ANALYTIC ENERGIES AND WAVE FUNCTIONS OF TWO-DIMENSIONAL SCHRÖDINGER EQUATION: TWO-DIMENSIONAL FOURTH-ORDER POLYNOMIAL POTENTIAL

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Dedicated to Professor Rudolf Zahradník on the occasion of his 80th birthday.

Direct method for searching analytic solutions of the two-dimensional Schrödinger equation with a two-dimensional fourth-order polynomial potential is presented. Analytic formulas for the energies and wave functions of the ground state and excited state are found. Obtained results can not be in general reduced to two one-dimensional cases.

Keywords: Analytic solution; Anharmonic oscillator; Polynomial potential; Schrödinger equation; Quantum chemistry.

In this paper, our goal is to generalize the algebraic method presented in[1–3] for searching the analytic solutions of the one-dimensional Schrödinger equation to the two-dimensional case. As the simplest case, an example of the analytic solution of the two-dimensional Schrödinger equation with the fourth-order polynomial potential is presented.

The problem of the one-dimensional Schrödinger equation with the fourth-order polynomial potential can be solved in different ways, see for example[4–8]. An obvious method of solving the two-dimensional Schrödinger equation is the separation of variables which is applicable in special cases only. Another exact methods for solving the Schrödinger equation with the two-dimensional fourth-order polynomial potential have been presented in the framework of the non-Hermitian models[9,10] or supersymmetric models[11]. The two-dimensional fourth-order polynomial potential can also be solved using some approximate methods[12–14].

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Our method represents a new algebraic approach, in which the two-dimensional Schrödinger equation is solved without the separation of variables and no symmetry of the problem is assumed.

First we summarize briefly the results of refs[1–3]. There, the solutions of the one-dimensional Schrödinger equation

$$-\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x) \tag{1}$$

was searched in the form of the linear combinations of the functions ψ_m

$$\psi(x) = \sum_m c_m \psi_m(x) \tag{2}$$

where

$$\psi_m(x) = f(x)^m h(x) . \tag{3}$$

Here, $f(x)$ is a given function and the function $h(x)$ can be obtained from the formula

$$h(x) = \exp\left(-\int \frac{\sum_m h_m (f)^m}{\sum_m f_m (f)^m} \, df\right) . \tag{4}$$

Coefficients h_m can be found by the method described in[2]. The formula (*4*) has been derived under very general assumptions and allows to find ground state wave functions of all usual one-dimensional analytically solvable potentials.

It has been proved in[2] that to obtain analytic solutions, the potential V must have the form

$$V(x) = \sum_m V_m f(x)^m \tag{5}$$

and the function $h(x)$ is the ground-state wave function. Using this approach, it is possible to take different forms of the function $f(x)$ and to test whether the Schrödinger equation with the potential V of the form (*5*) has analytical solutions obeying the corresponding boundary condition.

Now we will discuss generalization of this approach to the two-dimensional case.

GENERALIZATION TO TWO-DIMENSIONAL CASE

Few generalizations of Eqs (*2*)–(*3*) to two dimensions have been examined. Successful approach is to assume the solutions of the Schrödinger equation

$$-\Delta\psi(x,y) + V(x,y)\psi(x,y) = E\psi(x,y) \tag{6}$$

where $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ in the form

$$\psi(x,y) = \sum_{m,n} c_{mn}\psi_{mn}(x,y) \tag{7}$$

where

$$\psi_{mn}(x,y) = f(x)^m\, g(y)^n\, h(x,y)\,. \tag{8}$$

Here, the functions $f(x)$, $g(y)$ and $h(x,y)$ have an analogous meaning as the functions $f(x)$ and $h(x)$ in Eqs (*2*)–(*3*).

