Multi-point quasi-rational approximants for the energy eigenvalues of two-power potentials

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Analytic approximants for the eigenvalues of the one-dimensional Schrödinger equation with potentials of the form $V(x) = x^a + \lambda x^b$ are found using a multi-point quasi-rational approximation technique. This technique is based on the use of the power series and asymptotic expansion of the eigenvalues in λ, as well as the expansion at intermediate points. These expansions are found through a system of differential equations. The approximants found are valid and accurate for any values of $\lambda > 0$ (with $b > a$). As an example, the technique is applied to the quartic anharmonic oscillator.

Keywords: Polynomial potentials; quasi-rational approximants; anharmonic oscillators; eigenvalues; eigenfunctions.

Se determinaron aproximaciones analíticas para los valores propios de la ecuación unidimensional de Schrödinger con potenciales de la forma $V(x) = x^a + \lambda x^b$, usando la técnica de los aproximantes quasi-racionales a múltiples puntos. Esta técnica se basa en el uso de una serie potencial y una expansión asintótica de los valores propios en potencias de λ, así como la expansión en puntos intermedios. Estos expansiones se determinaron a través de un sistema de ecuaciones diferenciales. Las aproximaciones encontradas son válidas y precisas para cualquier valor de $\lambda > 0$ (con $b > a$). Como un ejemplo, la técnica se aplica al oscilador anarmónico de cuarto grado.

Descriptores: Potenciales polinómicos; aproximantes cuasi-racionales; osciladores anarmónicos; autovalores; autofunciones.

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1. Introduction

There are many techniques that have been developed with the purpose of solving the Schrödinger equation since it was first introduced more than eighty years ago. One might think that after so many years this should be a closed subject, yet this area of research is still being pursued nowadays by a number of physicists in the world. There are still many potentials of interest for which no exact solution is known and, moreover, new potentials that seem to model the behavior of physical systems, such as a set of different molecules interacting with each other or with an external field, are still being proposed from time to time, which prompts physicist to study them in more detail. A recent example of this can be found in Ref. 5.

Since one cannot find exact solutions for many of the most interesting potentials, one is left with one of two options: (1) use a numerical method or (2) try to find an approximate analytic solution. The last option is particularly appealing, since in many situations it is possible to use precise approximate solutions in the same way as the exact ones. Approximate analytic solutions can be obtained by different methods for both, the energy eigenvalues and eigenfunctions of the Schrödinger equation, although more methods can be found in the literature for the eigenvalues than for the eigenfunctions. In either case, there are hundreds of publications devoted to this subject, and it would be impossible to make justice by citing them all. Some of the most recent ones can be found in Refs. 1 to 12.

An analytic approximant should be a function of the parameters of the potential that comes very close to the values of the exact solutions (found numerically) when evaluated at any particular point in the parameter space. The usefulness of a particular method used to obtain these approximants will depend on the precision of the approximations as well as the simplicity of the analytic expressions.

In this paper, a new method is proposed for finding analytic approximants to the energy eigenvalues of the one-dimensional Schrödinger equation with two-power potentials, *i.e.*, potentials of the form $V(x) = x^a + \lambda x^b$ [13-18], valid for any (positive) values of the parameter λ. This kind of potentials are of great theoretical interest, since they include potentials such as the quartic and sextic anharmonic oscillators, and they are a good choice to test new methods before applying them to other problems that might be more interesting from a phenomenological point of view, such as radial potentials in three dimensions.

The method we are proposing here is based on the multi-point quasi-rational approximation technique, which has been successfully applied before to similar kinds of problems involving differential equations [19-24]. This technique consists in using the expansions of the function to be approx-

imated around different values of the parameters in the differential equation where this function appears, in order to write an approximant in terms of rational functions of these parameters combined with auxiliary ones. The approximant will then have almost the same expansions around the different chosen values of the parameters. The auxiliary functions are usually needed in order to match the behavior of the quantity to be approximated when the parameters go to infinity, which normally cannot be done solely using rational functions as in a Pade's approximation.

