot\boldsymbol{s}^{(1)},\quad \boldsymbol{\Omega}=\boldsymbol{\Omega}_{\rm MDM}+\boldsymbol{\Omega}_{\rm EDM},\\
\boldsymbol{\Omega}_{\rm MDM}&=\frac{e}{m}\left[-\beta\left(\frac{m}{\epsilon}+a\right)\boldsymbol{B}+\beta\frac{a}{\epsilon(\epsilon+m)}(\boldsymbol{p}\cdot\boldsymbol{B})\boldsymbol{p}+\frac{1}{\epsilon}\left(\frac{m}{\epsilon+m}+a\right)\boldsymbol{p}\times\boldsymbol{E}\right],\\
\boldsymbol{\Omega}_{\rm EDM}&=-\frac{e\eta}{2m}\left[\beta\boldsymbol{E}-\beta\frac{(\boldsymbol{p}\cdot\boldsymbol{E})\boldsymbol{p}}{\epsilon(\epsilon+m)}+\frac{\boldsymbol{p}\times\boldsymbol{B}}{\epsilon}\right],\quad \epsilon=\sqrt{m^2+\boldsymbol{p}^2},
\end{aligned} \tag{44}$$

where

$$\beta=\begin{pmatrix}\mathfrak{I} & 0\\ 0 & -\mathfrak{I}\end{pmatrix},\quad \boldsymbol{s}^{(1)}=\begin{pmatrix}\boldsymbol{S}^{(1)} & 0\\ 0 & \boldsymbol{S}^{(1)}\end{pmatrix}, \tag{45}$$

$a=(g-2)/2$, $g=2mc\mu/(e\hbar)$, and $\eta=2mcd/(e\hbar)$. Here $\boldsymbol{S}^{(1)}=(S_i^{(1)})$ is the conventional 3×3 spin matrix for spin-1 particles and $\mathfrak{I}$ is the 3×3 unit matrix. The wave function has six components. The matrix β may be removed if one considers positive-energy states and disregards the zero lower spinor-like part of the FW wave function.

Evidently, the definition of the position operator as the radius vector in the FW representation remains valid for spin-0 and spin-1 particles. The use of the FW transformation for a description of a relativistic spin-0 particle in gravitational fields and noninertial frames [89] confirms this definition of the position operator. The fundamental spin operator for a spin-1 particle in the FW representation is the matrix (45).

The basic role of the FW representation in nonstationary QM has been shown in Ref. [90]. The classical time-dependent energy corresponds to the time-dependent expectation value of the energy operator. The latter is the Hamiltonian in the Schrödinger QM and the FW representation (but not in the Dirac representation) [90]. The energy expectation values are defined by [90]

$$E(t)=\int\Psi^\dagger_{\rm FW}(\boldsymbol{r},t)\mathcal{H}_{\rm FW}(t)\Psi_{\rm FW}(\boldsymbol{r},t)dV. \tag{46}$$

In the Dirac representation,

$$E(t)=\int\Psi^\dagger_{D}(\boldsymbol{r},t)\widetilde{\mathcal{H}}(t)\Psi_{D}(\boldsymbol{r},t)dV, \tag{47}$$

where $\widetilde{\mathcal{H}}(t)$ is the energy operator which defines the energy expectation values by averaging. It does not coincide with the Dirac Hamiltonian and is equal to [90]

$$\widetilde{\mathcal{H}}(t) = \mathcal{H}_D + \frac{e\hbar}{8}\left\{\frac{1}{\epsilon'(\epsilon'+m)}, [-i\{\epsilon', \boldsymbol{\gamma}\cdot\dot{\boldsymbol{A}}\} - 2im\boldsymbol{\gamma}\cdot\dot{\boldsymbol{A}} + \boldsymbol{\Sigma}\cdot(\boldsymbol{\pi}\times\dot{\boldsymbol{A}} - \dot{\boldsymbol{A}}\times\boldsymbol{\pi})]\right\}$$
$$+ i\frac{e\hbar}{8}\left\{\frac{1}{\epsilon'^2(\epsilon'+m)}, [(\boldsymbol{\pi}\cdot\dot{\boldsymbol{A}})(\boldsymbol{\gamma}\cdot\boldsymbol{\pi}) + (\boldsymbol{\gamma}\cdot\boldsymbol{\pi})(\dot{\boldsymbol{A}}\cdot\boldsymbol{\pi})]\right\}, \tag{48}$$

where $\mathcal{H}_D$ is the Dirac Hamiltonian, $\epsilon' = \sqrt{m^2+\boldsymbol{\pi}^2}$, and dots denote time derivatives.

The contribution to the energy expectation values given by the two last terms in Eq. (48) can be rather important. This equation shows that the Dirac Hamiltonian does not correspond to the classical one in the nonstationary case [90].

In fact, the difference between the position operator (33) and the radius vector $\boldsymbol{r}$ in the Dirac representation is very important. The assumption that $\boldsymbol{r}$ is the true Dirac position operator leads to the misleading conclusion that the quantity $\varrho_D = \Psi_D^\dagger(\boldsymbol{r})\Psi_D(\boldsymbol{r})$ is the probability density that the particle is at the point $\boldsymbol{r}$ and the quantity $e\Psi_D^\dagger(\boldsymbol{r})\Psi_D(\boldsymbol{r})$ describes the electron charge distribution. This assumption also results in a calculation of incorrect expectation values of operators. We will discuss these problems in Sec. VII.

Thus, the consideration of a Dirac particle in external fields leads to results fully supporting the conclusions made in the precedent section. An analysis of spin-0 and spin-1 particles in external fields also presents arguments in favor of these conclusions. In contrast to the results for a free particle presented in Sec. III, the particle spin motion in electric and magnetic field is sensitive to the Thomas effect [64] and unambiguously shows that the fundamental spin operator is defined in the particle rest frame. The analysis presented excludes the possibility of a definition of this operator in the instantaneously accompanying frame.

V. RELATIVISTIC OPERATORS OF THE POSITION AND SPIN

The rest-frame spin $\boldsymbol{s}$ and the four-component one a^μ do not exhaust the list of relativistic spin operators. The spin can also be represented by the antisymmetric tensor (see Ref. [59], Sec. 29)

$$S^{\mu\nu} = \frac{1}{m}e^{\mu\nu\alpha\beta}a_\alpha p_\beta. \tag{49}$$

Similarly to the OAM, the spatial part (components S^{ij}) of this antisymmetric tensor forms the three-component vector $\boldsymbol{\zeta}$ with the following transformation properties (see Ref. [59], Sec. 29):

$$\boldsymbol{\zeta}^{(0)} = \boldsymbol{s}, \quad \zeta_\parallel = \zeta^{(0)}, \quad \zeta_\perp = \frac{\epsilon}{m}\zeta^{(0)},$$
$$\boldsymbol{\zeta} = \frac{\epsilon}{m}\boldsymbol{\zeta}^{(0)} - \frac{(\boldsymbol{\zeta}^{(0)}\cdot\boldsymbol{p})\boldsymbol{p}}{m(\epsilon+m)}, \tag{50}$$

where $\boldsymbol{\zeta}^{(0)}$ characterizes the particle rest frame. Evidently, the vectors $\boldsymbol{a}$ and $\boldsymbol{\zeta}$ differ. The quantity $\boldsymbol{\zeta}$ defines the three-component *laboratory-frame* spin and can be written in the form

$$\boldsymbol{\zeta} = \boldsymbol{s} - \frac{\boldsymbol{p}\times(\boldsymbol{p}\times\boldsymbol{s})}{m(\epsilon+m)}. \tag{51}$$

