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Precise analytical approximations of the eigenvalues of the decatic anharmonic potential

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Precise analytical approximations of the eigenvalues of the decatic anharmonic potential

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Abstract. Precise analytical approximations have been determined for the eigenvalues of the ground state of the decatic anharmonic potential $x^2 + \lambda x^{10}$ in the one-dimensional Schrödinger equation. The results have been found using the technique multipoint quasi-rational approximation (MPQA). With the new method, power and asymptotic expansions have been determined. The analytic function here obtained is derived connecting both expansions. The maximum relative error of the best analytical approximation here determined is 0.04. However, most of the relative errors for other values of λ, are smaller than 1% (less than 0.01).

1 Introduction

The eigenvalues of anharmonic potentials appear in many applications, such as Molecular Physics [1,2], Phonon Interaction [3] and String Vibrations [4]. For this reason, it is important to mention some physical applications, in the analysis of the decatic potential, demonstrated that Quantum monochromy occurs at a critical point in the energy spectrum. Y recently, by solving the Bohr Hamiltonian, they determined critical point nuclei for the isotopic chains Pd, Ru, Cd, Ba and Xe [5,6]. The particular case of the decatic anharmonic potential $x^2 + \lambda x^{10}$ will be treated here, general analytical solution not known. Numerical computation is the general way to obtain eigenvalues for this kind of potential. In this work a precise analytic solution for the ground state will be determined.
Most of the theories carry out the treatment of the Schrödinger equation with small values of the parameter λ, and for large values of λ are determined numerically. With the new method here described this problem is solved. The technique applied is the multi-point quasi-rational approximation (MPQA) [7,8]. In the method, the potential and asymptotic expansions must be determined for small and large values of λ. Finally, an analytical approximation $E_{ap}(\lambda)$ for the eigenvalues will be described as a bridge function between both the potential and asymptotic expansions [9].

2 Theorical Treatment

Consider is the ground state of the Schrödinger stationary equation in one-dimension with decatic potential [8],

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 + \alpha x^{10}\right)\psi(x) = E\psi(x), \tag{1}$$

where $\hbar$ is the reduced Planck constant, m the mass of the particle and ω the angular frequency. Using as atomic units ($\hbar = m = \omega = 1$), and the conventional change of variables, this equation can be written as follow,

$$\left(-\frac{d^2}{dx^2} + x^2 + \lambda x^{10}\right)\psi(x) = E\psi(x). \tag{2}$$

It is assumed as usual that the perturbation parameter λ is positive. The main idea is the construction of an approximant function $E_{ap}(\lambda)$ for the energy levels, based on the new multi-point quasi-rational approximation (MPQA) method [7-9].

2.1 *Potentials Series*

For small values of λ, the expansion for eigenvalues $E(\lambda)$ and eigenfunctions $\psi(x)$, are written as,

$$E(\lambda) = \sum_{k=0}^{\infty} E_k \lambda^k, \qquad \psi(x) = \sum_{k=0}^{\infty} \psi_k(x)\lambda^k. \tag{3}$$

Now Eq.(2) is expanded, thus the E_k and $\psi_k(x)$, are defined as:

$$\begin{aligned} L\psi_0(x) &= E_0\psi_0(x) \\ \vdots &= \vdots \\ L\psi_l(x) + x^{10}\psi_{l-1} &= \sum_{k=0}^{l} E_k\psi_{l-k}(x), \quad l > 1, \end{aligned} \tag{4}$$

where the operator $L = \left(\left(-d^2/dx^2\right) + x^2\right)$.The term $L\psi_0(x) = E_0\psi_0(x)$, has an exact solution with the energy ground state $E_0 = 1$ and the eigenfunction $\psi_0(x) \propto exp(-x^2/2)$.
The coefficients E_k, are determined by numerical procedures, specifically using the shooting method to solve the system of differential equations. The results for the first four terms are,

$$E_0 = 1; \quad E_1 = 0.368049; \quad E_2 = -0.0441781; \quad E_3 = 0.00361862; \quad E_4 = -0.000715894. \tag{5}$$

2.2 *Asymptotic Expansion*

The idea now is to consider expansions for large values of λ. To carry out this condition, a mechanism of variable change has been introduced.

