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

D. Diaz Almeida^{a,*}, P. Martin^b

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

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ABSTRACT

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

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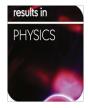
Introduction

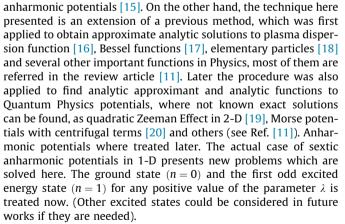
Harmonic potentials with sextic anharmonic terms has been treated for several authors [1–7]. This kind of potential play an important role in spectra of molecules such as ammonia and hydrogen bounded-solids [8,9], and they might be considered as a potential model for quark confinement in Quantum Chromodynamics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

In recent works, asymptotic Taylor expansion method has been used as an alternative approach to energy eigenvalue problems of

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

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

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

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

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

Theoretical treatment and power series

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

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

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

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

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

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

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

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

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

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

$$L\psi_k + \chi^6 \psi_{k-1} = \sum_{q=0}^k E_{k-q} \psi_q \quad \text{for } k \ge 1,$$
(5)

where, the operator L is defined as

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

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

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

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

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

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

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

Asymptotic expansion

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Changing now from $\tilde{\lambda}$ to λ , and following the procedure described in previous section (Section "Theoretical treatment and power series"), the asymptotic expansion will be written as

$$\tilde{E} = \lambda^{1/4} \sum_{k=0}^{\infty} \frac{E_{2k}}{\lambda^k} + \lambda^{-1/4} \sum_{k=0}^{\infty} \frac{E_{2k+1}}{\lambda^k}$$
(16)

There are two expansions, now for \tilde{E} , one with factor $\lambda^{1/4}$ and another, with the factor $\lambda^{-1/4}$. The structure of the expansion given by Eq. (16), has negative integer powers of λ multiplied by fractional power of λ . This means that the approximants to be built, must be divided in a fractional similar way in order to match the behavior of each piece.

Development of the approximation method through the sextic anharmonic oscillator and its application

The main problem in the MPOA technique is to design the structure of the approximations in terms of some parameters. In the Pade method only rational functions are used and they usually consider power series. Now the situation is more complicated, because the rational functions are combined with auxiliary ones, in such a way that the power and the asymptotic expansions, Eqs. (4) and (16), can be reproduced. In this way, the approximation function should be a bridge connecting in an efficient way both expansions, power and asymptotic. Thus though the auxiliary functions $\lambda^{-1/4}$ could be right from the asymptotic point of view, it would not be adequated for the power series, and it must be replaced for $(1 + \mu\lambda)^{-\frac{1}{4}}$, where μ is an arbitrary positive parameter to be determined later. This auxiliary function introduces and inconvenient point for $\mu_1 = -1/\lambda$. However, this point is sited in the negative axis of λ , and since here positive λ is considered, then, there is not problem with this unsuitable point. In (Tables 1 and 2), the coefficients for both the power series and the asymptotic expansions is presented for the ground state as well as for the first excited state of the sextic anharmonic oscillator.

The analysis presented above shows that the simplest form for the approximant is given by

$$E_{app}(\lambda) = (1+\mu\lambda)^{1/4} \frac{P_a(\lambda)}{Q(\lambda)} + (1+\mu\lambda)^{-1/4} \frac{P_b(\lambda)}{Q(\lambda)},$$
(17)

where the polynomials $P_a(\lambda), P_b(\lambda)$ are

$$P_a(\lambda) = \sum_{k=0}^{N} a_k \lambda^k, \tag{18a}$$

$$P_b(\lambda) = \sum_{k=0}^{N} b_k \lambda^k, \tag{18b}$$

and

$$Q(\lambda) = 1 + \sum_{k=1}^{N} q_k \lambda^k, \quad (q_0 = 1)$$
 (19)

In summary the approximant was constructed using rational function multiplied by auxiliary ones, chosen in such a way matching

 Table 1

 Power series coefficients for the ground state and the first odd excited state of the sextic anharmonic oscillator.

Coeffis.	n = 0	n = 1
E ₀	1	3
E_1	15/8	105/8
E_2	-3495/128	-47145/128
E ₃	1239675/1024	27817125/1024
E_4	-3342323355/32768	-110913018405/32768

Table 2

Coefficients of the asymptotic expansion of the eigenvalues for the sextic anharmonic oscillator obtained solving the differential equation, Eq. (13), using the shooting method.

