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Quantum contextuality for a relativistic spin-1/2 particle

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The quantum predictions for a single nonrelativistic spin-1/2 particle can be reproduced by noncontextual hidden variables. Here we show that quantum contextuality for a relativistic electron moving in a Coulomb potential naturally emerges if relativistic effects are taken into account. The contextuality can be identified through the violation of noncontextuality inequalities. We also discuss quantum contextuality for the free Dirac electron as well as the relativistic Dirac oscillator.

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I. INTRODUCTION

Noncontextual hidden variable theories assume that the results of measurements are independent of which other compatible observables are jointly measured [1]. The Kochen-Specker (KS) theorem [2] states that noncontextual hidden variables cannot reproduce the predictions of quantum mechanics for systems of dimension $d \geqslant 3$. This is known as quantum contextuality and is state-independent: For any dimension $d \geqslant 3$, there are universal sets of quantum observables which prove contextuality for any state of the system. Moreover, it has recently been shown that for any physical system of $d \geqslant 3$ there is an inequality satisfied by any noncontextual hidden variable theory but which is violated, for any quantum state, by a universal set of quantum observables [3,4]. Recent experiments have confirmed state-independent quantum contextuality [5,6]. The significance of these results can be summarized in the statement that, for systems of dimension higher than two, there are no "classical" (i.e., noncontextual) states [4].

However, there still remains a debate on whether quantum contextuality can be defined on systems of dimension two such as a single spin-1/2 particle. Using the standard approach of the KS theorem, based on von Neumann projective measurements, it is impossible to define contextuality on a single qubit, since every qubit observable is only compatible with itself and hence only appears in one measurement context. By adopting positive operator-valued measurements, Cabello [7] and Nakamura [8] have shown that a single qubit exhibits a form of contextuality. However, Grudka and Kurzyński [9] have criticized this approach by pointing out that the contextuality in Refs. [7,8] is different than the contextuality in the KS theorem. The issue of whether a single spin-1/2 particle can exhibit KS contextuality remains a pending problem.

Here we adopt a completely different perspective. We start with a specific physical qubit: the spin of an electron. Within the framework of nonrelativistic quantum mechanics, the spin of an electron is treated as a two-dimensional system and does not exhibit KS contextuality. However, the situation dramatically changes when special relativity is taken into account.

By requiring the relativistic wave equation to be a first-order differential equation with respect to time and spatial coordinates and Lorentz-invariant under space-time transformations, Dirac discovered his famous equation. For an electron moving in a potential $V(r)$, its relativistic Hamiltonian is given by

$$H = c\,\vec{\alpha}\cdot\vec{p} + \beta Mc^2 + V(r), \tag{1}$$

with $\vec{\alpha} = \sigma_x \otimes \vec{\sigma}$ and $\beta = \sigma_z \otimes \mathbb{1}$, $\vec{p}$ being the linear momentum, $\vec{r}$ the coordinate, $r = |\vec{r}|$, M the rest mass of the electron, c the speed of light in vacuum, $\vec{\sigma}$ the vector of Pauli matrices, and $\mathbb{1}$ the 2×2 identity matrix. The angular momentum should be a conserved quantity for the Hamiltonian H. However, the orbital angular momentum $\vec{L} = \vec{r} \times \vec{p}$ does not commute with H unless one adds it up with a quantity $\vec{S} = \frac{\hbar}{2}\vec{\Sigma}$, with $\vec{\Sigma} = \mathbb{1} \otimes \vec{\sigma}$ and $\hbar$ the Planck constant. The quantity $\vec{S}$ is nothing but the intrinsic spin angular momentum. From $\vec{S}^2 = \frac{3}{4}\hbar^2$ one may determine that its spin value is $\frac{1}{2}$. Consequently, the spin-1/2 angular momentum has a natural origin within relativistic quantum mechanics. According to Landau and Lifshitz, "this property of elementary particles [the spin] is peculiar to quantum mechanics $(\cdots)$ and therefore has in principle no classical interpretation" [10]. An immediate question arises: Is there KS contextuality for a single spin-1/2 particle moving in the potential $V(r)$ within the framework of relativistic quantum mechanics?

