

Summation of the eigenvalue perturbation series by multi-valued Padé approximants: application to resonance problems and double wells

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Abstract. Quadratic Padé approximants are used to obtain energy levels both for the anharmonic oscillator $x^2/2 - \lambda x^4$ and for the double well $-x^2/2 + \lambda x^4$. In the first case, the *complex*-valued energy of the resonances is reproduced by summation of the *real* terms of the perturbation series. The second case is treated formally as an anharmonic oscillator with a purely imaginary frequency. We use the expansion around the central maximum of the potential to obtain a complex perturbation series on the unphysical sheet of the energy function. Then, we perform an analytical continuation of this solution to the neighbouring physical sheet taking into account the supplementary branch of quadratic approximants. In this way we can reconstruct the *real* energy by summation of the *complex* series. Such an unusual approach eliminates the double degeneracy of states that makes ordinary perturbation theory (around the minima of the double-well potential) incorrect.

As a rule, perturbation series for energy levels in quantum mechanics have a zero radius of convergence. So, generalized summation methods that enable one to continue a Taylor series outside of its circle of convergence are commonly used. The classical example is the divergence of the perturbation series for the anharmonic oscillator (Bender and Wu 1973) and the summability of this series by Padé approximants (Loeffel *et al* 1969).

In general, the energy levels represent the sheets of some multi-valued analytic function. The natural generalization of the ordinary Padé approximants to the case of multi-valued functions is a quadratic Padé approximant (QPA) introduced by Shafer (1974). The ‘diagonal’ QPA to the function $f(z)$ is defined as a double-valued solution of a quadratic equation:

$$f_{[N,N,N]}(z) = (2A)^{-1}[-B \pm (B^2 - 4AC)^{1/2}] \quad (1)$$

where A , B and C are polynomials of degree N which satisfy

$$A(z)f^2(z) + B(z)f(z) + C(z) = o(z^{3N+1}). \quad (2)$$

Thus, $f_{[N,N,N]}(z)$ can be computed from the first $3N + 2$ terms of the Taylor expansion for $f(z)$.

This type of approximant is a special case of the generalized Padé–Hermite approximant extensively studied by Della Dora and Di-Crescenzo (1979). The coefficients of Padé–Hermite polynomials are determined by solving the system of linear algebraic equations.

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Together with QPA, Common (1982) considered 'integral' and 'differential' Padé-Hermite approximants also having branch-point structure.

The main branch of QPA re-generates the Taylor expansion for the initial function up to the order z^{3N+1} . It transfers to the second sheet at square-root branch points where the discriminant becomes zero. So, QPA can approximate both poles and cuts. Moreover, it can reconstruct to some extent the neighbouring sheets of the multi-valued function. Numerical results of Short (1979) indicate that QPA provides a practical method for the analytic continuation of a function from one Riemann sheet to another.

In the first part of this paper we apply the QPA to the function having a cut on the positive real axis; this is the case when the ordinary Padé approximants fail to converge because of an accumulation of poles on the cut (Baker 1975). The function to be approximated is a complex energy of resonances, $E = E_r \pm i\Gamma/2$, the plus sign corresponding to the incoming wave, and the minus sign corresponding to the outgoing wave boundary conditions. The real part E_r defines a position of the level, and Γ is its width. This approach is not completely new. Earlier, QPA were applied to the quasi-stationary states in a Yukawa potential (Sergeev and Sherstyuk 1984) and for a Stark effect in a hydrogen atom (Vainberg *et al* 1987). More ingenious summation procedures such as the modification of Padé approximants (Reinhardt 1982) and the Padé-Borel method (Franceschini *et al* 1985) were also considered for a Stark effect.