The quantities $\boldsymbol{l}$ and $\boldsymbol{s}$ forming the total angular momentum $\boldsymbol{j}$ have different physical meanings. The OAM $\boldsymbol{l}$ is the spatial part of the antisymmetric tensor $L^{\mu\nu} = (-\boldsymbol{\kappa}, -\boldsymbol{l})$ with $\boldsymbol{\kappa} = (\boldsymbol{q}\mathcal{H} + \mathcal{H}\boldsymbol{q})/2 - t\boldsymbol{p}$ and is noninvariant relative to Lorentz transformations. The rest-frame spin $\boldsymbol{s}$ is invariant relative to such transformations. It is natural to constitute the total angular momentum from spatial parts of the two antisymmetric tensors, $L^{\mu\nu}$ and $S^{\mu\nu}$:

$$J^{\mu\nu} = L^{\mu\nu} + S^{\mu\nu} = x^\mu p^\nu - x^\nu p^\mu + S^{\mu\nu}. \tag{52}$$

Since the spatial part of $S^{\mu\nu}$ is presented by the vector $\boldsymbol{\zeta}$, the definition of this vector is analogous to the definition of the total angular momentum $\boldsymbol{j}$. Equation (27) shows that the corresponding operators of the position and OAM should be redefined in order to avoid a change of the operator $\boldsymbol{j}$:

$$\boldsymbol{j} = \boldsymbol{l} + \boldsymbol{s} = \boldsymbol{\mathcal{L}} + \boldsymbol{\zeta}, \quad \boldsymbol{\mathcal{L}} = \boldsymbol{\mathcal{X}}\times\boldsymbol{p}. \tag{53}$$

Equations (51) and (53) specify the position operator $\boldsymbol{\mathcal{X}}$ [1,38,40]. In the FW representation [1,38,40],

$$\boldsymbol{\mathcal{X}}_{\rm FW} = \boldsymbol{x} + \frac{\boldsymbol{s}\times\boldsymbol{p}}{m(\epsilon+m)}, \quad \boldsymbol{\mathcal{L}}_{\rm FW} = \boldsymbol{\mathcal{X}}_{\rm FW}\times\boldsymbol{p}, \tag{54}$$

where $\boldsymbol{x}$ is the FW center-of-charge position operator and the spin operator $\boldsymbol{\zeta}_{\rm FW} = \boldsymbol{\zeta}$ is given by Eq. (51).

In the Dirac representation [1,38],

$$\boldsymbol{\mathcal{X}}_D = \boldsymbol{r} + i\left[\frac{\boldsymbol{\gamma}}{2m} - \frac{(\boldsymbol{\gamma}\cdot\boldsymbol{p})\boldsymbol{p}}{2m\epsilon^2}\right], \quad \boldsymbol{\mathcal{L}}_D = \boldsymbol{\mathcal{X}}_D\times\boldsymbol{p}, \tag{55}$$

$$\boldsymbol{\zeta}_D = \frac{\boldsymbol{\Sigma}}{2} - i\frac{\boldsymbol{\gamma}\times\boldsymbol{p}}{2m}, \tag{56}$$

where $\boldsymbol{r}$ is the Dirac position operator. Certainly, $\boldsymbol{\mathcal{X}}_D\times\boldsymbol{p} + \boldsymbol{\zeta}_D = \boldsymbol{\mathcal{X}}_{\rm FW}\times\boldsymbol{p} + \boldsymbol{\zeta} = \boldsymbol{j}$.

The Dirac and FW position operators have the same form, $\boldsymbol{r} = (x, y, z)$ and $\boldsymbol{x} = (x, y, z)$. However, they define different physical quantities; see Eq. (33). Only the FW position operator ("mean position operator" [3]) is the quantum-mechanical counterpart of the classical position variable $\boldsymbol{R} = (X, Y, Z)$ [3].

In the framework of *covariant* spin physics, the operator $\boldsymbol{q}$ should define the position of the center of mass. In this case, its determination is based on the use of the *laboratory-frame* spin $\boldsymbol{\zeta}$ and OAM $\boldsymbol{\mathcal{X}}\times\boldsymbol{p}$ and of the corresponding position operator $\boldsymbol{\mathcal{X}}$. Therefore, just the operator $\boldsymbol{q} = \boldsymbol{\mathcal{X}}$ characterizes the center of mass of a particle. By virtue of Eq. (54), the positions of the center of mass and the center of charge (or the mass point for an uncharged particle; see Sec. III) differ.

The corresponding classical variables are very similar. In classical physics, the center-of-mass position, the corresponding OAM, and the laboratory-frame spin are given by

$$\boldsymbol{\mathcal{X}} = \boldsymbol{R} + \frac{\boldsymbol{S}\times\boldsymbol{P}}{m(H+m)}, \quad \boldsymbol{\mathcal{L}} = \boldsymbol{\mathcal{X}}\times\boldsymbol{P}, \quad \boldsymbol{\zeta} = \boldsymbol{S} - \frac{\boldsymbol{P}\times(\boldsymbol{P}\times\boldsymbol{S})}{m(H+m)}. \tag{57}$$

More recent investigations [41,42,57,58,91] have confirmed the validity of results obtained in Refs. [1,38,40] and have given important substantiations of the meaning of the operator $\boldsymbol{\mathcal{X}}$. In particular, the shift of the center of mass relative to the center of charge manifests itself in spin-orbit and spin-spin effects in gravitational interactions [41]. The shift $\boldsymbol{\mathcal{X}}_{\rm FW} - \boldsymbol{x} = \boldsymbol{s}\times\boldsymbol{p}/[m(\epsilon+m)]$ naturally appears in the original quantum-mechanical approach expounded in Refs. [42,91].

Since Eq. (52) is covariant and it leads *only* to the relation $\boldsymbol{j} = \boldsymbol{\mathcal{L}} + \boldsymbol{\zeta}$ (but not to any different relation like $\boldsymbol{j} = \boldsymbol{l} + \boldsymbol{s}$), the covariant spin physics should be based on the operators $\boldsymbol{\mathcal{X}}, \boldsymbol{\mathcal{L}}, \boldsymbol{\zeta}$. In the general case, equations of momentum and spin dynamics obtained with the operators and *any different* set of fundamental operators (e.g., $\boldsymbol{x}, \boldsymbol{l}, \boldsymbol{s}$) are noncovariant. This fact (first noted in Refs. [41,42,91]) does not mean that the use of different sets can result in some mistakes. In particular, the correct utilization of the conventional operators $\boldsymbol{x}, \boldsymbol{l}, \boldsymbol{s}$ is ensured by Eq. (53). While equations of motion obtained with these operators can be noncovariant, such a noncovariance does not lead to any fallacy.

