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Towards Classification of Separable Pauli Equations

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We extend our approach, used to classify separable Schrödinger equations [1], to the case of the (1+3)-dimensional Pauli equations for a spin-$\frac{1}{2}$ particle interacting with the electromagnetic field. As a result, we get eleven classes of the vector-potentials of the electromagnetic field providing separability of the corresponding Pauli equations. It is shown, in particular, that the necessary condition for the Pauli equation to be separable is that it must be equivalent to the system of two Schrödinger equations and, furthermore, the magnetic field must be independent of the spatial variables.

1 Introduction

The quantum mechanical system consisting of a spin-$\frac{1}{2}$ charged particle interacting with the electro-magnetic field is described in a non-relativistic approximation by the Pauli equation (see, e.g., [2])

$$(p_0 - p_a p_a + e\vec{\sigma}\vec{H})\psi(t,\vec{x}) = 0, \tag{1}$$

where $\psi(t,\vec{x})$ is the two-component complex-valued function, e stands for the electric charge of particle. Here we use the notations

$$p_0 = i\frac{\partial}{\partial t} - eA_0(t,\vec{x}), \qquad p_a = -i\frac{\partial}{\partial x_a} - eA_a(t,\vec{x}), \qquad a = 1,2,3,$$

where $A = (A_0, A_1, A_2, A_3)$ is the vector-potential of the electro-magnetic field, $\vec{H} = \mathrm{rot}\ \vec{A}$ is the magnetic field, $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Hereafter the summation over the repeated Latin indices from 1 to 3 is understood.

Clearly, system (1) with arbitrary functions A_0, A_a, $(a = 1,2,3)$ is not separable. On the other hand, there do exist configurations of the electro-magnetic field providing separability of the Pauli equation. So a natural question arises whether it is possible to get a systematic description of all the possible curvilinear coordinate systems and vector-potentials A such that equation (1) is integrable by the variable separation. One of the principal objectives of the present paper is to provide an efficient way for answering these kinds of questions for systems of partial differential equations (PDEs). The approach used is the further extension of the method developed in our paper [1], where the problem of separation of variables in the Schrödinger equation has been solved.

For a solution to be found we adopt the following separation Ansatz:

$$\psi(t,\vec{x}) = Q(t,\vec{x})\varphi_0(t)\prod_{a=1}^{3}\varphi_a\left(\omega_a(t,\vec{x}),\vec{\lambda}\right)\chi, \tag{2}$$

where Q, φ_μ, $(\mu = 0,1,2,3)$ are non-singular 2×2 matrix functions of the given variables and χ is an arbitrary two-component constant column. What is more, the usual condition of commutativity of the matrices φ_μ is imposed, i.e.

$$[\varphi_\mu,\ \varphi_\nu] = \varphi_\mu\varphi_\nu - \varphi_\nu\varphi_\mu = 0, \qquad \mu,\nu = 0,1,2,3. \tag{3}$$

We say that the Pauli equation (1) is separable in a coordinate system t, $\omega_a = \omega_a(t,\vec{x})$, $(a = 1,2,3)$, if the separation Ansatz (2) reduces PDE (1) to four matrix ordinary differential equations (ODEs) for the functions φ_μ, $(\mu = 0,1,2,3)$

$$\begin{aligned} &i\varphi_0' = -\left(P_{00}(t) + P_{0b}(t)\lambda_b\right)\varphi_0, \\ &\varphi_a'' = \left(P_{a0}(\omega_a) + P_{ab}(\omega_a)\lambda_b\right)\varphi_a, \quad a = 1,2,3, \end{aligned} \tag{4}$$

where $P_{\mu\nu}$ $(\mu,\nu = 0,1,2,3)$ are some smooth 2×2 matrix functions of the given variables, λ_1, λ_2, λ_3 are separation constants and, what is more,

$$\operatorname{rank}\, \|P_{\mu a}\|_{\mu=0}^{3}\,{}_{a=1}^{3} = 6. \tag{5}$$

The condition (5) secures essential dependence of a solution with separated variables on the separation constants λ_1, λ_2, λ_3.

Next, we introduce the equivalence relation on the set of all coordinate systems providing separability of Pauli equation. We say that two coordinate systems t, ω_1, ω_2, ω_3 and $\tilde{t}$, $\tilde{\omega}_1$, $\tilde{\omega}_2$, $\tilde{\omega}_3$ are equivalent if the corresponding Ansätze (2) are transformed one into another by

- the continuous transformations from the Lie transformation group, admitted by the Pauli equation (1),
- the reversible transformations of the form

$$\begin{aligned} &t \to \tilde{t} = f_0(t), \qquad \omega_i \to \tilde{\omega}_a = f_a(\omega_a), \qquad a = 1,2,3, \\ &Q \to \tilde{Q} = Q l_0(t) l_1(\omega_1) l_2(\omega_2) l_3(\omega_3), \end{aligned} \tag{6}$$

  where $f_0, \ldots, f_3$ are some smooth functions and $l_0, \ldots, l_3$ are some smooth 2×2 matrix functions of the given variables.

