Multi-point quasi-rational approximants for the energy eigenvalues of potentials of the form $V(x) = Ax^a + Bx^b$

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Analytic approximants for the eigenvalues of the one-dimensional Schrödinger equation with potentials of the form $V(x) = Ax^a + Bx^b$ 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 $\lambda = A^{-\frac{a+b}{a+b}}B$, 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 value of $\lambda$. As examples, the technique is applied to the quartic and sextic anharmonic oscillators.

I. 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 [1]. 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.

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 potentials of the form \( V(x) = Ax^a + Bx^b \). This kind of potentials are perhaps not the most interesting ones from a phenomenological point of view, but they are certainly of theoretical interest, since they include such potentials as the quartic and sextic anharmonic oscillators, and in any case, they are a good choice to test new methods before applying them to more interesting problems.

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. This technique consists in using the expansions of the function to be approximated 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 in 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 is, of course, the Schrödinger equation

\[
\left(-\frac{d^2}{dx^2} + Ax^a + Bx^b\right)\psi = E\psi.
\] (1)

In this case, we have too parameters, \( A \) and \( B \), which will be assumed to be both 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 $b > a \geq 2$. As it is very well known [14], one can make this equation to depend on only one parameter by making the changes, $x = A^{-\frac{a}{a+b}}x'$ and $E' = A^{-\frac{b}{a+b}}E$, which leads to

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

(2)

where $\lambda = A^{-\frac{b}{a+b}}B$. From now on we will drop the primes and rename $x' \rightarrow x$ and $E' \rightarrow E$. The energy eigenvalues $E$ will depend on the parameter $\lambda$. Our goal is to find an approximating function for $E(\lambda)$ for each energy level, using expansions around different values of $\lambda$, including the power series (perturbative expansion around $\lambda = 0$), and the asymptotic expansion ($\lambda \rightarrow \infty$). In sections II and III a neat way to find these expansions will be shown using a system of coupled differential equations, which in the case of the power series provides an interesting alternative to standard perturbation methods, since here the perturbed eigenvalue can be found using only the corresponding unperturbed state, instead of using the whole unperturbed eigenvalue spectrum as in the usual quantum mechanics perturbation theory. In sections IV and V the construction of the approximants will be shown, using the quartic and sextic anharmonic oscillators as examples. These approximants will be found for the ground state energy eigenvalues, as well as the first and second excited levels. The important point of our technique is that the same approximant will be valid and accurate for any value of $\lambda$ (including large and small values).

II. POWER SERIES

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

$$E = E_0 + E_1\lambda + E_2\lambda^2 + \cdots,$$

$$\psi = \psi_0 + \psi_1\lambda + \psi_2\lambda^2 + \cdots.$$

One would like to find the coefficients $E_0, E_1, E_2 \ldots$. This can be done introducing these expansions in equation (2), and demanding it to be satisfied at every order in $\lambda$, which leads to the following system of differential equations

$$L\psi_0 = E_0\psi_0,$$

(5)
\[ L\psi_1 + x^b \psi_0 = E_0 \psi_1 + E_1 \psi_0 , \]  
\[ L\psi_2 + x^b \psi_1 = E_0 \psi_2 + E_1 \psi_1 + E_2 \psi_0 , \]  
\[ \vdots \]  
\[ L\psi_n + x^b \psi_{n-1} = \sum_{k=0}^{n} E_{n-k} \psi_k , \]  
where

\[ L = -\frac{d^2}{dx^2} + x^a \]  

It is important to note that, since \( \lambda \) is arbitrary, many of the properties of the eigenfunction \( \psi \) will be inherited by the functions \( \psi_0, \psi_1 \ldots \). For example, given that for bound states, the function \( \psi \) should fall off quickly for large values of \( x \), so should the expansion functions \( \psi_k \). Also, if the function \( \psi \) has definite parity, then the functions \( \psi_k \) will all have the same parity as \( \psi \).

The coefficients in the expansion of the energy can be found by solving numerically the differential equations one by one (using, for example, the shooting method). For instance, one could solve equation (5), obtaining then a numerical value for the coefficient \( E_0 \), together with a numerical solution for \( \psi_0 \). For a bound state, one should find a solution for a range of values in \( x \) where the fall off to zero of \( \psi_0 \) can be seen. Then one can make a very precise fit (a large polynomial in \( x \)) for \( \psi_0 \) within this range, and use this fit as an input to solve equation (6). This then leads to a numerical value for \( E_1 \), and a numerical solution for \( \psi_1 \), and in principle, the procedure can be repeated until one has as many coefficients \( E_k \) as one desires.