The Pauli-Lubanski four-vector (see Refs. [56,58])

$$W^\mu = \tfrac{1}{2} e^{\alpha\beta\nu\mu} p_\alpha J_{\beta\nu} \tag{58}$$

is also widely used as a relativistic spin operator. It is easy to check that the four-vectors ma^μ and W^μ are equivalent. The tensor of the total angular momentum is given by Eq. (52). The tensor of the OAM does not contribute to the Pauli-Lubanski vector. For an extended object like an atom, the spin tensor involves the *internal* OAM (for example, the OAM of an electron in an atom). In this case, Eqs. (35), (52), and (58) lead to the relation

$$W^\mu = ma^\mu. \tag{59}$$

In the FW representation,

$$W^\mu = (W^0, \boldsymbol{W}) = \left[\frac{\boldsymbol{p}\cdot\boldsymbol{\Sigma}}{2}, \frac{m\boldsymbol{\Sigma}}{2} + \frac{\boldsymbol{p}(\boldsymbol{p}\cdot\boldsymbol{\Sigma})}{2(\epsilon+m)}\right]. \tag{60}$$

A spinning particle is characterized by the two Casimir invariants (Casimir operators of the Poincaré group):

$$p^\mu p_\mu = m^2, \quad W^\mu W_\mu = -m^2\boldsymbol{s}^2 = -m^2 s(s+1)\mathcal{I}, \tag{61}$$

where $\mathcal{I}$ is the unit matrix. It has been noted at the end of Sec. III that the rest-frame spin $\boldsymbol{s}$ is invariant relative to Lorentz boosts. Therefore, the square of the spin operator is the Casimir invariant and the Lorentz scalar and $\boldsymbol{s}$ is the correct spin operator.

It has been obtained in Ref. [56] that the only spin operator satisfying the required commutation relations has the form

$$\boldsymbol{s}' = \frac{1}{m}\left(\frac{|p_0|}{p_0}\boldsymbol{W} - W_0\frac{\boldsymbol{p}}{|p_0|+m}\right) = \frac{1}{m}\left(\boldsymbol{W} - W_0\frac{\boldsymbol{p}}{p_0+m}\right). \tag{62}$$

The total energy is expected to be positive. It has been noted in Ref. [56] that this operator is *equivalent* to the rest-frame spin operator $\boldsymbol{s}$. In Ref. [56], nevertheless, the operators $\boldsymbol{s}$ and $\boldsymbol{s}'$ are defined by different formulas. The use of Eqs. (36), (59), and (62) shows that $\boldsymbol{s}' = \boldsymbol{s}$. This result has been first obtained by Ryder [55] (see also Ref. [58]). Therefore, the transformation of the operator $\boldsymbol{s}'$ to the Dirac representation leads to the operator (34). The operator (62) is also useful in the quantum field theory [92].

In Refs. [58,93–96], the projected spin operator has been considered. It is possible to project some operators onto positive- and negative-energy subspaces, eliminating the cross terms corresponding to the electron-positron transitions. In particular, the projected radius vector operator is given by [58,93,94,96]

$$\boldsymbol{\mathfrak{R}} = \Pi^+\boldsymbol{r}\Pi^+ + \Pi^-\boldsymbol{r}\Pi^-, \tag{63}$$

where the projectors are given by

$$\Pi^\pm = \frac{1}{2}U_{\rm FW}^\dagger(1\pm\beta)U_{\rm FW} = \frac{1}{2}\left(1 \pm \beta\frac{m}{\epsilon}\right) \pm \frac{\boldsymbol{\alpha}\cdot\boldsymbol{p}}{2\epsilon}.$$

In the Dirac and FW representations, the projected operators of the radius vector (position) and spin are equal to

$$\boldsymbol{\mathfrak{R}}_D = \boldsymbol{r} - \frac{\boldsymbol{\Sigma}\times\boldsymbol{p}}{2\epsilon^2} + i\frac{m\boldsymbol{\gamma}}{2\epsilon^2}, \quad \boldsymbol{\mathfrak{R}}_{\rm FW} = \boldsymbol{x} - \frac{\boldsymbol{\Sigma}\times\boldsymbol{p}}{2\epsilon(\epsilon+m)} \tag{64}$$

and

$$\boldsymbol{\mathfrak{S}}_D = \frac{1}{2\epsilon^2}[m^2\boldsymbol{\Sigma} + \boldsymbol{p}(\boldsymbol{p}\cdot\boldsymbol{\Sigma}) - im\boldsymbol{\gamma}\times\boldsymbol{p}],$$
$$\boldsymbol{\mathfrak{S}}_{\rm FW} = \frac{m\boldsymbol{\Sigma}}{2\epsilon} + \frac{\boldsymbol{p}(\boldsymbol{p}\cdot\boldsymbol{\Sigma})}{2\epsilon(\epsilon+m)}, \tag{65}$$

respectively [58,93–96]. The projected OAM operator is given by

$$\boldsymbol{\mathfrak{L}}_D = \boldsymbol{\mathfrak{R}}_D\times\boldsymbol{p}, \quad \boldsymbol{\mathfrak{L}}_{\rm FW} = \boldsymbol{\mathfrak{R}}_{\rm FW}\times\boldsymbol{p}. \tag{66}$$

Despite the assertion in Ref. [96] that the projected spin operator "corresponds to the spatial part of the Pauli-Lubanski four-vector," the two vectors substantially differ ($\boldsymbol{\mathfrak{S}}_{\rm FW} = \boldsymbol{W}/\epsilon \neq \boldsymbol{W}/m$). This conclusion follows also from Eq. (16) in Ref. [96]. In Pryce's classification [1], the projected operators of the position and spin correspond to the case (c). When our denotations are used, the classical counterpart of the projected position operator obtained by Pryce [1] reads [cf. Eqs. (27) and (64)]

$$\mathfrak{R}^i = \frac{tP^i + J^{i0}}{H}, \quad \boldsymbol{\mathfrak{R}} = \frac{t\boldsymbol{P} + \boldsymbol{K}}{H} = \boldsymbol{R} - \frac{\boldsymbol{S}\times\boldsymbol{P}}{H(H+m)}. \tag{67}$$

It has been asserted in Ref. [96] (p. 5) that the expectation value of the projected position operator "for a single-electron state corresponds to the center of the probability density (center of charge)." However, Eqs. (64) and (67) unambiguously show that the projected position depends on the spin. Therefore, this assertion is not correct. It can be added that the operator $\boldsymbol{\mathfrak{R}}$ substantially differs from the center-of-mass position operator $\boldsymbol{\mathcal{X}}$ (the quantities $\boldsymbol{\mathcal{X}}_{\rm FW} - \boldsymbol{x}$ and $\boldsymbol{\mathfrak{R}}_{\rm FW} - \boldsymbol{x}$ have even opposite signs). The projected and laboratory-frame spin operators are also substantially different. In the general case, this circumstance results in the noncovariance of equations of motion based on the projected operators.

Nevertheless, the projected operators are needed for the description of Berry phase effects. In this case, the noncommutativity of components of the projected position operator is important and defines the Berry curvature [95–100].

