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ON THE BOREL SUMMATION OF PERTURBATIVE SERIES

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The method of the Borel summation of perturbative series is described in detail and applied to the calculation of the ground state energy of an anharmonic oscillator. We have found a good agreement with the results obtained by different methods.

I. INTRODUCTION

There is only a small number of problems in physics which are exactly solvable. Most frequently approximative methods have to be used. Typical examples of this type are the perturbative series in quantum mechanics (or in the quantum field theory). There are defficulties with the perturbative expansions when the perturbation is in a certain sense large.

As an example of such a situation we can take a harmonic oscillator with the perturbation λx^4, which is "large" the respect to the harmonic potential $x^2/2$. The coefficients a_n in the perturbative expansion $\sum_0^\infty a_n \lambda^n$ of some quantity (e.g. the ground state energy) are well defined but the expansion is the asymptotical one being divergent for $\lambda \neq 0$ and for a small λ the first few terms in the expansion give only a rough estimate of the quantity in question. The perturbative expansion should be summed in a suitable generalized sense to extract the non-trivial information contained in the coefficients a_n.

The standard method of the resummability of some divergent series is the Borel method based on the following observation. Let the formal expansion of a function is given

$$E(\lambda) = \sum_0^\infty a_n \lambda^n. \qquad (1)$$

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Instead of investigating the $E(\lambda)$ directly we can investigate its Borel transform $F(x)$ defined by the relation

$$E(\lambda) = \frac{1}{\lambda}\int_0^\infty e^{-x/\lambda} F(x)\,dx,\ \lambda > 0. \tag{2}$$

The essence is that if $E(\lambda)$ is given by the formula (1), then for $F(x)$ we have the expansion

$$F(x) = \sum_0^\infty b_n x^n, \quad b_n = a_n/n!. \tag{3}$$

This is a consequence of the equality

$$n! = \lambda^{-n-1}\int_0^\infty x^n e^{-x/\lambda}\,dx, \quad \lambda > 0. \tag{4}$$

Evidently the convergence properties of the series (3) are better than those of the original expansion (1).

As a simple example let us take the series

$$E(\lambda) = \sum_0^\infty (-1)^n \lambda^n \tag{5}$$

which for $|\lambda| < 1$ converges (to the function $1/(1+\lambda)$), whereas for $|\lambda| > 1$ it is divergent. How to find its sum, e.g., for $\lambda = 2$? Using Eqs. (1) to (4) for $\lambda > 0$ we can write

$$E(\lambda) = \frac{1}{\lambda}\sum_0^\infty \frac{(-1)^n}{n!}\int_0^\infty x^n e^{-x/\lambda}\,dx = \\ = \frac{1}{\lambda}\int_0^\infty e^{-x/\lambda}\sum_0^\infty \frac{(-1)^n}{n!} x^n\,dx. \tag{6}$$

By interchanging the order of summation and integration we have used the fact that the last series converges for every x to the function

$$F(x) = \sum_0^\infty \frac{(-1)^n}{n!} x^n = e^{-x}. \tag{7}$$

For $\lambda > 0$ we then have

$$E(\lambda) = \frac{1}{\lambda}\int_0^\infty e^{-x/\lambda} e^{-x}\,dx = \frac{1}{1+\lambda}.$$

This is just the result which can be obtained by the analytic continuation of the sum in Eq. (5) valid for $|\lambda| < 1$.

In general we cannot explicitly sum the expansion (3) (as in (7)) and we should use some approximations: the approximative values $E_N(\lambda)$ of $E(\lambda)$ can be obtained using in (3) suitable approximations $F_N(x)$ instead of $F(x)$. If these approximations share the properties

i) $F_N(x) \to F(x)$ for $N \to \infty$ for almost any $x \in (0, \infty)$,

ii) the functions $e^{-x/\lambda} F_N(x)$ (for a given $\lambda > 0$) have an integrable majorant,

then the quantities

$$E_N(\lambda) = \frac{1}{\lambda}\int_0^\infty e^{-x/\lambda} F_N(x)\,dx \tag{8}$$

converge to $E(\lambda)$ (since we can take the limit in the integrand).

