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Information Content of the Born Series[1]

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ABSTRACT

It is a commonplace observation that if one tries to extrapolate a function to points far away from the region where the function is known, the results may be very sensitive to slight changes in the known values. A numerical example is used to show how very serious this problem may become when one attempts to extrapolate the Born series for scattering by strong potentials.

INTRODUCTION

The subject of perturbation theory, and particularly the Born series for general scattering problems, is given very great weight in most studies of quantum mechanics. As students we are told that the method is useful only when the perturbation is weak, yet so often we see the Born approximation used when the interaction is in fact strong. The excuses for this are that (a) the computation of a low-order Born approximation is the simplest calculation one can do, and (b) in some problems, e.g., quantum field theory, it may be the only well-definied procedure we have for doing any calculations at all. Recently there have appeared some very interesting attempts to build a proper theoretical basis for the use of Born calculations in strong interactions. In particular the analysis of Weinberg [1] for the case of potential scattering has shown

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what the divergence of the Born series really means. Now other authors [2, 3] are proposing to use such methods as the Padé approximation to carry the useful range of the Born series well beyond its ordinary limits. In this paper we shall suggest via the study of an example how unpractical this program may be.

I. The Example

For a numerical example we have studied the scattering by an attractive Yukawa potential at zero energy. The Schrodinger equation is

$$\left(-\frac{1}{r}\frac{d^2}{dr^2}r - g\frac{\exp(-r)}{r} - k^2\right)\psi(r) = 0, \tag{1}$$

and the Born series for the scattering amplitude (purely s-wave at $k = 0$) is

$$f(g) = \sum_{n=1}^{\infty} g^n T_n. \tag{2}$$

In Appendix A we describe how the terms T_n were calculated; the results are shown in Table I. The first four terms may be easily calculated analytically, and we conclude that the computer outputs shown in this Table are accurate to six or seven figures. At first one would imagine that this list of terms of the Born series contains a great deal of useful information. However, we shall now see that this is not the case.

In Table I are also shown ratios of successive terms T_n, and we see that beyond $n = 13$ these ratios do not change (within the accuracy which we have available here). This may be understood as follows. We know [1] that the function $f(g)$ has simple poles at those (positive) values of g for which the potential becomes just strong enough to accommodate one more bound state. Suppose these critical values of g are ordered

$$g_1 < g_2 < g_3 < \cdots, \tag{3}$$

then we may expect to represent the scattering amplitude in the functional form

$$f(g) = -g\left[\frac{r_1}{g-g_1} + \frac{r_2}{g-g_2} + \frac{r_3}{g-g_3} + \cdots\right]. \tag{4}$$

TABLE I

COMPUTED VALUES OF TERMS OF THE BORN SERIES FOR ZERO ENERGY SCATTERING IN A YUKAWA POTENTIAL. ALSO SHOWN ARE RATIOS OF SUCCESSIVE TERMS

n	T_n	$R_n = T_n/T_{n-1}$
1	1.00000000	
2	0.49999981	0.49999981
3	0.28768183	0.57536387
4	0.16989880	0.59057884
5	0.10094108	0.59412477
6	$0.60060339 \times 10^{-1}$	0.59500387
7	$0.35749587 \times 10^{-1}$	0.59522785
8	$0.21281215 \times 10^{-1}$	0.59528563
9	$0.12668721 \times 10^{-1}$	0.59530063
10	$0.75417472 \times 10^{-2}$	0.59530454
11	$0.44896442 \times 10^{-2}$	0.59530558
12	$0.26727114 \times 10^{-2}$	0.59530584
13	$0.15910809 \times 10^{-2}$	0.59530592
14	$0.94717993 \times 10^{-3}$	0.59530593
15	$0.56386181 \times 10^{-3}$	0.59530591
16	$0.33567026 \times 10^{-3}$	0.59530589
17	$0.19982649 \times 10^{-3}$	0.59530592
18	$0.11895789 \times 10^{-3}$	0.59530593
19	$0.70816337 \times 10^{-4}$	0.59530588
20	$0.42157384 \times 10^{-4}$	0.59530590
21	$0.25096540 \times 10^{-4}$	0.59530592

