Perturbation calculations for infrared-divergent problems

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A method for performing numerical calculations on problems subject to infrared divergences is presented. The method is illustrated by examples from nonrelativistic quantum mechanics.

INTRODUCTION

In this paper we shall describe a procedure for solving, in the context of perturbation theory, problems subject to infrared divergences. We have in mind infrared divergences of the type which result from the presence of long-range attractive forces such as exist in the harmonic oscillator and are thought to exist in QCD, rather than the somewhat artificial infrared divergences such as exist in QED. In the present paper we shall formulate the method for, and apply it to, problems in potential theory; specifically the potentials x^2 and $|x|$. In later papers we shall describe the application of the method to problems in quantum field theory. The objective of the work is similar to that of Ref. 1.

The basic idea of the method is simply described: We place the problem in a box which allows us to formulate perturbation theory. Although the terms of the perturbation series will diverge as the box size increases, any quantity we wish to calculate will appear as a power series in the box size. We use Padé techniques to evaluate this function at an infinite box size or, more precisely, at a sufficiently large box size such that the answer we obtain is close to the value at an infinite box size. The idea is as follows: we put the problem in a box to formulate perturbation theory then remove the box and observe the interaction make its own box.

FORMULATION OF THE METHOD

We wish to solve the problem

$$\left[-\frac{d^2}{dx^2}+x^2\right]\Psi=E\Psi\ . \tag{1}$$

Imposing upon ourselves the restriction that we solve the problem in perturbation theory using $-d^2/dx^2$ as the unperturbed operator and x^2 as the perturbing operator (we shall also consider the potential $|x|$).

To formulate perturbation theory we place the problem in a box: $-L<x<L$. The series for the energy takes the form

$$E=\frac{E_0}{L^2}+L^2E_1+L^6E_2+L^{10}E_3+\cdots \tag{2}$$

or

$$L^2E=E_0+L^4E_1+L^8E_2+L^{12}E_3+\cdots\ . \tag{3}$$

Defining $y\equiv L^4$ we have

$$\sqrt{y}E=E_0+yE_1+y^2E_2+y^3E_3+\cdots\ . \tag{4}$$

We wish to sum this series and take the limit as $y\to\infty$. If we form ordinary Padé approximants to (4) we cannot obtain an approximant which is asymptotic to $\sqrt{y}$ and thus cannot take the limit of the infinite box size. We can circumvent this difficulty in several ways: We can square both sides of (4) then form Padé approximants which are asymptotic to y thus obtaining a finite energy in the limit of the infinite box size; alternately we can form quadratic approximants[2] to (4), that is, approximants of the form

$$\sqrt{y}E\approx\frac{-B\pm(B^2-4AC)^{1/2}}{2A}\ , \tag{5}$$

where A, B, and C are polynomials in y. If the orders of A, B, and C are suitably chosen [$O(A)=O(B)=O(C)-1$, for example], we obtain an approximation to $\sqrt{y}E$ which is asymptotic to $\sqrt{y}$ and can thus obtain a finite energy in the limit of the infinte box size. It is this last process we shall study most in this paper.

Having manipulated the expressions into a form such that we can take the limit of the infinite box size we must confess that we do not intend to do so. The procedure of taking the limit $y\to\infty$ for a finite order of the Padé approximant is known to give poor resuts. As we shall see below, the manipulations which lead to an approximation for the energy (or wave function) which has the correct asymptotic form are valuable even though we do not take the limit of infinite box size. The discussion of the inadvisability of taking the limit of infinite box size for finite orders of approximant can be summarized as follows: If we fix the box size L and refer to an approximant of order N as $P(N,L)$ [N is an index which increases as we proceed, in some predetermined fashion, through the Padé table incorporating more information from the perturbation series for larger N; in the case of Eq. (5), for example, N might be the order of C, A and B being of order $N-1$] we may hope that

$$\lim_{N\to\infty}P(N,L)\to E(L)\ , \tag{6}$$

where $E(L)$ is the exact energy for the box size L. We would like to find

$$\lim_{L\to\infty}\lim_{N\to\infty}P(N,L)=\lim_{L\to\infty}E(L)=E\ . \tag{7}$$

If we took the limit $L\to\infty$ for each approximant

TABLE I. The results for the ground-state energy using quadratic Padé approximants. For L_0 see the text.

