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

Short title: Summation of the eigenvalue perturbation series

Name of author: A. V. Sergeev

Address of establishment where work was carried out:

S.I.Vavilov State Optical Institute, Tuchkov Per. 1, 199034 Saint Petersburg, Russian Federation

e-mail sergeev@soi.spb.su

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

A. V. Sergeev

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 complex perturbation series on the unphysical sheet of the energy function. Then, we perform analytic continuation of this solution to the neighbor 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 unusual approach eliminates double degeneracy of states that makes the ordinary perturbation theory (around the minima of the double well potential) to be incorrect.

Text

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

A. V. Sergeev

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 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 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,

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

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

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

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

The main branch of QPA regenerates 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 at some extent the neighbor 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 the 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. The present approach is not quite new. Earlier, QPA were applied to the quasistationary states in 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 modification of Padé approximants (Reinhardt 1982) and 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,

$$V(x) = x^2/2 - \lambda x^4. \tag{3}$$

The expansion for the energy

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

where n is a quantum number, can be easily computed up to higher orders. To calculate "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 diagonal Padé sequence. Two values of QPA prove to be complex-conjugate unless the parameter λ is too small. We present the values of QPA in the Table 1, retaining only the stabile digits which are common for three approximants [12,12,12], [13,13,13] and [14,14,14]. Our results appear slightly more accurate than the earlier numerical results of Drummond (1982) which are also given in the Table 1.

Table 1

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

$$U(x) = g(x^2/2 - x^4) \tag{5}$$

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

	Ground state, $n = 0$		First excited state, $n = 1$	
λ	Real	Imaginary	Real	Imaginary
0.01	0.98442767	0.0000000	2.92028216	0.000000
0.02	0.96745124 0.96745124[a]	0.00000060 0.00000060[a]	2.82710262	0.00008903
0.05	0.90067290 0.90067[a]	0.00669328 0.00669[a]	2.448334	0.153195
0.1	0.794881 0.7949[a]	0.089412 0.0894[a]	2.19290	0.67732
0.2	0.72882 0.7288[a]	0.27735 0.2773[a]	2.1652	1.3905
0.5	0.7477 0.7477[a]	0.6100 0.6100[a]	2.41	2.51
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).

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