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On the dynamic symmetry of the stationary Schrödinger equation

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Abstract. The symmetry of the two- and three-dimensional Schrödinger equation is analysed in terms of second-order differential operators which commute with the Hamiltonian of the solutions of the stationary Schrödinger equation. A set of equations for the coefficients of the symmetry operators is formulated and a general form for the structure of the symmetry operators is obtained. Symmetry operators have been found for the cases of some potentials. The effect of the symmetry raising at zero energy is described.

1. Introduction

Analysis of the dynamic symmetry of the stationary Schrödinger equation is of considerable interest in connection with such problems as the separation of variables (Miller 1977), the degeneration of energy levels and their classification, the derivation of a complete set of quantum numbers (Barut and Raczka 1977) and the calculation of matrix elements in the basis of the wavefunctions of coherent states (Malkin and Man'ko, 1979). Group properties of differential equations, which are the basis for an analysis of the dynamic symmetry, have been the object of many investigations. All the papers in this field may be tentatively divided into two groups: in the first group use is made of the criterion of invariance (Lie 1881, Ovsjannikov 1978, Meinhardt 1981); in the other group the notion of the symmetry operator $\hat{S}$ and operator equation for $\hat{S}$ is utilised (Winternitz *et al* 1966, Miller 1977, Barut and Raczka 1977). The second way, which is traditional for the solution of linear problems of mathematical physics and quantum mechanics, is accepted in this paper.

The work of Winternitz *et al* (1966) is the closest to the approach adopted in the present analysis. However, that paper deals only with the symmetry of the two-dimensional stationary Schrödinger equation, where the operators of the symmetry $\hat{S}$ identically commute with the Hamiltonian $\hat{H}: [\hat{S}, \hat{H}] = 0$. In the present work a more general definition of the symmetry operator is used, $[\hat{S}, \hat{H}]\psi = 0$ if $\hat{H}\psi = E\psi$ (Malkin and Man'ko 1965), with both two- and three-dimensional Schrödinger equations being analysed. In an earlier paper (Voronin *et al* 1982) an analysis of the symmetry of a three-dimensional stationary Schrödinger equation was made with the help of second-order differential symmetry operators identically commuting with the Hamiltonian.

It follows then that the symmetry operator, as defined in this paper, allows one solution of the stationary Schrödinger equation to be transformed into another at the same energy. Thus, the symmetry properties, investigated in this paper, describe the degeneration of the energy levels. It should also be noted that the symmetry operators used, which are second-order differential operators, prevent us from making a comprehensive analysis of the symmetry properties because the class of such operators is limited. However, the usefulness of this class of operators has been proved by analyses of many problems of quantum mechanics and mathematical physics (Barut and Raczka 1977, Miller 1977).

2. The basic system of equations

Let us introduce the n-dimensional Schrödinger equation

$$\hat{H}\psi = E\psi \tag{2.1}$$

where the Hamiltonian $\hat{H}$, in the corresponding units, may be written as

$$\hat{H} = -\Delta_r + V(\boldsymbol{r}) = -\partial^2/\partial x^s \partial x^s + V(\boldsymbol{r}) \tag{2.2}$$

$\boldsymbol{r} = (x^1, \ldots, x^n)$ and the repeated indices imply summation. It is now necessary to determine such second-order differential operators, called symmetry operators,

$$\hat{S} = A^{ij}(\boldsymbol{r})\, \partial^2/\partial x^i \partial x^j + B^k(\boldsymbol{r})\, \partial/\partial x^k + C(\boldsymbol{r}) \tag{2.3}$$

which commute with the Hamiltonian (2.2) on a set of solutions for equation (2.1). As $[\hat{S}, \hat{H}]$ and $\hat{H} - E$ are differential operators of orders 3 and 2 respectively, it is sufficient for them to vanish on the same set of functions

$$[\hat{S}, \hat{H}] = \hat{U}(\hat{H} - E) \tag{2.4}$$

where

$$\hat{U} = a^l(\boldsymbol{r})\, \partial/\partial x^l + b(\boldsymbol{r}) \tag{2.5}$$

is some first-order differential operator.

Substituting (2.2), (2.3) and (2.5) into (2.4) and equating coefficients of the same operators results in the following system of linear partial differential equations for the real functions A^{ij}, B^k, C, a^l and b:

$$\partial A^{ij}/\partial x^k + \partial A^{kj}/\partial x^i + \partial A^{ki}/\partial x^j = -\tfrac{1}{2}(a^k\delta_{ij} + a^i\delta_{kj} + a^j\delta_{ki}) \qquad i, j, k = 1, 2, \ldots, n \tag{2.6a}$$

$$\partial^2 A^{kl}/\partial x^s\, \partial x^s + \partial B^k/\partial x^l + \partial B^l/\partial x^k = -b\delta_{kl} \qquad k, l = 1, 2, \ldots, n \tag{2.6b}$$

$$2A^{ij}\, \partial V/\partial x^j + \partial^2 B^i/\partial x^s\, \partial x^s + 2\, \partial C/\partial x^i = a^i(V - E) \qquad i = 1, 2, \ldots, n \tag{2.6c}$$

$$B^k\, \partial V/\partial x^k + A^{ij}\, \partial^2 V/\partial x^i\, \partial x^j + \partial^2 C/\partial x^s\, \partial x^s = a^l\, \partial V/\partial x^l + b(V - E). \tag{2.6d}$$

Note that the system of equations (2.6) with the appropriate coefficients of $\hat{S}$ and $\hat{U}$ operators can be considered as equations for the potential V, which allows the given symmetry operator $\hat{S}$.