N \ L	2	2.5	3	3.5	4	5	6	L_0
1	1.080 087	1.034 322	1.062 486	1.106 487	1.138 33	1.213 04	1.356	1.7
2	1.074 926	1.010 095	1.003 156	1.011 957	1.033 70	1.108 89	1.199	3.3
3	1.074 922	1.009 908	1.000 802	1.000 405	1.002 70	1.127	1.127	4.4
4	1.074 922	1.009 908	1.000 782	1.000 023	1.002 70	1.030 96	0.585	3.9
5	1.074 922	1.009 908	1.000 782	1.000 036	1.000 02	1.00149	1.04	3.5
6	1.074 922	1.009 908	1.000 782	1.000 036	0.999 99	0.999 48	0.950	4.5

$P(N,L)$, then studied the sequence as N increased to as large a value as we could manage we would be attempting to study

$$\lim_{N\to\infty}\lim_{L\to\infty} P(N,L)\ . \tag{8}$$

The interchange of limits is observed in practice to give poor results. Carroll, Baker, and Gammel[3] suggest the alternate procedure:

$$\lim_{N\to\infty} P(N,L_N)\ , \tag{9}$$

where the sequence of values L_N goes to ∞ as N does. To apply this procedure we need some method of choosing the sequence L_N; Carroll, Baker, and Gammel[3] suggest looking at the singularities of the approximants as we shall discuss below.

Other methods for extracting the limit of a large box size for problems like this have been presented; some rather sophisticated techniques are discussed in Ref. 4. It is not the purpose of the present paper to compare the various techniques or to make any judgment as to which is best. We shall content ourselves with the following observations: (1) there exists a sequence L_N for which the procedure given above works well; (2) an appropriate sequence can be found by sophisticated procedures, rather mundane practical methods, or even experimental methods; (3) we can choose a sequence L_N rather different from the optimum one and still obtain a good answer for the energy or wave function we wish to calculate.

RESULTS

First we consider the ground-state energy for the harmonic oscillator. We perturb about the function

$$\psi_0=\frac{1}{\sqrt{L}}\cos\frac{\pi x}{2L} \tag{10}$$

to construct a series of the form (4). We then use approximants of the form (5) to produce the numbers given in Table I. In the table L is the box size and N is the order of the polynomial C (A and B have order $N-1$; the number of terms in the perturbation series needed to form an approximant of order N is $3N$). The numbers in the table show results anticipated by the above discussion: For small values of the box size we find rapid convergence to the correct value for that box size; for larger values of the box size we find slower convergence to the correct value for that box size but a converged answer closer to the correct value for infinite box size. Thus, if we have a small number of terms we should choose a small box size to obtain convergence, for a larger number of terms we should choose a larger box size to get an answer closer to that for infinite box size. Looking at the table we see that an approximately optimum sequence of box sizes would be $L_1=2.5$, $L_2=3$, $L_3=L_4=3.5$, and $L_5=L_6=4$. The real message of the table, however, is that we almost always get a good answer, even if we have only a few terms in the perturbation series and even if we choose a value of L substantially different from the optimum one. The meaning of the last column, labeled L_0, will be discussed below when we describe procedures for selecting the sequence L_N for problems where we do not know the correct answer.

In Table II we give results which make definite our earlier statement that it is advantageous to use an approximant with the correct asymptotic behavior even if we do not take the limit of infinite box size. For Table II we have used the same series as that used for Table I [having the form (4)] but have simply used the diagonal Padé approximants to evaluate the right-hand side (RHS) so the approximation for the energy would go to zero at infinite box size. The results shown in Table II are hardly awful and we could use them to get a good result if we had a

TABLE II. The results for the ground-state energy using ordinary Padé approximants.