Coeffis.	n = 0	n = 1
\tilde{E}_0	1.144802449	4.3385987182
\tilde{E}_1	0.316606042	1.2866508137
\tilde{E}_2	-0.007874753	-0.4797062708
\tilde{E}_3	0.001694326	0.0714618752
\tilde{E}_4	-0.000058640	-0.0002161802
\tilde{E}_5	0.00009989	0.0000251953

the asymptotic behavior of the eigenvalues. In this way changing, λ by $(1 + \mu\lambda)$ inside the roots, the correct behavior for $\lambda \to \infty$ and for $\lambda = 0$ are obtained. In general, the form of a quasi-rational approximant is mainly determined by the asymptotic expansion. This choice for the auxiliary functions requires that the degree of the polynomials at the numerator must be the same as the ones in the denominator. Then, for simplicity, a common denominator $Q(\lambda)$ for the two parts of the approximant has been chosen, since any other choice would lead to a system of non-linear equations for the a_k 's, b_k 's and q_k 's, and the determination of the approximant would be unnecessarily complicated.

The coefficients of the polynomials in the approximant have to be found using power series, asymptotic expansion and the expansion around some positive intermediate points λ_{β} ($0 < \lambda_{\beta} < \infty$). There is some freedom in chosen the terms of each expansion, as long as the total number of equations from both expansions is equaled to the total number of coefficients in the approximant. In general, the approximant will have higher precision with higher degree.

For the ground state, the eigenfunctions are even in x, so must be the functions $\tilde{\psi}_k$ (and the same applies for ψ_k and $\psi_k^{(\beta)}$). The initial condition to be used are $\tilde{\psi}_k(0) = 1$ and $\tilde{\psi}'_k(0) = 0$. Conversely, for the first excited level the eigenfunction is odd in x, so the conditions were $\tilde{\psi}_k(0) = 0$ and $\tilde{\psi}'_k(0) = 1$.

Now it is necessary to obtain a right number of equations for the parameters of the approximant. To do this, n_0 terms will be taken from the power series (around $\lambda = 0$) and n_a terms from the asymptotic expansion, thus

$$\left(\sum_{k=0}^{N} q_k \lambda^k \right) \left(\sum_{k=0}^{n_0} E_k \lambda^k \right) = (1 + \mu \lambda)^{1/4} \left(\sum_{k=0}^{N} a_k \lambda^k \right)$$
$$+ (1 + \mu \lambda)^{-1/4} \left(\sum_{k=0}^{N} b_k \lambda^k \right)$$
(20)

Furthermore, the expansions around intermediate points will also be used with the change $\lambda = \lambda_{\beta_i}$, that is,

Table 3

Coefficients of the series at different intermediate points from the first two energy levels for the sextic anharmonic potential $V(x) = x^2 + \lambda x^6$. Values obtained solving the Schrödinger equation, Eq. (2), by shooting method.

Coeffis.	n = 0	n = 1
$E(\lambda = 0.5)$	1.300986965	4.4636830989
$E(\lambda = 1)$	1.435624613	5.0333959502
$E(\lambda = 2)$	1.609931940	5.7493477662
$E(\lambda = 5)$	1.912453821	6.9608571533
$E(\lambda = 20)$	2.564644694	9.5120884929
$E(\lambda = 50)$	3.159021221	11.8057799890
$E(\lambda = 100)$	3.716974733	13.9462066273

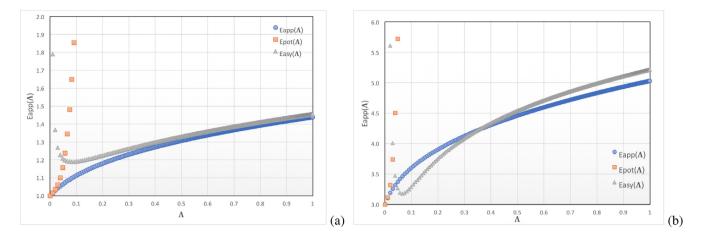


Fig. 1. Eigenvalues for the sextic anharmonic oscillator as a function of $\Lambda = \lambda/(1 + \lambda)$: single point shows the power series, triangle points are for the asymptotic expansion and plane line for the approximant: (a) ground state, and (b) the first excited state.

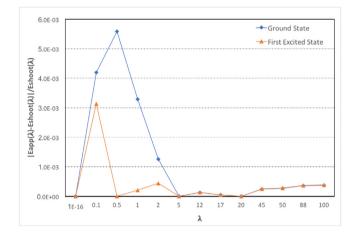


Fig. 2. Comparison of the relative errors for the eigenvalues given by the approximant and the exact eigenvalues determined by the shooting method for the ground state and the first excited state of the sextic anharmonic oscillator.

Table 4

Approximant coefficients for the ground state and the first odd excited state of the sextic anharmonic potential $V(x) = x^2 + \lambda x^6$, using polynomials of degree three for $\mu = 2$.

