# Summation of Rayleigh–Schrödinger perturbation series by algebraic Padé approximants: anharmonic oscillators

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**Abstract.** Padé approximants, quadratic approximants, and their higher degree algebraic generalizations are used to sum the divergent eigenvalue perturbation series for quantum anharmonic oscillators. Approximants of different degree are compared regarding their accuracy and the rate of convergence. Summation of hundreds of terms of the perturbation series gives an evidence that quadratic approximants converge much faster than ordinary Padé approximants, and cubic approximants converge still faster. The fourth, fifth and higher degree approximants (up to the 20th degree) converge faster and faster, especially on the second sheet of Riemann surface of the energy function.

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## 1. Introduction

The quartic anharmonic oscillator

$$H = \frac{p^2}{2} + \frac{x^2}{2} + \lambda x^4 \tag{1}$$

is a well-known example of divergent perturbation theory (Bender and Wu 1969). Perturbation series for the ground-state energy

$$E(\lambda) = \frac{1}{2} + \frac{3}{4}\lambda - \frac{21}{8}\lambda^2 + \frac{333}{16}\lambda^3 - \frac{30885}{128}\lambda^4 + ... \tag{2}$$

that can be calculated to high orders (Bender and Wu 1973, Vrscay and Cizek 1986, Turbiner and Ushveridze 1988) is commonly used for testing of various summation procedures that transform the divergent partial sums into convergent approximants (Reid 1967, Graffi *et al* 1970, Seznec and Zinn-Justin 1978, Caswell 1978, Dmitrieva and Plindov 1980, Drummond 1981, Weniger 1993). Here, the series (2) as well as the energy series for cubic, sextic, and octic anharmonic oscillators are used as a ground for numerical testing of the efficiency of Padé approximants and their algebraic generalizations such as quadratic, cubic, and higher degree approximants.

By definition, $[M, N]$ Padé approximant to the series $E(\lambda)$ is a rational function

$$E_{[M,N]}(\lambda) = \frac{p_0 + p_1\lambda + ... + p_M\lambda^M}{1 + q_1\lambda + q_2\lambda^2 + ... + q_N\lambda^N} \tag{3}$$

having the same $M+N+1$ first coefficients of Maclaurin expansion as the function $E(\lambda)$ (Basdevant 1972, Baker 1975). It is defined also as a solution of the linear equation

$$P(\lambda) - Q(\lambda)E_{[M,N]}(\lambda) = 0, \tag{4}$$

where $P$ and $Q$ are polynomials of degrees $M$ and $N$ respectively which satisfy

$$P(\lambda) - Q(\lambda)E(\lambda) = O(\lambda^{M+N+1}). \tag{5}$$

Padé approximants and related continued fractions have long history (Brezinski 1991). There is a theory of Stieltjes functions dealing with convergence of Padé approximants (Bender and Orszag 1978). It was proved that the function $\lambda^{-1}(E(\lambda) - \frac{1}{2})$ for the quartic oscillator belongs to the class of Stieltjes functions. As a result, the series (2) is Padé summable for all complex $\lambda$ when $|\arg\lambda| < \pi$ (Simon 1970, Loeffel *et al* 1969).

For $\lambda < 0$ the energy (2) turnes into the double-valued complex energy of resonances $E = E_0 \pm \mathrm{i}\Gamma/2$, where $E_0$ is a position of the energy level, and $\Gamma$ is its width. The plus and minus signs correspond to the incoming and outgoing wave boundary conditions respectively. The function $E(\lambda)$ has a cut along the negative real axis (Bender and Wu 1969). Padé approximants simulate a cut by a sequence of poles (Baker 1975) that

deteriorate the convergence near the cut. For negative $\lambda$, Padé approximants to the series (2) don't converge.

A natural generalization of the ordinary Padé approximant to the case of at least double-valued functions is a quadratic Padé approximant (Shafer 1974). The $[L, M, N]$ quadratic approximant is defined as a solution of the quadratic equation

$$A(\lambda) + B(\lambda)E_{[L,M,N]}(\lambda) + C(\lambda)E^2_{[L,M,N]}(\lambda) = 0, \tag{6}$$

where $A$, $B$ and $C$ are polynomials of degree $L$, $M$ and $N$ respectively which satisfy

$$A(\lambda) + B(\lambda)E(\lambda) + C(\lambda)E^2(\lambda) = O(\lambda^{L+M+N+2}). \tag{7}$$

We don't know any general theory of convergence of quadratic approximants. The convergence seems provable rigorously only for the simplest functions like $e^\lambda$ or $(1+\lambda)^{1/3}$ when the expression for an arbitrary quadratic approximant is known (Shafer 1974). Applicability of quadratic approximants for various functions of physical interest was justified numerically (Short 1979, Jeziorski *et al* 1980, Lin and Bergersen 1981, Common 1982, Mayer and Tong 1985, De'Bell 1992, Goodson *et al* 1992, Hamer *et al* 1992). These approximants do not need to simulate the branch cut by a sequence of poles; for the series (2) they actually converge on the cut at $\lambda < 0$ (Sergeev 1995).