N \ L	3	3.5	4	4.5	5	5.5	6
1	0.952 427 8	0.879 770 8	0.784 00	0.682 95	0.588 93	0.507	0.438
2	0.929 232 9	0.856 974 0	0.761 45	0.661 69	0.569 59	0.490	0.422
3	0.998 951 3	0.986 960 4	0.954 52	0.897 79	0.824 10	0.744	0.665
4	1.000 957	1.002 219	1.011 12	1.033 23	1.071 8	1.126	1.194
5	1.000 758	0.999 489 4	0.995 92	0.984 29	0.959 92	0.922	0.871
6	1.000 782	1.000 00	0.999 46	0.996 74	0.988 55	0.972	0.944
7	1.000 781	0.999 994 5	0.999 41	0.996 54	0.98802	0.971	0.943
8	1.000 782	1.000 030	0.999 85	0.99879	0.994 77	0.985	0.967

reasonably good guess for the optimum box size. We noticed, however, that when using the results of Table II the quality of our answer would be much more sensitive to the value we choose for the box size than would be the case for Table I. The advantage of using an approximant with the correct asymptotic form is added stability of the answer for differing choices of box size.

We now turn to the problem of using our method to calculate the wave function. The perturbation series for the wave function takes the form

$$\Psi(x)\approx\frac{1}{\sqrt{L}}\Psi_0(x)+\frac{L^4}{\sqrt{L}}\sum_i a_i\cos\frac{(i+\frac{1}{2})\pi x}{L}+\frac{L^8}{\sqrt{L}}\sum b_i\cos\frac{(i+\frac{1}{2})\pi x}{L}+\cdots . \quad (11)$$

The procedure we shall use to evaluate the wave function at a particular value of x is nearly equivalent to multiplying through by $\sqrt{L}$ and using Padé approximants to evaluate the resulting RHS; the slight difference from this procedure is that we shall not expand the cosine functions as a power series in L. The procedure is easier to understand than to state: We define a new variable $\hat{L}$ and replace (11) with

$$\Psi(x)=\frac{1}{\sqrt{L}}\Psi_0(x)+\frac{L^4}{\sqrt{L}}\sum_i a_i\cos\frac{(i+\frac{1}{2})\pi x}{\hat{L}}+\frac{L^8}{\sqrt{L}}\sum b_i\cos\frac{(i+\frac{1}{2})\pi x}{\hat{L}}+\cdots . \quad (12)$$

We then multiply through by $\sqrt{L}$ and choose particular values for x and $\hat{L}$ to get

$$\sqrt{L}\,\Psi(x_0)=\Psi_0+y\Psi_1+y^2\Psi_2+\cdots \quad (y\equiv L^4) . \quad (13)$$

We then form the diagonal Padé approximants to the RHS of (13) and evaluate them at $L=\hat{L}$ (the asymptotic form of this approximant is not quite correct but it is wrong by only $L^{-1/2}$ whereas those used to create Table II were wrong by L^{-2}). The results of this procedure are shown in Table III for values of the box size ranging from 2.5 to 4 as indicated. The column labeled [1,1] results from a Padé approximant whose numerator and denominator are both linear functions (thus, the perturbation series through second order is used). The column labeled [8,8] results from the use of 17 terms in the perturbation series. The column labeled Ψ is the value of the exact wave function for infinite box size. The column labeled L_0 is the magnitude of the location of the pole in the [1,1] approximant; usually the pole is on the negative L axis, for those cases shown in parentheses it is on the positive L axis. The use of L_0 will be discussed in the section below.

The results in Table III show that the wave function is computed quite well. Lest the reader strain his eyes looking we point out that the one rather poor number is for $L=4$, the [1,1] column, and $x=1.5$. As seen in the L_0 column the reason is that a "spurious pole" at $L=3.3$ has crept into the approximant and our value of L $(=4)$ is sufficiently close to the pole that we obtain a poor result.

We now turn to the question of whether or not we can calculate excited states. The first excited state is the lowest state of odd pariy; thus it is not connected to any state of lower energy by the interaction Hamiltonian. For this reason the first excited state may have stability properties which make it particularly easy to calculate. We shall therefore turn our attention to the second excited state.

In Table IV we show the results of applying the quadratic Padé method to the series for the energy of the second excited state. As can be seen, the convergence is not as good as was obtained for the case of the ground state.

TABLE III. The wave function for the ground state. For L_0 see the text.