In our case, the differential equation we are interested in, of course, the Schrödinger equation

$$\left(-\frac{d^2}{dx^2}+x^a+\lambda x^b\right)\psi = E\psi\,. \tag{1}$$

In this case, we have one parameter, λ, which will be assumed to be positive to simplify the treatment, though the method can be used without this restriction. It is also assumed that a and b are positive integers, and $b > a \geq 2$. The energy eigenvalues E will depend on the parameter λ. Our goal is to find an approximating function for $E(\lambda)$ for each energy level, using expansions around different values of λ, including the power series (perturbative expansion around $\lambda = 0$), and the asymptotic expansion ($\lambda \to \infty$). The first part of the method follows the lines described in Ref. 25, where a perturbation theory is used in such a way that the perturbed terms are obtained using the eigenvalues and eigenfunctions of the corresponding unperturbed hamiltonian, instead of the whole spectrum of unperturbed states. In the present treatment, this part corresponds to our expansion around $\lambda = 0$. We have extended the method presented in Ref. 25 to include expansions around points different from the origin ($\lambda = 0$). An extension of the method has also been performed to obtain the asymptotic expansion corresponding to $\lambda \to \infty$.

The main part of our method consists in the simultaneous use of all expansions in λ, in order to obtain a unique quasi-rational function in this parameter, which gives good accuracy for *any value* of $\lambda > 0$. Here is where the multipoint quasi-rational approximation technique is used. This quasi-rational approximation acts as a bridge connecting the expansions around different values of λ.

This paper is organized as follows. In Secs. 2 and 3 we describe the method presented in Ref. 25 and its extension to arbitrary values of λ. In Sec. 4, the construction of the approximants will be shown, using the quartic anharmonic oscillator as an example. These approximants will be found for the ground state energy eigenvalues, as well as the first and second excited levels.

2. Power series

The expansion of the energy eigenvalues and eigenfunctions around $\lambda = 0$ can be written as

$$E = \sum_{k=0}^{\infty} E_k \lambda^k\,, \quad \psi = \sum_{k=0}^{\infty} \psi_k \lambda^k\,. \tag{2}$$

One would like to find the coefficients E_0, E_1, $E_2 \ldots$. This can be done introducing these expansions in (1), and demanding it to be satisfied at every order in λ, which leads to the following system of differential equations [25]

$$L\psi_0 = E_0\psi_0\ , \tag{3}$$

$$L\psi_1 + x^b\psi_0 = E_0\psi_1 + E_1\psi_0\ , \tag{4}$$

$$L\psi_2 + x^b\psi_1 = E_0\psi_2 + E_1\psi_1 + E_2\psi_0\ , \tag{5}$$

$$\vdots \qquad\qquad \vdots$$

$$L\psi_n + x^b\psi_{n-1} = \sum_{k=0}^{n} E_{n-k}\psi_k\,, \quad \text{for} \quad n \geq 1\,, \tag{6}$$

where

$$L = -\frac{d^2}{dx^2} + x^a \tag{7}$$

It is important to note that, since λ is arbitrary, many of the properties of the eigenfunction ψ will be inherited by the functions ψ_0, $\psi_1 \ldots$. For example, given that for bound states, the function ψ should fall off quickly for large values of x, so should the expansion functions ψ_k. Also, if the function ψ has definite parity, then the functions ψ_k will all have the same parity as ψ.

The coefficients in the expansion of the energy can be found by solving numerically the system of differential equations (using, for example, the shooting method).