In the same spirit an algebraic approximant of arbitrary degree $M$ (Brak and Guttmann 1990), or "$M$-power" approximant (Short 1979) is defined by the equation

$$\sum_{k=0}^{M} A^{(k)}(\lambda)E^k_{[p_0,p_1,...,p_M]}(\lambda) = 0, \tag{8}$$

where $A^{(k)}(\lambda)$ are polynomials in $\lambda$ of degree $p_k$ $(k = 0, 1, ..., M)$ which satisfy

$$\sum_{k=0}^{M} A^{(k)}(\lambda)E^k(\lambda) = O(\lambda^{p-1}), \tag{9}$$

where $p = \sum_{k=0}^{M}(p_k + 1)$ is a total number of polynomial coefficients. This is a special case of more general approximation scheme (Hermite 1893, Padé 1894) known as Padé–Hermite approximants (Della Dora and Di-Crescenzo 1979, Della Dora 1981). We use algebraic approximants for the energy of anharmonic oscillators which is a multi-valued function of the coupling parameter (Shanley 1986).

The paper of Short (1979) is probably the closest prototype of the present study. There, similar multi-valued approximants were designed to incorporate into approximation scheme a branch-point structure of Feinman matrix elements. For the simple example of the multi-valued function $\ln(1 - z)$, Short (1979) observed that the quadratic approximants reduce the errors by roughly two orders of magnitude compared with Padé approximants. Then, he found a similar improvement in accuracy of quadratic and especially cubic approximants for certain Feinman integrals. He noted also that the quadratic approximants approximate $f(z)$ on two Riemann sheets. "Thus, starting

from the power series containing information on only one sheet, we are able to obtain convergent results on two sheets of $f(z)$; the quadratic approximants therefore continue the function from one Riemann sheet to another" (p. 172). "Using multi-valued approximants, we can obtain a certain amount of information on the unphysical sheet together with very good results on the physical sheet" (p. 175). Here, we give still more convincing evidence of the power of algebraic approximants extending calculations to extremely high orders of perturbation theory.

## 2. Calculation of algebraic approximants at large orders

The $[p_0, p_1, ..., p_M]$ approximant is calculated usually by solving the system of $p-1$ linear homogeneous equations for $p$ coefficients of the polynomials $A^{(0)}$, $A^{(1)}$,..., $A^{(M)}$ (Della Dora and Di-Crescenzo 1979). This system follows from (9) after expanding of its left-hand side in powers of $\lambda$ and putting to zero the coefficients of $\lambda^0$, $\lambda^1$, ..., $\lambda^{p-2}$. Any solution may be multiplied by a common factor; under the condition $A^{(0)}(0) = 1$ the solution is generally unique.

For ordinary Padé approximants, the $[L, M]$ approximants with $L = M$ ("diagonal" approximants) or $L \sim M$ are known to be more accurate than the approximants with $L >> M$ or $L << M$ (Baker 1975). We believe that quadratic and higher degree approximants with near equal indexes are also the most accurate. Here, we use a special algorithm for such approximants that is much faster and needs much less memory at large orders than solving the system of linear equations (Sergeev 1986).

Our algorithm is based on successive calculation of polynomials $A_N^{(k)}(\lambda)$ ($k = 0, 1, ..., M$) and remainder functions

$$R_N(\lambda) = \lambda^{-N} \sum_{k=0}^{M} A_N^{(k)}(\lambda) E^k(\lambda). \tag{10}$$

for $N = 0, 1, 2, ....$

At initial steps of our calculation for $N = 0, 1, ..., M$, we set the polynomials $A_N^{(k)}(\lambda)$ to constants

$$A_N^{(k)}(\lambda) = C_N^k [-E(0)]^{N-k}, \tag{11}$$

where $C_N^k$ are binomial coefficients, $C_N^k = N!/[k!(N-k)!]$ if $k \leq N$ or zero otherwise. Corresponding remainder functions are

$$R_N(\lambda) = \lambda^{-N} [E(\lambda) - E(0)]^N. \tag{12}$$

Subsequent recursive steps ($N = M+1, M+2, ...$) are threefold. First, define subsidiary (auxiliary?) polynomials $A_{N,0}^{(k)}$ ($k = 0, 1, ..., M$) and a subsidiary remainder function $R_{N,0}$ as

$$A_{N,0}^{(k)}(\lambda) = \lambda A_{N-M-1}^{(k)}(\lambda), \tag{13}$$

$$R_{N,0}(\lambda) = R_{N-M-1}(\lambda). \tag{14}$$

Second, define subsequently for $p = 1, 2, ..., M$ another subsidiary polynomials and remainder functions as

$$A^{(k)}_{N,p}(\lambda) = A^{(k)}_{N,p-1}(\lambda)R_{N-M+p-1}(0) - R_{N,p-1}(0)A^{(k)}_{N-M+p-1}(\lambda), \tag{15}$$

$$R_{N,p}(\lambda) = \lambda^{-1}[R_{N,p-1}(\lambda)R_{N-M+p-1}(0) - R_{N,p-1}(0)R_{N-M+p-1}(\lambda)]. \tag{16}$$

And third, calculate

$$A^{(k)}_N(\lambda) = A^{(k)}_{N,M}(\lambda), \tag{17}$$

$$R_N(\lambda) = R_{N,M}(\lambda). \tag{18}$$

Equations (11) – (18) are very feasible for computer programming.