In this work, we provide an affirmative answer to this question and demonstrate that contextuality of a single hydrogen atom (i.e., a relativistic electron moving in the Coulomb potential) naturally emerges from a relativistic treatment. We

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prove that all eigenstates of the relativistic hydrogen atom violate a noncontextuality inequality. The contextuality of the free Dirac electron and the Dirac oscillator is also discussed based on the measurability of the observables.

II. QUANTUM CONTEXTUALITY FOR THE RELATIVISTIC HYDROGEN ATOM

It is interesting to study the quantum contextuality of a relativistic electron moving in a Coulomb potential. This is just a model of a single relativistic hydrogen atom (RHA). The corresponding Dirac Hamiltonian reads

$$H_{\rm rha} = c\,\vec{\alpha}\cdot\vec{p} + \beta Mc^2 - \frac{\hbar c a}{r}, \tag{2}$$

with $a = e^2/\hbar c \simeq 1/137.036$ being the fine structure constant and e the electric charge. The energy spectrum is given by the Sommerfeld formula

$$\frac{E}{Mc^2} = \left(1 + \frac{a^2}{(n - |\kappa| + \sqrt{\kappa^2 - a^2})^2}\right)^{-1/2}, \quad |\kappa| = (j + 1/2) = 1,2,3,\ldots, \quad n = 1,2,3,\ldots \tag{3}$$

The common eigenfunctions of $\{H_{\rm rha}, \vec{J}^2, J_z\}$ are twofold Krammer's degeneracies [11,12], i.e.,

$$|\psi^{+}_{njm_j}(\vec{r})\rangle = \frac{1}{\sqrt{\mathcal{N}}}\begin{pmatrix} if(r)\phi^{A}_{jm_j} \\ g(r)\phi^{B}_{jm_j}\end{pmatrix}, \tag{4a}$$

$$|\psi^{-}_{njm_j}(\vec{r})\rangle = \frac{1}{\sqrt{\mathcal{N}}}\begin{pmatrix} if(r)\phi^{B}_{jm_j} \\ g(r)\phi^{A}_{jm_j}\end{pmatrix}, \tag{4b}$$

where $K|\psi^{\pm}_{njm_j}(\vec{r})\rangle = \pm|\kappa||\psi^{\pm}_{njm_j}(\vec{r})\rangle$, with $K = \beta(\vec{\Sigma}\cdot\vec{L}/\hbar + 1)$ being the Dirac operator, $K^2 = \vec{J}^2/\hbar^2 + 1/4$, and $\vec{J} = \vec{L} + \vec{S}$ the total angular momentum operator. $|\psi^{\pm}_{njm_j}(\vec{r})\rangle$ corresponds to $\kappa = \pm(j + 1/2)$, $j = l \pm 1/2$, and m_j runs from $-j$ to j. For $n = |\kappa|$, κ only takes $j + 1/2$, or $j = n - 1/2$. $\mathcal{N} = \int_0^{+\infty} r^2[f^2(r) + g^2(r)]dr$ is the normalization constant. The exact solutions of $f(r)$ and $g(r)$ are [11,12]

$$f(r) = \sqrt{Mc^2 + E}[-\tilde{n}\ {}_1F_1(1-\tilde{n},2\nu+1,\rho) + (Mc^2 a\lambda + \kappa)\,{}_1F_1(-\tilde{n},2\nu+1,\rho)]\ \rho^{\nu-1}e^{-\rho/2}, \tag{5a}$$

$$g(r) = \sqrt{Mc^2 - E}[\tilde{n}\ {}_1F_1(1-\tilde{n},2\nu+1,\rho) + (Mc^2 a\lambda + \kappa)\,{}_1F_1(-\tilde{n},2\nu+1,\rho)]\ \rho^{\nu-1}e^{-\rho/2}, \tag{5b}$$

where $\tilde{n} = n - |\kappa|$, $\nu = \sqrt{\kappa^2 - a^2}$, $\rho = 2r/\hbar c\lambda$, ${}_1F_1(p;q;z) = 1 + \frac{p}{q}\frac{z}{1!} + \frac{p(p+1)}{q(q+1)}\frac{z^2}{2!} + \cdots$ is confluent hypergeometric function, $\lambda = 1/\sqrt{M^2c^4 - E^2}$, and

