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Analytic Solutions of Multi-Dimensional Schrödinger Equation

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Abstract. There exists a part of mathematical physics that aims to find new potentials for which the Schrödinger equation has analytical solution. One method of this searching for one-dimensional Schrödinger equation was presented in [1], [2]. Our goal is to generalize this method to a multi-dimensional case.

Introduction

It was assumed in [1], [2] that the wave functions are linear combinations of the functions in the form

$$\psi_m(x) = f(x)^m h(x), \tag{1}$$

where $f(x)$ and $h(x)$ are general functions.

It has been proved that in this case the potential must have the form

$$V(x) = \sum_m f(x)^m \tag{2}$$

and the function $h(x)$ is the ground state wave function. It is possible to choose function $f(x)$ and test if the Schrödinger equation with some potential of the form (2) has analytical solutions.

Now we search for generalization to a multi-dimensional case.

Generalization to multi-dimensional case

Wave functions

It is possible to suggest few generalizations of the assumption (1) to n-dimensional case, but the most straightforward is to suppose that wave functions are linear combinations of functions

$$\psi_{m_1,m_2,\ldots,m_n} = f_1(x_1)^{m_1} f_2(x_2)^{m_2} \ldots f_n(x_n)^{m_n} h(x_1, x_2, \ldots, x_n). \tag{3}$$

General discussion is very complicated in this case. Now we will confine ourselves to a two-dimensional case

$$\psi_{m,n} = f(x)^m g(y)^n h(x, y). \tag{4}$$

We will discuss this problem in cartesian coordinates. It is possible to discuss the problem in the polar coordinates, but it is more complicated than a cartesian case, because it is necessary to include a cyclic condition for the angle coordinate in this case.

Potential

We tried to generalize the potential form to

$$V(x, y) = \sum_m \sum_n V_{mn} f(x)^m g(y)^n. \tag{5}$$

We will discuss only the case when $f(x) = x$ and $g(y) = y$. It means that potential is a polynomial in the variables x and y.

Function h

A differential equation for function $h(x)$ was found in [1], [2]. In the one-dimensional case this function is determined for the given function $f(x)$. We have not found an analogical result for the two-dimensional case. But we know that some polynomial potentials in one-dimensional case have the ground state in form of an exponential of a polynomial. That is why we will suppose that the function $h(x,y)$ has the form

$$h(x,y) = \psi_0(x,y) = \exp\left(\sum_{m,n} c_{mn} f(x)^m g(y)^n\right) = \exp\left(\sum_{m,n} c_{mn} x^m y^n\right), \tag{6}$$

where c_{mn} are numerical coefficients.

Bound states for two-dimensional quadratic potential

We assume that the potential has a form

$$V(x,y) = V_{20}x^2 + V_{02}y^2 + V_{11}xy + V_{10}x + V_{01}y. \tag{7}$$

This potential has bound states if and only if

$$V_{20} > 0 \tag{8}$$

$$V_{02} > 0 \tag{9}$$

$$(V_{11})^2 \leq 4V_{20}V_{02}. \tag{10}$$

It will occur if and only if the potential (7) is a positive definite quadratic form. Therefore, we can diagonalize this quadratic form and separate partial Schrödinger equation with independend variables x and y to two ordinary Schrödinger equations for two harmonic oscillators. It means that this problem is always analytically solvable, but we tested to use the mentioned method of solving this problem. It means that we tested whether our assumptions are correct.

Let us assume that the ground state wave function is an exponential of a polynomial as we have mentioned above

$$h(x,y) = \exp\left(-c_{20}x^2 - c_{02}y^2 - c_{11}xy - c_{10}x - c_{01}y\right). \tag{11}$$

Here we have written conventional minus signs in the exponential.

The function $h(x,y)$ must obey the Schrödinger equation

$$-\triangle h(x,y) + V(x,y)h(x,y) = Eh(x,y). \tag{12}$$

We want to find the potential $V(x,y)$ that is why we will rewrite the Schrödinger equation into the form

$$V(x,y) - E = \frac{\triangle h(x,y)}{h(x,y)}. \tag{13}$$

Substituting (7) and (11) into (13) we get an equation with polynomials at both sides

$$\begin{aligned} V_{20}x^2 & + V_{02}y^2 + V_{11}xy + V_{10}x + V_{01}y - E \\ = & \quad (4\,c_{20}{}^2 + c_{11}{}^2)\,x^2 + (4\,c_{02}{}^2 + c_{11}{}^2)\,y^2 + (4\,c_{11}\,c_{02} + 4\,c_{20}\,c_{11})\,x\,y \\ + & \quad (4\,c_{10}\,c_{20} + 2\,c_{01}\,c_{11})\,x + (4\,c_{01}\,c_{02} + 2\,c_{10}\,c_{11})\,y - 2\,c_{20} + c_{10}{}^2 - 2\,c_{02} + c_{01}{}^2. \end{aligned} \tag{14}$$

