Hermiticity and self-adjointness in quantum mechanics

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Abstract

It is shown that Hamiltonians in the geveralized Feshbach-Villars and Foldy-Wouthuysen representations which describe a scalar particle interacting with electromagnetic fields in the Minkowski spacetime are non-Hermitian but self-adjoint. This property attributing to special relativity if curvilinear coordinates are used remains valid in general relativity. Thus, the quantum mechanics is, in the general case, non-Hermitian but self-adjoint.

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I. INTRODUCTION

The relativistic quantum mechanics (QM) of a scalar (spin-0) particle interacting with electromagnetic fields in Riemannian spacetimes can be presented in the Schrödinger-like form. For this purpose, the relativistic Foldy-Wouthuysen (FW) transformation should be applied.

This transformation is one of powerful methods of contemporary QM. A great advantage of the FW representation demonstrated in the seminal paper [1] is the simple form of operators corresponding to classical observables. In this representation, the Hamiltonian and all operators are even, i.e., block diagonal (diagonal in two spinors for a Dirac particle or in two spinor-like wave functions for particles with other spins). Relations between the operators in the FW representation are similar to those between the respective classical quantities. The form of quantum-mechanical operators for relativistic particles in external fields is the same as in the nonrelativistic quantum theory. The passage to the classical limit usually reduces to a replacement of operators in quantum-mechanical Hamiltonians and equations of motion with the corresponding classical quantities [2]. Thanks to these properties, the FW representation provides the best possibility of obtaining a meaningful classical limit of relativistic QM not only for the stationary case [1–4] but also for the nonstationary one [5–7]. The relativistic FW transformation allows one to obtain a compact Schrödinger-like form of relativistic Hamiltonians. Various methods of such a transformation have been developed in Refs. [8–11] and some specific methods are successfully used in quantum chemistry (see Refs. [12–19] and references therein). In this paper, we apply the method of the relativistic FW transformation expounded in Ref. [11]. This method is general because it is applicable to relativistic particles with any spin in arbitrarily strong external fields. The relativistic FW Hamiltonian is expanded in powers of the Planck constant. In this Hamiltonian, terms proportional to the zero and first powers of the Planck constant are determined exactly, while lower-order terms are not specified.

In previous investigations of relativistic QM of a scalar particle in Riemannian spacetimes, the FW transformation has been used in Refs. [20–23]. In Ref. [22], electromagnetic interactions have also been taken into account. The results obtained in these works are revised in the present study because we use and substantiate different approach to a derivation of the FW Hamiltonian.

Our notations correspond to Refs. [21–23]. We denote world and spatial indices by Greek and Latin letters $\alpha, \mu, \nu, \ldots = 0, 1, 2, 3$ and $i, j, k, \ldots = 1, 2, 3$, respectively. Tetrad indices are denoted by Latin letters from the beginning of the alphabet, $a, b, c, \ldots = 0, 1, 2, 3$. Temporal and spatial tetrad indices are distinguished by hats. The signature is $(+---)$. Commas and semicolons before indices denote partial and covariant derivatives, respectively. Repeated Greek indices and the Latin indices from the beginning of the alphabet are summed over the values $0, 1, 2, 3$. Repeated Latin indices $i, j, k, \ldots, \widehat{i}, \widehat{j}, \widehat{k}, \ldots$ are summed over the values $1, 2, 3$. The tetrad indices are raised and lowered with the flat Minkowski metric, $\eta_{\mu\nu} = \mathrm{diag}(1, -1, -1, -1)$. The Ricci scalar curvature is defined by $R = g^{\mu\nu}R_{\mu\nu} = g^{\mu\nu}R^{\alpha}{}_{\mu\alpha\nu}$ where $R^{\alpha}{}_{\mu\beta\nu} = \partial_\beta \Gamma^{\alpha}{}_{\mu\nu} - \ldots$ is the Riemann curvature tensor. The matrices ρ_1, ρ_2, ρ_3 coincide with the corresponding Pauli matrices (see Subsec. II C). However, they act on two components of bispinor-like wave functions in the generalized Feshbach-Villars representation. 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, $[\ldots, \ldots]$ and $\{\ldots, \ldots\}$, denote commutators and anticommutators, respectively. For any function of coordinates, $f_{,\mu} \equiv \partial_\mu f \equiv \partial f/(\partial x^\mu)$.