		$L=2.5$					$L=3$		
x	[1,1]	[8,8]	Ψ	L_0	x	[1,1]	[8,8]	Ψ	L_0
0	0.751	0.751	0.751	3.4	0	0.751	0.751	0.751	3.4
0.5	0.664	0.662	0.663	3.2	0.5	0.667	0.663	0.663	3.3
1	0.449	0.452	0.456	(5.8)	1	0.476	0.455	0.456	2.0
1.5	0.234	0.237	0.244	3.2	1.5	0.239	0.243	0.244	3.5
2	0.083	0.088	0.102	2.9	2	0.088	0.101	0.102	3.1
2.5	0	0	0.033	3.1	2.5	0.016	0.030	0.033	2.9
					3	0	0	0.008	2.9
		$L=3.5$					$L=4$		
x	[1,1]	[8,8]	Ψ	L_0	x	[1,1]	[8,8]	Ψ	L_0
0	0.751	0.751	0.751	3.4	0	0.751	0.751	0.751	3.4
0.5	0.665	0.663	0.663	3.3	0.5	0.655	0.663	0.663	3.4
1	0.481	0.456	0.456	2.8	1	0.488	0.456	0.456	3.0
1.5	0.227	0.244	0.244	4.4	1.5	0.469	0.244	0.244	(3.3)
2	0.088	0.102	0.102	3.3	2	0.094	0.102	0.102	3.5
2.5	0.005	0.033	0.033	3.0	2.5	0.004	0.033	0.033	3.2
3	−0.017	0.008	0.008	2.9	3	−0.034	0.008	0.008	3.0
3.5	0	0	0.002	3.1	3.5	−0.029	0.002	0.002	2.9
					4	0	0	0.0002	3.1

TABLE IV. The results for the energy of the second excited stae. For L_0 see the text.

N \ L	2.5	3	3.5	4	4.5	5	5.5	6	L_0
1	5.557	5.462	6.194	8.14					
2	5.473	5.076	4.942	4.66	3.55				3.6
3	5.473	5.083	5.025	5.13	5.45	6.00	6.75	7.76	9.2
4	5.473	5.084	5.014	5.044	5.15	5.33	5.57	5.82	3.3
5	5.473	5.082	5.008	5.001	5.00	5.02	5.04	5.07	3.4
6	5.473	5.082	5.008	5.001	5.01	5.03	5.06	5.08	3.3

Furthermore, for the cases $N=1$ and 2 there is a branch point on the positive real axis, and for values of L greater than that we get a complex energy. This may be an instance where the more sophisticated methods of extracting the limit of large L might prove valuable.[4,5] Still, with a reasonable choice for L_N we can get a good answer; if we wish to know that the answer is about 5 we can make do with very few terms in the series; with a handful of terms we can get a three- or four-figure accuracy.

In Table V we show the results for the second-excited-state wave function. The format is the same as for Table III. The accuracy with which the method calculates this more complicated wave function is really quite remarkable.

As a final example we show, in Table VI, the results for the ground-state energy for the potential $|x|$. For those who do not carry the zeros of Airy functions to lots of figures around in their head we have given the correct answer in the table caption. Since the potential $|x|^{\alpha}$ in the limit of large α is the box itself one should expect that our method would provide better convergence for larger α. Looking at Table VI we see that this effect is not dramatic between $\alpha=2$ and $\alpha=1$; the results in Table VI are nearly as good as those in Table I.

CHOOSING A VALUE FOR L

Having convinced ourselves, we hope, that if we can choose an appropriate value for L we can use the method to calculate a good answer, we now turn to the question of how to choose L. A procedure suggested in Ref. 3 is to study the singularities of the Padé approximants and choose L to be some value of the order of the magnitude of the distance the farthest the singularity is from the origin. In general we are advised to ignore singularities in the physical region (here the positive real axis) and to choose a value somewhat smaller than the relevant distance.[6] In Table I in the column labeled L_0 we give a number equal to 0.75 times the magnitude of the singular point having a negative real part which is farthest from the origin. If we use these numbers for the sequence L_N we obtain an estimate for the energy: 1.03; 1.008; 1.06; 1.002; 1.000 04; 0.9998. While not lying precisely on our optimum sequence for L_N the sequence we obtain in this fashion gives satisfactory results.

