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Fundamental operators in Dirac quantum mechanics

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Abstract. Old achievements and more recent results in a solution of problem of the position and spin in relativistic quantum mechanics are considered. It is definitively shown that quantum-mechanical counterparts of the classical position and spin variables are the position and spin operators in the Foldy-Wouthuysen representation (but not in the Dirac one). The probabilistic interpretation is valid only for Foldy-Wouthuysen wave functions.

1. Introduction

A very important problem of relativistic quantum mechanics (QM) is a determination of the position and spin operators. A transition to relativistic QM leads to a dependence of these fundamental operators on a representation. Pryce [1] has shown the nontriviality of forms of the position and spin operators for a spin-1/2 particle and has obtained some possible forms. In the manifold of positive-energy wave functions in the Dirac representation, Newton and Wigner [2] have determined localized eigenfunctions and the position operator having commuting components. Foldy and Wouthuysen have shown [3] its equivalence to the radius vector operator in the Foldy-Wouthuysen (FW) representation. It has been established [3] 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 $\boldsymbol{s} = \hbar\boldsymbol{\Sigma}/2$ in the *Foldy-Wouthuysen* (FW) representation. These conclusions which are also based on the results obtained by Pryce [1] and Newton and Wigner [2] have been confirmed in a lot of publications.

Unfortunately, these achievements were not reflected in textbooks and were missed by many researchers. The short analysis of the problem has been given in Ref. [4]. In the present work, we reproduce well-known (but sometimes 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 new arguments given by a contemporary development of theory of the FW transformation.

Our analysis is based on Refs. [4, 5]. We use the system of units $\hbar = 1,\ c = 1$ but include $\hbar$ and c explicitly when this inclusion clarifies the problem. The square and curly brackets, $[\dots,\dots]$ and $\{\dots,\dots\}$, denote commutators and Poisson brackets, respectively. The standard denotations of Dirac matrices are applied (see, e.g., Ref. [6]).

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2. Connection between fundamental classical variables and operators of relativistic quantum mechanics

One of great achievements of QM in the last century was a determination of a definitive connection between fundamental classical variables and operators of relativistic QM. For a Dirac particle, this connection is nontrivial because it corrupts the connection between energy, momentum, and velocity. The consideration was based on the Poincaré group (inhomogeneous Lorentz group [1]). This group is formed by ten independent *fundamental quantities* $P_\mu = (H, \boldsymbol{P})$, $J_{\mu\nu}$ $(\mu, \nu = 0, 1, 2, 3)$ defining the four-momentum and the total angular momentum and characteristic for the dynamical system [1, 7, 8, 9]. The antisymmetric tensor $J_{\mu\nu}$ is defined by the two vectors, $\boldsymbol{J}$ and $\boldsymbol{K}$. The fundamental quantities are 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, 7, 8, 9, 10, 11, 12, 13]. These ten generators satisfy the following Poisson brackets [1, 7, 8, 9, 10, 11, 12]:

$$\begin{gathered}\{P_i, P_j\} = 0, \quad \{P_i, H\} = 0, \quad \{J_i, H\} = 0, \quad \{J_i, J_j\} = e_{ijk}J_k, \quad \{J_i, P_j\} = e_{ijk}P_k, \\ \{J_i, K_j\} = e_{ijk}K_k, \quad \{K_i, H\} = P_i, \quad \{K_i, K_j\} = -e_{ijk}J_k, \quad \{K_i, P_j\} = \delta_{ij}H.\end{gathered} \tag{1}$$

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. For a free particle, Eq. (1) describes the Lie algebra of classical motion 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:

$$\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}, \qquad \boldsymbol{L} \equiv \boldsymbol{Q} \times \boldsymbol{P}. \tag{2}$$

There is some 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, 8, 9]:

$$\{Q_i, P_j\} = \delta_{ij}, \quad \{Q_i, J_j\} = e_{ijk}Q_k, \quad \{Q_i, K_j\} = \frac{1}{2}\left(Q_j\{Q_i, H\} + \{Q_i, H\}Q_j\right) - t\delta_{ij}. \tag{3}$$

It follows from Eqs. (1) – (3) that

$$\{L_i, P_j\} = e_{ijk}P_k, \qquad \{S_i, P_j\} = 0. \tag{4}$$

Equations (1) – (4) 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 Poisson brackets for the *conventional* particle position are equal to zero:

$$\{Q_i, Q_j\} = 0. \tag{5}$$

The property (5) is equivalent to the commutativity of operators of the particle position components and is not trivial (see Ref. [1, 9]). Other sets of fundamental variables violating Eq. (5) can also be used [1]. Equations (1) – (5) describe a classical Hamiltonian system.

