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ON COMPLETE SETS OF OBSERVABLES

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A method is proposed for writing down n − 1 linearly independent second order differential operators which commute with the Hamiltonian and with each other in any coordinate system in which the variables of the corresponding Schrödinger equation in a Riemann space R_n can be separated. The separation constants are the eigenvalues of the operators. The discrete and continuous spectra of the hydrogen atom are considered as examples. It is shown that operators quadratic in the generators of the group of space motions correspond to coordinate systems in which the variables in the wave equation can be separated.

1. INTRODUCTION

POTENTIALS possessing higher symmetries play an essential part in the various nuclear models and can also be useful in the dynamical models in the theory of elementary particles. The problem arises of finding the operators commuting with the Hamiltonian, which are defined in each of the coordinate systems where variables can be separated and subsequently constructing Lie algebras from these operators. In this article a complete set of commuting operators is obtained in an explicit form by means of a general method. Their number is obviously equal to the rank of a group for every coordinate system where the variables separate in the Schrödinger equation and in the wave equation, in the space of relativistic velocities. Since the Schrödinger equation admits separation of variables in the same coordinate systems where the separation of variables of the wave equation in Euclidean space can be obtained, we discuss the last case. A transition to the operators that correspond to the separation of variables in the Schrödinger equation is simple.

We consider also a complete set of commuting operators in a three-dimensional space of constant positive and negative curvature, for a free motion (wave equation). These operators can be applied to the solution of the physical problem of Coulomb interaction between two bodies in the case of discrete and continuous spectrum respectively.

According to Olevskiĭ [1], in a three-dimensional Riemann space of constant positive curvature there are six coordinate systems, in which the wave equation admits a complete separation of variables. Therefore, for the hydrogen atom (discrete spectrum), for which the symmetry group is the group of motions of a space of constant positive curvature, realized on the three-dimensional sphere in a four-dimensional space introduced by Fock [2], six different complete sets of quantum numbers which are the eigenvalues of some operators, are possible.

In the case of a continuous spectrum the symmetry group of the problem is the homogeneous Lorentz group (the group of motions of the three-dimensional Lobachevskiĭ space [2]. There are 34 coordinate systems in which the variables of the wave equation can be separated in this space [1]. Thus, in the case of the continuous spectrum of the hydrogen atom there are 34 sets of quantum numbers, which are eigenvalues of the operators for which the explicit form is given below.

2. SEPARATION OF VARIABLES IN THE SCHRÖDINGER EQUATION AND SETS OF COMMUTING OPERATORS

Consider a generalized, time independent Schrödinger equation with an arbitrary number $n \geq 2$ of independent variables:

$$F[u] \equiv \Delta_2 u + (E - V) u = 0. \tag{1}$$

Δ_2 is the second differential Beltrami parameter (the Beltrami-Laplace operator) relative to the fundamental form of the Riemann space.

In this space

$$ds^2 = g_{ii}(dx^i)^2, \quad g = \det(g_{ij}) \neq 0,$$
$$\Delta_2 u = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i}\left(\sqrt{g}\, g^{ij} \frac{\partial u}{\partial x^j}\right). \tag{2}$$

Equation (1) is the eigenvalue equation of the energy operator $\hat{H}$

$$\hat{H}u \equiv (-\Delta_2 + V)u = Eu. \qquad (1')$$

Let us formulate the conditions under which Eq. (1) admits the separation of variables in the system of coordinates $(x^1, z^2, \ldots, x^n)$ in the space R_n. Equation (1) admits a complete separation of variables if it has solutions in the form of the product

$$u = \prod_{i=1}^{n} u_i(x^i), \qquad (3)$$

where each of the functions $u_i(x^i)$ is a solution of an ordinary second-order differential equation.

Equation (1) admits in the coordinate system $(x^1, x^2, \ldots, x^n)$ a complete separation of variables if and only if there are n^2 functions $\varphi_{ij} = \varphi_{ij}(x^i)$ and 2n functions $f_i = f_i(x^i)$, $\chi_i = \chi_i(x^i)$, $i, j = 1, 2, \ldots, n$, which satisfy the conditions

$$\frac{1}{g_{ii}} = (\varphi^{-1})_{i1}, \quad \sqrt{g}\det(\varphi^{-1}) = \prod_{i=1}^{n} f_i, \quad i = 1, 2, \ldots, n, \quad (4)$$

where φ is the Stäckel determinant[3] i.e., the determinant with elements $\varphi_{ij} = \varphi_{ij}(x^i)$.

