Two roles of relativistic spin operators

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Operators that are associated with several important quantities, such as angular momentum, play a double role: they are both generators of the symmetry group and ‘‘observables.’’ The analysis of different splittings of angular momentum into ‘‘spin’’ and ‘‘orbital’’ parts reveals the difference between these two roles. We also discuss a relation of different choices of spin observables to the violation of Bell inequalities.

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Spin degrees of freedom appear in a variety of applications in quantum information theory and foundations of quantum mechanics [1,2], and usually are analyzed nonrelativistically. In a relativistic domain an observable of choice is the helicity $\mathbf{S}\cdot\mathbf{p}$, which is well defined for particles with sharp momentum (for beams in accelerators typical spread to energy ratios are about 10^{-3}–10^{-4} [5]). Nevertheless, there is also an interest in spin operators in general [6–10].

In this paper, we consider two standard spin operators for massive spin-$\frac{1}{2}$ particles, the rest-frame spin and the Dirac spin operator $\mathbf{\Sigma}$ that is associated with the spin of moving particles as seen by a stationary observer [3]. These two quantities can serve as prototypes (or building blocks) for various alternative ‘‘spin operators’’ that appear in the literature [7,8].

Spin and many other operators play a double role: they are symmetry generators and at the same time are ‘‘observables’’ in a sense of von Neumann measurement theory. In most cases, both in classical and quantum physics, there is no need to distinguish between these two roles, a notable exception being Koopmanian formulation of classical mechanics, where the generators of symmetries and observables are represented by different operators [1,11].

We begin from a review of necessary concepts and present a list of properties that an operator should satisfy in order to be called ‘‘spin.’’ Then we show that even if $\mathbf{\Sigma}$ is a discrete-degrees-of-freedom part of the generator of rotation, it is impossible to construct one-particle Hilbert-space operator that gives the same statistics and satisfies the spin operator requirements. This is similar to the analysis of van Enk and Nienhuis of splitting angular-momentum operator of electromagnetic field into spin and orbital parts. They show that both are measurable quantities, but neither of them satisfies commutation relations of the angular-momentum operator [9]. Finally, we discuss how a choice of the spin operator affects a degree of violation of the Bell-type inequalities.

For the sake of simplicity, we consider only states with a well-defined momentum. A nonzero spread in momentum has important consequences for quantum information theory but is irrelevant for our present subject and is described elsewhere [12]. We set $\hbar=c=1$.

Following Wigner [13] the Hilbert space is

$$\mathcal{H}=\mathbb{C}^2\otimes L^2(\mathbb{R}^3,d\mu(p)),\quad d\mu(p)=\frac{1}{(2\pi)^3}\frac{d^3\mathbf{p}}{(2p^0)},\tag{1}$$

where $p^0=\sqrt{m^2+\mathbf{p}^2}$. The generators of the Poincaré group are represented by

$$P^\mu=p^\mu,\tag{2a}$$

$$\mathbf{K}=-ip^0\nabla_{\mathbf{p}}-\frac{\mathbf{p}\times\mathbf{S}}{m+p^0},\tag{2b}$$

$$\mathbf{J}=-i\mathbf{p}\times\nabla_{\mathbf{p}}+\mathbf{S},\tag{2c}$$

where the angular momentum is split into orbital and spin parts, respectively. We label basis states $|\sigma,p\rangle$. Pure state of definite momentum and arbitrary spin will be labeled as $\binom{\alpha}{\beta}|p\rangle$.

Lorentz transformation Λ, $y^\mu=\Lambda^\mu_\nu x^\nu$, induces a unitary transformation of states. In particular,

$$U(\Lambda)|\sigma,p\rangle=\sum_\xi D_{\xi\sigma}[W(\Lambda,p)]|\xi,\Lambda p\rangle,\tag{3}$$

where $D_{\xi\sigma}$ are the matrix elements of a unitary operator D which corresponds to a Wigner rotation $W(\Lambda,p)$. The Wigner rotation itself is given by

$$W(\Lambda,p):=L^{-1}_{\Lambda p}\Lambda L_p\,,\tag{4}$$

where L_p is a standard pure boost that takes a standard momentum $k_R=(m,0,0,0)$ to a given momentum p. Explicit formulas of L_p are given, e.g., in Refs. [4,14].