Of course, the applicability of this method is limited by the numerical precision with which the differential equations are solved, and since the method is iterative, the numerical errors from the first \( n \) equations will be propagated to the solution of equation \( n + 1 \). For this reason, one would expect the precision of \( E_k \) to be lower for larger values of \( k \).

The numerical values of the coefficients \( E_k \) can also be found directly using the solutions of the first \( k - 1 \) differential equations, without solving the \( k \)-th one. For example, if one has already obtained \( E_0 \) and \( \psi_0(x) \), one can multiply both sides of equation (6) by \( \psi_0(x) \), and integrating in \( x \) it is possible to show that

\[ E_1 = \frac{\int_{-\infty}^{\infty} dx x^b \psi_0^2}{\int_{-\infty}^{\infty} dx \psi_0^2} , \]  

(10)
which coincides with the expression obtained using standard perturbation methods. The same procedure can be repeated for all the other equations, leading to

$$E_n = \frac{\int_{-\infty}^{\infty} dx \left( x^b \psi_{n-1} - \sum_{k=1}^{n-1} E_{n-k} \psi_k \right) \psi_0}{\int_{-\infty}^{\infty} dx \psi_0^2}. \quad (11)$$

This way of finding $E_k$ is more precise, since the number of differential equation to be solved is $k - 1$. In practice, the integrals are taken within a range of $x$ where the functions $\psi_k(x)$ have already fallen to very small values.

On the other hand, equation (5) 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

$$\psi_1(x) = (p_0 + p_1 x + p_2 x^2 + p_3 x^3 + p_4 x^4) \exp(-x^2/2). \quad (12)$$

When this is introduced in equation (11), 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

$$p_1 = 0, \quad p_2 = -\frac{3}{8}, \quad p_3 = 0, \quad p_4 = -\frac{1}{8}, \quad E_1 = \frac{3}{4}, \quad (13)$$

and it can be seen that $p_0$ 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 $\psi_2, \psi_3, \text{etc.},$ writing

$$\psi_n = \left( \sum_{k=0}^{4n} p_k x^k \right) \exp(-x^2/2). \quad (14)$$

We obtain

$$E_0 = 1, \quad E_1 = \frac{3}{4}, \quad E_2 = -\frac{21}{16}, \quad E_3 = \frac{333}{64}, \quad E_4 = -\frac{30885}{1024}. \quad (15)$$

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’s call \( \lambda_\alpha = \lambda - \alpha \), then we can write
\[
\left(-\frac{d^2}{dx^2} + x^a + \alpha x^b + \lambda_\alpha x^b\right)\psi = E\psi ,
\]
and now we can expand around \( \lambda_\alpha = 0 \) (i.e. around \( \lambda = \alpha \)).

\[
E = E_0^\alpha + E_1^\alpha \lambda_\alpha + E_2^\alpha \lambda_\alpha^2 + \cdots ,
\]
(17)

\[
\psi = \psi_0^\alpha + \psi_1^\alpha \lambda_\alpha + \psi_2^\alpha \lambda_\alpha^2 + \cdots .
\]
(18)

The following set of equations is obtained

\[
L_\alpha \psi_0^\alpha = E_0^\alpha \psi_0^\alpha
\]
(19)

\[
L_\alpha \psi_1^\alpha + x^b \psi_0^\alpha = E_0^\alpha \psi_1^\alpha + E_1^\alpha \psi_0^\alpha ,
\]
(20)

\[
L_\alpha \psi_2^\alpha + x^b \psi_1^\alpha = E_0^\alpha \psi_2^\alpha + E_1^\alpha \psi_1^\alpha + E_2^\alpha \psi_0^\alpha ,
\]
(21)

\[
\vdots \quad \vdots
\]

\[
L_\alpha \psi_n^\alpha + x^b \psi_{n-1}^\alpha = \sum_{k=0}^{n} E_{n-k}^\alpha \psi_k^\alpha ,
\]
(22)

where
\[
L_\alpha = -\frac{d^2}{dx^2} + x^a + \alpha x^b .
\]
(23)