The potential V must have the form

$$V = \sum_{i=1}^{n} (\varphi^{-1})_{i1}\chi_i(x^i), \qquad (5)$$

and (1) can be represented as

$$F[u] = \sum_{i=1}^{n} (\varphi^{-1})_{i1} F_i[u] = 0. \qquad (6)$$

Here F_i is a linear differential operator of second order in the i-th independent variable, and corresponds to the separated equations $(i, j = 1, \ldots, n)$:

$$F_i[u] \equiv \frac{1}{f_i}\frac{\partial}{\partial x^i}\left[f_i \frac{\partial u}{\partial x^i}\right] + (\alpha_j \varphi_{ij} + \chi_i)u = 0, \qquad (7)$$

where $\alpha_1 = E$ and $\alpha_2, \ldots, \alpha_n$ are separation constants.

On the basis of the form (6), we construct a complete set of commuting operators in every coordinate system in which (1) admits separation of variables. The following theorem is valid.

Assume that in the coordinate system $(x^1, x^2, \ldots, x^n)$ of the space R_n Eq. (1) admits a complete separation of variables. Then there are $n - 1$ linearly independent differential operators of second order, $\hat{X}_k$, $k = 2, 3, \ldots, n$, which commute with the Hamiltonian $\hat{H}$ and with each other:

$$\hat{X}_k = -\sum_{i=1}^{n} (\varphi^{-1})_{ik}\left[\frac{\partial^2}{(\partial x^i)^2} + \frac{1}{f_i}\frac{\partial f_i}{\partial x^i}\frac{\partial}{\partial x^i} + \chi_i\right] \qquad (8)$$

$(k = 2, 3, \ldots, n)$. The separation constants $\alpha_2, \alpha_3, \ldots, \alpha_n$ are the eigenvalues of these operators.

$$\hat{X}_k u = \alpha_k u, \quad k = 2, 3, \ldots, n. \qquad (9)$$

Let us introduce a determinant $|A^{ij}|$ associated with the Stäckel determinant $|\varphi_{ij}|$, and in which every element φ_{ij} is replaced with its cofactor A^{ij}. The linear independence of the operators (9) is a consequence of the fact that the determinant

$$A = \det|A^{ij}| = (\det|\varphi^{ij}|)^{n-1} = \varphi^{n-1}$$

is different from zero when $\varphi \neq 0$. Obviously

$$A^{ij} = A^{ij}(x^1, \ldots, x^{i-1}, x^{i+1}, \ldots, x^n). \qquad (10)$$

To prove the theorem we use an expression known from linear algebra

$$A^{ik}A^{jl} - A^{il}A^{jk} = (-1)^{i+j+l+k}\varphi d^{ijkl}, \qquad (11)$$

where

$$d = d(x^1, \ldots, x^{i-1}, x^{i+1}, \ldots, x^{j-1}, x^{j+1}, \ldots, x^n) \qquad (12)$$

is the minor of order $n - 2$, obtained from the determinant by deleting the i-th and j-th rows and k-th and l-th columns ($i < j$ and $k < l$).

Consider the operators X_k, which correspond to the equations

$$X_k[u] \equiv \sum_{i=1}^{n} \frac{A^{ik}}{\varphi} F_i[u] = 0, \quad k = 1, 2, \ldots, n \qquad (13)$$

(for k = 1 we have, obviously, the operator F). Let us show that the operators X_k commute with one another, i.e.,

$$[X_k, X_l] = 0. \qquad (14)$$

Indeed ($k < l$),

$$[X_k, X_l] = \sum_{i,j=1}^{n}\left[\frac{A^{ik}}{\varphi}F_i, \frac{A^{jl}}{\varphi}F_j\right]$$

$$= \sum_{i=1}^{n}\left[\frac{A^{ik}}{\varphi}F_i, \frac{A^{il}}{\varphi}F_i\right] + \sum_{\substack{i,j=1\\ i\neq j}}^{n}\left[\frac{A^{ik}}{\varphi}F_i, \frac{A^{jl}}{\varphi}F_j\right].$$

