Symbolic-numeric Solution of the Two-dimensional Schrödinger Equation with Double-well Potential

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Abstract. In this work the self-consistent basis method for solving the two-dimensional stationary Schrödinger equation is presented. The solution shows a potential energy surface with two local minima and a unique saddle point. We have developed a symbolic-numeric algorithm and Maple program (SELFA) that realizes the computation. The low part of energy spectrum and corresponding wave functions for the C_{2v} invariant Hamiltonian were also calculated by means of this program.

1 Introduction

For solving an eigenvalue problem, in particular the Schrödinger equation, there are many different methods, for example: diagonalization method [1, 2, 3], quasi-classical approaches [4, 5, 6], different variants of perturbation theory [7, 8], finite element method [9], generalized continuous analog of the Newton method [10], normal form methods [11, 12, 13, 14], the so-called $1/N$ expansion [15], oscillator representation method [16], variation and operation methods [17, 18, 19, 20], symplectic method [21].

As is known, when a dimension of the considered system is increased, the complexity of the differential Schrödinger operator for which an eigenvalue problem is solved results in a concomitant increase in numerical difficulties. Besides this, the accuracy of energy spectra and wave functions calculated decreases if the quantum system allows the existence of dynamical chaos in its classical limit [22].

In Ref. [23] the invariant of the two-dimensional polynomial C_{3v} Schrödinger's equation shows that the potential energy surface (PES) has the only minimum. The self-consistent basis method [24, 25] was used to obtain the solution.

In this paper we consider the C_{2v} symmetric Hamiltonian with four parameters. The parameters were chosen in such a way that PES has two local minima and a unique saddle point (see Fig. 1). On the one hand this choice of the PPE results in simplifying the solution of the Schrödinger equation in comparison with that PES that have more than two local minima. On the other hand, this choice results in the possibility that tunneling effects and classical chaos may exist and affect the properties of the energy spectrum and wave functions.

2 Main equations

In this report the self-consistent basis method is used to solve the eigenvalue problem for the C_{2v} invariant Schrödinger operator

$$\hat{H}(x,y,\hat{p}_x,\hat{p}_y) = \frac{1}{2}(\hat{p}_x^2+\hat{p}_y^2)+V(x,y), \tag{1}$$

where the potential energy surface (PES)

$$V(x,y) = \frac{a}{2}(x^2+y^2) - \frac{a^{'}}{2}x^2 + bx^2y^2 + c(x^2+y^2)^2, \tag{2}$$

has two local minima for $a = 1.8490$, $a^{'} = 8.257825$, $b = -0.287070$, $c = 0.375509$ (see Fig. 1).

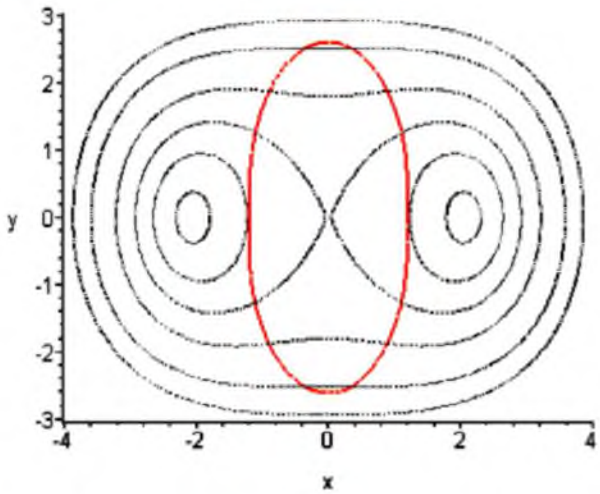

Figure 1: Isolines of the PES (dotted) and the Gaussian curvature zero line (continuous) for Eq. (2).

