Analytic approximants for the energy eigenvalues of anharmonic potentials

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SUMMARY

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 use of quasi-rational approximants found from these expansions at various points. The technique is applied explicitly to the ground state of the quartic anharmonic oscillator.

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 esta 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 armónico de grado cuatro.

KEYWORDS / anharmonic potentials / quasirational approximations / Solutions of wave equations: bound states

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

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}\,\mathrm{x}^2}+\mathrm{A}\,\mathrm{x}^2+\mathrm{B}\,\mathrm{x}^4\right)\psi=\mathrm{E}\,\psi \quad , \tag{1}$$

Redefining x as $\mathrm{x}\to\mathrm{A}^{-1/4}\,\mathrm{x}$ and $\mathrm{E}\to\mathrm{A}^{-1/2}\,\mathrm{E}$, and taking $\lambda=B\,A^{-3/2}$, we obtain a Schrödinger equation depending on only one parameter

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}\,\mathrm{x}^2}+\mathrm{x}^2+\lambda\,\mathrm{x}^4\right)\psi=\mathrm{E}\,\psi \quad . \tag{2}$$

The approximants will be functions of this parameter, $\mathrm{E}=\mathrm{E}(\lambda)$, 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 $E = E_0 + E_1 \lambda + E_2 \lambda^2 + ...$, $\psi = \psi_0 + \psi_1 \lambda + \psi_2 \lambda^2 + ...$ Introducing these expressions for E and ψ in equation (2), and asking it to be satisfied at every order in λ, leads to a system of differential equations,

$$\mathrm{L}\psi_0 = \mathrm{E}_0 \psi_0 \quad , \tag{3}$$

$$\mathrm{L}\psi_1 + \mathrm{x}^4 \psi_0 = \mathrm{E}_0 \psi_1 + \mathrm{E}_1 \psi_0 \quad , \tag{4}$$

$$\begin{matrix} \mathrm{L}\psi_2 + \mathrm{x}^4 \psi_1 = \mathrm{E}_0 \psi_2 + \mathrm{E}_1 \psi_1 + \mathrm{E}_2 \psi_0 \\ \vdots \qquad\qquad \vdots \end{matrix} \quad , \tag{5}$$

$$\mathrm{L}\psi_\mathrm{n} + \mathrm{x}^4 \psi_{\mathrm{n}-1} = \sum_{\mathrm{k}=0}^{\mathrm{n}} \mathrm{E}_{\mathrm{n}-\mathrm{k}} \psi_\mathrm{k} \quad , \tag{6}$$

where $\mathrm{L} = -\frac{\mathrm{d}^2}{\mathrm{d}\,\mathrm{x}^2} + \mathrm{x}^2$. The coefficients $E_0, E_1, ...$, as well as the functions $\psi_0, \psi_1, ...$ of the power series, can be easily found since $\mathrm{L}\psi_0 = \mathrm{E}_0 \psi_0$ can be solved exactly. In the case of the ground state, $\mathrm{E}_0 = 1$ and $\psi_0 = \exp(-\mathrm{x}^2/2)$. E_1 and ψ_1 can be found writing $\psi_1(\mathrm{x}) = \left(1 + \mathrm{p}_1 \mathrm{x} + \mathrm{p}_2 \mathrm{x}^2 + \mathrm{p}_3 \mathrm{x}^3 + \mathrm{p}_4 \mathrm{x}^4\right) \psi_0(\mathrm{x})$. When this is introduced in equation 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 $\mathrm{p}_\mathrm{i}'\mathrm{s}$ is obtained, whose solution is $\mathrm{p}_1 = 0$, $\mathrm{p}_2 = 3/8$, $\mathrm{p}_3 = 0$, $\mathrm{p}_4 = -1/8$ and $\mathrm{E}_1 = 3/4$. The same procedure can be repeated for ψ_2, ψ_3, etc., writing $\psi_n = \psi_0 \sum_{k=0}^{n} p_k \, x^k$. We obtain $E_0 = 1$, $E_1 = 3/4$, $E_2 = -21/16$, $E_3 = 333/64$, $E_4 = -30885/1024$. 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 $\lambda_a = 0$. Doing this, one can find a system of equations similar to the one shown above, but now the operator L becomes $L \to L_a = -\frac{d^2}{dx^2} + x^2 + \alpha x^4$. 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

$$\left(-\frac{d^2}{dy^2} + \tilde{\lambda}\, y^2 + y^4 \right) \psi = \tilde{E}\, \psi \quad . \tag{7}$$

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

$$\tilde{L}\, \tilde{\psi}_0 = \tilde{E}_0\, \tilde{\psi}_0 \quad , \tag{8}$$

$$\tilde{L} \tilde{\psi}_1 + y^4 \tilde{\psi}_0 = \tilde{E}_0 \tilde{\psi}_1 + \tilde{E}_1 \tilde{\psi}_0 \quad , \tag{9}$$

$$\begin{aligned} \tilde{L} \tilde{\psi}_2 + y^4 \tilde{\psi}_1 &= \tilde{E}_0 \tilde{\psi}_2 + \tilde{E}_1 \tilde{\psi}_1 + \tilde{E}_2 \tilde{\psi}_0 \\ \vdots \qquad & \qquad \vdots \end{aligned} \tag{10}$$

$$\tilde{L} \tilde{\psi}_n + y^4 \tilde{\psi}_{n-1} = \sum_{k=0}^{n} \tilde{E}_{n-k} \tilde{\psi}_k \quad , \tag{11}$$

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

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

In other words, the eigenvalue E goes as $\approx \lambda^{1/3}$ when $\lambda \to \infty$. The coefficients $\tilde{E}_0$, $\tilde{E}_1$, $\tilde{E}_2$,..., 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 the $n-$th coefficient can be found multiplying the differential equation for $\tilde{\psi}_n$ by $\tilde{\psi}_0$ and integrating in y. One obtains

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

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 parameter λ, together with auxiliary functions that allow to reproduce the behavior at $\lambda \to \infty$

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

where $P_a(\lambda) = \sum_{k=0}^{n} a_k \lambda^k$, $P_b(\lambda) = \sum_{k=0}^{n} b_k \lambda^k$, $P_c(\lambda) = \sum_{k=0}^{n} c_k \lambda^k$ 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 λ, $\tilde{\lambda}$ or λ_a, with the corresponding expansions after multiplying both, the expansion and the approximant by the denominator $Q(\lambda)$ of the later.

Results and conclusions

In the case of the ground state, for the asymptotic expansion the differential equations (8)-(11) were solved numerically and the following values for the coefficients were found $\tilde{E}_0 = 1.06036194$, $\tilde{E}_1 = 0.36202294$, $\tilde{E}_2 = -0.034510565$, $\tilde{E}_3 = 0.00515693$ 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 term in the expansion of the eigenvalue at these intermediate points. Taking $n = 3$ and $\mu = 2$, we found

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

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 $V(x) = A\,x^a + B\,x^b$, or even radial potentials of the same form. This will be discussed in future publications.

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