In consequence of (10) the first sum is zero. Regrouping the terms in the second sum we obtain

$$[X_k, X_l] = \sum_{\substack{i=1\\ j>i}}^{n}\left\{\left[\frac{A^{ik}}{\varphi}F_i, \frac{A^{jl}}{\varphi}F_j\right] + \left[\frac{A^{jk}}{\varphi}F_j, \frac{A^{il}}{\varphi}F_i\right]\right\}$$

$$= \sum_{\substack{i=1\\ j>i}}^{n}\left[\left(\frac{A^{ik}}{\varphi}F_i\frac{A^{jl}}{\varphi}F_j - \frac{A^{il}}{\varphi}F_i\frac{A^{jk}}{\varphi}F_j\right)\right.$$

$$\left. - \left(\frac{A^{jl}}{\varphi}F_j\frac{A^{ik}}{\varphi}F_i - \frac{A^{jk}}{\varphi}F_j\frac{A^{il}}{\varphi}F_i\right)\right]$$

$$= \sum_{\substack{i=1\\ j>i}}^{n}\left(\frac{1}{\varphi}F_i\frac{A^{ik}A^{jl} - A^{il}A^{jk}}{\varphi}F_j\right.$$

$$-\frac{1}{\varphi}F_j\frac{A^{ik}A^{jl}-A^{il}A^{jk}}{\varphi}F_i\Big)=\sum_{\substack{i=1\\ j>i}}^{n}\Big(\frac{1}{\varphi}F_i\,d^{ijkl}F_j-\frac{1}{\varphi}F_j\,d^{ijkl}F_i\Big)(-1)^{i+j+k+l}=0.$$

It is easy to see that the equations $X_k[u]=0$ are the eigenvalue equations of the operators (8). The separation constants α_k turn out to be the eigenvalues.

3. THE HYDROGEN ATOM. POSSIBLE SETS OF THE QUANTUM NUMBERS

As an example of the utilization of the proposed method of constructing the possible sets of quantum numbers, we consider various sets of observables in the case of the discrete and continuous spectra of the hydrogen atom.

Fock[2] has shown that the Schrödinger equation for the hydrogen atom in momentum representation

$$\frac{\mathbf{p}^2}{2}\Psi(\mathbf{p})-\frac{1}{2\pi^2}\int\frac{\Psi(\mathbf{p}')\,d\mathbf{p}'}{|\mathbf{p}-\mathbf{p}'|^2}=E\Psi(\mathbf{p}) \qquad (15)$$

expressed in terms of the new variables

$$\xi_i=\frac{2p_0p_i}{p_0^2+\mathbf{p}^2},\quad i=1,2,3;\qquad \xi_4=\frac{p_0^2-\mathbf{p}^2}{p_0^2+\mathbf{p}^2}; \qquad (16)$$

where $p_0=\sqrt{-2E}$, and in which the unknown function is replaced by

$$\Phi(\mathbf{p})=\frac{\pi}{2\sqrt{2}}p_0^{-5/2}(p_0^2+\mathbf{p}^2)\Psi(\mathbf{p})$$

assumes a form of an integral equation for the spherical functions of a four-dimensional sphere (discrete spectrum), i.e., it becomes equivalent to a wave equation in a three-dimensional Riemann space of constant positive curvature. Similarly, the wave functions of the continuous spectrum are determined by a wave equation in Lobachevskiĭ space.

We present here sets of operators, defined in each of 34 coordinate systems in which the variables of this equation can be separated.[1)]

1–2. $X_2=\frac{\partial^2}{\partial\rho_2^2},\qquad X_3=\frac{\partial^2}{\partial\rho_3^2};$

3. $X_2=\frac{4P^{1/2}(\rho_1)}{\rho_1-\rho_2}\frac{\partial}{\partial\rho_1}\Big(P^{1/2}(\rho_1)\frac{\partial}{\partial\rho_1}\Big)-\frac{4P^{1/2}(\rho_2)}{\rho_1-\rho_2}\frac{\partial}{\partial\rho_2}\Big(P^{1/2}(\rho_2)\frac{\partial}{\partial\rho_2}\Big),$

$X_3=\frac{\rho_2P^{1/2}(\rho_1)}{\rho_1-\rho_2}\frac{\partial}{\partial\rho_1}\Big(P^{1/2}(\rho_1)\frac{\partial}{\partial\rho_1}\Big)-\frac{\rho_1P^{1/2}(\rho_2)}{\rho_1-\rho_2}\frac{\partial}{\partial\rho_2}\Big(P^{1/2}(\rho_2)\frac{\partial}{\partial\rho_2}\Big),$

$P(\rho)\equiv(\rho-a)(\rho-b)(\rho-c);$

4–9[2)].

