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# Continuum limit of lattice approximation schemes

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Boundary-layer perturbation theory problems are inherently singular. However, it is known that discretizing the problem by introducing a lattice may convert such problems into regular perturbation problems. The singular nature of boundary-layer problems is then relegated to and hidden in the continuum limit, the subtle limit in which the lattice spacing tends to zero. If the lattice is introduced cavalierly, then extrapolating to zero lattice spacing gives a sequence of extrapolants that at first approaches the correct limit and then veers off, thereby revealing the asymptotic nature of such problems. However, discretizing the problem following the procedures described here yields lattice approximations that have a smooth and regular continuum limit. These ideas are illustrated by three nonlinear ordinary differential equations: the cubic equation that describes instantons, an oscillator equation having a quadratic nonlinearity, and the Blasius equation. © 1997 American Institute of Physics. [S0022-2488(97)02307-4]

## I. INTRODUCTION

A powerful nonperturbative approach to the solution of quantum field theory is to discretize the theory by introducing a lattice. The advantage of this approach is that the lattice serves as a regulator; divergent quantities in the continuum theory become finite in the corresponding lattice theory. However, the lattice spacing must be removed at the end of the computation to obtain the solution to the original continuum theory. Removing the lattice spacing (taking the continuum limit of the lattice theory) is a highly nontrivial procedure.

In this paper we examine the problem of reconstructing the original continuum theory from a discrete lattice approximation in a simpler and more concrete context, namely, boundary-layer theory. A boundary-layer problem is a differential equation and an associated set of boundary conditions in which the highest derivative in the differential equation is multiplied by a small parameter  $\delta$ . The solution to a boundary-layer problem consists of two regions: an *inner* region, called a *boundary layer*, in which the solution is rapidly varying, and an *outer* region in which the solution is slowly varying. The width of the inner region vanishes as  $\delta \rightarrow 0$ . Boundary-layer problems are *singular* perturbation problems.<sup>1</sup> This means that the solution to the boundary-layer problem does not have a convergent Taylor series representation in powers of  $\delta$ .

When a boundary-layer problem is *discretized* by introducing a lattice with lattice spacing  $a$ , then the resulting problem often becomes a *regular* perturbation problem (one whose solution has the form of a Taylor series in powers of  $\delta^{2-4}$ ). This transformation from a singular to a regular perturbation problem is the differential-equation analog of the lattice regulation that occurs in the context of quantum field theory. The singular nature of the problem then resurfaces when the continuum limit of the discretized problem is taken. This singular limit is nontrivial. One cannot just set the parameter  $a$  to zero; rather, one must perform the delicate limit  $a \rightarrow 0$  using numerical extrapolation techniques. Extrapolation techniques that have been used in the past have been based on Padé approximation methods.

Unfortunately, the continuum limit  $a \rightarrow 0$  is so singular that, not surprisingly, the accuracy of numerical results that have been obtained in the past is not unimpressive. In fact, in very high

order approximations the numerical extrapolants typically approach the exact answer for a while and then veer off. Thus, there appears to be a maximally obtainable accuracy that cannot be improved by going to higher order in powers of  $\delta$ .

In this paper we propose a resolution to this dilemma. We note that there are *many* ways to discretize a differential equation problem. We enumerate several criteria that enable us to choose uniquely the optimal discretization scheme for the differential equation. The optimal scheme appears to have the advantage that the extrapolants to the continuum limit approach the  $a=0$  value *smoothly*. Thus, as the order of the approximation is increased, the numerical error in these extrapolants continues to decrease.

Our paper is organized very simply. In Sec. II we examine the instanton solution to a cubic nonlinear differential equation:

$$\delta^2 y''(x) = [y(x)]^3 - y(x). \quad (1.1)$$

The boundary conditions  $y(0)=0$  and  $y(\infty)=1$  give rise to a boundary layer at  $x=0$ ; the objective is to calculate the value of  $y'(0)$ . This problem has the virtue that the exact solution, called an instanton, is known analytically. We examine various discretization schemes for this problem, and we formulate a set of criteria for selecting the best of these schemes.

In Sec. III we study an oscillator having a quadratic nonlinearity:

$$\delta^2 y''(x) = [y(x)]^2 - 2y(x). \quad (1.2)$$

We seek soliton solutions satisfying the boundary conditions  $y(\pm\infty)=2$ . There are two *even-parity* solutions to this problem, a trivial constant solution  $y\equiv 2$ , and a nontrivial solution. Our objective here is to find the value of  $y(0)$  for the nontrivial solution. Again, the exact solution to this problem is known analytically.

Finally, in Sec. IV we look at the very difficult problem of a boundary-layer solution to the Blasius equation,

$$\delta y'''(x) + y(x)y''(x) = 0, \quad (1.3)$$

where  $y(0)=0$ ,  $y'(0)=0$ , and  $y'(\infty)=1$ . The goal here is to calculate the value of  $y''(0)$ . The solution to this third problem is not known analytically; it can only be obtained by using numerical methods.

We hope that the success of the lattice techniques discussed in this paper will inspire a re-examination of the strong-coupling lattice techniques that have been used in the past to study quantum field theory.<sup>5</sup> We feel that these improved discretization schemes will lead to dramatically improved numerical results in quantum field theory.

## II. BOUNDARY-LAYER APPROXIMATION TO AN INSTANTON

In this section we consider the boundary-value problem,

$$\delta^2 y''(x) = [y(x)]^3 - y(x), \quad y(0)=0, \quad y(\infty)=1. \quad (2.1)$$

The solution to this equation is called an *instanton*. This instanton arises in the context of a semiclassical approximation to the functional integral representing a  $\phi^4$  Euclidean quantum field theory.

The exact closed-form solution to the problem in Eq. (2.1) is known:

$$y(x) = \tanh\left(\frac{x}{\delta\sqrt{2}}\right). \quad (2.2)$$

Observe that when  $\delta \ll 1$  the solution exhibits a *boundary layer* (a narrow region of rapid variation) at the origin  $x=0$ ; as  $\delta \rightarrow 0$ , the solution becomes discontinuous at  $x=0$ . The solution is slowly varying elsewhere.

