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MATCHING SOLUTIONS BASED ON SMALL AND LARGE δ APPROACHES

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ABSTRACT

Two-point Padé and quasifractional approximations are matched in order to achieve uniform and suitable analytical solution. The introduced approach is applied to Thomas-Fermi and Schrödinger equations.

1. INTRODUCTION

In order to extract mostly required full information from a truncated perturbation series different summation methods are applied [1-7]. Unfortunately, those methods not always give the proper answer, especially if the number of truncated series terms is low [1-3, 5]. It occurs that very often more effective become the two-point Padé approximations. As it has been pointed out in reference [8] "There are cases in which both weak coupling and strong coupling expansions can be constructed. In such a case, it should be possible to apply summation techniques that use simultaneously information from the weak coupling as well as from the strong coupling expansion. Obviously, such a dual approach should at least in principle be capable of producing better results than a summation technique which only uses information from either the weak coupling or the strong coupling expansion".

If both a weak coupling and a strong coupling expansion is available, it is an obvious idea to use two-point Padé approximations (TPPA).

Evidently, the TPPA is also not a panacea. For example, one of the bottle neck's of the TPPA method is related to the presence of logarithmic components in numerous asymptotic expansions. Van Dyke [5] wrote: "A technique analogous to rational functions is needed to improve the utility of series containing logarithmic terms. No striking results have yet been achieved. We give an example of partial success". This problem is the most essential for the TPPAs, since one of the

limits ($\varepsilon \rightarrow 0$ or $\varepsilon \rightarrow \infty$) for a real physical problems gives expansions with logarithmic terms or other complicated functions. It is worth noting that in some cases the obstacles may be overcome by using an approximate method of TPPAs construction by taking as limit points not $\varepsilon = 0$ and $\varepsilon = \infty$, but some small and large (but finite) values [9]. On the other hand Martin and Baker [10] (see also [11]) proposed the so called quasifractional approximations (QAs). Let us suggest that we have perturbation approach in powers of ε for $\varepsilon \rightarrow 0$ and asymptotic expansions $F(\varepsilon)$ containing, for example, logarithm for $\varepsilon \rightarrow \infty$. By definition QA is a ratio R with unknown coefficients a_i, b_i , containing both powers of ε and $F(\varepsilon)$. The coefficients a, b are chosen in such a way, that (a) the expansion of R in powers of ε match the corresponding perturbation expansion; and (b) the asymptotic behaviour of R for $\varepsilon \rightarrow \infty$ coincides with $F(\varepsilon)$.

Quasifractional approximations include the a priori known elements of an analytical structure of solution. This main advantage sometimes leads directly to get qualitatively required results [12, 13].

2. ALGEBRAIC EQUATION

We begin with simple example [14, 15] of the following algebraic equation

$$x^n + x = 1. \quad (1)$$

We consider a positive root to equation (1).
We get

$$\begin{aligned} n=1 \quad x &= 0.5, \\ n=2 \quad x &= 0.5(\sqrt{5}-1) \approx 0.618034, \\ n=5 \quad x &= 0.76359. \end{aligned} \quad (2)$$

The small δ method is defined by an introduction of the artificial parameter in the following way

$$x(\delta) = 0.5 + 0.25 \ln 2\delta - 0.125 \ln 2\delta^2 + \dots \quad (3)$$

The radius of convergence of the series (3) is equal to 1, and for $\delta=1$ the first three terms of (3) gives $x=0.58664$. The error related to exact values equals $\sim 5.1\%$. For $\delta > 1$, for instance for $\delta=4$, one needs to include large number of the terms of the series (3) and apply the Padé transformation [14].

The series (1) can be transformed to the analytically equivalent form

$$x = 0.5 \exp(0.5 \ln 2\delta + \dots) \quad (4)$$

The alternative asymptotics related to artificial large parameter can be constructed for $n \rightarrow \infty$ [15]. Introducing $y = x^n$ and taking into account the series

$$y^{2/n} = 1 + \frac{1}{n} \ln y + \dots,$$

one gets

$$y \approx \left(\frac{\ln n}{n} \right)^n, \quad (5)$$

$$y \approx \left(\frac{\ln n - \ln \ln n}{n} \right)^{1/n}, \quad (6)$$

and so on.

