THE FK OPERATOR METHOD FOR TWO-DIMENSIONAL SEXTIC DOUBLE WELL OSCILLATOR

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ABSTRACT

The FK operator method is used for solving the Schrödinger equation of a two dimensional sextic double well oscillator. We obtain the exact numerical energies for any quantum states with the precision of up to six decimal places. The FORTRAN program for automatically calculating the solutions is made and tested for the states of the principal quantum number up to hundreds.

Keywords: operator method, Schrödinger equation, energy, sextic double well oscillator.

TÓM TẮT

Phương pháp toán tử FK cho dao động tử dạng hố thế đôi với số hạng phi điều hòa bậc sáu hai chiều

Phương pháp toán tử FK được sử dụng để giải phương trình Schrödinger cho dao động tử dạng hố thế đôi với số hạng phi điều hòa bậc sáu hai chiều. Chúng tôi thu được nghiệm số cho bài toán với độ chính xác đến sáu chữ số thập phân cho trạng thái lượng tử bất kì và giá trị bất kì của tần số dao động. Chương trình tính toán tự động trên ngôn ngữ lập trình FORTRAN được xây dựng và được kiểm chứng cho các trạng thái có số lượng tử chính lên đến hàng trăm.

Từ khóa: phương pháp toán tử, phương trình Schrödinger, năng lượng, dao động tử hố thế đôi bậc sáu.

1. Introduction

The anharmonic oscillator is one of the simplest quantum models which finds extensive application in various areas of physics as well as chemistry: atomic and molecular physics, quantum chemistry, condensed matter physics, particle physics, statistical physics, quantum field theory and cosmology. However, solutions of the above problems cannot be found using exact calculation methods. Hence, developing approximate calculation methods for these systems interests many physicists [4]. Among anharmonic oscillator models, the double well oscillator, obtained by changing the harmonic term $\frac{1}{2}\omega^2 x^2$ into $-\frac{1}{2}\omega^2 x^2$, can be used for modeling of two-state systems, such as the interpretation of the infrared spectra of the NH_3 molecule, infrared and Raman spectra of the hydrogen-bonded systems, inversion characteristics of isomers, structural phase transitions, polarizability of perovskite ferroelectrics, formation of noble-gas monolayers on a graphite substrate, macroscopic quantum coherence in

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superconducting Josephson devices, switching and storage devices in computers, and so on [1, 3, 10]. Various methods have been applied for finding the energy of the system in the case of one-dimensional space [2, 3, 9, 10]. In addition, the work [3] showed an interesting point that the exact analytical solutions exist for the case of one-dimensional sextic double well oscillator in some constrained conditions. For the case of higher dimensional spaces, the less attention has been given because of the presence of angular-momentum states that make the problem more complicated [2].

The FK operator method (FK-OM) [5, 6] is an *ab initio* method for solving the Schrödinger equation of non-perturbative systems. It allows to obtain exact numerical solutions (energies and wave-functions) for systems with arbitrary intensity of external field. This method was development successfully for various systems in atomic physics, condense matter physics, field theory, and so on [6-8].

In this work, we apply the FK-OM to solving the Schrödinger equation of a two-dimensional sextic double well oscillator (2D-SDWO) in order to obtain the exact numerical solutions. These results are also the base for the follow-up research to find if the problem has exact analytical solutions similarly to the case one-dimensional space, and if have, what conditions it must satisfy to have these solutions.

The paper is divided into three main sections. In section 2 we present the FK-OM and apply the method to the problem of 2D-SDWO. Section 3 is for the obtained results and discussion. Section 4 concludes the paper.

2. FK operator method for two-dimensional sextic double well oscillator

The 2D-SDWO potential has the form:

$$V(x,y) = -\frac{m\omega^2}{2}(x^2+y^2) + \frac{\lambda}{8}(x^2+y^2)^3, \tag{1}$$

in which the harmonic term is negative $-m\omega^2/2 < 0$; here m, ω and λ are the mass, the oscillation frequency and the coefficient of sextic anharmonic term of the 2D-SDWO, respectively.