$X_2=\frac{4P^{1/2}(\rho_1)}{\rho_2-\rho_1}\frac{\partial}{\partial\rho_1}\Big(P^{1/2}(\rho_1)\frac{\partial}{\partial\rho_1}\Big)-\frac{4P^{1/2}(\rho_2)}{\rho_2-\rho_1}\frac{\partial}{\partial\rho_2}\Big(P^{1/2}(\rho_2)\frac{\partial}{\partial\rho_2}\Big),$

$X_3=\frac{\rho_2P^{1/2}(\rho_1)}{\rho_2-\rho_1}\frac{\partial}{\partial\rho_1}\Big(P^{1/2}(\rho_1)\frac{\partial}{\partial\rho_1}\Big)-\frac{\rho_1P^{1/2}(\rho_2)}{\rho_2-\rho_1}\frac{\partial}{\partial\rho_2}\Big(P^{1/2}(\rho_2)\frac{\partial}{\partial\rho_2}\Big);$

10. $X_2=-\frac{\partial^2}{\partial\theta^2}-\cot\theta\frac{\partial}{\partial\theta}-\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2},\quad X_3=-\frac{\partial^2}{\partial\varphi^2};$

11.* $X_2=-\frac{\partial^2}{\partial\rho_1^2}-\operatorname{cth}\rho_1\frac{\partial}{\partial\rho_1}-\frac{1}{\operatorname{sh}^2\rho_1}\frac{\partial^2}{\partial\rho_2^2}\quad X_3=-\frac{\partial^2}{\partial\rho_2^2};$

12.† $X_2=-\frac{\partial^2}{\partial\rho_1^2}-\operatorname{th}\rho_1\frac{\partial}{\partial\rho_1}-\frac{1}{\operatorname{ch}^2\rho_1}\frac{\partial^2}{\partial\rho_2^2}\qquad X_3=-\frac{\partial^2}{\partial\rho_2^2};$

13. $X_2=-\frac{\partial^2}{\partial\rho_1^2}+\frac{\partial}{\partial\rho_1}-e^{2\rho_1}\frac{\partial^2}{\partial\rho_2^2},\qquad X_3=-\frac{\partial^2}{\partial\rho_2^2};$

14. $X_2=-\frac{\partial^2}{\partial\rho_1^2}-\frac{1}{\rho_1}\frac{\partial}{\partial\rho_1}-\frac{1}{\rho_1^2}\frac{\partial^2}{\partial\rho_2^2},\qquad X_3=-\frac{\partial^2}{\partial\rho_2^2};$

15. $X_2=\frac{1}{\cos2\rho_2-\operatorname{ch}2\rho_1}\Big(\frac{\partial^2}{\partial\rho_1^2}+\frac{\partial^2}{\partial\rho_2^2}\Big),$

$X_3=\frac{1}{\cos2\rho_2-\operatorname{ch}2\rho_1}\Big(\cos2\rho_2\frac{\partial^2}{\partial\rho_1^2}+\operatorname{ch}2\rho_1\frac{\partial^2}{\partial\rho_2^2}\Big);$

16. $X_2=-\frac{1}{\rho_1^2+\rho_2^2}\Big(\frac{\partial^2}{\partial\rho_1^2}+\frac{\partial^2}{\partial\rho_2^2}\Big),$

$X_3=-\frac{\rho_2^2}{\rho_1^2+\rho_2^2}\frac{\partial^2}{\partial\rho_1^2}-\frac{\rho_1^2}{\rho_1^2+\rho_2^2}\frac{\partial^2}{\partial\rho_2^2};$

17–27. $X_2=\frac{1}{2}\frac{\partial^2}{\partial\rho_3^2},$

$$X_3=\frac{(\rho_2-\alpha)P^{1/2}(\rho_1)}{(\rho_2-\rho_1)(\rho_1-\alpha)^{1/2}}\frac{\partial}{\partial\rho_1}\Big[P^{1/2}(\rho_1)(\rho_1-\alpha)^{1/2}\frac{\partial}{\partial\rho_1}\Big]-\frac{(\rho_1-\alpha)P^{1/2}(\rho_2)}{(\rho_2-\rho_1)(\rho_2-\alpha)^{1/2}}\frac{\partial}{\partial\rho_2}\Big[P^{1/2}(\rho_2)(\rho_2-\alpha)^{1/2}\frac{\partial}{\partial\rho_2}\Big]-\frac{\rho_2+\rho_1-2\alpha}{2(\rho_2-\alpha)(\rho_1-\alpha)}\frac{\partial^2}{\partial\rho_3^2}.$$

28–34. $X_2=\frac{(\rho_3+\rho_2)Q^{1/2}(\rho_1)}{(\rho_1-\rho_2)(\rho_1-\rho_3)}\frac{\partial}{\partial\rho_1}\Big(Q^{1/2}(\rho_1)\frac{\partial}{\partial\rho_1}\Big)$

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1)The sets of commuting operators in the systems 1, 10, 11 and 14 in the space of relativistic velocities were discussed in the article of Winternitz et al.[4], for the systems C, S, H, and O, respectively. The wave functions of continuous spectrum of the hydrogen atom in one of the coordinate systems have been discussed by Perelomov and Popov[5].