It follows from this equations that

$$\begin{aligned}
V_{20} &= 4\,{c_{20}}^2 + {c_{11}}^2, && (15)\\
V_{02} &= 4\,{c_{02}}^2 + {c_{11}}^2, && (16)\\
V_{11} &= 4\,c_{11}\,c_{02} + 4\,c_{20}\,c_{11}, && (17)\\
V_{10} &= 4\,c_{10}\,c_{20} + 2\,c_{01}\,c_{11}, && (18)\\
V_{01} &= 4\,c_{01}\,c_{02} + 2\,c_{10}\,c_{11}, && (19)\\
E &= 2\,c_{20} - {c_{10}}^2 + 2\,c_{02} - {c_{01}}^2. && (20)
\end{aligned}$$

Now we can evaluate coefficients V_{ij} and the ground state energy E if we know coefficients c_{ij}. But a normal task is reversal. For a given potential we want to evaluate the wave function and energy. We need to solve the system of equations (15)-(19) with respect to the coefficients c_{ij}. It is possible, but the resulting formulas are complicated. We have chosen the simpler way. We have expressed the coefficient c_{11} and found two solutions for its square. It means that there exist four solutions for c_{11}

$$(c_{11})^2 = \frac{(V_{11})^2}{4}\frac{V_{02} + V_{20} + \sqrt{4V_{20}V_{02} - (V_{11})^2}}{(V_{20} - V_{02})^2 + (V_{11})^2} \qquad (21)$$

or

$$(c_{11})^2 = \frac{(V_{11})^2}{4}\frac{V_{02} + V_{20} - \sqrt{4V_{20}V_{02} - (V_{11})^2}}{(V_{20} - V_{02})^2 + (V_{11})^2}. \qquad (22)$$

Now for the chosen solution we can express other coefficients c_{ij} as

$$\begin{aligned}
c_{01} &= \frac{1}{2}\,\frac{-V_{10}\,c_{11} + \sqrt{V_{20} - {c_{11}}^2}\,V_{01}}{\sqrt{V_{02} - {c_{11}}^2}\,\sqrt{V_{20} - {c_{11}}^2} - {c_{11}}^2}, && (23)\\
c_{10} &= \frac{1}{2}\,\frac{-V_{01}\,c_{11} + \sqrt{V_{02} - {c_{11}}^2}\,V_{10}}{\sqrt{V_{02} - {c_{11}}^2}\,\sqrt{V_{20} - {c_{11}}^2} - {c_{11}}^2}, && (24)\\
c_{02} &= \frac{1}{2}\sqrt{V_{02} - {c_{11}}^2}, && (25)\\
c_{20} &= \frac{1}{2}\sqrt{V_{20} - {c_{11}}^2}. && (26)
\end{aligned}$$

If we evaluate these coefficients, we can determine the ground state wave function from the formula (11) and its energy from (20).

Bound states for two-dimensional quartic potential

Now the potential is assumed in the form

$$\begin{aligned}
V(x,y) &= V_{40}x^4 + V_{04}y^4 + V_{31}x^3y + V_{13}xy^3 + V_{22}x^2y^2 && (27)\\
&+ V_{30}x^3 + V_{03}y^3 + V_{21}x^2y + V_{12}xy^2\\
&+ V_{20}x^2 + V_{02}y^2 + V_{11}xy + V_{10}x + V_{01}y.
\end{aligned}$$

Let us try to find the ground state wave function as an exponential function of a cubic polynomial as it is in the one-dimensional case

$$h(x,y) = \exp\left(-c_{30}x^3 - c_{03}y^3 - c_{21}x^2y - c_{12}xy^2 - c_{20}x^2 - c_{02}y^2 - c_{11}xy - c_{10}x - c_{01}y\right). \quad (28)$$