The column labeled L_0 in Table III provides somewhat similar information (we recall that the number given there is the location of the pole in the [1,1,] approximant, the location usually being on the negative real axis but oc-

TABLE V. The wave function for the second excited state. For L_0 see the text.

		$L=2.5$					$L=3$		
x	[1,1]	[8,8]	Ψ	L_0	x	[1,1]	[8,8]	Ψ	L_0
0	0.266	0.266	0.266	2.5	0	0.266	0.266	0.266	2.5
0.5	0.105	0.104	0.117	3.2	0.5	0.113	0.115	0.117	2.9
1	−0.180	−0.183	−0.161	3.7	1	−0.145	−0.165	−0.161	3.5
1.5	−0.296	−0.295	−0.302	3.1	1.5	−0.295	−0.301	−0.302	3.7
2	−0.181	−0.186	−0.252	(3.5)	2	−0.260	−0.241	−0.252	3.2
2.5	0	0	−0.134	4.9	2.5	−0.086	−0.110	−0.134	(1.7)
					3	0	0	−0.050	(4.5)
		$L=3.5$					$L=4$		
x	[1,1]	[8,8]	Ψ	L_0	x	[1,1]	[8,8]	Ψ	L_0
0	0.266	0.266	0.266	2.5	0	0.266	0.266	0.266	2.5
0.5	0.104	0.117	0.117	3.0	0.5	0.084	0.116	0.117	2.8
1	−0.103	−0.161	−0.161	3.7	1	−0.055	−0.163	−0.161	3.4
1.5	−0.263	−0.301	−0.301	3.5	1.5	−0.200	−0.299	−0.301	3.7
2	−0.261	−0.250	−0.252	2.5	2	−0.230	−0.248	−0.252	3.5
2.5	−0.196	−0.132	−0.134	(4.1)	2.5	−0.173	−0.132	−0.134	(2.9)
3	0.025	−0.045	−0.050	3.4	3	−0.151	−0.049	−0.050	(2.7)
3.5	0	0	−0.017	4.9	3.5	0.126	−0.013	−0.017	(4.9)
					4	0	0	−0.003	4.9

TABLE VI. The results for the energy of the ground state for a linear potential. The correct answer is 1.018 793.

N \ L	3	4	5	6	7	8	9
1	1.040 927	1.043 807	1.049 88	1.043 07	1.026 07	1.004	0.979
2	1.031 392	1.021 217	1.029 09	1.045 68	1.066 36	1.086	1.103
3	1.031 309	1.109 357	1.019 25	1.022 19	1.032 07	1.054	1.093
4	1.031 309	1.019 339	1.018 76	1.017 69	1.004 47	1.162	1.099
5	1.031 309	1.019 339	1.018 81	1.018 83	1.019 30	1.022	1.036
6	1.031 309	1.019 339	1.018 81	1.018 80	1.018 90	1.020	1.030
7	1.031 309	1.019 339	1.018 81	1.018 81	1.019 03	1.021	1.029

casionally, for those values shown in parentheses, being on the positive real axis). While there is a considerable range of values, using the Carroll-Baker-Gammel rule one would probably choose a value of L somewhere between 2.5 and 3; that would be an appropriate choice for the [1,1] and would give a good esimate of the wave function out to distances where it is quite small.

Another method for choosing L, less elegant but in some cases perhaps more practical, is to examine the behavior of the approxmiate wave function. In Fig. 1 we plot the ground-state wave function for the harmonic oscillator as predicted by the [1,1] approximant for various values of the box size. For $L=1.5$ the wave function appears entirely boxlike; for $L=2.5$ there is clear evidence of something inside the box containing the wave function; for $L=3$ the box wall is clearly having little effect on the system. Looking at this information we would choose a value of L between 2.5 and 3 and expect that if we could obtain a converged answer for that value of L the answer would be close to that at infinite box size. That is certainly the case for the problems presented here.