The $N$-th algebraic approximant $E_N(\lambda)$ ($N = M, M+1, ...$) is defined by the equation

$$\sum_{k=0}^{M} A^{(k)}_N(\lambda)E^k_N(\lambda) = 0. \tag{19}$$

For $M = 1$ our algorithm reduces to the method of continued fractions (Bender and Orszag 1978). Our functions $E_N(\lambda)$ are identical to truncated continued fractions that are members of "stepwise" Padé sequence $[0,0]$, $[1,0]$, $[1,1]$, $[2,1]$,... Equations (15) are three-term recurrence relations for numerators and denominators of continued fractions. The first 105 coefficients of the continued fraction for the series (2) were listed by Vrscay and Čížek (1986) who studied their large-order behaviour.

For $M = 2$, our algorithm is equivalent to the method of Mayer and Tong (1985). It generates a sequence of quadratic approximants $[0,0,0]$, $[1,0,0]$, $[1,1,0]$, $[1,1,1]$, $[2,1,1]$, ...

For arbitrary $M = 1, 2, 3, ...$ the functions $A_N(\lambda)$ are algebraic approximants

$$[\ \underbrace{L, L, L, ..., L,}_{K+1}\ \underbrace{L-1, L-1, ..., L-1}_{M-K}\ ] \tag{20}$$

where $L$ satisfies the equation $N = L(M+1) + K$ with $0 \le K \le M$. They are listed in the table 1.

The approximant (20) has $M$ branches representing roots of the polynomial (19). Let us consider asymptotic behavior of approximants at $\lambda \to 0$ and at $\lambda \to \infty$.

It follows from (**??**) that $E(0)$ is a root of a polynomial $P(E) = \sum_{k=0}^{M} A^{(k)}_N(0)E^k$ ($N \ge M$). We don't consider here the case of a multiple root when $E(0)$ is also a root of a polynomial $dP/dE$ (it may occur accidentally, but is rare in practice). Then, according to a theorem of Baker (Baker and Graves-Morris 1995, p. 534) the root of the equation (19) specified by $E_N(0) = E(0)$ differs from the defining series $E(\lambda)$ by an error at worst $O(\lambda^N)$. This root will be referred as a *main* branch. It is used commonly as a

**Table 1.** Sequences of algebraic approximants generated by recurrence relations (15) for different degrees $M$.

| $N$ | $M=1$ | $M=2$ | $M=3$ | $M=4$ | $M=5$ | ... |
|---|---|---|---|---|---|---|
| 1 | $[0,0]$ | | | | | |
| 2 | $[1,0]$ | $[0,0,0]$ | | | | |
| 3 | $[1,1]$ | $[1,0,0]$ | $[0,0,0,0]$ | | | |
| 4 | $[2,1]$ | $[1,1,0]$ | $[1,0,0,0]$ | $[0,0,0,0,0]$ | | |
| 5 | $[2,2]$ | $[1,1,1]$ | $[1,1,0,0]$ | $[1,0,0,0,0]$ | $[0,0,0,0,0,0]$ | |
| 6 | $[3,2]$ | $[2,1,1]$ | $[1,1,1,0]$ | $[1,1,0,0,0]$ | $[1,0,0,0,0,0]$ | |
| 7 | $[3,3]$ | $[2,2,1]$ | $[1,1,1,1]$ | $[1,1,1,0,0]$ | $[1,1,0,0,0,0]$ | |
| ... | | | | | | |
| 100 | $[50,49]$ | $[33,33,32]$ | $[25,24,24,24]$ | $[20,19,19,19,19]$ | $[16,16,16,16,16,15]$ | |
| ... | | | | | | |

"generalized" sum of the first $N$ terms of the series (up to the term of an order $\lambda^{N-1}$). It approximates the function on the main sheet of Riemann surface. Supplementary branches may be useful for approximating of the second, third etc. sheets of Riemann surface.

At the opposite limit $\lambda \to \infty$, the approximant $E_N(\lambda)$ is defined asymptotically by an equation

$$\sum_{k=0}^{K} A_{N,0}^{(k)} E_N^k(\lambda) + \lambda^{-1} \sum_{k=K+1}^{M} A_{N,0}^{(k)} E_N^k(\lambda) = 0, \tag{21}$$

where $A_{N,0}^{(k)}$ are coefficients of polynomials $A_N^{(k)}(\lambda)$ before the leading term. Let us prove that $K$ branches of the approximant $E_N(\lambda)$ tend to constants, and another $M-K$ branches behave like $\lambda^{1/(M-K)}$. Generally, solution of the equation (21) behaves at large $\lambda$ like $c\lambda^{\alpha}$ with some constants $c$ and $\alpha$. Below, we consider three opportunities: $\alpha = 0$, $\alpha > 0$, and $\alpha < 0$. If $\alpha = 0$, then at the leading order in $\lambda$ we have $\sum_{k=0}^{K} A_{N,0}^{(k)} c^k = 0$ that has $K$ solutions in respect to $c$. If $\alpha > 0$, then at the leading order in $\lambda$ we have $A_{N,0}^{(K)} c^K \lambda^{\alpha K} + \lambda^{-1} A_{N,0}^{(M)} c^M \lambda^{\alpha M} = 0$ that has $M-K$ nonzero solutions if $\alpha = (M-K)^{-1}$ and none solutions for another $\alpha$. If $\alpha < 0$, then at the leading order in $\lambda$ we have $A_{N,0}^{(0)} = 0$ that has no solutions. As a result, we find that there are $K$ solutions for $\alpha = 0$ plus $M-K$ solutions for $\alpha = (M-K)^{-1}$.