Our objective in this section is to use a lattice approximation to determine the value of  $y'(0)$ . Of course, from Eq. (2.2) we already know the exact answer:

$$y'(0) = \frac{1}{\delta\sqrt{2}}. \quad (2.3)$$

There are many ways to discretize the differential equation in Eq. (2.1). For example, an apparently natural way to introduce a lattice is to replace this differential equation by the difference equation,

$$\epsilon(y_{n+1} - 2y_n + y_{n-1}) = y_n^3 - y_n, \quad (2.4)$$

where

$$\epsilon \equiv \frac{\delta^2}{a^2}. \quad (2.5)$$

The underlying reason for introducing the variable  $\epsilon$  is that it is *dimensionless*. We emphasize that the limit of zero lattice spacing does not make sense because one cannot take a dimensional quantity such as  $a$  to be “small.” This is because one can always redefine the units so that the dimensional quantity has exactly the same numerical size. One can only take the lattice limit *relative to another quantity* in the theory having the same dimensions as  $a$ ; this other quantity is  $\delta$ . Thus, the continuum limit of the theory is achieved by performing the limit  $\epsilon \rightarrow \infty$ .

There is another limit in the theory, namely,  $\epsilon \rightarrow 0$ . We borrow some terminology from quantum field theory<sup>6</sup> and refer to this limit as the *ultralocal* limit. In the ultralocal limit the kinematic (derivative) terms on the left side of Eq. (2.1) vanish and there is a balance of the local terms on the right side. In the language of boundary-layer theory, this limit is called the *outer limit*.

The calculational procedure is now to treat the lattice spacing  $a$  as being *fixed* and  $\delta$  as small, or equivalently, to treat the parameter  $\epsilon$  as small. Then, at each lattice point  $n$  we expand  $y_n$  as a series in powers of  $\epsilon$ . Finally, from the power series for  $y_1$  and  $y_0$ , we try to recover the derivative  $y'(0)$ .

We do not describe the details of this calculation here because they are given in Refs. 2 and 3. However, in brief, we incorporate the boundary conditions by requiring that  $y_0=0$  and that  $y_\infty=1$ . Second, we observe that at  $\epsilon=0$  (the ultralocal limit of the lattice problem) there is a simple solution  $y_0=0$  and  $y_n=1$  ( $n>0$ ). Next, we expand about this unperturbed solution and obtain a series expansion for  $y_n$  for each value of  $n$ :

$$\begin{aligned} y_0 &= 0, \\ y_1 &= 1 - \frac{1}{2}\epsilon + \frac{1}{8}\epsilon^2 - 0\epsilon^3 + \frac{11}{28}\epsilon^4 + \dots, \\ y_2 &= 1 - \frac{1}{4}\epsilon^2 + \frac{5}{16}\epsilon^3 - \frac{15}{32}\epsilon^4 + \dots, \\ y_3 &= 1 - \frac{1}{8}\epsilon^3 + \frac{9}{32}\epsilon^4 + \dots, \\ y_4 &= 1 - \frac{1}{16}\epsilon^4 + \dots, \end{aligned} \quad (2.6)$$

and so on.

The boundary-layer structure at the origin  $x=0$  is incorporated in this discrete problem in an interesting fashion: Observe that the first dependence on  $\epsilon$  in the power series for  $y_n$  occurs at the  $\epsilon^n$  term. Thus, as  $n$  increases, the  $\epsilon$  dependence becomes weaker; this is the lattice version of the *outer region* where the solution to the boundary-layer problem is a slowly varying function of  $x$ . As  $n$  tends to  $\infty$ ,  $y_n$  has the degenerate power series 1 and the boundary condition at  $x=\infty$  is correctly incorporated.

We must now calculate  $y'(0)$  in the continuum limit. Since the lattice representation of  $y'(x)$  is  $\lim_{a \rightarrow 0} (y_{n+1} - y_n)/a$ , we have from Eq. (2.6),

$$\begin{aligned}
 y'(0) &= \lim_{\epsilon \rightarrow \infty} \frac{1}{a} (y_1 - y_0) = \lim_{\epsilon \rightarrow \infty} \frac{1}{a} \left( 1 - \frac{1}{2} \epsilon + \frac{1}{8} \epsilon^2 - 0 \epsilon^3 + \frac{11}{28} \epsilon^4 + \dots \right) \\
 &= \frac{1}{\delta} \lim_{\epsilon \rightarrow \infty} \sqrt{\epsilon} \left( 1 - \frac{1}{2} \epsilon + \frac{1}{8} \epsilon^2 - 0 \epsilon^3 + \frac{11}{28} \epsilon^4 + \dots \right). \tag{2.7}
 \end{aligned}$$

If we compare this structure with the exact answer in Eq. (2.3), we see that the factor of  $1/\delta$  is, of course, correct. However, it is not at all obvious how to obtain the numerical result,

$$\frac{1}{\sqrt{2}} = \lim_{\epsilon \rightarrow \infty} \sqrt{\epsilon} \left( 1 - \frac{1}{2} \epsilon + \frac{1}{8} \epsilon^2 - 0 \epsilon^3 + \frac{11}{28} \epsilon^4 + \dots \right). \tag{2.8}$$

We have now encountered a very difficult problem associated with the interchange of limits. In principle, we must first obtain the perturbation expansion to all orders in powers of  $\epsilon$  and sum the series. Second, we must take the limit  $\epsilon \rightarrow \infty$ . Unfortunately, it is not possible to perform the limits in this order because one can only obtain a *finite* number of terms in any perturbation expansion for a nontrivial problem. Thus, the question is this: How can one make sense of Eq. (2.8) when there are only a limited number of terms known in the series? A number of solutions to this problem have been suggested and studied;<sup>7-9</sup> all of the approaches involve the use of Padé approximations.