We can see that the approximants $F_N(x)$ should satisfy some conditions and moreover in practical applications only a finite number of coefficients in expansion is known. We therefore formulate the problem as follows: using the coefficients $a_0, a_1, \ldots, a_N$ find the best approximation $F_N(x)$ to $F(x)$ (and simultaneously the best approximation $E_N(\lambda)$ to $E(\lambda)$). In literature such questions are usually only outlined and the problem is not optimized.

The construction of approximants is described in the Sect. 2. The Sect. 3 is devoted to applications and the last, Sect. 4, contains the concluding remarks.

II. THE BOREL METHOD

Let us consider the formal power series with alternating signs

$$E(\lambda) = \sum_0^\infty a_n \lambda^n \tag{9}$$

in which for a large n there holds

$$a_n \sim (-R)^n n^\alpha n!. \tag{10}$$

Here α and $R > 0$ are real numbers. Due to alternating signs in Eq. (10) one can show that there exists the function $E(\lambda)$ holomorphic in the complex λ-plane with the cut $(-\infty, 0)$, which has the formal power expansion (9) for $\lambda > 0$ (see [1] and [2], where one can find a detailed dicussion of the divergent series).

The problem now is to sum up the divergent series (9). The method of the Padé approximants is frequently used: one finds such coefficients $b_0, \ldots, b_L$ and $c_1, \ldots, c_N$ that there holds

$$P_N^L(\lambda) = \frac{b_0 + b_1\lambda + \ldots + b_L\lambda^L}{1 + c_1\lambda + \ldots + c_N\lambda^N} = \sum_0^{L+N} a_n\lambda^n + 0(\lambda^{L+N+1}).$$

One can show [2] that outside the cut $(-\infty, 0\rangle$ the Padé approximants $P_N^{N+J}(\lambda)$

converge for $N \to \infty$ (and $J \geqslant -1$ fixed) to the function $E(\lambda)$. In this method the cut is approximated by poles in the denominator of the Padé approximant $P_N^L(\lambda)$.

In what follows, we describe the method of the Borel summation, which works with approximants having correct analytical properties, i.e., the approximants are holomorphic in the complex cut-plane. In this method one works instead of with the divergent series (9) with its Borel transform

$$F(x) = \sum_0^\infty b_n x^n, \quad b_n = a_n/n!. \tag{11}$$

This expansion converges in the complex x-plane in the disc $|x| < R$ to the holomorphic function. One can show (see, e.g., [1]) that $F(x)$ could be analytically continued outside the disc to the x-plane with the cur $(-\infty, -R\rangle$. The analytical properties of $F(x)$ are shown in Fig. 1a.

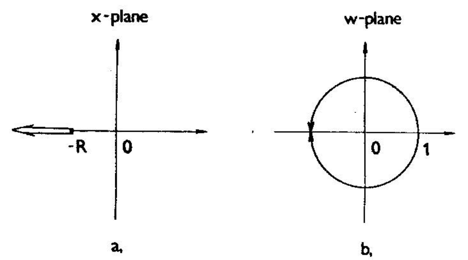

Fig. 1. The conformal mapping of the cut x-plane onto the unit disc in the w-plane.

We shall now construct the approximants $F_N(x)$ converging to $F(x)$ for all $x \geqslant 0$. Moreover, we shall require the linear dependence of $F_N(x)$ on $a_0, a_1, \ldots, a_N$ (the linearity requirement is a consequence of the linearity between $E(\lambda)$ and $F(x)$).

Such approximants could be constructed as follows. The complex x-plane with the cut $(-\infty, R\rangle$ is by the mapping

$$w = f(x) = \frac{\sqrt{(1 + x/R)} - 1}{\sqrt{(1 + x/R)} + 1} \tag{12}$$

conformally mapped onto the unit disc $|w| < 1$ in the w-plane, see Fig. 1b (in Eq. (12), the square root has the cut $(-\infty, -R\rangle$ and is positive for $x \in (-R, +\infty)$). The inverse mapping is

$$x = g(w) = 4Rw/(1 - w)^2. \tag{13}$$

The function $\Phi(w) = F(g(w))$ is holomorphic in the disc $|w| < 1$ and it could be expanded into the power series so that the partial sums

$$\Phi_N(w) = \sum_0^N c_n w^n \tag{14}$$

for $|w| < 1$ converge to the $\Phi(w) = \sum_0^\infty c_n w^n$. In the variable x it means that the approximants

$$F_N(x) = \sum_0^N c_n f^n(x) \tag{15}$$

converge in the cut x-plane (and especially for x real and positive) to the function

$$F(x) = \sum_0^\infty c_n f^n(x). \tag{16}$$

It remains to express the coefficients c_n as linear combinations of $b_0, \ldots, b_n$. In the neighbbourrhood of $w = 0$ both expansions (11) and (16) are convergent, i.e.