## 3. Results

### *3.1. A simple example of a multi-valued function*

Firstly, we consider the summation of the series

$$F(\lambda) = 1 - \frac{1}{2}\lambda + \frac{1}{3}\lambda^2 - \frac{1}{4}\lambda^3 + \frac{1}{5}\lambda^2 - \frac{1}{6}\lambda^3 + ... \tag{22}$$

that is an expansion of an infinitely-valued function $\lambda^{-1}\ln(1+\lambda)$.

We found that algebraic approximants can approximate both the principal sheet and neigbor complex sheets of the logarithmic function giving $F_n(\lambda) = \lambda^{-1}\left[\ln(1+\lambda) + 2\pi n\mathrm{i}\right]$ with integer $n$ as a result of summation. The convergence appears to be similar to geometric progression:

$$|F_{\{M,N\}}(\lambda) - F_n(\lambda)| \sim C_{M,n}^{-N}(\lambda) \tag{23}$$

Coefficients $C_{M,n}(\lambda)$ for several $M$, $n$, and $\lambda$ were found by numerical fitting, and a general analytic formula in agreement with numerical results was conjectured:

$$C_{M,n}(\lambda) = \left| \frac{1 - (1+\lambda)^{\frac{1}{M+1}} \exp\left(\frac{2\pi\mathrm{i}}{M+1}\left[\frac{M+1}{2}\right]\right)}{1 - (1+\lambda)^{\frac{1}{M+1}} \exp\left(\frac{2\pi\mathrm{i}}{M+1}n\right)} \right| \tag{24}$$

where $\left[\frac{M+1}{2}\right]$ stands for an integer part of a number $\frac{M+1}{2}$. Here, $|n| \leq \frac{M-1}{2}$, and there is no convergence outside this range of $n$ for positive real $\lambda$. So, approximants of the $M$-th degree can approximate $2\left[\frac{M-1}{2}\right] + 1$ branches of the logarithmic function corresponding to $n = -\left[\frac{M-1}{2}\right], -\left[\frac{M-1}{2}\right] + 1, ..., \left[\frac{M-1}{2}\right]$. A coefficient $C_{1,0}(\lambda) = \left[(1+\lambda)^{\frac{1}{2}} + 1\right]\left[(1+\lambda)^{\frac{1}{2}} - 1\right]^{-1}$ agrees with a theoretical estimate of rate of convergence of continued fractions to the series (22) (Bender and Orszag 1978).

Dependence on $M$ in (24) is almost linear, $C_{M,n}(\lambda) \sim 2\left[\ln^2(1+\lambda) + 4\pi^2 n^2\right]^{-1/2} M$. Increasing of the degree $M$ always increases $C_{M,n}(\lambda)$ and improves the convergence.

Apart from dependence of the accuracy on $N$, we study also the dependence on $M$, the degree of approximants, i. e. we consider accuracy in rows in the table 1. The dependence of the accuracy on $M$ is shown on a figure 1. Optimum degrees of approximants built from the same number of perturbation series coefficients correspond to maxima on the curves. The optimum degree increases with $N$, but the increasing is uneven because of fluctuations of the curves around shallow maxima.

Evaluation of the optimum degree is of particular interest. For a given value of $N$, $M$ varies from 1 to $N$. We give arguments that optimum $M$ cannot be neither small nor large. Increasing of $C_M$ in (**??**) with $M$ means that for sufficiently large $N > N_M$ an accuracy of the $M+1$-th degree approximants is better than $M$-th degree approximants. So for large $N$, the accuracy firstly increases with $M$ as long as $N > N_M$, that may be

attributed to adding new sheets to Riemann surface of approximants. To understand decrease of the accuracy for large $M$, let us expand polynomials $A^{(k)} = \sum_{l=0}^{p_k} a_{k,l}\lambda^l$ and rewrite the equation defining $F_{\{M,N\}}$ as

$$\sum_{k=0}^{M}\sum_{l=0}^{p_k} a_{k,l}F_{\{M,N\}}^k\lambda^l = 0, \tag{25}$$

where $p_k = L = [N/(M+1)]$ if $k \le K = N - L(M+1)$ or $L-1$ otherwise, $[N/(M+1)]$ denotes integer part of a number $N/(M+1)$. After collecting the terms with the same powers of $\lambda$, (25) reads

$$\sum_{l=0}^{L} B^{(l)}(F_{\{M,N\}})\lambda^l = 0, \tag{26}$$

where $B^{(l)}(F_{\{M,N\}}) = \sum_{m=0}^{m_l} a_{m,l}F_{\{M,N\}}^m$, $m_l = M$ for $l < L$, $m_L = K$. For higher $M$, the degree $L$ becames too small for satisfactory approximation of the inversion function, and as a result the accuracy decreases. For extreme value $M = N$, $L = 0$, and the approximant is a constant, $F_{\{M,N\}}(\lambda) = F(0)$ that obviously is poor. For $N/2 \le M < N$, equation (26) is equivalent to

$$\lambda = -\frac{B^{(0)}(F_{\{M,N\}})}{B^{(1)}(F_{\{M,N\}})}. \tag{27}$$

It means that inversion of the function $F(\lambda)$ is approximated by a rational function. However, the inversion of the function $F(\lambda)$ has infinitely many square root branch point (roots of an equation $F = 1 + \ln F + 2n\pi\mathrm{i}$ with integer $n$). For $N/3 \le M < [N/2]$, equation (26) reads

$$B^{(0)}(F_{\{M,N\}}) + \lambda B^{(1)}(F_{\{M,N\}}) + \lambda^2 B^{(2)}(F_{\{M,N\}}) = 0. \tag{28}$$