Equations (1) – (5) allow one to obtain the following Poisson brackets [1, 9, 14]

$$\{Q_i, L_j\} = e_{ijk}Q_k, \quad \{Q_i, S_j\} = 0, \quad \{P_i, S_j\} = 0, \quad \{L_i, L_j\} = e_{ijk}L_k, \quad \{S_i, S_j\} = e_{ijk}S_k. \tag{6}$$

Evidently,

$$\{L_i, S_j\} = 0. \tag{7}$$

The main variables of a free spinning particle in CM are specified by Eqs. (2) and

$$H=\sqrt{m^2+\boldsymbol{P}^2},\qquad \boldsymbol{K}=\boldsymbol{Q}H-\frac{\boldsymbol{S}\times\boldsymbol{P}}{m+H}-t\boldsymbol{P} \tag{8}$$

(see also Refs. [11, 12] and Eq. (A.23) in Ref. [15]). In Refs. [9, 10, 15, 13], the last term in the relation for $\boldsymbol{P}$ has been missed. The Poisson brackets (6) and (7) show that the variable $\boldsymbol{Q}$ defined by Eq. (5) 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. A violation of the condition (5) leads to a dependence of $\boldsymbol{Q}$ on the spin.

The well-known deep connection between the Poisson brackets in classical mechanics (CM) and the commutators in QM remains valid *in any representation*. The commutation relations for free spinning Dirac fermions allow one to establish definitive forms of operators in the Dirac and FW representations corresponding to basic classical variables.

In CM, the position vector satisfying Eq. (5) 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 (8) (which is spin-independent for a free particle) and the corresponding FW Hamiltonian [3]

$$\mathcal{H}_{FW}=\beta\sqrt{m^2+\boldsymbol{p}^2},\qquad \boldsymbol{p}\equiv-i\hbar\frac{\partial}{\partial\boldsymbol{r}}. \tag{9}$$

The lower spinor of the FW wave function Ψ_{FW} is equal to zero if the total particle energy is positive. The Hamiltonian (9) results from the FW transformation of the Dirac Hamiltonian

$$\mathcal{H}_D=\beta m+\boldsymbol{\alpha}\cdot\boldsymbol{p}. \tag{10}$$

The remaining operators read

$$\boldsymbol{j}=\boldsymbol{l}+\boldsymbol{s},\quad \boldsymbol{l}\equiv\boldsymbol{q}\times\boldsymbol{p},\quad \boldsymbol{K}=\frac{1}{2}(\boldsymbol{q}\mathcal{H}+\mathcal{H}\boldsymbol{q})-\frac{\boldsymbol{s}\times\boldsymbol{p}}{m+\mathcal{H}}-t\boldsymbol{p}, \tag{11}$$

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

The operators being counterparts of fundamental classical variables should satisfy the relations [cf. Eqs. (1) – (7)]

$$\begin{gathered}
[p_i,p_j]=0,\quad [p_i,\mathcal{H}]=0,\quad [j_i,\mathcal{H}]=0,\quad [j_i,j_j]=ie_{ijk}j_k,\quad [j_i,p_j]=ie_{ijk}p_k,\\
[j_i,K_j]=ie_{ijk}K_k,\quad [K_i,\mathcal{H}]=ip_i,\quad [K_i,K_j]=-ie_{ijk}j_k,\quad [K_i,p_j]=i\delta_{ij}\mathcal{H},\\
[q_i,K_j]=\tfrac{1}{2}\left(q_j\left[q_i,\mathcal{H}\right]+\left[q_i,\mathcal{H}\right]q_j\right)-it\delta_{ij},\quad [q_i,p_j]=i\delta_{ij},\quad [q_i,j_j]=ie_{ijk}q_k,\\
[q_i,s_j]=0,\quad [s_i,p_j]=0,\quad [l_i,s_j]=0,\quad [l_i,l_j]=ie_{ijk}l_k,\quad [s_i,s_j]=ie_{ijk}s_k,
\end{gathered} \tag{12}$$

$$[q_i,q_j]=0. \tag{13}$$

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. (12) 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 $\boldsymbol{p},\mathcal{H}_{FW},\boldsymbol{j},\boldsymbol{K},\boldsymbol{q},\boldsymbol{s}$ 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. (12), (13) are now satisfied. Thus, the counterparts of the classical Hamiltonian, the position vector, the orbital angular momentum (OAM), and the spin are the operators $\mathcal{H}_{FW}$, $\boldsymbol{x}$, $\boldsymbol{x}\times\boldsymbol{p}$, 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 (11) with $\boldsymbol{q}=\boldsymbol{x}$.

Evidently, the Hamiltonian (9) commutes with the OAM and spin operators.