Expressed as polar coordinates, $x = r\cos\varphi$, $y = r\sin\varphi$, Eqs. (1)-(2) we have

$$\hat{H}(r,\varphi)\psi(r,\varphi) = E\psi(r,\varphi), \tag{3}$$

$$\hat{H}(r,\varphi) = -\frac{1}{2}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right)+\frac{r^2}{2}+\frac{br^3}{2}\sin 3\varphi + cr^4. \tag{4}$$

A regular and bounded solution of the partial eigenvalue problem for Eqs.(3)-(4) can be found in the form of the following Fourier series:

$$u(r,\varphi) = \sqrt{r}\psi(r,\varphi) = \frac{A_0(r)}{2} + \sum_{l=1}^{n}[A_l(r)\cos l\varphi + B_l(r)\sin l\varphi]. \qquad (5)$$

Projecting the unknown solution $u(r,\varphi)$ onto basis functions, $\sin l'\varphi$ and $\cos l'\varphi$ $(l' = 1, ..., n)$, we have four linear systems of second-order ordinary differential equations (ODE), the consequence of a discrete symmetry, C_{2V}, of the Hamiltonian (4), which correspond to four irreducible representations:

$$\begin{aligned}
&\mathrm{A}_1: \ u(r,\varphi)=\frac{A_0(r)}{2}+\sum_{l=1} A_{2l}(r)\cos 2l\varphi,\\
&\mathrm{A}_2: \ u(r,\varphi)=\sum_{l=1} B_{2l}(r)\sin 2l\varphi,\\
&\mathrm{B}_1: \ u(r,\varphi)=\sum_{l=1} A_{2l+1}(r)\cos(2l+1)\varphi,\\
&\mathrm{B}_2: \ u(r,\varphi)=\sum_{l=1} B_{2l+1}(r)\sin(2l+1)\varphi.
\end{aligned}$$

As result we obtained the following infinite system for the second-order differential equations:

$$\begin{aligned}
&\mathrm{A}_1:\\
&A_0''+\alpha_0 A_0+2\beta A_2+2\gamma A_4=0,\\
&A_2''+\alpha_2 A_2+\beta(A_0+A_4)+\gamma(A_6+A_2)=0,\\
&A_l''+\alpha_l A_l+\beta(A_{l-2}+A_{l+2})+\gamma(A_{l-4}+A_{l+4})=0,\\
&\qquad\qquad l=4,6,8,\dots, \qquad (6)
\end{aligned}$$

$$\begin{aligned}
&\mathrm{A}_2:\\
&B_2''+(\alpha_2-\gamma)B_2+\beta B_4+\gamma B_6=0,\\
&B_4''+\alpha_4 B_4+\beta(B_2+B_6)+\gamma B_8=0,\\
&B_l''+\alpha_l B_l+\beta(B_{l-2}+B_{l+2})+\gamma(B_{l-4}+B_{l+4})=0,\\
&\qquad\qquad l=6,8,10,\dots, \qquad (7)
\end{aligned}$$

$$\begin{aligned}
&\mathrm{B}_1:\\
&A_1''+A_1\alpha_1+A_3(\beta+\gamma)+\gamma A_5=0,\\
&A_l''+A_l\alpha_l+\beta(A_{l-2}+A_{l+2})+\gamma(A_{l-4}+A_{l+4})=0,\\
&\qquad\qquad l=3,5,7,\dots, \qquad (8)
\end{aligned}$$

$$\begin{aligned}
&\mathrm{B}_2:\\
&B_1''+\alpha_1 B_1+\beta B_3+\gamma(B_5-B_3)=0,\\
&B_3''+\alpha_3 B_3+\beta(B_1+B_5)+\gamma(B_7-B_1)=0,\\
&B_l''+\alpha_l B_l+\beta(B_{l-2}+B_{l+2})+\gamma(B_{l+4}-B_{l-4})=0,\\
&\qquad\qquad l=5,7,9,\dots, \qquad (9)
\end{aligned}$$

where $\alpha_l = 2E - ((4l^2-1)/4)r^2 - ar^2 + (a'/2)r^2 - (b/4)r^4 - 2cr^4$, $\beta = (a'/4)r^2$, $\gamma = (b/8)r^4$.