3. Two-dimensional stationary Schrödinger equation

Let us introduce conventional notations for the two independent variables: $x = x^1$, $y = x^2$. Operators in this case may be written as

$$\hat{H} = -\partial^2/\partial x^2 - \partial^2/\partial y^2 + V(x, y) \tag{3.1}$$

$$\hat{S} = A^{11}\,\partial^2/\partial x^2 + 2A^{12}\,\partial^2/\partial x\,\partial y + A^{22}\,\partial^2/\partial y^2 + B^1\,\partial/\partial x + B^2\,\partial/\partial y + C \tag{3.2}$$

$$\hat{U} = a^1\,\partial/\partial x + a^2\,\partial/\partial y + b. \tag{3.3}$$

In (3.2) and in further calculations the matrix of coefficients A^{ij} is assumed to be symmetric ($A^{ij} = A^{ji}$), which apparently does not invalidate the general character of the analysis. In the two-dimensional case the system of equations (2.6) consists of ten equations

$$\partial A^{11}/\partial x = 2\,\partial A^{12}/\partial y + \partial A^{22}/\partial x = -\tfrac{1}{2}a^1 \tag{3.4a}$$

$$\partial A^{22}/\partial y = 2\,\partial A^{12}/\partial x + \partial A^{11}/\partial y = -\tfrac{1}{2}a^2 \tag{3.4b}$$

$$\Delta A^{11} + 2\,\partial B^1/\partial x = \Delta A^{22} + 2\,\partial B^2/\partial y = -b \tag{3.4c}$$

$$\Delta A^{12} + \partial B^2/\partial x + \partial B^1/\partial y = 0 \tag{3.4d}$$

$$2(A^{11}\,\partial V/\partial x + A^{12}\,\partial V/\partial y) + \Delta B^1 + 2\,\partial C/\partial x = a^1(V - E) \tag{3.4e}$$

$$2(A^{12}\,\partial V/\partial x + A^{22}\,\partial V/\partial y) + \Delta B^2 + 2\,\partial C/\partial y = a^2(V - E) \tag{3.4f}$$

$$A^{11}\,\partial^2 V/\partial x^2 + 2A^{12}\,\partial^2 V/\partial x\,\partial y + A^{22}\,\partial^2 V/\partial y^2 + B^1\,\partial V/\partial x + B^2\,\partial V/\partial y + \Delta C$$
$$= a^1\,\partial V/\partial x + a^2\,\partial V/\partial y + b(V - E). \tag{3.4g}$$

From (3.4a) – (3.4d)

$$(\partial/\partial x)\tfrac{1}{2}(A^{11} - A^{22}) = \partial A^{12}/\partial y \qquad (\partial/\partial y)\tfrac{1}{2}(A^{11} - A^{22}) = -\partial A^{12}/\partial x \tag{3.5}$$

$$\partial B^1/\partial x = \partial B^2/\partial y \qquad \partial B^1/\partial y = -\partial B^2/\partial x \tag{3.6}$$

follow. Equations (3.5) and (3.6) are Cauchy–Riemann conditions for two pairs of functions: $\tfrac{1}{2}(A^{11} - A^{22})$, A^{12} and B^1, B^2. This leads to

$$\tfrac{1}{2}(A^{11} - A^{22}) + \mathrm{i}A^{12} = f(z) \qquad B^1 + \mathrm{i}B^2 = g(z) \tag{3.7}$$

where $z = x + \mathrm{i}y$ and $f(z)$, $g(z)$, thus far, are arbitrary analytical functions of z. One can obtain the formula for determining C and the conditions which functions $f(z)$ and $g(z)$ would satisfy from (3.4e)–(3.4g). In order to express these results, it is convenient to introduce a potential V as a function of $z = x + \mathrm{i}y$ and $\bar{z} = x - \mathrm{i}y$. Let us take $W(z, \bar{z}) = V - E$. From the conditions of coincidence for equations (3.4e)–(3.4f) it follows that

$$\mathrm{Im}[(\partial^2/\partial z^2)(fW) + (\partial/\partial z)(f\,\partial W/\partial z)] = 0. \tag{3.8}$$

Equation (3.4g) gives

$$\mathrm{Re}[(\partial/\partial z)W(g - df/dz)] = 0. \tag{3.9}$$

Thus, the problem of finding the function $C(x, y)$ is reduced to that of restoring the function from well known components of its gradient. Using equations (3.4e) and (3.4f) gives

$$C(x, y) = -A^{11}(x, y_0)V(x, y_0)$$
$$+ A^{11}(x_0, y_0)V(x_0, y_0) - A^{22}(x, y)V(x, y) + A^{22}(x, y_0)V(x, y_0)$$
$$- \mathrm{Im}\left(\int_{x_0}^{x} f(\xi + \mathrm{i}y_0)\,\frac{\partial V(\xi, y)}{\partial y}\bigg|_{y_0} d\xi + \int_{y_0}^{y} f(x + \mathrm{i}\eta)\,\frac{\partial V(x, \eta)}{\partial x}\,d\eta\right)$$
$$+ \text{constant}. \tag{3.10}$$

Note, that the functions $f(z)$ and $g(z)$, satisfying conditions (3.8) and (3.9), must be defined with maximum generality. As follows from (3.7), the difference $A^{11}-A^{22}$ (but not each of the coefficients separately) may be found from $f(z)$. Thus one of these coefficients may be chosen arbitrarily. This degree of arbitrariness is due to the fact that a trivial symmetry operator

$$\hat{S}_0=\phi(x,y)(\hat{H}-E) \tag{3.11}$$

may be added to each operator of the symmetry $\hat{S}$. In the Lie algebra L of symmetry operators $\hat{S}$ a set of operators (3.11) forms the ideal I. In fact, only the factor algebra L/I of the non-trivial symmetries is of interest and will be considered in this paper (Miller 1977). To do this, it suffices to fix A^{22}, taking, for instance, $A^{22}=0$.