This *second kind* of quadratic approximants was introduced by Shafer (1974) who defined *two kinds* of quadratic approximants, either direct or by inversion. We expect that it works better than rational approximation (27) for multi-valued inversion functions such as the inversion of $F(\lambda)$. So, accuracy of the inversion function $\delta\lambda$ for $N/3 \le M < [N/2]$ is probably better than for $N/2 \le M < N$. Accuracy of the direct function $\delta F$ behaves similarly since $\delta F = \frac{dF}{d\lambda}\delta\lambda$.

Degrees of the polynomial (25) in variables $F_{\{M,N\}}$ and $\lambda$ ($M$ and $L$ respectively) became equal if $M = N/(M+1)$, or $M = (N+1)^{1/2} - 1$. These points are marked by asterisks on figure 1. Numerical evidence is that they roughly give the optimum degrees of approximants (marked by circles on figure 1).

### *3.2. The quartic anharmonic oscillator*

The first 41 coefficients of the series (2) were listed as rational numbers by Turbiner and Ushveridze (1988). We found exactly all coefficients up to the 600-th order. Recursive

calculations of approximants were done using multiple-precision arithmetic (5000 digits) because the algorithm is numerically unstable (Mayer and Tong 1985).

Accuracy of approximants is measured by a quantity $-\lg|E_N - E|$ roughly equal to the number of accurate digits after the decimal point. Dependence of the accuracy on $N$, the number of summed terms of the series (2), is shown on figures 2–4 for different $\lambda$.

The figure 2 refers to a bound state at $\lambda = \frac{1}{2}$. There, quadratic and especially cubic approximants converge much better than ordinary Padé approximants. Excellent convergence of cubic approximants for strong coupling constants can be attributed to the cubic-root singularity of the energy function at $\lambda = \infty$, $E(\lambda) \sim b_0\lambda^{1/3}$ (Tubiner and Ushveridze 1988, Guardiola *et al* 1992). Higher-degree approximants slightly improve the convergence. The 20-th degree approximants appear to converge up to 80 decimal places that is several times more than the most accurate result reported previously (Taşeli and Demiralp 1988). We found that at large $N$ $\ln|E_N - E| \sim -C_M N^{\alpha_M}$ where $\alpha_M = 0.5$, 0.55, and 0.65 for $M = 1$, 2, and 3 respectively. Note that convergence of Padé approximants for the series of factorials $\sum(-1)^k k!\lambda^k$ has similar behavior with $\alpha = 1/2$ (Bender and Orszag 1978).

The figure 3 compares the convergence for different $\lambda$ on a comlex circle $|\lambda| = 1/2$. Here we use third-degree polynomial fits to supress relatively small fluctuations of curves around regular trends. Convergence of algebraic approximants for $\lambda = \mathrm{i}/2$ is similar to $\lambda = \frac{1}{2}$, but the accuracy is slightly poorer. The physical meaning of imaginary coupling constants will be discussed below. At $\lambda = -\frac{1}{2}$, the potential does not support bound states. Padé approximants no longer converge, but quadratic and especially cubic approximants converge fairly good to a comlex energy of a quasi-stationary state. Note an appreciable improvement of convergence of higher-degree approximants.

Using the scaling transformation of the variable $x = x'\exp(-\pi\mathrm{i}/4)$ in the Hamiltonian (1), one can prove that the values of $\lambda = \exp(\frac{3}{2}\mathrm{i}\pi)\lambda'$ correspond to a double-well problem

$$H_{\mathrm{DW}} = \frac{p^2}{2} - \frac{x^2}{2} + \lambda' x^4 \tag{29}$$

with eigenvalues $E_{\mathrm{DW}}(\lambda') = -\mathrm{i}E(\lambda)$ (Crutchfield 1978, Seznec and Zinn-Justin 1978). These $\lambda$ lie on the second sheet of Riemann surface of the energy function under the cut $(-\infty, 0)$. The function $E(\lambda)$ can be calculated on the second sheet using the supplementary branch of quadratic approximants (Sergeev 1995). Here, we approximate the second branch of $E(\lambda)$ at $\lambda = -\mathrm{i}\lambda'$ by higher degree approximants also. The accuracy of results is shown on the figure 3 for $\lambda' = \frac{1}{2}$ and on a figure 4 for $\lambda' = 1/10$ and $\lambda' = 3/100$. Convergence improves significantly with the increasing of the degree of approximants, especially for smaller $\lambda'$. We explain this fact by the presence of an infinite sequence of square-root branch points near the line $\arg\lambda = \pm\frac{3}{2}\pi$ (Bender and Wu 1969).