We rewrite linear systems (6)–(9) in the form of a first-order ODE using a transformation of the above functions $A_i(r)$, $B_j(r)$ $(i,j=1,2)$ to new functions $z_k(r)$:

$$
\begin{aligned}
&\mathrm{A}_1: (A_l \to z_{l+1}, A_l' \to z_{l+2}, l=0,2,4,...),\\
&\mathrm{A}_2: (B_l \to z_{l-1}, B_l' \to z_l \quad, l=2,4,6,...),\\
&\mathrm{B}_1: (A_l \to z_l \quad, A_l' \to z_{l+1}, l=1,3,5,...),\\
&\mathrm{B}_2: (B_l \to z_l \quad, B_l' \to z_{l+1}, l=1,3,5,...),
\end{aligned}
$$

and we obtain the following system:

$$
\begin{aligned}
&\mathrm{A}_1:\\
&z_{l+1}' - z_{l+2} = 0, \qquad l=0,2,4,...,\\
&z_2' + \alpha_0 z_1 + 2\beta z_3 + 2\gamma z_5 = 0,\\
&z_4' + \alpha_2 z_3 + \beta(z_1+z_5) + \gamma(z_7+z_3) = 0,\\
&z_l' + \alpha_l z_{l+1} + \beta(z_{l-1}+z_{l+3}) + \gamma(z_{l-3}+z_{l+5}) = 0,\\
&\qquad\qquad l=4,6,8,\ldots,
\end{aligned}
\tag{10}
$$

$$
\begin{aligned}
&\mathrm{A}_2:\\
&z_{l-1}' - z_l = 0, \qquad l=2,4,6,...,\\
&z_2' + \alpha_2 z_1 + \beta z_3 + \gamma(z_5 - z_1) = 0,\\
&z_4' + \alpha_4 z_3 + \beta(z_1+z_5) + \gamma z_7 = 0,\\
&z_l' + \alpha_l z_{l-1} + \beta(z_{l-3}+z_{l+1}) + \gamma(z_{l-5}-z_{l+3}) = 0,\\
&\qquad\qquad l=6,8,10,\ldots,
\end{aligned}
\tag{11}
$$

$$
\begin{aligned}
&\mathrm{B}_1:\\
&z_l' - z_{l+1} = 0, \qquad l=1,3,5,...,\\
&z_2' + \alpha_1 z_1 + \beta z_3 + \gamma(z_3+z_5) = 0,\\
&z_{l+1}' + \alpha_l z_l + \beta(z_{l-2}+z_{l+2}) + \gamma(z_{l-4}+z_{l+4}) = 0,\\
&\qquad\qquad l=3,5,7,\ldots,
\end{aligned}
\tag{12}
$$

$$
\begin{aligned}
&\mathrm{B}_2:\\
&z_l' - z_{l+1} = 0, \qquad l=1,3,5,...,\\
&z_2' + \alpha_1 z_1 + \beta z_3 + \gamma(z_5 - z_3) = 0,\\
&z_4' + \alpha_3 z_3 + \beta(z_1+z_5) + \gamma(z_7 - z_1) = 0,\\
&z_{l+1}' + \alpha_l z_l + \beta(z_{l-2}+z_{l+2}) + \gamma(z_{l+4}+z_{l-4}) = 0,\\
&\qquad\qquad l=5,7,9,\ldots.
\end{aligned}
\tag{13}
$$

Truncating the system obtained (10)–(13) up to the $2Neq$ equations, we cast it as a finite homogeneous system of linear first-order ODE in the unknown functions $z_k(r)$, where the function α_l consists of an arbitrary eigenvalue E.

To solve the obtained eigenvalue problem numerically, one needs to define $2Neq$ initial condition data. From the general theory of linear ODE it is known that its general solution has the form of a linear combination:

$$
Z_j = \sum_{k=1}^{2Neq} C_k z_j^{(k)}, \tag{14}
$$

spanned the $2Neq$ linear-independent solutions

$$z^j = \{z_1^j, z_2^j, ..., z_{2Neq}^j\}, (j = 1, 2, ..., 2Neq), \quad (15)$$

for any system (10)–(13).