Let us consider some examples. It can be seen from the calculations that symmetry operators, not identically commuting with the Hamiltonian, exist only at a definite value of energy (most frequently at $E=0$). It is this case which will be considered here, since symmetry operators of the two-dimensional stationary Schrödinger equation, identically commuting with the Hamiltonian, are given by Winternitz *et al* (1966).

3.1. *Two-dimensional hydrogen atom at zero energy*

In this case we have

$$V(x,y)=-\alpha(x^2+y^2)^{-1/2}=-\alpha(z\bar{z})^{-1/2}=W(z,\bar{z}). \tag{3.12}$$

Condition (3.8) takes the form

$$\mathrm{Im}(\mathrm{d}^2f/\mathrm{d}z^2-(3/2z)\,\mathrm{d}f/\mathrm{d}z+(3/2z^2)f)=0. \tag{3.13}$$

Since the expression $\mathrm{d}^2f/\mathrm{d}z^2-(3/2z)\,\mathrm{d}f/\mathrm{d}z+(3/2z^2)f$ at $z\neq 0$ is an analytical function of z, the imaginary part of which is equal to zero, the analytical function itself may be equal only to a real constant. Thus, condition (3.8) becomes a differential equation for $f(z)$:

$$\mathrm{d}^2f/\mathrm{d}z^2-(3/2z)\,\mathrm{d}f/\mathrm{d}z+(3/2z^2)f=C_1 \tag{3.14}$$

where C_1 is a real constant. Solving equation (3.14) gives

$$f=2C_1z^2+(C_2+\mathrm{i}C_3)z+(C_4+\mathrm{i}C_5)z^{3/2} \tag{3.15}$$

where all C_i for $i=1,\ldots,5$ are real constants. Let us introduce a new analytical function

$$h(z)=g(z)-\mathrm{d}f/\mathrm{d}z. \tag{3.16}$$

From (3.9) it follows that

$$\mathrm{Re}(\mathrm{d}h/\mathrm{d}z-h/2z)=0. \tag{3.17}$$

As the expression $\mathrm{d}h/\mathrm{d}z-h/2z$ at $z\neq 0$ is an analytical function of z, the real part of which is equal to zero, the function $\mathrm{d}h/\mathrm{d}z-h/2z$ may be equal to an imaginary constant only

$$\mathrm{d}h/\mathrm{d}z-h/2z=2\mathrm{i}C_6 \tag{3.18}$$

where C_6 is a real constant. Using the relations (3.16) and (3.18), we obtain

$$\begin{aligned} h(z) &= 4\mathrm{i}C_6 z + (\tilde{C}_7 + \mathrm{i}\tilde{C}_8) z^{1/2} \\ g(z) &= C_2 + \mathrm{i}C_3 + (C_7 + \mathrm{i}C_8) z^{1/2} + 4(C_1 + \mathrm{i}C_6) z \end{aligned} \tag{3.19}$$

where $C_7 = \tilde{C}_7 + 3C_4/2$, $C_8 = \tilde{C}_8 + 3C_5/2$, and C_6, $\tilde{C}_7$, $\tilde{C}_8$, C_7, C_8 are real constants. Thus, in a general solution of (3.15) and (3.19) for f and g there are eight real constants, which give the corresponding eight symmetry operators. Since C_6 and C_1 give functionally dependent operators $\hat{L}_z = y\,\partial/\partial x - x\,\partial/\partial y$ and $\hat{L}_z^2$, only seven symmetry operators are independent:

$$\begin{aligned} \hat{X}_1 &= \hat{L}_z = y\,\partial/\partial x - x\,\partial/\partial y \\ \hat{X}_2 &= \hat{A}_x = x\,\partial^2/\partial y^2 - y\,\partial^2/\partial x\,\partial y - \tfrac{1}{2}\,\partial/\partial x + \tfrac{1}{2}\alpha x (x^2+y^2)^{-1/2} \\ \hat{X}_3 &= \hat{A}_y = y\,\partial^2/\partial x^2 - x\,\partial^2/\partial x\,\partial y - \tfrac{1}{2}\,\partial/\partial y + \tfrac{1}{2}\alpha y (x^2+y^2)^{-1/2} \\ \hat{X}_4 &= \mathrm{Re}\, z^{1/2}(\partial/\partial x - \mathrm{i}\partial/\partial y) \\ \hat{X}_5 &= \mathrm{Im}\, z^{1/2}(\partial/\partial x - \mathrm{i}\,\partial/\partial y) \\ \hat{X}_6 &= \mathrm{Re}\, z^{3/2}(\partial/\partial x - \mathrm{i}\,\partial/\partial y)\,\partial/\partial x + \alpha x\, \mathrm{Re}\, z^{-1/2} \\ \hat{X}_7 &= \mathrm{Im}\, z^{3/2}(\partial/\partial x - \mathrm{i}\,\partial/\partial y)\,\partial/\partial x + \alpha x\, \mathrm{Im}\, z^{-1/2}. \end{aligned} \tag{3.20}$$

Functions $C(x, y)$ in each symmetry operator are calculated from (3.10). The operators $\hat{A}_x$, $\hat{A}_y$ are the components of a two-dimensional Runge–Lenz vector. Note that the symmetry operators $\hat{X}_4$–$\hat{X}_7$ (unlike $\hat{X}_1$–$\hat{X}_3$) exist only at zero energy and commute with the Hamiltonian only on solutions of a corresponding Schrödinger equation. They are many-valued functions of coordinates.