$$x = \lambda^{-\frac{1}{12}} y; \qquad \widetilde{\lambda} = \lambda^{-\frac{1}{3}}; \qquad \widetilde{E} = \lambda^{-\frac{1}{6}} E, \tag{6}$$

these values are particular cases of the more general expressions described in previous works [8,9], here $a = 2$ and $b = 10$. In this way, replacing Eq.(6) into Eq.(2), the new Schrödinger equation will be,

$$\left(-\frac{d^2}{dy^2} + y^{10} + \widetilde{\lambda} y^2\right)\widetilde{\psi}(y) = \widetilde{E}\widetilde{\psi}(y). \tag{7}$$

The new expansions are:

$$\widetilde{E}(\widetilde{\lambda}) = \sum_{k=0}^{\infty} \widetilde{E}_k \widetilde{\lambda}^k, \qquad \widetilde{\psi}(y) = \sum_{k=0}^{\infty} \widetilde{\psi}_k(y)\widetilde{\lambda}^k. \tag{8}$$

The eigenvalues and eigenfunctions are obtained from the differential equations,

$$\widetilde{L}\widetilde{\psi}_l(y) + y^2\widetilde{\psi}_{l-1}(y) = \sum_{k=0}^{l} \widetilde{E}_k\widetilde{\psi}_{l-k}(y), \quad l > 1. \tag{9}$$

It is defined a new operator $\widetilde{L} = \left(-\left(d^2/dy^2\right) + y^{10}\right)$. Here the new values $\widetilde{E}_k$ are determined by numerical procedures, specifically here by the shooting method. Hence, the new values are,

$$\widetilde{E}_0 = 1.298844;\ \widetilde{E}_1 = 0.256464;\ \widetilde{E}_2 = -0.00100381;\ \widetilde{E}_3 = -0.000254016$$
$$\widetilde{E}_4 = -0.0000375953; \quad \widetilde{E}_5 = 0.000005063. \tag{10}$$

2.3 *Analytic Function Structure*

The asymptotic expansion will be written in terms of the variable λ instead of $\widetilde{\lambda}$. In this way, it is obtained

$$E(\lambda) \approx \lambda^{1/6} \sum_{k=0}^{\infty} \frac{\widetilde{E}_{3k}}{\lambda^k} + \lambda^{-1/6} \sum_{k=0}^{\infty} \frac{\widetilde{E}_{3k+1}}{\lambda^k} + \lambda^{-1/2} \sum_{k=0}^{\infty} \frac{\widetilde{E}_{3k+2}}{\lambda^k}. \tag{11}$$

Using polynomials of second degree a good accuracy is obtained. Thus the bridge function $E_{ap}(\lambda)$ is defined as:

$$E_{ap}(\lambda) = (1+\mu\lambda)^{\frac{1}{6}} \frac{a_0 + a_1\lambda + a_2\lambda^2}{1+q\lambda^2} + (1+\mu\lambda)^{-\frac{1}{6}} \frac{b_0 + b_1\lambda + b_2\lambda^2}{1+q\lambda^2} + (1+\mu\lambda)^{-\frac{1}{2}} \frac{c_0 + c_1\lambda + c_2\lambda^2}{1+q\lambda^2}. \tag{12}$$

Initially in equation (11), an undesirable singularity must be avoided, that is in the value of $\lambda = 0$. Thus, in the approximate function, λ is replaced by $(1+\mu\lambda)$, and this is way undesirable singularities are avoided, and μ is a new parameter to be determined.

2.4 *Determination of Parameters*

To determine the parameters equal number of terms from the power series and asymptotic expansion will be used. In this way from the power series the following equations are obtained,

$$\begin{aligned}
a_0 + b_0 + c_0 &= E_0 \\
(1/3)\,\mu\,(2a_0 + b_0) + a_1 + b_1 + c_1 &= (1/2)\,\mu E_0 + E_1 \\
(1/9)\,\mu^2\,(-a_0 - b_0) + (1/3)\,\mu\,(2a_1 + b_1) + a_2 + b_2 + c_2 &= \left((8q - \mu^2)/8\right) E_0 + (1/2)\,\mu E_1 + E_2 \\
(1/81)\,\mu^3\,(4a_0 + 5b_0) + (1/9)\,\mu^2\,(-a_1 - b_1) + (1/3)\,\mu\,(2a_2 + b_2) &= \left((8q\mu - \mu^3)/16\right) E_0 \\
&\quad + \left((8q - \mu^2)/8\right) E_1 + (1/2)\,\mu E_2 + E_3 \\
(1/243)\,\mu^4\,(7a_0 - 10b_0) + (1/81)\,\mu^3\,(4a_1 + 5b_1) + (1/9)\,\mu^2\,(-a_2 - b_2) &= -\left((16q\mu - 5\mu^4)/128\right) E_0 \\
&\quad + \left((8q\mu - \mu^3)/16\right) E_1 + \left((8q - \mu^2)/8\right) E_2 + (1/2)\,\mu E_3 + E_4.
\end{aligned} \tag{13}$$

