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Analytic approximants for the energy eigenvalues of anharmonic potentials

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Abstract

A technique is presented that allows to obtain analytic approximations for the energy eigenvalues of the one-dimensional Schrödinger equation with anharmonic potentials. This technique is based on an original way of obtaining perturbative expansions, together with the used of quasirational approximants found from these expansions at various points. The technique is applied explicitly to the ground state of the quartic anharmonic oscillator.

Keywords: anharmonic potentials, quasirational approximations.

Aproximantes analíticos para los autovalores de energía de potenciales anarmónicos

Resumen

Se presenta una técnica que permite obtener aproximaciones analíticas para los autovalores de energía de la ecuación de Schrödinger unidimensional con potenciales anarmónicos. La técnica está basada en una forma original de obtener expansiones perturbativas, junto con el uso de aproximantes cuasi-racionales obtenidos a partir de estas expansiones en varios puntos. La técnica es aplicada explícitamente al estado base del oscilador anarmónico de grado cuatro.

Palabras clave: potenciales anarmónicos, aproximaciones cuasi-racionales,

Introduction

The quantum anharmonic oscillator is one of the most studied potentials in the one-dimensional Schrödinger equation for which no exact analytic solution is known. Many techniques have been developed that allow to deal with the problem of finding the energy eigenvalues or even the eigenstates, either numerically or in an approximate analytic way, see for instance (1-11). The last alternative is particularly attractive, since it allows to obtain analytic expressions that can be used, in many contexts, in the same way as one would use the exact ones, if they existed. The present work goes in this direction. Of course, the usefulness of a particular technique depends on how precise the analytic approximations are, as well as the simplicity of the approximating functions themselves. It will be shown here that using the power series and asymptotic expansion of the energy eigenvalues (in the parameters of the potential), together with expansions at intermediate points, it is possible to build very precise and simple quasi-rational approximants for

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the energy eigenvalues of the quartic anharmonic oscillator. The Schrödinger equation for the quartic anharmonic oscillator is given by

$$\left(-\frac{d^2}{dx^2}+Ax^2+Bx^4\right)\psi = E\psi \qquad [1]$$

Redefining x as $x \to A^{-1/4}$ and E as $E \to A^{-1/2}$, and taking $\lambda = BA^{-3/2}$, we obtain a Schrödinger equation depending only of one parameter of the form:

$$\left(-\frac{d^2}{dx^2}+x^2+\lambda x^4\right)\psi = E\psi \qquad [2]$$

The approximants will be functions of this parameter, $E = E(\lambda)$, and they will be constructed demanding that its behavior almost matches that of the exact eigenvalues for $\lambda \to 0$ and $\lambda \to \infty$, as well as its behavior at possible intermediate points that can be chosen arbitrarily.

Power series

To find the power series, the energy can be expanded as $E = E_0 + E_1\lambda + E_2\lambda^2 + \ldots$, while the wavefunctions is given by $\psi = \psi_0 + \psi_1\lambda + \psi_2\lambda^2 + \ldots$. Introducing these expressions for E and ψ in eq. [2], in the case of non-degenerates eigenvalues, and asking it to be satisfied at every order in λ, leads to a system of differential equations,

$$L\psi_0 = E_0\psi_0 \qquad [3]$$

$$L\psi_1 + x^4\psi_0 = E_0\psi_1 + E_1\psi_0 \qquad [4]$$

$$L\psi_2 + x^4\psi_1 = E_0\psi_2 + E_1\psi_1 + E_2\psi_0 \qquad [5]$$

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$$L\psi_n + x^4\psi_{n-1} = \sum_{k=0}^{n} E_{n-k}\psi_k\,, \qquad [6]$$