In terms of classical mechanics (3.20) means that a move in a two-dimensional Coulomb potential with zero energy would be described by at least seven integrals of motion instead of three. Four of them are many-valued functions of coordinates.

3.2. Movement in the potential of a two-dimensional 'turn over' oscillator, $V = -\omega^2(x^2+y^2)$, at zero energy

Using the procedure described in the previous example we obtain the following symmetry operators:

$$\begin{aligned} \hat{X}_1 &= \hat{L}_z = y\,\partial/\partial x - x\,\partial/\partial y \\ \hat{X}_2 &= \partial^2/\partial x^2 + \omega^2 x^2 \\ \hat{X}_3 &= \partial^2/\partial x\,\partial y + \omega^2 xy \\ \hat{X}_4 &= \mathrm{Re}\, z^{-1}(\partial/\partial x - \mathrm{i}\,\partial/\partial y) \\ \hat{X}_5 &= \mathrm{Im}\, z^{-1}(\partial/\partial x - \mathrm{i}\,\partial/\partial y) \\ \hat{X}_6 &= \mathrm{Re}\,[z^{-2}(\partial/\partial x - \mathrm{i}\,\partial/\partial y)\,\partial/\partial x - z^{-3}(\partial/\partial x - \mathrm{i}\,\partial/\partial y) + \omega^2 x/z] \\ \hat{X}_7 &= \mathrm{Im}\,[z^{-2}(\partial/\partial x - \mathrm{i}\,\partial/\partial y)\,\partial/\partial x - z^{-3}(\partial/\partial x - \mathrm{i}\,\partial/\partial y) + \omega^2 x/z]. \end{aligned} \tag{3.21}$$

As in the previous example the symmetry operators $\hat{X}_1$–$\hat{X}_3$ also exist at any energy, while operators $\hat{X}_4$–$\hat{X}_7$ only exist if $E = 0$ with the regularity of coefficients breaking in the point $x = y = 0$.

It should be noted that neither the system of symmetry operators (3.20) nor the system (3.21) are closed with respect to commutation and, therefore, they do not form a Lie algebra. This is due to the limitation of the class of symmetry operators (2.9). The completion of sets (3.20) and (3.21) up to the bases of Lie algebra is not described by operators (2.3). However, the subsets of the first-order symmetry operators in (3.20) and (3.21) are closed with respect to the operation of commutation:

in (3.20)

$$[\hat{L}_z, \hat{X}_4] = -\tfrac{1}{2}\hat{X}_5 \qquad [\hat{L}_z, \hat{X}_5] = \tfrac{1}{2}\hat{X}_4 \qquad [\hat{X}_4, \hat{X}_5] = 0$$

in (3.21)

$$[\hat{L}_z, \hat{X}_4] = -2\hat{X}_5 \qquad [\hat{L}_z, \hat{X}_5] = 2\hat{X}_4 \qquad [\hat{X}_4, \hat{X}_5] = 0$$

and form a new, special Lie subalgebra, existing only at zero energy in the examples discussed.

4. Three-dimensional stationary Schrödinger equation

By introducing the independent variables x, y, z instead of x^1, x^2, x^3, operators $\hat{H}$, $\hat{S}$ and $\hat{U}$ can be written for a three-dimensional case ($n = 3$)

$$\hat{H} = -\partial^2/\partial x^2 - \partial^2/\partial y^2 - \partial^2/\partial z^2 + V(x, y, z) \tag{4.1}$$

$$\hat{S} = A^{11}\,\partial^2/\partial x^2 + A^{22}\,\partial^2/\partial y^2 + A^{33}\,\partial^2/\partial z^2 + 2A^{12}\,\partial^2/\partial x\,\partial y + 2A^{13}\,\partial^2/\partial x\,\partial z$$
$$+ 2A^{23}\,\partial^2/\partial y\,\partial z + B^1\,\partial/\partial x + B^2\,\partial/\partial y + B^3\,\partial/\partial z + C \tag{4.2}$$

$$\hat{U} = a^1\,\partial/\partial x + a^2\,\partial/\partial y + a^3\,\partial/\partial z + b. \tag{4.3}$$

The group of equations (2.6a) at $n = 3$ consists of the following ten equations

$$\begin{aligned}
&(\partial/\partial x)\tfrac{1}{2}(A^{11} - A^{22}) = \partial A^{12}/\partial y \qquad && (\partial/\partial y)\tfrac{1}{2}(A^{11} - A^{22}) = -\partial A^{12}/\partial x \\
&(\partial/\partial x)\tfrac{1}{2}(A^{11} - A^{33}) = \partial A^{13}/\partial z && (\partial/\partial z)\tfrac{1}{2}(A^{11} - A^{33}) = -\partial A^{13}/\partial x \\
&(\partial/\partial y)\tfrac{1}{2}(A^{22} - A^{33}) = \partial A^{23}/\partial z && (\partial/\partial z)\tfrac{1}{2}(A^{22} - A^{33}) = -\partial A^{23}/\partial y \\
&\partial A^{12}/\partial z + \partial A^{13}/\partial y + \partial A^{23}/\partial x = 0
\end{aligned} \tag{4.4}$$

$$a^1 = -2\,\partial A^{11}/\partial x \qquad a^2 = -2\,\partial A^{22}/\partial y \qquad a^3 = -2\,\partial A^{33}/\partial z. \tag{4.5}$$