On the other hand, Eq. (3) can be solved exactly for $a = 2$, since then it would be the Schrödinger equation for a harmonic oscillator. It can be shown that in this case, all the other equations in the system can also be solved exactly. For example, for the ground state $E_0 = 1$ and $\psi_0(x) \propto \exp(-x^2/2)$. If we take $b = 4$ (quartic anharmonic oscillator) the next function, $\psi_1(x)$, can be written as

$$\psi_1(x) = (p_0 + p_1x + p_2x^2 + p_3x^3 + p_4x^4)\exp\left(-x^2/2\right)\ .$$

When this is introduced in (4), the function $\exp(-x^2/2)$ 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_i's is obtained, whose solution is

$$p_1 = 0,\ \ p_2 = -\frac{3}{8}\,,\ \ p_3 = 0\,,\ \ p_4 = -\frac{1}{8}\,,\ \ E_1 = \frac{3}{4},$$

and it can be seen that p_0 is arbitrary, which means that just like for $\psi_0(0)$, the initial condition $\psi_1(0) = p_0$ is arbitrary (this will be the case for all the other functions in the expansion).

The same procedure can be repeated for ψ_2, ψ_3, etc., writing

$$\psi_n = \left(\sum_{k=0}^{4n} p_k x^k\right)\exp\left(-\frac{x^2}{2}\right)\ .$$

We obtain

$$E_0 = 1, \quad E_1 = \frac{3}{4}, \quad E_2 = -\frac{21}{16},$$
$$E_3 = \frac{333}{64}, \quad E_4 = -\frac{30885}{1024}.$$

This coincides with the results obtained by 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. The same can be done for other values of b.

Similar expansions can be found around any point other than $\lambda = 0$. Let us call $\lambda_\alpha = \lambda - \alpha$, then we can write

$$\left(-\frac{d^2}{dx^2} + x^a + \alpha x^b + \lambda x^b\right)\psi = E\psi \tag{8}$$

and now an expansion around $\lambda_\alpha = 0$ (*i.e.* around $\lambda = \alpha$) can be performed.

$$E = \sum_{k=0}^{\infty} E_k^a \, \lambda^k \qquad \psi = \sum_{k=0}^{\infty} \psi_k^a \, \lambda^k \tag{9}$$

Here the α in E_a and ψ_a is a label, not a power. The following set of equations is obtained

$$L_\alpha \psi_0^\alpha = E_0^\alpha \psi_0^\alpha \tag{10}$$
$$L_\alpha \psi_1^\alpha + x^b \psi_0^\alpha = E_0^\alpha \psi_1^\alpha + E_1^\alpha \psi_0^\alpha \, , \tag{11}$$
$$L_\alpha \psi_2^\alpha + x^b \psi_1^\alpha = E_0^\alpha \psi_2^\alpha + E_1^\alpha \psi_1^\alpha + E_2^\alpha \psi_0^\alpha \, , \tag{12}$$
$$\vdots \qquad\qquad \vdots$$
$$L^\alpha \psi_n^\alpha + x^b \psi_{n-1}^\alpha = \sum_{k=0}^{n} E_{n-k}^\alpha \psi_k^\alpha \, , \quad \text{for} \quad n \geq 1 \, , \tag{13}$$

where

$$L_\alpha = -\frac{d^2}{dx^2} + x^a + \alpha x^b \, . \tag{14}$$

Clearly, Eq. (10) will not have exact solutions for any values of a and b, so one is forced to find the coefficients numerically.

The coefficient E_k^α is actually $k!$ times the value of the k-th derivative of the function $E(\lambda)$ evaluated at $\lambda = \alpha$. One might find these derivatives directly, evaluating $E(\lambda)$ nearby $\lambda = \alpha$. However, this way of finding the coefficients becomes relatively difficult for higher derivatives, since then one needs to evaluate the function $E(\lambda)$ with increasing accuracy. The method proposed here can be viewed as an alternative and more accurate way to find these derivatives.