where we defined $L = -\frac{d^2}{dx^2} + x^2$. The coefficients $E_0, E_1, \ldots$, as well as the functions $\psi_0, \psi_1, \ldots$ of the power series, can be easily found since $L\psi_0 = E_0\psi_0$ can be solved exactly. In the case of the ground state, $E_0 = 1$ and $\psi_0 = \exp(-x^2/2)$. The wavefunctions ψ_1 can be written in the general form as $\psi_1(x) = (1 + p_1x + p_2x^2 + p_3x^3 + p_4x^4)\psi_0(x)$. When this is introduced in eq. [4], the function ψ_0 disappears and a relation between two polynomials is left. Since this relation must be satisfied at each order in x, a system of equations in E_1 and the p_1's is obtained, and whose solution is $p_1 = 0$, $p_2 = -3/8$, $p_3 = 0$, $p_4 = -1/8$ and $E_1 = 3/4$ The same procedure can be repeated for the other functions $\psi_2, \psi_3, \ldots$, writing in the form $\psi_n = \psi_0 \sum_{k=0}^{n} p_k x^k$. We obtain $E_0 = 1$, $E_1 = 3/4$, $E_2 = -21/6$, $E_3 = 333/64$, $E_4 = -30885/1024$. This coincides with the results that are obtained using the standard Rayleigh-Schrödinger perturbation method, with the advantage that no information about the eigenstates of energy levels different from the one being considered is required in order to obtain the terms of higher order. One can also find expansions at intermediate points defining $\lambda = a + \lambda_a$ and expanding E and ψ as power series around of $\lambda_a = 0$. Doing this, one can find a system of equations similar to the one shown above, but now the operator L becomes $L \to L_a = -d^2/dx^2 + x^2 + \alpha x^4$. This operator does not have any known exact solutions, so the coefficients must be found by solving the differential equations numerically.

Asymptotic series

We can do the change of variables $x = \lambda^{-1/6}y$, and defining $\tilde{\lambda} = \lambda^{-2/3}$ and $\tilde{E} = \lambda^{-1/3}E$, the Schrödinger equation becomes

$$\left(-\frac{d^2}{dy^2}+\tilde{\lambda}y^2+y^4\right)\psi = \tilde{E}\psi \qquad [7]$$

We can expand as before $\tilde{E} = \tilde{E}_0 + \tilde{E}_1\tilde{\lambda} + \tilde{E}_2\tilde{\lambda}^2 + \ldots$ and $\psi = \tilde{\psi}_0 + \tilde{\psi}_1\tilde{\lambda} + \tilde{\psi}_2\tilde{\lambda}^2 + \ldots$ which leads to the following system of equations:

$$\tilde{L}\tilde{\psi}_0 = \tilde{E}_0\tilde{\psi}_0 \quad [8]$$

$$\tilde{L}\tilde{\psi}_1 + y^2\tilde{\psi}_0 = \tilde{E}_0\tilde{\psi}_1 + \tilde{E}_1\tilde{\psi}_0 \quad [9]$$

$$\tilde{L}\tilde{\psi}_2 + y^2\tilde{\psi}_1 = \tilde{E}_0\tilde{\psi}_2 + \tilde{E}_1\tilde{\psi}_1 + \tilde{E}_2\tilde{\psi}_0 \quad [10]$$

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$$\tilde{L}\tilde{\psi}_n + y^2\tilde{\psi}_{n-1} = \sum_{k=0}^{n}\tilde{E}_{n-k}\tilde{\psi}_k \quad [11]$$

with $\tilde{L} = -\frac{d^2}{dy^2} + y^4$. The expansion of the energy leads to

$$E = \lambda^{1/3}\left(\tilde{E}_0 + \frac{\tilde{E}_1}{\lambda^{2/3}} + \frac{\tilde{E}_2}{\lambda^{4/3}} + \frac{\tilde{E}_3}{\lambda^2} + \ldots\right) \quad [12]$$

In other words, the eigenvalue E goes as $\approx\lambda^{1/3}$ when $\lambda \to \infty$. The coefficients $\tilde{E}_0, \tilde{E}_1, \tilde{E}_2, \ldots$ can be found solving the differential equations [8]-[11]. In particular, if we find up to the (n-1)-th function $\tilde{\psi}_{n-1}$ and up to the (n-1)-th coefficient $\tilde{E}_{n-1}$, then n-th coefficient can be found multiplying the differential equation for $\tilde{\psi}_n$ by $\tilde{\psi}_0$ and integrating in y. One obtains

$$\tilde{E}_n = \frac{\int_{-\infty}^{\infty} dy\left(y^2\tilde{\psi}_{n-1} - \sum_{k=1}^{n-1}\tilde{E}_{n-k}\tilde{\psi}_k\right)\tilde{\psi}_0}{\int_{-\infty}^{\infty} dy\tilde{\psi}_0^2} \quad [13]$$