Substituting (27) and (28) into (13) as it has been done for a quadratic potential, we get the formula for the ground state energy

$$E = -{c_{10}}^2 - {c_{01}}^2 + 2c_{02} + 2c_{20} \qquad (29)$$

and system of equations for the potential coefficients

$$
\begin{aligned}
V_{40} &= 9{c_{30}}^2 + {c_{21}}^2, && (30)\\
V_{04} &= 9{c_{03}}^2 + {c_{12}}^2, && (31)\\
V_{31} &= 12c_{30}c_{21} + 4c_{21}c_{12}, && (32)\\
V_{13} &= 12c_{03}c_{12} + 4c_{12}c_{21}, && (33)\\
V_{22} &= 6c_{30}c_{12} + 4{c_{12}}^2 + 4{c_{21}}^2 + 6c_{21}c_{03}, && (34)\\
V_{30} &= 12c_{20}c_{30} + 2c_{11}c_{21}, && (35)\\
V_{03} &= 12c_{02}c_{03} + 2c_{11}c_{12}, && (36)\\
V_{21} &= 4c_{21}c_{02} + 8c_{20}c_{21} + 6c_{30}c_{11} + 4c_{11}c_{12}, && (37)\\
V_{12} &= 4c_{12}c_{20} + 8c_{02}c_{12} + 6c_{03}c_{11} + 4c_{11}c_{21}, && (38)\\
V_{20} &= 2c_{01}c_{21} + {c_{11}}^2 + 4{c_{20}}^2 + 6c_{10}c_{30}, && (39)\\
V_{02} &= 2c_{10}c_{12} + {c_{11}}^2 + 4{c_{02}}^2 + 6c_{01}c_{03}, && (40)\\
V_{11} &= 4c_{01}c_{12} + 4c_{11}c_{02} + 4c_{20}c_{11} + 4c_{10}c_{21}, && (41)\\
V_{10} &= 4c_{10}c_{20} - 6c_{30} + 2c_{01}c_{11} - 2c_{12}, && (42)\\
V_{01} &= 4c_{01}c_{02} - 6c_{03} + 2c_{10}c_{11} - 2c_{21}. && (43)
\end{aligned}
$$

It is a system of 14 equations for 9 coefficients. It is clear that this system is not solvable in general. But for certain choice of potential coefficients some equations will get dependent and we get a regular system of equations. This problem is well known from one-dimensional case. Only some quartic potentials are analytically solvable in one-dimensional case. We are not surprised that the same is right in two-dimensional case.

The second problem is that equations (30)-(43) are not linear. We have found that there exist cases when the system has solution but we cannot get it by algebraical methods. In these cases the problem leads to algebraic equations of the order higher than four and that is why numerical methods are needed in these cases.

For example, we have proved that c_{12} must be equal to 0 or the equation

$$
\begin{aligned}
0 &= \frac{1}{256}\,{V_{13}}^8 + \left(-\frac{1}{8}\,V_{40}\,{V_{13}}^6 - \frac{1}{4}\,{V_{13}}^6\,V_{04}\right) c\mathit{2}_{12}\\
&+ \left(2\,{V_{13}}^4\,V_{04}\,V_{40} + 6\,{V_{13}}^4\,{V_{04}}^2 - \frac{1}{4}\,V_{31}\,{V_{13}}^5 + \frac{1}{8}\,{V_{31}}^2\,{V_{13}}^4 + {V_{40}}^2\,{V_{13}}^4 + \frac{3}{8}\,{V_{13}}^6\right) {c\mathit{2}_{12}}^2\\
&+ \big(32\,V_{40}\,{V_{13}}^2\,{V_{04}}^2 + 12\,{V_{31}}^2\,{V_{13}}^2\,V_{04} - 14\,{V_{13}}^4\,V_{04} + 4\,V_{31}\,{V_{13}}^3\,V_{40} - 64\,{V_{13}}^2\,{V_{04}}^3\\
&- 8\,V_{31}\,{V_{13}}^3\,V_{04} - 2\,{V_{31}}^2\,V_{40}\,{V_{13}}^2 - 32\,{V_{40}}^2\,{V_{13}}^2\,V_{04} - 4\,{V_{13}}^4\,V_{40}\big) {c\mathit{2}_{12}}^3\\
&+ \big(-4\,{V_{31}}^3\,V_{13} + {V_{31}}^4 + 256\,{V_{04}}^4 - 64\,V_{31}\,V_{13}\,V_{40}\,V_{04} + 32\,{V_{31}}^2\,{V_{04}}^2 - 32\,{V_{31}}^2\,V_{40}\,V_{04}\\
&+ 192\,V_{31}\,V_{13}\,{V_{04}}^2 + 32\,{V_{40}}^2\,{V_{13}}^2 + 160\,{V_{13}}^2\,{V_{04}}^2 - 6\,{V_{31}}^2\,{V_{13}}^2 + 4\,V_{31}\,{V_{13}}^3 + 9\,{V_{13}}^4\\
&- 512\,V_{40}\,{V_{04}}^3 + 256\,{V_{40}}^2\,{V_{04}}^2\big) {c\mathit{2}_{12}}^4\\
&+ \big(-32\,{V_{13}}^2\,V_{40} - 160\,{V_{13}}^2\,V_{04} + 64\,V_{31}\,V_{13}\,V_{40} - 512\,{V_{40}}^2\,V_{04} - 512\,{V_{04}}^3 - 96\,{V_{31}}^2\,V_{04}\\
&+ 32\,{V_{31}}^2\,V_{40} + 1024\,{V_{04}}^2\,V_{40} - 320\,V_{31}\,V_{13}\,V_{04}\big) {c\mathit{2}_{12}}^5\\
&+ \left(-512\,V_{40}\,V_{04} + 64\,{V_{13}}^2 + 64\,{V_{31}}^2 + 128\,V_{31}\,V_{13} + 256\,{V_{40}}^2 + 256\,{V_{04}}^2\right) {c\mathit{2}_{12}}^6 \qquad (44)
\end{aligned}
$$