$$\phi^{A}_{jm_j} = \frac{1}{\sqrt{2l+1}}\begin{pmatrix}\sqrt{l+m+1}\ Y_{lm}(\vartheta,\varphi) \\ \sqrt{l-m}\ Y_{l,m+1}(\vartheta,\varphi)\end{pmatrix}, \tag{6a}$$

$$\phi^{B}_{jm_j} = \frac{1}{\sqrt{2l+3}}\begin{pmatrix}-\sqrt{l-m+1}\ Y_{l+1,m}(\vartheta,\varphi) \\ \sqrt{l+m+2}\ Y_{l+1,m+1}(\vartheta,\varphi)\end{pmatrix}, \tag{6b}$$

where $m = m_j - 1/2$ and $Y_{lm}(\vartheta,\varphi)$ are the spherical harmonics.

Let us now consider the following noncontextuality inequality:

$$\mathcal{I} = \langle AB\rangle + \langle BC\rangle + \langle CD\rangle - \langle DA\rangle \leqslant 2, \tag{7}$$

where A, B, C, and D are observables taking values ±1, and the pairs (A,B), (B,C), (C,D), and (D,A) contain compatible observables. The inequality (7) is similar to the Clauser-Horne-Shimony-Holt (CHSH) Bell inequality, but does not make a distinction between compatible observables which are spacelike separated and those which are not [13]. It is therefore a noncontextuality inequality which can be tested on a noncomposite system. Indeed, this inequality has been used for testing contextuality on single photons [14] and single neutrons [15].

The quantum contextuality of a relativistic hydrogen atom is stated in the following theorem:

Theorem. All eigenstates of $H_{\rm rha}$ violate the noncontextuality inequality (7).

Proof. We introduce two sets of operators,

$$\vec{\Gamma} = (\Gamma_x,\Gamma_y,\Gamma_z) = (\gamma^0,\gamma^2\gamma^0,i\gamma^2), \tag{8a}$$

$$\vec{\Gamma}' = (\Gamma'_x,\Gamma'_y,\Gamma'_z) = (\gamma^3\gamma^5,i\gamma^3\gamma^1,\gamma^5\gamma^1), \tag{8b}$$

where $\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3$, and γ's are the Dirac γ matrices in the Weyl basis:

$$\gamma^0 = \begin{pmatrix}0 & \mathbb{1}\\ \mathbb{1} & 0\end{pmatrix}, \tag{9a}$$

$$\gamma^1 = \begin{pmatrix}0 & \sigma_x\\ -\sigma_x & 0\end{pmatrix}, \tag{9b}$$

$$\gamma^2 = \begin{pmatrix}0 & \sigma_y\\ -\sigma_y & 0\end{pmatrix}, \tag{9c}$$

$$\gamma^3 = \begin{pmatrix}0 & \sigma_z\\ -\sigma_z & 0\end{pmatrix}. \tag{9d}$$

Due to the anticommutative relations $\gamma^i\gamma^j = -\gamma^j\gamma^i$, $i \neq j$, it is easy to prove that $\vec{\Gamma}$ and $\vec{\Gamma}'$ commute.

The ground states are twofold degenerated. For the ground state $|\psi^{+}_{1,\frac{1}{2},\frac{1}{2}}(\vec{r})\rangle$, we choose the observables

$$A = \Gamma_x, \tag{10a}$$

$$B = \frac{1}{\sqrt{2}}(\Gamma'_x - \Gamma'_z), \tag{10b}$$

$$C = \Gamma_z, \tag{10c}$$

$$D = -\frac{1}{\sqrt{2}}(\Gamma'_x + \Gamma'_z). \tag{10d}$$

Quantum mechanically, the expectation value is given by

$$\langle AB\rangle = \int_0^{\infty} r^2 dr \int_0^{\pi} \sin\vartheta\, d\vartheta \int_0^{2\pi} d\varphi \langle\psi|AB|\psi\rangle, \tag{11}$$

with a similar expression for the other pairs. We obtain the quantum violation

$$\mathcal{I}^{\rm QM} = (1 + \sqrt{1 - a^2})\sqrt{2} \simeq 2.828\,39, \tag{12}$$

which is very close to $2\sqrt{2}$.