Clearly, equation (19) will not have exact solutions for any values of \( a \) and \( b \), so one is forced to find the coefficients numerically. Equations (10) and (11) will still be valid, but with the changes \( \psi_k \to \psi_k^\alpha \) and \( E_k \to E_k^\alpha \), i.e.,

\[
E_1^\alpha = \frac{\int_{-\infty}^{\infty} dx x^b (\psi_0^\alpha)^2}{\int_{-\infty}^{\infty} dx (\psi_0^\alpha)^2}
\]
(24)

and

\[
E_n^\alpha = \frac{\int_{-\infty}^{\infty} dx \left( x^b \psi_{n-1}^\alpha - \sum_{k=1}^{n-1} E_{n-k}^\alpha \psi_k^\alpha \right) \psi_0^\alpha}{\int_{-\infty}^{\infty} dx \psi_0^\alpha} .
\]
(25)

The coefficient \( E_k^\alpha \) is actually 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 \( \lambda = \alpha \), for example,

\[
E_1^\alpha = \frac{E(\lambda = \alpha) - E(\lambda = \alpha + \epsilon)}{\epsilon} .
\]
(26)

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, more accurate, easier and more efficient way to find these derivatives.
III. ASYMPTOTIC EXPANSION

Doing the change of variables $x = \lambda^{-\frac{1}{2}} y$, and defining $\tilde{\lambda} = \lambda^{-\frac{2}{4b}}$ and $\tilde{E} = \lambda^{-\frac{2}{4b}} E$, the Schrödinger equation becomes

$$\left( -\frac{d^2}{dy^2} + \tilde{\lambda} y^a + y^b \right) \psi = \tilde{E} \psi . \quad (27)$$

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

$$\tilde{E} = \tilde{E}_0 + \tilde{E}_1 \tilde{\lambda} + \tilde{E}_2 \tilde{\lambda}^2 + \cdots , \quad (28)$$
$$\psi = \tilde{\psi}_0 + \tilde{\psi}_1 \tilde{\lambda} + \tilde{\psi}_2 \tilde{\lambda}^2 + \cdots , \quad (29)$$

Introducing this in equation $(27)$ leads also to a system of differential equations

$$\tilde{L} \tilde{\psi}_0 = \tilde{E}_0 \tilde{\psi}_0 , \quad (30)$$
$$\tilde{L} \tilde{\psi}_1 + y^a \tilde{\psi}_0 = \tilde{E}_0 \tilde{\psi}_1 + \tilde{E}_1 \tilde{\lambda} \tilde{\psi}_0 , \quad (31)$$
$$\tilde{L} \tilde{\psi}_2 + y^a \tilde{\psi}_1 = \tilde{E}_0 \tilde{\psi}_2 + \tilde{E}_1 \tilde{\psi}_1 + \tilde{E}_2 \tilde{\psi}_0 , \quad (32)$$
$$\vdots \quad \vdots \quad \vdots$$
$$\tilde{L} \tilde{\psi}_n + y^a \tilde{\psi}_{n-1} = \sum_{k=0}^{n} \tilde{E}_{n-k} \tilde{\psi}_k , \quad (33)$$

where

$$\tilde{L} = -\frac{d^2}{dy^2} + y^b \quad (34)$$

Rewriting the asymptotic expansion in terms of $\lambda$ 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 $b = 4$), equation $(28)$ leads to

$$E = \lambda^{1/3} \left( \tilde{E}_0 + \frac{\tilde{E}_1}{\lambda^{2/3}} + \frac{\tilde{E}_2}{\lambda^{4/3}} + \frac{\tilde{E}_3}{\lambda^2} + \cdots \right)$$
$$= \lambda^{1/3} \sum_{k=0}^{\infty} \frac{\tilde{E}_{3k}}{\lambda^{2k}} + \lambda^{-1/3} \sum_{k=0}^{\infty} \frac{\tilde{E}_{3k+1}}{\lambda^{2k}} + \frac{1}{\lambda} \sum_{k=0}^{\infty} \frac{\tilde{E}_{3k+2}}{\lambda^{2k}}$$
$$= \lambda^{1/3} \sum_{k=0}^{\infty} \frac{\tilde{E}_{3k}}{\lambda^{2k}} + \lambda^{-1/3} \sum_{k=0}^{\infty} \frac{\tilde{E}_{3k+1}}{\lambda^{2k}}$$