For $n=2$ the formula (5) gives $x=0.58871$, which defines the error of $\sim 4.7\%$. For $n=5$ we have $x=0.79745$ with the error of $\sim 4.4\%$. The formula (6) for $n=5$ gives $x=0.74318$, with the error of $\sim 2.7\%$.

We construct a quasifractional approximation matching the first term of the series (3) and the asymptotics (5)

$$x \sim \left[\frac{0.5 + \delta \ln(\delta+1)}{1 + \delta(\delta+1)} \right]^{\frac{1}{1+\delta}}. \quad (7)$$

For $\delta=0$ the formula (7) gives exact value $x=0.5$ of the root. For $\delta=1$ we have $x=0.63065$, and the error $\sim 2\%$, whereas for $\delta=4$ we get $x=0.80137$ with the corresponding error $\sim 4.9\%$. The approximation accuracy can be increased using the formulas (4) and (6).

3. THOMAS-FERMI EQUATION

We consider a statistical model of a neutral atom governed by nonlinear Thomas-Fermi equation

$$\frac{d^2 \Phi(x)}{dx^2} = \frac{\Phi(x)^{3/2}}{\sqrt{x}} \quad (8)$$

with the boundary conditions

$$\Phi(0) = 1, \quad \Phi(\infty) = 0. \quad (9)$$

Here the function $\Phi(x)$ determines the joint nucleus and electrons charge density.

The boundary value problem (8), (9) do not have exact analytical solution. However, numerical solution can be found with great difficulty: in order to integrate from $x=0$ (using, for example, Runge-Kutta procedure) one must assume a value for $\partial\Phi(0)/\partial x$. If it is chosen to large, the solution will eventually become singular at some finite value of x in (8). On the other hand, if $\partial\Phi(0)/\partial x$ is chosen to small, the solution will cross below the x axis at some finite value of x and become complex. At the correct value $\partial\Phi(0)/\partial x = -1.5880710\dots$, the function $\Phi(x)$ decays smoothly and monotonically from $\Phi(0)=1$ to $\Phi(\infty)=0$. The number $\partial\Phi(0)/\partial x$ can be treated as a kind of eigenvalue. Its accurate calculation requires a large amount of computer time. This is not surprising because (8), (9) is a global problem whose solution is determined by boundary data from the widely separated points $x=0$ and $x=\infty$. Next we focus on evaluating $\Phi(x)$.

When $x \rightarrow 0$ there is a power series expansion [16]

$$\Phi(x) = 1 + a_1 x^{(1/2)} + a_2 x + a_3 x^{(3/2)} + \dots, \quad (10)$$

where coefficients a_i are determined from the iterative relations

$$\sum_{i=0}^j i(i-2)(5i-3j-6)a_i a_{j-i} = 0, \quad (11)$$

$$a_1 = 0, \quad a_2 = \frac{\partial\Phi(0)}{\partial x} = -1.5881, \quad a_3 = 4/3.$$

Sommerfeld developed asymptotic solution for $x \rightarrow \infty$ [16]:

$$\Phi(x) = (1 + 0.2783x^{0.772})^{-3.886}. \quad (12)$$

Let us point out that formula (12) satisfies the boundary conditions (9) at $x=0$, but it does not yield accurate results for small x . Sabirov proposed an empirical formula, valid for all values of x [16]:

$$\Phi(x) = \frac{144}{(x+b)^2} (1 + (1 + \alpha x^{(1/2)} + \beta x) \exp(-\gamma x^{(1/2)})), \quad (13)$$

where: $b=288^{(1/3)}$, $\alpha=\gamma=1.2098$, $\beta=-1.2247$. However, expression (13) at some points was matched to numerical data. Due to this, it may not be regarded as the universal solution.

Here we apply the method of quasifractional approximants. In the case $x \rightarrow 0$ we use five leading terms of series (8) up to x^2 order. For $x \rightarrow \infty$ a solution is obtained from expression (10) after asymptotically equivalent substitution

$$x^{0.772} \rightarrow x(1+x)^{-0.228}, \quad (14)$$

$$\Phi(x) = \left(1 + \frac{0.2783x}{(1+x)^{0.228}} \right)^{-3.886}. \quad (15)$$

On the basis of expansion (10) and formula (15), we derive the following QA:

$$\Phi(x) = \frac{1 + 0.1336x^{(1/2)} - 1.3038x + 0.9598x^{(3/2)} - 0.2523x^2 + x^{(5/2)}F'}{1 + 0.1336x^{(1/2)} + 0.2842x - 0.1614x^{(3/2)} + 0.0209x^2 + x^{(5/2)}F'} \quad (16)$$

$$\text{where: } F = (1 + 0.2783x(1+x)^{0.228})^{3.886}$$

Comparison with results of Sommerfeld (12) and Sabirov (13) is given in Table 1. The QA (16) provides us with the most accurate results for all values of x .