For the ground state $|\psi^{+}_{1,\frac{1}{2},-\frac{1}{2}}(\vec{r})\rangle$, we choose the observables $A = \Gamma_x$, $B = \frac{1}{\sqrt{2}}(\Gamma'_z - \Gamma'_x)$, $C = \Gamma_z$, and $D = \frac{1}{\sqrt{2}}(\Gamma'_x +$

Γ'_z), and obtain the same value for the quantum violation $\mathcal{I}^{\rm QM}$. This proves the case for the ground states.

For excited states with $\kappa > 0$, we consider the following observables: $A = \Gamma_y, B = -\sin\xi\ \Gamma'_y + \cos\xi\ \Gamma'_z, C = \Gamma_z, D = \sin\xi\ \Gamma'_y + \cos\xi\ \Gamma'_z$. Substituting them into Eq. (7) and using $\frac{1}{\mathcal{N}}\int_0^\infty r^2 f^2(r)dr = (1+\mu)/2$, $\frac{1}{\mathcal{N}}\int_0^\infty r^2 g^2(r)dr = (1-\mu)/2$, and $\mu = E/Mc^2$, the left-hand side of Eq. (7) becomes $2[-\frac{(2m+1)(\mu+2l+2)}{4l^2+8l+3}\cos\xi - \mu\sin\xi]$, which can reach

$$\mathcal{I}^{\rm QM} = 2\sqrt{\mu^2 + \frac{(2m+1)^2(\mu+2l+2)^2}{(4l^2+8l+3)^2}} \tag{13a}$$

$$> 2\sqrt{\mu^2 + \frac{(\mu+2l+2)^2}{(4l^2+8l+4)^2}} \tag{13b}$$

$$> 2\sqrt{1 + \frac{1-4a^2}{4(l+1)^2}} > 2. \tag{13c}$$

In step (13b), we take $m = 0$; in step (13c), μ takes the minimal value $\sqrt{1-a^2/\kappa^2}$ for $n = \kappa = l+1$.

For excited states with $\kappa < 0$, we choose the same observables as for the case of $\kappa > 0$. Then, the left-hand side of Eq. (7) becomes $2[\frac{(2m+1)(-\mu+2l+2)}{4l^2+8l+3}\cos\xi - \mu\sin\xi]$, which reaches the value

$$\mathcal{I}^{\rm QM} = 2\sqrt{\mu^2 + \frac{(2m+1)^2(2l+2-\mu)^2}{(4l^2+8l+3)^2}} \tag{14a}$$

$$> 2\sqrt{\mu^2 + \frac{(2l+1)^2}{(4l^2+8l+3)^2}} \tag{14b}$$

$$= 2\sqrt{1 + \frac{1}{(2l+3)^2} - \frac{a^2}{l^2+1}} > 2. \tag{14c}$$

In step (14b), we take $m = 0$; in step (14c), μ^2 takes the minimal value $\mu^2_{\rm min} > 1 - \frac{a^2}{1+l^2}$ for $n = l+1$. Therefore, the noncontextuality inequality (7) is always violated. This completes the proof. ■

Let us point out that the above test of quantum contextuality is state-dependent. By resorting to the Peres-Mermin square [1,16], we show that the quantum contextuality for the relativistic hydrogen atom can also be verified state-independently. The Peres-Mermin square contains nine observables:

$$P = \begin{pmatrix} \Sigma'_z & \Sigma_z & \Sigma_z\Sigma'_z \\ \Sigma_x & \Sigma'_x & \Sigma_x\Sigma'_x \\ \Sigma'_z\Sigma_x & \Sigma'_x\Sigma_z & \Sigma_y\Sigma'_y \end{pmatrix}, \tag{15}$$

where $\vec{\Sigma}' = (\Sigma'_x, \Sigma'_y, \Sigma'_z) = \vec{\sigma}\otimes\mathbb{1}$. Note that observables in the same row or column mutually commute. They violate the following noncontextuality inequality [3]:

$$\langle P_{11}P_{12}P_{13}\rangle + \langle P_{21}P_{22}P_{23}\rangle + \langle P_{31}P_{32}P_{33}\rangle + \langle P_{11}P_{21}P_{31}\rangle + \langle P_{12}P_{22}P_{32}\rangle - \langle P_{13}P_{23}P_{33}\rangle \leqslant 4, \tag{16}$$

where P_{ij} $(i,j = 1,2,3)$ are the corresponding matrix entries in Peres-Mermin square, and are dichotomic observables which commute with one another in the same correlator. One can verify that for noncontextual theories, the upper bound of the inequality is 4. However, quantum mechanics gives 6, regardless of details of the states. This state-independent advantage readily allows one to verify quantum contextuality for arbitrary four-spinor states (4a) and (4b).

