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Inversion of the perturbation series

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Abstract
We investigate the inversion of the perturbation series and its resummation, and prove that it is related to a recently developed parametric perturbation theory. Results for some illustrative examples show that in some cases series reversion may improve the accuracy of the results.

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1. Introduction

Perturbation theory yields the solution of a problem in the form of a power series of a properly chosen model (or dummy) parameter. When the convergence radius of this series is too small for the physical application, or the series converges too slowly, it is customary to resort to a resummation method that produces an approximant that improves the results. There are many approaches for that purpose; among them we mention Padé approximants, Borel summation, algebraic approximants, continued fractions, nonlinear transformations of the expansion parameter, etc [1–3].

The purpose of this paper is to investigate the application of a well–known mathematical method, named series reversion or series inversion [4–6], to perturbation theory. In section 2, we outline the main ideas of the approach, in section 3, we show the connection between the method of series reversion and a recently developed parametric perturbation theory [7–9]. In section 4, we compare the accuracy of resummation of the direct and inverse series for some illustrative examples. Finally, in section 5, we draw some conclusions about the usefulness of the approach.

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2. Inversion of series

Suppose that we are trying to estimate accurate values of an unknown function $E(g)$ from a few available coefficients of its power series:

$$E(g) = \sum_{j=0}^{\infty} E_j g^j. \tag{1}$$

When the convergence radius of this series is too small for the physical application, or the series converges too slowly, it is custommary to resort to a resummation method that produces an approximant $E \approx A_E^{[N]}(g)$ from the partial sum of order N: $S_N = E_0 + E_1 g + \cdots + E_N g^N$ [1–3].

It is always possible to invert the series (1) and obtain g in terms of $\Delta E = E - E_0$ [4–6]:

$$g = \Delta E \sum_{j=0}^{\infty} G_j \Delta E^j = \frac{\Delta E}{E_1} - \frac{E_2 \Delta E^2}{E_1^3} + \frac{\left(2E_2^2 - E_1 E_3\right)\Delta E^3}{E_1^5} + \cdots. \tag{2}$$

If we apply a resummation method to this series we obtain an approximation of the form $g \approx A_g^{[N]}(\Delta E)$. This strategy may give more accurate results than the former one if the radius of convergence or the region of utility of the series (2) is greater than that of the direct expansion (1). However, even in this favorable situation we are paying the price of having the inverse of the desired function.

In order to get some motivation for the use of the inverse series, consider the function

$$E = \sqrt{1+g} = 1 + \tfrac{1}{2}g - \tfrac{1}{8}g^2 + \cdots \tag{3}$$

that is real for all $g > -1$. The Taylor series about $g = 0$ converges only for $|g| < 1$ because of the branch point at $g = -1$. However, the inverse series $g = 2\Delta E + \Delta E^2$ converges for all ΔE suggesting that in some cases it is convenient to use the latter instead of the former.

3. Parametric perturbation theory

In what follows we show that the inversion of series is related to a recently developed parametric perturbation theory [7–9]. If we define the parameter $\rho = \Delta E/E_1$ then

$$g = \rho \sum_{j=0}^{\infty} G_j E_1^{j+1} \rho^j = \rho - \frac{E_2 \rho^2}{E_1} + \frac{\left(2E_2^2 - E_1 E_3\right)\rho^3}{E_1^2} + \cdots. \tag{4}$$

Application of a resummation method gives an expression for g in terms of the parameter ρ:

$$g \approx A_g^{[N]}(E_1 \rho) \tag{5}$$

which together with

$$E = E_0 + E_1 \rho \tag{6}$$

define an approximate parametric representation of $E(g)$. These equations are the basis of the so-called parametric perturbation theory developed recently by Amore [7–9] from a principle of absolute simplicity.

More precisely, in parametric perturbation theory one introduces an approximant $g = A^{[N]}(\rho)$ into the direct expansion (1) and chooses the approximant coefficients so that $E = b_0 + b_1 \rho + [\rho^{N+1}]$. Since the approximant is constructed so that $A^{[N]}(\rho) \approx \rho$ for $\rho \ll 1$ [7–9] then we realize that $b_0 = E_0$ and $b_1 = E_1$, and conclude that parametric perturbation theory is basically the inversion of the perturbation series.

In order to see the connection more clearly consider the trivial example (3) again. If we substitute $\rho + c_2\rho^2 + \cdots + c_N\rho^N$ for g into the series (3) and choose the coefficients c_j in order to remove the terms of order greater that one, we obtain $c_2 = 1/4$ and $c_j = 0$, $j > 2$. The resulting expressions $E = 1 + \rho/2$ and $g = \rho + \rho^2/4$ exactly agree with the inverse series shown above.