Analogously to Eq. (*5*), it is assumed that the potential has the form

$$V(x,y) = \sum_{m,n} V_{mn}\, f(x)^m\, g(y)^n\,. \tag{9}$$

BOUND STATES FOR TWO-DIMENSIONAL FOURTH-ORDER POLYNOMIAL POTENTIAL

In this paper, we discuss only the simplest case $f(x) = x$ and $g(y) = y$, i.e. the potential V is assumed in the form of a polynomial in the variables x and y

$$\begin{aligned} V(x,y) = {} & W_{40}^2 x^4 + W_{04}^2 y^4 + V_{31}x^3y + V_{13}xy^3 + V_{22}x^2y^2 + \\ & + V_{30}x^3 + V_{03}y^3 + V_{21}x^2y + V_{12}xy^2 + \\ & + V_{20}x^2 + V_{02}y^2 + V_{11}xy + V_{10}x + V_{01}y\,. \end{aligned} \tag{10}$$

Here, we denoted $W_{40} \equiv \sqrt{V_{40}}$, $W_{04} \equiv \sqrt{V_{04}}$, where we assume $V_{40} > 0$ and $V_{04} > 0$ which are necessary conditions for the existence of the bound states. The potential (*10*) can represent important physical potentials: coupled anharmonic oscillators, two-dimensional double-well problem and generalizations of these problems. In chemical physics, such potentials are important for example for description of the highly non-linear vibrational problems of nonrigid molecules. We note that the coupling terms proportional to x^3y, xy^3, x^2y^2, x^2y, xy^2 and xy prevent separation of the two-dimensional problem with the potential (*10*) to two independent one-dimensional problems. Therefore, the usual method based on separation of variables is not applicable here.

We have not found generalization of the formula (*4*) to two-dimensions. For this reason, another method of searching for the function $h(x,y)$ is used. It is known from[1–3] that in the one-dimensional case, the polynomial potentials lead to the function $h(x)$ in form of the exponential of a polynomial. Therefore, we assume the function $h(x,y)$ in the form

$$h(x,y) = \exp\left(-\sum_{m,n} d_{mn} f(x)^m \, g(y)^n\right) = \exp\left(-\sum_{m,n} d_{mn} x^m y^n\right) \qquad (11)$$

where d_{mn} are numerical coefficients to be found.

Ground States

By analogy with the one-dimensional case, it is assumed that the function $h(x,y)$ plays the role of the ground-state wave function. Substituting Eqs (*11*) and (*10*) into Eq. (*6*) and comparing the terms of the same order, we get the ground state energy

$$E = -d_{10}^2 - d_{01}^2 + 2d_{02} + 2d_{20} \qquad (12)$$

and a system of 14 equations for 9 unknown coefficients d_{ij}

$$W_{40}^2 = 9d_{30}^2 + d_{21}^2 \qquad (13)$$

$$W_{04}^2 = 9d_{03}^2 + d_{12}^2 \qquad (14)$$

$$V_{31} = 12d_{30}d_{21} + 4d_{21}d_{12} \quad (15)$$

$$V_{13} = 12d_{03}d_{12} + 4d_{12}d_{21} \quad (16)$$

$$V_{22} = 6d_{30}d_{12} + 4d_{12}^2 + 4d_{21}^2 + 6d_{21}d_{03} \quad (17)$$

$$V_{30} = 12d_{20}d_{30} + 2d_{11}d_{21} \quad (18)$$

$$V_{03} = 12d_{02}d_{03} + 2d_{11}d_{12} \quad (19)$$

$$V_{21} = 4d_{21}d_{02} + 8d_{20}d_{21} + 6d_{30}d_{11} + 4d_{11}d_{12} \quad (20)$$

$$V_{12} = 4d_{12}d_{20} + 8d_{02}d_{12} + 6d_{03}d_{11} + 4d_{11}d_{21} \quad (21)$$

$$V_{20} = 2d_{01}d_{21} + d_{11}^2 + 4d_{20}^2 + 6d_{10}d_{30} \quad (22)$$

$$V_{02} = 2d_{10}d_{12} + d_{11}^2 + 4d_{02}^2 + 6d_{01}d_{03} \quad (23)$$

$$V_{11} = 4d_{01}d_{12} + 4d_{11}d_{02} + 4d_{20}d_{11} + 4d_{10}d_{21} \quad (24)$$