II. FUNDAMENTALS OF CLASSICAL AND QUANTUM MECHANICS OF A SCALAR PARTICLE

It is instructive to consider basic classical and quantum-mechanical equations describing a scalar particle interacting with electromagnetic fields in Riemannian spacetimes. The Cartan torsion couples the spin but does not influence the momentum and the angular momentum (see Ref. [24]). Therefore, Hamiltonians and equations of motion for the *scalar* particle remain unchanged in Riemann-Cartan spacetimes with the same metric tensor.

A. Fundamentals of quantum mechanics of a scalar particle

Let us consider the complex scalar field ψ in the Minkowski spacetime. The Lagrangian density is given by

$$\mathcal{L} = \eta^{\mu\nu}(\partial_\mu \psi^\dagger)(\partial_\nu \psi) - m^2 \psi^\dagger \psi. \tag{1}$$

The action takes the form

$$S=\int\left[\eta^{\mu\nu}(\partial_\mu\psi^\dagger)(\partial_\nu\psi)-m^2\psi^\dagger\psi\right]d^4x. \tag{2}$$

The Euler-Lagrange equation reads

$$\partial_\mu\frac{\partial\mathcal{L}}{\partial(\partial_\mu\psi^\dagger)}=\frac{\partial\mathcal{L}}{\partial\psi^\dagger}. \tag{3}$$

As a result, one obtains the Klein-Gordon (KG) equation [25] for a free scalar particle:

$$(\partial^\mu\partial_\mu+m^2)\psi=0. \tag{4}$$

The gauge transformations of the electromagnetic field have the form

$$A_\mu\rightarrow A'_\mu=A_\mu-\partial_\mu\Lambda,\qquad \boldsymbol{A}\rightarrow\boldsymbol{A}'=\boldsymbol{A}+\boldsymbol{\partial}\Lambda,\qquad \Phi\rightarrow\Phi'=\Phi-\partial_0\Lambda, \tag{5}$$

where A_μ is the four-potential of this electromagnetic field. We use the denotations $A_\mu=(\Phi,-\boldsymbol{A})$, $\partial_\mu\equiv\partial/\partial x^\mu=(\partial_0,\boldsymbol{\partial})$, where $\boldsymbol{\partial}\equiv(\partial_i)$. We underline that the operator $\boldsymbol{\partial}$, in general, differs from the nabla operator $\boldsymbol{\nabla}$ in special relativity (SR) and their components can even have different dimensions. The difference between these operators is important for curvilinear coordinates in the Minkowski spacetime (see Sec. II A). In the general case, the partial derivatives in Eq. (4) should be replaced with the covariant derivatives.

The Lagrangian of a scalar particle in an electromagnetic field should be invariant under the local gauge transformation

$$\Psi\rightarrow\Psi'=\exp{(ie\Lambda)}\Psi. \tag{6}$$

It is well-known that this condition results in lengthening the partial derivatives:

$$\partial_\mu\rightarrow\mathcal{D}_\mu=\partial_\mu+ieA_\mu. \tag{7}$$

The Lagrangian and the KG equation in the electromagnetic field are given by

$$\mathcal{L}=\eta^{\mu\nu}(\mathcal{D}_\mu\psi^\dagger)(\mathcal{D}_\nu\psi)-m^2\psi^\dagger\psi, \tag{8}$$

$$\left(\mathcal{D}^\mu\mathcal{D}_\mu+m^2\right)\psi=0. \tag{9}$$

For a scalar particle in Riemannian spacetimes, a passage from the Minkowski spacetime to the Riemannian one defined by the metric tensor $g_{\mu\nu}$ consists in a replacement of the partial derivative ∂_μ with the covariant derivative of general relativity (GR) $\mathfrak{D}_\mu$ and the volume d^4x with the covariant volume $\sqrt{-g}\,d^4x$. Here $g = \det g_{\mu\nu}$. The covariant derivatives of the scalar ϕ, the covariant vector J_ν and the contravariant vector K_ν are given by