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

$$E = \lambda^{1/4} \left( \tilde{E}_0 + \frac{\tilde{E}_1}{\lambda^{1/2}} + \frac{\tilde{E}_2}{\lambda^{3/2}} + \frac{\tilde{E}_3}{\lambda^2} + \cdots \right)$$
$$= \lambda^{1/4} \sum_{k=0}^{\infty} \frac{\tilde{E}_{2k}}{\lambda^{k}} + \lambda^{-1/4} \sum_{k=0}^{\infty} \frac{\tilde{E}_{2k+1}}{\lambda^{k}} .$$
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 $\lambda$, multiplied by a rational power of $\lambda$. 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 two sections.

IV. APPROXIMANTS FOR THE QUARTIC ANHARMONIC OSCILLATOR

For the quartic anharmonic oscillator $[15, 16, 17, 18, 19]$, the approximants for the energy eigenvalues can be written in the following form

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

(37)

where

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

(38)

and

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

(39)

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 positive values of $\lambda$. 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 $\mu$ has been included, which can be adjusted in order to improve the precision of the approximant.

With this choice 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 equation (37), 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 $p_k$’s and $q_k$’s, making the determination of the approximant unnecessarily complicated.

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 section II, the values of the coefficients for the power series are exact. The values of the coefficients for the asymptotic expansion were obtained by solving equations (30)-(33) 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 $\psi_k$ and $\psi^c_k$), 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 $\lambda$ (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 $\alpha_i$ ($i = 1, 2, \ldots$), 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 $\sum n_i + n_0 + n_a = 4N + 3$. Using the power series at $\lambda = 0$ one can write

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

(40)

Taylor-expanding each side of this equation in $\lambda$, and demanding it to be satisfied at every order up to $\lambda^{n_0}$, 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
TABLE I: Exact coefficients of the power series for the first three energy levels of the quartic anharmonic oscillator.

| Coefficients | $n = 0$ | $n = 1$ | $n = 2$ |
|--------------|--------|--------|--------|
| $E_0$        | 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.

| Coefficients | $n = 0$ | $n = 1$ | $n = 2$ |
|--------------|--------|--------|--------|
| $\tilde{E}_0$ | 1.060361944892 | 3.7996728480480 | 7.455697915983 |
| $\tilde{E}_1$ | 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 |

$\lambda = \lambda_{\alpha i} + \alpha_i$, one can write

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

(41)

If one demands this equation to be satisfied at every order in $\lambda_{\alpha i}$ 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

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

(42)
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

$$\left(1 + \sum_{k=1}^{N} q_k \lambda^{N-k} \right) \sum_{k=0}^{\infty} \tilde{E}_{3k} \lambda^{2k} = (\lambda' + \mu)^{1/3} \sum_{k=0}^{N} a_k \lambda^{N-k} , \quad (43)$$

$$\left(1 + \sum_{k=1}^{N} q_k \lambda^{N-k} \right) \sum_{k=0}^{\infty} \tilde{E}_{3k+1} \lambda^{2k} = (\lambda' + \mu)^{-1/3} \sum_{k=0}^{N} b_k \lambda^{N-k} , \quad (44)$$

$$\left(1 + \sum_{k=1}^{N} q_k \lambda^{N-k} \right) \sum_{k=0}^{\infty} \tilde{E}_{3k+2} \lambda^{2k} = \frac{1}{\lambda' + \mu} \sum_{k=0}^{N} c_k \lambda^{N-k} . \quad (45)$$

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 $\lambda$), 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

$$\frac{|E_{\text{app}} - E_{\text{shooting}}|}{E_{\text{shooting}}} . \quad (46)$$

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

$$\left. \frac{|E_{\text{app}} - E_{\text{shooting}}|}{E_{\text{shooting}}} \right|_{\lambda = 0.17} = 1.05 \times 10^{-6} . \quad (47)$$

The relative error decreases rapidly for smaller values of $\lambda$, and of course, it also decreases when $\lambda$ increases until it finds the next node at $\lambda = 0.5$. After that, the relative error never
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.

