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Eigenvalues and eigenfunctions of the anharmonic oscillator $V(x, y) = x^2y^2$

Research Article

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Abstract: We obtain sufficiently accurate eigenvalues and eigenfunctions for the anharmonic oscillator with potential $V(x, y) = x^2y^2$ by means of three different methods. Our results strongly suggest that the spectrum of this oscillator is discrete in agreement with early rigorous mathematical proofs and against a recent statement that cast doubts about it

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1. Introduction

Some time ago Bender et al. [1] stated that it is not known if the spectrum of the anharmonic oscillator potential $V(x, y) = x^2y^2$ is discrete. Several years earlier Simon [2] had given five proofs that the spectrum of such oscillator is indeed discrete. The reason why at first sight one may suspect that this model does not support bound states is outlined in Simon's paper [2].

We are not aware of any calculation of the eigenvalues and eigenfunctions of that anharmonic oscillator. For this reason we will provide some reasonably accurate results in this paper. In section 2 we outline the application of the Rayleigh-Ritz variational method taking into account the point-group symmetry of the oscillator. In section 3 we discuss two approaches based on the moments of the Hamiltonian operator: the Rayleigh-Ritz method in the Krylov space (RRK) [3] (and references therein) and the connected-moments expansion (CMX) [4, 5]. In section 4 we compare and discuss the results obtained by the three approaches and draw conclusions.

2. Rayleigh-Ritz variational method

As stated in the introduction, we are interested in the eigenvalues and eigenfunctions of the anharmonic oscillator

$$H = p_x^2 + p_y^2 + x^2y^2. \tag{1}$$

In this section we outline the application of the well known Rayleigh-Ritz variational method. We choose products $\varphi_{mn}(x, y) = \phi_m(x)\phi_n(y)$ of eigenfunctions $\phi_n(q)$, $n = 0, 1, \ldots$, of the harmonic oscillator $H = p_q^2 + q^2$ as a

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suitable basis set.

Like the Pullen-Edmonds Hamiltonian[6] the Hamiltonian (1) is invariant under the symmetry operations of the point group C_{4v} [7, 8]. Therefore, the appropriate basis functions are

$$\begin{array}{ll} \varphi^{+}_{2m\,2n}(x,y),\ m,n=0,1,\ldots & A_1 \\ \varphi^{-}_{2m+1\,2n+1}(x,y),\ m\neq n=0,1,\ldots & A_2 \\ \varphi^{-}_{2m\,2n}(x,y),\ m\neq n=0,1,\ldots & B_1 \\ \varphi^{+}_{2m+1\,2n+1}(x,y),\ m,n=0,1,\ldots & B_2 \\ \{\varphi_{2m\,2n+1}(x,y),\varphi_{2m+1\,2n}(x,y)\},\ m,n=0,1,\ldots & E \end{array}, \tag{2}$$

where

$$\begin{aligned} \varphi^{+}_{mn}(x,y) &= \frac{1}{\sqrt{2(1+\delta_{mn})}}\left(\varphi_{mn}+\varphi_{nm}\right), \\ \varphi^{-}_{mn}(x,y) &= \frac{1}{\sqrt{2}}\left(\varphi_{mn}-\varphi_{nm}\right). \end{aligned} \tag{3}$$

An obvious advantage of using point-group symmetry is that we diagonalize the Hamiltonian matrix $\mathbf{H}^S$ (with matrix elements $\left\langle\varphi^S_{mn}\right| H \left|\varphi^S_{m'n'}\right\rangle$) for each irreducible representation $S=A_1,A_2,B_1,B_2,E$ separately. The reason is that $\left\langle\varphi^S_{mn}\right| H \left|\varphi^{S'}_{m'n'}\right\rangle=0$ when $S\neq S'$ so that functions of different symmetry do not mix [7, 8]. What is more: we can even split the calculation for the two-dimensional irreducible representation E into its two components, which decreases the dimension of the matrices still further. Thus, point-group symmetry simplifies all the calculations and enables us to interpret the results more clearly. We will refer to this Rayleigh-Ritz method with the harmonic-oscillator basis set as RRHO. As usual we calculate the eigenvalues of each matrix $\mathbf{H}^S$ for increasing dimension until convergence. In this way we estimate the number of reliable digits in the results. One can easily calculate the Hamiltonian matrix elements analytically by means of the well known mathematical properties of the eigenfunctions of the harmonic oscillator.