The simplest approach is to treat the perturbation parameter  $\epsilon$  as small ( $\epsilon \ll 1$ ) and to conduct a sequence of algebraic manipulations whose objective is to change the form of the right side of Eq. (2.8) to one that has a limit as  $\epsilon \rightarrow \infty$ . With each manipulation we retain the terms of the series in Eq. (2.8) to order  $\epsilon^N$ , where  $N$  is the number of terms that we have calculated in perturbation theory. First, we square the right side of Eq. (2.8) to eliminate the fractional power of  $\epsilon$ . This gives a structure of the form

$$\epsilon \sum_{k=0}^N A_k \epsilon^k, \tag{2.9}$$

where the numbers  $A_k$  are obtained by squaring the series in Eq. (2.8) term-by-term. We emphasize that consistency demands that we truncate the squared series after the  $\epsilon^N$  term. Next, we invert the  $A$ -series term-by-term and again truncate the resulting series after the  $\epsilon^N$  term:

$$\frac{\epsilon}{\sum_{k=0}^N B_k \epsilon^k}. \tag{2.10}$$

We now raise the expression in Eq. (2.10) to the power  $N$ :

$$\frac{\epsilon^N}{\sum_{k=0}^N C_k \epsilon^k}. \tag{2.11}$$

Observe that the continuum limit  $\epsilon \rightarrow \infty$  now exists! In this limit the right side of Eq. (2.11) becomes  $1/C_N$ . Finally, we compensate for having raised the right side of Eq. (2.9) to the powers 2 and  $N$  by taking the  $2N$ th root of this limit; we *define* the  $N$ th *extrapolant*  $L_N$  by

$$L_N \equiv (C_N)^{1/2N}. \quad (2.12)$$

Clearly, the hope is that as  $N \rightarrow \infty$ , the  $N$ th extrapolant  $L_N$  will tend to the correct limit  $1/\sqrt{2} = 0.70711\dots$ . However, what we actually observe is that the extrapolants approach the correct limit for a while and then veer away from this limit. Specifically, as  $N$  increases from 1, the extrapolants  $L_N$  seem to be approaching the correct limit monotonically:  $L_1 = 1.0$ ,  $L_2 = 0.84090$ ,  $L_3 = 0.78193$ ,  $L_4 = 0.75724$ ,  $L_5 = 0.74076$ ,  $L_6 = 0.73121$ ,  $L_7 = 0.72393$ ,  $L_8 = 0.71905$ ,  $L_9 = 0.71515$ ,  $L_{10} = 0.71231$ . The extrapolants continue to decrease until they *undershoot* the exact value. Eventually, the extrapolants reach a broad, flat minimum in 24th order:  $L_{24} = 0.70198$ . The relative error between this value and the exact answer is less than 1%. Then the extrapolants gradually rise; they recross the value 0.70711 at 41st order and continue rising. This behavior is strongly reminiscent of the behavior of the sequence of partial sums of an asymptotic (divergent) series. Apparently, there is no advantage to going to higher order in powers of  $\epsilon$ . We believe that underlying this behavior is the fact that we are solving a boundary-layer problem, which is a *singular* perturbation problem.

The purpose of this paper is to remedy this serious divergence problem. We will do so by using a superior lattice approximation. We begin by using the well-known fact that a lattice approximation to a differential equation may be regarded as a *higher order derivative perturbation* of that differential equation. An example of a higher order derivative perturbation of the differential equation  $y''(x) = [y(x)]^3 - y(x)$  is

$$\epsilon^2 y''''(x) + y''(x) = [y(x)]^3 - y(x), \quad (2.13)$$

where  $\epsilon$  is a small parameter.

Introducing a lattice is merely another way to perturb an equation. On a lattice of lattice spacing  $a$  we make the replacement

$$\begin{aligned} y''(x) &\rightarrow D^2 y(x) \equiv a^{-2} [y(x+a) - 2y(x) + y(x-a)] \\ &= y''(x) + \frac{1}{12} a^2 y''''(x) + \frac{1}{360} a^4 y''''''(x) + \dots \end{aligned} \quad (2.14)$$

Note that either of the above equations is a *singular perturbation* of  $y''(x) = [y(x)]^3 - y(x)$  because higher derivatives are multiplied by powers of the small parameter. However, we can use the Lie symmetry of the underlying unperturbed nonlinear equation  $y''(x) = [y(x)]^3$  to eliminate small parameter factors multiplying the higher derivatives. This equation is invariant under

$$x \rightarrow \alpha x, \quad y(x) \rightarrow \frac{1}{\alpha} y(x). \quad (2.15)$$

Thus, if we choose  $\alpha = \epsilon$  in Eq. (2.13) or  $\alpha = a$  in  $D^2 y(x) = [y(x)]^3 - y(x)$ , we obtain the equations

$$y''(x) + y''''(x) = [y(x)]^3 - \epsilon^2 y(x) \quad (2.16)$$

and

$$y''(x) + \frac{1}{12}y''''(x) + \frac{1}{360}y''''''(x) + \dots = [y(x)]^3 - a^2y(x). \quad (2.17)$$

These equations appear to be *regular* perturbation problems because the higher derivatives are no longer multiplied by factors of the perturbation parameter. However, this is not really so because the singular behavior has been shifted to the point  $z = \infty$ , where  $x = \epsilon z$ .

It can be proved<sup>10</sup> that *all* solutions except the trivial solution  $y(x) = 0$  to these equations are *not* regular at  $z = \infty$ . Indeed, in the  $(y, y')$ -phase plane [the two-dimensional projection of the full  $(y, y', y'', y''', \dots)$ -phase space] the phase portrait of (2.17) exhibits chaotic behavior.<sup>10</sup>

Exactly the same arguments can be made if the cubic nonlinear term in Eq. (2.13) or in the corresponding discretized equation is replaced by the quadratic nonlinear term  $[y(x)]^2$ . For this case the nonlinear equation  $y''(x) = [y(x)]^2$  is invariant under the Lie symmetry,

$$\begin{aligned} x &\rightarrow \alpha x, \\ y(x) &\rightarrow \frac{1}{\alpha^2}y(x). \end{aligned} \quad (2.18)$$

Again there is no nontrivial regular solution at  $z = \infty$ . [A central-difference discretization of Eq. (1.2) is equivalent to the Hénon map that is known to exhibit chaotic behavior.]

A necessary condition for there to be a smooth continuum limit is that at  $z = \infty$  there exist a nontrivial regular solution (in the form of a Taylor series in powers of  $1/z$ ); such a solution would not exhibit chaotic behavior. It is the rigorously demonstrated nonexistence of such a regular solution at  $z = \infty$  that probably prevents us from extrapolating smoothly to the continuum limit of the lattice approximation in Eq. (2.14). However, if we could find a discretization scheme that respects the discrete Lie symmetry, then the Taylor series at  $z = \infty$  would truncate and we would have a regular solution. (Of course, the mere existence of a solution that is regular at  $z = \infty$  does not in itself guarantee that the solution we seek will be regular. However, we immediately reject all other discretization schemes because they are associated with chaotic behavior.)