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, 9, 11, 12, 13, 14] which is inverse with respect to the FW one. The Dirac operators of the position ("mean position" [3]) and the spin ("mean spin angular momentum" [3]) are equal to [1, 3, 16]

$$\boldsymbol{q}=\boldsymbol{X}=\boldsymbol{r}-\frac{\boldsymbol{\Sigma}\times\boldsymbol{p}}{2\epsilon(\epsilon+m)}+\frac{i\boldsymbol{\gamma}}{2\epsilon}-\frac{i(\boldsymbol{\gamma}\cdot\boldsymbol{p})\boldsymbol{p}}{2\epsilon^2(\epsilon+m)}, \tag{14}$$

$$\boldsymbol{\mathcal{S}}=\frac{m}{2\epsilon}\boldsymbol{\Sigma}-i\frac{\boldsymbol{\gamma}\times\boldsymbol{p}}{2\epsilon}+\frac{\boldsymbol{p}(\boldsymbol{\Sigma}\cdot\boldsymbol{p})}{2\epsilon(\epsilon+m)}, \quad \epsilon=\sqrt{m^2+\boldsymbol{p}^2}. \tag{15}$$

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.* 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. The Newton-Wigner (NW) method [2] (see also Ref. [17]) occupies a special place among them. Newton and Wigner have investigated localized states for elementary systems. They have shown [2] that the operator (14) (NW position operator) 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. 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 [18, 19, 20, 21, 22, 23, 24, 25, 26].

The equivalence of the classical spin $\boldsymbol{S}$ and the FW mean-spin operator has also been proven in Refs. [18, 24, 25, 26, 27, 28, 29, 30]. A rather important result has been obtained by Fradkin and Good [30]. They not only have confirmed Eq. (15) for the spin operator in the Dirac representation but 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 $\boldsymbol{s}$ defines the rest-frame spin [30] and is, certainly, invariant relative to Lorentz boosts.

Dirac particles in (1+1) dimensions have been considered in Refs. [31, 32]. In the FW representation, wavepackets described by the (1+1)-dimensional Dirac equation also behave much more like a classical particle than in the Dirac representation [31, 32].

Thus, the correct forms of conventional operators of the position and spin of a free Dirac particle are defined by Eqs. (14) and (15) in the Dirac representation. In the FW representation, these operators are equal to the radius vector $\boldsymbol{x}$ and to the spin operator $\hbar\boldsymbol{\Sigma}/2$.

3. Classical limit for a Dirac fermion in external fields

Contemporary relativistic QM presents important additional arguments in favor of the conclusions made in the previous section. Relativistic methods giving compact relativistic FW Hamiltonians for any energy [33, 34, 35, 36, 37, 38, 39, 40] 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 use of this representation reduces finding the classical limit to the replacement of operators in the Hamiltonian and quantum-mechanical equations of motion by the respective classical variables [41]. This property leads

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to the conclusion that the quantum-mechanical counterparts of the classical variables are the corresponding operators *in the FW representation.*

It Ref. [30], the equation of spin motion has been derived *in the Dirac representation* and its classical limit has been obtained. A particle with an anomalous magnetic moment (AMM) has been considered and the initial Dirac-Pauli equation has been used. In the classical limit, Fradkin and Good have obtained the equation [30] coinciding with the famous classical Thomas-Bargmann-Michel-Telegdi one [42, 43]. The presence of the Thomas term shows that the both equations are derived for the rest-frame spin $\boldsymbol{S}$ but not for the spin in the lab 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 interaction of a spin-1/2 particle possessing the AMM μ' and the electric dipole moment (EDM) d with electromagnetic fields has been described in Ref. [44]. To compare the position and spin operators with their classical counterparts, the weak-field approximation can be used and terms in the relativistic FW Hamiltonian [44] proportional to $\hbar^2$ and defining contact interactions can be disregarded. For the uniform fields, the gauge $\Phi = -\boldsymbol{E}\cdot\boldsymbol{x}$, $\boldsymbol{A} = (\boldsymbol{B}\times\boldsymbol{x})/2$ can be applied. In this case, the general Hamiltonian derived in Ref. [44] takes the form [4]