The three relations (4.5) actually define the coefficients a^1, a^2, a^3. The first six equations in (4.4) are Cauchy–Riemann conditions for the corresponding variables. General solutions of these equations are

$$\begin{aligned}
&\tfrac{1}{2}(A^{11} - A^{22}) + \mathrm{i}A^{12} = f(x + \mathrm{i}y, z) \\
&\tfrac{1}{2}(A^{11} - A^{33}) + \mathrm{i}A^{13} = g(x + \mathrm{i}z, y) \\
&\tfrac{1}{2}(A^{22} - A^{33}) + \mathrm{i}A^{33} = h(y + \mathrm{i}z, x)
\end{aligned} \tag{4.6}$$

where $f(\cdot, \cdot)$, $g(\cdot, \cdot)$ and $h(\cdot, \cdot)$ are analytical functions of two variables. From (4.4) and (4.6) two functional couplings for f, g and h are obtained:

$$\mathrm{Im}\,(\partial f/\partial z + \partial g/\partial y + \partial h/\partial x) = 0 \tag{4.7}$$

$$\mathrm{Re}\,(f - g + h) = 0. \tag{4.8}$$

Using functions f, g and h, the group of equations (2.6b) may be expressed as:

$$\begin{aligned} &\mathrm{Re}\, \partial^2 f/\partial z^2 + \partial B^1/\partial x - \partial B^2/\partial y = 0 \\ &\mathrm{Re}\, \partial^2 g/\partial y^2 + \partial B^1/\partial x - \partial B^3/\partial z = 0 \\ &\mathrm{Re}\, \partial^2 h/\partial x^2 + \partial B^2/\partial y - \partial B^3/\partial z = 0 \end{aligned} \qquad (4.9a)$$

$$\begin{aligned} &\mathrm{Im}\, \partial^2 f/\partial z^2 + \partial B^2/\partial x + \partial B^1/\partial y = 0 \\ &\mathrm{Im}\, \partial^2 g/\partial y^2 + \partial B^3/\partial x + \partial B^1/\partial z = 0 \\ &\mathrm{Im}\, \partial^2 h/\partial x^2 + \partial B^3/\partial y + \partial B^2/\partial z = 0. \end{aligned} \qquad (4.9b)$$

One of the equations (4.9a) is the result of two other equations and the condition (4.8). However, in order to give the whole system (4.9) a more compact complex form, three equations are written in (4.9a). Let us introduce the new complex functions

$$B^{12} = B^1 + \mathrm{i}B^2 \qquad B^{13} = B^1 + \mathrm{i}B^3 \qquad B^{23} = B^2 + \mathrm{i}B^3. \qquad (4.10)$$

Multiplying each of equations (4.9b) by i and adding to the corresponding equation (4.9a) a system of three complex equations would result instead of (4.9)

$$\begin{aligned} &\partial B^{12}/\partial x + \mathrm{i}\, \partial B^{12}/\partial y + \partial^2 f/\partial z^2 = 0 \\ &\partial B^{13}/\partial x + \mathrm{i}\, \partial B^{13}/\partial z + \partial^2 g/\partial y^2 = 0 \\ &\partial B^{23}/\partial y + \mathrm{i}\, \partial B^{23}/\partial z + \partial^2 h/\partial x^2 = 0. \end{aligned} \qquad (4.11)$$

The following is a general solution of the system (4.11)

$$\begin{aligned} &B^{12} = \tilde{f}(x + \mathrm{i}y, z) - x\, \partial^2 f/\partial z^2 \\ &B^{13} = \tilde{g}(x + \mathrm{i}z, y) - x\, \partial^2 g/\partial y^2 \\ &B^{23} = \tilde{h}(y + \mathrm{i}z, x) - y\, \partial^2 h/\partial x^2 \end{aligned} \qquad (4.12)$$

where $\tilde{f}(\cdot,\cdot)$, $\tilde{g}(\cdot,\cdot)$ and $\tilde{h}(\cdot,\cdot)$ are analytical functions of two variables. Due to (4.10), the following conditions must evidently be satisfied:

$$\mathrm{Re}\,(B^{12} - B^{13}) = 0 \qquad \mathrm{Im}(B^{13} - B^{23}) = 0 \qquad \mathrm{Re}\, B^{23} = \mathrm{Im}\, B^{12} \qquad (4.13)$$

which are three functional couplings for $\tilde{f}$, $\tilde{g}$ and $\tilde{h}$. As has been mentioned in the previous section, classes of equivalent symmetry operators, forming a factor algebra L/I in relation to the ideal of trivial symmetries $\phi(x, y, z)(\hat{H} - E)$, are under consideration. Since one of the diagonal coefficients A^{ii} of the operator representing any of these classes may be taken as arbitrary, A^{22} may be chosen equal to 0 without reducing the generality. In this case from (2.6b) at $k = l = 2$ it follows that

$$b = -2\, \partial B^2/\partial y. \qquad (4.14)$$

In order to deduce mathematical consequences from the five functional couplings (4.7), (4.8) and (4.13) it suffices to analyse the case when A^{ij} and B^k are regular functions at the point $x = y = z = 0$ and to expand the functions f, g, h, $\tilde{f}$, $\tilde{g}$ and $\tilde{h}$ as