It is well known [4] that for a pure rotation $\mathcal{R}$ the three-dimensional Wigner rotation matrix is the rotation itself,

$$W(\mathcal{R},p)=\mathcal{R},\quad \forall p=(E(\mathbf{p}),\mathbf{p}).\tag{5}$$

As a result, Wigner's spin operators are nothing else but halves of Pauli matrices (tensored with the identity of L^2).

A useful corollary of Eqs. (3) and (4) is a property of the rest-frame spin. If an initial state (in the rest frame) is

$$|\Psi\rangle=\alpha\left|\frac{1}{2},k_R\right\rangle+\beta\left|-\frac{1}{2},k_R\right\rangle,\tag{6}$$

with $|\alpha|^2+|\beta|^2=1$, then a pure boost Λ leads to

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$$U(\Lambda)|\Psi\rangle=\begin{pmatrix}\alpha\\ \beta\end{pmatrix}|\Lambda k_R\rangle. \tag{7}$$

A Pauli-Lubanski vector is an important quantity that is constructed from the group generators [14],

$$w_\varrho=\frac{1}{2}\epsilon_{\lambda\mu\nu\varrho}P^\lambda M^{\mu\nu}, \tag{8a}$$

$$w_0=-\mathbf{P}\cdot\mathbf{J},\quad \mathbf{w}=P^0\mathbf{J}+\mathbf{P}\times\mathbf{K}, \tag{8b}$$

where $M^{12}=J^3, M^{01}=K^1$, etc. In particular, it helps in splitting spin out of the angular momentum,

$$\mathbf{S}=\frac{1}{m}\left(\mathbf{w}-\frac{w^0\mathbf{P}}{P^0+m}\right). \tag{9}$$

For a particle with definite four-momentum p, this formula just says that the components of a spin operator are three spacelike components of the Pauli-Lubanski operator at the rest frame,

$$S_k=(L_p^{-1}w)_k. \tag{10}$$

We take three following properties as defining a natural relativistic extension of the spin observable.

(1) The triple of operators $\mathbf{S}$ reduces in the rest frame to a nonrelativistic expression $\mathbf{w}_R/m$.

(2) It is a three-vector

$$[J_j,S_k]=i\epsilon_{jkl}S_l. \tag{11}$$

(3) It satisfies spin commutation relation

$$[S_j,S_k]=i\epsilon_{jkl}S_l. \tag{12}$$

A simple lemma (the proof can be found in Ref. [14]) shows that this operator is unique, under one technical assumption.

Lemma 1. The only triple of operators $\mathbf{S}$ that satisfies the above assumptions, and in addition is a linear combination of the operators w^μ, is given by Eq. (9).

To discuss Dirac spin operators we need more elements of field-theoretical formalism. States of definite spin and momentum are created from the vacuum by creation operators $|\sigma,p\rangle=\hat{a}^\dagger_{\sigma p}|0\rangle$, while antiparticles are created by $\hat{b}^\dagger_{\sigma p}$. We use the following normalization convention:

$$\langle\sigma,p|\xi,q\rangle=(2\pi)^3(2p^0)\delta_{\sigma\xi}\delta^{(3)}(\mathbf{p}-\mathbf{q}). \tag{13}$$

Field operators are usually written with Dirac spinors. A Hilbert space and unitary representation on it can be constructed from the bispinorial representation of the Poincaré group. To this end we take positive-energy solutions of Dirac equation, which form a subspace of the space of all four-component spinor functions $\Psi=\Psi^\lambda(p)$, $\lambda=1,\ldots,4$. A Lorentz-invariant inner product becomes positive definite and the subspace of positive-energy solutions becomes a Hilbert space. The generators in this representation are

$$P^\mu=p^\mu,\quad J^{\mu\nu}=L^{\mu\nu}+S^{\mu\nu}, \tag{14}$$

where

$$L^{lm}=i\left(p^l\frac{\partial}{\partial p_m}-p^m\frac{\partial}{\partial p_l}\right), \tag{15a}$$

$$L^{0m}=ip^0\frac{\partial}{\partial p_m},\quad S^{\mu\nu}=\frac{i}{4}[\gamma^\mu,\gamma^\nu]. \tag{15b}$$

A double infinity of plane-wave positive-energy solutions of the Dirac equation (functions $u_p^{(1/2)}$ and $u_p^{(-1/2)}$ that are proportional to $e^{-ip\cdot x}$) is a basis of this space. Basis vectors of Wigner and Dirac Hilbert spaces are related by [14]

$$u_p^{(1/2)}\Leftrightarrow\left|\frac{1}{2},p\right\rangle,\quad u_p^{(-1/2)}\Leftrightarrow\left|-\frac{1}{2},p\right\rangle. \tag{16}$$