Remark 1. In nonrelativistic quantum mechanics, there are no enough compatible observables for a single spin-1/2 particle to establish the inequalities (7) and (16). Here we provide an intuitive reason why it is possible for the case in relativistic quantum mechanics. Let us focus on the operator $\vec{\Sigma} = \mathbb{1}\otimes\vec{\sigma}$. One finds that it possesses a very nice property: the eigenvalues are $+1$ and -1 (or equivalently its square is a 4×4 unit matrix). Moreover, one easily observes that any operator of the form $\mathcal{O}\otimes\mathbb{1}$ commutes with $\vec{\Sigma}$. If one requires the eigenvalues of $\mathcal{O}\otimes\mathbb{1}$ are also $+1$ and -1, then the general form of the operator is

$$\vec{\Sigma}' = \mathcal{V}\vec{\sigma}\mathcal{V}^\dagger\otimes\mathbb{1}, \tag{17}$$

with $\mathcal{V}$ the 2×2 unitary matrix. The components of $\vec{\Sigma}$ and $\vec{\Sigma}'$ can be used to construct the nine observables in the Mermin-Peres square [see Eq. (15), where we have simply set $\mathcal{V} = \mathbb{1}$], therefore the standard KS theorem is applicable for the relativistic spin-1/2 particle by violation of the state-independent noncontextuality inequality (16).

Moreover, it can be verified directly that the operator $\vec{\Sigma}\cdot\vec{n}$ commutes with the operator $\vec{\Sigma}'\cdot\vec{n}'$, where $\vec{n}$, $\vec{n}'$ are some directions in the three-dimensional space. In general, up to a unitary transformation $\mathcal{U}$, the two operators

$$\vec{\Gamma}\cdot\vec{n} = \mathcal{U}\ \vec{\Sigma}\ \mathcal{U}^\dagger\cdot\vec{n}, \tag{18a}$$

$$\vec{\Gamma}'\cdot\vec{n}' = \mathcal{U}\ \vec{\Sigma}'\ \mathcal{U}^\dagger\cdot\vec{n}', \tag{18b}$$

are commutative. Thus $(\vec{\Gamma}\cdot\vec{n}, \vec{\Gamma}'\cdot\vec{n}')$ is a compatible pair of observables. By choosing an appropriate unitary transformation $\mathcal{U}$, one may arrive at the operators $\vec{\Gamma}$ and $\vec{\Gamma}'$ as in Eq. (8a) and Eq. (8b). Then the construction of observables A, B, C, D in the inequality (7) is as follows:

$$A = \vec{\Gamma}\cdot\vec{n}_a, \quad C = \vec{\Gamma}\cdot\vec{n}_c, \tag{19a}$$

$$B = \vec{\Gamma}'\cdot\vec{n}'_b, \quad D = \vec{\Gamma}'\cdot\vec{n}'_d. \tag{19b}$$

It is easy to check that eigenvalues of A, B, C, D are ± 1, and (A,B), (B,C), (C,D), (D,A) are compatible pairs. For the observables (10a)–(10d)), we have chosen the directions as $\vec{n}_a = (1,0,0)$, $\vec{n}'_b = (\cos\theta, 0, -\sin\theta)$, $\vec{n}_c = (0,0,1)$, $\vec{n}'_d = (-\cos\theta, 0, -\sin\theta)$. Thus the standard KS theorem is also applicable for the relativistic spin-1/2 particle by violation of the CHSH-like noncontextuality inequality of Eq. (7).

Remark 2. The eigenstates of the observables (10a)–(10d) are superpositions of eigenstates of $H_{\rm rha}$, whose eigenenergies (3) are all positive. This makes the observables (10a)–(10d) in principle measurable. Let us take observable A for an example. Assume its eigenstates are $|u_i\rangle, (i = 1,2,3,4)$, then each $|u_i\rangle$ can be expanded as $|u_i\rangle = \sum_\ell (c^+_\ell|\psi^+_\ell\rangle + c^-_\ell|\psi^-_\ell\rangle)$, with $|\psi^\pm_\ell\rangle$ eigenstates (4a) and (4b), respectively, and ℓ denoting indices njm_j.