Table 1. Function $\Phi(x)$ for different values of x .

x	Numerical data	Sommerfeld's solution (3.5)	Sabirov's formula (3.6)	The QA (3.9)
0	1	1	1	1
0.1	0.8820	0.8360	0.8890	0.8820
0.5	0.6070	0.5560	0.6140	0.6110
1	0.4240	0.3850	0.4240	0.4310
2	0.2430	0.2210	0.2370	0.2450
3	0.1570	0.1430	0.1510	0.1560
4	0.1080	0.0990	0.1050	0.1070
5	0.0788	0.0720	0.0744	0.0772
10	0.0243	0.0230	0.0264	0.0235
15	0.0108	0.0102	0.0126	0.0104
25	0.0035	0.0033	0.0043	0.0033
40	0.0011	0.0011	0.0014	0.0011

4. LARGE δ METHOD

The problem of a strong coupling in the quantum theory belongs to one of the most important. In particular a special attention is focused on construction of the successive asymptotics to the Schrödinger equation

$$\psi_{xx} + x^{2N}\psi - E\psi = 0, \quad (17)$$

$$\psi(\pm\infty) = 0 \text{ for } N \rightarrow \infty. \quad (18)$$

In this work the new approach is developed which yields a series construction using directly the powers $1/N$ and achieving a success in low terms of perturbation approach.

For $N \rightarrow \infty$, from (17) and (18), we get

$$\psi_{xx} + E\psi = 0,$$

$$\psi(\pm 1) = 0.$$

A solution to the above problem defines the following energy levels

$$E_n = 0.25\pi^2(n+1)^2, \quad n=0,1,2,\dots$$

A comparison of E_0 with exact values (see Table 2) shows, that an acceptable accuracy is achieved only for large N , and therefore one needs to improve the solution.

Table 2. A comparison of the exact values of $E_0(N)$ obtained numerically¹⁸ with the predicted values obtained via various methods.

N	E_0 exact ¹⁸	(4.11)	Error %	(4.15)
1	1.0000	0.9100	9.00	160.65
2	1.0604	1.0422	1.72	4.1673
4	1.2258	1.2385	1.04	1.6678
10	1.5605	1.5831	0.81	1.6383
50	1.1052	2.1074	0.10	2.1094
200	2.3379	2.3382	0.02	2.3382
500	2.4058	2.4032	0.01	2.40586
1500	2.4431	2.4428	0.01	2.44309
3500	2.4558	2.4555	0.01	2.45576

Error %	(4.16)	Error %	(6.1)	Error %
15965.3	4.4729	347.292	1.0	0
292.992	1.9514	84.026	0.9974	5.9364
36.0619	1.5080	23.024	1.17446	4.1882
4.98517	1.6255	4.1654	1.5398	1.33
0.2012	2.1091	0.1840	2.1035	0.079
0.011	2.3381	0.011	2.3376	0.006
0.002	2.4058	0.002	2.4058	-0
-0	2.4431	-0	2.4431	-0
-0	2.4558	-0	2.4558	-0

Let us consider the function

$$\varphi = x^{2N} \text{ for } 0 \leq x \leq 1.$$

The series of $1/N$ of the function φ for large N reads

$$\begin{aligned} \varphi &= \delta(x-1)(2N+1)^{-1} - \delta^{(1)}(x-1)(2N+1)^{-1}(2N+2)^{-1} + \dots \\ &\dots - \delta^{(2N-1)}(x-1)(2N+1)^{-1}(2N+2)^{-1} \dots \\ &\dots \times (2N+i)^{-1} + \dots = \sum_{i=0}^{\infty} (-1)^i \delta^{(i)}(x-1) \times \\ &\times (2N+1)^{-1}(2N+2)^{-1} \dots (2N+i)^{-1}, \end{aligned} \quad (19)$$

where: $\delta(x)$ is the Dirac's function.