For convenience, the dimensionless Schrödinger equation has been used:

$$\left\{-\frac{1}{2}\Delta_{x,y} - \frac{\omega^2}{2}(x^2+y^2) + \frac{1}{8}(x^2+y^2)^3\right\}\Psi(x,y) = E\,\Psi(x,y), \tag{2}$$

in which the units of mass, energy and frequency are $\sqrt[8]{\hbar^2/\lambda m}$, $\sqrt[4]{\lambda\hbar^6/m^3}$ and $\sqrt[4]{\lambda\hbar^2/m^3}$, respectively.

We will apply the FK-OM with four basic steps to obtain the exact numerical solution for the problem as follows: (1) rewrite the Schrödinger equation in the algebraic representation of the two-dimensional Dirac creation and annihilation operators. Note that the considered system is two-dimensional on the surface Oxy, so the projectile of angular momentum on the axis Oz is conservative. Hence, we will use

such new creation and annihilation operators that the operator $\hat{L}_z$ is diagonalized; (2) use the idea of the perturbation theory to find the zero-order approximate solutions, in which the Hamiltonian is divided into two parts. The main part contains only the terms of neutral operators which have the same number of creation and annihilation operators. The eigen-functions of this part are those of harmonic oscillator. The rest terms belong to the perturbative part; (3) establish the basic set of eigen-functions in the form of the wave-functions of the two-dimensional harmonic oscillator. This set is also the wave-function of $\hat{L}_z$ because the creation and annihilation operators are chosen in order that this operator is diagonalized. Note that in step (1), we put a free parameter α into the creation and annihilation operators. So the two divided parts of the Hamiltonian depend on the value of α but the total Hamiltonian does not, which helps to regulate the rate of convergence of the method via choosing appropriate value of α; (4) Use the perturbation theory schemes to obtain exact numerical solutions. The calculation results will be presented in bellows.

First, we will transform the Schrödinger equation (2) into the algebraic form. We use the two-dimensional Dirac creation and annihilation operators defined as follows:

$$\begin{aligned} \hat{a} &= \sqrt{\frac{\alpha}{2}}\left(x+\frac{1}{\alpha}\frac{\partial}{\partial x}\right), & \hat{a}^{+} &= \sqrt{\frac{\alpha}{2}}\left(x-\frac{1}{\alpha}\frac{\partial}{\partial x}\right), \\ \hat{b} &= \sqrt{\frac{\alpha}{2}}\left(y+\frac{1}{\alpha}\frac{\partial}{\partial y}\right), & \hat{b}^{+} &= \sqrt{\frac{\alpha}{2}}\left(y-\frac{1}{\alpha}\frac{\partial}{\partial y}\right), \end{aligned} \tag{3}$$

in which α is a free parameter. These operators satisfy the following commutative relation:

$$\left[\hat{a},\hat{a}^{+}\right]=\left[\hat{b},\hat{b}^{+}\right]=1, \tag{4}$$

other commutators equal zero.

The projectile of angular momentum on Oz-axis has the form:

$$\hat{L}_z=-i\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)=-i\left(\hat{a}^{+}\hat{b}-\hat{a}\hat{b}^{+}\right). \tag{5}$$

For diagonalizing this operator, we choose new creation and annihilation operators so that $\hat{L}_z$ can be rewritten under the form of neutral operator:

$$\begin{aligned} \hat{u}^{+} &= \frac{1}{\sqrt{2}}(\hat{a}^{+}+i\hat{b}^{+}), & \hat{u} &= \frac{1}{\sqrt{2}}(\hat{a}-i\hat{b}), \\ \hat{v}^{+} &= \frac{1}{\sqrt{2}}(\hat{a}^{+}-i\hat{b}^{+}), & \hat{v} &= \frac{1}{\sqrt{2}}(\hat{a}+i\hat{b}). \end{aligned} \tag{6}$$

These new operators also satisfy the commutative relations similar to the formula (4):

$$\left[\hat{u},\hat{u}^{+}\right]=\left[\hat{v},\hat{v}^{+}\right]=1. \tag{7}$$

Now, the projectile of the angular momentum on Oz-axis can be rewritten as follow:

$$\hat{L}_z=\hat{u}^{+}\hat{u}-\hat{v}^{+}\hat{v}. \tag{8}$$

Thus, we obtain the Hamiltonian in algebraic representation of creation and annihilation operators (6):