Thus, we can select three sets of fundamental FW operators, $\boldsymbol{x}, \boldsymbol{l}, \boldsymbol{s}$, $\boldsymbol{\mathcal{X}}, \boldsymbol{\mathcal{L}}, \boldsymbol{\zeta}$, and $\boldsymbol{\mathfrak{R}}, \boldsymbol{\mathfrak{L}}, \boldsymbol{\mathfrak{S}}$. Other fundamental operators in these sets coincide. The three sets are self-consistent but the operators in these sets have different meanings. For a charged particle, the first set defines the conventional operators of the center-of-charge position, the OAM, and the rest-frame spin. These operators satisfy Eq. (28). While the NW position operators in the Dirac representation ($\boldsymbol{X}$) and in the FW one ($\boldsymbol{x}$) do not exactly determine the center-of-mass position of an ensemble of spinning particles; they define the center-of-charge position of this ensemble (see Sec. III).

The second set characterizes the center-of-mass position, the *corresponding* OAM, and the laboratory-frame spin. The quantity $\boldsymbol{\mathcal{X}}$ defines the center-of-mass position of an ensemble of spinning particles. However, the Cartesian components of the operator $\boldsymbol{\mathcal{X}}$ do not commute and the standard commutation relations for the components of the OAM and spin are not satisfied either:

$$[\mathcal{X}_i, \mathcal{X}_j] \neq 0, \quad [\mathcal{L}_i, \mathcal{L}_j] \neq ie_{ijk}\mathcal{L}_k, \quad [\zeta_i, \zeta_j] \neq ie_{ijk}\zeta_k, \quad i \neq j; \quad [\mathcal{L}_i, \zeta_j] \neq 0 \quad \text{for any } i, j. \tag{68}$$

The third set defines the projected operators and is useful for the description of the Berry phase effects. For the operators forming this set, the commutation relations are similar to Eq. (68):

$$[\mathfrak{R}_i, \mathfrak{R}_j] \neq 0, \quad [\mathfrak{L}_i, \mathfrak{L}_j] \neq ie_{ijk}\mathfrak{L}_k, \quad [\mathfrak{S}_i, \mathfrak{S}_j] \neq ie_{ijk}\mathfrak{S}_k, \quad i \neq j; \quad [\mathfrak{L}_i, \mathfrak{S}_j] \neq 0 \quad \text{for any } i, j. \tag{69}$$

Certainly, explicit forms of the commutators in Eqs. (68) and (69) differ.

It can be easily shown that the first set is much more convenient than the second and third sets. Besides a commutative geometry, an important reason is a definition of electromagnetic and other interactions. It is very important that the electromagnetic fields act on charges and currents. Therefore, *the electromagnetic interactions are defined by the center-of-charge position but not by the center-of-mass one*. The interaction energy depends on the fields in the center-of-charge point but not in the center-of-mass one. The same situation takes place for gravitational, inertial, and weak interactions. In all quantum-mechanical equations describing the gravitational and inertial interactions (see Refs. [69–79,89] and references therein), the radius vector relates to the position of the mass point coinciding with the center of charge for charged particles with negligible EDMs. Equations of motion obtained with the first (conventional) set of fundamental operators are fully right while some of these equations can be noncovariant [42,91]. When the weak interaction is considered in the framework of QM [101–103], the situation is the same. As a result, there is no reason for a wide use of the second and third sets of fundamental operators for a description of the fundamental interactions. In particular, these operators are useless for relativistic quantum chemistry and physics of heavy atoms. Nevertheless, we agree with Refs. [42,91] that the noncovariance of equations of motion can be avoided by passing to the center-of-mass position. For this purpose, the second set of fundamental operators is useful. Another exception is a determination of the Berry phase effects with the third set. In other cases, one needs to apply the first set of fundamental operators.

The necessity of using the mathematical tool of noncommutative geometry significantly complicates all derivations with the second and third sets. Further, the laboratory-frame spin $\boldsymbol{\zeta}$, the corresponding OAM $\boldsymbol{\mathcal{L}}$, and the projected operators $\boldsymbol{\mathfrak{L}}$ and $\boldsymbol{\mathfrak{S}}$ are momentum dependent. As a result, the commutation relations for their components given by Eqs. (68) and (69) are not similar to the commutation relations (28) for the components of the total angular momentum $\boldsymbol{j}$. In addition, the use of the above-mentioned operators prevents one from introducing the quantum numbers l and s connected with the *conventional* operators $\boldsymbol{l}$ and $\boldsymbol{s}$. Only the conventional operators belonging to the first set satisfies the commutation relations similar to those for the total angular momentum [see Eq. (28)].

The consideration of relativistic operators of the position and spin carried out in this section leads to the conclusions which agree with the results obtained in Refs. [38,40,42,55–58,91]. However, our conclusions contradict the conclusions which have been made in Refs. [9,10,28,29,95,96,104–107] and are widely used in physics of twisted electrons and relativistic quantum chemistry. The analysis of the latter conclusions launched in this section will be finalized in Sec. VI.

VI. RELATED PROBLEMS OF RELATIVISTIC QUANTUM MECHANICS

In this section, we analyze and correct two common errors: a probabilistic interpretation of a wave function in the Dirac representation and an assertion about an existence of SOI for a free particle. We also discuss the problem of *Zitterbewegung*.

A. Probabilistic interpretation of a wave function

Unfortunately, many scientists suppose that the Dirac representation corrupting the connection among energy, momentum, and velocity provides the right distribution of the probability density and the FW representation restoring the Schrödinger picture of relativistic QM distorts this density. While this point of view is not correct, it is presented in almost all papers on twisted (vortex) electrons and, moreover, prevails in publications devoted to some other problems. In particular, the probabilistic interpretation of the wave function in the Dirac representation is commonly used in relativistic quantum chemistry (see below). Of course, this situation is not satisfactory.

It is generally accepted that nonrelativistic Schrödinger QM admits a probabilistic interpretation of the wave function. The classical center-of-charge position $\boldsymbol{R}$ corresponds to the Schrödinger position operator (the radius vector $\boldsymbol{x}$). In the relativistic case, the classical center-of-charge position is a counterpart of the FW position operator which is also equal to the radius vector $\boldsymbol{x}$. This property has been first established in Ref. [3] and unambiguously follows from our analysis. As a result, just the FW wave function being an expansion of the Schrödinger wave function on the relativistic case admits the

probabilistic interpretation. The wave function in the Dirac representation cannot have such an interpretation [11] because the Dirac radius vector $\boldsymbol{r}$ is not the counterpart of the classical position.

It can also be noted that the components of the Schrödinger position operator commute. Therefore, any quantum-mechanical approach based on a position operator with *noncommuting* components cannot be a relativistic extension of the Schrödinger QM. In Sec. V, we have considered the sets of operators, $\boldsymbol{\mathcal{X}}$, $\boldsymbol{\mathcal{L}}$, $\boldsymbol{\zeta}$ and $\mathfrak{R}$, $\mathfrak{L}$, $\mathfrak{S}$, containing the laboratory-frame spin $\boldsymbol{\zeta}$ and the projected operators, respectively. The components of the position operators are noncommuting in the both sets. As a result, the quantum-mechanical approaches based on these sets lead to wave functions which cannot be relativistic extensions of the Schrödinger wave functions and cannot have a *direct* probabilistic interpretation. However, wave functions based on the above-mentioned (second and third) sets of operators can be derived from the FW wave functions. For any set of fundamental operators, the classical limit of the FW Hamiltonian coincides with the *corresponding* classical Hamiltonian. While the Hamiltonians are equal for different sets, their functional dependencies on the corresponding operators of the position, OAM, and spin vary. It can be added that the Schrödinger-Pauli spin operator satisfies the commutation relations (28) which remain valid for the FW spin operator but are violated for the operators $\boldsymbol{\zeta}$ and $\mathfrak{S}$.