Here, we illustrate the convergence of QPA for the oscillator with negative quartic anharmonicity

$$V(x) = x^2/2 - \lambda x^4. \quad (3)$$

The expansion for the energy

$$E(\lambda) = n + \frac{1}{2} - \frac{3}{4}(2n^2 + 2n + 1)\lambda - \frac{1}{8}(34n^3 + 51n^2 + 59n + 21)\lambda^2 - \dots \quad (4)$$

where n is a quantum number, can be easily computed up to higher orders. To calculate a 'diagonal' QPA we use a fast algorithm based on a four-term recurrence relation (Mayer and Tong 1985, Sergeev 1986) and resembling the method of continued fractions for the diagonal Padé sequence. Two values of the QPA prove to be complex conjugate except where the parameter λ is too small. We present the values of the QPA in table 1, retaining only the stable digits which are common for the three approximants [12,12,12], [13,13,13] and [14,14,14]. Our results appear to be slightly more accurate than the earlier numerical results of Drummond (1982) which are also given in table 1.

Further, we note that the problem in question can be converted into a problem with the potential

$$U(x) = g(x^2/2 - x^4) \quad (5)$$

by the scaling $x \rightarrow \lambda^{-1/2}x$. The corresponding eigenvalues depending on a coupling constant are

$$\varepsilon(g) = g^{1/2}E(g^{-1/2}). \quad (6)$$

So, the large g limit is in a close relation with the small λ asymptotics for the initial potential $V(x)$.

For positive g , $\varepsilon(g)$ gives the complex energy of resonances. The behaviour at large g is

$$\varepsilon(g) = (n + \frac{1}{2})g^{1/2} - \frac{3}{4}(2n^2 + 2n + 1) - \frac{1}{8}(34n^3 + 51n^2 + 59n + 21)g^{-1/2} - \dots \quad (7)$$

Table 1. The double energy of resonances $2E$ (to make an easier comparison with previous results) obtained by summation of the perturbation series for a potential $x^2/2 - \lambda x^4$ by QPA.

λ	Ground state, $n = 0$		First excited state, $n = 1$	
	Real	Imaginary	Real	Imaginary
0.01	0.984 427 67	0.000 0000	2.920 282 16	0.000 000
0.02	0.967 451 24	0.000 000 60	2.827 102 62	0.000 089 03
	0.967 451 24 ^a	0.000 000 60 ^a		
0.05	0.900 672 90	0.006 693 28	2.448 334	0.153 195
	0.900 67 ^a	0.006 69 ^a		
0.1	0.794 881	0.089 412	2.192 90	0.677 32
	0.7949 ^a	0.0894 ^a		
0.2	0.728 82	0.277 35	2.1652	1.3905
	0.7288 ^a	0.2773 ^a		
0.5	0.7477	0.6100	2.41	2.51
	0.7477 ^a	0.6100 ^a		
1.0	0.8297	0.9097	2.78	3.53
2.0	0.964	1.260	3.3	4.73
5.0	1.23	1.84	4.3	6.8

^a The results obtained by Runge-Kutta integrations (Drummond 1982).

When g is negative, $\varepsilon(g)$ represents the bound-state energy in a double-well potential having an asymptotic expansion in powers of $(-g)^{-1/2}$:

$$\varepsilon_{\pm}(g) = \frac{g}{16} + \frac{\sqrt{2}}{2}(2n+1)(-g)^{1/2} - (3n^2+3n+1) - \frac{\sqrt{2}}{4}(34n^3+51n^2+35n+9)(-g)^{-1/2} - \dots \tag{8}$$

This is equivalent to the expansion studied by Damburg and Propin (1971). The index \pm denotes the parity of states. So, the levels are not defined without ambiguity by the series, and difficulties arise if we try to sum expansion (8). Borel resummation gives a complex result coinciding with the energy of a resonance in a quite different problem (Seznec and Zinn-Justin 1979). Here, we hope to overcome the difficulty related to double degeneracy of states by summation of expansion (7) for negative values of g (the parameter of the expansion will be $i(-g)^{-1/2}$). Of course, the main branch of function (7) yields some unphysical complex eigenvalues if $g < 0$. We conjecture that this function can be analytically continued so that its second branch would give a real bound-state energy.