The above series (19) is obtained in the following way. First we use Laplace transform [17] (p is Laplace transform parameter):

$$\varphi \rightarrow p^{-2N-1} \gamma(2N+1, p).$$

Then we construct a series in relation to $1/(2N+1)$ of the obtained expression. Finally, we successively return back to the originals, in the space of generalized functions (more details are given, for instance, in reference [18]).

In the space $0 \leq x \leq 1$ the equation (17) has the form

$$\psi_{1xx} + \varphi\psi_1 - E\psi_1 = 0. \quad (20)$$

We look to its solutions in the following forms

$$\psi = \sum_{i=0}^{\infty} \psi_{1i} (2N+1)^{-1} \dots (2N+1+i)^{-1},$$

$$E = \sum_{i=0}^{\infty} E^{(i)} (2N+1)^{-1} \dots (2N+1+i)^{-1}.$$

Then, after splitting in relation to $(2N+1)^{-1}$, we get the following recurrent system of equations

$$-\psi_{10xx} - E^{(0)}\psi_{10} = 0, \quad (21)$$

$$-\psi_{1ixx} - E^{(i)}\psi_{1i} - E^{(i-1)}\psi_{10} + \delta(x-1)\psi_{10} = 0. \quad (22)$$

A solution to equation (21) in the case of symmetry in relation to the line $x=0$ has the form (an anti-symmetrical case is treated in the similar way):

$$\psi_1 = C \cos \lambda x,$$

$$\lambda = (E^{(0)})^{1/2}. \quad (23)$$

Let us consider now the space $x > 1$. In this case (in zero approximation) the term $E\psi_2$ can be omitted, and we obtain

$$\psi_{2xx} - x^{2N}\psi_2^{(0)} = 0. \quad (24)$$

We need to apply the decay condition of the form

$$\psi_2^{(0)} \rightarrow 0 \quad \text{for } x \rightarrow \infty. \quad (25)$$

A solution to equation (24) using the boundary condition (25) reads

$$\psi_2^{(0)} = C_1 x^{1/2} K_\nu(\nu x^{N+1}),$$

where: K_ν is the Bessel function, $\nu = 0.5/(N+1)$.

For $x=1$ the solutions ψ_1 and ψ_2 should be matched, and therefore for $x=1$ we get

$$\psi_1^{(i)} = \psi_2^{(i)},$$

$$\psi_{1x}^{(i)} = \psi_{2x}^{(i)}, \quad i = 0, 1, 2, \dots \quad (26)$$

The condition (26) for $i=0$ yields the following transcendental equation

$$-c \operatorname{tg} \lambda = \frac{4\lambda K_\nu(\nu)}{2K_\nu(\nu) - K_{1-\nu}(\nu) - K_{1+\nu}(\nu)} \quad (27)$$

for unknown λ . The minimal real solutions to this equation for different values of N are given in Table 2. They prove a high accuracy of the applied method.

Now we consider the problem related to construction of the successive approximations in the space $x > 1$. We define $\psi_2 = \bar{\psi}(\bar{x})$, where $\bar{x} = x^{N+1}/(N+1)$, and the following equation is obtained

$$\bar{\psi}_{\bar{x}\bar{x}} + N\bar{x}^{-N-1}\bar{\psi}_{\bar{x}} + E\bar{x}^{-2N}\bar{\psi} - \bar{\psi} = 0, \quad (28)$$

which defines the function $\bar{\psi}$. The functions x^{-2N} and x^{-N-1} are developed into the series of $1/(2N+1)$ and $1/(N+2)$ in a similar to earlier presented way, and they read

$$x^{-2N} = \sum_{i=0}^{\infty} (-1)^i \delta^{(i)} (1-1/x)(2N+1)^{-1} \times \dots (2N+1+i)^{-1}, \quad (29)$$

$$x^{-N-1} = \sum_{i=0}^{\infty} (-1)^i \delta^{(i)} (1-1/x)(N+2)^{-1} \times \dots (N+1+i)^{-1}. \quad (30)$$

Substituting expression (29) and (30) into equation (28) and matching in relation to $1/N$ we get a successive recurrent equations with the solutions defining the boundary conditions for $\psi_1^{(i)}$.