$$V_{10} = 4d_{10}d_{20} - 6d_{30} + 2d_{01}d_{11} - 2d_{12} \quad (25)$$

$$V_{01} = 4d_{01}d_{02} - 6d_{03} + 2d_{10}d_{11} - 2d_{21} \quad (26)$$

It is seen also that all coefficients d_{ij}, where $i + j > 3$ must equal zero. As in the one-dimensional case[3], the system of Eqs (*13*)–(*26*) is solvable only for certain values of the potential coefficients V_{mn}.

To get the function ψ_0 quadratically integrable in the whole plane (x,y), a similar method as in[3] is used. The function h and the potential V are modified to the form depending on $|x|$ and $|y|$

$$\psi_0(x,y) = h(x,y) = \exp(-d_{30}|x|^3 - d_{03}|y|^3 - d_{21}x^2|y| - d_{12}|x|y^2 - d_{20}x^2 - d_{02}y^2 - d_{11}|xy| - d_{10}|x| - d_{01}|y|) \qquad (27)$$

$$V(x,y) = W_{40}^2 x^4 + W_{04}^2 y^4 + V_{31}|x|^3 y + V_{13}x|y|^3 + V_{22}x^2y^2 + V_{30}|x|^3 + V_{03}|y|^3 + V_{21}x^2|y| + V_{12}|x|y^2 + V_{20}x^2 + V_{02}y^2 + V_{11}|xy| + V_{10}|x| + V_{01}|y| \,. \qquad (28)$$

In this case, the only problem is that the potential (*28*) and the wave function (*27*) have not continuous derivatives at the coordinate axes, as already known from the one-dimensional case (see ref.[3]).

General discussion of the solutions of the system of Eqs (*13*)–(*26*) will be published elsewhere. In this paper, only the simplest case $V_{13} = V_{31} = 0$ and $d_{21} = d_{12} = 0$ will be discussed. In this case, Eqs (*15*)–(*16*) are fulfilled automatically, Eq. (*17*) yields

$$V_{22} = 0 \qquad (29)$$

and Eqs (*13*)–(*14*) have the solution

$$d_{30} = \frac{W_{40}}{3} \qquad (30)$$

$$d_{03} = \frac{W_{04}}{3} \,. \qquad (31)$$

Here, to get d_{30} and d_{03} positive, the positive signs of the square roots are taken. With this choice, the wave function (*27*) behaves as $\exp(-|x|^3 - |y|^3)$ and is quadratically integrable in the whole plane (x,y).

Now, the remaining system of Eqs (*18*)–(*26*) has a solution if and only if

$$\frac{V_{21}}{W_{40}} = \frac{V_{12}}{W_{04}} \equiv X \tag{32}$$

$$V_{11} = \frac{V_{30}X}{2W_{40}} + \frac{V_{03}X}{2W_{04}} \tag{33}$$

$$V_{10} = \frac{4W_{04}^2 V_{02} - V_{03}^2 - V_{12}^2}{8W_{04}^3} X + \frac{4W_{40}^2 V_{20} - V_{30}^2 - V_{21}^2}{8W_{40}^4} V_{30} - 2W_{40} \tag{34}$$

$$V_{01} = \frac{4W_{40}^2 V_{20} - V_{30}^2 - V_{21}^2}{8W_{40}^3} X + \frac{4W_{04}^2 V_{02} - V_{03}^2 - V_{12}^2}{8W_{04}^4} V_{03} - 2W_{04} \tag{35}$$