Coeffis.	n = 0	n = 1		
<i>a</i> ₀	8.3786952759	657.31747745		
<i>a</i> ₁	17.253086792	-827.31301406		
a2	330.33033420	4157.4219687		
a3	6.1575633825	2093.7260144		
b_0	-7.3786952759	-654.31747745		
b_1	39.775013122	513.84782811		
b_2	123.55100908	2064.8581374		
b ₃	2.4083108233	524.96798410		
q_1	63.031795191	109.74243049		
q_2	343.98675636	1274.7360399		
q_3	6.3964033200	573.88895241		

$$\begin{split} \left(1 + \sum_{k=1}^{N} q_k \lambda_{\beta_i}^k \right) E(\lambda_{\beta_i}) &= (1 + \mu \lambda_{\beta_i})^{1/4} \left(\sum_{k=0}^{N} a_k \lambda_{\beta_i}^k \right) \\ &+ (1 + \mu \lambda_{\beta_i})^{-1/4} \left(\sum_{k=0}^{N} b_k \lambda_{\beta_i}^k \right), \end{split}$$
(21)

where $E(\lambda_{\beta_i})$ are obtained by numerical computation from the differential equation using, for instance, the shooting method.

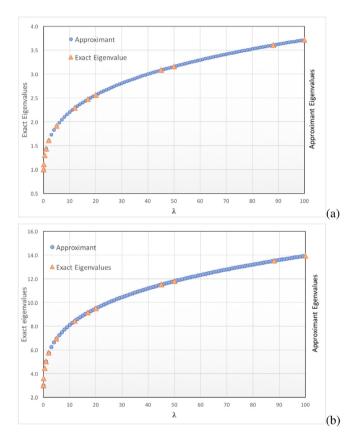


Fig. 3. Comparison of the exact eigenvalues calculated using the shooting method with those determined by the approximant for the ground state of sextic anharmonic oscillator in terms of λ with $\mu = 2$.

Finally, for the asymptotic expansion, the change $\lambda' = 1/\lambda$ is required as well as to match the expansion with the approximant for each of the two pieces in which it is divided. Therefore, it is obtained

$$\left(\sum_{k=0}^{N} q_{N-k} \lambda^{\prime k}\right) \left(\sum_{k=0}^{\infty} \tilde{E}_{2k} \lambda^{\prime k}\right) = \left(1 + \frac{\lambda^{\prime}}{\mu}\right)^{1/4} \sum_{k=0}^{N} a_{N-k} \lambda^{\prime k}$$
(22)

$$\left(\sum_{k=0}^{N} q_{N-k} \dot{\lambda}^{\prime k}\right) \left(\sum_{k=0}^{\infty} \tilde{E}_{2k+1} \dot{\lambda}^{\prime k}\right) = \left(1 + \frac{\lambda^{\prime}}{\mu}\right)^{-1/4} \sum_{k=0}^{N} b_{N-k} \dot{\lambda}^{\prime k}$$
(23)

The number of terms taken from the asymptotic expansion will be n_a , that is, the terms \tilde{E}_k with $k > n_a$ are not needed to be calculated. A set of n_a linear equations for the coefficients of the approximant will be obtained. Thus, the procedure has to be done in such a way that the number of equation should be equal to the number of unknown coefficients.

Results and discussion

In Table 4, the values of the coefficients of the approximant are shown for both the ground state and the first excited level of the sextic anharmonic potential, using polynomials of degree three and choosing $\mu = 2$. Each of the eleven coefficients for the ground state approximant were obtained using the first four terms from the power series (around $\lambda = 0$), the first five terms of the asymptotic expansion, and the values of *E* for $\lambda = 5$ and $\lambda = 20$. For the first excited state the eleven coefficients were obtained using four equation from the power series as well as four of the asymptotic expansion and the last three equations correspond to the *E* values for $\lambda = 0.5$, $\lambda = 5$, and $\lambda = 20$. (The coefficient values are shown in the Table 3). Thus the eleven parameters in the rational function were determined as a function of μ through eleven linear algebraic equations.

high precision with some values of the asymptotic expansion. The variable is $\Lambda = \lambda/(1 + \lambda)$ in order to compress all the values of λ in the interval (0, 1).

Despite of a few minor differences between the curves, the approximant for both ground and first excited states in fact achieved the recovery of the eigenvalues for any values of $\lambda > 0$, effectively, acting as a bridge connecting the expansions around different values of λ . For large values of this parameter the approximant for the sextic anharmonic oscillator had a difference about 1% for the ground state and 3.5% for the first odd excited state both respect to the asymptotic expansion.