Therefore, the assertion that the quantity $\varrho_D(\boldsymbol{r}) = \Psi_D^\dagger(\boldsymbol{r})\Psi_D(\boldsymbol{r})$ is the probability density of the particle position [9,10,104] is not correct. In fact, the probability density of the particle position is equal to $\varrho(\boldsymbol{x}) = \varrho_{\rm FW}(\boldsymbol{x}) = \Psi_{\rm FW}^\dagger(\boldsymbol{x})\Psi_{\rm FW}(\boldsymbol{x})$ [11,108]. This statement has also been made in Refs. [34,79] and has been implicitly used in Refs. [7,8,109,110]. The basic role of the FW representation for a particle in nonstationary fields has been properly shown in Ref. [90] (see also Sec. IV).

The quantities ϱ_D and $\varrho_{\rm FW}$ can significantly differ [10,11,111,112]. A general connection between the Dirac and FW wave functions at the exact FW transformation has been obtained in Ref. [112]. In this case, upper spinors in the two representations differ only by constant factors and lower FW spinors vanish. An origin of the difference between ϱ_D and $\varrho_{\rm FW}$ is clear from the following derivation. Since $\Psi_{\rm FW} = U_{\rm FW}\Psi_D$ and $U_{\rm FW}$ is a self-adjoint unitary operator, the integration of the probability density results in

$$\int \varrho_{\rm FW} dV = \int \Psi_{\rm FW}^\dagger \Psi_{\rm FW} dV = \int \left(\Psi_D^\dagger U_{\rm FW}^{-1}\right)(U_{\rm FW}\Psi_D) dV$$
$$= \int \Psi_D^\dagger \left(U_{\rm FW}^{-1} U_{\rm FW}\Psi_D\right) dV = \int \Psi_D^\dagger \Psi_D dV = 1,$$

where the operator $U_{\rm FW}^{-1}$ in $(\Psi_D^\dagger U_{\rm FW}^{-1})$ and $(U_{\rm FW}^{-1}U_{\rm FW}\Psi_D)$ acts to the left and to the right, respectively. However, the self-adjointness of operators manifests at the integration but cannot be used in any fixed point of a domain of definition. Therefore,

$$\Psi_{\rm FW}^\dagger \Psi_{\rm FW} = \left(\Psi_D^\dagger U_{\rm FW}^{-1}\right)(U_{\rm FW}\Psi_D) \neq \Psi_D^\dagger \Psi_D$$

and $\varrho_{\rm FW} \neq \varrho_D$.

The probabilistic interpretation of the FW wave function allows one to calculate expectation values of all operators. In particular, the mean squared radius $\langle r^2\rangle$ and the quadrupole moment tensor Q_{ij} are given by

$$\langle r^2\rangle = \int \Psi_{\rm FW}^\dagger \boldsymbol{x}^2 \Psi_{\rm FW} dV,$$
$$Q_{ij} = \int \Psi_{\rm FW}^\dagger (3x_i x_j - \boldsymbol{x}^2\delta_{ij})\Psi_{\rm FW} dV. \tag{70}$$

In relativistic quantum chemistry, the term "FW transformation" is used for the original transformation by Foldy and Wouthuysen [3] and the relativistic FW transformation is called the "Douglas-Kroll-Hess transformation." The latter transformation can be carried out with any needed accuracy. For this purpose, analytical or numerical calculations can be fulfilled. In contemporary relativistic quantum chemistry, the point of view contradictory to our analysis is generally accepted (see Sec. 15.2 in Ref. [28] and Refs. [29,105,106]). It is supposed that expectation values of operators are defined in the *Dirac* representation. In this case, the use of the FW representation needs the transformation of operators to the FW representation and expectation values of *transformed* operators are determined. The expectation values of any operator A in the Dirac and FW representations are defined by

$$\langle A\rangle \equiv \langle A_D\rangle = \int \Psi_D^\dagger A \Psi_D dV$$
$$= \int \Psi_{\rm FW}^\dagger (U_{\rm FW} A U_{\rm FW}^{-1})\Psi_{\rm FW} dV = \int \Psi_{\rm FW}^\dagger A' \Psi_{\rm FW} dV,$$
$$\tilde{A} \equiv \langle A_{\rm FW}\rangle = \int \Psi_{\rm FW}^\dagger A \Psi_{\rm FW} dV, \quad A' = U_{\rm FW} A U_{\rm FW}^{-1}. \tag{71}$$

The difference

$$PCE(A) = \langle A\rangle - \tilde{A} \tag{72}$$

is called the "picture change error" [28,29,105,106]. For example, the formula used for a calculation of the quadrupole moment tensor reads

$$Q_{ij} = \int \Psi_D^\dagger (3x_i x_j - \boldsymbol{r}^2\delta_{ij})\Psi_D dV. \tag{73}$$

Our analysis unambiguously shows that this definition is not correct. The picture change error is, indeed, equal to zero and the expectation values of all operators should be defined in the FW representation. Therefore, all results obtained in relativistic quantum chemistry with Eq. (72) should be reconsidered.

B. Spin-orbit interaction for a free particle

The analysis presented in Secs. III and IV shows the correspondence between the classical rest-frame spin $\boldsymbol{S}$, the Pauli spin, and the FW mean-spin operator ($\boldsymbol{s} = \hbar\boldsymbol{\Sigma}/2$ in the FW representation). This correspondence has been discovered by Foldy and Wouthuysen [3] and has been shown in Refs. [32,37,39,46–54]. Evidently, the FW mean-spin operator commutes with the FW Hamiltonian (25) and the FW mean-OAM operator ($\boldsymbol{l} = \boldsymbol{x}\times\boldsymbol{p}$ in the FW representation). Therefore, the SOI cannot exist for the conventional rest-frame spin operator $\boldsymbol{s}$ and the corresponding OAM operator $\boldsymbol{l}$. In the Dirac representation, the operator $\hbar\boldsymbol{\Sigma}/2$ does not commute with the Dirac Hamiltonian. However, it does not describe the conventional spin defined by Eq. (34). Thus,

applying the first set of fundamental operators (see Sec. V) leads to the nonexistence of the SOI.

In Refs. [95,96,107], the existence of the SOI for a free Dirac particle has been claimed. This statement is based on the assumption that the quantum-mechanical counterparts of the position, OAM, spin, and other fundamental classical variables are the corresponding operators in the *Dirac* representation. However, it has been explicitly shown in numerous publications considered in detail in Secs. III–V that these counterparts are the corresponding operators in the FW representation, $\boldsymbol{x}, \boldsymbol{l}, \boldsymbol{s}$. In relation to the spin, it has been made in Refs. [3,4,46,50,51,54–57]. The connection between the classical and quantum-mechanical descriptions of the spin has been expounded in Secs. III–V. All these results contradict to the key statement in Ref. [96] that the spin is defined by the operator $\boldsymbol{s}_D = \hbar\boldsymbol{\Sigma}/2$ in the *Dirac* representation.