and its solution is

$$d_{20} = \frac{V_{30}}{4W_{40}} \tag{36}$$

$$d_{02} = \frac{V_{03}}{4W_{04}} \tag{37}$$

$$d_{11} = \frac{X}{2} \tag{38}$$

$$d_{10} = \frac{4W_{40}^2 V_{20} - V_{30}^2 - V_{21}^2}{8W_{40}^3} \tag{39}$$

$$d_{01} = \frac{4W_{04}^2 V_{02} - V_{03}^2 - V_{12}^2}{8W_{04}^3} . \tag{40}$$

The potential satisfying all the conditions $V_{31} = V_{13} = 0$ and Eq. (*29*), Eqs (*32*)–(*35*) can be in general written as

$$
\begin{aligned}
V_0(x,y) = {} & W_{40}^2 x^4 + W_{04}^2 y^4 + V_{30}|x|^3 + V_{03}|y|^3 + W_{40} X x^2 |y| + W_{04} X |x| y^2 + \\
& + V_{20} x^2 + V_{02} y^2 + \frac{X}{2}\left(\frac{V_{30}}{W_{40}} + \frac{V_{03}}{W_{04}}\right)|xy| + \\
& + \left(\frac{4W_{04}^2 V_{02} - W_{04}^2 X^2 - V_{03}^2}{8W_{04}^3} X + \frac{4W_{40}^2 V_{20} - W_{40}^2 X^2 - V_{30}^2}{8W_{40}^4} V_{30} - 2W_{40}\right)|x| + \\
& + \left(\frac{4W_{40}^2 V_{20} - W_{40}^2 X^2 - V_{30}^2}{8W_{40}^3} X + \frac{4W_{04}^2 V_{02} - W_{04}^2 X^2 - V_{03}^2}{8W_{04}^4} V_{03} - 2W_{04}\right)|y|
\end{aligned}
\qquad (41)
$$

where W_{40} and W_{04} are arbitrary positive real numbers and V_{30}, V_{03}, V_{20}, V_{02} and X are arbitrary real numbers. Substituting all formulas for the coefficients d_{ij}, i.e. Eqs (*30*)–(*31*), (*36*)–(*38*) and (*39*)–(*40*) into Eqs (*12*) and (*27*) we get the formula for the ground state wave function for the potential (*41*) in the form

$$
\begin{aligned}
\psi_0(x,y) = \exp\Bigg(& -\frac{W_{40}}{3}|x|^3 - \frac{W_{04}}{3}|y|^3 - \frac{V_{30}}{4W_{40}} x^2 - \frac{V_{03}}{4W_{04}} y^2 - \frac{X}{2}|xy| - \\
& - \frac{4W_{40}^2 V_{20} - W_{40}^2 X^2 - V_{30}^2}{8W_{40}^3}|x| - \frac{4W_{04}^2 V_{02} - W_{04}^2 X^2 - V_{03}^2}{8W_{04}^3}|y|\Bigg).
\end{aligned}
\qquad (42)
$$

The corresponding ground state energy reads

$$
\begin{aligned}
E_0 = {} & \frac{V_{30}}{2W_{40}} + \frac{V_{03}}{2W_{04}} - \\
& - \frac{(4W_{40}^2 V_{20} - W_{40}^2 X^2 - V_{30}^2)^2}{64W_{40}^6} - \frac{(4W_{04}^2 V_{02} - W_{04}^2 X^2 - V_{03}^2)^2}{64W_{04}^6} .
\end{aligned}
\qquad (43)
$$

It is seen that the resulting wave function (*42*) is quadratically integrable in the whole plane (x,y). If $X \neq 0$, the potential (*41*) contains three cross terms (proportional to $x^2|y|$, $|x|y^2$ and $|xy|$) and, in general, it cannot be reduced to two independent one-dimensional potentials. Note that if $X = 0$, i.e. if the coupling terms are absent, the potential (*41*) has the form of the sum of two one-dimensional potentials discussed in[3].