To calculate unknown coefficients C_k in Eq. (14), one needs to take into account appropriate boundary conditions placed on functions $A_i(r)$ and $B_j(r)$ that correspond to the general solution with odd index, i.e. $Z_{2j-1}(r)$ $(j = 1, 2, ..., Neq)$. Then conditions $Z_{2j-1}(0) = 0$ and $Z_{2j-1}(\infty) = 0$ lead to a system of algebraic equations with respect to unknown coefficients C_k. A nontrivial solution of this system is calculated by setting to zero the corresponding determinant, $D(E) = |z_j^k(E)| = 0$. Roots of this determinant give us the low part of the energy spectrum $E = E_j, (j = 1, 2, 3, \ldots, Neq)$ for the two-dimensional Schrödinger equation (3)-(4) under consideration. For given E_j we also construct the corresponding eigenfunction.

3 Results

Grounded in the self-consistent basis method [23, 24, 25, 26, 27], a symbolic-numeric algorithm and Maple program have been developed to solve the Schrödinger equation (3) with Hamiltonian (4).

For all four state types A_1, B_1, A_2, B_2, the energy spectrum E_n and wave functions were calculated. In the Table below, values of the lowest energy levels are presented, while in Figure 2 the structure of its localization in double-well potential is shown. In Figures 3 and 4 some profiles and isolines of the wave functions are plotted.

Table. The energy spectrum of the Hamiltonian (1)-(2).

n	E_n	Type	n	E_n	Type	n	E_n	Type
0	-3.898 809	A_1	9	1.346 141	B_2	18	4.365 241	A_2
1	-3.897 242	B_1	10	1.529 112	A_2	19	5.300 808	B_1
2	-1.423 213	B_2	11	2.056 203	B_1	20	5.667 120	A_1
3	-1.419 615	A_2	12	3.242 163	B_2	21	5.940 909	B_2
4	-0.903 803	A_1	13	3.684 687	A_1	22	6.293 753	B_2
5	-0.807 265	B_1	14	3.773 432	A_1	23	6.683 205	A_2
6	1.160 673	A_1	15	3.918 503	B_2	24	6.735 355	B_1
7	1.196 685	B_1	16	3.923 146	A_2	25	6.740 105	A_1
8	1.217 782	A_1	17	4.039 048	B_1	26	6.907 529	B_1

4 Conclusion and Acknowledgments

A program, SELFA, grounded in the self-consistent basis method, was implemented in MAPLE to solve the two-dimensional Schrodinger equation. The

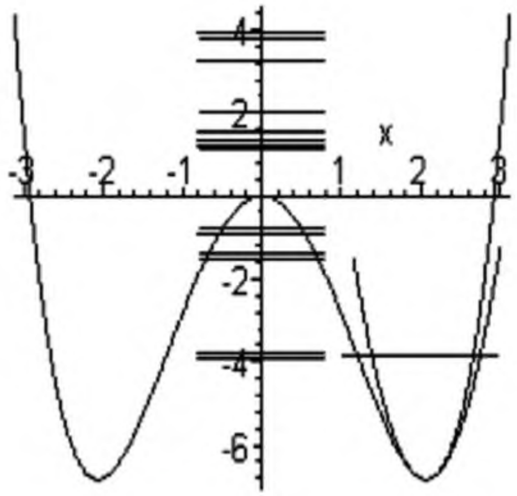

Figure 2: Structure of the energy level localization in double-well potential $V(x, y = 0)$.

efficiency of this program is shown on the C2V symmetric Hamiltonian with two local minimuma, for which the lowest energy levels and wave functions are calculated. Further applications of SELFA include solving the eigenvalue problem for different Hamilton operators, studying tunneling effects, and avoiding crossing phenomena of eigenenergies. An appropriate development of this approach can also be done within the framework of the Kantorovich method using a self-consistent basis with r as a parameter, taking into account the discrete symmetry of Hamiltonian under consideration.

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References

[1] Wilkinson J.H., Reinsch C. - *Handbook for Automatic Computation, Vol.2, Linear Algebra.* Heidelberg New York Springer-Verlag Berlin, 1971.

[2] Golub G.H., Van Loan Ch.F. - *Matrix Computations.* The John Hopkins University Press Baltimore and London, 1989.

[3] Banerjee K. - *General anharmonic oscillators.* Proc. R. Soc. Lond., Vol.A364, 1978, 265-275.

[4] Fröman N., Fröman O. - *JWKB Approximation.* North-Holland Publishing Company, Amsterdam, 1965.