In some cases one easily estimates a range of utility of the parametric representation of $E(g)$. For example, suppose that we know that $\mathrm{d}E/\mathrm{d}g < 0$ (> 0), then $E_1 < 0$ (> 0). In both cases the range of utility of the approximant $g \approx A^{[N]}(\rho)$ is determined by the conditions $\rho > 0$ and $\mathrm{d}g/\mathrm{d}\rho > 0$.

4. Examples

As an illustrative example we consider the integral

$$E(g) = \int_0^\infty \mathrm{e}^{-x^2 - gx^4}\,\mathrm{d}x. \tag{7}$$

The formal expansion

$$E(g) = \frac{\sqrt{\pi}}{2}\left(1 - \frac{3g}{4} + \frac{105g^2}{32} - \frac{3465g^3}{128} + \frac{675\,675g^4}{2048} - \frac{43\,648\,605g^5}{8192} + \cdots\right) \tag{8}$$

is known to diverge for all values of g [2] which is reflected by the form of the expansion coefficients $E_n = (-1)^n\Gamma(2n + 1/2)/[2(n!)]$. We can rewrite the inverse expansion

$$g(\Delta E) = -\frac{8\Delta E}{3\sqrt{\pi}} + \frac{280\Delta E^2}{9\pi} - \cdots \tag{9}$$

in terms of the parameter $\rho = -3\sqrt{\pi}\Delta E/8$ as

$$g(\rho) = \rho + \frac{35\rho^2}{8} + \frac{35\rho^3}{16} + \frac{17\,675\rho^4}{256} - \frac{263\,095\rho^5}{256} + \cdots. \tag{10}$$

In this case we have

$$E(\rho) = \frac{\sqrt{\pi}}{2} - \frac{3\sqrt{\pi}\rho}{8}. \tag{11}$$

The pair of equations for $g(\rho)$ and $E(\rho)$ are a parametric representation of the function $E(g)$.

For simplicity we restrict to series of order five with the purpose of illustrating some ways of constructing the approximants. In order to determine the range of applicability of the ρ-series we take into consideration that $\mathrm{d}g/\mathrm{d}\rho > 0$ for all $\rho > 0$. Therefore, we assume that it may be reasonable to use the parametric representation for all $0 < \rho < \rho_m$, where ρ_m is the smallest positive root of $\mathrm{d}g/\mathrm{d}\rho = 0$. In the case of the partial sum of order five (10) we have $\rho_m = 0.1659$ that leads to $g_m = g(\rho_m) = 0.2194$. Table 1 shows that the parametric representation embodied in equations (10) and (11) yields better results than the direct g-power series (8), at least for all $g < g_m$.

We can improve the accuracy of the results by means of resummation methods. For simplicity we try Padé approximants [1, 2] built from the g-series and ρ-series of order five shown above. Since $E(g \to \infty) = 0$ we choose the [2/3] Padé approximant

$$E \approx \frac{2\sqrt{\pi}(115\,460\,139g^2 + 28\,532\,448g + 1163\,200)}{141\,105\,195g^3 + 534\,788\,100g^2 + 117\,619\,392g + 4652\,800}. \tag{12}$$

The [2/3] Padé approximant for the inverse series

$$g = \frac{16\rho(219\,707\rho + 15\,640)}{26\,152\,805\rho^3 - 11\,137\,140\rho^2 + 2420\,512\rho + 250\,240} \tag{13}$$

Table 1. Series expansions of order five for the integral (7).

g	ρ	Equation (8)	Equation (10)	Exact
0.04	0.227 268 254	0.863 022 3905	0.863 217 2917	0.863 228 1022
0.08	0.221 197 9138	0.835 883 9701	0.844 769 0498	0.844 994 1504
0.12	0.213 865 426	0.750 015 5805	0.828 552 4745	0.829 688 3134
0.16	0.204 317 9764	0.452 537 4722	0.750 422 8564	0.816 422 8001
0.2	0.189 165 5735	-0.365 537 6234	0.760 494 2069	0.804 680 5576

Table 2. Padé approximants [2/3] for the integral (7).

g	ρ	Equation (12)	Equation (13)	Exact
0.1	0.074 198 513 29	0.836 884 189	0.836 909 3852	0.837 042 9277
0.2	0.124 755 604	0.803 286 224	0.803 305 5939	0.804 680 5576
0.3	0.166 889 096	0.776 055 4974	0.775 300 7175	0.780 043 4542
0.4	0.206 990 6611	0.752 362 5938	0.748 646 4025	0.760 035 8198
0.5	0.251 505 9286	0.731 012 4346	0.719 058 431	0.743 155 4088
0.6	0.392 980 645	0.711 393 8594	0.625 024 4038	0.728 543 9429

Table 3. Padé approximant [2/3] for the g-series and [3/2] for the inverse series of the integral (7).

g	ρ	Equation (12)	Equation (14)	Exact
0.1	0.074 045 208 14	0.836 884 189	0.837 011 2825	0.837 042 9277
1	0.307 904 2644	0.644 683 1837	0.681 572 1382	0.684 213 4278
10	0.604 380 6547	0.214 262 8036	0.484 513 1183	0.460 980 4743
100	0.706 145 4902	0.028 014 053 74	0.416 873 0654	0.277 288 4009
1000	0.719 672 7352	0.002 890 400 973	0.407 881 9088	0.159 480 8649
10 000	0.721 073 2433	0.000 289 961 386	0.406 951 0328	0.090 335 022 45

presents a maximum at $\rho_m = 0.360$ where $g_m = 0.607$. Table 2 shows that the Padé approximant for the direct series is more accurate than the one for the inverse series.