Excited States

Using the notation

$$p(x,y) = \sum_{m,n=0}^{m+n \leq N} c_{m,n} x^m y^n \tag{44}$$

where c_{mn} are coefficients to be found, Eq. (*7*) can be rewritten into the form

$$\psi(x,y) = p(x,y)h(x,y) \tag{45}$$

where $h(x,y) = \psi_0(x,y)$ is given by Eq. (*42*). Substituting Eq. (*45*) into Eq. (*6*) we get

$$\frac{\Delta p + \frac{\partial p}{\partial x}\frac{\partial h}{\partial x}\frac{2}{h} + \frac{\partial p}{\partial y}\frac{\partial h}{\partial y}\frac{2}{h}}{p} + \frac{\Delta h}{h} = V - E\,. \tag{46}$$

In this equation, V and $\Delta h/h$ are polynomials in the variables x and y. For this reason, the first fraction in Eq. (*46*) must be possible to modify to a polynomial. Therefore, it must exist a polynomial $a(x,y)$ satisfying the equation

$$\Delta p + \frac{\partial p}{\partial x}\frac{\partial h}{\partial x}\frac{2}{h} + \frac{\partial p}{\partial y}\frac{\partial h}{\partial y}\frac{2}{h} = pa\,. \tag{47}$$

Calculating the orders of the polynomials and their derivatives in this equation, it can be shown that a must be a first-order polynomial for arbitrary N, i.e. a must have a form

$$a(x,y) = a_{10}x + a_{01}y + a_{00}\,. \tag{48}$$

Substituting Eqs (*42*), (*44*) for a given order N and Eq. (*48*) into Eq. (*47*) and comparing the terms of the same order a system of equations for the unknowns c_{ij} and a_{ij} is obtained. For $N = 1$, this system of equations has the form

$$0 = 2c_{10}W_{40} + c_{10}a_{10} \tag{49}$$

$$0 = 2c_{01}W_{04} + c_{01}a_{01} \tag{50}$$

$$0 = c_{10}a_{01} + c_{01}a_{10} \tag{51}$$

$$0 = \frac{c_{10}V_{30}}{W_{40}} + c_{01}X + c_{10}a_{00} + c_{00}a_{10} \tag{52}$$

$$0 = \frac{c_{01}V_{03}}{W_{04}} + c_{10}X + c_{01}a_{00} + c_{00}a_{01} \tag{53}$$

$$0 = \frac{V_{30}^2 c_{10}}{4W_{40}^3} + \frac{V_{03}^2 c_{01}}{4W_{04}^3} + \frac{X^2 c_{10}}{4W_{40}} + \frac{X^2 c_{01}}{4W_{04}} - \frac{V_{20}c_{10}}{W_{40}} - \frac{V_{02}c_{01}}{W_{04}} - c_{00}a_{00}\,. \tag{54}$$

The system of Eqs (*49*)–(*54*) has a solution only if the condition

$$V_{20} - V_{02} = \frac{W_{04}^2 X^2 + 3V_{30}^2 - 2W_{04}V_{30}X}{8W_{40}^2} - \frac{W_{40}^2 X^2 + 3V_{03}^2 - 2W_{40}V_{03}X}{8W_{04}^2} \tag{55}$$

is fulfilled. If this condition is fulfilled, the system of Eqs (*49*)–(*54*) has an infinite number of solutions leading to the same potential and energy and to physically equivalent wave functions differing by the normalization factor only. One of the solutions is

$$p(x,y) = W_{40}x - W_{04}y + \frac{W_{40}X - V_{03}}{4W_{04}} - \frac{W_{04}X - V_{30}}{4W_{40}} \tag{56}$$

$$a(x,y) = -2W_{40}x - 2W_{04}y + \frac{X}{2}\left(\frac{W_{40}}{W_{04}} + \frac{W_{04}}{W_{40}}\right) - \frac{V_{30}}{2W_{40}} - \frac{V_{03}}{2W_{04}} . \tag{57}$$