| Coefficients $E_0(\lambda)$ | $n = 0$ | $n = 1$ | $n = 2$ |
|------------------------------|---------|---------|---------|
| $\lambda = 1/2$             | 1.241854043136 | 4.051932338617 | 7.396900686938 |
| $\lambda = 1$               | 1.392351580103 | 4.64881282723 | 8.65504982254 |
| $\lambda = 2$               | 1.607541348124 | 5.475784646286 | 10.35858364736 |
| $\lambda = 5$               | 2.018340657447 | 7.013479298703 | 13.467730394819 |
| $\lambda = 20$              | 3.009944947791 | 10.643215959124 | 20.694110927154 |

becomes higher than $2 \times 10^{-7}$. For the first and second excited level, the maximum error around $\lambda \approx 0.2$, was about $8 \times 10^{-7}$ and $2.4 \times 10^{-6}$, respectively, and after the node at $\lambda = 0.5$ this error is never higher than $4 \times 10^{-8}$. In fact, the relative error decreases quite rapidly in the case of the first and second excited levels for large values of $\lambda$, 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 $\mu$ 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 $\mu$ 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 other restriction in $\mu$. Among all of the values of $\mu$ 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
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.

| Coefficients | $n = 0$ | $n = 1$ | $n = 2$ |
|--------------|---------|---------|---------|
| $a_0$        | -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 | 4.8022464913 | 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 |

V. APPROXIMANTS FOR THE SEXTIC ANHARMONIC OSCILLATOR

For the sextic anharmonic oscillator \[20, 21\], the asymptotic expansion consists of only two pieces, so the approximant can be written as

$$E_{\text{app}}(\lambda) = (1 + \mu \lambda)^{1/4} \frac{P_a(\lambda)}{Q(\lambda)} + (1 + \mu \lambda)^{-1/4} \frac{P_b(\lambda)}{Q(\lambda)},$$  \hspace{1cm} (48)

where $P_a(\lambda)$, $P_b(\lambda)$ and $Q(\lambda)$ are given in equations \[38\] and \[39\]. The corresponding coefficients $a_k$, $b_k$ and $q_k$ are found in a similar way as we did for the quartic anharmonic oscillator. For approximants of degree $N$, we will have $3N + 2$ coefficients, so taking $n_0$ coincide with the values of $E(\lambda)$ and its derivatives at more points. This last possibility is studied in the next example.
TABLE V: Exact coefficients of the power series for the first three energy levels of \( V(x) = x^2 + \lambda x^6 \).

| Coefficients | \( n = 0 \) | \( n = 1 \) | \( n = 2 \) |
|--------------|-------------|-------------|-------------|
| \( E_0 \)    | 1           | 3           | 5           |
| \( E_1 \)    | 15/8        | 105/8       | 375/8       |
| \( E_2 \)    | -3495/128   | -47145/128  | -295095/128 |
| \( E_3 \)    | 1239675/1024 | 27817125/1024 | 276931275/1024 |
| \( E_4 \)    | -334232355/32768 | -110913108405/32768 | -1626954534555/32768 |

The first few coefficients of the power series at \( \lambda = 0 \) and the asymptotic expansion, obtained using the systems of differential equations described in sections II and III are shown in tables V and VI, respectively. As expected, the coefficients of the power series are exact, and the coefficients of the asymptotic expansion are obtained numerically.

The degree of the polynomials in the approximant was first chosen to be \( N = 5 \). The coefficients of the approximants were calculated choosing different intermediate points (nodes)
TABLE VI: Coefficients of the asymptotic expansion obtained solving the differential equations using the shooting method for $V(x) = x^2 + \lambda x^6$.

for the first three energy levels, together with the first four terms of the power series and the first five terms of the asymptotic expansion. For the ground state, the intermediate points were $\lambda = 0.1$, $\lambda = 0.2$, $\lambda = 0.5$, $\lambda = 1$, $\lambda = 2$, $\lambda = 5$ and $\lambda = 10$, and only the energy eigenvalues at those point were used, i.e., we didn’t pick any of the derivatives at these points. Furthermore, we chose $\mu = 1/2$. For the first and second excited level, we used $E_{0}^{1}$, $E_{0}^{2}$, $E_{0}^{5}$, $E_{0}^{10}$, $E_{0}^{20}$, $E_{0}^{0.1}$, $E_{1}^{0.1}$ and $E_{0}^{0.01}$, with $\mu = 0.95$. Notice that in these cases, the derivative at $\lambda = 0.1$, i.e., $E_{1}^{0.1}$, has also been used. With these choices, the values of the coefficients in the approximants are given in table VII. With these approximants, the highest relative errors were obtained around small values of $\lambda$. Specifically, at $\lambda = 0.014$ the relative error for the ground state eigenvalue is $2.55 \times 10^{-5}$. For even smaller values of $\lambda$, this error decreases rapidly. For $1 < \lambda < 5$ that maximum error is $1.3 \times 10^{-7}$, and for $\lambda > 5$ the maximum error was $7 \times 10^{-8}$, decreasing rapidly for large values of $\lambda$.