$$\hat{H}=-\frac{\alpha}{4}\left(\hat{M}^{+}-\hat{N}+\hat{M}\right)-\frac{\omega^2}{4\alpha}\left(\hat{M}^{+}+\hat{N}+\hat{M}\right)+\frac{1}{64\alpha^3}\left(\hat{M}^{+}+\hat{N}+\hat{M}\right)^3, \tag{9}$$

in which $\hat{M}^{+}=2\hat{u}^{+}\hat{v}^{+}$, $\hat{N}=2\hat{u}^{+}\hat{u}+2\hat{v}^{+}\hat{v}+2$ and $\hat{M}=2\hat{u}\hat{v}$. These operators are the elements of a closed algebra with the commutative relations as follows:

$$\left[\hat{M},\hat{N}\right]=4\hat{M},\quad \left[\hat{M},\hat{M}^{+}\right]=2\hat{N},\quad \left[\hat{N},\hat{M}^{+}\right]=4\hat{M}^{+}, \tag{10}$$

which are the tools for latter algebraic calculation.

Next, we will establish an orthogonal basic set of wave function for calculation of matrix element of Hamiltonian. The eigen-functions of two-dimensional harmonic oscillator will be used:

$$\left|n_1,n_2\right\rangle=\frac{1}{\sqrt{n_1!n_2!}}\left(\hat{u}^{+}\right)^{n_1}\left(\hat{v}^{+}\right)^{n_2}\left|0(\alpha)\right\rangle, \tag{11}$$

in which $\left|0(\alpha)\right\rangle$ is vacuum state defined as follows:

$$\hat{u}\left|0(\alpha)\right\rangle=0,\quad \hat{v}\left|0(\alpha)\right\rangle=0,\quad \left\langle 0(\alpha)\middle|0(\alpha)\right\rangle=1. \tag{12}$$

The wave-functions (11) are also the eigen-functions of the angular momentum $\hat{L}_z$ with the eigen-value *m* which is the quantum magnetic number:

$$\hat{L}_z\left|n_1,n_2\right\rangle=m\left|n_1,n_2\right\rangle,\ \left(m=0,\pm1,\pm2,..\right). \tag{13}$$

For convenience, we use two basic sets of wave function depending on the value of *m* as follows:

- For $m\geq 0$: we use two quantum numbers *m* and $n=n_2$, then the wave functions (11) become:

$$\left|n,m\right\rangle=\frac{1}{\sqrt{n!\left(n+\left|m\right|\right)!}}\left(\hat{u}^{+}\right)^{n+|m|}\left(\hat{v}^{+}\right)^{n}\left|0(\alpha)\right\rangle, \tag{14}$$

- For $m \le 0$: we use two quantum numbers m and $n = n_1$, then the wave functions (11) become:

$$|n,m\rangle = \frac{1}{\sqrt{n!(n+|m|)!}}\left(\hat{u}^+\right)^n\left(\hat{v}^+\right)^{n+|m|}|0(\alpha)\rangle, \tag{15}$$

in which $n = 0,1,2,...; |m| = 0,1,2,....$

For further calculation, we use the following action formulae:

$$\begin{aligned}
&\hat{M}^+|n,m\rangle = 2\sqrt{(n+1)(n+|m|+1)}\,|n+1,m\rangle,\\
&\hat{M}|n,m\rangle = 2\sqrt{n(n+|m|)}\,|n-1,m\rangle,\\
&\hat{N}|n,m\rangle = 2(2n+|m|+1)|n,m\rangle.
\end{aligned} \tag{16}$$

Finally, we obtain the non-zero matrix elements of Hamiltonian for calculation the exact numerical solutions as follows:

$$\begin{aligned}
H^m_{n,n} &= (2n+|m|+1)\left\{\frac{\alpha^2-\omega^2}{2\alpha}+\frac{1}{8\alpha^3}\left[6n(n+|m|)+(2n+|m|+2)(2n+|m|+3)\right]\right\},\\
H^m_{n,n+1} &= \left(\frac{3}{8\alpha^3}\left[n(n+|m|)+(2n+|m|+2)(2n+|m|+3)\right]-\frac{\alpha^2+\omega^2}{2\alpha}\right)\sqrt{(n+1)(n+|m|+1)},\\
H^m_{n,n+2} &= \frac{3}{8\alpha^3}(2n+|m|+3)\sqrt{(n+1)(n+|m|+1)(n+2)(n+|m|+2)},\\
H^m_{n,n+3} &= \frac{1}{8\alpha^3}\sqrt{(n+1)(n+|m|+1)(n+2)(n+|m|+2)(n+3)(n+|m|+3)}.
\end{aligned} \tag{17}$$

The other non-zero matrix elements can be deduced based on the symmetric property: $H^m_{n,n+s} = H^m_{n+s,n}$.