3. Asymptotic expansion

Doing the change of variables

$$x = \lambda^{-\frac{1}{2+b}} y,$$

and defining

$$\tilde{\lambda} = \lambda^{-\frac{2+a}{2+b}}$$

and

$$\tilde{E} = \lambda^{-\frac{2}{2+b}} E,$$

the Schrödinger equation becomes

$$\left(-\frac{d^2}{dy^2} + \tilde{\lambda} y^a + y^b\right)\psi = \tilde{E}\psi \, . \tag{15}$$

One can expand now $\tilde{E}$ and ψ in a similar way as before,

$$\tilde{E} = \sum_{k=0}^{\infty} \tilde{E}_k \lambda^k \, , \quad \psi = \sum_{k=0}^{\infty} \tilde{\psi}_k \tilde{\lambda}_k \, , \tag{16}$$

Introducing this in (15) leads also to a system of differential equations

$$\tilde{L}\tilde{\psi}_0 = \tilde{E}_0 \tilde{\psi}_0 \, , \tag{17}$$
$$\tilde{L}\tilde{\psi}_1 + y^a \tilde{\psi}_0 = \tilde{E}_0 \tilde{\psi}_1 + \tilde{E}_1 \tilde{\psi}_0 \, , \tag{18}$$
$$\tilde{L}\tilde{\psi}_2 + y^a \tilde{\psi}_1 = \tilde{E}_0 \tilde{\psi}_2 + \tilde{E}_1 \tilde{\psi}_1 + \tilde{E}_2 \tilde{\psi}_0 \, , \tag{19}$$
$$\vdots \qquad\qquad \vdots$$
$$\tilde{L}\tilde{\psi}_n + y^a \tilde{\psi}_{n-1} = \sum_{k=0}^{n} \tilde{E}_{n-k} \tilde{\psi}_k \, , \quad \text{for} \quad n \geq 1 \, , \tag{20}$$

where

$$\tilde{L} = -\frac{d^2}{dy^2} + y^b \tag{21}$$

Rewriting the asymptotic expansion in terms of λ instead of $\tilde{\lambda}$, it is clear that the form of the expansion depends on the particular potential to be considered. In the case of the quartic anharmonic oscillator ($a = 2$ and $b = 4$), Eq. (16) leads to

$$E = \lambda^{1/3} \sum_{k=0}^{\infty} \frac{\tilde{E}_{3k}}{\lambda^{2k}} + \lambda^{-1/3} \sum_{k=0}^{\infty} \frac{\tilde{E}_{3k+1}}{\lambda^{2k}} + \frac{1}{\lambda} \sum_{k=0}^{\infty} \frac{\tilde{E}_{3k+2}}{\lambda^{2k}} \, . \tag{22}$$

while in the case of the sextic anharmonic oscillator ($a = 2$ and $b = 6$), we obtain

$$E = \lambda^{1/4} \sum_{k=0}^{\infty} \frac{\tilde{E}_{2k}}{\lambda^k} + \lambda^{-1/4} \sum_{k=0}^{\infty} \frac{\tilde{E}_{2k+1}}{\lambda^k} \, . \tag{23}$$

In general, the expansions will have this structure, *i.e.*, they can be divided in a few pieces, each one consisting in a series of negative integer powers of λ, multiplied by a rational power of λ. For this reason, the approximants that we will build must also be divided in a similar way, in order to match the behavior of each piece. This will be seen explicitly in the next section.

4. Approximants for the Quartic Anharmonic Oscillator

For the quartic anharmonic oscillator [26-30], the approximant for the energy eigenvalues can be written in the following form

$$E_{\rm app}(\lambda) = (1+\mu\lambda)^{1/3}\frac{P_a(\lambda)}{Q(\lambda)} + (1+\mu\lambda)^{-1/3}\frac{P_b(\lambda)}{Q(\lambda)} + \frac{1}{1+\mu\lambda}\frac{P_c(\lambda)}{Q(\lambda)}, \quad (24)$$

where

$$P_a(\lambda) = \sum_{k=0}^{N} a_k\lambda^k,$$

$$P_b(\lambda) = \sum_{k=0}^{N} b_k\lambda^k, \quad P_c(\lambda) = \sum_{k=0}^{N} c_k\lambda^k,$$