The [3/2] Padé approximant

$$g = \frac{\rho(15\,904 + 318\,204\rho + 747\,223\rho^2)}{15\,904 + 248\,624\rho - 375\,297\rho^2} \tag{14}$$

exhibits a pole at $\rho_0 = 0.721$ and we can therefore use this parametric representation for all $0 < g < \infty$ when $0 < \rho < \rho_0$. The main limitation of this approach is that $E(g \to \infty) = E_0 + E_1\rho_0 = 0.407$. Table 3 shows that the inverse series is slightly more accurate for small g but leads to a wrong limit. On the other hand, the direct series approaches the correct limit too fast as $1/g$.

The approximants so far used do not take into consideration the asymptotic behavior $E(g) \sim g^{-1/4}$ as $g \to \infty$. In the case of the direct series, we may calculate $[N/N+1](g)$ Padé approximants for $E(g)^4$ and then use $[N/N+1](g)^{1/4}$ as a reasonable approximation; for example

$$E \approx \frac{\sqrt{\pi}}{2}\left(\frac{116\,949g^2 + 27\,216g + 1060}{218\,277g^3 + 190\,647g^2 + 30\,396g + 1060}\right)^{1/4}. \tag{15}$$

Table 4. Improved Padé approximants [2/3] for the integral (7).

g	ρ	Equation (15)	Equation (16)	Exact
0.1	0.073 564 026 68	0.836 944 5716	0.837 331 1095	0.837 042 9277
1	0.289 244 6121	0.671 580 9835	0.693 974 6529	0.684 213 4278
10	0.582 853 7448	0.419 825 1659	0.498 821 4137	0.460 980 4743
100	0.037 234 840 95	0.239 386 0646	0.861 478 0364	0.277 288 4009
1000	0.037 373 191 61	0.134 810 1326	0.861 386 0789	0.159 480 8649
10 000	0.037 373 191 61	0.075 820 233 69	0.861 386 0789	0.090 335 022 45

Table 5. Improved Padé approximant [3/2] for the inverse series of the integral (7).

g	ρ	Equation (17)
0.1	0.074 043 457 42	0.837 012 4462
1	0.317 028 1954	0.675 507 7332
10	0.809 151 3837	0.348 408 1181
100	0.005 450 129 21	0.882 604 387
1000	0.005 450 129 21	0.882 604 387
10 000	0.005 450 129 21	0.882 604 387

We do not know how to obtain reasonable approximants for the inverse series; for that reason we try Amore's approach $g(\rho) = \rho[N/N+1](\rho)^5$; for example,

$$g = \frac{-1048\,576\rho(24\,078\,737\,127\rho^2 + 4884\,321\,032\rho + 161\,747\,680)^5}{(240\,656\,732\,281\rho^3 - 321\,691\,293\,064\rho^2 - 75\,884\,668\,992\rho - 2587\,962\,880)^5} \tag{16}$$

constructed from the ρ-series of order six. One realizes that this is the parametric perturbation approach proposed by Amore [7–9] for this particular case. In the neighborhood of the pole $\rho = \rho_0$ closest to origin this approximant behaves as $g \approx K_0(\rho - \rho_0)^{-5}$ so that $E(g) \approx E_0 + E_1\rho_0 + E_1 K_0^{1/5} g^{-1/5}$. We appreciate that this parametric representation tends to a wrong limit (because $E_0 + E_1\rho_0 \neq 0$ in general) and in a wrong way. Table 4 shows that these approximants are more accurate than the previous ones, as expected, and that the direct series is clearly better than the inverse one. Note that the parametric representation gives the wrong limit $E(g \to \infty) = 0.861$. Besides, remember that we need perturbation coefficients of order five and six of the direct and reverse series, respectively, in the construction of such approximants.

Following the same philosophy we have also tried [3/2] approximants for the reverse series

$$g = \frac{\rho(583\,627\,586\,759\rho^3 + 767\,002\,386\,296\rho^2 + 44\,364\,247\,040\rho - 265\,333\,760)^5}{32\,768(290\,961\,289\,397\rho^2 + 5574\,551\,760\rho - 33\,166\,720)^5}. \tag{17}$$

Table 5 shows that this parametric representation yields better results than the preceding one, but it also leads to a wrong limit: $E(g \to \infty) = 0.883$.