must be fulfilled. The symbol $c\mathit{2}_{12}$ means the square of c_{12}. Equation (44) is an algebraic equation of the sixth order for the unknown $c\mathit{2}_{12}$.

The third problem is the asymptotic behaviour of the solution. For example if $c_{03} > 0$ and $c_{30} > 0$, the function $h(x, y)$ can be normalized on the first quadrant but not on the other ones. It means that we must solve the system of equations (30)-(43) separately on all quadrants and we must hope that these solutions are possible to match.

It has been said that it is not possible to find the general exact solution of the equations (30)-(43). But we have found it can be done for some special cases.

For example, we have solved the equations (30)-(43) for the case when $V_{13} = 0$, $V_{31} = 0$ and $V_{22} = 0$, if we suppose that $c_{21} = 0$ and $c_{12} = 0$. The solution is

$$c_{30} = \frac{Z}{3}, \tag{45}$$

$$c_{03} = \frac{Y}{3}, \tag{46}$$

$$c_{20} = \frac{1}{4}\frac{V_{30}}{Z}, \tag{47}$$

$$c_{02} = \frac{1}{4}\frac{V_{03}}{Y}, \tag{48}$$

$$c_{11} = X, \tag{49}$$

$$c_{01} = \frac{(-V_{01}V_{30} + 2XZV_{10} + 4XZ^2 - 2V_{30}Y)Y}{4X^2ZY - V_{03}V_{30}}, \tag{50}$$

$$c_{10} = \frac{(-V_{10}V_{03} + 2XYV_{01} + 4XY^2 - 2V_{03}Z)Z}{4X^2ZY - V_{03}V_{30}}, \tag{51}$$

where

$$Z = \pm\sqrt{V_{40}}, \tag{52}$$

$$Y = \pm\sqrt{V_{04}}, \tag{53}$$

$$X = \frac{1}{2}\frac{V_{12}}{Y}, \tag{54}$$

$$X = \frac{1}{2}\frac{V_{21}}{Z}, \tag{55}$$

$$X = \frac{V_{11}ZY}{V_{30}Y + V_{03}Z}, \tag{56}$$

$$X = \pm\frac{1}{2}\frac{\sqrt{4V_{20}Z^2 - 8c_{10}Z^3 - (V_{30})^2}}{Z}, \tag{57}$$

$$X = \pm\frac{1}{2}\frac{\sqrt{4V_{02}Y^2 - 8c_{01}Y^3 - (V_{03})^2}}{Y} \tag{58}$$

The signs in the equations (52) and (53) can be chosen according to the quadrant where the wave function is to be normalized. There exist five equations for the coefficient X. The potential and the signs in equations (57) and (58) must be chosen to get the same five terms on the right sides of equations (54)-(58).

The energy of the ground state is

$$E = \frac{1}{2}\frac{V_{30}}{Z} + \frac{1}{2}\frac{V_{03}}{Y} - \frac{(-V_{10}V_{03} + 2YXV_{01} + 4Y^2X - 2V_{03}Z)^2Z^2}{(4X^2ZY - V_{03}V_{30})^2} - \frac{(-V_{01}V_{30} + 2XZV_{10} + 4Z^2X - 2V_{30}Y)^2Y^2}{(4X^2ZY - V_{03}V_{30})^2}. \tag{59}$$

An example of the potential that fulfills the conditions listed above is

$$V(x,y) = 9x^4 + 12x^3 + 9x^2 - 2x + 9y^4 + 12y^3 + 9y^2 - 2y + 6x^2y + 6xy^2 + 8xy. \tag{60}$$

From the equations (45)-(51) with respect to the equations (52)-(58) we can get its ground state wave function, which can be normalized on the first quadrant

$$h(x,y) = e^{\left(-x^3 - x^2 - \frac{2}{3}x - y^3 - y^2 - \frac{2}{3}y - xy\right)}. \tag{61}$$

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