A discrete part of $S^{\mu\nu}$ ($\Sigma^1/2\equiv S^{23}$, etc.) is a Dirac spin operator. In standard or Weyl representations, it looks like

$$\mathbf{\Sigma}=\begin{pmatrix}\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma}\end{pmatrix}. \tag{17}$$

It is possible to say that different propositions for spin operators are different ways to split $\mathbf{J}$. However, a momentum-dependent Foldy-Wouthuysen transformation takes $\mathbf{\Sigma}$ to the spinor representation of $\mathbf{S}$ [3,14]. Hence, we see that the difference is essentially in a covariant treatment.

A field operator is constructed with the help of plane-wave solutions of Dirac equations [3,4,14],

$$\hat{\phi}(x)=\sum_{\sigma=1/2,-1/2}\int d\mu(p)(e^{ix\cdot p}v_p^\sigma\hat{b}^\dagger_{\sigma p}+e^{-ix\cdot p}u_p^\sigma\hat{a}_{\sigma p}), \tag{18}$$

where v_p^σ are negative-energy plane-wave solutions of Dirac equation.

Using field transformation properties it is a standard exercise to get the following expression for Dirac spin operator [15]:

$$\hat{\mathbf{\Sigma}}=::\int d^3x\,\hat{\phi}^\dagger(x)\frac{\mathbf{\Sigma}}{2}\hat{\phi}(x)::, \tag{19}$$

where :: designates a normal ordering. Wigner spin is given by

$$\hat{\mathbf{S}}=\frac{1}{2}\sum_{\eta,\zeta}\boldsymbol{\sigma}_{\eta\zeta}\int d\mu(p)(\hat{a}^\dagger_{\eta p}\hat{a}_{\zeta p}+\hat{b}^\dagger_{\eta p}\hat{b}_{\sigma p}). \tag{20}$$

An interpretation of $\hat{\mathbf{\Sigma}}$ and $\hat{\mathbf{S}}$ as observables is based on the analysis of one-particle states with well-defined momentum and an arbitrary spin, such as $|\Psi\rangle=\binom{\alpha}{\beta}|p\rangle\equiv\psi|p\rangle$. A corresponding Dirac spinor for this state is $\Psi_p=\alpha u_p^{(1/2)}+\beta u_p^{(-1/2)}$.

An expectation value of Wigner spin operator is just a nonrelativistic rest-frame expression

$$\overline{\mathbf{s}}=\frac{\langle\Psi|\hat{\mathbf{S}}|\Psi\rangle}{\langle\Psi|\Psi\rangle}=\psi^\dagger\frac{\boldsymbol{\sigma}}{2}\psi. \tag{21}$$

The transformation properties of momentum eigenstates Eq. (7), Lemma 1, and the fact that Wigner spin operator commutes with the Hamiltonian lead to the association of $\hat{\mathbf{S}}$ with a conserved quantity rest-frame spin.

Dirac spin $\boldsymbol{\Sigma}$ is associated with the spin of a moving particle. A quantity

$$\overline{\mathbf{s}^D}=\frac{\langle\Psi|\hat{\boldsymbol{\Sigma}}|\Psi\rangle}{\langle\Psi|\Psi\rangle}=\Psi_p^\dagger\frac{\boldsymbol{\Sigma}}{4E(\mathbf{p})}\Psi_p \tag{22}$$

is interpreted as an expectation value of the spin of a moving particle with momentum $\mathbf{p}$ [3]. It reduces to its nonrelativistic value for $\mathbf{p}\rightarrow\mathbf{0}$ and particle's helicity can be calculated with either of the operators.

While from Lemma 1 it is clear that $\boldsymbol{\Sigma}$ does not define spin operators on the one-particle Hilbert space, it is instructive to see how it fails to do so. En route we construct $\boldsymbol{\mathcal{S}}$, a one-particle Hilbert-space restriction of $\hat{\boldsymbol{\Sigma}}$. To this end we derive a necessary and sufficient condition for three expectation values to be derivable from the three operators that satisfy spin commutation relations.