It is instructive to discuss why this statement leads to the SOI for a free particle. The use of the projected operators analyzed in Sec. V considerably simplifies the consideration of the SOI. There is some similarity between operators in the Dirac representation and the corresponding projected operators. For any localized particle state, they have the same expectation values [93,96]. In particular, the spin operator in the *Dirac* representation $\boldsymbol{s}_D$ transformed to the FW representation takes the form [3]

$$\mathfrak{s}_{D\to\mathrm{FW}} = \frac{m\boldsymbol{\Sigma}}{2\epsilon} + \frac{\boldsymbol{p}(\boldsymbol{p}\cdot\boldsymbol{\Sigma})}{2\epsilon(\epsilon+m)} + \frac{i\boldsymbol{\gamma}\times\boldsymbol{p}}{2\epsilon}. \tag{74}$$

Its similarity to the projected spin operator in the FW representation $\mathfrak{S}_{\mathrm{FW}}$ defined by Eq. (65) is evident. Since the lower FW spinor for positive-energy states and the upper FW spinor for negative-energy ones are equal to zero, the expectation values of the operators $\mathfrak{S}_{\mathrm{FW}}$ and $\mathfrak{s}_{D\to FW}$ coincide. Certainly, they also coincide with the expectation values of these operators in the Dirac representation, $\langle\mathfrak{S}_D\rangle$ and $\langle\boldsymbol{s}_D\rangle$.

It is worth mentioning that the Dirac operators and the corresponding projected ones are not equivalent. In particular, the Dirac spin operator satisfies the standard algebra $[(s_D)_i, (s_D)_j] = ie_{ijk}(s_D)_k$ $(i, j, k = 1, 2, 3)$. Its square is equal to $\boldsymbol{s}_D^2 = s(s+1)\mathcal{I} = 3\mathcal{I}/4$, where $\mathcal{I}$ is the 2×2 unit matrix. The Dirac position operator has commutative components $([r_i, r_j] = 0)$. These properties remain valid in any representation. The corresponding projected operators do not satisfy these properties [see Eq. (69)]. Because of the nonequivalence of the Dirac and projected operators and the inconsistency of the former operators with any fundamental classical variables, the Dirac operators are useless. In contrast to them, the projected operators may be useful for a solution of some physical problems. However, their application needs noncommutative geometry (see Sec. V).

The connection between the expectation values of the Dirac spin operator and the rest-frame spin (e.g., "mean spin angular momentum" [3]) follows from Eqs. (65) and (74) and is given by Eq. (7) in Ref. [96]:

$$\langle\boldsymbol{s}_D\rangle = \frac{m}{\epsilon}\langle\boldsymbol{s}\rangle + \frac{\boldsymbol{p}(\boldsymbol{p}\cdot\langle\boldsymbol{s}\rangle)}{\epsilon(\epsilon+m)}. \tag{75}$$

In disagreement with Ref. [96], the Dirac spin operator and the projected spin substantially differ from the spatial parts of the four-component spin operator and the Pauli-Lubanski four-vector, $\boldsymbol{a}$ and $\boldsymbol{W} = m\boldsymbol{a}$, respectively. This fact has already been mentioned in Sec. V.

The opposite statement presented in Ref. [96] is rather strange because Eqs. (15) and (16) in this paper give the correct relation between the projected and Pauli-Lubanski operators, $\mathfrak{S}_{\mathrm{FW}} = \boldsymbol{W}/\epsilon$ [see also Eq. (60) in Sec. V].

It is also claimed in Ref. [96] that the projected operators are covariant. However, the results obtained in Refs. [38,40–42,91] unambiguously show that covariant equations of motion can be obtained *only* with the laboratory-frame spin $\boldsymbol{\zeta}$ and the corresponding operators of the position and OAM, $\boldsymbol{\mathcal{X}}$ and $\boldsymbol{\mathcal{L}}$. These quantities form the *second* set of fundamental operators (see Sec. V). As a result, the use of the projected operators of the position, OAM, and spin leads to noncovariant equations of motion for the spin and momentum in the presence of external fields. Even if some equations of spin motion are covariant, it is not so in the general case. This conclusion remains valid for the corresponding operators in the Dirac representation, $\boldsymbol{r}, \boldsymbol{l}_D, \boldsymbol{s}_D$. Moreover, even the application of $\boldsymbol{a}$ as *a spin part of the total angular momentum* $\boldsymbol{j}$ with the corresponding redefinition of the position operator cannot result in covariant equations of motion. In this case, $\boldsymbol{j} = \boldsymbol{\varrho}\times\boldsymbol{p} + \boldsymbol{a}$, where $\boldsymbol{\varrho}$ is the corresponding position operator. The quantities $\boldsymbol{a}$ and $\boldsymbol{j}$ are covariant. However, $\boldsymbol{a}$ is a spatial part of a four-vector and $\boldsymbol{j}$ is formed by spatial components of an antisymmetric tensor. Therefore, the quantities $\boldsymbol{a}$ and $\boldsymbol{j}$ are dissimilar and their simultaneous use does not lead to the covariant equations of motion. The problem of the covariant fundamental operators and the covariant equations of motion has been definitively solved in Refs. [38,40]. However, these papers are not cited in Ref. [96].

We should also mention that Eq. (7) in Ref. [96] coinciding with Eq. (75) in the present study has nothing in common with "the Lorentz boost to the rest frame." It describes the connection between the expectation values of the Dirac spin $\langle\boldsymbol{s}_D\rangle$ (defined as $\langle\boldsymbol{S}\rangle$ in Ref. [96]) and the FW (rest-frame) spin $\langle\boldsymbol{s}\rangle$. The Lorentz boosts define only the connections between the expectation values of the FW spin and the spatial parts of either the four-component spin vector ($\langle\boldsymbol{a}\rangle$) or the antisymmetric spin tensor ($\langle\boldsymbol{\zeta}\rangle$). These connections are given by

$$\langle\boldsymbol{a}\rangle = \langle\boldsymbol{s}\rangle + \frac{\boldsymbol{p}(\boldsymbol{p}\cdot\langle\boldsymbol{s}\rangle)}{m(\epsilon+m)},$$
$$\langle\boldsymbol{\zeta}\rangle = \frac{\epsilon}{m}\langle\boldsymbol{s}\rangle - \frac{\boldsymbol{p}(\boldsymbol{p}\cdot\langle\boldsymbol{s}\rangle)}{m(\epsilon+m)}. \tag{76}$$

Evidently, they substantially differ from the connection described by Eq. (75) (Eq. (7) in Ref. [96]).