Taylor series:

$$\begin{pmatrix} f \\ \tilde{f} \end{pmatrix} = \sum_{k,l=0}^{\infty} \begin{pmatrix} f_{kl} \\ \tilde{f}_{kl} \end{pmatrix} (x+\mathrm{i}y)^k z^l \qquad \begin{pmatrix} g \\ \tilde{g} \end{pmatrix} = \sum_{k,l=0}^{\infty} \begin{pmatrix} g_{kl} \\ \tilde{g}_{kl} \end{pmatrix} (x+\mathrm{i}z)^k y^l$$
$$\begin{pmatrix} h \\ \tilde{h} \end{pmatrix} = \sum_{k,l=0}^{\infty} \begin{pmatrix} h_{kl} \\ \tilde{h}_{kl} \end{pmatrix} (y+\mathrm{i}z)^k x^l. \tag{4.15}$$

Substituting series (4.15) into equations (4.7), (4.8) and (4.13) gives recurrence relations for coefficients $f_{kl}, \ldots, \tilde{h}_{kl}$. Analysis of these recurrence relations shows that series (4.15) are cut off. The functions f, g and h appear to be fourth-order polynomials and $\tilde{f}$, $\tilde{g}$ and $\tilde{h}$ third-order polynomials in x, y, z. As a result of very long calculations it was found that all coefficients of these polynomials are defined by 46 arbitrarily chosen real constants and hence, the general symmetry operator (2.3) may be written as a linear combination of 46 basis operators of the type (2.3).

Let us introduce the following designations for the ten first-order basis operators obtained as described above:

$$\begin{aligned} &\hat{X}_1 = \partial/\partial x \qquad \hat{X}_2 = \partial/\partial y \qquad \hat{X}_3 = \partial/\partial z \\ &\hat{X}_4 = z\,\partial/\partial y - y\,\partial/\partial z \qquad \hat{X}_5 = x\,\partial/\partial z - z\,\partial/\partial x \\ &\hat{X}_6 = y\,\partial/\partial x - x\,\partial/\partial y \qquad \hat{X}_7 = x\,\partial/\partial x + y\,\partial/\partial y + z\,\partial/\partial z \\ &\hat{X}_8 = (x^2-y^2-z^2)\,\partial/\partial x + 2xy\,\partial/\partial y + 2xz\,\partial/\partial z + x \\ &\hat{X}_9 = 2xy\,\partial/\partial x + (y^2-x^2-z^2)\,\partial/\partial y + 2yz\,\partial/\partial z + y \\ &\hat{X}_{10} = 2xz\,\partial/\partial x + 2yz\,\partial/\partial y + (z^2-x^2-y^2)\,\partial/\partial z + z. \end{aligned} \tag{4.16a}$$

Using the methods described above, the general symmetry operator may be given in the form

$$\hat{X} = \lambda_0 + \sum_{\alpha=1}^{10} \lambda_\alpha \hat{X}_\alpha + \sum_{\alpha,\beta\in\Omega} \lambda_{\alpha\beta}\hat{X}_\alpha\hat{X}_\beta + C(x, y, z) \tag{4.16b}$$

where $\lambda_0, \lambda_\alpha, \lambda_{\alpha\beta}$ are real constants, $C(\cdot,\cdot,\cdot)$ is a function of coordinates, the form of which depends upon the potential, and Ω is a set consisting of 35 pairs (α, β):

$$\begin{aligned} \Omega = \{&1, 1; 1, 2; 1, 3; 1, 4; 1, 5; 1, 7; 2, 3; 2, 5; 2, 7; 2, 8; 3, 3; 3, 4; \\ &3, 5; 3, 7; 3, 8; 3, 9; 4, 4; 4, 7; 4, 9; 4, 10; 5, 5; 5, 7; 5, 8; 5, 9; 5, 10; 6, 6; \\ &6, 7; 6, 8; 6, 9; 6, 10; 8, 8; 8, 9; 8, 10; 9, 9; 9, 10\}. \end{aligned} \tag{4.17}$$

It should be noted, that the choice of the set Ω is not unique; instead of (4.17) any other set from the 35 pairs (α, β) may be chosen without invalidating the linear independence of the elements

$$1, \qquad \hat{X}_\alpha\ (\alpha = 1, \ldots, 10), \qquad \hat{X}_\alpha\hat{X}_\beta\ (\alpha, \beta \in \Omega). \tag{4.18}$$

The main property of Ω is that any class of equivalent operators, represented by an element $\hat{X}_\alpha\hat{X}_\beta$ $(\alpha, \beta = 1, \ldots, 10)$ belongs to the linear space with basis (4.18).

From (4.16a) it follows that all symmetry operators of the first-order X_α $(\alpha = 1, \ldots, 10)$ may be represented as

$$\hat{X}_\alpha = B_\alpha^k\,\partial/\partial x^k + C_\alpha \qquad \alpha = 1, \ldots, 10 \tag{4.19}$$

where summing over k is from 1 to 3, with $x^1=x$, $x^2=y$, $x^3=z$. All B^k_α and C_α coefficients are defined uniquely by (4.16a) and (4.19). Substituting (4.19) into (4.16b) and using (2.3) and (2.4) gives

$$A^{ij}=\tfrac{1}{2}\sum_{\alpha,\beta\in\Omega}\lambda_{\alpha\beta}(B^i_\alpha B^j_\beta+B^j_\alpha B^i_\beta) \tag{4.20}$$

$$B^k=\sum_{\alpha=1}^{10}\lambda_\alpha B^k_\alpha+\sum_{\alpha,\beta\in\Omega}\lambda_{\alpha\beta}(C_\alpha B^k_\beta+C_\beta B^k_\alpha+B^l_\alpha\,\partial B^k_\beta/\partial x^l).$$