On the other way from the asymptotic expansion the equations are:

$$a_2 = \mu^{-1/6} q \widetilde{E}_0; \qquad b_2 = \mu^{1/6} q \widetilde{E}_1; \qquad c_2 = \mu^{1/2} q \widetilde{E}_2$$
$$a_1 = \mu^{-1/6} q \left(-\frac{1}{6\mu}\widetilde{E}_0 + \widetilde{E}_3\right); \qquad c_1 = \mu^{1/2} q \left(\frac{1}{2\mu}\widetilde{E}_2 + \widetilde{E}_5\right). \tag{14}$$

The equations obtained are linear in all parameters, except for the parameter μ. The value μ is not determined by any of this equations. The criterion that is assumed is to search for the optimal value μ that produces the lowest maximum relative error, with positive values of q.

3 Results

The solutions to the system of equations (13) and (14) provide all the parameters a_k, b_k, c_k and q as a function of μ. In particular q it is given by:

$$q = \frac{\left(-22.27 + 159.47\mu - 636.16\mu^2 + 110.42\mu^3 + 15\mu^4\right)}{1374.1 - 16217\mu - 14400\mu^4 + 25229\mu^{11/6} + 2585.2\mu^{13/6} - 4\mu^{15/6} - 0.24\mu^{17/6} - 0.00049\mu^{21/6}}. \quad (15)$$

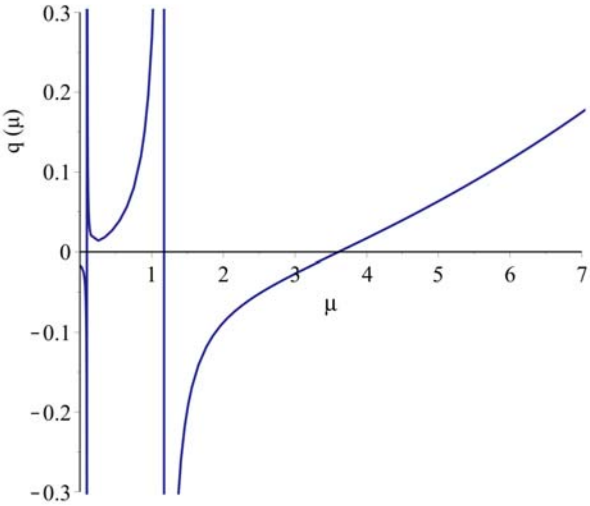

Figure 1: Plot of q as a function of μ. For the intervals $0.2 \le \mu \le 1.2$ and $3.7 \le \mu \le 7.0$, the values of q verify that $q > 0$.

The parameter μ has been considered until now as unknown. The way to determine it is by looking for the optimal value μ_0 between the values $0.2 \le \mu \le 1.2$ and $3.7 \le \mu \le 7.0$ that produces the lowest maximum relative error. In this way, $\mu_0 = 6.6$ is found and the maximum relative error using this value is 0.04. The plot of the relative errors in function of λ are shown in Fig. 2, and the eigenvalues as a function of λ, are shown in Fig. 3.

$$\begin{aligned} E_{ap}(\lambda) &= (1+6.6\lambda)^{\frac{1}{6}} \frac{\left(0.413 - 0.00362\lambda + 0.142\lambda^2\right)}{(1+0.150\lambda^2)} \\ &+ (1+6.6\lambda)^{-\frac{1}{6}} \frac{\left(0.659 + 0.403\lambda + 0.0528\lambda^2\right)}{(1+0.150\lambda^2)} \\ &+ (1+6.6\lambda)^{-\frac{1}{2}} \frac{\left(-0.0724 - 0.0000274\lambda - 0.000387\lambda^2\right)}{(1+0.150\lambda^2)}. \end{aligned} \quad (16)$$

The equation represents the final form of the approximant for the ground state of the decatic anharmonic potential.

