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Improvement of an Extrapolation Scheme for Strong-Coupling Expansion in Quantum Field Theory

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By letting the lattice spacing a approach zero as the order n of perturbation theory increases in such a way that the product na remains fixed, we substantially improve the numerical predictions. The approximation scheme described here is superior to conventional Padé approximation.

In a previous paper[1] we proposed a Padé-like scheme for extrapolating to the zero-lattice-spacing limit of a $g\varphi^4$ field theory expanded in powers of $g^{-1/2}$ on a lattice. In this paper we show that this scheme becomes inadequate when the order of perturbation theory is sufficiently large. We propose an improved extrapolation method which appears to be free of the flaws of the scheme in Ref. 1.

The extrapolation scheme used in Ref. 1 is described below. For a $g\varphi^4$ theory in d-dimensional space-time, the dimensionless expansion parameter x that always appears in the $g^{-1/2}$ expansion is

$$x = 1/g^{1/2}a^{2-d/2}, \tag{1}$$

where a is the lattice spacing. The expansion on the lattice of some physical quantity Q such as a Green's function or any energy level has the general form

$$Q = a^{\alpha} g^{\beta} \sum_{n=0}^{\infty} \gamma_n x^n, \tag{2}$$

where α, β, and γ_n are pure numbers. α and β fix the naive dimensions of Q. (For simplicity, we are considering only a theory with zero bare mass.) With use of (1), the series in (2) takes the form

$$Q = g^{\beta-\alpha/(4-d)} x^{2\alpha/(d-4)} \sum_{n=0}^{\infty} \gamma_n x^n. \tag{3}$$

Next we compute the dimensionless numerical quantity

$$N(x) = (Q/g^{\beta-\alpha/(4-d)})^{(d-4)/2\alpha}$$
$$= x\sum_{n=0}^{\infty}\delta_n x^n = x/\sum_{n=0}^{\infty}\epsilon_n x^n, \quad (4)$$

where the new series coefficients δ_n and ϵ_n are obtained by raising the power series in (3) to the power $(d-4)/2\alpha$ and then inverting it.

Assuming that $d<4$, (1) implies that the zero-lattice-spacing limit $a\to 0$ corresponds to the limit $x\to\infty$. The problem is to extrapolate $N(x)$ to $N(\infty)$ when only a finite number of coefficients ϵ_n are known. The extrapolation procedure consists of generating a sequence of extrapolants N_1, N_2, N_3,... which hopefully approach the exact answer $N(\infty)$. The nth extrapolant N_n is computed by raising the last expression in (4) to the nth power, truncating the series after the x^n term, taking the limit $x\to\infty$, and taking the nth root:

$$N_n \equiv \left\{ \lim_{x\to\infty} \frac{x^n}{\left[\left(\sum_{i=0}^{\infty}\epsilon_i x^i\right)^n\right]_{\text{truncated after } x^n \text{ term}}} \right\}^{1/n}. \quad (5)$$

In Ref. 1 we used this extrapolation technique to compute various known quantities in a $g\varphi^4$ field theory with $d=1$. For example, if $E(g)$ is the ground-state energy of the anharmonic oscillator whose Euclidean-space Lagrangian is given by $L=\frac{1}{2}(\partial\varphi)^2+\frac{1}{4}g\varphi^4$, then[2]

$$4g(dE/dg) = (0.569473\ldots)g^{1/3}. \quad (6)$$

We computed in Ref. 1 the first five approximants to the coefficient of $g^{1/3}$ in (6): $N_1=0.6242$, $N_2=0.5861$, $N_3=0.5754$, $N_4=0.5717$, and $N_5=0.5707$. These five numbers suggest that the entire sequence of approximations is rapidly and monotonically approaching the correct limit in (6).

However, we have now calculated on a computer seven more approximants: $N_6=0.5708$, $N_7=0.5712$, $N_8=0.5717$, $N_9=0.5720$, $N_{10}=0.5721$, $N_{11}=0.5719$, and $N_{12}=0.5719$.

Thus, these extrapolants appear to behave like the partial sums of a divergent asymptotic series; they approach the exact answer for a while and and then veer off. We must conclude that the extrapolation procedure used in Ref. 1 is inadequate. This Letter proposes a modification of this procedure which appears to give a *convergent* sequence of extrapolants.

The idea for this modification was suggested to us in a short paper by Carroll, Baker, and Gam-

TABLE I. Comparison of the old extrapolation scheme in (5) with the improved extrapolation scheme in (7) for $g\varphi^4$ theory in one space-time dimension. The quantity being calculated is $4g(dE/dg)/g^{1/3}$, where E is the ground-state energy. The exact value of this quantity is 0.569473.... Observe that in the old scheme the approximants approach the correct answer for a while and then veer off. The improved extrapolation scheme approaches the exact answer monotonically and thus may be further extrapolated to a limiting value.