and

$$Q(\lambda) = 1 + \sum_{k=1}^{N} q_k\lambda^k = \sum_{k=0}^{N} q_k\lambda^k, \quad (q_0 = 1),$$

that is, the approximant is constructed using rational functions multiplied by auxiliary ones, conveniently chosen in order to match the asymptotic behavior of the eigenvalues. Furthermore, since the power series is also going to be used, it should be possible to Taylor-expand these functions around non-negative values of λ, and in particular around $\lambda = 0$. It is for this last reason that the auxiliary functions are not chosen directly as the factors of $\lambda^{1/3}$, $\lambda^{-1/3}$ and $1/\lambda$ that appear multiplying each one of the three pieces that make up the asymptotic expansion. Instead, we do the change $\lambda \to (1+\mu\lambda)$ inside these roots, which, of course, still gives the right behavior for $\lambda \to \infty$. An arbitrary factor of $\mu > 0$ has also been included, which can be adjusted in order to improve the precision of the approximant. In general, the form of a quasi-rational approximant is mainly determined by the asymptotic expansion. As another example, based on Eq. (23), an approximant for the sextic anharmonic oscillator [31,32] can be written as

$$E_{\rm app}(\lambda) = (1+\mu\lambda)^{1/4}\frac{P_a(\lambda)}{Q(\lambda)} + (1+\mu\lambda)^{-1/4}\frac{P_b(\lambda)}{Q(\lambda)}. \quad (25)$$

With these choices of auxiliary functions the degrees of the polynomials in the numerator must be the same as the ones in the denominator. In principle, this can be done independently for each one of the three pieces in (24), *i.e.* $P_a(\lambda)$, $P_b(\lambda)$ and $P_c(\lambda)$ could be chosen with different degrees, and in that case, different denominators matching the degree of each one of these polynomials would be needed. For simplicity, a denominator $Q(\lambda)$ common to all three pieces has been chosen, and so all polynomials have the same degree. As it will be understood later, any other choice would lead to a system of non-linear equations in the a_k's, b_k's, c_k's and q_k's, making the determination of the approximant unnecessarily complicated.

TABLE I. Exact coefficients of the power series for the first three energy levels of the quartic anharmonic oscillator

Coeffs.	$n=0$	$n=1$	$n=2$
E_0	1	3	5
E_1	3/4	15/4	39/4
E_2	-21/16	-165/16	-615/16
E_3	333/64	3915/64	20079/64
E_4	-30885/1024	-520485/1024	-3576255/1024
E_5	916731/4096	21304485/4096	191998593/4096

TABLE II. Coefficients of the asymptotic expansion for the eigenvalues of the quartic anharmonic oscillator obtained solving the differential equations using the shooting method

Coeffs.	$n=0$	$n=1$	$n=2$
$\tilde{E}_0$	1.060361944	3.799672848	7.455697916
$\tilde{E}_1$	0.362022935	0.901605953	1.244714261
$\tilde{E}_2$	-0.034510565	-0.057483095	-0.046601602
$\tilde{E}_3$	0.005195593	0.005492673	0.000958945
$\tilde{E}_4$	-0.000831127	-0.000513914	-0.000831127

The coefficients of the polynomials in the approximant are found using the power series, asymptotic expansion and the expansions around intermediate points ($0 < \alpha < \infty$), whose calculation was explained in the previous two sections. One is free to choose as many terms from each expansion as one desires, as long as the total number of terms from all expansions equals the total number of coefficients in the approximant. If the degree of the polynomials is N, the total number of coefficients will be $4N+3$. In general, the approximants will have higher precision for higher N.