Equation (4) gives the following representation for the Born terms:

$$T_n = \frac{r_1}{(g_1)^n} + \frac{r_2}{(g_2)^n} + \frac{r_3}{(g_3)^n} + \dots, \tag{5}$$

so that for large n we expect the ratios

$$R_n = T_n/T_{n-1} = g_1^{-1} + 0[(g_1/g_2)^n] \tag{6}$$

to approach g_1^{-1} quite rapidly as n increases. We can thus pick out from the tail end of Table I the value

$$g_1 = +\ 1.679809, \tag{7}$$

which is, to the best of our knowledge, the most accurate determination of this critical number. The residue is found to be

$$r_1 = 1.349179. \tag{8}$$

We would now like to look at the higher terms of (4) by considering

$$f'(g) = f(g) + \frac{gr_1}{g - g_1} \tag{9}$$

or

$$T_n' = T_n - \frac{r_1}{(g_1)^n}. \tag{10}$$

When we carry out this subtraction the lower half of the data in Table I disappears (to 7 or 8 figures), and what remains allows us to find the second pole to only a few tenths of 1% accuracy:

$$g_2 = +6.47, \qquad r_2 = 0.780. \tag{11}$$

Again subtracting this second pole term, what remains is just enough to indicate that g_3 is around $+20$ (to one significant figure).

What conclusions do we draw from the above numerical game? The Born series is an expansion about $g = 0$. By knowing the analytical structure of the function $f(g)$ we can use the terms T_n to learn about $f(g)$ outside the radius of convergence (g_1) of the series; however, if we try to stretch too far away, the predictions become very sensitive to the accuracy with which the terms T_n are known. (The tail wags the dog.) Now we turn to another method of using the data of Table I.

II. The Padé Approximation

A popular method for extending the usefulness of a power series expansion is the Padé method [4]. At the Nth approximation we represent the Born series (2) by the quotient of polynomials

$$P_N(g) = \frac{\sum_{n=0}^{N} a_n g^{n+1}}{1 + \sum_{n=1}^{N} b_n g^n}, \tag{12}$$

where the coefficients a_n and b_n are determined by fitting the power series expansion of $P_N(g)$ to the first $2N + 1$ terms of (2). The results of this procedure are shown in Fig. 1. The heavy curve shows the correct function $f(g)$ as obtained by directly integrating the Schrodinger equation, and the double arrows indicate the positions of the first four

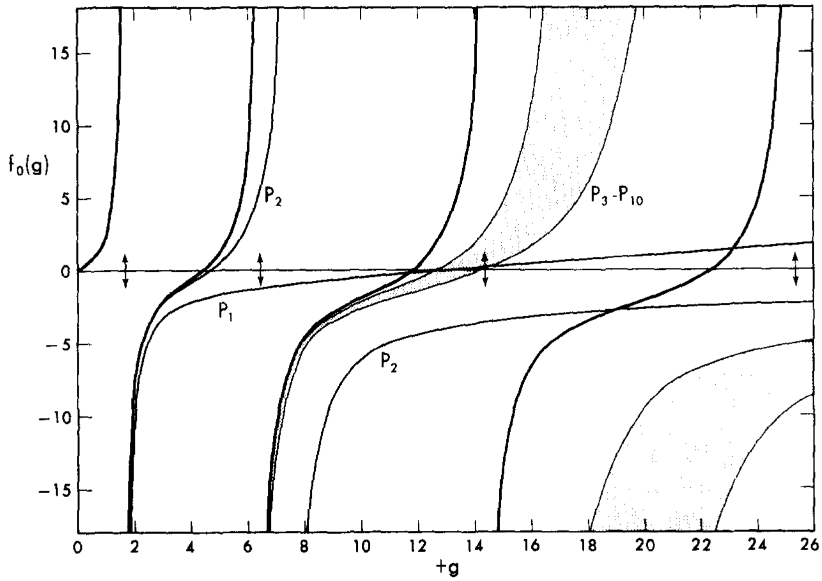

FIG. 1. Successive Padé approximations to the zero energy scattering amplitude for a Yukawa potential, as a function of the potential strength parameter g. The heavy curve is the exact result.

poles. The Padé approximants were determined using as inputs the values of T_n given in Table I. P_1 is seen to locate the first pole (g_1) fairly well, but it is not useful much beyond that point. The curve P_2 is better, giving g_2 accurate to about 15%. All the higher order approximants, $N = 3$ through 10, are contained within the shaded region. The separate curves do not converge smoothly within this region, but rather jump about; this is presumably due to the imperfect numerical accuracy of the input numbers T_n and the numerical process for evaluating P_N. On the basis of these curves one would predict g_3 to be around 19, but with a rather large uncertainty; this is essentially the same conclusion as was drawn in the previous section. Actually $g_3 = 14.4$, and we must conclude that the prediction of the Padé method for this problem are useless beyond about $g = 11$. (Near $g = 14$ we would predict an antiresonance, when in fact there is a resonance.)