[5] Maslov V.P., Fedoryuk M.V. - *Kvaziklassicheskie pribligheniya dlya uravnenii kvantovoi mekhaniki.* Nauka, Moskva, 1976.

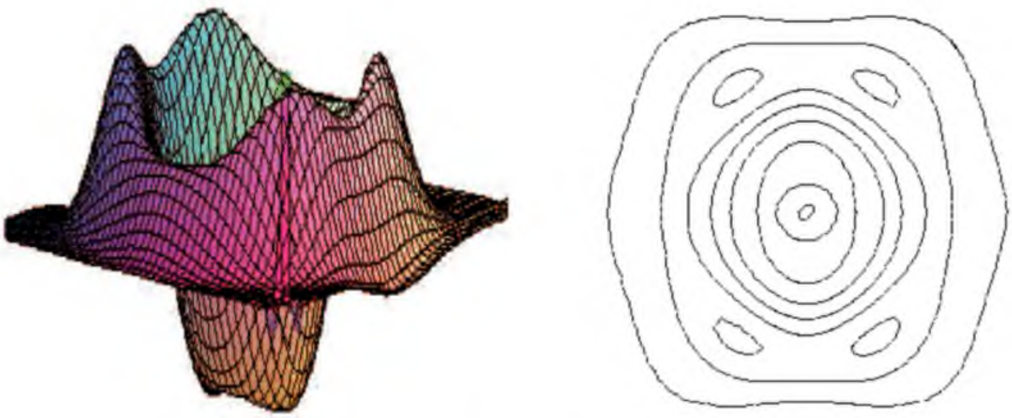

Figure 3: Surface and isolines the wave function of A_1-type with energy $E = 1.160673$.

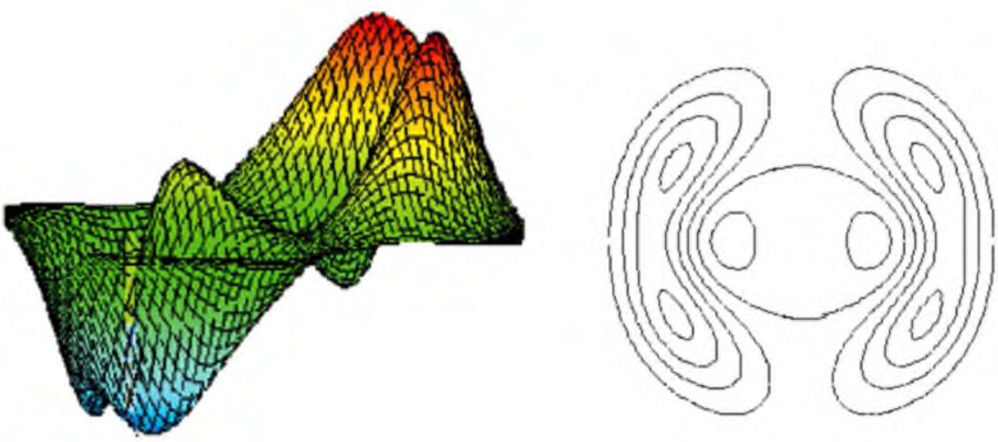

Figure 4: Surface and isolines the wave function of B_1-type with energy $E = -0.807265$.

[6] Born M. - *Vorlesungen über atommechanik.* Vol.1, Berlin, 1925.

[7] Bethe H.A. - *Intermediate quantum mechanics.* W. A. Benjamin, inc. New York, Amsterdam, 1964.

[8] Flügge S. - *Practical quantum mechanics.* Vol.1,2, Springer-Verlag, Berlin - Heidelberg - New York, 1971.

[9] Abrashkevich A.G., Abrashkevich D.G., Kaschiev M.S., Puzynin I.V. - *FESSDE, a program for the finite-element solution of the coupled-channel Schroedinger equation using high-order accuracy approximations.* Comp. Phys. Commun., Vol.85, 1995, 65-74.

[10] Puzynin I.V. et.al. - *Obobshennyi nepreryvnyi analog metoda Newtona dlya chislennogo issledovaniya nekotoryh nelineinyh kvantovo-polevyh modelei.* Physics of elementary particles and atomic nuclei. Vol.30(1), 1999, 210-265.