In this region, the energy function becomes an essentially infinitely-valued function. We believe that the existance of infinitely many sheets makes higher degree approximants more effective like for the logarithmic function (subsection 3.1). The point $\lambda = -\mathrm{i}/10$ lies closer to the singularity of the largest absolute value $\lambda_0 = \pm 0.0319934 - 0.0367596\mathrm{i}$ (Shanley 1986) and to another ones (see a figure 5) than $\lambda = -\mathrm{i}/2$. So, higher-degree approximants are especially effective in this case. The point $\lambda = -0.03\mathrm{i}$ is surrounded by several singularities (see the figure 5). Approximants of lower degrees (less than four) no longer converge, but the 20-th degree approximants still converge to a purely imaginary result

$$E(\frac{3}{100}\mathrm{e}^{\frac{3}{2}\mathrm{i}\pi}) = \mathrm{i}E_{\mathrm{DW}}(\lambda') = -1.411\,819\,732\,54\mathrm{i} \tag{30}$$

corresponding to the ground state energy in the double well. Moreover, another branch of the 20-th degree approximant at higher orders ($N > 300$) converge to $-0.312\,162\,1\mathrm{i}$ corresponding to the excited $n = 2$ state energy in the double well (these two branches join at the square-root branch point $\lambda_0$ near the point $\lambda = -0.03\mathrm{i}$ where the function $E(\lambda)$ is evaluated).

The main branch of the function $E(\lambda)$ at $\lambda = -\mathrm{i}\lambda'$ (summable by single-valued Padé approximants) corresponds to complex energy of the barrier resonance in the double well, $E^{\mathrm{r}}_{\mathrm{DW}}(\lambda') = -\mathrm{i}E(-\mathrm{i}\lambda')$. The small-coupling expansion

$$E^{\mathrm{r}}_{\mathrm{DW}}(\lambda') = \frac{-\mathrm{i}}{2} + \frac{3}{4}\lambda' - \frac{21}{8}\mathrm{i}\lambda'^2 + \frac{333}{16}\mathrm{i}\lambda'^3 + \ldots \tag{31}$$

represents a formal Rayleigh–Schrödinger perturbation series for the anharmonic oscillator $\frac{1}{2}\omega^2 x^2 + \lambda' x^4$ with an imaginary frequency $\omega = -\mathrm{i}$. A similar perturbation theory for resonances was recently used by Fernández (1996). Such broad resonances with the real part of the energy near the potential maximum are associated with chemical reaction thresholds (Friedman and Truhlar 1991, Friedman *et al* 1995).

The cases $\lambda = 100$ and $\lambda = 10^6$ displayed at the bottom of the figure 4 refer to a strong-coupling region when $E(\lambda) \sim b_0\lambda^{1/3}$. Since Padé and quadratic approximants fail to approximate cubic-root singularities, their convergence is very slow. Convergence of cubic and higher degree approximants is as good as for $\lambda = -1/2$. The 20-th degree approximants of the form $[L, L, ..., L, L-1, L-1, L-1]$ ($N = 21L + 17$) are marked by crosses on the figure 4. Their accuracy is considerably better than the averaged accuracy of the 20-th degree approximants (solid line) because they always have correct $\sim \lambda^{1/3}$-behavior at large $\lambda$ (see the last paragraph of the section 2).

The case $\lambda = -1/1000$ displayed on the figure 6 corresponds to a quasistationary state with extremely small width, $\Im E = \pm 4.319 \cdot 10^{-144}$. An error introduced by Padé approximants decreases with $N$ until it reaches $\sim |\Im E|$. Then it holds steady on this level. For sufficiently small $N$ when quadratic approximants are still real, they have near the same error as Padé approximants. Then after appearing of an

imaginary part (when their discriminants become negative) accuracy of quadratic approximants continues to rise. Partial sums (also given on figure 6) reach the highest accuracy $|E_N - E| = 1.00023|\Im E|$ at $N = 333$ when $|E^{(N+1)}\lambda^{N+1}|$ attains its minimum $(1.887 \cdot 10^{-145})$. Here, accuracy of all algebraic approximants is also $\sim |\Im E|$.

### *3.3. The cubic anharmonic oscillator*

The harmonic oscillator with a cubic distortion $gx^3$ is a prototypical system exhibiting resonances. Its complex eigenvalues were studied both analytically and numerically (Drummond 1981, Alvarez 1988).

Since odd-order terms of the energy series in $g$ are zero (because the energy is an even function of $g$), we define the coupling constant as $\lambda = g^2$ and arrive to the series with non-zero coefficients at any term $\sim \lambda^k$ $(k = 0, 1, 2, ...)$:

$$E(\lambda) = \frac{1}{2} - \frac{11}{8}\lambda - \frac{465}{32}\lambda^2 - \frac{39709}{128}\lambda^3 - \frac{19250805}{2048}\lambda^4 + ... \tag{32}$$

Convergence of algebraic approximants to the function (32) at $\lambda = 1/4$ (see a figure 7) looks similar to that to the function (2) for the quartic anharmonic oscillator at $\lambda = -1/2$ (see the figure 3). However, improving of the convergence for the fourth and for the fifth degree approximants is more appreciable in comparison with the latter case. We explain this fact by the presence of the fifth order root singularity at infinity, $E(\lambda) \sim \exp(-\mathrm{i}\pi/5)\lambda^{1/5}$ (Alvares 1988).