$$\mathfrak{D}_\mu\psi \equiv \psi_{;\mu} = \partial_\mu\psi, \qquad \mathfrak{D}_\mu j_\nu \equiv J_{\nu\,;\mu} = \partial_\mu J_\nu - \left\{{\rho \atop \nu\mu}\right\} J_\rho,$$
$$\mathfrak{D}_\mu K^\nu \equiv K^\nu_{;\mu} = \partial_\mu K^\nu + \left\{{\nu \atop \rho\mu}\right\} K^\rho,$$

where

$$\left\{{\rho \atop \nu\mu}\right\} = \frac{1}{2}g^{\rho\lambda}\left(g_{\lambda\nu,\mu} + g_{\lambda\mu,\nu} - g_{\nu\mu,\lambda}\right) \tag{10}$$

are the Christoffel symbols. We will use the formula for the covariant divergence:

$$g^{\mu\nu}\mathfrak{D}_\mu(A_\nu) = \mathfrak{D}_\mu(A^\mu) \equiv A^\mu_{;\mu} = \frac{1}{\sqrt{-g}}\partial_\mu(\sqrt{-g}A^\mu). \tag{11}$$

The Lagrangian obtained can also be added by the term $\lambda R\psi^\dagger\psi$ ($\lambda = const$) describing the coupling with the scalar curvature. In this case, the Lagrangian and the action take the form

$$\mathcal{L} = g^{\mu\nu}(\partial_\mu\psi^\dagger)(\partial_\nu\psi) - (m^2 - \lambda R)\psi^\dagger\psi, \qquad S = \int\sqrt{-g}\mathcal{L}d^4x. \tag{12}$$

The corresponding KG equation reads

$$(\Box + m^2 - \lambda R)\psi = 0, \qquad \Box \equiv g^{\mu\nu}\mathfrak{D}_\mu\mathfrak{D}_\nu = \frac{1}{\sqrt{-g}}\partial_\mu\sqrt{-g}g^{\mu\nu}\partial_\nu. \tag{13}$$

For the minimal coupling, $\lambda = 0$. However, this choice of λ is not satisfactory for a number of reasons (see Refs. [20, 21, 26, 27] and references therein). It has been proven in Refs. [28, 29] that the addition of the above-mentioned term with $\lambda = 1/6$ leads to the conformal invariance of the KG equation for a massless particle. The sign of the Penrose-Chernikov-Tagirov term [28, 29] depends on the definition of R.

In Riemannian spacetimes, electromagnetic interactions of a scalar particle can be described as well as in the Minkowski spacetime. The Lagrangian (12) is invariant under the local gauge transformation (6) when the replacement (7) is made. As a result, electromagnetic interactions of a scalar particle in Riemannian spacetimes are defined by

$$\mathcal{L} = g^{\mu\nu}(\mathcal{D}_\mu\psi^\dagger)(\mathcal{D}_\nu\psi) - (m^2 - \lambda R)\psi^\dagger\psi, \tag{14}$$

$$(g^{\mu\nu}D_\mu D_\nu + m^2 - \lambda R)\psi = 0, \qquad D_\mu = \mathfrak{D}_\mu + ieA_\mu. \tag{15}$$

The operator acting on the scalar wave function is given by

$$g^{\mu\nu}D_\mu D_\nu = \frac{1}{\sqrt{-g}}\mathcal{D}_\mu\sqrt{-g}g^{\mu\nu}\mathcal{D}_\nu. \tag{16}$$

The covariant derivatives $\mathfrak{D}_\mu$ and D_μ commute with the metric tensor in Riemannian spacetimes. Therefore, Eq. (15) can be divided by g^{00} and can be presented in the equivalent form

$$\left[\left(D_0+\frac{g^{0i}}{g^{00}}D_i\right)^2+\frac{G^{ij}}{g^{00}}D_iD_j+\frac{m^2-\lambda R}{g^{00}}\right]\psi=0,\qquad G^{ij}=g^{ij}-\frac{g^{0i}g^{0j}}{g^{00}}. \tag{17}$$

This form is convenient for a comparison with the classical description presented in Subsec. II B. Equation (15) is an initial equation for further derivations.