As it can be seen, in both the quartic and sextic anharmonic oscillators, the region of $\lambda$ where it is more difficult to achieve high accuracy is for $\lambda < 0.5$. We tried also approximants of degree 6 for the sextic anharmonic oscillator, and it was possible to reduce the relative error in this region by a factor of 1/2. The coefficients of the approximants can be found in table VIII. For $n = 0, 2$, we used $\mu = 1/2$, while for $n = 1$, we used $\mu = 1$. For $n = 0$ the approximant was built using the first four terms of the power series around $\lambda = 0$ and the first five terms of the asymptotic series, together with $E_{0}^{1}$, $E_{0}^{2}$, $E_{0}^{5}$, $E_{0}^{10}$, $E_{0}^{20}$, $E_{1}^{1/2}$, $E_{0}^{0.2}$, $E_{0}^{0.1}$, $E_{1}^{0.1}$ and $E_{0}^{0.01}$. For $n = 1, 2$, the same terms were taken, except that the fourth term of the power series around $\lambda = 0$ was replaced by $E_{2}^{1/2}$ (i.e. the second derivative at $\lambda = 1/2$). The improvement in the accuracy of the approximants for $\lambda < 0.5$ is related to
TABLE VII: Coefficients for the approximants of the first three energy eigenvalues of $V(x) = x^2 + \lambda x^6$, using polynomials of degree 5.

| Coefficients | $n = 0$ | $n = 1$ | $n = 2$ |
|--------------|---------|---------|---------|
| $a_0$        | -228343.425175410234 | -1455854.05235538211 | -1636184.16769173318 |
| $a_1$        | -51504.186680287753 | -523067.617460085793 | -319382.170585718291 |
| $a_2$        | -3246.30836836582236 | -82992.9062424631909 | -76246.268053710652 |
| $a_3$        | 17641.2930769775453 | 564652.836765077747 | 842519.3872436837 |
| $a_4$        | 40455.7925641666977 | 121783.949326608282 | 156879.990271492461 |
| $a_5$        | 25845.5374941939783 | 3765927.01323457233 | 1037731.04646700931 |
| $b_0$        | 108718.883825186570 | 1215348.7606881283 | 1098149.56754718475 |
| $b_1$        | 12471.9577982789445 | 211783.949326608282 | 461008.702437356268 |
| $b_2$        | 8971.90069757654071 | 247389.200455627253 | 461008.702437356268 |
| $b_3$        | 12714.5141045106691 | 765825.922719107915 | 1349548.74023090975 |
| $b_4$        | 4915.62090727820199 | 607633.680665566723 | 1008252.48843727777 |
| $q_1$        | 126.840851046236208 | 245.543619745344247 | 306.370961578640294 |
| $q_2$        | 3258.74684448027568 | 13846.7357289482276 | 20215.7966313260916 |
| $q_3$        | 21339.120242371419 | 208223.456783358953 | 314306.763606766761 |
| $q_4$        | 39515.8524539180998 | 853339.703125454811 | 1215186.64688146943 |
| $q_5$        | 18984.428445198520 | 856945.745673868394 | 1129173.69341497105 |

having used more terms in the expansions around points in this region, including first and second derivatives.