$$\sum_0^\infty b_n g^n(w) = \sum_0^\infty c_k w^k \tag{17}$$

(in the l. h. s. we put $x = g(w)$). The powers $g^n(w)$ are holomorphic for $|w| < 1$ and one can easily show that

$$g^n(w) = \sum_n^\infty g_k^{(n)} w^k, \tag{18}$$

where

$$g_k^{(n)} = (4R)^n (k + n - 1)!/(k - n)!. \tag{19}$$

From Eqs. (17)—(19) the desired relation is

$$c_k = \sum_0^k b_n g_k^{(n)}. \tag{20}$$

The Eq. (20) now determines the approximants (15) in terms of the coefficients $b_0, b_1, \ldots, b_N$.

The conditions i) and ii) mentioned in the introduction imposed on $F_N(x)$ are satisfied under weak assumptions about the behaviour of $F(x)$ on the cut i.e.

Table 1

The approximants $E_N(\lambda) - 1$ compared with the exact values $E(l) - 1$

N	$\lambda = 0.001$	$\lambda = 1.0$	$\lambda = 5.0$
1	−0.000186680	−0.109620	−0.259146
2	−0.000186662	−0.105196	−0.238472
3	−0.000186662	−0.106862	−0.252244
4	−0.000186662	−0.106629	−0.249383
5	−0.000186662	−0.106713	−0.251419
6	−0.000186662	−0.106698	−0.250839
7	−0.000186662	−0.106705	−0.251265
8	−0.000186662	−0.106704	−0.251130
9	−0.000186662	−0.106705	−0.251230
10	−0.000186662	−0.106704	−0.251171
Exact value	−0.000188768	−0.106723	−0.251241

about the $\Phi(w)$ on the circle $|w| = 1$. If e.g. $|F(x)| \leqslant M$ for $x \in (-\infty, -R\rangle$, then $|c_n| \leqslant M$ and one has $x \in (0, \infty)$ the estimate

$$|F(x) - F_N(x)| \mathrm{e}^{-x/\lambda} \leqslant \frac{M}{2}\left(1 + \sqrt{1 + \frac{x}{R}}\right) \mathrm{e}^{-x/\lambda} f^{N+1}(x).$$

where $f(x)$ is given in Eq. (12). This quarantees the required convergence. The corresponding Borel approximants

$$E_N(\lambda) = \sum_0^N c_n d_n(\lambda) \tag{21}$$

converge to the function $E(\lambda)$ given in Eq. (2). In the expression (21)

$$d_n(\lambda) = \frac{1}{\pi} \int_0^\infty \mathrm{e}^{-x/\lambda} f^n(x) \, \mathrm{d}x. \tag{22}$$

Now we shall test our method on the function

$$E(\lambda) = \sqrt{\frac{2}{\pi}} \int_0^\infty \exp\left(-\frac{1}{2}x^2 - \frac{\lambda}{16}x^4\right) \mathrm{d}x. \tag{23}$$

Expanding the factor $\exp\left(-\frac{\lambda}{16}x^4\right)$ we obtain a formal power expansion

$$E(\lambda) = 1 + \sum_1^\infty a_n \lambda^n$$

with the coefficients

$$a_n = (-1)^n n! \prod_{k=1}^n \left(1 - k^{-1} + \frac{3}{16}k^{-2}\right)$$

which has the asymptotics $a_n \sim -1)^n n!$. We can directly use the method described above. Table 1 contains approximative values $E_N(\lambda)$ for $N = 1, 2, \ldots, 10$, which are compared with $E(\lambda)$ obtained directly by numerical integration of (23).

