Results in Physics 8 (2018) 140–145

Contents lists available at ScienceDirect

Results in Physics

journal homepage: www.journals.elsevier.com/results-in-physics

Analytic approximate eigenvalues by a new technique. Application to sextic anharmonic potentials

D. Diaz Almeida [a,*], P. Martin [b]

[a] Centro de Desarrollo Energético Antofagasta (CDEA), Av. Angamos 601, Antofagasta 1270300, Chile
[b] Departamento de Física, Universidad de Antofagasta, Av. Angamos 601, Antofagasta 1270300, Chile

ARTICLE INFO

Article history:
Received 18 July 2017
Received in revised form 9 November 2017
Accepted 11 November 2017
Available online 26 November 2017

Keywords:
Eigenvalue
Sextic anharmonic potential
Ground state
Quantum mechanics
Anharmonic oscillator

ABSTRACT

A new technique to obtain analytic approximant for eigenvalues is presented here by a simultaneous use of power series and asymptotic expansions is presented. The analytic approximation here obtained is like a bridge to both expansions: rational functions, as Padé, are used, combined with elementary functions are used. Improvement to previous methods as multipoint quasirational approximation, MPQA, are also developed. The application of the method is done in detail for the 1-D Schrödinger equation with anharmonic sextic potential of the form $V(x) = x^2 + \lambda x^6$ and both ground state and the first excited state of the anharmonic oscillator.

Introduction

Harmonic potentials with sextic anharmonic terms has been treated for several authors [1–7]. This kind of potential play an important role in spectra of molecules such as ammonia and hydrogen bounded-solids [8,9], and they might be considered as a potential model for quark confinement in Quantum Chromodynamics [10]. An analytic solution of the one dimensional (1-D) Schrödinger equation of this quantum mechanical system is not actually known, and numerically computation is the usual way to obtain the eigenvalues of the equation, as well as perturbation techniques around the harmonic potential. This leads to approximations which are usually good for small values of the perturbative parameter λ. However, improvements in a recient technique denoted as multi-point quasi-rational approximant (MPQA), will allow to obtain precise analytic approximations for any value of the parameter λ, using simultaneously power series and asymptotic expansions [11–14]. The present new technique uses rational approximants, as Pade's method, but combined with other auxiliary functions as fractional powers, exponentials, trigonometricals and others elementary functions [12].

In recent works, asymptotic Taylor expansion method has been used as an alternative approach to energy eigenvalue problems of anharmonic potentials [15]. On the other hand, the technique here presented is an extension of a previous method, which was first applied to obtain approximate analytic solutions to plasma dispersion function [16], Bessel functions [17], elementary particles [18] and several other important functions in Physics, most of them are referred in the review article [11]. Later the procedure was also applied to find analytic approximant and analytic functions to Quantum Physics potentials, where not known exact solutions can be found, as quadratic Zeeman Effect in 2-D [19], Morse potentials with centrifugal terms [20] and others (see Ref. [11]). Anharmonic potentials where treated later. The actual case of sextic anharmonic potentials in 1-D presents new problems which are solved here. The ground state $(n = 0)$ and the first odd excited energy state $(n = 1)$ for any positive value of the parameter λ is treated now. (Other excited states could be considered in future works if they are needed).

Eigenvalues of sextic anharmonic potentials in 1-D with the form $V(x) = x^2 + \lambda x^6$ are study now. No general analytic solutions to this problem is known, although particular analytical solutions can be found when the parameters obey certain relations, potentials so called quasi-exactly-solvable, see for instance a good list of references in [6]. Perturbation theory leads to power expansions, which are only usually good for small values of λ. In the case of anharmonic quartic potentials general method for any positive λ was presented in previous works [12], using power series and asymptotic expansions. An improvement of this technique is presented here using the two previous expansions as well as

* Corresponding author.
E-mail addresses: daniel.diaz@uantof.cl (D. Diaz Almeida), pmartin@usb.com (P. Martin).

https://doi.org/10.1016/j.rinp.2017.11.019
2211-3797/© 2017 Published by Elsevier B.V.

additional power series around some intermediate points $\lambda_i, 0 < \lambda_i < \infty$. Thus now besides to use the power series around $\lambda = 0$ and asymptotic expansions, new power series around intermediate points between zero and infinity are also include.

The accuracy of the analytic form here obtained is very good for every positive value of the parameter λ. The analytic approximation is more elaborated than that for the quartic anharmonic potential, but the accuracy is about the same and also a similar number of terms has been used. The highest relative error of the approximant for the ground state is about $5 * 10^{-3}$, but this error is usually smaller than 10^{-5} for most of values of λ. Despite numerical calculation allows to determine the eigenvalue for any given value of λ, the formula now developed determines the value of any λ in a very simple way even with an usual pocket calculator, and with accuracy high enough for most of the applications. Furthermore, the approximate expression can be differenciated or integrated if it is required.