3. Moments methods

In this section we discuss two methods based on the moments of the Hamiltonian operator

$$\mu_j=\frac{\langle\varphi|\,H^j\,|\varphi\rangle}{\langle\varphi|\,\varphi\rangle}, \tag{4}$$

where φ is a properly chosen reference function.

The first one is the Rayleigh-Ritz variational method in the Krylov space (RRK) spanned by the non-orthogonal basis set of functions

$$f_j=H^j\varphi,\ j=0,1,\ldots, \tag{5}$$

which has been successfully applied to the Pullen-Edmonds Hamiltonian [3]. In this case we solve the eigenvalue matrix equation $(\mathbf{H}-E\mathbf{S})\,\mathbf{C}=\mathbf{0}$, where $H_{ij}=\langle f_i|\,H\,|f_j\rangle=\mu_{i+j+1}$, $S_{ij}=\langle f_i|\,f_j\rangle=\mu_{i+j}$ and $\mathbf{C}$ is a column matrix with the coefficients of the expansion of the approximate eigenfunction. We increase the dimension of the matrices until we obtain the desired accuracy.

The second approach is the connected-moments expansion (CMX) developed by Cioslowski [4] who tested it on the ground state of the Pullen-Edmonds Hamiltonian. Amore and Fernández [3] carried out a calculation of much larger order on the ground and excited states by means of the compact and most elegant formula developed by Knowles [5] that we also use in this paper. The procedure is straightforward: we calculate the connected moments I_j from the moments of the Hamiltonian operator (4) and then estimate the eigenvalues by means of the expression developed by Knowles [5] (see also the paper by Amore and Fernández [3] for additional details)

For the application of both moments methods we resort to the following reference functions

$$\begin{aligned} \varphi_{A_1} &= \exp\left(-a\left[x^2+y^2\right]\right) \\ \varphi_{A_2} &= xy(x^2-y^2)\exp\left(-a\left[x^2+y^2\right]\right) \\ \varphi_{B_1} &= (x^2-y^2)\exp\left(-a\left[x^2+y^2\right]\right) \\ \varphi_{B_2} &= xy\exp\left(-a\left[x^2+y^2\right]\right) \\ \varphi_E &= \left\{\begin{array}{l} x\exp\left(-a\left[x^2+y^2\right]\right) \\ y\exp\left(-a\left[x^2+y^2\right]\right) \end{array}\right. . \end{aligned} \tag{6}$$

In this way we can obtain the lowest eigenvalue for every symmetry species, a property that was not considered in the first applications of the method [4, 5]. Note that the reference function φ_{A_2} was inadvertently omitted in the application of these methods to the Pullen-Edmonds Hamiltonian [3].

4. Results and discussion

We carried out all the calculations in this paper by means of computer algebra software. In particular, we obtained the RRHO eigenvalues by means of the Maple command “Eigenvalues”. In the case of RRK we first obtained the secular polynomial by means of the Derive command “det” and its real roots by means of “nsolutions”. We also resorted to the Derive “det” command to obtain the determinant that appears in the CMX formula derived by Knowles [5].

Table 1 shows results for the lowest eigenvalues obtained by the three methods outlined above. As it is usual in quantum molecular calculations the number before the

Table 1. First eigenvalues of the anharmonic oscillator (1) calculated by means of the three methods discussed in sections 2 and 3.

State	RRHO	RRK	CMX
$1A_1$	1.10822315759	1.108224	1.10822
$1E$	2.37863782934	2.37869	2.376
$1B_1$	3.05608115466	3.0563	3.055
$2A_1$	3.5149490453	3.518	
$2E$	4.09346927636	4.10	
$2B_1$	4.75277240183	4.78	
$3A_1$	4.98496358748	5.07	
$1B_2$	5.01127928154	5.01127930	5.0112
$3E$	5.498979516	5.7	
$3B_1$	6.1448192750	6.5	
$4A_1$	6.237128106		
$4E$	6.67235007		
$5E$	7.1810983		
$4B_1$	7.37557348		
$5A_1$	7.381759978		
$6E$	7.999		
$1A_2$	8.074373925386	8.0743745	8.0738