Formulae (4.20) give general expressions for regular coefficients A^{ij} and B^k, containing 45 constants λ_α ($\alpha=1,\ldots,10$) and $\lambda_{\alpha\beta}$ ($\alpha,\beta\in\Omega$). These expressions should then be used in four equations (2.6c) and (2.6d), which contain the potential V. Three conditions of coincidence of these equations follow from the group of the equations (2.6c),

$$(\partial/\partial x^k)[a^i(V-E)-\Delta B^i-2A^{ij}\,\partial V/\partial x^j]=(\partial/\partial x^i)[a^k(V-E)-\Delta B^k-2A^{kl}\,\partial V/\partial x^l]$$
$$ik=12,13,23 \qquad (x^1,x^2,x^3)\equiv(x,y,z) \tag{4.21}$$

with the formula for C being

$$C(x,y,z)=\int_{x_0}^{x}[\tfrac{1}{2}a^1(V-E)-\tfrac{1}{2}\Delta B^1-A^{1j}\,\partial V/\partial x^j]_{\substack{x=\xi\\ y=y_0,z=z_0}}\,\mathrm{d}\xi$$
$$+\int_{y_0}^{y}[\tfrac{1}{2}a^2(V-E)-\tfrac{1}{2}\Delta B^2-A^{2j}\,\partial V/\partial x^j]_{\substack{y=\eta\\ z=z_0}}\,\mathrm{d}\eta \tag{4.22}$$
$$+\int_{z_0}^{z}[\tfrac{1}{2}a^3(V-E)-\tfrac{1}{2}\Delta B^3-A^{3j}\,\partial V/\partial x^j]_{z=\zeta}\,\mathrm{d}\zeta+\text{constant}.$$

Calculating ΔC with the help of (2.6c) and substituting this expression into (2.6d) leads to

$$(V-E)(\tfrac{1}{2}\,\partial a^k/\partial x^k-b)-\tfrac{1}{2}\,\partial\Delta B^k/\partial x^k+(B^k-\partial A^{kl}/\partial x^l-\tfrac{1}{2}a^k)\,\partial V/\partial x^k=0. \tag{4.23}$$

Relations (4.21) and (4.23) must be fullfilled identically for independent variables $x=x^1$, $y=x^2$, $z=x^3$. This condition permits all equations for 45 constants λ_α ($\alpha=1,\ldots,10$) and $\lambda_{\alpha\beta}$ ($\alpha,\beta\in\Omega$) to be obtained as well as the symmetry operators of the stationary Schrödinger equation with a particular potential to be found.

Let us now consider some examples. In the case of $V=-\tilde{\alpha}/\sqrt{x^2+y^2+z^2}$ and $V=-\omega^2(x^2+y^2+z^2)$, two-dimensional analogues of which were considered in § 3, additional symmetry operators at $E=0$ have not been found. Next, consider the example of a potential, which permits the symmetry operator, commuting with the Hamiltonian only on the solutions of the corresponding stationary Schrödinger equation.

Let only one constant λ_{67} differ from zero in the operator $\hat{X}$ (4.16b), so that

$$\hat{X}=\hat{X}_6\hat{X}_7+C(x,y,z). \tag{4.24}$$

The potential, permitting the operator (4.24), is then conveniently found in the form

$$V=r^{-2}\phi(z/r)+\theta(x,y,z) \tag{4.25}$$

where $r^2=x^2+y^2$, and $\phi(\cdot)$ is an arbitrary function. At $E=0$ the potential $V_0=r^{-2}\phi(z/r)$ allows both first-order symmetry operators $\hat{X}_6$ and $\hat{X}_7$: $[\hat{X}_6,\hat{H}]=0$,

$[\hat{X}_7, \hat{H}] = -2\hat{H}$. We are to find such functions $\theta(x, y, z)$ and $C(x, y, z)$ for which the potential (4.25) would allow the second-order symmetry operator (4.24) with $C(x, y, z) \neq 0$. The potential (4.25) must satisfy three equations (4.21) and equation (4.23). Considering that $V_0 = r^{-2}\phi(z/r)$ satisfies these equations with A^{ij} and B^k, defined by (4.24), the following four equations for θ can be derived from (4.21) and (4.23):

$$y\,\partial\theta/\partial x - x\,\partial\theta/\partial y = 0 \tag{4.26a}$$

$$\tfrac{1}{2}(x^2-y^2)(\partial^2\theta/\partial x^2 - \partial^2\theta/\partial y^2) + 2xy\,\partial^2\theta/\partial x\,\partial y + \tfrac{1}{2}xz\,\partial^2\theta/\partial x\,\partial z + \tfrac{1}{2}yz\,\partial^2\theta/\partial y\,\partial z$$
$$+3x\,\partial\theta/\partial x + 3y\,\partial\theta/\partial y + z\,\partial\theta/\partial z + 2\theta = 0 \tag{4.26b}$$

$$\tfrac{1}{2}yz\,(\partial^2\theta/\partial x^2 - \partial^2\theta/\partial z^2) - \tfrac{1}{2}xz\,\partial^2\theta/\partial x\,\partial y - xy\,\partial^2\theta/\partial x\,\partial z$$
$$+\tfrac{1}{2}(x^2-y^2)\,\partial^2\theta/\partial y\,\partial z - \tfrac{1}{2}z\,\partial\theta/\partial y - \tfrac{3}{2}y\,\partial\theta/\partial z = 0 \tag{4.26c}$$

$$\tfrac{1}{2}xz\,(\partial^2\theta/\partial y^2 - \partial^2\theta/\partial z^2) - \tfrac{1}{2}yz\,\partial^2\theta/\partial x\,\partial y - \tfrac{1}{2}(x^2-y^2)\,\partial^2\theta/\partial x\,\partial z$$
$$-xy\,\partial^2\theta/\partial y\,\partial z - \tfrac{1}{2}z\,\partial\theta/\partial x - \tfrac{3}{2}x\,\partial\theta/\partial z = 0. \tag{4.26d}$$