2)Systems 4-9 are combined, because the corresponding expressions for systems 5-9 either coincide with the same expressions in 4 as in systems 5 and 6, or represent particular cases of these systems. This remark is valid also for systems 1-2, 17-27, 28-34.

*cth = coth; sh = sinh.

†th = tanh; ch = cosh.

$$+\frac{(\rho_1+\rho_3)Q^{1/2}(\rho_2)}{(\rho_1-\rho_2)(\rho_3-\rho_2)}\frac{\partial}{\partial\rho_2}$$

$$\times\left(Q^{1/2}(\rho_2)\frac{\partial}{\partial\rho_2}\right)+\frac{(\rho_2+\rho_1)Q^{1/2}(\rho_3)}{(\rho_2-\rho_3)(\rho_1-\rho_3)}\frac{\partial}{\partial\rho_3}\left(Q^{1/2}(\rho_3)\frac{\partial}{\partial\rho_3}\right),$$

$$X_3=\frac{\rho_2\rho_3Q^{1/2}(\rho_1)}{(\rho_1-\rho_2)(\rho_3-\rho_1)}\frac{\partial}{\partial\rho_1}\left(Q^{1/2}(\rho_1)\frac{\partial}{\partial\rho_1}\right)$$

$$+\frac{\rho_1\rho_3Q^{1/2}(\rho_2)}{(\rho_1-\rho_2)(\rho_2-\rho_3)}\frac{\partial}{\partial\rho_2}$$

$$\times\left(Q^{1/2}(\rho_2)\frac{\partial}{\partial\rho_2}\right)+\frac{\rho_1\rho_2Q^{1/2}(\rho_3)}{(\rho_2-\rho_3)(\rho_3-\rho_1)}\frac{\partial}{\partial\rho_3}\left(Q^{1/2}(\rho_3)\frac{\partial}{\partial\rho_3}\right),$$

$$Q(\rho)\equiv(\rho-a)(\rho-b)(\rho-c)(\rho-d).$$

The designations 1–34 correspond to the classification of Olevskiĭ[1]. The systems 1, 3, 10, 17, 18 and 28 refer also to a space of constant positive curvature (discrete spectrum of hydrogen atom).

4. ELLIPSOIDAL COORDINATES AND THE GROUP OF MOTIONS OF SPACE

Consider, for example, the operators corresponding to the separation of variables in the wave equation in a three-dimensional Euclidean space. In this case, as is well known, there are eleven coordinate systems in which variables can be separated, consisting of confocal quadric surfaces and their degenerate forms. It turns out that the operators that correspond to conserved quantities and have definite values in the states described by the corresponding systems of eigenfunctions are quadratic polynomials in the generators of the group of motions of the Euclidean space. For the purpose of illustration let us give the expressions for these operators in the three most general coordinate systems (i.e., not cylindrical and not coordinates of rotation) in which the variables in the wave equation can be separated—conical, paraboloidal, and ellipsoidal. A full account of the results is given in[6]. **P** and **L** are here the operators of linear and angular momentum respectively.

I. Conical coordinates:

$$X_2=L_x^2+L_y^2+L_z^2,\qquad X_3=b^2L_y^2+c^2L_z^2.$$

II. Paraboloidal coordinates:

$$X_2=\tfrac14L_z^2+\tfrac12b(L_xP_y+P_yL_x)-\tfrac12c(L_yP_x+P_xL_y)$$
$$-bcP_z^2=\tfrac14L_z^2-bcP_z^2+[\mathbf{LQ}]_z-[\mathbf{QL}]_z,$$

$$\mathbf{Q}=\tfrac12c\mathbf{P}_x+\tfrac12b\mathbf{P}_y+\mathbf{P}_z,$$

$$X_3=\tfrac12[\mathbf{LP}]_z-\tfrac12[\mathbf{PL}]_z-c(P_x^2+P_z^2)-b(P_y^2-P_z^2).$$

III. Ellipsoidal coordinates:

$$X_2=b^2L_y^2+c^2L_z^2+b^2c^2P_x^2,$$

$$X_3=-L_x^2-L_y^2-L_z^2-(c^2+b^2)P_x^2-c^2P_y^2-b^2P_z^2.$$

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