Order n	Old Approximant N_n from (5)	New Approximant N_n from (7)
1	0.624162	0.477788
2	0.586107	0.535128
3	0.575408	0.548817
4	0.571738	0.554843
5	0.570704	0.558673
6	0.570754	0.561548
7	0.571199	0.563809
8	0.571687	0.565563
9	0.572027	0.566845
10	0.572123	0.567683
11	0.571947	0.568114
12	0.571532	0.568195

TABLE II. Comparison of the old extrapolation scheme in (5) with the new extrapolation scheme in (7) for $4g(dE/dg)/[g\ln(1+x)]$ in a two-dimensional $g\varphi^4$ theory. [We are dividing by the series for $\ln(1+x)$ and computing the coefficient of the logarithmic divergence.] Just as in the case $d=1$ the old extrapolants in column 2 appear to approach an answer and then veer off while the new extrapolants in column 3 appear to converge monotonically. For comparison, in column 4 we have divided by $\ln(2+x)$. Note that the results are not sensitive to the particular choice of logarithms.

Order n	Old Approximant[a] N_n	New Approximant[b] N_n	New Approximant[c] N_n
1	0.4537	0.3121	0.1961
2	0.4429	0.3639	0.2961
3	0.4256	0.3766	0.3263
4	0.4224	0.3858	0.3563
5	0.4232	0.3932	0.3727
6	0.4243	0.3987	0.3827
7	0.4257	0.4031	0.3906
8	0.4274	0.4069	0.3965
9	0.4292	0.4102	0.4015
10	0.4311	0.4132	0.4060
11	0.4332	0.4161	0.4102
12	0.4359	0.4189	0.4142

[a]From Eq. (5).
[b]From Eq. (7), with division by $\ln(1+x)$.
[c]From Eq. (7), with division by $\ln(2+x)$.

mel.[3] They examined the question of when it is correct to compute $f(\infty)$ by expanding $f(x)$ in a Taylor series $f(x)=\sum a_n x^n$, computing the diagonal Padé approximant $P_n{}^n(x)$, and taking the limit $x\to\infty$ for n fixed. The correct order of limits is of course to fix x, to take $n\to\infty$ (which cannot be done unless all the a_n are known), and then to take $x\to\infty$. For some functions $f(x)$, it is incorrect to interchange the two limits $n\to\infty$ and $x\to\infty$: For $f(x)=e^{-x}$, $P_1{}^1(\infty)=-1$, $P_2{}^2(\infty)=1$, $P_3{}^3(\infty)=-1$, ... Carroll, Baker, and Gammel[3] propose (without proof) a recipe for computing $e^{-\infty}=0$ from the diagonal Padé approximants of the Taylor series; namely, that $P_n{}^n(x)$ be evaluated at $x=x_n$, where x_n is a sequence of points approaching ∞. For the simple choice $x_n=n$, there is a vast improvement in the convergence: $P_1{}^1(1)=\frac{1}{3}$, $P_2{}^2(2)=\frac{1}{7}$, and $P_3{}^3(3)=\frac{7}{145}$. However, no general prescription is given in Ref. 3 for how one might determine the optimal sequence x_n.[4]

There is a physical reason why one might expect the extrapolation procedure in Ref. 1 to break down. In nth-order perturbation theory on the lattice, the nth coefficient α_n in (2) is a sum of Feynman-like diagrams having at most n adjacent vertices. Since the distance between vertices is the lattice spacing a, the physical size of the largest diagram is na. However, the extrapolation prescription in Ref. 1 consists of fixing n and letting $x\to\infty$ (which is equivalent to $a\to 0$); so the spatial extent of all diagrams in each order approaches zero in this limit. But physical quantities, like masses or energies, are not fixed by the very-short-distance behavior of Green's functions, but reflect some of the long-distance features as well. Thus, it would not be surprising to find that the extrapolation procedure in Ref. 1 ultimately leads to a divergent result.

The above argument suggests an improved extrapolation procedure. To describe spatially extended features, we should take $a\to 0$ in such a way that na is held fixed. Thus, rather than taking the limit $x\to\infty$ in (5), we redefine N_n as

$$N_n \equiv \left\{ \frac{(x_n)^n}{\left\{ \left[\sum_{i=0}^{n} \epsilon_i (x_n)^i \right]^n \right\}_{\text{truncated after } x^n \text{ term}}} \right\}^{1/n}, \tag{7}$$

where for large n, x_n grows like $n^{2-d/2}$ [see (1)]. For simplicity we take $x_n=n^{2-d/2}$. For example, when $d=1$ we take $x_n=n^{3/2}$. The results for $4g(dE/dg)/g^{1/3}$ are given in Table I. When $d=2$, the quantity $4g(dE/dg)/g$ is logarithmically divergent (E is the vacuum expectation value of the energy density). If, as is discussed in Ref. 1, we divide by the Taylor series expansion of $\ln(1+x)$, we find that the extrapolants for this ratio appear to approach a constant, which is the numerical coefficient of the divergence.