III. APPLICATION TO THE ANHARMONIC OSCILLATOR

We shall determine the ground state energy $E(\lambda)$ of the anharmonic oscillator which corresponds to the normalized solution of the Schrödinger equation

$$\left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}x^2 + \lambda x^4\right)\Psi(x) = E\Psi(x) \tag{24}$$

with the lowest eigenvalue $E = E(\lambda)$. This problem cannot be solved exactly but the perturbative expansion

$$E(\lambda) = \frac{1}{2} + \sum_1^\infty a_n \lambda^n \tag{25}$$

is well known. In Ref. [3] the coefficients $a_1, a_2, \ldots, a_{75}$ in (25) were calculated. In Table 2 we give first 10 coefficients which we shall need later. Moreover, in [3] there is derived the asymptotic formula in which the dominant term is

$$a_n \sim (-3)^n n^{-1/2} n!. \tag{26}$$

Table 2

The perturbative coefficients for the ground state energy of the anharmonic oscillator

n	a_n	n	a_n
1	0.750000	6	−0.639828 10^5
2	−0.262500 10^1	7	0.132973 10^7
3	0.208125 10^2	8	−0.314482 10^8
4	−0.241289 10^3	9	0.833541 10^9
5	0.358090 10^4	10	−0.244789 10^{11}

From (26) it follows that our method is applicable. In Table 3 we give the approximants $E_N(\lambda)$ for $N = 1, 2, \ldots, 10$ and for different values of λ.

For the sake of completeness it is useful to describe briefly alternative methods used in [4] and [5], [6]. According to the former method [4], the

Table 3

The Borel approximants $E_N(\lambda) - 1/2$

N	$\lambda = 0.01$	$\lambda = 0.1$	$\lambda = 0.5$	$\lambda = 1.0$
1	0.00493942	0.0456778	0.1790112	0.292322
2	0.00493146	0.0450384	0.1704716	0.271344
3	0.00493178	0.0452482	0.1791938	0.302256
4	0.00493178	00452342	0.1774836	0.293796
5	0.00493178	0.0452358	0.1780510	0.297654
6	0.00493178	0.0452358	0.1780018	0.297200
7	0.00493178	0.0452358	0.1780108	0.297312
8	0.00493178	0.0452358	0.1780062	0.297236
9	0.00493178	0.0452358	0.1780098	0.297318
10	0.00493178	0.0452358	0.1780082	0.297272
N	$\lambda = 3.0$	$\lambda = 5.0$	$\lambda = 10.0$	$\lambda = 50.0$
1	0.548358	0.691076	0.894380	1.332250
2	0.483392	0.593046	0.739564	1.017578
3	0.631570	0.854202	1.229618	2.322664
4	0.570958	0.731258	0.960072	1.405536
5	0.611126	0.824060	1.195054	2.409000
6	0.604400	0.806422	1.143916	2.138580
7	0.606754	0.813376	1.166844	2.287100
8	0.604510	0.805980	1.139138	2.069160
9	0.607826	0.818176	1.190676	2.557840
10	0.605258	0.807660	1.140716	1.990442

Schrödinger equation (24) is first rewritten in the infinite matrix form

$$\sum_0^\infty H_{nk} \Psi_k = E \Psi_n, \quad n = 0, 1, 2, \dots \tag{27}$$

in the linear harmonic oscillator basis. The eigenvalues E correspond to zeros of the determinant

$$\det(H_{nk} - E\delta_{nk}) = 0. \tag{28}$$

In [4] the infinite matrix was approximated by the finite $m \circ m$ matrix and for any m the lowest solution $E^{(m)}$ of (28) was calculated. This m was successively increased up to a stable value $E^{(m)} \doteq E(\lambda)$. For $\lambda < 1$ it was enough to take $m \lesssim 20$. For $\lambda > 1$ in [4], the starting point was the equation

$$\left(-\frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}\omega^2 y^2 + y^4 \right) \varphi(y) = \varepsilon \varphi(y) \tag{29}$$

Table 4

The comparise of our values of the ground state energy $E(\lambda) = E_{10}(\lambda)$ with the same quantity determined in [4] and [5]

λ	$E_{10}(\lambda)$	$E(\lambda)$ from [4]	$E(\lambda)$ from [5]
0.1	0.54524	0.55915	
0.5	0.67801	0.69618	0.7017
1.0	0.79727	0.80377	0.8125
10.0	1.64072	1.50497	1.5313
50.0	2.49044	2.49971	

and similarly as before the lowest eigenvalue $\varepsilon = \varepsilon(\omega)$ was numerically determined. A simple scaling argument then gives

$$E(\lambda) = \lambda^{1/3} \varepsilon(\lambda^{-1/3}). \tag{30}$$

A different approach was proposed in Refs. [5], [6], where in the framework of the path-integral method an accurate estimate was found of the effective potential $W(x, \beta)$ defined by

$$\sum_{n=0}^{\infty} \exp(-\beta E_n) = \int \frac{dx}{\sqrt{2\pi}} \exp[-\beta W(x, \beta)].$$

The ground state energy was then calculated as

$$E_0 = \min_{\beta \to \infty} W(x, \beta).$$

The method was applied to the anharmonic oscillator in Ref. [5].