This equivalence relation splits the set of all possible coordinate systems into equivalence classes. In a sequel, when presenting the lists of coordinate systems enabling us to separate variables in Pauli equation we will give only one representative for each equivalence class.

The principal steps of the procedure of variable separation in Pauli equation (1) are as follows:

1. We insert the Ansatz (2) into the Pauli equation and express the derivatives φ_0', φ_a'' in terms of the functions φ_0, φ_a, φ_a' $(a = 1,2,3)$ using equations (4).
2. We split the expression obtained by φ_0, φ_a, φ_a', λ_a $(a = 1,2,3)$ using the commutativity condition (3) and get an over-determined system of nonlinear PDEs for unknown functions A_0, A_a, Q, ω_a.
3. Integrating the obtained system yields all the possible configurations of the vector-potentials of the electro-magnetic field providing separability of the Pauli equation and the corresponding coordinate systems.

Having performed the first two steps of the above algorithm we obtain the system of nonlinear matrix PDEs

$$(i)\ \ \frac{\partial\omega_b}{\partial x_a}\frac{\partial\omega_c}{\partial x_a} = 0, \qquad b \neq c, \quad b,c = 1,2,3;$$

$$(ii)\quad \sum_{a=1}^{3} P_{ab}(\omega_a)\frac{\partial\omega_a}{\partial x_c}\frac{\partial\omega_a}{\partial x_c} = P_{0b}(t), \qquad b=1,2,3;$$

$$(iii)\quad 2\left(\frac{\partial Q}{\partial x_b} - ieQA_b\right)\frac{\partial\omega_a}{\partial x_b} + Q\left(i\frac{\partial\omega_a}{\partial t} + \Delta\omega_a\right) = 0, \qquad a=1,2,3;$$

$$(iv)\quad Q\sum_{a=1}^{3} P_{a0}(\omega_a)\frac{\partial\omega_a}{\partial x_b}\frac{\partial\omega_a}{\partial x_b} + i\frac{\partial Q}{\partial t} + \Delta Q - 2ieA_b\frac{\partial Q}{\partial x_b}$$
$$+\left(-P_{00}(t) - ie\frac{\partial A_b}{\partial x_b} - eA_0 - e^2A_bA_b + e\vec{\sigma}\vec{H}\right)Q = 0.$$

So the problem of variable separation in the Pauli equation reduces to integrating system of nonlinear PDEs for eight unknown functions A_0, A_1, A_2, A_3, Q, ω_1, ω_2, ω_3 of four variables t, $\vec{x}$. What is more, some coefficients are arbitrary matrix functions, which are to be determined while integrating system of PDEs (i)–(iv). We have succeeded in constructing the general solution of the latter, which yields, in particular, all the possible vector-potentials $A(t,\vec{x}) = (A_0(t,\vec{x}),\ldots,A_3(t,\vec{x}))$ such that Pauli equation (1) is solvable by the method of separation of variables. Due to the space limitations we are unable to present the full integration details, since the computations are very involved. The integration procedure is basically very much similar to that for classifying separable Schrödinger equations [1] (though the matrix case is considerably more difficult to handle). So that, we restrict ourselves to giving the list of the final results.

2 Principal results

Integration of the system PDEs (i)–(ii) yields the most general forms of coordinate systems t, $\vec{\omega}$ that provide separability of the Pauli equation. The general solution $\vec{\omega} = \vec{\omega}(t,\vec{x})$ of system of equations (i)–(ii) has been constructed in [1]. It is given implicitly within the equivalence relation (6) by the following formulae:

$$\vec{x} = \mathcal{T}(t)\mathcal{L}(t)\left(\vec{z}(\vec{\omega}) + \vec{v}(t)\right). \tag{7}$$

Here $\mathcal{T}(t)$ is the time-dependent 3×3 orthogonal matrix with the Euler angles $\alpha(t)$, $\beta(t)$, $\gamma(t)$:

$$\mathcal{T}(t) = \begin{pmatrix} \cos\alpha\,\cos\beta - \sin\alpha\,\sin\beta\cos\gamma & -\cos\alpha\,\sin\beta - \sin\alpha\,\cos\beta\cos\gamma & \sin\alpha\,\sin\gamma \\ \sin\alpha\,\cos\beta + \cos\alpha\,\sin\beta\cos\gamma & -\sin\alpha\,\sin\beta + \cos\alpha\,\cos\beta\cos\gamma & -\cos\alpha\,\sin\gamma \\ \sin\beta\,\sin\gamma & \cos\beta\,\sin\gamma & \cos\gamma \end{pmatrix}; \tag{8}$$