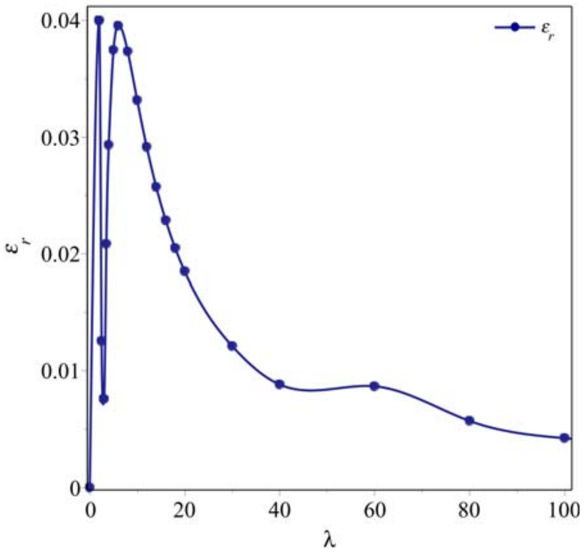

Figure 2: Relative errors ε_r (discrete dots) of the approximation function as a function of the parameter λ. It is shown that the maximum relative error is 0.04 in the optimal values of $\mu_0 = 6.6$ and $\lambda = 2$.

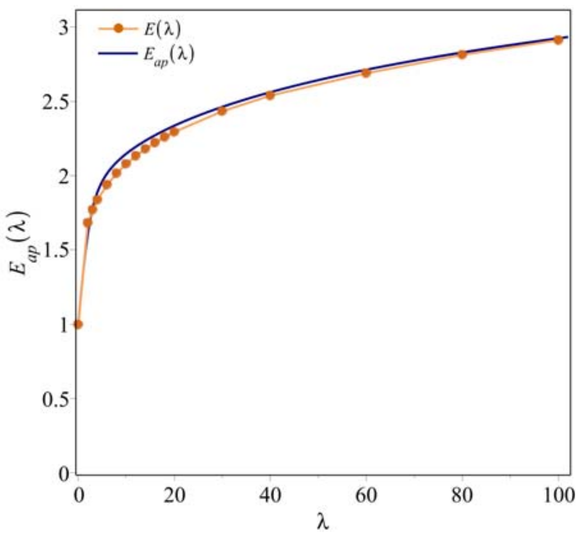

Figure 3: Comparison between the exact eigenvalues $E(\lambda)$ (discrete dots) and the approximation function $E_{ap}(\lambda)$ (solid line) for the anharmonic potential $x^2 + \lambda x^{10}$ in terms of the parameter λ.

4 Conclusions

A technique has been developed to determine precise analytic solutions of the eigenvalues of the ground state of the Schrödinger equation with anharmonic potential $x^2 + \lambda x^{10}$. The ground state eigenvalues have been considered here. With the technique, the power series and asymptotic expansion have been obtained as a function of the parameter λ. Both series determine the structure of the approximation function for the eigenvalues. The analytic function is built with polynomials of degree two. In this way the maximum relative error was 0.04.

References

[1] Fernandez F. M. and Tipping R. H., 1999 *J. Molec. Struct.* **488**, 157-161.

[2] Piccini G. and Sauer J., 2014 *J. Chem.* **10**, 2479-2487.

[3] Wang W., Tinka Gammel J., Bishop A. and Salkola M., 1996 *Phys. Rev. Lett.* **76**, 3598-3601.

[4] Jaradat A., Obeidat A., Gharaibeh M., Aledealat K., Khasawinah K., Qaseer M. and Rousan A., 2018 *IJRAE* **12**, 10372-10375.

[5] Dong S. A., 2002 *J. Theor. Phys.* **41**, 89-99.

[6] Sobhani H., Hassanabadi H., Bonatsos D., Cui S., Feng Z. and Draayer J. P., 2020 *Eur. Phys. J.* **A56**, 1-10.

[7] De Freitas A., Martín P., Castro E. and Paz J. L., 2007 *Phys. Rev. Lett.***A362**, 371-376.

[8] Martín P., Castro E., and Paz J. L., 2012 *Rev. Mexicana Física* **58**, 301-307.

[9] Martín P., Diaz Almeida D. and Maass F., 2020 *Results in Phys.* **18**, 1-4.