The fact that the approximants become less accurate for small values of $\lambda$ may be related to the analytic properties of the exact function $E(\lambda)$ [15], although this is far from clear. As it is well known, the perturbative expansion (i.e., the power series around $\lambda = 0$) is divergent for any $\lambda \neq 0$. However, in previous works where quasi-rational approximants have been used, it has been found that the main factor determining the accuracy of an approximant is the accuracy of the coefficients in the expansions used to build it. For example, in references [22] and [23] series with radius of convergence equal to zero were used, yet the approximants were very accurate because the coefficients of these series were determined with very high
precision.

| Coefficients | $n = 0$ | $n = 1$ | $n = 2$ |
|--------------|--------|--------|--------|
| $a_0$        | 10662630.6230456957 | -4140725.8249895087 | -190986117.577446118 |
| $a_1$        | -792418.407061574860 | -3392187.29848733455 | -9634761.79985940628 |
| $a_2$        | -770199.048057820101 | -691764.158783859149 | -1118886.9611306088 |
| $a_3$        | -30901.7803416591912 | 352514.275425898392 | 582001.151582893834 |
| $a_4$        | 663802.804751486527  | 1809854.68977494829 | 4102541.85172044638 |
| $a_5$        | 1304251.65718790436  | 3042011.16842997607 | 6466260.98769018109 |
| $a_6$        | 768824.185718239332  | 443056.032781395005 | 2682339.1191005685 |
| $b_0$        | -10662629.6230456957 | 4140728.8249895087 | 190986122.577446118 |
| $b_1$        | -18730301.9075998957 | 5463158.61490945598 | 144095348.88473491 |
| $b_2$        | 1312291.68171628629  | 1901041.02272365822 | 29373600.914712753 |
| $b_3$        | 289403.682268640790  | 314656.648970897322 | 1721958.42036808095 |
| $b_4$        | 312257.358605665963  | 547382.135140547781 | 658971.157529230082 |
| $b_5$        | 397391.953291475945  | 540767.205553174330 | 644912.329241756943 |
| $b_6$        | 146224.401105478984  | 73344.3715121889572 | 189069.456358376232 |
| $q_1$        | 207.057939859483339  | 198.176309122347673 | 230.798303579776449 |
| $q_2$        | 10393.8027931755210  | 9463.18894774927319 | 11496.2792134605234 |
| $q_3$        | 157632.217425587120  | 133763.388618245199 | 150748.225437877810 |
| $q_4$        | 775120.602962958890  | 586955.795810181245 | 587462.21822778458 |
| $q_5$        | 1249527.64792219401  | 727254.753026886137 | 723876.01523016534 |
| $q_6$        | 564727.576025957156  | 102119.617954584846 | 248600.057576103110 |

TABLE VIII: Coefficients for the approximants of the first three energy eigenvalues of $V(x) = x^2 + \lambda x^6$, using polynomials of degree 6.

VI. CONCLUSIONS

In this paper, it has been shown that accurate approximants for the energy eigenvalues of potentials of the form $V(x) = Ax^a + Bx^b$ 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 $\lambda$. 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 $\lambda$, together with the asymptotic expansion. These expansions are 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 examples, approximants for the lowest energy levels of the quartic and sextic anharmonic oscillators were obtained. The approximants were fairly simple, since the degree of the polynomials used was not too high. In particular, for the quartic anharmonic oscillator, it was shown that it is possible to obtain approximants with polynomials of degree 3 for which the relative error is not higher than $\sim 3 \times 10^{-6}$. In the case of the sextic anharmonic, polynomials of degree 5 and 6 were tried, and it was shown that in the second case it was possible to improve the accuracy for $\lambda < 0.5$ while maintaining the accuracy for larger values of $\lambda$.

In this technique, one has a lot of freedom choosing the intermediate points, as well as how many terms from each one of the series to take. This gives a lot of possibilities to try to reduce relative errors, and it would be interesting to study if it is possible to do this systematically. It would also be interesting to try to find methods that allow to improve the accuracy of the coefficients in the expansions. For example, if better numerical solutions for the expansion functions can be found, this should lead to better coefficients and therefore to better approximants. As it was mentioned before, 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. For simplicity, here we have limited ourselves to the use of the shooting method to solve the systems of differential equations. On the other hand, the first equation in each one of the systems, i.e., equations (5), (19) and (30) are just regular Schrödinger equations, and many methods have been developed that allow to obtain the corresponding eigenvalues with very high precision [5, 17, 18, 19, 24, 25, 26, 27, 28, 29, 30]. In fact, we could have used any of these methods to obtain the coefficients $E_0^{\alpha}$ and $\tilde{E}_0$, but it is not clear how to extend these methods to solve the remaining equations in the systems. In the future, we plan to study these issues in more detail, and apply this technique to other potentials of interest, both in
physics as well as chemistry.

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