Consider six 2×2 spin-density matrices with Bloch vectors $\pm\hat{\mathbf{z}},\pm\hat{\mathbf{x}}$, and $\pm\hat{\mathbf{y}}$. These density matrices are

$$\rho_z=\begin{pmatrix}1&0\\0&0\end{pmatrix},\quad \rho_x=\begin{pmatrix}\frac{1}{2}&\frac{1}{2}\\ \frac{1}{2}&\frac{1}{2}\end{pmatrix},\quad \rho_y=\begin{pmatrix}\frac{1}{2}&-\frac{i}{2}\\ \frac{i}{2}&\frac{1}{2}\end{pmatrix}, \tag{23}$$

etc. We are looking for three Hermitian 2×2 matrices $\mathcal{S}_k$ the expectation values of which on the above states are the prescribed numbers $\overline{s_k}(\rho_l)$,

$$\overline{s_k}(\rho_l)=\mathrm{tr}(\mathcal{S}_k\rho_l),\quad k=1,2,3;\quad \pm l=\pm x,\pm y,\pm z. \tag{24}$$

We decompose these matrices in terms of Pauli matrices,

$$\mathcal{S}_k=\sum_{n=0}^{3}s_{kn}\sigma_n, \tag{25}$$

where σ_0 is an identity. It is easy to see that

$$\mathrm{tr}(\rho_l\sigma_n)=\delta_{ln},\qquad n=1,2,3. \tag{26}$$

Therefore, $\overline{s_k}(\rho_l)=s_{k0}+s_{kl}$. If instead of spin states ρ_l we take their orthogonal complements ρ_{-l} we see that all $s_{k0}=0$, so

$$\mathcal{S}_k=\sum_l\overline{s_k}(\rho_l)\sigma_l. \tag{27}$$

We want these operators to satisfy spin commutation relations $[\mathcal{S}_j,\mathcal{S}_k]=i\epsilon_{jkl}\mathcal{S}_l$. Therefore,

$$\overline{s_j}(\rho_m)\overline{s_k}(\rho_n)[\sigma_m,\sigma_n]=2i\epsilon_{jkl}\overline{s_l}(\rho_p)\sigma_p \tag{28}$$

holds and the summation is understood over the repeated indices. As a result, we establish the following lemma.

Lemma 2. A necessary and sufficient condition for a triple of probability distributions on spin-$\frac{1}{2}$ states with the expectation values $\overline{\mathbf{s}}=(\overline{s_1},\overline{s_2},\overline{s_3})$ to be derived from a triple of matrices that satisfy spin commutation relations is

$$\overline{s_j}(\rho_m)\overline{s_k}(\rho_n)\epsilon_{mnp}=\epsilon_{jkl}\overline{s_l}(\rho_p), \tag{29}$$

where the three states ρ_p are the pure states with Bloch vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$, respectively.

We apply this technique to a relativistic spin. Six states ρ are taken to be spin parts of zero-momentum states. Consider them in a frame where they have a momentum $\mathbf{p}=p(n_x,n_y,n_z)$. Expectation values of $\mathbf{s}^D$ in that frame are calculated according to Eq. (22). For ρ_z we get

$$\overline{\mathbf{s}^D}(\rho_z)=\frac{1}{2}\frac{1}{p^2+m(m+\sqrt{m^2+p^2})}\times(n_xn_zp^2,n_yn_zp^2,m^2+n_z^2p^2+m\sqrt{m^2+p^2}), \tag{30}$$

and analogous expressions for other states. From Eq. (27) we see that $\boldsymbol{\mathcal{S}}$ is given by

$$\mathcal{S}_k=\sum_l\overline{s_k^D}(\rho_l)\sigma_l. \tag{31}$$

However, a simple calculation reveals that, e.g.,

$$[\mathcal{S}_x(\mathbf{p}),\mathcal{S}_y(\mathbf{p})]\neq i\mathcal{S}_z(\mathbf{p}), \tag{32}$$

and the equality is recovered only in the nonrelativistic limit. It is not just a problem of combining three operators into three-vector. If we write $n_z=\cos\theta$, we find that the eigenvalues of $\mathcal{S}_z$ are

$$s_\pm=\pm\frac{1}{2}\frac{\sqrt{E^2(\mathbf{p})+m^2+\mathbf{p}^2\cos2\theta}}{\sqrt{2}E(\mathbf{p})}. \tag{33}$$

A triple of operators $\mathcal{S}_j\otimes1_{L^2}$ is a restriction of $\hat{\boldsymbol{\Sigma}}$ that operates on the Fock space $\mathcal{F}(\mathcal{H})=\oplus_nS^-(\mathcal{H}^{\otimes n})$ to the one-particle space $\mathcal{H}$. In the process of restriction the essential spin operator properties are lost, even if the resulting operators are the legitimate observables, similarly to Ref. [9].