B. Connection between classical and quantum-mechanical descriptions

To establish the right approach to a construction of QM of a scalar particle in curved spacetimes, we need to compare basic classical and quantum-mechanical equations.

In classical mechanics, the convoluted generalized four-momentum is equal to $p_\mu p^\mu=m^2$. This equation can be presented in the form

$$g^{\mu\nu}p_\mu p_\nu-m^2=0. \tag{18}$$

As $p_\mu=\partial S/(\partial x^\mu)$ (S is the action), one obtains the Hamilton-Jacobi equation:

$$g^{\mu\nu}\frac{\partial S}{\partial x^\mu}\frac{\partial S}{\partial x^\nu}-m^2=0. \tag{19}$$

Since $H\equiv p_0=\partial S/(\partial x^0)$ is the classical Hamiltonian, it satisfies the equation [30]

$$H=\left(\frac{m^2-G^{ij}p_ip_j}{g^{00}}\right)^{1/2}-\frac{g^{0i}p_i}{g^{00}},\qquad G^{ij}=g^{ij}-\frac{g^{0i}g^{0j}}{g^{00}}. \tag{20}$$

To take into account electromagnetic interactions, one needs to pass to the kinetic four-momentum $\pi_\mu=p_\mu-eA_\mu$. In this case, Eq. (18) takes the form

$$g^{\mu\nu}\pi_\mu\pi_\nu-m^2=0 \tag{21}$$

and the classical Hamiltonian reads [30]

$$H=\left(\frac{m^2-G^{ij}\pi_i\pi_j}{g^{00}}\right)^{1/2}-\frac{g^{0i}\pi_i}{g^{00}}+eA_0. \tag{22}$$

The classical equations (18), (19), and (21) are similar to the KG equations (15) and (17). The connection between the Hamiltonian (22) and Eq. (17) is evident.

We need to specify the momentum operator. In classical physics, the coordinate and momentum are canonical variables satisfying the Hamilton equations

$$\frac{dx^i}{dt}=-\frac{\partial H}{\partial p_i},\qquad \frac{dp_i}{dt}=\frac{\partial H}{\partial x^i}. \tag{23}$$

In the Minkowski spacetime, SR is commonly used and the classical equations of motion contain the nabla operator $[\boldsymbol{r}=(x^i),\ \boldsymbol{p}=-(p_i)]$:

$$\frac{d\boldsymbol{r}}{dt}=\frac{\partial H}{\partial \boldsymbol{p}},\qquad \frac{d\boldsymbol{p}}{dt}=-\frac{\partial H}{\partial \boldsymbol{r}}=-\boldsymbol{\nabla}H. \tag{24}$$

The corresponding quantum-mechanical equations are given by

$$\frac{d\boldsymbol{r}}{dt}=\frac{i}{\hbar}[\mathcal{H},\boldsymbol{r}],\qquad \frac{d\boldsymbol{p}}{dt}=\frac{i}{\hbar}[\mathcal{H},\boldsymbol{p}]. \tag{25}$$

It has been proven in Ref. [2] that quantum-mechanical equations of motion *in the FW representation* are similar to their classical counterparts. A comparison of classical and quantum-mechanical equations in the framework of SR shows that Eq. (25) takes the form (24) on condition that the momentum operator of SR in the FW representation is defined by

$$\boldsymbol{P}=-i\hbar\nabla. \tag{26}$$

In this case,

$$\frac{d\boldsymbol{r}}{dt}=\frac{\partial \mathcal{H}}{\partial \boldsymbol{P}},\qquad \frac{d\boldsymbol{P}}{dt}=-\frac{\partial \mathcal{H}}{\partial \boldsymbol{r}}=-\nabla\mathcal{H}. \tag{27}$$

In GR, the connection between classical and quantum-mechanical equations of motion results in

$$\frac{dx^i}{dt}=-\frac{\partial \mathcal{H}}{\partial p_i},\qquad \frac{dp_i}{dt}=\frac{\partial \mathcal{H}}{\partial x^i},\qquad p_i=i\hbar\partial_i,\qquad \boldsymbol{p}=-i\hbar\boldsymbol{\partial}. \tag{28}$$

The form of the momentum operator of GR is very important. For example, it would be wrong to suppose that $\boldsymbol{p}=-i\hbar\boldsymbol{\mathfrak{D}}$, where $\boldsymbol{\mathfrak{D}}=(\mathfrak{D}_i)$. Since $g^{\mu\nu}_{;i}=0$, the operator $\boldsymbol{\mathfrak{D}}$ commutes with the Hamiltonian at the absence of electromagnetic interactions and therefore conserves.