[11] Swimm R.T., Delos J.B. - *Semiclassical calculation of vibrational energy levels for non-separable systems using Birkhoff-Gustavson normal form.* J. Chem. Phys. Vol.71, 1979, 1706-1716.

[12] Ali M.K. - *The quantum normal form and its equivalents.* J. Math. Phys., Vol.26(10), 2565-2572.

[13] Robnik M. - *Algebraic quantization of the Birkhoff-Gustavson normal form.* J. Phys.A: Math.Gen., Vol.17, 1984, 109-130.

[14] Chekanov N.A. - *Kvantovanie normalnoi formy Bikgofa-Gustavsona.* Jadernaya fizika, Vol.50(8), 1989, 344-346.

[15] Jaffe L. - *Large N limits as classical mechanics.* Rev. Mod. Phys. Vol.54, 1982, 407.

[16] Dineykhan M. and Efimov G.V. - *The Schrödinger equation for bound state systems in the oscillator representation.* Reports of Math. Phys., Vol.6(2/3), 1995, 287-308.

[17] Collatz L. - - *Eigenwertaufgaben mit technischen anwendungen.* Akademische verlagsgesellschaft geest & portig K.-G., Leipzig, 1963.

[18] Jafarpour M., Afshar D. - *Calculation of energy eigenvalues for the quantum anharmonic oscillator with a polynomial potential.* J. Phys. A: Math. Gen., Vol.35, 2002, 87-92.

[19] Ivanov I.A. - *Sextic and octic anharmonic oscillator: connection between strong-coupling and weak-coupling expansions.* J. Phys. A: Math. Gen. Vol.31, 1998, 5697-5704.

[20] Ivanov I.A. - *Link between the strong-coupling and weak-coupling asymptotic perturbation expansions for the quartic anharmonic oscillator.* J. Phys. A: Math. Gen. Vol.31, 1998, 6995-7003.

[21] Liu X.S., Su L.W., Ding P.Z. Intern. J. - *Quantum Chem.* 2002, 1-11.

[22] Bolotin Yu.L., Gonchar V.Yu., Tarasov V.N., Chekanov N.A. - *The transition regularity-chaos-regularity and statistical properties of wave function.* Phys. Lett., Vol.A144(8,9), 1990, 459-461.

[23] Belyaeva I.N., Ukolov Yu.A., Chekanov I.N., Ukolov Yu.A. - *Vycheslenie energeticheskogo spectra i volnovyh funkziiobobschennogo gamiltoniana Henon-Heiles metodom samosoglasovanno bazisa.* Vestnik Hersonskogo gosudarstvennogo tekhnicheskogo universiteta, Vol.2(22), 2005, 43-47.

[24] Vinitsky S.I., Inopin E.V., Chekanov N.A. - *Reshenie dvumernogo uravneniya Schredingera v samosoglasovannom basise.* Preprint JINR-P4-93-150, Dubna, 1993, 12.

[25] Chekanov N.A., Ukolov Yu.A. - *Chislennoe reshenie statsionarnogo uravneniya Schredingera v priblizhenii samosoglasovannogo basisa.* International Seminar "Super-computations and computer simulation", Sarov, Russian federal nuclear center – All Russian research institute of experimental physics, 2004, 100-102.

[26] Belyaeva I.N., Ukolov Yu.A., Chekanov N.A. - *Vestnik Kherson. Gosudarst. Techn. Univer.*, Vol.2(22), 2005, 43-47.

[27] Belyaeva I.N., Chekanov N.A, Gusev A.A., Rostovtsev V.A., Ukolov Yu.A., Uwano Y and Vinitsky S.I. - *A MAPLE symbolic-numeric program for solving the 2D-eigenvalue problem by a self-consistent basis method.* Lecture Notes in Computer Science, Vol.3718, 2005, 32-39.

[28] Vinitsky S.I., Gerdt V.P., Gusev A.A., Kaschiev M.S., Rostovtsev V.A., Samoilov V.N., Tyupikova T.V., and Chuluunbaatar O. - *A symbolic-numerical algorithm for the computation of matrix elements in the parametric eigenvalue problem.* Programming and Computer Software, Vol. 33, 2007, 105-116.