If one requires fixed outcomes $\pm\frac{1}{2}$ they are possible to achieve at the price of introducing a two-outcome positive operator-valued measure (POVM) [1,2]. The expectation value $\overline{s_k^D}$ implies that the probabilities of the outcomes $\pm\frac{1}{2}$ are

$$p_k^\pm(\rho_l)=\frac{1}{2}[1\pm2\overline{s_k^D}(\rho_l)]. \tag{34}$$

Using the operators $\mathcal{S}_k$ we can construct projectors $\mathcal{P}_k^\pm$ on the one-particle Hilbert space, which correspond to projectors $\hat{P}_k^\pm$ on the Fock space. They are

$$\mathcal{P}_k^{\pm}=\frac{1}{2}(1\pm 2\mathcal{S}_k). \quad (35)$$

By a simple inspection we find that, e.g.,

$$\mathcal{P}_z^{+}\mathcal{P}_z^{-}\neq 0, \quad (36)$$

and the orthogonality is recovered only in the limit $\mathbf{p}\to\mathbf{0}$. Since $\mathcal{P}_k^{\pm}>0$ and $\mathcal{P}_k^{+}+\mathcal{P}_k^{-}=1$ we indeed have a two-outcome POVM.

From these results we learn that being a representation of a symmetry generator does not necessarily imply that this operator is also an observable with "usual" properties. We have two distinct representations of su(2) algebra on the spin-$\frac{1}{2}$ Fock space, $\hat{\mathbf{S}}$ and $\hat{\boldsymbol{\Sigma}}$. However, only one of them preserves defining commutation relations when restricted to the one-particle Hilbert space.

Now let us consider a relation of different spin operators to the maximal violation of Bell inequalities [1,2]. Consider the Clauser-Horne [16] version of Bell inequalities, where two pairs of operators describe pairs of possible tests (A_1 and A_2 for the first particle, B_1 and B_2 for the second). In each test, two possible outcomes are conventionally labeled "+" and "−." Probabilities of these outcomes, e.g., for the first particle, are given as expectations $p_i^{\pm}=\mathrm{tr}(E_i^{\pm}\rho)$, where positive operators $E_i^{\pm}$ form a two-outcome POVM, $E_i^{+}+E_i^{-}=1$. The four operators A_i, B_i are defined similarly to Eq. (36). In particular, $A_1=2E_i-1$, and the absence of a factor $\frac{1}{2}$ is conventional.

It was shown by Summers and Werner [17] that the inequalities are maximally violated only if each couple of operators generates spin commutation relations. In particular, the operators A_i have to satisfy $A_i^2=1$ and $A_1A_2+A_2A_1=0$, and operators B_i are similarly constrained. Hence, defining $A_3:=-(i/2)[A_1,A_2]$ one indeed reproduces commutation relations of Pauli matrices.

Now assume that these operators are realized as $A_i=2\mathbf{a}_i\cdot\boldsymbol{\mathcal{S}}$, etc., where $\mathbf{a}_i$ is a unit vector. Then Eq. (33) shows that generically there will be less than maximal violations of the inequalities.

Czachor [7] considers a different spin operator, $\tilde{\mathbf{S}}$, which is a suitably normalized Pauli-Lubanski operator $\mathbf{w}$. Then $A_i=2\mathbf{a}_i\cdot\tilde{\mathbf{S}}$, so

$$A_i=2\left[\frac{m}{p^0}\mathbf{a}_i+\left(1-\frac{m}{p^0}\right)(\mathbf{a}\cdot\mathbf{n})\mathbf{n}\right]\cdot\mathbf{S}\equiv 2\boldsymbol{\alpha}(\mathbf{a},\mathbf{p})\cdot\mathbf{S}, \quad (37)$$

where $\mathbf{S}$ is the Wigner spin operator and $\mathbf{n}=\mathbf{p}/|\mathbf{p}|$. The length of the auxiliary vector $\boldsymbol{\alpha}$ is

$$|\boldsymbol{\alpha}|=\frac{\sqrt{(\mathbf{p}\cdot\mathbf{a})^2+m^2}}{p^0}, \quad (38)$$

so we see that generically $A_i^2=\boldsymbol{\alpha}^2 1<1$. This provides a simple explanation of the lower than maximal Einstein-Podolsky-Rosen correlations reported in Ref. [7] (and, accordingly, weak or no violations of Bell-type inequalities).

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