$\vec{v}(t)$ stands for the vector-column whose entries $v_1(t)$, $v_2(t)$, $v_3(t)$ are arbitrary smooth functions of t; $\vec{z} = \vec{z}(\vec{\omega})$ is given by one of the eleven formulas

1. Cartesian coordinate system,
   $z_1 = \omega_1, \quad z_2 = \omega_2, \quad z_3 = \omega_3, \quad \omega_1,\omega_2,\omega_3 \in \mathbb{R}.$
2. Cylindrical coordinate system,
   $z_1 = e^{\omega_1}\cos\omega_2, \quad z_2 = e^{\omega_1}\sin\omega_2, \quad z_3 = \omega_3, \quad 0 \le \omega_2 < 2\pi, \quad \omega_1,\omega_3 \in \mathbb{R}.$
3. Parabolic cylindrical coordinate system,
   $z_1 = (\omega_1^2 - \omega_2^2)/2, \quad z_2 = \omega_1\omega_2, \quad z_3 = \omega_3, \quad \omega_1 > 0, \quad \omega_2,\omega_3 \in \mathbb{R}.$

4. Elliptic cylindrical coordinate system,
   $z_1 = a\cosh\omega_1\cos\omega_2, \quad z_2 = a\sinh\omega_1\sin\omega_2, \quad z_3 = \omega_3,$
   $\omega_1 > 0, \quad -\pi < \omega_2 \le \pi, \quad \omega_3 \in \mathbb{R}, \quad a > 0.$
5. Spherical coordinate system,
   $z_1 = \omega_1^{-1}\operatorname{sech}\omega_2\cos\omega_3, \quad z_2 = \omega_1^{-1}\operatorname{sech}\omega_2\sin\omega_3, \quad z_3 = \omega_1^{-1}\tanh\omega_2,$
   $\omega_1 > 0, \quad \omega_2 \in \mathbb{R}, \quad 0 \le \omega_3 < 2\pi.$
6. Prolate spheroidal coordinate system,
   $z_1 = a\operatorname{csch}\omega_1\operatorname{sech}\omega_2\cos\omega_3, \quad z_2 = a\operatorname{csch}\omega_1\operatorname{sech}\omega_2\sin\omega_3,$
   $z_3 = a\coth\omega_1\tanh\omega_2, \quad \omega_1 > 0, \quad \omega_2 \in \mathbb{R}, \quad 0 \le \omega_3 < 2\pi, \quad a > 0. \qquad (9)$
7. Oblate spheroidal coordinate system,
   $z_1 = a\csc\omega_1\operatorname{sech}\omega_2\cos\omega_3, \quad z_2 = a\csc\omega_1\operatorname{sech}\omega_2\sin\omega_3,$
   $z_3 = a\cot\omega_1\tanh\omega_2, \quad 0 < \omega_1 < \pi/2, \quad \omega_2 \in \mathbb{R}, \quad 0 \le \omega_3 < 2\pi, \quad a > 0.$
8. Parabolic coordinate system,
   $z_1 = e^{\omega_1+\omega_2}\cos\omega_3, \quad z_2 = e^{\omega_1+\omega_2}\sin\omega_3, \quad z_3 = \left(e^{2\omega_1} - e^{2\omega_2}\right)/2,$
   $\omega_1, \omega_2 \in \mathbb{R}, \quad 0 \le \omega_3 \le 2\pi.$
9. Paraboloidal coordinate system,
   $z_1 = 2a\cosh\omega_1\cos\omega_2\sinh\omega_3, \quad z_2 = 2a\sinh\omega_1\sin\omega_2\cosh\omega_3,$
   $z_3 = a(\cosh 2\omega_1 + \cos 2\omega_2 - \cosh 2\omega_3)/2, \quad \omega_1, \omega_3 \in \mathbb{R}, \quad 0 \le \omega_2 < \pi, \quad a > 0.$
10. Ellipsoidal coordinate system,
   $$z_1 = a\,\frac{1}{\operatorname{sn}(\omega_1,\, k)}\operatorname{dn}(\omega_2,\, k')\operatorname{sn}(\omega_3,\, k), \quad z_2 = a\,\frac{\operatorname{dn}(\omega_1,\, k)}{\operatorname{sn}(\omega_1,\, k)}\operatorname{cn}(\omega_2,\, k')\operatorname{cn}(\omega_3,\, k),$$
   $$z_3 = a\,\frac{\operatorname{cn}(\omega_1,\, k)}{\operatorname{sn}(\omega_1,\, k)}\operatorname{sn}(\omega_2,\, k')\operatorname{dn}(\omega_3,\, k),$$
   $0 < \omega_1 < K, \quad -K' \le \omega_2 \le K', \quad 0 \le \omega_3 \le 4K, \quad a > 0.$
11. Conical coordinate system,
   $z_1 = \omega_1^{-1}\operatorname{dn}(\omega_2,\, k')\operatorname{sn}(\omega_3,\, k), \quad z_2 = \omega_1^{-1}\operatorname{cn}(\omega_2,\, k')\operatorname{cn}(\omega_3,\, k),$
   $z_3 = \omega_1^{-1}\operatorname{sn}(\omega_2,\, k')\operatorname{dn}(\omega_3,\, k), \quad \omega_1 > 0, \quad -K' \le \omega_2 \le K', \quad 0 \le \omega_3 \le 4K;$