Construction of the approximants

Taking into account the form of the asymptotic series, one can write an approximant in terms of rational functions depending on the parameters λ, together with auxiliary functions that allow to reproduce the behavior at $\lambda \to \infty$ of the form:

$$E_{app} = (1+\mu\lambda)^{1/3}\frac{P_a(\lambda)}{Q(\lambda)} + (1+\mu\lambda)^{-1/3}\frac{P_b(\lambda)}{Q(\lambda)} + (1+\mu\lambda)^{-1}\frac{P_c(\lambda)}{Q(\lambda)} \quad [14]$$

Where we have defined the following relationship:

$$P_a(\lambda) = \sum_{k=0}^{n} a_k\lambda^k\ ,\ P_b(\lambda) = \sum_{k=0}^{n} b_k\lambda^k\ ,$$

$$P_c(\lambda) = \sum_{k=0}^{n} c_k\lambda^k$$

and $Q(\lambda) = 1 + \sum_{k=1}^{n} q_k\lambda^k$. Here μ is a free parameter that can be adjusted in order to improve the precision of the approximant, and n defines its size, which will depend on the total number of terms used from each series. The coefficients a_k, b_k, c_k and q_k can be obtained expanding the auxiliary functions and equating, order by order in $\lambda, \tilde{\lambda}$ or λ_a, with the corresponding expansions after multiplying both, the expansion and the approximant by the denominator $Q(\lambda)$ of the later.

The way how we arrive to Eq. [14] is explained in previous works (1, 5, 9), however we will explain the main ideas here. First we are using polynomials of the same degree in numerator and denominator because of the asymptotic expansion starts with the fractional power potential 1/3, with is smaller than one. Now in order to obtain the first term of the asymptotic expansions, we cannot use $\lambda^{1/3}$ because, in this way, we are introducing a ramification point in $\lambda = 0$, which is not in the actual function, since the first term of the power series start with a constant value. Now the simplest way to go around this problem, is to use $(1+\mu\lambda)^{1/3}$ instead of $\lambda^{1/3}$. In this way if $\mu > 0$, then the singularity for λ will be $\lambda = -1/\mu$, which is out of our

region of interest, $\lambda \geq 0$. Introducing the auxiliary function $(1+\mu\lambda)^{1/3}$ we get all the powers of the asymptotic expansions of the form $\lambda^{(1/3-n)}$, but in order to get all the terms in the asymptotic expansions we have to introduce the second and third rational function in the right hand side of Eq. [14]. The singularities of the additional auxiliary functions are in the same point $\lambda = -1/\mu$, which means that if the free parameter μ is chosen always a positive number, there is not any problem in the region of interest for λ, which is $\lambda \geq 0$, as were explain before.

Results and conclusions

In the case of the ground state, for the asymptotic expansion the differential eqs. [8]-[11] were solved numerically, using a program in Mathematica with 16 digits of precision, and the following values for the coefficients we found $\tilde{E}_0 = 1.06036194$, $\tilde{E}_1 = 0.362022294$, $\tilde{E}_2 = 0.034510565$, $\tilde{E}_3 = 0.00515693$ and $\tilde{E}_4 = -0.000831127$. The technique was applied forcing the approximant to coincide with the exact eigenvalues at the points $\lambda = 1/2$, $\lambda = 1$, $\lambda = 2$, $\lambda = 5$ and $\lambda = 10$. This is equivalent to using only the first terms in the expansion of the eigenvalue at these intermediate points. Taking $n = 3$ and $\mu = 2$, we found:

$$E_{app} = \left[(1+2\mu)^{1/3}(1.058825793 + 11.26748564\lambda + 76.32694079\lambda^2 + 192.69010099\lambda^3) + (1+2\mu)^{1/3} \times 1.457146273 + 15.2056452\lambda + 76.17650183\lambda^2 + 104.4306642\lambda^3) + (1+2\mu)^{-1}(1.515972066 + 7.475347279\lambda + 16.227055764\lambda^2 + 15.80267791\lambda^3)\right] \times \left[1 + 21.05910003\lambda + 128.8506322\lambda^2 + 228.954205\lambda^3\right]^{-1} \quad [15]$$

With this approximant, the maximum percent error obtained was of the order of $\approx 10^{-4}\%$ for all values of λ in the range $[0,\infty)$. The technique described here can be applied also to other energy levels, as well as to any potential of the form $V(x) = Ax^a + Bx^b$, or even radial potentials of the same form. This will be discussed in future publications, as well as the case of degenerate eigenvalues.

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