C. Self-adjointness and Hermiticity in quantum mechanics of a scalar particle

The self-adjointness and Hermiticity are important properties of operators. Conventional QM uses self-adjoint operators. The self-adjointness of Hamiltonians secures the reality of their eigenvalues and the orthogonality of their eigenfunctions. It also opens a possibility of unitary transformations of Hamiltonians and the eigenfunctions. While self-adjoint operators are Hermitian, there is also a room for non-Hermitian QM (see Ref. [31] and references therein). Hereinafter, ρ_1, ρ_2, and ρ_3 are the Pauli matrices:

$$\rho_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \rho_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \rho_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{29}$$

For a scalar particle, the normalization of the two-component wave function in the Feshbach-Villars (FV) representation [32]

$$\Psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \tag{30}$$

is given by

$$\int \Psi^\dagger \rho_3 \Psi dV = 1. \tag{31}$$

The FV Hamiltonian is pseudo-Hermitian (more exactly, ρ_3-pseudo-Hermitian): $\mathcal{H}^\ddagger = \rho_3 \mathcal{H}^\dagger \rho_3 = \mathcal{H}$. The FW transformation eliminates the lower and upper components of the wave function for states with positive and negative energies, respectively. The FW Hamiltonian should be Hermitian. A difference between the Hermiticity of the initial Hamiltonians for fermions and the ρ_3-pseudo-Hermiticity of the corresponding Hamiltonians for bosons disappears after the FW transformation. These properties indicate the unification of relativistic QM for particles with different spins in the FW representation [33]. In connection with this unification, we can mention the existence of bosonic symmetries of the standard Dirac equation [34–40].

Evidently, the operator $\Box$ in Eq. (13) is self-adjoint [20] because $g^{\mu\nu}_{;\rho} = 0$ and $g^{\mu\nu}\mathfrak{D}_\mu\mathfrak{D}_\nu = \mathfrak{D}_\nu\mathfrak{D}_\mu g^{\mu\nu}$. Nevertheless, its explicit form (13) is non-Hermitian because $(1/\sqrt{-g})\partial_\mu\sqrt{-g} \neq \partial_\mu$. For this reason, the appropriate nonunitary transformation

$$\psi = \frac{1}{\sqrt{g^{00}\sqrt{-g}}}\psi' \tag{32}$$

removing this non-Hermicity has been carried out in all previous studies [20–23]. The operator acting on ψ' is Hermitian. The above-mentioned argument shows that this nonunitary transformation is superfluous. Certainly, any nonunitary transformation changes the form of the final Hamiltonian.

Fortunately, the problem of necessity of the additional nonunitary transformation of the operator $\Box$ can be definitely solved. For this purpose, we will consider curvilinear coordinates in the Minkowski spacetime and will compare the results obtained in SR and GR.

III. CURVILINEAR COORDINATES IN THE MINKOWSKI SPACETIME: SPECIAL RELATIVITY VERSUS GENERAL RELATIVITY

The use of curvilinear coordinates in the Minkowski spacetime clearly shows a difference between the descriptions of a scalar particle in SR and GR. The nabla operator used in SR is not equivalent to the operator $\boldsymbol{\partial}\equiv(\partial_i)$. These operators differ in multiple actions and actions on vectors. They can even have different dimensions. For the Cartesian coordinates, $\nabla=\boldsymbol{\partial}$. However, the difference between these operators is important in other cases, in particular, for the cylindrical and spherical coordinates. For the cylindrical coordinates (ρ,ϕ,z), the nabla operator is defined by

$$\nabla=\frac{\partial}{\partial\rho}\boldsymbol{e}_\rho+\frac{1}{\rho}\frac{\partial}{\partial\phi}\boldsymbol{e}_\phi+\frac{\partial}{\partial z}\boldsymbol{e}_z. \tag{33}$$