The methods used in [4], [5] are different from ours and consequently we can use the results obtained in [4], [5] as a test of our method. The results are compared in Table 4.

IV. CONCLUDING REMARKS

Let us investigate in more detail the problem of the optimization of approximants $F_N(x)$. Instead of using the mapping (12), we can use any confformal mapping $w = \tilde{f}(x)$ of a suitable domain $\tilde{D}$ onto the unit disc, which has the property $\tilde{f}(0) = 0$. The domain D should not contain the cur $(-\infty, -R\rangle$, but it should contain the half-line $\langle 0, \infty)$. The approximants then are

$$\tilde{F}_N(x) = \sum_0^N \tilde{c}_n \tilde{f}^n(x), \tag{31}$$

where the coefficients $\tilde{c}_n$ are determined by the comparison of the expansions

$$\sum_0^\infty b_n x^n = \sum_0^\infty \tilde{c}_n \tilde{f}^n(x)$$

in the neighbourhood of $x = 0$.

The approximants (31) are convergent in the domain $\tilde{D}$, i.e. $\tilde{F}_N(x) \to F(x)$ as $N \to \infty$ for $x \in \tilde{D}$. This means that to a larger domain $\tilde{D}$ there corresponds a larger domain of convergence of (31). Moreover, it was proved in [7] that the convergence $\tilde{F}_N(x) \to F(x)$ inside $\tilde{D}$ is asymptotically faster if $\tilde{D}$ is larger. The optimal $\tilde{D}$ then corresponds to the maximal admissible domain D, which is just the cut-plane assumed in Sect. 2.

Finally we note that a slight improvement of the described method is possible. Let us rewrite the asymptotic estimate (10) as

$$a_n \sim (-R)^{-n} \Gamma(1 + n + \alpha), \tag{32}$$

where the Γ-function is defined by the formula

$$\Gamma(z) = \int_0^\infty x^{z-1} e^{-x} \, dx$$

(the Eq. (31) follows from the fact that for a large n there holds $\Gamma(1 + n + \alpha) \doteq n! \, (n/e)^\alpha$). Instead of (2) it is more appropriate to use the generalized Borel transform $\tilde{F}(x)$ defined by

$$E(\lambda) = \lambda^{-1-\alpha} \int_0^\infty e^{-x/\lambda} x^\alpha \tilde{F}(x) \, dx. \tag{33}$$

The optimal approximants to $\tilde{F}(x)$ are

$$\tilde{F}_N(x) = \sum_0^N c_n f^n(x) \tag{34}$$

with $f(x)$ given by (12). The corresponding approximants of $E(\lambda)$ are

$$\tilde{E}_N(\lambda) = \sum_0^N c_n \tilde{d}_n(\lambda), \tag{35}$$

where

$$\tilde{d}_n(\lambda) = \lambda^{-1-\alpha} \int_0^\infty e^{-x/\lambda} x^\alpha f^n(x) \, dx. \tag{36}$$

The described modification improves the convergence $\tilde{F}_N(x) \to F(x)$ mainly in the neighbourhood of the cut $(-\infty, -R\rangle$. Since (33) contains integration over the interval $(0, \infty)$, the use of the modified Borel transformation has only a weak influence on the results.

Our aim was not to present a deep theory but to show how to proceed in practical applications using the method of the Borel summation. We applied it to the calculation of the ground state energy of an anharmonic oscillator starting from the divergent perturbative expansion. The method is quite simple, numerically modest and we have found a nice agreement with the results obtained by different methods.

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О СУММАЦИИ БОРЕЛА ДЛЯ РЯДОВ ТЕОРИИ ВОЗМУЩЕНИЙ

В статье детально описывается метод суммации Борела для рядов теории возмущений и его применение для вычисления энергии основного состояния ангармонического осциллятора. Получено хорошее согласие с результатами, которые были достигнуты другим методом.