We summarize the above remarks in the form of a general criterion.

*Criterion 1: One must discretize the nonlinear term in the differential equation so that the resulting discrete difference equation has the same (singular) scaling solution (that is, the same Lie symmetry) as the original differential equation.*

We apply this criterion to Eq. (2.1) as follows: Neglecting the linear term, which in the scaled equation (2.17) is multiplied by the small parameter  $a^2$ , we observe that there is a singular scaling solution to  $\delta^2 y''(x) = [y(x)]^3$  of the form  $y(x) = c/x$ , where  $c$  is a constant. Thus, we seek to discretize the nonlinear term  $[y(x)]^3$  so that the difference equation has a solution of the form  $c/n$ . The choice of difference equation is now unambiguous; there is a unique cubic term that respects the Lie symmetry:

$$\epsilon(y_{n+1} - 2y_n + y_{n-1}) = \frac{1}{2}(y_{n+1} + y_{n-1})y_n^2. \quad (2.19)$$

[As we show in Sec. III for the case of a quadratic nonlinearity, we seek an exact solution of the form  $y_n = c/n(n+1)$ .]

The above criterion does not provide any guidance about how to discretize the linear term in the differential equation. Lacking guidance, we might choose

$$\epsilon(y_{n+1} - 2y_n + y_{n-1}) = \frac{1}{2}(y_{n+1} + y_{n-1})y_n^2 - y_n, \quad (2.20)$$



which is the simplest scheme. However, this choice is unacceptable as we now show. Consider the ultralocal ( $\epsilon=0$ ) equation:

$$\frac{y_{n+1}+y_{n-1}}{2}y_n^2-y_n=0. \quad (2.21)$$

The natural solution to Eq. (2.21) at  $n=0$  is

$$y_0=0, \quad (2.22)$$

because it incorporates the boundary condition  $y(0)=0$ . Next, we examine Eq. (2.21) at  $n=1$ ; this equation reads as  $y_2y_1^2=2y_1$ . Let

$$y_1=\alpha, \quad (2.23)$$

where  $\alpha$  is arbitrary. Then,

$$y_2=\frac{2}{\alpha}. \quad (2.24)$$

Next, we examine Eq. (2.21) at  $n=2$ ; this equation reads as  $(y_3+y_1)y_2^2=2y_2$ , whence

$$y_3=0. \quad (2.25)$$

If we continue this process, we obtain  $y_4=\beta$ , where  $\beta$  is arbitrary,  $y_5=2/\beta$ ,  $y_6=0$ ,  $y_7=\gamma$ , where  $\gamma$  is arbitrary,  $y_8=2/\gamma$ ,  $y_9=0$ , and so on. We reject the discretization in Eq. (2.20) because it gives a sequence of  $y_n$  at  $\epsilon=0$  that does not have a continuum limit; rather, it has a choppy, fluctuating structure.

To determine an acceptable discretization of Eq. (2.1), we formulate a second criterion.

*Criterion 2: The unperturbed ultralocal solution to the difference equation in the outer region must be smooth so that it will have a continuum limit.*

Imposing this criterion *uniquely* determines a discretization for Eq. (2.1):

$$\epsilon(y_{n+1}-2y_n+y_{n-1})=\frac{1}{2}(y_{n+1}+y_{n-1})y_n^2-\frac{1}{2}(y_{n+1}+y_{n-1}). \quad (2.26)$$

The ultralocal solution to this equation satisfies Criterion 2:

$$y_0=0, \quad y_n=1(n>0). \quad (2.27)$$

Although this ultralocal solution is not smooth at  $n=0$ , this jump discontinuity does not violate Criterion 2 because this jump is in the boundary-layer (inner) region and not in the outer region.

Next, we expand  $y_n$  for each  $n$  as a series in powers of  $\epsilon$  and obtain the analog of Eq. (2.6):

$$\begin{aligned}
y_0 &= 0, \\
y_1 &= 1 - \epsilon + \frac{3}{2}\epsilon^2 - \frac{5}{2}\epsilon^3 + \frac{35}{8}\epsilon^4 + \dots, \\
y_2 &= 1 - \frac{1}{2}\epsilon^2 + \epsilon^3 - \frac{13}{8}\epsilon^4 + \dots, \\
y_3 &= 1 - \frac{1}{4}\epsilon^3 + \frac{3}{4}\epsilon^4 + \dots, \\
y_4 &= 1 - \frac{1}{8}\epsilon^4 + \dots,
\end{aligned} \tag{2.28}$$

and so on. If we now determine the extrapolants  $L_N$  from these new series, we obtain a dramatic improvement; not only does  $L_N$  converge to the exact answer as  $N \rightarrow \infty$ , but  $L_N$  equals the exact answer for all  $N$ :

$$L_N = \frac{1}{\sqrt{2}} \text{ (all } N). \tag{2.29}$$

We are able to verify this result because while it is extremely rare to find an exact solution to a nonlinear equation, we have succeeded in solving the difference equation (2.26) *exactly and in closed form* for all values of  $\epsilon$ :

$$\begin{aligned}
y_0 &= 0, \quad y_1 = \frac{1}{\sqrt{2\epsilon+1}}, \quad y_2 = \frac{\sqrt{2\epsilon+1}}{\epsilon+1}, \\
y_3 &= \frac{3\epsilon+2}{(\epsilon+2)\sqrt{2\epsilon+1}}, \quad y_4 = \frac{(2\epsilon+2)\sqrt{2\epsilon+1}}{\epsilon^2+4\epsilon+2}, \\
y_5 &= \frac{5\epsilon^2+10\epsilon+4}{(\epsilon^2+6\epsilon+4)\sqrt{2\epsilon+1}}, \quad y_6 = \frac{(3\epsilon^2+8\epsilon+4)\sqrt{2\epsilon+1}}{\epsilon^3+9\epsilon^2+12\epsilon+4},
\end{aligned} \tag{2.30}$$

and so on. In general, for all  $n$  we have

$$y_n = \frac{(\sqrt{2\epsilon+1}+1)^n - (\sqrt{2\epsilon+1}-1)^n}{(\sqrt{2\epsilon+1}+1)^n + (\sqrt{2\epsilon+1}-1)^n}, \tag{2.31}$$

which is the lattice version of the hyperbolic tangent function in Eq. (2.2).<sup>11</sup>