Using the scaling transformation $x = \omega^{1/2}x'$, one can prove that $\omega E(\omega^{-5}\lambda)$ is an eigenvalue in a potential $\omega^2 x^2/2 + \lambda^{1/2}x^3$. Particularly for $\omega = \exp(-\pi\mathrm{i}/2)$, $-\mathrm{i}E(\mathrm{e}^{\frac{5}{2}\mathrm{i}\pi}\lambda)$ is an eigenvalue in a potential $-x^2/2 + \lambda^{1/2}x^3$. A shift transformation reduces this modified potential to the initial potential,

$$-\frac{1}{2}x^2 + \lambda^{1/2}x^3 = \frac{1}{2}x'^2 + \lambda^{1/2}x'^3 - \frac{1}{54\lambda}, \tag{33}$$

where $x' = x + 1/(3\lambda^{1/2})$, and the eigenvalues in a modified potential differ from initial ones only by a shift,

$$-\mathrm{i}E(\mathrm{e}^{\frac{5}{2}\mathrm{i}\pi}\lambda) = E(\lambda) - \frac{1}{54\lambda}. \tag{34}$$

So, $E(\lambda) = -\mathrm{i}E(\lambda') + \frac{1}{54\lambda}$, where $\lambda' = \exp(\frac{5}{2}\mathrm{i}\pi)\lambda$. The point $\lambda'$ lies on the second sheet of Riemann surface under the cut $(0, \infty)$. $E(\lambda')$ can be rewritten as $E'(\mathrm{i}\lambda)$ where $E'$ means the second branch of the function $E$. Thus, the eigenvalues can be calculated by two different ways. They can be found by direct summation of the series $E(\lambda)$ (on the principal sheet), and they can be found by calculating the second branch of approximants at $\lambda' = \mathrm{i}\lambda$. Such approach is equivalent to expansion of the potential $-x^2/2 + \lambda^{1/2}x^3$ over its local maximum and developing a complex perturbation theory

for an upturned harmonic oscillator with a purely imaginary frequency with subsequent summation of the perturbation series on the second sheet.

At $\lambda = \frac{1}{4}\exp(5\mathrm{i}\pi/2)$ (see the figure 7), higher degree approximants considerably improve the convergence. However, the accuracy of results for $\lambda = \frac{1}{4}\exp(5\mathrm{i}\pi/2)$ is less than for $\lambda = \frac{1}{4}$, and the second way of calculation of $E(\lambda)$ appears impractical (for this particular $\lambda$).

The bottom of the figure 7 ($\lambda = 100$) refers to a strong-coupling regime $E(\lambda) \sim \exp(-\mathrm{i}\pi/5)\lambda^{1/5}$. Here, the fifth and higher degree approximants considerably improve the convergence, because they can approximate singularities like $\lambda^{1/5}$. The 20-th degree approximants $[L, L, ..., L, L-1, L-1, L-1, L-1, L-1]$ ($N = 21L + 15$) are marked by crosses on the figure 7. They always behave like $\sim \lambda^{1/5}$ at $\lambda \to \infty$ (see the last paragraph of the section 2), and their accuracy is much better than averaged accuracy of the series of the 20-th degree approximants listed in the table 1 (solid line on the figure 7).

### *3.4. Sextic and octic anharmonic oscillators*

Perturbation theory for sextic ($\lambda x^6$) and octic ($\lambda x^8$) anharmonic oscillators is strongly divergent (leading factors are $(2k)!$ and $(3k)!$ respectively, where $k$ is the order of the perturbation theory). As a result, Padé approximants converge very slowly for the sextic oscillator (even at small $\lambda$) and fail to converge for the octic oscillator (Graffi and Grecchi 1978).

We found that quadratic, cubic, and fourth degree approximants for the sextic anharmonic oscillator converge considerably better than Padé approximants (figure 8) although their convergence is uneven.

The problem of the octic oscillator is interesting because $[N, N]$ and $[N+1, N]$ sequences of Padé approximants converge to different limits giving lower and upper bounds to the energy (Austin 1984). We found that diagonal quadratic approximants converge also to a wrong limit slightly different from the energy, but the achieved number of correct digits is roughly 2.5 times greater than for diagonal Padé approximants, see the figure 9. Diagonal cubic approximants seem to converge to a wrong limit also, but their accuracy is still greater (an upper curve on the figure 9).

The obtained accuracy both for sextic and for octic oscillators exceeds the accuracy of Levin's transformation of "renormalized series" (Weniger *et al* 1993).

## 4. Conclusion

Algebraic approximants of at least third degree are found very effective for summing of the perturbation series for quantum anharmonic oscillators both on the main sheet and on neighbour sheets of Riemann surface. Generally, eigenvalues (of the given symmetry)

are branches of a single multi-valued function. So, large-degree algebraic approximants that can reproduce several sheets of a multi-valued analytic function starting from Taylor expansion on the main sheet look promising for another quantum-mechanical perturbation problems.