The values of the first few terms in the power series (around $\lambda = 0$) for the first three energy levels (labeled by n) of the quartic anharmonic oscillator are shown in Table I, while the values of the first few terms in the asymptotic expansion are shown in Table II. Notice that in accordance with what was discussed in Sec. 2, the values of the coefficients for the power series are exact. The values of the coefficients for the asymptotic expansion were obtained by solving Eqs. (17)-(20) using the shooting method. For the ground state ($n = 0$) and the second excited level ($n = 2$), the eigenfunctions are even in x, and as mentioned before, so must be the functions $\tilde{\psi}_k$ (and the same applies to ψ_k and ψ_k^α), so the initial conditions used in those cases were $\tilde{\psi}_k(0) = 1$ and $\tilde{\psi}_k'(0) = 0$. For the first excited level the eigenfunction is odd in x, so the conditions were $\tilde{\psi}_k(0) = 0$ and $\tilde{\psi}_k'(0) = 1$. One might feel uneasy about the propagation of errors from one differential equation to the next, but it can be checked numerically that the accuracy of the energy eigenvalues for large

values of λ (or small values of $\tilde{\lambda}$) improves as one includes higher terms in the expansion, which gives us confidence that the precision of the coefficients is acceptable.

Let's choose a few intermediate points α_i ($i = 1, 2, \ldots$), and let's take n_i terms from the expansion around each one of these points. Let's also take n_0 terms from the power series (around $\lambda = 0$) and n_a terms from the asymptotic expansion. It will be assumed that $\sum_i n_i + n_0 + n_a = 4N + 3$. Using the power series at $\lambda = 0$ one can write

$$Q(\lambda)\sum_{k=0}^{n_0} E_k\lambda^k = (1+\mu\lambda)^{1/3}P_a(\lambda) + (1+\mu\lambda)^{-1/3}P_b(\lambda) + \frac{1}{1+\mu\lambda}P_c(\lambda)\ , \quad (26)$$

Taylor-expanding each side of this equation in λ, and demanding it to be satisfied at every order up to λ^{n_0}, one obtains a set of n_0 linear equations in the coefficients of the approximant. Likewise, one can use the expansions at the intermediate points, and doing the change $\lambda = \lambda_{\alpha_i} + \alpha_i$, one can write

$$\left(1 + \sum_{k=1}^{N} q_k(\lambda_{\alpha_i} + \alpha_i)^k\right)\sum_{k=0}^{n_i} E_k^{\alpha_i}\lambda_{\alpha_i}^k = (1+\mu(\lambda_{\alpha_i}+\alpha_i))^{1/3}\sum_{k=0}^{N} a_k(\lambda_{\alpha_i}+\alpha_i)^k + (1+\mu(\lambda_{\alpha_i}+\alpha_i))^{-1/3}\sum_{k=0}^{N} b_k(\lambda_{\alpha_i}+\alpha_i)^k + \frac{1}{1+\mu(\lambda_{\alpha_i}+\alpha_i)}\sum_{k=0}^{N} c_k(\lambda_{\alpha_i}+\alpha_i)^k \quad (27)$$

If one demands this equation to be satisfied at every order in λ_{α_i} up to $\lambda_{\alpha_i}^{n_i}$, one obtains a set of n_i linear equations in the coefficients. Finally, one can use the asymptotic expansion. For this we need to do the change $\lambda' = 1/\lambda$, and match the expansion with the approximant for each one of the three pieces in which it is divided. For example, since

$$(1+\mu\lambda)^{1/3}\frac{P_a(\lambda)}{Q(\lambda)} = \lambda^{1/3}(\mu+\lambda')^{1/3}\frac{\sum_{k=0}^{N} a_k\lambda'^{N-k}}{\sum_{k=0}^{N} q_k\lambda'^{N-k}}\ ,$$

one can compare the term multiplying $\lambda^{1/3}$ in the right hand side of this equation with the term multiplying the same factor in the asymptotic expansion. Doing the same also for the other two pieces leads to

$$\sum_{k=0}^{N} q_k\lambda'^{N-k}\sum_{k=0}^{\infty}\tilde{E}_{3k}\lambda'^{2k} = (\lambda'+\mu)^{1/3}\sum_{k=0}^{N} a_k\lambda'^{N-k},$$

$$\sum_{k=0}^{N} q_k\lambda'^{N-k}\sum_{k=0}^{\infty}\tilde{E}_{3k+1}\lambda'^{2k} = (\lambda'+\mu)^{-1/3}\sum_{k=0}^{N} b_k\lambda'^{N-k},$$