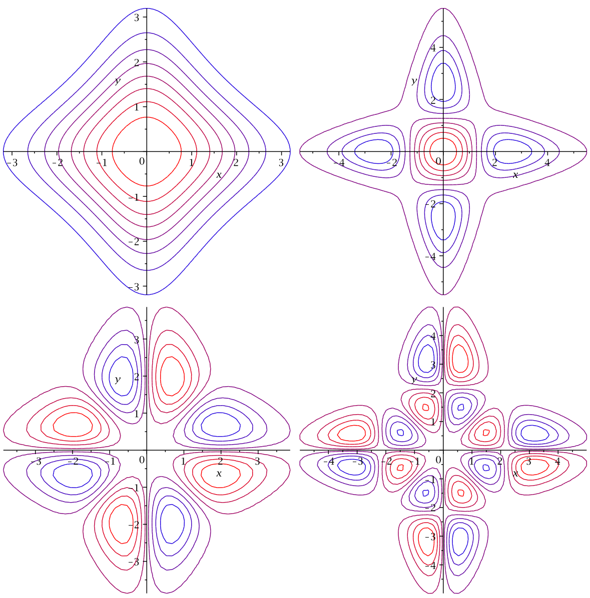

Figure 1. Contour lines for the eigenfunctions $1A_1$, $2A_1$, $1A_2$ and $2A_2$

symmetry symbol indicates the energy order; for example the energy of $1A_1$ is smaller that that of $2A_1$ and so forth. The RRHO ones are the most accurate because they are based on basis sets of dimension $D \leq 1035$. The RRK and CMX results were obtained with smaller basis sets because their purpose is merely to verify the RRHO results. The CMX is the less reliable of the three methods as argued elsewhere [3] but it is a suitable independent test because it is not based on the variational method.

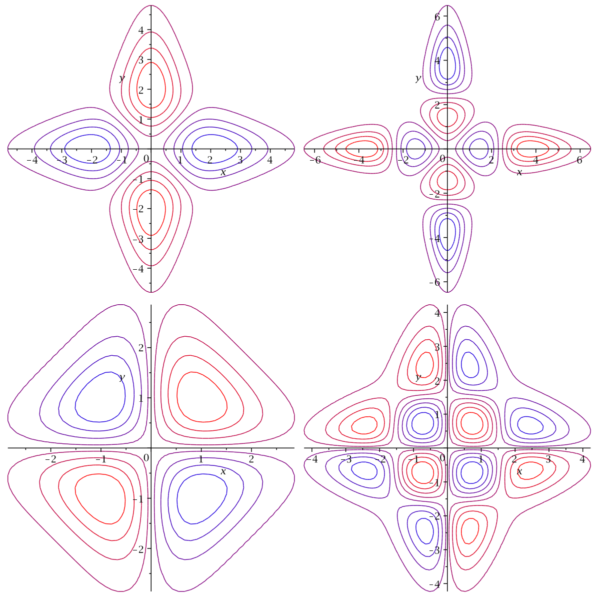

Figure 2. Contour lines for the eigenfunctions $1B_1$, $2B_1$, $1B_2$ and $2B_2$

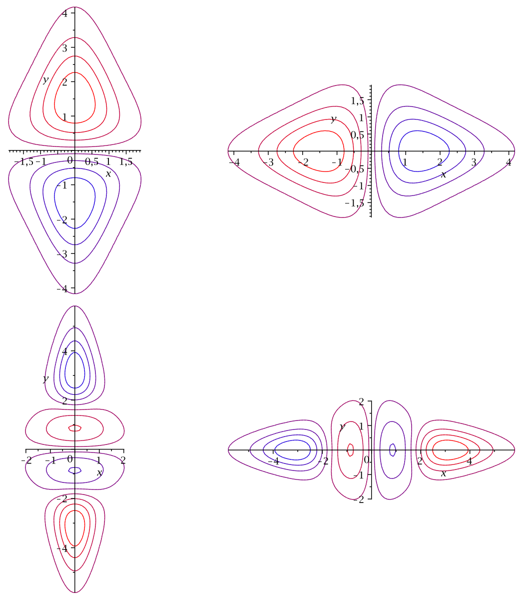

Figure 3. Contour lines for the two-fold degenerate eigenfunctions $1E$ and $2E$

It is possible to improve the RRK and CMX results by choosing α conveniently; however, here we simply chose $\alpha = 1$ that is not optimal for all the states. Figures 1, 2 and 3 show contour lines for some of the states of the anharmonic oscillator obtained by means of the RRHO. The two variational methods appear to converge rather slowly but smoothly from above as expected for such approaches. Numerical instabilities appeared for the greatest RRHO matrices and we estimated the eigenvalues from the best results that satisfied the well known variational inequality $E^{(D+m)} < E^{(D)}$. The CMX does not give upper bounds but it approached the variational results satisfactorily. No anomalous behaviour was detected that could suggest that the spectrum is not discrete. Therefore, present numerical results support the mathematical proofs given by Simon [2] and stand against the claim raised by Bender et al. [1].

Acknowledgments

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