Our next comment relates to one of principal Pryce's assumptions [1] that a choice of the fundamental variables $\boldsymbol{Q}, \boldsymbol{L}, \boldsymbol{S}$ is not unique and the use of different sets of these variables is possible. The revision of this assumption made in Ref. [96] is unsubstantiated. The authors of this paper have considered the first and third sets of fundamental operators and have concluded that only the latter set of these operators correctly and exhaustively describes physical phenomena. However, it is clear from Ref. [1] and subsequent publications that the use of the ten-parameter Poincaré group leaves a room for different definitions of the position and spin operators satisfying Eqs. (18) and (27). Of course, useful

definitions should have appropriate substantiations. Nevertheless, *all* well-substantiated position, OAM, and spin operators are correct. We have analyzed the three sets of fundamental operators. Each of them is useful for a description of some physical phenomena and dynamical equations for the spin and momentum obtained with all the sets should agree. Furthermore, any other set of fundamental operators (even based on a confusion) leads to correct dynamical equations. Certainly, different sets are not equally convenient. We mentioned above that the second and third sets of fundamental operators are not useful for relativistic quantum chemistry and physics of heavy atoms. The preferences of the first set are the commutative geometry, simple commutation relations, and the independence of potentials and strengths of external fields from the momentum and spin of the particle. These preferences are seen from the following example. When the first set is used, the scalar potential of an electric field in the FW representation has the simple form $\phi(\boldsymbol{x})$. For the set of projected operators, it is given by $\phi(\mathfrak{R}_{\rm FW} + \frac{\mathfrak{S}_{\rm FW}\times \boldsymbol{p}}{m(\epsilon+m)})$. While the potential $\phi(\mathfrak{R}_{\rm FW})$ incorporates the SOI with an external electric field [96], the need for use of noncommutative geometry makes this set to be inconvenient.

The analysis fulfilled unambiguously shows that there is not the SOI if the terms "spin" and "OAM" denote the *conventional* rest-frame spin operator $\boldsymbol{s}$ and the corresponding OAM operator $\boldsymbol{l}$. Since different definitions of the fundamental operators of the position, OAM, and spin are admissible, the existence or nonexistence of the SOI for free particles depends on these definitions. More precisely, the SOI does not exist for the conventional fundamental operators containing the first set but exists for the operators forming other sets. However, it would be misleading to assert that the SOI exists but to omit the specification that this effect takes place, e.g., for projected operators based on noncommutative geometry and specific commutation relations. We also underline that the fundamental classical variables correspond to the related fundamental operators in the FW representation while the Dirac representation distorts these operators.

We should also comment the statement [96] that the FW representation "cannot be used for massless particles." The application of relativistic methods of the FW transformation explicitly shows the inaccuracy of this statement. Even the early paper by Blount [22] has been demonstrated (despite some imperfections) the validity of the FW representation in the massless limit $m \to 0$. The appropriateness of the FW representation in the massless limit is also clearly seen from Eqs. (13)–(15), (37), (41), (43), (44), and (48) [113]. The only important difference between the FW transformations for massive and massless particles is the loss of classical interpretation of the spin operator $\boldsymbol{s} = \hbar\boldsymbol{\Sigma}/2$ when $m = 0$. It can be added that the FW representation has been used for the photon in Refs. [110,114].

Nevertheless, we should note that particle physics does not support the smooth transition to the massless limit. Spin-0 and spin-1/2 particles can be considered as exceptions. For the photon, the FW transformation significantly differs from that for massive spin-1 particles [88]. It is well known that massive spin-1 particles can have the helicity $0, \pm 1$ but the photon cannot exist in a helicity zero state. The rest-frame spin of massive spin-1 particles is described by the 3×3 matrix (45). Its use for a fixed momentum direction allows one to obtain the three above-mentioned eigenvalues of the helicity operator. However, this matrix cannot reproduce the two helicity eigenvalues ±1 of the photon. While the matrix (45) is also applied for the photon [114–116], a possibility to connect it with the photon spin seems to be, at least, doubtful. This simple analysis shows a deep difference between massless particles with the spins 1/2 and 1. Therefore, results obtained for the photon cannot be directly applied to a massless spin-1/2 particle. For the photon, the laboratory-frame spin operator leading to the SOI can be used.

We should also note that QM cannot provide for an exhaustive description of massless particles. For this purpose, the mathematical tool of quantum field theory is needed. Nevertheless, some specific properties of massless particles can be studied in the framework of QM. In this case, the FW transformation can be helpful even for the photon (see Refs. [110,114]).

C. *Zitterbewegung*

Zitterbewegung is a well-known effect consisting of a superfast trembling motion of a free Dirac particle first described by Schrödinger [117]. This effect is also known for a scalar particle [118,119]. Our preceding analysis perfectly agrees with the conclusions about the origin and observability of this effect made in Refs. [119–121].

As is well known, the Dirac velocity operator is given by

$$\boldsymbol{v}_D \equiv \frac{d\boldsymbol{r}}{dt} = i[\mathcal{H}_D, \boldsymbol{r}] = \boldsymbol{\alpha}. \tag{77}$$

This operator is time dependent:

$$\frac{d\boldsymbol{\alpha}}{dt} = i[\mathcal{H}_D, \boldsymbol{\alpha}] = i\{\boldsymbol{\alpha}, \mathcal{H}_D\} - 2i\boldsymbol{\alpha}\mathcal{H}_D = 2i(\boldsymbol{p} - \boldsymbol{\alpha}\mathcal{H}_D). \tag{78}$$

The problem is usually considered in the Heisenberg picture:

$$\boldsymbol{v}_D(t) = e^{i\mathcal{H}_D t}\boldsymbol{\alpha}e^{-i\mathcal{H}_D t}. \tag{79}$$

In the Schrödinger picture, the result is the same. We suppose that the eigenvalues of the momentum and Hamiltonian operators are $\mathfrak{p}$ and H, respectively. In this case, Eq. (78) can be presented in terms of the Dirac velocity operator:

$$\frac{d\boldsymbol{v}_D}{dt} = 2i(\mathfrak{p} - \boldsymbol{v}_D H). \tag{80}$$

Its integration shows the oscillatory behavior of the Dirac velocity:

$$\boldsymbol{v}_D(t) = \left[\boldsymbol{v}_D(0) - \frac{\mathfrak{p}}{H}\right]e^{-2iHt} + \frac{\mathfrak{p}}{H}. \tag{81}$$

The evolution of the Dirac position operator is given by

$$\boldsymbol{r}_D(t) = \boldsymbol{r}_D(0) + \frac{\mathfrak{p}t}{H} + \frac{i}{2H}\left[\boldsymbol{v}_D(0) - \frac{\mathfrak{p}}{H}\right](e^{-2iHt} - 1). \tag{82}$$

For a free scalar (spin-0) particle, the initial Feshbach-Villars Hamiltonian reads [122]

$$\mathcal{H}_{FV} = \rho_3 m + (\rho_3 + i\rho_2)\frac{\boldsymbol{p}^2}{2m}. \tag{83}$$

The velocity operator in the Feshbach-Villars representation is equal to

$$\boldsymbol{v}_{FV} = (\rho_3 + i\rho_2)\frac{\boldsymbol{p}}{m}. \tag{84}$$

The corresponding acceleration operator is defined by the equation similar to Eq. (78) [119]:

$$\frac{d\boldsymbol{v}_{FV}}{dt} = i[\mathcal{H}_{FV}, \boldsymbol{v}_{FV}] = i\{\boldsymbol{v}_{FV}, \mathcal{H}_{FV}\} - 2i\boldsymbol{v}_{FV}\mathcal{H}_{FV}$$
$$= 2i(\boldsymbol{p} - \boldsymbol{v}_{FV}\mathcal{H}_{FV}). \tag{85}$$