A function in the most general form, satisfying four equations (4.26), may be written as

$$\theta(x, y, z) = (1/r^2)\phi_1(z/r) + (\gamma/r^2)\ln r \tag{4.27}$$

where $r^2 = x^2 + y^2$, $\phi_1(\cdot)$ an arbitrary function, γ is a constant. The first term on the right hand side (4.27) is, however, of no importance, since it may be included in the term $r^{-2}\phi(z/r)$ of (4.25). Thus, the potential of interest has the form

$$V = (1/r^2)\phi(z/r) + (\gamma/r^2)\ln r \qquad \gamma \neq 0. \tag{4.28}$$

Calculating $C(x, y, z)$ in terms of (4.22) yields

$$\hat{X} = \hat{X}_6\hat{X}_7 + \tfrac{1}{2}\gamma\tan^{-1}(y/x). \tag{4.29}$$

It can be seen that the symmetry operator (4.29) satisfies the commutation relation

$$[\hat{X}, \hat{H}] = -2\hat{X}_6\hat{H}. \tag{4.30}$$

It should be noted that the axially symmetric potential (4.28) at $E \neq 0$ permits only one first-order symmetry operator $\hat{X}_6$, which identically commutes with the Hamiltonian. At $E = 0$ the potential (4.28) permits the non-commuting Lie algebra $(1, \hat{X}_6, \hat{X})$:

$$[\hat{X}_6, \hat{X}] = -\tfrac{1}{2}\gamma \tag{4.31}$$

with $\hat{X}$, as follows from (4.30), commuting with the Hamiltonian only on solutions of the corresponding stationary Schrödinger equation $\hat{H}\psi = 0$.

5. Conclusions

In both two- and three-dimensional cases, additional symmetry operators (which are, in terms of classical mechanics, additional integrals of motion) may appear when motion occurs with a specific energy. Naturally the origin of energy reference is chosen so that this specific energy is $E = 0$. Additional symmetry operators, existing only at $E = 0$, commute with the Hamiltonian only on solutions of a corresponding stationary Schrödinger equation. The symmetry operators, existing at all energies, identically commute with the Hamiltonian. With additional symmetry operators a specific Lie subalgebra may appear to exist in these problems only at $E=0$. Combination of all first and second-order symmetry operators, is not closed as a rule, with respect to commutation and does not form a Lie algebra, this being due to the limitation of the class of second-order symmetry operators.

In the two-dimensional case the structure of symmetry operators substantially depends on the fact that some linear combinations of operator coefficients are analytical functions of the complex variable $z=x+\mathrm{i}y$:

$$\tfrac{1}{2}(A^{11}-A^{22})+\mathrm{i}A^{12}=f(z) \qquad B^1+\mathrm{i}B^2=g(z).$$

In the most non-trivial (from the mathematical point of view) cases the potential, which is not identically equal to zero, allows up to seven non-trivial symmetry operators. Hence the analytical functions $f(z)$ and $g(z)$ satisfy some differential equations, the form of which depends on the potential. The specific nature of the two-dimensional case is that potential which is identically equal to zero at $E=0$ (Laplace equation) permits an infinite-dimensional Lie algebra, with the functions $f(z)$ and $g(z)$ being arbitrary.

In the three-dimensional case the number of second-order symmetry operators with regular coefficients is always limited and never exceeds 45. All the 45 symmetry operators are permited only when the potential is identically equal to zero at $E=0$ (Laplace equation). In this case ten symmetry operators $\hat{X}_\alpha$ ($\alpha=1,\ldots,10$) do not contain double differentiation and are, in fact, first-order operators. The other 35 operators can be presented in the form $\hat{X}_\alpha\hat{X}_\beta$. The mutual second-order symmetry operator, which depends on the 45 constants, has the following structure

$$\hat{X}=C(x,y,z)+\sum_{\alpha=1}^{10}\lambda_\alpha\hat{X}_\alpha+\sum_{\alpha,\beta\in\Omega}\lambda_{\alpha\beta}\hat{X}_\alpha\hat{X}_\beta$$

where λ_α, $\lambda_{\alpha\beta}$ are constants, $C(x,y,z)$ is a function of coordinates, the form of which depends on the potential, and Ω is some set of pairs (α,β) consisting of 35 elements. For each particular potential not all λ_α, $\lambda_{\alpha\beta}$ constants will be independent, and the number of symmetry operators, resulting from independent constants, is determined by the symmetry properties of the potential.

It should be noted that the problem of symmetry operators for a three-dimensional stationary Schrödinger equation with irregular coefficients (in one or more points) has not been considered in this work and remains to be solved.

Using these results one may not only examine the symmetry of the stationary Schrödinger equation with a given potential, but may also find potentials which possess certain properties of symmetry. Thus, the potential

$$V=(1/r^2)\phi(z/r)+(\gamma/r^2)\ln r,$$

taken as an example in § 4, leaves only λ_6 arbitrary at all energies and, thus, permits only the symmetry operator $\hat{X}_6$ which identically commutes with the Hamiltonian. Under the condition of zero energy there is a second arbitrary constant λ_{67} that is not equal to zero, and this gives an additional second-order symmetry operator, which commutes with the Hamiltonian only for solutions of a corresponding stationary

Schrödinger equation. It should be stressed that in this case symmetry operators form a non-commutative Lie algebra, which in the example considered exists only if the energy is equal to zero.

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