Things need not always work as neatly as shown in Fig. 1. In Fig. 2(a) we show similar plots for the second-excited-state wave function. For the [1,1] approximant we can tell that the $L=2.5$ wave function is boxlike but the spurious singularities make interpretation of the wave function for larger L somewhat difficult. While we might guess that a value of around 3.5 would be appropriate, it would be difficult to have great confidence on the basis of these plots. If we have a few more terms in the perturbation series and can form the [3,3] approximant the situation is much clearer as we see in Fig. 2(b); although there are still spurious singularities they are much less inconveniently placed. If we have lots of terms and can form the [8,8] approximant the situation is quite clear as we see in Fig. 2(c).

A final method for choosing L we shall mention is simply to incorporate experimental information with the calculations. We expect that convergence will always be faster for smaller values of L. Physically we expect, and the present calculations bear this out, that once the size of the box becomes larger than the size of the object whose properties we are trying to calculate, the effects of the box walls will rapidly diminish. For many objects of interest we know the relevant size parameter. For instance, we know the size of hadrons; if we wished to do a calculation in QCD using the method we would therefore choose to study some value, or range of values, of L which is slightly larger than the hadron radius.

The best method for choosing L will depend on the amount of information available and on the objectives of the calculation. In the situation where only a few terms in the perturbation expansion are available, the calculator knows the length scale of the object being calculated, and the objective of the calculation is a result of modest accuracy (such as would be the case for a first calculation of a mass spectrum from QCD) one should choose a value of L 20—30% larger than the size of the object; if the

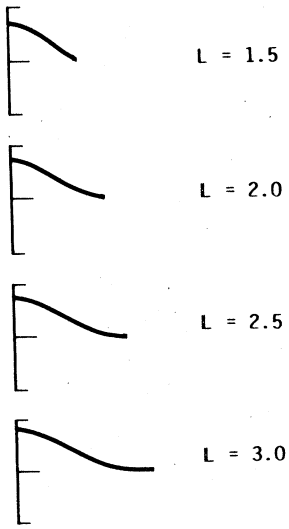

FIG. 1. The ground-state wave function as calculated by the [1,1] approximant for various values of the box size.

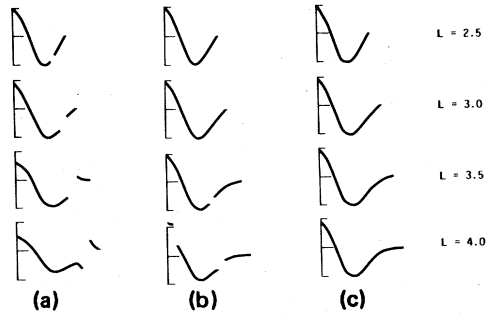

FIG. 2. The second-excited-state wave function as calculated by the [1,1] (a), [3,3] (b), and [8,8] (c) approximants for various values of the box size.

method is going to work at all this value of L will be appropriate. If one has enough terms in the series to construct at least three or four approximations and one knows the size of the object, one should construct a table such as Table I for values of L ranging from the characteristic size to a few times that size. One can choose L by picking the largest value for which good convergence is observed down the column. In either case one should plot the singularities of the approximants; if they conform to the Carroll-Baker-Gammel rule one can have added confidence in the results. One should also plot the approximants for the wave function to see that the expected inflection point is suitably inside the chosen value of L. For problems in field theory the wave function may be pointlike and this last procedure will not be available; we shall discuss such problems in a later paper. Finally, if one has a large number of terms but no estimate of the size of the object one should plot the location of the singularities of the approximants. If the method is working well there will be a characteristic magnitude for these points. (They will tend to lie at poles or on cuts of the approximated function; if such behavior is not observed when a large number of terms is available the procedure is probably not working very well.) One should construct a table such as Table I for values of L ranging over the values characteristic of the magnitude of the singularities. If the method is working one will observe good convergence for the columns under small values of L, less good convergence for larger values. One chooses the largest value for which good convergence is observed. In such a case one can obtain an estimate of the accuracy of the final result by observing the apparent degree of convergence down the column under the chosen value of L and across the bottom row out to that column.

DISCUSSION

In this paper we have presented a method for doing numerical calculations for problems subject to infrared divergences due to the presence of interactions which become stronger at larger distances. In the present paper we have given examples of problems from potential theory. For these problems the method works very well. In a later paper we shall show that the method also works well for a model quantum field theory which is also subject to infrared divergences of the type we are interested in.

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