For the spherical coordinates (r,θ,ϕ)

$$\nabla=\frac{\partial}{\partial r}\boldsymbol{e}_r+\frac{1}{r}\frac{\partial}{\partial\theta}\boldsymbol{e}_\theta+\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\boldsymbol{e}_\phi. \tag{34}$$

The action of the nabla on a scalar is trivial but its convolution with a vector (divergence) in these coordinates is nontrivial and has the form

$$\begin{gathered}\nabla\cdot\boldsymbol{\mathfrak{T}}=\frac{1}{\rho}\frac{\partial(\rho\mathfrak{T}_\rho)}{\partial\rho}+\frac{1}{\rho}\frac{\partial\mathfrak{T}_\phi}{\partial\phi}+\frac{\partial\mathfrak{T}_z}{\partial z},\\ \nabla\cdot\boldsymbol{\mathfrak{T}}=\frac{1}{r^2}\frac{\partial(r^2\mathfrak{T}_r)}{\partial r}+\frac{1}{r\sin\theta}\frac{\partial(\sin\theta\mathfrak{T}_\theta)}{\partial\theta}+\frac{1}{r\sin\theta}\frac{\partial\mathfrak{T}_\phi}{\partial\phi}.\end{gathered} \tag{35}$$

The operator $\boldsymbol{P}^2=-\hbar^2\Delta$ acts on the scalar wave function. The Laplace operator is defined by

$$\Delta=\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}+\frac{\partial^2}{\partial z^2} \tag{36}$$

and

$$\Delta=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \tag{37}$$

for the cylindrical and spherical coordinates, respectively.

Definitions of the kinetic momentum in SR and GR also differ. In SR, the use of the curvilinear coordinates instead of the Cartesian ones does not change the dependence of the

FW Hamiltonian on $\boldsymbol{P}^2$ and $\boldsymbol{\Pi}^2=(\boldsymbol{P}-e\boldsymbol{\mathcal{A}})^2$. This property follows from the connection between relativistic ans nonrelativistic QM and can be illustrated by the Landau problem (a charged particle in a uniform magnetic field [41, 42]). Certainly, the metric tensor describes the Minkowski spacetime $\eta_{\mu\nu}$. In GR, a nontrivial form of the metric tensor can also lead to different dimensions of the vectors $\boldsymbol{\mathcal{A}}$ and $\boldsymbol{A}$. An appropriate choice of a tetrad establishes a connection between these vectors:

$$e^i_{\hat{j}}A_i=A_{\hat{j}},\qquad \widehat{\boldsymbol{A}}=\boldsymbol{\mathcal{A}}.$$

For any curvilinear coordinates, $g^{00}=1,\ g^{0i}=0\ (i=1,2,3)$.

We can now specify a description of a scalar particle in the cylindrical and spherical coordinates.

A. Cylindrical coordinates

For the cylindrical coordinates in the Minkowski spacetime, the metric is given by

$$g_{\mu\nu}=\mathrm{diag}(1,-1,-\rho^2,-1),\qquad \sqrt{-g}=\rho. \tag{38}$$

Evidently,

$$\Delta=-\frac{1}{\sqrt{-g}}\partial_i\sqrt{-g}g^{ij}\partial_j.$$

The only nontrivial component of the appropriate tetrad is $e^2_{\hat{2}}=1/\rho$. Therefore, $\mathcal{A}_\rho=A_\rho=A^\rho$, $\mathcal{A}_\phi=A_\phi/\rho=\rho A^\phi$, $\mathcal{A}_z=A_z=A^z$. We can also check that $\boldsymbol{\mathcal{A}}\cdot\boldsymbol{\nabla}=g^{ij}A_i\partial_j$. We should also take into account the covariant divergence (11). In the considered case, $g^{00}\mathfrak{D}_0A_0=\mathfrak{D}_0A^0=\partial_0A^0$ and Eq. (11) takes the form

$$g^{ij}\mathfrak{D}_i(A_j)=\mathfrak{D}_i(A^i)=\frac{1}{\sqrt{-g}}\partial_i(\sqrt{-g}A^i)=\frac{1}{\rho}\frac{\partial(\rho A^\rho)}{\partial\rho}+\frac{\partial A^\phi}{\partial\phi}+\frac{\partial A^z}{\partial z}=\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{A}}. \tag{39}$$