and $\mathcal{L}(t)$ is the 3×3 diagonal matrix

$$\mathcal{L}(t) = \begin{pmatrix} l_1(t) & 0 & 0 \\ 0 & l_2(t) & 0 \\ 0 & 0 & l_3(t) \end{pmatrix},$$

where $l_1(t), l_2(t), l_3(t)$ are arbitrary non-zero smooth functions, that satisfy the following condition:

- $l_1(t) = l_2(t)$ for the partially split coordinate systems (cases 2–4 from (9)),
- $l_1(t) = l_2(t) = l_3(t)$ for non-split coordinate systems (cases 5–11 from (9)).

Here we use the standard notations for the trigonometric, hyperbolic and Jacobi elliptic functions, k $(0 < k < 1)$ being the module of the latter and $k' = \left(1 - k^2\right)^{1/2}$.

With this result in hand it is not difficult to integrate the remaining equations (*iii*) and (*iv*) from the system under study, since they can be regarded as the algebraic equations for the functions $A_a(t, \vec{x})$, $(a = 1, 2, 3)$ and $A_0(t, \vec{x})$, correspondingly. The principal results can be summarized as follows. The necessary condition for the Pauli equation (1) to be separable is that it is gauge equivalent to the Pauli equation with following space-like components of the vector-potential $A(t,\vec{x})$ of the electro-magnetic field

$$\vec{A}(t,\vec{x}) = \frac{1}{2}\begin{pmatrix} 0 & -H_3(t) & H_2(t) \\ H_3(t) & 0 & -H_1(t) \\ -H_2(t) & H_1(t) & 0 \end{pmatrix}\vec{x} = \frac{1}{2}\vec{H}(t)\times\vec{x}. \tag{10}$$

So that the magnetic field $\vec{H}$ is independent of the spatial variables and related to the Euler angles $\alpha(t)$, $\beta(t)$, $\gamma(t)$ of the matrix $\mathcal{T}(t)$ (8) through the following formulae:

$$eH_1 = -\dot{\gamma}(t)\cos\alpha(t) - \dot{\beta}(t)\sin\alpha(t)\sin\gamma(t),$$
$$eH_2 = -\dot{\gamma}(t)\sin\alpha(t) + \dot{\beta}(t)\cos\alpha(t)\sin\gamma(t),$$
$$eH_3 = -\dot{\alpha}(t) - \dot{\beta}(t)\cos\gamma(t).$$

Next, keeping in mind that $\vec{H}$ depends on t only, we make in (1) the change of variables

$$\psi = U(t)\tilde{\psi},$$

where $U(t)$ is a unitary 2×2 matrix function satisfying the matrix ODE

$$iU_t = (-e\vec{\sigma}\vec{H})U$$

with the initial condition $U(0) = I$. This transformation splits the separable Pauli equation into two Schrödinger equations, i.e. the term $e\vec{\sigma}\vec{H}$ is cancelled.

Summing up we conclude that the Pauli equation (1) admits separation of variables if and only if it is equivalent to the system of two Schrödinger equations. Moreover the space-like components A_1, A_2, A_3 of the vector-potential of the electro-magnetic field are linear in the spatial variables and given by (10).