The results are given in Table II. How sensitive are the approximants to our choice of logarithm? In Table II we give the extrapolants that arise after dividing by $\ln(2+x)$. These extrapolants are also monotonic and appear to approach

TABLE III. Comparison of the old and new extrapolation schemes for the ground-state energy of the harmonic oscillator (see Ref. 5). The tabulated numbers are approximants to $2E/m=1$. Both sequences of extrapolants seem to be approaching 1, but the improved sequence is monotonic while the old sequence is irregular. For the new sequence of approximants, requiring that $na=1$ gives $x_n=n^2$.

Order n	Old Sequence of Approximants (see Ref. 5)	New Sequence of Approximants with $x_n=n^2$
1	0.6000	0.3750
2	0.8847	0.6783
3	0.7937	0.7147
4	0.8812	0.8086
5	0.8681	0.8220
6	0.9039	0.8617
7	0.9037	0.8715
8	0.9221	0.8924
9	0.9246	0.8999
10	0.9353	0.9124
11	0.9382	0.9181
12	0.9449	0.9262

TABLE IV. Padé approximants for $4g(dE/dg)/g^{1/3}$ with $d=1$. Observe that the Padé sequence is greatly improved by evaluating it at $x=x_n=n^{3/2}$. However, it is still not nearly as smooth as the sequence in the right-hand column in Table I.

Padé approximant	$[P_{n+1}{}^n(x)]_{x=\infty}$	$[P_{n+1}{}^n(x)]_{x=x_n=n^{3/2}}$
$P_1{}^0$	0.6242	0.4778
$P_2{}^1$	0.5594	0.5209
$P_3{}^2$	0.5770	0.5579
$P_4{}^3$	0.4007	0.5240
$P_5{}^4$	0.5682	0.5626
$P_6{}^5$	0.5633	0.5605

TABLE V. Padé approximants for $4g(dE/dg)/[g\ln(1+x)]$ with $d=2$. As in Table IV, the Padé sequence at $x=x_n=n$ is not as smooth as the sequence in column 3 in Table II.

Padé Approximant	$[P_{n+1}^{n}(x)]_{x=\infty}$	$[P_{n+1}^{n}(x)]_{x=x_n=n}$
P_0^1	0.4537	0.3121
P_2^1	0.4674	0.3823
P_3^2	0.4224	0.3858
P_4^3	0.4300	0.4018
P_5^4	0.4738	0.4191
P_6^5	0.4190	0.4014

TABLE VI. Padé approximants for the ground-state energy of the harmonic oscillator (see Ref. 5). As in Table III, the tabulated numbers are the approximants to $2E/m=1$. These Padé approximants are not as good as the extrapolants in Table III.

Padé Approximant	$[P_{n+1}^{n}(x)]_{x=\infty}$	$[P_{n+1}^{n}(x)]_{x=x_n=n^2}$
P_1^0	0.6000	0.3750
P_2^1	0.7575	0.6226
P_3^2	0.8194	0.7677
P_4^3	0.8582	0.8283
P_5^4	0.8837	0.8630
P_6^5	0.9008	0.8854

the same limit as the approximants in the third column of Table II. Because $\ln(1+x)$ is slowly varying, Table II does not rule out an admixture of $\ln^2$ divergence.

We have also examined the effect of the improved extrapolation scheme on a calculation of the ground-state energy E of the harmonic oscillator whose Lagrangian is given by[5] $\frac{1}{2}(\partial\varphi)^2+\frac{1}{2}m^2\varphi^2$. In Table III we list the first twelve extrapolants for $2E/m=1$. Observe that the old extrapolants approach 1 in an uneven fashion while the improved extrapolants approach 1 monotonically.

For all the models we have examined we find that the improved extrapolants approach their limits smoothly and monotonically.[6] This is particularly advantageous because there are many numerical techniques available for accelerating the convergence of smooth monotonic sequences to their limits (Richardson extrapolation, Shanks transformation, and so on).

Finally, the improved extrapolation scheme has several advantages over a conventional Padé approximation. [We have in mind here a $P_{n+1}^{n}(x)$ Padé approximation for the series $\sum\delta_n x^n$ in (4).] The main advantage is that there are twice as many extrapolants and so it is easier to extrapolate to the limit of the sequence. In addition we find that the improved extrapolants converge more rapidly and are smoother than the Padé approximanants, regardless of whether $P_{n+1}^{n}(x)$ is evaluated at $x=\infty$ or at (see Tables IV–VI) $x=x_n$.

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3 A. Carroll, G. A. Baker, and J. L. Gammel, Nucl. Phys. B129, 361 (1977).

4 It is suggested in Ref. 3 that one should determine the sequence x_n by looking for the poles of the Padé approximants. However, this method does not define the sequence x_n very clearly and it seems to give spurious results for some models.

5 The details of this calculation are given by C. M. Bender, F. Cooper, G. S. Guralnik, R. Roskies, D. H. Sharp, and M. L. Silverstein, Phys. Rev. D (to be published).

6 It is, of course, not true that whenever x_n grows like $n^{2-d/2}$ the extrapolants are monotonic. For example, if we had chosen $x_n=100n^{2-d/2}$, then for small n the results would have been indistinguishable from the behavior with $x_n=\infty$, which is always monotonic.