In Fig. 2, a comparison of the relative errors of the approximant for both ground state and first excited state are shown as a function of the parameter λ . It is easy to observe that the large relative error is for small values of λ , which is also a consequence of the different behavior of the coefficients in both expansions, where the highest is $5.6 * 10^{-3}$ for $\lambda = 0.5$, for the ground state, and $3.1 * 10^{-3}$ with $\lambda = 0.1$, for the first excited level. It is clear that the relative errors were very small for large values of λ , with at least one order of magnitude below the highest relative errors. Furthermore, from $\lambda = 5$ to $\lambda = 100$ the presicion of the approximants is nearly the same. Eqs. (25) and (26), represent the final form of the approximant for the two first energy levels, the ground state and the first odd excited state, respectively, with $\mu = 2$.

$$E_{app}(\lambda) = (1+2\lambda)^{-\frac{1}{4}} \frac{(-7.37869527+39.77501312\lambda+123.55100908\lambda^{2}+2.40831082\lambda^{3})}{(1+63.03179519\lambda+343.98675636\lambda^{2}+6.39640332\lambda^{3})} + (1+2\lambda)^{\frac{1}{4}} \frac{(8.37869527+17.25308679\lambda+330.33033420\lambda^{2}+6.15756338\lambda^{3})}{(1+63.03179519\lambda+343.98675636\lambda^{2}+6.39640332\lambda^{3})}$$
(25)

$$E_{app}(\lambda) = (1+2\lambda)^{-\frac{1}{4}} \frac{(-654.31747745+513.84782811\lambda+2064.85813740\lambda^{2}+524.96798410\lambda^{3})}{(1+109.74243049\lambda+1274.73603995\lambda^{2}+573.88895241\lambda^{3})} + (1+2\lambda)^{\frac{1}{4}} \frac{(657.31747745-827.31301406\lambda+4157.42196879\lambda^{2}+2093.72601442\lambda^{3})}{(1+109.74243049\lambda+1274.73603995\lambda^{2}+573.88895241\lambda^{3})}$$
(26)

The expansion around intermediate points are very important, since they allowed to build approximants with higher precision for polynomials of any degree by imposing them to coincide with the exact eigenvalues at these points. Therefore, not only the relative error of the approximant at these points are zero but it helps also to decrease the error in intermediate points. The relative error is defined as

$$\frac{|E_{app} - E_{shooting}|}{E_{shooting}}$$
(24)

In Fig. 1, a comparison between the power series, asymptotic expansion and the approximant for both ground state (Fig. 1a) and first odd excited state (Fig. 1b) are presented. Clearly, it is shown that the approximant will coincide with the power series for small values of λ , and with the asymptotic expansion for large ones. However, the coincidence with the asymptotic expansion is better than the power series for the ground state due to the fast increment of the power series coefficients and the decrement of the asymptotic expansion ones. On the other hand, Fig. 1b exhibits the behavior of the approximant for the first excited state compared to both power and asymptotic expansions for the eigenvalues of the sextic anharmonic potential which match accurately with the power series for small values of the parameter λ and with

In the above equations the coefficients a's, b's, and q's, with only eight decimal digits instead of ten digits as in Table 4 are written since that is enough to obtain the same relative errors.

In Fig. 3, it is shown the eigenvalues calculated with the approximant, compared with the values obtained numerically by the shooting method as shown in Table 3. At this scale, there is not difference between the exact and the approximated eigenvalues.

Conclusion

In this work an improvement and extension has been performed of the MPQA method described in previous papers [11– 14,16–20]. The new technique has been applied to obtain approximations for the ground state of the 1-D Schrödinger equation with sextic anharmonic potential, $V(x) = x^2 + \lambda x^6$, where λ is an arbitrary parameter. Building the approximant as a degree three polynomial, the accuracy of the approximant is high with a relative error less than 5 * 10⁻³. The higher the polynomial degree, the better the precision of the approximant.

In order to apply this technique, an expansion in terms of the parameter λ of the eigenvalues has been determined through an auxiliary system of differential equations, which can be considered as a Taylor series of the eigenvalues in terms of λ . The correspond-

ing asymptotic expansion has been found using a similar auxiliary system of equations, but now in terms of a right new parameter $\tilde{\lambda} = \lambda^{-\frac{1}{2}}$. So that, the idea of the approximant is to build a function using rational functions together with auxiliary ones, as a bridge between Taylor and asymptotic expansions.

For the potential here considered the coefficients of the Taylor series increase very quickly, and in contrast those of the asymptotic expansion decrease faster. This is the reason, that the highest relative errors are found for small values λ , and for large λ these are smaller at least in one order of magnitude. In addition to the above described expansions as it is usually done in MPQA method, and additional condition have to be imposed to the approximant, which must have exact values for two intermediate points, $\lambda = 5$ and $\lambda = 20$, for example.

The approximant here found is good for any positive value of λ , which is an important advantage compared with polynomials approximations, which are usually good in an interval of the variable λ . Furthermore, the relative errors are so small, that the approximant here found for the eigenvalues, can be used in most of the applications of this potential.

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