For the potential (5), the analytic properties of bound and resonance energies as functions of the coupling constant were studied extensively by Shanley (1989). Using a complex scaling argument he found that the quantum levels in a potential and its inversion are intimately related. Here, we are going to exploit the fact that the energies of both types of states are joined at branch points. So, one of these energies can be obtained from another energy by analytic continuation.

As a justification for our conjecture, let us temporarily consider a much simpler prototype model with a pair of zero range potentials:

$$U(x) = g[\delta(x - 1) + \delta(x + 1)]. \tag{9}$$

The equation for the energy function is

$$k(i + \tan k) = 2g \quad E(g) = k^2/2 \tag{10}$$

(the odd parity states are not regarded here but they may be treated similarly). Because the energies both for resonances ($g > 0$) and for bound states ($g < 0$) may be obtained from the same general equation (10), they represent different branches of a single multi-valued function.

If $g < 0$, it is convenient to rewrite equation (10) using a customary notation $x = -ik$:

$$x(1 + \operatorname{th}x) = -2g \quad E = -x^2/2. \quad (11)$$

Equation (11) has a single real solution so only one bound state exists; its energy tends to $-g^2/2$ when $g \rightarrow -\infty$.

It will be instructive to observe what happens to this ground-state energy as g moves along the real axis. When g becomes positive, the bound state smoothly transforms into a virtual state without any singularity. When g reaches a branch point $g_{\text{br}} = 0.1392$, this is the solution of the transcendental equation $2g + \ln(2g) + 1 = 0$, the complex-conjugate energies of resonances arise as a result of a collision of two virtual levels and the energy has a square-root singularity. At a large g limit, the problem is equivalent to the rectangular-shape potential with infinitely high walls, and the ground-state energy is $\pi^2/8$.

The zero-range model (9) is also an instructive example regarding the summability of the perturbation series. For negative g the energy behaves as

$$\varepsilon(g) = -\frac{g^2}{2} - g^2 e^{2g} - \left(\frac{g^2}{2} + 2g^3\right) e^{4g} - (2g^3 + 6g^4) e^{6g} - \dots \quad g \rightarrow -\infty. \quad (12)$$

If we try to expand (12) in negative powers of g and then sum the expansion we obtain the wrong answer $-g^2/2$ because we neglect exponentially small terms.

In the opposite limit, the large g behaviour of the energy takes the form of an expansion in powers of $1/g$:

$$\varepsilon(g) = \frac{\pi^2}{8} - \frac{\pi^2}{8} g^{-1} + \frac{\pi^2}{32} (3 \pm i\pi) g^{-2} + \dots \quad g \rightarrow \infty. \quad (13)$$

The series (13) can be summed at large $|g|$ to an analytic function. For negative g , the real solution (12) having an essential singularity at infinity can be obtained by analytic continuation of this function along a contour embracing the point g_{br} .

Now let us consider the double well

$$V_{\text{DW}}(x) = -x^2/2 + \lambda x^4 \quad (14)$$

that is related to the coupling problem (5) for negative g . We expect that the spectral Riemann surface for problem (5) has a structure resembling the case of the zero-range model (9). So, treating (14) formally as a perturbed harmonic oscillator with a frequency $\omega = i$ ($\omega = -i$ would be equally suitable), we obtain the expansion on the unphysical sheet of the energy function:

$$E'_{\text{DW}}(\lambda) = (n + \frac{1}{2})i - \frac{3}{4}(2n^2 + 2n + 1)\lambda + \frac{1}{8}(34n^3 + 51n^2 + 59n + 21)i\lambda^2 + \dots \quad (15)$$