$$
\begin{gathered}
\mathcal{H}_{FW} = \beta\sqrt{m^2 + \left(\boldsymbol{p} - \tfrac{e}{2}\boldsymbol{B}\times\boldsymbol{x}\right)^2} - e\boldsymbol{E}\cdot\boldsymbol{x} + \boldsymbol{\Omega}\cdot\boldsymbol{s}, \quad \boldsymbol{\Omega} = \boldsymbol{\Omega}_{MDM} + \boldsymbol{\Omega}_{EDM},\\
\boldsymbol{\Omega}_{MDM} = \tfrac{e}{m}\left[-\beta\left(\tfrac{m}{\epsilon} + a\right)\boldsymbol{B} + \beta\tfrac{a}{\epsilon(\epsilon+m)}(\boldsymbol{p}\cdot\boldsymbol{B})\boldsymbol{p} + \tfrac{1}{\epsilon}\left(\tfrac{m}{\epsilon+m} + a\right)\boldsymbol{p}\times\boldsymbol{E}\right],\\
\boldsymbol{\Omega}_{EDM} = -\tfrac{e\eta}{2m}\left[\beta\boldsymbol{E} - \beta\tfrac{(\boldsymbol{p}\cdot\boldsymbol{E})\boldsymbol{p}}{\epsilon(\epsilon+m)} + \tfrac{\boldsymbol{p}\times\boldsymbol{B}}{\epsilon}\right], \quad \boldsymbol{s} = \tfrac{\boldsymbol{\Sigma}}{2}, \quad \epsilon = \sqrt{m^2 + \boldsymbol{p}^2},
\end{gathered}
\tag{16}
$$

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 equation of spin motion is given by

$$
\frac{d\boldsymbol{s}}{dt} = \frac{1}{2}\frac{d\boldsymbol{\Sigma}}{dt} = \frac{1}{2}(\boldsymbol{\Omega}_{MDM} + \boldsymbol{\Omega}_{EDM})\times\boldsymbol{\Sigma}. \tag{17}
$$

The operator $\boldsymbol{\Omega}_{MDM}$ is in compliance with the operator of the angular velocity of spin rotation in the Dirac representation obtained in Ref. [30]. The Hamiltonian (16) is similar to the corresponding classical Hamiltonian. The operator $\boldsymbol{\Omega}$ also corresponds to the classical expression for the angular velocity of spin rotation (see Refs. [45, 46, 47] and references therein).

A consideration of a Dirac particle in gravitational fields and noninertial frames also shows that the FW position and spin operators are the quantum-mechanical counterparts of the corresponding classical variables. This statement has been definitively proven in many papers devoted to this problem [48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58].

The basic role of the FW representation in nonstationary QM has been proven in Ref. [59]. 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 in the FW representation (but not in the Dirac representation) [59]. The energy expectation values are defined by [59] $E(t) = \int \Psi^\dagger_{FW}(\boldsymbol{r},t)\mathcal{H}_{FW}(t)\Psi_{FW}(\boldsymbol{r},t)dV$. In the Dirac representation, $E(t) = \int \Psi^\dagger_D(\boldsymbol{r},t)\widetilde{\mathcal{H}}(t)\Psi_D(\boldsymbol{r},t)dV$, where $\widetilde{\mathcal{H}}(t)$ is the energy operator which defines the energy expectation values by averaging. Since $\widetilde{\mathcal{H}}(t)$ does not coincide with the Dirac Hamiltonian and the difference is not small, the Dirac Hamiltonian does not correspond to the classical one in the nonstationary case [59].

4. Probabilistic interpretation of a wave function

The difference between the position operator (14) and the radius vector $\boldsymbol{r}$ in the Dirac representation is very important. 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, $\boldsymbol{R}$ is a counterpart of the FW position operator equal to the radius vector operator $\boldsymbol{x}$. This property unambiguously follows from our analysis and has been first established in Ref. [3]. 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 [4, 5] because the Dirac radius vector $\boldsymbol{r}$ is not a counterpart of the classical position.

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 [60, 61, 62] is therefore incorrect. In fact, the probability density of the particle position is equal to $\varrho(\boldsymbol{x}) = \varrho_{FW}(\boldsymbol{x}) = \Psi_{FW}^\dagger(\boldsymbol{x})\Psi_{FW}(\boldsymbol{x})$ [4, 5]. This statement has also been made in Refs. [11, 58] and has been implicitly used in Refs. [63, 64, 65, 66]. In expressions for $\varrho_D(\boldsymbol{r})$ and $\varrho_{FW}(\boldsymbol{x})$, the variables $\boldsymbol{r}$ and $\boldsymbol{x}$ are identical. The quantities ϱ_D and ϱ_{FW} can significantly differ [4, 62, 67, 68]. A general connection between the Dirac and FW wave functions at the exact FW transformation has been obtained in Ref. [68]. In this case, upper spinors in the two representations differ only by constant factors and lower FW spinors vanish.

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

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

and $\varrho_{FW} \neq \varrho_D$. The probabilistic interpretation of the FW wave function allows one to calculate expectation values of all position-dependent operators, e.g., the mean squared radius and the quadrupole moment.

5. Summary
We have fulfilled the analysis of problem of the position and spin in Dirac QM. This analysis unambiguously shows that the quantum-mechanical counterparts of the classical position and spin are the position and spin operators in the FW representation (but not in the Dirac one). A consideration of a Dirac fermion in external fields presents important additional arguments in favor of this conclusion. The probabilistic interpretation is valid only for FW wave functions. 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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