### III. OSCILLATOR WITH A QUADRATIC NONLINEARITY

In this section we show how to use the criteria formulated in Sec. II to find the correct discretization of the nonlinear equation,

$$\delta^2 y''(x) = [y(x)]^2 - 2y(x), \quad (3.1)$$

subject to the boundary conditions

$$y(\pm\infty) = 2. \quad (3.2)$$

Because Eq. (3.1) has a translation symmetry, there is an infinite number of soliton solutions to this problem, all parameterized by the location of the center (minimum value) of the wave. To eliminate this translation ambiguity, we impose the further condition that  $y(x)$  be an *even* function of  $x$ . There are exactly two solutions that satisfy this additional requirement, a trivial constant solution,

$$y(x) \equiv 2, \quad (3.3)$$

and a nontrivial solution that can be given exactly in terms of the hyperbolic tangent function,

$$y(x) = -1 + 3 \left[ \tanh\left(\frac{x}{\delta\sqrt{2}}\right) \right]^2. \quad (3.4)$$

Our objective will be to find the numerical value of  $y(0)$ ; from the above two equations we know that the exact answers are  $y(0) = 2$  and  $y(0) = -1$ .

Like the boundary-value problem considered in Sec. II, the differential equation in Eq. (3.1) is a boundary-layer problem. From the exact solution in Eq. (3.4) we know that the boundary layer occurs at the origin and has thickness  $\delta$ .

We introduce a lattice according to the principles formulated in Sec. II. First, we observe that the nonlinear differential equation  $\delta^2 y''(x) = [y(x)]^2$  has a scale invariance (a Lie symmetry) and admits singular, double-pole solutions of the form

$$y(x) = \frac{c}{x^2}, \quad (3.5)$$

where  $c$  is a constant. The lattice equivalent of a double pole is the function  $1/n(n+1)$  [or, more generally,  $1/(n+\alpha)(n+1+\alpha)$ ] and *not*  $1/n^2$ , as one might naively think. In general, the lattice equivalent of the continuum function  $x^{-k}$  is

$$f_k = \frac{1}{(n+\alpha)(n+1+\alpha)(n+2+\alpha)(n+3+\alpha)\dots(n+k-1+\alpha)}. \quad (3.6)$$

To understand this equivalence we observe that the analogy of the continuum equation

$$\frac{d}{dx} x^{-k} = -kx^{-k-1}, \quad (3.7)$$

is

$$Df_k = -kf_{k+1}, \quad (3.8)$$

where  $D$  is the discrete derivative (first difference) operator.

Now we apply Criterion 1 of Sec. II. Since we are looking for a symmetric solution to Eq. (3.1), we represent  $y''(x)$  by a *symmetric* double difference:  $a^{-2}(y_{n+1} - 2y_n + y_{n-1})$ . When we take the second difference of the solution  $y_n = 1/(n+\alpha)(n+1+\alpha)$ , we obtain

$$\frac{1}{(n-1+\alpha)(n+\alpha)(n+1+\alpha)(n+2+\alpha)}, \tag{3.9}$$

apart from a multiplicative constant. There are exactly *two* symmetric quadratic lattice structures that we could use on the right side of the equation to produce the result in Eq. (3.9) from  $y_n = 1/(n+\alpha)(n+1+\alpha)$ ; the structure  $y_{n+1}y_{n-1}$  gives

$$\frac{1}{(n-1+\alpha)(n+\alpha)(n+1+\alpha)(n+2+\alpha)}, \tag{3.10}$$

and  $y_n(y_{n+1}+y_n+y_{n-1})$  gives

$$\frac{3}{(n-1+\alpha)(n+\alpha)(n+1+\alpha)(n+2+\alpha)}. \tag{3.11}$$

(Recall that Criterion 1 does not place any requirements on the linear term.) We conclude that the most general symmetric difference equation satisfying Criterion 1 is

$$\epsilon(y_{n+1} - 2y_n + y_{n-1}) = +Qy_{n+1}y_{n-1} - Ry_{n+1} + y_{n-1} - Sy_n, \tag{3.12}$$

where

$$\epsilon = \frac{\delta^2}{a^2}. \tag{3.13}$$

The arbitrary constants  $P$ ,  $Q$ ,  $R$ , and  $S$  in Eq. (3.12) obey two constraints: Since the coefficient of the quadratic term in Eq. (3.1) is 1, we have

$$3P + Q = 1, \tag{3.14}$$

and since the coefficient of the linear term in Eq. (3.1) is  $-2$ , we have

$$2R + S = 2. \tag{3.15}$$

Next we impose Criterion 2 (smoothness of the ultralocal solution in the outer region). Criterion 2 states that outside the boundary layer at  $x=0$  ( $n=0$  on the lattice) the unperturbed solution must have a slowly varying continuum limit. We therefore seek an ultralocal ( $\epsilon=0$ ) solution of the form

$$y_0 = \xi, \quad y_n = 2(n \neq 0). \tag{3.16}$$

For  $n=0$  this gives the constraint

$$0 = \xi(4 + \xi)P + 4Q - 4R - \xi S, \tag{3.17}$$

and for  $n=1$  this gives

$$0 = 2(4 + \xi)P + 2\xi Q - (2 + \xi)R - 2S. \tag{3.18}$$

When  $n > 1$ , we obtain the condition  $0 = 6P + 2Q - 2R - S$ , which is already true by virtue of Eqs. (3.14) and (3.15).