The complex expansion coefficient can be easily found using the relation

$$E'_{\text{DW}}(\lambda) = iE(-i\lambda) \quad (16)$$

and expansion (4). Then, we calculate QPA. Numerical evidence is that the second (supplementary) branch of the QPA is rather close to the bound-state energy, but the results are not as perfect as in the case of the anharmonic oscillator. One of the reasons may be the fact that the actual expansion of the energy (from the perturbation theory around the minima of a double-well potential) has a pole at $\lambda = 0$:

$$E_{\text{DW}}^{\pm}(\lambda) = -\frac{1}{16\lambda} + \frac{\sqrt{2}}{2}(2n + 1) - (3n^2 + 3n + 1)\lambda - \frac{\sqrt{2}}{4}(34n^3 + 51n^2 + 35n + 9)\lambda^2 - \dots \tag{17}$$

simply because the potential has no minimum when $\lambda = 0$. QPA defined by equation (1) has no such pole unless $A(0) = 0$.

In order to account for this pole, we also calculate a slightly modified QPA that is defined by equations (1) and (2) with the substitution $A(z) \rightarrow zA(z)$. Two branches of QPA are given in table 2. The supplementary branch of QPA is proved to approximate the exact ground-state energy (found by numerical integration of the Schrödinger equation) to within an accuracy of about 0.01 unless the parameter λ becomes too small or too large. The surprising result is that the *real* energy can be calculated by summation of the *complex* perturbation series (cf with the former resonance problem when the *complex* energy was obtained by summation of the *real* perturbation series). The accuracy is expected to rise if an essential singularity of the energy at $\lambda = 0$ and the cubic-root singularity at $\lambda = \infty$ could be incorporated by a further modification of QPA.

Table 2. Summation of the complex perturbation series on the unphysical sheet of the energy function for the double-well potential. Modified QPA [12,12,12] is presented.

λ	Main branch		Supplementary branch	
	Real	Imaginary	Real	Imaginary
0.1	-0.064 750 96	0.517 142 56	-0.150 -0.1541 ^a	-0.020
0.15	-0.088 616 72	0.530 293 58	0.004 -0.0026 ^a	0.002
0.2	-0.108 735 33	0.543 574 55	0.086 0.0850 ^a	0.005
0.3	-0.141 576 05	0.568 993 43	0.192 0.1960 ^a	0.000
0.5	-0.190 392 9	0.614 013 8	0.330 0.3288 ^a	-0.005
0.7	-0.227 162	0.652 653	0.425 0.4173 ^a	-0.002
1.0	-0.270 343	0.702 275	0.522 0.5148 ^a	0.009
1.5	-0.325 10	0.770 56	0.625 0.6329 ^a	0.017
2.0	-0.3680	0.8274	0.698 0.7230 ^a	0.010
3.0	-0.435	0.9204	0.822 0.8608 ^a	-0.024
5.0	-0.532	1.062	1.056 1.0564 ^a	-0.090

^a Exact ground-state energy in a double well.

The physical interpretation of the complex quantity obtained from the main branch of QPA remains unclear for us because there are no resonances for such a problem. The only conjecture we can suppose is that it is very close to the energy of the broad unstable resonance in the modified inverse-well potential

$$V_{\text{IW}}(x) = \begin{cases} -x^2/2 + \lambda x^4 & |x| \leq 1/2\sqrt{\lambda} \\ -1/16\lambda & |x| > 1/2\sqrt{\lambda}. \end{cases} \quad (18)$$

The complex expansion around the central maximum invites further applications for other symmetrical potentials. Generally, the method may be useful for the cases when the energy has exponentially small terms neglected by perturbation theory. An example is the Killingbeck potential

$$V(r) = -1/r + 2\lambda r + 2\lambda^2 r^2 \quad (19)$$

having a finite asymptotic expansion for the ground-state energy

$$E(\lambda) = -1/2 + 3\lambda \quad (20)$$

but its sum was proved not to be identical to the energy when $\lambda < 0$ (Killingbeck 1978).

In one dimension, the simplest way to obtain the energy remains a direct integration of the Schrödinger equation. Nevertheless, the method may be of a practical importance for multi-dimensional potentials, where the coefficients of the perturbation expansion can also be exactly computed up to an arbitrary order.

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