The polylogarithm function

$$Li_s(z) = \frac{z}{\Gamma(s)} \int_0^\infty \frac{t^{s-1}}{e^t - z}\, dt \tag{18}$$

Table 6. Values of $Li_{3/2}(g)$ for g close to 1 obtained from Padé approximants on the direct and inverse series. Exact figures are underlined for comparison.

g	$[6/7](g)$	$[5/6](\rho)$	Exact
0.999 999	2.380 740 506	2.608 744 256	2.608 831 900
0.999 99	2.380 591 082	2.601 153 011	2.601 179 942
0.9999	2.379 099 267	2.577 063 920	2.577 071 427
0.999	2.364 418 183	2.501 706 883	2.501 708 465
0.99	2.237 103 024	2.271 659 944	2.271 660 077
0.9	1.614 336 255	1.614 438 528	1.614 438 529

appears in several fields of theoretical physics, for example, in the Bose–Einstein and Fermi–Dirac distributions [10]. The Taylor expansion of this function about $z = 0$ yields the series

$$Li_s(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^s}. \tag{19}$$

In this case the inverse series gives more accurate results than the direct one and, consequently, we draw the same conclusion regarding the Padé approximants constructed from them. Table 6 shows that the Padé approximant $[5/6](\rho)$ for the former series gives considerably more accurate results than the $[6/7](g)$ Padé approximant for the latter one.

The formal Taylor series about $g = 0$ for the function

$$E(g) = \int_0^{\infty} \frac{\mathrm{e}^{-x}}{1 + gx}\,\mathrm{d}x \tag{20}$$

is divergent as shown by its coefficients $E_n = (-1)^n n!$. The asymptotic behavior at $g \gg 1$ is given by

$$E(g) \approx \frac{\ln(g) - \gamma}{g} + \frac{\ln(g) - \gamma + 1}{g^2} + \cdots \tag{21}$$

where $\gamma = 0.577\,215\,6649\ldots$ is Euler's constant. In this case the inverse series is more accurate than the direct one, and exactly the same situation takes place for their corresponding Padé approximants.

As another illustrative example consider the function $E(g)$ defined by $g = E\,\mathrm{e}^{-E}$. The power series $E(g) = g + g^2 + 3g^2/2 + \cdots$ converges for $g < \mathrm{e}^{-1}$ which is reflected by the form of the expansion coefficients $E_n = n^{n-1}/n!$, $n \geqslant 1$. On the other hand, the inverse series $g = E - E^2 + \cdots + (-1)^{n-1}E^n/(n-1)! + \cdots$ converges for all E and is therefore preferable for practical applications. However, it is not always true that the inverse series have greater convergence radius than the direct one; simply consider the function $E(g) = g\,\mathrm{e}^{-g}$, where the role of the variables has been reversed. In this case parametric perturbation theory will perform poorer than standard perturbation theory.

5. Conclusions

In this paper, we investigated the usefulness of the inversion of the perturbation series and its resummation. Our simple examples show that in some cases it is convenient to resort to the inverse series, but in others the straightforward perturbation series is expected to provide better results. We have also proved that the recently proposed parametric perturbation theory [7–9], based on the principle of absolute simplicity, consists of a convenient modification and resummation of the inverse series. Therefore, in some cases this approach will not perform better than well-known resummation methods on the direct series. In addition to it, parametric perturbation theory exhibits two disadvantages: producing the inverse of the desired function, and the difficulty of deriving the correct asymptotic limit and behavior when it is known.

References

[1] Bender C M and Orszag S A 1978 *Advanced Mathematical Methods for Scientists and Engineers* (New York: McGraw-Hill)

[2] Arteca G A, Fernández F M and Castro E A 1990 *Large Order Perturbation Theory and Summation Methods in Quantum Mechanics* (New York: Springer)

[3] Fernández F M 2000 *Introduction to Perturbation Theory in Quantum Mechanics* (Boca Raton: CRC Press)

[4] Ahlfors L V 1953 *Complex Analysis* (New York: McGraw-Hill)

[5] Morse P M and Feshbach H 1953 *Methods of Theoretical Physics* (New York: McGraw-Hill)

[6] Abramowitz M and Stegun I A 1972 *Handbook of Mathematical Functions* (New York: Dover)

[7] Amore P 2007 A new approach to resummation *Parametric Perturbation Theory* (*Preprint* 0705.1166)

[8] Amore P 2007 Going beyond perturbation theory *Parametric Perturbation Theory* (*Preprint* 0705.1168)

[9] Amore P 2007 *Phys. Rev.* D **76** 076001

[10] McQuarrie D A 1976 *Statistical Mechanics* (New York: Harper and Row)