Next, a simultaneous solution to the systems (22) and (28) gives a possibility to define the improved values of E . Using the successive matching the following function has been obtained [19]

$$E_n(N) = \frac{\pi^2}{4} (n+1)^2 (2N)^{-1} \Gamma\left(\frac{N}{N+1}\right)^2 \left(\sum_{i=0}^{\infty} A_i(n) N^{-i} \right)^2, \quad (31)$$

where:

$$A_0(n) = 1; \quad A_1(n) = 0; \quad A_2(n) = 1 - 0.5\xi(2);$$

where ξ denotes the Riemann's ξ -function. In Table 2 the calculating results of $E_0(N)$ using the formula (31) with five first terms and then the Padé approximant (2) are reported [19].

Using only first term of the series (31) we obtain

$$E_0(N) = \frac{\pi^2}{4} (2N)^{-1} \Gamma\left(\frac{N}{N+1}\right)^2. \quad (32)$$

The calculation results using formula (32) are presented in Table 2.

Let us compare two methods [19, 20]. In the reference [19] a successive procedure of matching of asymptotic series is presented. However, at least five first series terms are needed and then the Padé approximation is applied in order to get good results.

A direct matching of solutions in different zones with the yielded transcendental equation [20] solution gives suitable results already in the first step of approximation (see Table 2).

5. SCHRÖDINGER EQUATION: SMALL δ APPROACH

We consider the following form of the Schrödinger equation

$$\psi_{xx} - x^{2+\delta}\psi + E\psi = 0.$$

Using the series

$$x^{2\delta} = 1 + \delta \ln(x^2) + \dots$$

we develop the being sought both eigenfunction ψ and the eigenvalue E into the series

$$\psi = \psi_0 + \delta\psi_1 + \delta^2\psi_2 + \dots \quad (33)$$

$$E = E_0 + \delta E_1 + \delta^2 E_2 + \dots \quad (34)$$

In result we get the following recurrent system of boundary value problems related to eigenvalues

$$\psi_{0xx} - x^2\psi_0 + E_0\psi_0 = 0, \quad (35)$$

$$\psi_{1xx} - x^2\psi_1 + E_0\psi_1 + E_1\psi_0 = x^2\psi_0 \ln(x^2), \quad (36)$$

$$|\psi_i| \rightarrow 0 \text{ for } |x| \rightarrow \infty, \quad i = 1, 2, 3, \dots \quad (37)$$

A solution to the boundary value problem (35), (37) has the form

$$E_0^{(n)} = 2n + 1; \quad \psi_0^{(n)} = \bar{c} x^{1/2} H_n(x), \quad n = 0, 1, 2, \dots$$

The boundary value problem (36), (37) yields

$$E_1^{(n)} = \frac{\int_{-\infty}^{\infty} x^2 e^{-x^2} H_n^2(x) \ln(x^2) dx}{\sqrt{\pi} 2^n n!}.$$

For $n=0$ we get $H_0(x) = 1$ and (see [17])

$$\int_{-\infty}^{\infty} x^2 \ln x e^{-x^2} dx = \frac{\sqrt{\pi}}{8} (2 - 2 \ln 2 - C),$$

where: $C = 0.577215\dots$ is the Euler's constant.

Therefore

$$E_0^{(0)} = 1 + \frac{1}{16} (2 - 2 \ln 2 - C) \delta + \dots \quad (38)$$

2. MATCHING PROCEDURE

Matching for small and large δ can be obtained in various ways. The most simply procedure is related to matching of formula (32) and of the first term of the series (38) related to eigenvalue for small δ .

Using the solution

$$E_0(N) \sim \frac{\pi + \Gamma\left(\frac{N}{N+1}\right)^2}{4(2N + \alpha)^{N+1}}, \quad (39)$$

we get $\alpha = \pi^2 \Gamma(1.25) - 2 \approx 6.946$. The computational results due to formula (39) are given in Table 2.

The second possibility concerns a matching of solutions (34) and (31).

2. CONCLUSION

It has been shown that the matching using two-point Padé approximations and quasifractional approximations can be widely used during construction of the $1/N$ expansions. The presented approach is also applicable to the strong coupling

problems and even in all cases, where two limiting series in relations to any parameter can be constructed [21].

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