The structure of the time-like component of the vector-potential $A(t,\vec{x})$ providing separability of Pauli equation is determined by the form of the corresponding coordinate systems $\omega_a(t,\vec{x})$, $a = 1,2,3$:

$$\begin{aligned} eA_0(t,\vec{x}) &= \sum_{a=1}^{3} F_{a0}(\omega_a)\frac{\partial\omega_a}{\partial x_b}\frac{\partial\omega_a}{\partial x_b} + T_0(t) - e^2A_bA_b \\ &\quad - \frac{1}{4}\sum_{a=1}^{3}\left(\ddot{l}_a l_a(z_a+v_a)^2 + 2l_a(l_a\ddot{v}_a + 2\dot{l}_a\dot{v}_a)(z_a+v_a) + l_a^2\dot{v}_a^2\right), \end{aligned} \tag{11}$$

where $F_{10}(\omega_1)$, $F_{20}(\omega_2)$, $F_{30}(\omega_3)$, $T_0(t)$ are arbitrary smooth functions defining the explicit form of the reduced equations (4); A_1, A_2, A_3 are given by (10); z_1, z_2, z_3 are the functions given in the list (9); and $l_a(t)$, $v_a(t)$, $\alpha(t)$, $\beta(t)$, $\gamma(t)$ are arbitrary smooth functions defining the form of the new coordinate system (7).

Thus there are eleven classes of separable Pauli equations corresponding to eleven classes of coordinate system (7). For instance, the general form of the time-like component of the vector-potential $A(t,\vec{x})$ providing separability of Pauli equation in the spherical coordinate system reads as

$$\begin{aligned} eA_0 &= T_0(t) + l_1^{-2}\omega_1^4F_{10}(\omega_1) + l_1^{-2}\omega_1^2\cosh^2\omega_2\,(F_{20}(\omega_2) + F_{30}(\omega_3)) \\ &\quad - e^2A_bA_b - \frac{1}{4}\sum_{a=1}^{3}\left(\ddot{l}_1 l_1(z_a+v_a)^2 + 2l_1(l_1\ddot{v}_a + 2\dot{l}_1\dot{v}_a)(z_a+v_a) + l_1^2\dot{v}_a^2\right), \end{aligned}$$

z_1, z_2, z_3 being given by the formulae 5 from (9).

The Pauli equation (1) for the class of functions $A_0(t,\vec{x})$, $\vec{A}(t,\vec{x})$ defined by (10), (11) under arbitrary $T_0(t)$, $F_{a0}(\omega_a)$ and arbitrarily fixed functions $\alpha(t)$, $\beta(t)$, $\gamma(t)$, $v_a(t)$, $l_a(t)$, $a=1,2,3$ separates in exactly one coordinate system. Properly specifying the functions $F_{\mu 0}(\omega_a)$, $\mu=0,1,2,3$ may yield additional possibilities for variable separation in the corresponding Pauli equation. What we mean is that for some particular forms of the vector-potential $A(t,\vec{x})$ (10), (11) there might exist several coordinate systems (7) enabling to separate the corresponding Pauli equation. Note that the quantum mechanical models possessing this property are called super-integrable (see, e.g., [3]).

As an illustration, we consider the problem of separation of variables in the Pauli equation (1) for a particle moving in the constant magnetic field. Namely, we fix the following form of the vector-potential:

$$2e\vec{A} = \begin{pmatrix} 0 & -c & 0 \\ c & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \vec{x}, \qquad eA_0 = \frac{q}{|\vec{x}|} - \frac{c^2}{12}\left(x_1^2 + x_2^2 - 2x_3^2\right), \tag{12}$$

where $q=\text{const}$. As a direct check shows, this vector-potential satisfies the vacuum Maxwell equations without currents

$$\Box A_0 - \frac{\partial}{\partial t}\left(\frac{\partial A_0}{\partial t} + \operatorname{div}\vec{A}\right) = 0,$$
$$\Box \vec{A} + \operatorname{grad}\left(\frac{\partial A_0}{\partial t} + \operatorname{div}\vec{A}\right) = \vec{0},$$

where $\Box = \partial^2/\partial t^2 - \Delta$ is the d'Alembert operator. Therefore, vector-potential (12) is the natural generalization of the standard Coulomb potential, that is obtained from (12) under $c \to 0$.

The Pauli equation (1) with potential (12) separates in three coordinate systems

$$\vec{x} = \mathcal{T}(t)\vec{z},$$

where $\mathcal{T}$ is the time-dependent 3×3 orthogonal matrix (8), with the Euler angles

$$\alpha(t) = -ct, \qquad \beta = \text{const}, \qquad \gamma = \text{const}$$

and $\vec{z}$ is one of the following coordinate systems:

1) spherical (formula 5 from the list (9));
2) prolate spheroidal (formula 6 from the list (9));
3) conical (formula 11 from the list (9)).

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