The equations (3.14), (3.15), (3.17), and (3.18) determine uniquely the arbitrary constants in the lattice equation (3.12):

$$\begin{aligned} P &= \frac{2}{2-\xi}, & Q &= \frac{\xi+4}{\xi-2}, \\ R &= \frac{2\xi+4}{\xi-2}, & S &= \frac{2\xi+12}{2-\xi}. \end{aligned} \quad (3.19)$$

It appears as if all that remains is for us to substitute Eq. (3.19) into Eq. (3.12) and to expand  $y_n$  for each  $n$  as series in powers of  $\epsilon$ . However, as we now show, this procedure is not quite as straightforward as in Sec. II because here we encounter a subtlety with regard to the form of the regular perturbation expansion. In particular, if we attempt to expand  $y_n$  as a series in powers of  $\epsilon$ , we reach an immediate contradiction! Let

$$\begin{aligned} y_0 &= \xi + a_0\epsilon + O(\epsilon^2), \\ y_n &= 2 + a_n\epsilon + O(\epsilon^2) \quad (n \neq 0). \end{aligned} \quad (3.20)$$

Now, for  $n=0$  we obtain

$$2 - \xi + a_0 + a_1 + a_{-1} = 0, \quad (3.21)$$

and for  $n=1$  we have

$$\xi - 2 + (\xi + 4)a_2 = 0. \quad (3.22)$$

For  $n > 1$  we get simply

$$a_2 = 0, \quad a_3 = 0, \quad a_4 = 0, \quad (3.23)$$

and so on. Hence, from Eqs. (3.21)–(3.23) we have  $\xi=2$  and we are forced to conclude that there is *no boundary layer* at  $x=0$ .

There are two ways to avoid this problem. The first is to recognize that because the boundary layer in the continuum differential equation is thick [of size  $\delta = O(\sqrt{\epsilon})$  and not  $O(\epsilon)$ ], the boundary layer on the lattice must be made thicker. Thus, we replace Eq. (3.16) by

$$y_0 = \xi_1, \quad y_{\pm 1} = \xi_2, \quad y_n = 2 \quad (n \neq 0, \pm 1). \quad (3.24)$$

We have examined this approach in detail and have verified that it works successfully; in fact, with the choice in Eq. (3.24) we are able to find all the terms in the perturbation series and to sum the perturbation series to all orders in closed form. However, we do not pursue this approach further here because there is a second procedure that is simpler and more natural. Since the thickness of the boundary layer in the continuum is of order  $\delta$ , we seek an expansion of  $y_n$  for each  $n$  as a series in powers of  $z = \sqrt{\epsilon}$ . Thus, we replace Eq. (3.20) by

$$\begin{aligned} y_0 &= \xi + a_0z + b_0z^2 + c_0z^3 + O(z^4), \\ y_n &= 2 + a_nz + b_nz^2 + c_nz^3 + O(z^4) \quad (n \neq 0). \end{aligned} \quad (3.25)$$

With this *ansatz* we obtain the following series representations in powers of  $z = \sqrt{\epsilon}$  on the lattice:

$$y_0 = \xi + a_0z + \frac{(\xi-2)(\xi+12)}{4}z^2 + \frac{(\xi-2)^2(\xi+8)}{2a_0}z^3 + \frac{(\xi-2)(\xi+4)(\xi+6)}{16}z^4 + \dots,$$

$$\begin{aligned}
 y_{\pm 1} &= 2 - \frac{a_0}{2}z + \frac{(2-\xi)}{2}z^2 - \frac{(\xi-2)^2(\xi+6)}{4a_0}z^3 - \frac{(\xi-2)(\xi+6)}{8}z^4 + \dots, \\
 y_{\pm 2} &= 2 - \frac{a_0}{4}z^3 + O(z^4), \quad y_{\pm 3} = 2 + O(z^5), \\
 y_{\pm 4} &= 2 + O(z^7), \quad y_{\pm 5} = 2 + O(z^9), \quad y_{\pm 6} = 2 + O(z^{11}),
 \end{aligned}
 \tag{3.26}$$

and so on, where  $(a_0)^2 = 2(\xi - 2)^2$ .

We have been able to carry out this analysis to *all* orders in powers of  $z$  and to sum the series in closed form. We are especially interested in  $y_0$ . For this case the odd terms and the even terms in the series have completely different structures. For even powers in  $z$  we have

$$\begin{aligned}
 \{y_0\}_{\text{even}} &= \xi + \frac{(\xi-2)(\xi+12)}{4}z^2 + \frac{(\xi-2)(\xi+4)(\xi+6)}{16}z^4 + \frac{(\xi-2)^2(\xi+4)(\xi+6)}{64}z^6 \\
 &\quad + \frac{(\xi-2)^3(\xi+4)(\xi+6)}{256}z^8 + \frac{(\xi-2)^4(\xi+4)(\xi+6)}{1024}z^{10} + \dots, \\
 &= \xi + \frac{(\xi-2)(\xi+12)}{4}z^2 + \frac{(\xi-2)(\xi+4)(\xi+6)}{16}z^4 \sum_{k=0}^{\infty} \left[ \frac{(\xi-2)z^2}{4} \right]^k \\
 &= \xi + \frac{(\xi-2)(\xi+12)}{4}z^2 + \frac{(\xi-2)(\xi+4)(\xi+6)z^4}{16-4(\xi-2)z^2}.
 \end{aligned}
 \tag{3.27}$$

The odd powers of  $z$  in the series for  $y_0$  are somewhat more complicated:

$$\begin{aligned}
 \{y_0\}_{\text{odd}} &= a_0z + a_0 \frac{(\xi+8)}{4}z^3 + a_0 \frac{\xi^2+6\xi}{16}z^5 + a_0 \frac{\xi^3+4\xi^2-12\xi-16}{64}z^7 + \dots, \\
 &= za_0 \sum_{k=0}^{\infty} \mathcal{P}_k(\xi) \left( \frac{z^2}{4} \right)^k,
 \end{aligned}
 \tag{3.28}$$

where  $\mathcal{P}_k$  is the set of polynomials in the variable  $\xi$ :

$$\begin{aligned}
 \mathcal{P}_0 &= 1, \\
 \mathcal{P}_1 &= \xi + 8, \\
 \mathcal{P}_2 &= \xi^2 + 6\xi, \\
 \mathcal{P}_3 &= \xi^3 + 4\xi^2 - 12\xi - 16, \\
 \mathcal{P}_4 &= \xi^4 + 2\xi^3 - 20\xi^2 + 8\xi + 64, \\
 \mathcal{P}_5 &= \xi^5 - 24\xi^3 + 48\xi^2 + 48\xi - 192,
 \end{aligned}
 \tag{3.29}$$

and so on.