TABLE III. First coefficient (energy eigenvalues) of the series at different intermediate points for the first three energy levels with $V(x) = x^2 + \lambda x^4$. These values were obtained using the shooting method

Coeffs.	$n=0$	$n=1$	$n=2$
$E_0(\lambda{=}1/2)$	1.24185404314	4.05193233862	7.39690068694
$E_0(\lambda{=}1)$	1.39235158010	4.64881282723	8.65504998225
$E_0(\lambda{=}2)$	1.60754134812	5.47578464629	10.3585833647
$E_0(\lambda{=}5)$	2.01834065745	7.01347929870	13.4677303948
$E_0(\lambda{=}20)$	3.00994494779	10.6432159591	20.6941109272

$$\sum_{k=0}^{N} q_k\lambda'^{N-k}\sum_{k=0}^{\infty}\tilde{E}_{3k+2}\lambda'^{2k} = \frac{1}{\lambda'+\mu}\sum_{k=0}^{N} c_k\lambda'^{N-k}.$$

Here the number of terms taken in each expansion is determined by n_a, that is, one would not allow any $\tilde{E}_k$ with $k > n_a$ in the sums. In this way, one gets a set of n_a linear equations for the coefficients of the approximant.

In Table IV, the values of the coefficients of the approximants are shown for the first three energy levels, using polynomials of degree three. There are fifteen coefficients in each approximant, and they were obtained using the first five terms of the power series (around $\lambda = 0$), the first five terms of the asymptotic expansion, and the first term of the series around $\lambda = 0.5$, $\lambda = 1$, $\lambda = 2$, $\lambda = 5$ and $\lambda = 20$ (which are shown for the three energy levels in Table III). This means that we are only using the exact energy eigenvalue around these intermediate points, and forcing the approximant built with the power series and asymptotic expansion to furthermore coincide with these "exact" eigenvalues at these points. This not only brings the relative error of the approximant at these points down to zero (they become nodes of the relative error as a function of λ), but also helps to decrease the error in between these points. The relative error is defined using as target the eigenvalues obtained numerically through the shooting method, *i.e.*, the relative error is given by

$$\frac{|E_{\rm app} - E_{\rm shooting}|}{E_{\rm shooting}}\ . \quad (28)$$

The highest relative error with these approximants was obtained for relatively small values of λ. Specifically, the maximum relative error was obtained around $\lambda \approx 0.2$. In the case of the ground state, the highest relative error was

$$\left.\frac{|E_{\rm app} - E_{\rm shooting}|}{E_{\rm shooting}}\right|_{\lambda=0.17} = 1.05\times10^{-6}\ . \quad (29)$$

The relative error decreases rapidly for smaller values of λ, and of course, it also decreases when λ increases until it finds the next node at $\lambda = 0.5$. After that, the relative error never becomes higher than 2×10^{-7}. For the first and second excited level, the maximum error around $\lambda \approx 0.2$, was about 8×10^{-7} and 2.4×10^{-6}, respectively, and after the node at

TABLE IV. Coefficients for the approximants of the first three energy eigenvalues of $V(x) = x^2 + \lambda x^4$, using polynomials of degree 3

Coeffs.	$n = 0$	$n = 1$	$n = 2$
a_0	-235.587774594	3.26113271857	-46.3903727540
a_1	129.192528081	45.7861842084	118.622015136
a_2	819.219808968	347.592601172	906.778841942
a_3	4083.20247083	1023.55148495	3353.40199807
b_0	49.9309955808	4.80222464913	8.35806073416
b_1	374.551951382	43.2593054339	113.555378592
b_2	1181.63222463	259.439145729	536.540936096
b_3	2212.93937770	385.537761596	888.696857827
c_0	186.656779013	-5.06335736770	43.0323120198
c_1	208.866219507	-20.7666223608	48.6886778830
c_2	-423.418335743	-35.6233569984	-59.8483255497
c_3	-334.866518168	-39.0190739652	-52.8167275564
q_1	148.201294158	24.5427291322	29.7104983824
q_2	1782.00574019	171.823102857	247.681714807
q_3	4851.65727491	339.396077796	566.683604101