We suppose that the eigenvalues of the momentum and Hamiltonian operators are $\mathfrak{p}$ and H, respectively. As a result, the final equations of dynamics of the free scalar particle [119] are equivalent to the corresponding equations for the Dirac particle:

$$\boldsymbol{v}_{FV}(t) = \left[\boldsymbol{v}_{FV}(0) - \frac{\mathfrak{p}}{H}\right]e^{-2iHt} + \frac{\mathfrak{p}}{H}, \tag{86}$$

$$\boldsymbol{r}_{FV}(t) = \boldsymbol{r}_{FV}(0) + \frac{\mathfrak{p}t}{H} + \frac{i}{2H}\left[\boldsymbol{v}_{FV}(0) - \frac{\mathfrak{p}}{H}\right](e^{-2iHt} - 1). \tag{87}$$

However, it has been pointed out [49] that the operators $\boldsymbol{p}$ and $\boldsymbol{v}$ can be proportional for free particles with any spin. The proportionality of these operators vanishing the acceleration ($d\boldsymbol{v}/(dt) = 0$) can be achieved by the FW transformation. In the FW representation, the Dirac Hamiltonian takes the form (25) and the velocity operator is given by

$$\boldsymbol{v}_{\mathrm{FW}} = \beta\frac{\boldsymbol{p}}{\sqrt{m^2 + \boldsymbol{p}^2}} = \frac{\boldsymbol{p}}{\mathcal{H}_{\mathrm{FW}}}. \tag{88}$$

Similar relations can be obtained for particles with any spin.

It has been shown in Ref. [119] that *Zitterbewegung* is the result of the interference between positive- and negative-energy states. It disappears for the "mean position operator" [3], the position operator in the FW representation [119–121]. "*Zitterbewegung* was found to be a feature of a particular choice of coordinate operator associated with Dirac's formulation of relativistic electron theory" [120] (p. 334). It can be removed by carrying out the unitary transformation to the FW representation. Experiments do not distinguish between equally valid but different representations leading to the same observables and the transition to the FW representation does not change the physics [121]. It can be concluded that *Zitterbewegung* is not an observable [121].

Our analysis fully agrees with this conclusion. The derivations presented in this subsection show that *Zitterbewegung* is an effect attributed to the Dirac and Feshbach-Villars position and velocity operators but not to the corresponding FW operators. However, just the FW position and velocity operators are the quantum-mechanical counterparts of the classical position and velocity. In the Dirac representation, these quantum-mechanical counterparts are defined by the operators $\boldsymbol{X}$ [see Eq. (33)] and $d\boldsymbol{X}/(dt)$. For the latter operators, *Zitterbewegung* does not take place in any representation. Our analysis shows that the Dirac and Feshbach-Villars position and velocity operators are not the quantum-mechanical counterparts of the classical position and velocity and, in accordance with Ref. [121], *Zitterbewegung* cannot be observed.

However, there exists an effect which is more or less similar to *Zitterbewegung*. Feshbach and Villars [122] have obtained the eigenfunctions of the mean position operator $\boldsymbol{X}$ and have proven that they are not localized in the configuration space but are extended over a radius of the order of the Compton wavelength. These eigenstates are the narrowest possible free wave packets composed only of positive energy states whose behavior agrees with the nonrelativistic (Schrödinger) pattern. The nonlocality of the particle position takes also place for spinning particles [120,123]. It has been emphasized by Sakurai [123] that "the nonlocality of $\boldsymbol{X}$ is the price we must pay" for the absence of *Zitterbewegung*. This indirect connection between the nonlocality of the particle position and *Zitterbewegung* has also been considered in other works (see, e.g., Refs. [124–126]). The nonlocality of the particle position manifests in the Darwin interaction defined by Eq. (14).

VII. DISCUSSION AND SUMMARY

The goal of the present study is a change of the paradoxical contemporary situation in the relativistic QM when the forms of the position and spin operators securely established sixty years ago are "forgotten" while incorrect and unsubstantiated definitions of these operators are widely used. The Dirac representation distorts the connection among the energy, momentum, and velocity operators. Therefore, it is too optimistic to believe that the Dirac operators of the position and spin, $\boldsymbol{r}$ and $\boldsymbol{s}_D$, are relativistic extensions of the corresponding Schrödinger-Pauli operators and quantum-mechanical counterparts of the classical position and spin. Indeed, there are not any serious arguments in favor of this point of view which has been proclaimed in Refs. [9,10,28,29,104–106] and has been explicitly or implicitly presented in almost all papers devoted to twisted electrons. Some exceptions, in particular, Refs. [7,8,109,110], are not numerous. Paradoxically, the correct results obtained for the position and spin operators sixty years ago were widely discussed [3,4,31–35,39,46–57]. Nevertheless, the researchers holding the opposite point of view never carefully considered the arguments obtained in the above-mentioned publications in favor of a definition of the fundamental operators in the FW representation. The proof of this definition carried out in Refs. [3,4,31–35,39,46–57] is straightforward (see Sec. III).

More recent achievements allowing one to perform the FW transformation for relativistic scalar and spinning particles in external fields (see Sec. II) have allowed us to give important arguments in support of this definition. We have shown in Sec. IV that the position and spin operators corresponding to the conventional classical variables (the radius vector $\boldsymbol{R}$ and the rest-frame spin $\boldsymbol{S}$) are the FW operators $\boldsymbol{x}$ and $\boldsymbol{s} = \hbar\boldsymbol{\Sigma}/2$ and their transforms to other representations, including the Dirac representation. This property remains valid in the presence of external fields. Our analysis unambiguously shows that the fundamental spin operator is defined in the particle rest frame but not in the instantaneously accompanying one.

The main result of the present study is the comparative analysis of alternative definitions of the position and spin operators. Certainly, the use of the Dirac position operator $\boldsymbol{r}$ as a quantum-mechanical counterpart of the classical position variable brings confusion. A determination of the probability density with Dirac eigenfunctions [9,10,104] distorts the

electron charge distribution in a free space and atoms. In relativistic quantum chemistry, a calculation of expectation values with FW eigenfunctions but with FW transforms of *Dirac* operators [28,29,105,106] leads to incorrect results due to unnecessary corrections for the picture change errors.

A calculation of expectation values of the spin with the Dirac spin operator $\boldsymbol{s}_D$ [95,96,107] has similar consequences. As a result, the illusory effect of the SOI appears. The SOI does not exist for a free particle if the terms "spin" and "OAM" define the *conventional* spin and OAM operators which, in particular, satisfy the commutation relations $[s_i, s_j] = ie_{ijk}s_k$, $[l_i, l_j] = ie_{ijk}l_k$, $[l_i, s_j] = 0$. Other definitions of these operators are possible, but all of them do not satisfy these commutation relations and are based on noncommutative geometry. For such definitions, the spin-orbit interaction can exist. The Dirac spin operator has the same expectation values as the projected spin operator. Both of them substantially differ from the two covariant spin operators given by the spatial parts of the four-component spin vector and the antisymmetric spin tensor, $\boldsymbol{a}$ and $\boldsymbol{\zeta}$, respectively. Unfortunately, Refs. [95,96,107] present the misleading conclusion about the SOI. The problem of the SOI is a matter of a definition of the spin. The conventional QM based on commutative geometry leads to the nonexistence of the SOI.

We can conclude that the basic representation in relativistic QM is the FW one because it provides for a direct similarity between the relativistic quantum-mechanical operators and the classical variables.

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