Formulas for the potential, wave function and energy of the excited state are obtained by substituting Eqs (*42*) and (*56*) to Eqs (*45*)–(*46*). The resulting formulas are

$$V_1(x,y) = W_{40}^2x^4 + W_{04}^2y^4 + V_{30}|x|^3 + V_{03}|y|^3 + W_{40}Xx^2|y| + W_{04}X|x|y^2 +$$
$$+ V_{20}x^2 + V_{02}y^2 + \frac{X}{2}\left(\frac{V_{30}}{W_{40}} + \frac{V_{03}}{W_{04}}\right)|xy| + \tag{58}$$
$$+\left(\frac{4W_{04}^2V_{02} - W_{04}^2X^2 - V_{03}^2}{8W_{04}^3}X + \frac{4W_{40}^2V_{20} - W_{40}^2X^2 - V_{30}^2}{8W_{40}^4}V_{30} - 4W_{40}\right)|x| +$$
$$+\left(\frac{4W_{40}^2V_{20} - W_{40}^2X^2 - V_{30}^2}{8W_{40}^3}X + \frac{4W_{04}^2V_{02} - W_{04}^2X^2 - V_{03}^2}{8W_{04}^4}V_{03} - 4W_{04}\right)|y|$$

and

$$\psi_1(x,y) = \left(W_{40}x - W_{04}y + \frac{W_{40}X - V_{03}}{4W_{04}} - \frac{W_{04}X - V_{30}}{4W_{40}}\right)\times$$
$$\times \exp\left(-\frac{W_{40}}{3}|x|^3 - \frac{W_{04}}{3}|y|^3 - \frac{V_{30}}{4W_{40}}x^2 - \frac{V_{03}}{4W_{04}}y^2 - \frac{X}{2}|xy| - \right. \tag{59}$$
$$\left. - \frac{4W_{40}^2V_{20} - W_{40}^2X^2 - V_{30}^2}{8W_{40}^3}|x| - \frac{4W_{04}^2V_{02} - W_{04}^2X^2 - V_{03}^2}{8W_{04}^3}|y|\right)$$

$$E_1 = \frac{V_{30}}{W_{40}} + \frac{V_{03}}{W_{04}} - \frac{X}{2}\left(\frac{W_{40}}{W_{04}} + \frac{W_{04}}{W_{40}}\right) - \qquad (60)$$
$$- \frac{(4W_{40}^2 V_{20} - W_{40}^2 X^2 - V_{30}^2)^2}{64W_{40}^6} - \frac{(4W_{04}^2 V_{02} - W_{04}^2 X^2 - V_{03}^2)^2}{64W_{04}^6} .$$

The formulas (*58*)–(*60*) are valid only if the condition (*55*) is fulfilled. It is seen that the wave function (*59*) is quadratically integrable in the whole plane (x,y).

Our analysis indicates that the appropriate system of equations has no solution for $N > 1$.

It is seen that if $X \neq 0$, the potential V_1 cannot be in general transformed into the sum of two independent one-dimensional potentials. Therefore, there are analytic solutions of the two-dimensional Schrödinger equation with the fourth-order polynomial potential that cannot be obtained by the separation of variables.

Note that if $X = 0$, i.e. if the coupling terms are absent, the potential (*41*) has the form of the sum of two one-dimensional potentials discussed in[3].

CONCLUSIONS

In this paper, we have discussed analytic solutions of the two-dimensional Schrödinger equation in cases when other known methods like the separation of variables are unusable. This problem appears to be rather difficult and, for this reason, we have made several additional assumptions. For the sake of generality, we have used the algebraic method of the solution of the Schrödinger equation. The advantage of this approach is its generality not relying on the special properties (like the symmetry, supersymmetry, etc.) of the problem. Our method is generalization of the one-dimensional approach used in[1–3]. It appears in analogy with the one-dimensional case that the analytic solutions of the Schrödinger equation exist for the two-dimensional fourth-order polynomial potentials only for certain values of the potential coefficients. Analytic formulas for the wave functions and energies of the ground state and one excited state have been found.

It has been shown that there exist analytic solutions of the two-dimensional Schrödinger equation that cannot be obtained by the separation of the variables leading to two independent one-dimensional problems. Generalization of the presented method to other types of potentials is in progress.

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