$\lambda = 0.5$ this error is never higher than 4×10^{-8}. In fact, the relative error decreases quite rapidly in the case of the first and second excited levels for large values of λ, although it does so more slowly in the case of the ground state.

In all these approximants, we chose $\mu = 2$. This parameter is arbitrary except for one restriction: The approximants should not have any defects, that is, there should not be any poles in the approximant (positive roots of $Q(\lambda)$) with the corresponding nearby zeros. Notice in Table IV that with this choice of μ all of the coefficients of $Q(\lambda)$ are positive, which will, of course, guarantee that it has no roots for $\lambda > 0$. Other choices of μ may lead to mixed negative and positive coefficients in $Q(\lambda)$, which will in general lead to positive real roots in this polynomial. Other than that, there is no restriction in μ. Among all of the values of μ that allow to keep the approximant free of defects, one is free to choose the one that minimizes the relative errors.

Other than improving the numerical method used to obtain the coefficients of the expansions, there are several ways in which the maximum relative error of the approximants can be decreased for all energy levels. The easiest one is to move one of the nodes. For example, one may choose the approximant to have a node at $\lambda = 0.2$ instead of $\lambda = 0.5$. If this is done, it can be seen that the maximum relative error is reduced by about a half for all energy levels. Another possibility is to use the derivatives of $E(\lambda)$ at some of the intermediate points. Finally, one may try an approximant of higher degree, allowing it to coincide with the values of $E(\lambda)$ and its derivatives at more points

5. Conclusions

In this paper, it has been shown that accurate analytic approximants for the energy eigenvalues of potentials of the form $V(x) = x^a + \lambda x^b$ can be found using a multi-point quasi-rational approximation technique. The approximants are constructed using rational functions, together with auxiliary functions introduced to be able to reproduce the behavior of the eigenvalues for large λ. The coefficients of the rational functions are found using the power series of the eigenvalues, not only at $\lambda = 0$, but also for arbitrary finite values of λ, together with the asymptotic expansion. These expansions can be found using a system of differential equations, which in the case of the power series at $\lambda = 0$, represents an alternative way to find the perturbative expansion, as shown in Ref. 25. As an example, approximants for the lowest energy levels of the quartic anharmonic oscillator were obtained. The approximants were fairly simple, since the degree of the polynomials used was not too high. In particular, it was shown that it is possible to obtain approximants with polynomials of degree 3 for which the relative error is not higher than $\sim 3 \times 10^{-6}$.

The method can be applied to other values of a and b in $V(x) = x^a + \lambda x^b$, such as the sextic anharmonic oscillator ($a = 2$, $b = 6$), or even to potentials with no exact solution for $\lambda = 0$, such as $V(x) = x^4 + \lambda x^6$ (as long as one is able to solve the system of differential equations numerically). It should not be difficult to extend this method to radial potentials of the form $V(r) = r^a + \lambda r^b$.

For simplicity, here we have limited ourselves to the use of the shooting method to solve the systems of differential equations. It would be interesting to try to find other methods that allow to improve the numerical accuracy of the coefficients in the expansions. If better numerical solutions for the expansion functions can be found, this should lead to better coefficients and therefore to better approximants. Experience with quasi-rational approximants has shown that the accuracy of the coefficients in the expansions is the main factor influencing the accuracy of multi-point quasi-rational approximations. In the future, we plan to study this and other issues in more detail, and apply this technique to other potentials of interest, both in physics as well as in chemistry.

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