Algebraic approximants are expected to be useful also for numerical study of singularities and an analytic structure of the eigenvalues in a complex plane of coupling constants that is important for evaluation of transition probabilities in adiabatic processes (Grozdanov and Solov'ev 1990).

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## Figure captions

**Figure 1.** Dependence of the accuracy on the degree of algebraic approximants on the principal sheet and on a complex sheet of the function $F(\lambda) = \lambda^{-1} \ln(1+\lambda)$. For each curve, the number of summed terms of the series is the same. A typical curve has a maximum corresponding to the optimum degree marked by a circle. The points $M = (N+1)^{1/2} - 1$ with equal degrees $M$ and $L = [N/(M+1)]$ are marked by asterisks. They appear to lie near the maxima.

**Figure 2.** Accuracy of algebraic approximants for the ground-state energy of the quartic anharmonic oscillator at $\lambda = \frac{1}{2}$ (a bound state). The accuracy is measured by a number of correct digits (after the decimal point) defined as $-\lg|E_N - E|$. $N$ is the number of summed terms of the perturbation series.

**Figure 3.** Accuracy of algebraic approximants for the quartic anharmonic oscillator at different $\lambda$ on a complex circle $|\lambda| = 1/2$. To make general trends more clear, the curves are smoothed by third degree polynomial fits (cf with figure 2). Dotted lines are Padé approximants, dashed lines are quadratic approximants, dot-dashed lines are cubic approximants, double dot-dashed lines are fourth degree approximants, and solid lines are 20-th degree approximants. Verticale scale is different for different $\lambda$. At $\lambda = -\frac{1}{2}$ (a quasistationary state), Padé approximants fail to converge. At $\lambda = \frac{1}{2}\exp(\frac{3}{2}\mathrm{i}\pi)$ (on the second sheet of Riemann surface), Padé approximants are not defined because they are single-valued functions.

**Figure 4.** Accuracy of algebraic approximants for the quartic anharmonic oscillator at small and at large $\lambda$. The curves are smoothed by third degree polynomial fits. Padé, quadratic, cubic, fourth degree, and 20-th degree approximants are marked by the same way as on the figure 3. At $\lambda = \frac{1}{10}\exp(\frac{3}{2}\mathrm{i}\pi)$ and at $\lambda = \frac{3}{100}\exp(\frac{3}{2}\mathrm{i}\pi)$, considerable improvement of convergence of the 20-th degree approximants comparing with lower degree approximants is related to a complex analytic structure of the energy function on the second sheet, see the next figure 5. At $\lambda = 100$ and at $\lambda = 10^6$, the 20-th degree approximants for $N = 21L + 17$ ($L = 1, 2, ...$) that have correct cubic root behavior at large $\lambda$ are marked by crosses while diagonal approximants are marked by circles.

**Figure 5.** Positions of several square-root branch points of largest absolute value on the second sheet of Riemann surface near the line $\arg\lambda = \frac{3}{2}\pi$ found numerically by Shanley (1986). The cut separating this sheet from the main sheet of Riemann surface goes along the negative real axis (broad line).

**Figure 6.** Accuracy of algebraic approximants for a long-living quasistationary state of the quartic anharmonic oscillator. Padé, quadratic, and cubic approximants are marked by the same way as on the figure 3, partial sums are marked by a solid line. Accuracy of quartic and higher degree approximants is a little better than cubic approximants so that the difference would be hardly visible in the scale of this figure.

**Figure 7.** Accuracy of algebraic approximants for the cubic anharmonic oscillator. The curves are smoothed by the third degree polynomial fits. Dashed lines are quadratic approximants, dot-dashed lines are cubic approximants, double dot-dashed lines are fourth degree approximants, dotted lines are fifth degree approximants, and solid lines are 20-th degree approximants. Padé approximants don't converge because the state is quasistationary (with a complex energy), but Padé approximants are real. The point $\lambda = \frac{1}{4}\exp(\frac{5}{2}\mathrm{i}\pi)$ is on the second sheet of Riemann surface. The energy at $\lambda = \frac{1}{4}\exp(\frac{5}{2}\mathrm{i}\pi)$ is closely related to the energy at $\lambda = \frac{1}{4}$ according to (34). However, the accuracy of approximants at $\lambda = \frac{1}{4}\exp(\frac{5}{2}\mathrm{i}\pi)$ does not reach that at $\lambda = \frac{1}{4}$. The case $\lambda = 100$ refers to a strong coupling regime. The 20-th degree approximants at $N = 21L + 15$ $(L = 1, 2, ...)$ that have correct $\lambda^{1/5}$ behavior at $\lambda \to \infty$, are marked by crosses while diagonal approximants are marked by circles.

**Figure 8.** Accuracy of algebraic approximants for the the sextic anharmonic oscillator at $\lambda = \frac{1}{10}$. Theoretically, Padé approximants converge, but in practice their convergence is very slow. Quadratic, cubic, and fourth degree approximants converge much faster, although the convergence is uneven.

**Figure 9.** Accuracy of diagonal algebraic approximants for the octic anharmonic oscillator at $\lambda = \frac{1}{100}$. Diagonal Padé approximants converge to 0.5272 (99.1% of the exact energy), diagonal quadratic approximants converge to 0.532 105 (100.0002%), and diagonal cubic approximants appear to converge to 0.532 103 926 (99.999 999 7%).