III. QUANTUM CONTEXTUALITY FOR THE FREE DIRAC ELECTRON AND THE RELATIVISTIC DIRAC OSCILLATOR

Let us discuss here the KS contextuality for a free Dirac electron. For $V(r) = 0$, we have the Hamiltonian of the free

Dirac electron from Eq. (1) as

$$H_{\mathrm{e}} = c\,\vec{\alpha}\cdot\vec{p} + \beta Mc^2. \tag{20}$$

For simplicity, we assume that the electron is moving in the z direction. For a given momentum $\vec{p} = \hbar k\hat{e}_z$, energy $E = \sqrt{M^2c^4 + \hbar^2c^2k^2}$, and helicity $\vec{\Sigma}\cdot\vec{p} = \pm\hbar k$, the four-spinor eigenstate reads

$$|\Psi_e^{\pm}(k)\rangle = \frac{1}{\sqrt{\mathcal{N}_e}}\begin{pmatrix}\chi^{\pm}\\ \frac{c\hbar k}{Mc^2+E}\chi^{\pm}\end{pmatrix}e^{ikz}, \tag{21}$$

where the two-spinors $\chi^+ = \binom{1}{0}, \chi^- = \binom{0}{1}$ are the spin-up and spin-down states of σ_z, respectively, and $\mathcal{N}_e = 2E/(Mc^2 + E)$ is the normalization constant. If one adopts the following observables:

$$A' = \gamma^0, \tag{22a}$$
$$B' = (\cos\theta\gamma^3 + \sin\theta\gamma^1)\gamma^5, \tag{22b}$$
$$C' = i\gamma^2, \tag{22c}$$
$$D' = (-\cos\theta\gamma^3 + \sin\theta\gamma^1)\gamma^5, \tag{22d}$$

with $\theta = \arctan(\frac{Mc^2}{E})$. Then for the state $|\Psi_e^+(k)\rangle$, the quantum prediction reads

$$\mathcal{I}^{\mathrm{QM}} = 2\sqrt{2 - \frac{c^2\hbar^2k^2}{E^2}} = 2\sqrt{2 - \frac{v^2}{c^2}}, \tag{23}$$

which beats the upper bound of the noncontextuality inequality (7) for any $v < c$, where $v = c^2|\vec{p}|/E$ is the velocity of the electron. However, this does not imply the KS contextuality of H_{e} is identified. Because the eigenstates of observables (22a)–(22d) are superpositions of both positive and negative energy wave functions (i.e., both electron and positron states) for nonzero momentum, this hinders the measurability of the observables [17,18]. The same discussion also applies for the relativistic Dirac oscillator,

$$H_{\mathrm{RDO}} = c\,\vec{\alpha}\cdot(\vec{p} - iM\omega\beta\vec{r}) + \beta Mc^2, \tag{24}$$

whose eigenenergies can also be positive and negative [19].

IV. CONCLUSIONS

Although the existence of KS contextuality for a single spin-1/2 particle remains a disputed problem within nonrelativistic quantum mechanics, here we have shown that KS contextuality for an electron moving in the Coulomb potential naturally emerges within a relativistic treatment. Within this approach, we have explored the quantum contextuality of the relativistic hydrogen atom through violations of noncontextuality inequalities. We have proven that all eigenstates of the atom violate noncontextuality inequalities. This confirms that contextuality exists in the domain of relativistic quantum mechanics.

A distinction between relativistic and nonrelativistic quantum mechanics is that negative energies of antiparticles may emerge in the former. Given a relativistic Hamiltonian, if a Hermitian operator cannot be expanded by the eigenstates of Hamiltonian with positive energy alone, then it cannot be viewed as a measurable observable. In nonrelativistic quantum mechanics, the KS contextuality only depends on the dimension of the system, i.e., any system with $d \geqslant 3$ has contextuality. Nonetheless, in the framework of relativistic quantum mechanics, when investigating the KS contextuality one has to additionally take the measurability of observables into account. Although to some extent the four-spinor states can be viewed as a four-dimensional system, the dimension of the relativistic system itself does not guarantee the existence of the KS contextuality. We expect further developments of contextuality in relativistic quantum mechanics in the near future.

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