These polynomials satisfy the simple difference equation

$$\mathcal{P}_{k+1} = (\xi - 2)\mathcal{P}_k + T_k,
 \tag{3.30}$$

where  $T_k$  ( $k=0,1,2,3,4,\dots$ ) is the sequence of numbers 10, 16, -16, 32, -64, 0, 1536, -16896, 146432, -1171456, . . . . An exact, closed-form expression for  $T_k$  is

$$T_k = \frac{(k-5)(-8)^k}{\sqrt{\pi}(k+1)!} \Gamma\left(k - \frac{1}{2}\right). \quad (3.31)$$

Hence, an explicit formula for  $\mathcal{P}_k$  is

$$\mathcal{P}_k = (\xi-2)^k + \sum_{j=0}^{k-1} T_j (\xi-2)^{k-j-1}. \quad (3.32)$$

If we substitute Eq. (3.32) into Eq. (3.28) and perform the double summation, we obtain

$$\{y_0\}_{\text{odd}} = \frac{2a_0z(2+3z^2)\sqrt{1+2z^2}}{4-(\xi-2)z^2}. \quad (3.33)$$

Finally, combining the even and odd parts of  $y_0$  and eliminating  $z$  and  $a_0$  in favor of  $\epsilon$ , we have

$$y_0 = \xi + \frac{(\xi-2)\epsilon}{4-\epsilon(\xi-2)} \left[ 12\epsilon + \xi + 12 - (8+12\epsilon) \sqrt{1 + \frac{1}{2\epsilon}} \right]. \quad (3.34)$$

Observe that when  $\xi=2$ , we have  $y_0=2$  for any  $\epsilon$ ; thus, we have found the trivial solution to the problem. On the other hand, when  $\xi \neq 2$ , in the limit of zero lattice spacing we obtain

$$y_0 = -1 - \frac{19\xi+58}{(8\xi-16)\epsilon} + O(\epsilon^{-2}) \quad (\epsilon \rightarrow \infty). \quad (3.35)$$

Thus, in the limit as  $\epsilon \rightarrow \infty$  we recover the nontrivial boundary-layer solution to the problem.

It is startling indeed that we have managed once again to find the exact, closed-form solution to a nonlinear second order difference equation. It is quite remarkable that imposing Criteria 1 and

2 on the nonlinear differential equations in Secs. II and III has led us to formulate discrete nonlinear difference equations that can be solved exactly and in closed form; any other discretizations yield difference equations for which there is virtually no hope of finding exact solutions.<sup>12</sup>

#### IV. BLASIUS EQUATION

The Blasius equation is a nonlinear third order differential equation that arises in the description of a fluid flowing along a flat plate:

$$\delta y'''(x) + y(x)y''(x) = 0, \quad (4.1)$$

where  $y(x)$  satisfies the boundary conditions

$$y(0) = 0, \quad y'(0) = 0, \quad y'(\infty) = 1. \quad (4.2)$$

Our goal is to show that

$$y''(0) = 0.46960 \dots / \sqrt{\delta}. \quad (4.3)$$

This is an extremely difficult boundary-value problem that not only has no known analytical solution but also is extremely difficult to solve numerically.

In Refs. 2 and 3 this problem was considered but the discretization scheme that was used there gave only moderately good and not excellent results. The discretization was exactly what one might choose in the absence of the criteria developed in Sec. II:

$$\begin{aligned} y(x) &\rightarrow y_n, \\ y''(x) &\rightarrow (y_{n+1} - 2y_n + y_{n-1})/a^2, \\ y'''(x) &\rightarrow (y_{n+1} - 3y_n + 3y_{n-1} - y_{n-2})/a^3. \end{aligned}$$

Using as boundary conditions  $y_{-1} = y_0 = 0$ , a lattice series for  $y_1$  in powers of the scaled small parameter  $\delta$  was obtained to 38th order. From this series a sequence of lattice extrapolants was obtained. The lattice extrapolants  $E_N$  form a monotonically decreasing sequence:  $E_1 = 0.7071/\sqrt{\delta}$ ,  $E_2 = 0.5945/\sqrt{\delta}$ ,  $E_3 = 0.5583/\sqrt{\delta}$ ,  $E_4 = 0.5401/\sqrt{\delta}$ ,  $E_5 = 0.5292/\sqrt{\delta}$ , and so on. Although this sequence continues to decrease, it is not obvious whether it approaches the correct answer in Eq. (4.3); indeed it appears to level off at a value that is about 5% too high:  $E_{25} = 0.4953/\sqrt{\delta}$ ,  $E_{26} = 0.4950/\sqrt{\delta}$ ,  $E_{37} = 0.4928/\sqrt{\delta}$ ,  $E_{38} = 0.4927/\sqrt{\delta}$ .

In this paper we discretize the Blasius equation following the procedures described in Secs. II and III. First, we make the replacement

$$y'''(x) \rightarrow (f_{n+3} - 3f_{n+2} + 3f_{n+1} - f_n)/a^2. \quad (4.4)$$

Here,  $a$  is the lattice spacing and for convenience we perform a scaling  $y_n = af_n$ . Next, we consider the nonlinear term and make the replacement:

$$\begin{aligned} y(x)y''(x) &\rightarrow Pf_{n+2}f_{n+3} + (1-2Q-P)f_nf_{n+1} + (1-3Q)f_nf_{n+3} - 3Qf_{n+1}f_{n+2} \\ &\quad + (6Q+2P-2)f_nf_{n+2} + (2Q-2P)f_{n+1}f_{n+3}, \end{aligned} \quad (4.5)$$

where  $P$  and  $Q$  are arbitrary parameters. This expression is the *most general* discretization of  $y(x)y''(x)$  using quadratic terms at the lattice points  $n, n+1, n+2, n+3$  such that the following two requirements are satisfied.



(1) Criterion 1: The Blasius equation has the Lie symmetry scaling solution  $y = c/x$ . If we substitute the lattice equivalent  $f_n = 1/n$  into Eq. (4.5), we get  $2[n(n+1)(n+2)(n+3)]$  for all  $P$  and  $Q$ . This is the same structure that one gets when one substitutes  $f_n = 1/n$  into the right side of Eq. (4.4).

(2) Criterion 2: For  $f_n = An + B$  (any linear function), the result vanishes; hence, we obtain a smooth ultralocal solution in the outer region (away from the boundary layer at  $n=0$ ).