The reason why we get unreliable predictions at large g is that the input values of the Born terms are not exact. One expects to pay some price for finite numerical accuracy, but it is very sobering to realize just how sensitive the distant extrapolation is to very small changes in the values of the Born terms.

We have not attempted a numerical analysis of this procedure to answer such questions as "How is it that the number $g_3/g_1 \cong 8.6$ implies the numerical error figure $\sim 10^7$?" The Padé method has been very successful in other problems [4][2] of finding a singularity in a function, given several terms of its power series about some distant origin. Perhaps the difficulty with the scattering problem is that one can say nothing about $f(g)$ for $g \to \infty$, and this lack of constraint on P_N leads to the troubles we have found.

III. Summary

While our example was taken from potential scattering, we are not really interested in solving such simple (two-) one-body problems: any method works, and directly integrating the Schroinger equation is still the easiest method to answer all numerical questions. The hard and interesting problems we think of involve several bodies interacting with strong forces. What we want to calculate are bound state eigenvalues and scattering state phase shifts. The Born series is not at all useful in finding the former. Let us now consider the practicalities of the latter calculation. If we have to consider N bodies in 3-dimensional space, then the nth order Born term requires the evaluation of n-fold integrals each in $3(N - 1)$ dimensions. The integrands may be simple or complicated depending on the particular form for the Green's function and the interaction, but one must expect to be forced to use computing machines to make any significant headway. If the interaction is really strong, then one must go to quite high order Born terms. The calculation of each of these becomes steadily harder and harder; therefore one expects to obtain the higher Born terms with *less and less* numerical accuracy. The whole point of our example is then to show that one might never

[2] Some mention of the problem of numerical accuracy—as distinct from the formal analysis of convergence of the Padé method—may be found in the paper by G. A. Baker, Jr., G. S. Rushbrooke, and H. E. Gilbert, *Phys. Rev.* **135**, A1272 (1964).

solve the problem this way, since *greater and greater* numerical accuracy is needed to extrapolate the Born series far away from $g = 0$.

Appendix A

In general the nth term of the Born series looks like

$$\int \varphi' \, VGVG...VGV\varphi, \quad V \text{ appears } n \text{ times.} \tag{A1}$$

At zero energy the Green's function is given by

$$G(r', r) = \frac{1}{4\pi r_>} \tag{A2}$$

and the plane wave functions φ are simply unity. So we are led to consider the recursively defined functions

$$F_n(r) = \int_0^\infty r'^2 dr' \, \frac{1}{r_>} \, \frac{\exp(-r')}{r'} \, F_{n-1}(r'); \; F_0 = 1. \tag{A3}$$

Next we make a Laplace transform

$$F_n(r) = \int_0^\infty dp \exp(-pr) \, u_n(p), \tag{A4}$$

so that we have the system

$$u_n(p) = \int_{(p,1)_<}^\infty \frac{dq}{q^2} \, u_{n-1}(q - 1), \tag{A5}$$

where the desired terms of the Born series are given by

$$T_n = u_n(1). \tag{A6}$$

The first few terms are easily found analytically,

$$u_0 = \delta(p)$$

$$\begin{aligned} u_1 &= \theta(1 - p) \\ u_2 &= \theta(2 - p) \left[\left(\frac{1}{p} - \frac{1}{2} \right) \theta(p - 1) + \frac{1}{2} \theta(1 - p) \right], \end{aligned} \tag{A7}$$

and the higher ones are obtained by numerical integration. A sequence of mesh sizes were used and the final results were obtained by extrapolation to zero mesh size.

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4. See the review article by G. A. BAKER *in* "Advances in Theoretical Physics," Vol. 1. Academic Press, New York (1965).