In the next section, Section "Theoretical treatment and power series", of the paper, the way to obtain a power series in λ for the eigenvalue is derived, as an extension of the MPQA method. The way to obtain an asymptotic series is more elaborated and it is develop in Section "Asymptotic expansion". The analysis of both the power series and asymptotic expansion, leads to the form of the approximate for the actual potential, which will be two rational functions combined with fractional powers, and its application will be considered in Section "Development of the approximation method through the sextic anharmonic oscillator and its application" for both the ground state and the first excited state. The determination of the parameters, results and discussion of the accuracy for the approximant will be performed in Section "Results and discussion". Section "Conclusion", finally, is devoted to the Conclusion.

Theoretical treatment and power series

The equation of interest, is the Schrödinger equation given by:

$$\left(-\frac{\hbar}{2m}\frac{d^2}{dz^2} + \frac{1}{2}m\omega^2 z^2 + \alpha z^6\right)\psi = E\psi, \tag{1}$$

This equation is usually written using atomic units ($\hbar = m = \omega = 1$), and a conventional change of variables as

$$\left(-\frac{d^2}{dx^2} + x^2 + \lambda x^6\right)\psi = \epsilon\psi, \tag{2}$$

This equation, Eq. (2), is a particular case of more general equation considered in previous paper [11,12]

$$\left(-\frac{d^2}{dx^2} + x^a + \lambda x^b\right)\psi = E\psi \tag{3}$$

The perturbative parameter λ is assume to be positive in order to simplify the treatment. The eigenvalues will depend on this parameters.

For small values of λ, the expansion for the energy eigenvalues and eigenfunctions around $\lambda = 0$, are written as

$$E = \sum_{k=0}^{\infty} E_k \lambda^k, \quad \psi = \sum_{k=0}^{\infty} \psi_k \lambda^k, \tag{4}$$

where the sub-index k represent the perturbation order of the energy level of the system. Introducing the expansions given by Eq. (4), and demanding to be satisfied at every order in λ, the following system of differential equations is obtained [11,12]

$$L\psi_k + x^6\psi_{k-1} = \sum_{q=0}^{k} E_{k-q}\psi_q \quad for\ k \geqslant 1, \tag{5}$$

where, the operator L is defined as

$$L = -\frac{d^2}{dx^2} + x^2. \tag{6}$$

It is important to note that, since λ is arbitrary, the associated wave functions $\psi_0, \psi_1, ..,$ will have the same properties than the eigenfunction ψ.

For the ground state $E_0 = 1$, and $\psi_0(x) \propto \exp(-x^2/2)$. Following a similar procedure than in Ref. [12], the solution for ψ will be

$$\psi_k = \left(\sum_{q=0}^{6k} p_q x^q\right)\exp\left(-\frac{x^2}{2}\right) \quad para\ k \geq 1, \tag{7}$$

where the p_q's are coefficients of an arbitrary polynomial to be determined.

An extension and improvement of previous method can be done in the case of expansion around intermediate points λ_β (where, $0 < \lambda_\beta < \infty$). Hence, calling $\lambda_\beta = \beta$, the equations will be written as

$$\left(-\frac{d^2}{dx^2} + x^2 + \lambda_\beta x^6\right)\psi(x, \lambda_\beta) = E(\lambda_\beta)\psi(x, \lambda_\beta), \tag{8}$$

Asymptotic expansion

An extension of the method have been done in order to obtain an expression for the asymptotic expansion corresponding to $\lambda \to \infty$. In this case, the following change of variables has to be done [11,12]

$$x = \lambda^\alpha y, \quad with \quad \alpha = -\frac{1}{2+b}, \tag{9}$$

where b is defined in Eq. (3), and in this work, $b = 6$. Therefore, the new Schrödinger equation, will be

$$\left(-\frac{d^2}{dy^2} + \tilde{\lambda}y^2 + y^6\right)\tilde{\psi} = \tilde{E}\tilde{\psi}, \tag{10}$$

where, the new variables, $\tilde{\lambda}$ and $\tilde{E}$, are given by

$$\tilde{\lambda} = \lambda^{-\frac{2+a}{2+b}} = \lambda^{-\frac{1}{2}}; \quad \tilde{E} = \lambda^{-\frac{2}{a+b}}E = \lambda^{-\frac{1}{4}}E. \tag{11}$$

So that, the perturbative solution of Eq. (10) will be

$$\tilde{E} = \sum_{k=0}^{\infty} \tilde{E}_k \tilde{\lambda}^k, \quad \tilde{\psi_n} = \sum_{k=0}^{\infty} \tilde{\psi}_k \tilde{\lambda}^k. \tag{12}$$

resulting in a system of equations analog to that developed for the power series in λ

$$\tilde{L}\tilde{\psi}_k + y^2\tilde{\psi}_{k-1} = \sum_{q=0}^{k} \tilde{E}_{k-q}\tilde{\psi}_q \quad for\ k \geq 1, \tag{13}$$

where, now, the operator $\tilde{L}$ is written as

$$\tilde{L} = -\frac{d^2}{dy^2} + y^6. \tag{14}$$

In this way, the expansion given by Eq. (12) for $\tilde{E}$ can be re-written in terms of $\tilde{\lambda}$ instead of λ. In the case of sextic anharmonic oscillator ($a = 2$ and $b = 6$) it is obtained

$$E = \lambda^{-2\alpha} \sum_{k=0}^{\infty} \tilde{\lambda}^k \tilde{E}_k \tag{15}$$