We now take

$$\epsilon = \frac{\delta}{a^2}. \quad (4.6)$$

Thus, we have to solve

$$\begin{aligned} \epsilon(f_{n+3} - 3f_{n+2} + 3f_{n+1} - f_n) + Pf_{n+2}f_{n+3} + (1-2Q-P)f_nf_{n+1} + (1-3Q)f_nf_{n+3} \\ - 3Qf_{n+1}f_{n+2} + (6Q+2P-2)f_nf_{n+2} + (2Q-2P)f_{n+1}f_{n+3} = 0, \end{aligned} \quad (4.7)$$

subject to the three boundary conditions  $f_0 = 0$ ,  $f_1 = 0$ ,  $\lim_{n \rightarrow \infty} f_{n+1} - f_n = 1$ , and our objective is to show that

$$\lim_{\epsilon \rightarrow \infty} \sqrt{\epsilon} f_2 = 0.46960. \quad (4.8)$$

We begin our analysis by looking at the case  $n=0$ . This gives the equation

$$\epsilon(f_3 - 3f_2) + Pf_2f_3 = 0. \quad (4.9)$$

Assuming that  $f_2$  and  $f_3$  are nonzero when  $\epsilon=0$ , we are compelled to choose  $P=0$ . This fixes one of the two arbitrary parameters. With  $P=0$  we have

$$\begin{aligned} \epsilon(f_{n+3} - 3f_{n+2} + 3f_{n+1} - f_n) + (1-2Q)f_nf_{n+1} + (1-3Q)f_nf_{n+3} - 3Qf_{n+1}f_{n+2} \\ + (6Q-2)f_nf_{n+2} + (2Q)f_{n+1}f_{n+3} = 0. \end{aligned} \quad (4.10)$$

To determine the parameter  $Q$  we note that there is one more symmetry of the Blasius equation that we have not yet used, namely, reflection symmetry. Equation (4.1) is symmetric under the discrete symmetry,

$$x \rightarrow -x, \quad y \rightarrow -y.$$

While reflection symmetry is not a Lie symmetry, it does seem natural to impose this symmetry here because it uniquely fixes the value of the remaining arbitrary parameter  $Q$ . On the lattice this symmetry takes the form

$$\begin{aligned} f_n &\rightarrow -f_{n+3}, & f_{n+1} &\rightarrow -f_{n+2}, \\ f_{n+2} &\rightarrow -f_{n+1}, & f_{n+3} &\rightarrow -f_n. \end{aligned}$$

Requiring that Eq. (4.10) be invariant under this symmetry gives the value  $Q=1/2$ .

For this case, let

$$f_n = a_n + \epsilon b_n + \epsilon^2 c_n + \epsilon^3 d_n + \dots \quad (4.11)$$

In the ultralocal limit ( $\epsilon=0$ ),  $a_n$  satisfies

$$a_{n+3} = a_{n+2} \frac{3a_{n+1} - 2a_n}{2a_{n+1} - a_n}. \quad (4.12)$$

This equation gives the sequence

$$a_0 = 0,$$

$$a_1 = 0, \quad a_2 = x, \quad a_3 = 3x,$$

$$a_4 = 9x/2, \quad a_5 = 63x/10, \quad a_6 = 63x/8, \quad a_7 = 77x/8, \quad (4.13)$$

where  $x$  is an arbitrary parameter.

The exact formula for  $a_n$  is

$$a_{2n} = \frac{2x\Gamma(1/4)\Gamma(n-1/4)\Gamma(n+1/2)}{\Gamma(3/4)\Gamma(1/2)\Gamma(n-3/4)\Gamma(n)},$$

$$a_{2n+1} = \frac{2x\Gamma(1/4)\Gamma(n+3/4)\Gamma(n+1/2)}{\Gamma(3/4)\Gamma(1/2)\Gamma(n+1/4)\Gamma(n)}. \quad (4.14)$$

Now we impose the requirement that  $\lim_{n \rightarrow \infty} a_{n+1} - a_n = 1$ . This fixes the value of  $x$ :

$$x = \frac{\Gamma(3/4)\Gamma(1/2)}{\Gamma(1/4)} = 0.5990701173677961. \quad (4.15)$$

Next, we examine the solution to first order in  $\epsilon$ . Note that  $b_n$  satisfies the equation

$$0 = a_{n+3} - 3a_{n+2} + 3a_{n+1} - a_n + a_{n+1}b_{n+3} + a_{n+3}b_{n+1} + a_n b_{n+2} + a_{n+2}b_n - \frac{1}{2}a_n b_{n+3} - \frac{1}{2}a_{n+3}b_n - \frac{3}{2}a_{n+1}b_{n+2} - \frac{3}{2}a_{n+2}b_{n+1}. \quad (4.16)$$

The first few values of  $b_n$  are

$$b_0 = 0, \quad b_1 = 0, \quad b_2 = y, \quad b_3 = 3y, \quad b_4 = 9y/2 + 3/2, \quad b_5 = 63y/10 + 89/50,$$

$$b_6 = 63y/8 + 51/16, \quad b_7 = 77y/8 + 4697/1296, \quad (4.17)$$

where  $y$  is an arbitrary parameter.

The sequence  $b_n$  consists of two parts. The part multiplying  $y$  is just  $a_n$  (the homogeneous solution). To isolate the second part, we write

$$b_n = \frac{y}{x} a_n + z_n. \quad (4.18)$$

Now, as  $n \rightarrow \infty$ , we can show that

$$b_n \sim \frac{y}{x} n + nL, \quad (4.19)$$

where  $L = 0.9272586576$ . Hence,  $y = -x(0.9272586576)$ . Thus, to first order in powers of  $\epsilon$  we have

$$f_2 = x(1 - 0.9272586576\epsilon + \dots). \quad (4.20)$$

We can now use this result to obtain the *first* extrapolant  $E_1$  to the value of  $y''(0)$ :

$$\begin{aligned} E_1 &= \frac{1}{\sqrt{\delta}} \lim_{\epsilon \rightarrow \infty} x \sqrt{\epsilon} (1 - 0.9272586576\epsilon) \\ &= \frac{x}{\sqrt{\delta}} \lim_{\epsilon \rightarrow \infty} \frac{\sqrt{\epsilon}}{1 + 2(0.9272586576)\epsilon} \\ &= \frac{x}{\sqrt{\delta}} (0.7343187) = \frac{1}{\sqrt{\delta}} (0.43990837). \end{aligned} \quad (4.21)$$

When we compare this number with 0.46960 (exact) we see that our result is 6.3% low. This first order result is already comparable in accuracy with that obtained in Refs. 2 and 3 in 38th order!

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