3. Results and analysis

The computational program in FORTRAN 90 permits to obtain exact numerical energies and wave-functions of 2D-SDWO for any state and any oscillation frequency. This program is tested for the quantum number of up to 500. Some results are shown in the Table 1 with the precision of up to six decimal places. For this problem, the convergence zone of the free parameter α are rather wide. The precision of obtained solutions can be increased if the value of this parameter is investigated more carefully as in the work [7, 8]. The program with these improvements will be published in the journals specified for publishing codes.

Table 1. *The energies of 2D-SDWO in different states and with different values of oscillation frequency. The energies in bold text are predicted the exact analytical solutions of the problem*

n	$m = 0,\ \omega = 2.$	$m = 0,\ \omega = \sqrt{5}.$	$\lvert m\rvert = 3,\ \omega = 3.$	$\lvert m\rvert = 100,\ \omega = 100.$
0	**-1.414214E+00**	**-2.000000E+00**	**-6.000000E+00**	-3.847569E+05
1	**1.414214E+00**	**2.000000E+00**	3.521549E-07	-3.845569E+05
2	5.315649E+00	6.605241E+00	**6.000000E+00**	-3.843569E+05
3	1.052921E+01	1.223973E+01	1.246183E+01	-3.841570E+05
4	1.675396E+01	1.880020E+01	1.958590E+01	-3.839571E+05
5	2.384386E+01	2.617903E+01	2.739994E+01	-3.837572E+05
6	3.170412E+01	3.429697E+01	3.587924E+01	-3.835574E+05
7	4.026593E+01	4.309356E+01	4.498910E+01	-3.833576E+05
8	4.947621E+01	5.252089E+01	5.469567E+01	-3.831578E+05
9	5.929236E+01	6.253985E+01	6.496834E+01	-3.829580E+05
10	6.967924E+01	7.311776E+01	7.577999E+01	-3.827583E+05
11	8.060717E+01	8.422677E+01	8.710661E+01	-3.825586E+05
12	9.205067E+01	9.584280E+01	9.892689E+01	-3.823589E+05
13	1.039876E+02	1.079448E+02	1.112218E+02	-3.821593E+05
14	1.163983E+02	1.205140E+02	1.239744E+02	-3.819597E+05
15	1.292654E+02	1.335338E+02	1.371691E+02	-3.817601E+05
16	1.425733E+02	1.469892E+02	1.507920E+02	-3.815606E+05
17	1.563079E+02	1.608665E+02	1.648303E+02	-3.813610E+05
18	1.704564E+02	1.751533E+02	1.792723E+02	-3.811615E+05
19	1.850070E+02	1.898383E+02	1.941071E+02	-3.809621E+05
20	1.999488E+02	2.049110E+02	2.093248E+02	-3.807626E+05

In the work [3] for the problem in one-dimensional space, the authors showed that the states which correspond to the case of exact analytical solutions have the same values of energies with the opposite signs $\pm E$. In the results given above, the energies printed in bold text are also in the form of $\pm E$. In addition, these values compose a mathematical beauty. For examples, the case $m = 0,\ \omega = 2,$ and $n = 0,1$ corresponding to the energy $E = \pm 1.414214 = \pm\sqrt{2}$; the case $m = 0,\ \omega = \sqrt{5},$ and $n = 0,1$ corresponding to the energy $E = \pm 2.0$; and the case $\lvert m\rvert = 3,\ \omega = 3,$ and $n = 0,2$ corresponding to the energy $E = \pm 6.0$. Hence, we predict that these states are also corresponding to the exact analytical energies of the 2D-SDWO. This prediction will be confirmed in the follow-up research.

4. Conclusion

In this work, using the FK-OM, the exact numerical solutions for the 2D-SDWO are obtained with the precision of up to six decimal places for any state and any value of oscillation frequency. The program can be upgraded to reach higher precision results. Some results under the form of $\pm E$ are expected being the exact analytical of the problem, which need further research.

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