As a result, we obtain the important relation

$$\boldsymbol{\Pi}^2=-g^{ij}D_iD_j. \tag{40}$$

The operator $\boldsymbol{\Pi}^2$ enters the Schrödinger Hamiltonian. The Schrödinger representation (used only in the nonrelativistic approximation) and the FW representation are identical. Therefore, the operator $\boldsymbol{\Pi}^2$ and its counterpart in GR enter the FW Hamiltonians as well. This means that any nonunitary transformation of the wave function is not suitable in this case. Otherwise, the cylindrical coordinates are covered by the nonunitary transformation (32) $\left(g^{00}\sqrt{-g}=\rho\right)$. As a result, this transformation should not be performed for the cylindrical coordinates.

B. Spherical coordinates

For the spherical coordinates in the Minkowski spacetime, the metric is given by

$$g_{\mu\nu}=\operatorname{diag}(1,-1,-r^2,-r^2\sin^2\theta),\qquad \sqrt{-g}=r^2|\sin\theta|. \tag{41}$$

In this case, the relation

$$\Delta=-\frac{1}{\sqrt{-g}}\partial_i\sqrt{-g}g^{ij}\partial_j$$

is also valid. The nontrivial components of the appropriate tetrad are $e^2_{\hat{2}}=1/r$, $e^3_{\hat{3}}=1/(r\sin\theta)$. Therefore, $\mathcal{A}_r=A_r=A^r$, $\mathcal{A}_\theta=A_\theta/r=rA^\theta$, $\mathcal{A}_\phi=A_\phi/(r\sin\theta)=r\sin\theta A^\phi$. We can check that $\boldsymbol{\mathcal{A}}\cdot\boldsymbol{\nabla}=g^{ij}A_i\partial_j$. We should also take into account the covariant divergence (11). For the spherical coordinates, $g^{00}\mathfrak{D}_0A_0=\mathfrak{D}_0A^0=\partial_0A^0$ and Eq. (11) takes the form

$$g^{ij}\mathfrak{D}_i(A_j)=\mathfrak{D}_i(A^i)=\frac{1}{\sqrt{-g}}\partial_i(\sqrt{-g}A^i)=\frac{1}{r^2}\frac{\partial(r^2A^r)}{\partial r}+\frac{1}{\sin\theta}\frac{\partial A^\theta}{\partial\theta}+\frac{\partial A^\phi}{\partial\phi}=\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{A}}. \tag{42}$$

As a result, the relation (40) is also satisfied for the spherical coordinates in the Minkowski spacetime.

For the spherical coordinates, the operator $\boldsymbol{\Pi}^2$ is defined by Eqs. (34), (35), and (37). This definition of $\boldsymbol{\Pi}^2$ is widely used in Schrödinger QM and, therefore, it should be applied in the FW representation in relativistic QM. For the spherical coordinates, the nonunitary transformation (32) is also nontrivial: $\sqrt{g^{00}\sqrt{-g}}=r\sqrt{|\sin\theta|}$. As a result, this nonunitary transformation of the wave function is not suitable for the spherical coordinates either.

C. Inappropriateness of extra nonunitary transformations of the Klein-Gordon equation and the Feshbach-Villars Hamiltonian

The results obtained in this section show that FW Hamiltonians containing the Laplace operator in the cylindrical and spherical coordinates should not be subjected to a nonunitary transformation. For a particle in electromagnetic fields, this operator corresponds to the operator $-\boldsymbol{\Pi}^2$ or, equivalently, to the operator $g^{ij}D_iD_j$. We can definitively state the uselessness of the nonunitary transformation (32) in QM of a scalar particle with the determination of a Hamiltonian form of the KG equation. For this purpose, the results obtained in Refs. [21, 22, 43] can be used. For curvilinear coordinates, Eq. (15) takes the form

$$(D_0^2+T)\psi=0,\qquad T=g^{ij}D_iD_j+m^2=m^2+\frac{1}{\sqrt{-g}}\mathcal{D}_i\sqrt{-g}g^{ij}\mathcal{D}_j. \tag{43}$$

The generalized Feshbach-Villars (GFV) transformation has the form [21, 22, 43]

$$\psi=\phi+\chi,\qquad i\partial_0\psi=N(\phi-\chi), \tag{44}$$

where N is an arbitrary nonzero real parameter. For the original Feshbach-Villars transformation [32], this parameter is equal to the particle mass m. The functions ϕ and χ form the two-component wave function in the GFV representation, $\Psi=\begin{pmatrix}\phi\\ \chi\end{pmatrix}$. Equation (44) allows one to obtain the explicit form of this wave function [43]:

$$\Psi=\frac{1}{2}\begin{pmatrix}\psi+\dfrac{i}{N}\dfrac{\partial\psi}{\partial t}\\ \psi-\dfrac{i}{N}\dfrac{\partial\psi}{\partial t}\end{pmatrix}. \tag{45}$$

The exact Hamiltonian in the GFV representation is defined by [43]

$$i\frac{\partial\Psi}{\partial t}=\mathcal{H}\Psi,\quad \mathcal{H}=\rho_3\frac{N^2+T}{2N}+i\rho_2\frac{-N^2+T}{2N}, \tag{46}$$

where ρ_i $(i=1,2,3)$ are the Pauli matrices. When $A_0=0$ and the magnetic field is static, the subsequent FW transformation is exact and the FW Hamiltonian is given by [21–23, 43]

$$\mathcal{H}_{FW}=\rho_3\sqrt{T}. \tag{47}$$

In all previous studies, a nonunitary transformation of the operator T to a Hermitian form has been used. This transformation has been carried out either for the Feshbach-Villars Hamiltonian [20, 21, 23] or for the initial KG equation (15) [22]. In the considered case, the result is the same and consists in the FW Hamiltonian

$$\mathcal{H}'_{FW}=\rho_3\sqrt{T'},\qquad T'=m^2+\frac{1}{\sqrt{g^{00}\sqrt{-g}}}\mathcal{D}_i\sqrt{-g}g^{ij}\mathcal{D}_j\frac{1}{\sqrt{g^{00}\sqrt{-g}}}. \tag{48}$$

A simple calculation shows that

$$T'=-\frac{\partial^2}{\partial\rho^2}-\frac{1}{4\rho^2}-\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}-\frac{\partial^2}{\partial z^2} \tag{49}$$

for the cylindrical coordinates and

$$T' = -\frac{\partial^2}{\partial r^2} - \frac{1}{r^2}\left(\frac{\partial^2}{\partial\theta^2} + \frac{1+\sin^2\theta}{4\sin^2\theta}\right) - \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \tag{50}$$

for the spherical ones. It can be checked that $T = m^2 - \Delta$ and $T' \neq m^2 - \Delta$ when $A_0 = 0$ and the magnetic field is static. Thus, the extra nonunitary transformation leading to the operator T' is inappropriate.

It is very natural to extend the conclusion about an inappropriateness of the extra nonunitary transformation of the initial KG equation or the Feshbach-Villars Hamiltonian on an arbitrary spacetime metric. Therefore, the FW Hamiltonians describing a scalar particle in Riemannian spacetimes and containing the operator $g^{ij}D_iD_j$ should not be transformed. The approach used in Refs. [20–23] is based on the nonunitary transformation (32). Since this approach covers the cylindrical and spherical coordinates, the transformation (32) should not be fulfilled. Therefore, the results obtained in Refs. [20–23] should be revised.

IV. CONCLUSIONS

The fulfilled consideration of a scalar particle interacting with electromagnetic fields in the Minkowski spacetime allows us to make some conclusions which are also valid for general relativity. We have seen that the natural and correct form of the GFV and FW Hamiltonians in non-Hermitian but self-adjoint. This property is even attributed to SR if curvilinear coordinates are used and remains valid in GR. Thus, the QM is, in the general case, non-Hermitian but self-adjoint.

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