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Solution of a general one-turning-point Schrödinger equation using lattice extrapolation techniques

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In this paper a recently proposed lattice approach to the solution of boundary-layer problems is applied to the one-turning-point WKB problem. The introduction of the lattice converts the singular-differential-equation perturbation problem to a regular perturbation problem. The singular nature of the WKB problem is restored when the lattice spacing is extrapolated to zero. Accurate numerical results are obtained for several cases of interest.

Lattice methods have played an important role in the derivation of strong-coupling expansions in quantum field theory, and various Padé-type schemes have been used to extrapolate the lattice strong-coupling expansion to the continuum. In recent papers, lattice methods have also been used as a means of finding approximate solutions to singular boundary-layer problems.[1] In Ref. 1, it was shown that the introduction of a lattice converts a singular perturbation problem into a regular perturbation problem, which can then be solved to very high order using a (convergent) perturbation series. The inherently singular nature of the problem resurfaces when the lattice perturbation series is extrapolated back to the continuum (zero lattice spacing).

It was recently suggested to us by Russell Pack that a one-turning-point WKB problem would provide an interesting testing ground for the methods developed in Ref. 1. Therefore, in this brief paper we give a lattice analysis of a generalized one-turning-point problem.

By a one-turning-point problem we mean a Schrödinger boundary-value problem of the form

$$\epsilon^2 y''(x) = s(x)y(x)\,, \tag{1}$$

where ϵ is a small positive parameter and $s(x)$ has one zero, which with no loss of generality can be located at the origin. A region in which $s(x)>0$ is called a classically forbidden region and we assume, again without loss of generality, that $s(x)>0$ for $x>0$. We seek the solution to (1) which satisfies the boundary conditions

$$y(0)=1 \quad\text{and}\quad y(+\infty)=0\,. \tag{2}$$

Near the origin, $s(x)$ is assumed to have the asymptotic form

$$s(x) \sim \alpha x^\beta \quad (\alpha, \beta > 0)\,. \tag{3}$$

It is clear that if (3) is substituted into (1), the variable x can be scaled to eliminate α from the problem.

To illustrate the lattice methods discussed in Ref. 1, and the assertion that lattice methods reduce singular perturbation problems to regular perturbation problems, we consider the following simple singular boundary-value problem:

$$\epsilon^2 y''(x) = x^\beta y(x) \tag{4}$$

with $y(0)=1$, $y(+\infty)=0$, in which $s(x)$ is everywhere equal to its asymptotic behavior at the origin. Our objective will be to compute $y'(0)$. The value of $y'(0)$, which is a nontrivial consequence of the two widely separated boundary conditions, is crucial because, together with the value of $y(0)$, it determines all of the Taylor coefficients of $y(x)$ at the origin.

We have chosen to solve the problem (4) because (4) has an exact analytic solution to which the lattice results can be compared. The solution to the differential equation (4) which decays exponentially as $x\to+\infty$ is

$$y(x) = C\epsilon^{-1/(\beta+2)} x^{1/2} K_{1/(\beta+2)}\left(\frac{2}{(\beta+2)\epsilon} x^{(\beta+2)/2}\right). \tag{5}$$

Requiring that $y(0)=1$ determines the constant $C = 2(\beta+2)^{-1/(\beta+2)}\Gamma(1/(\beta+2))$. Finally, evaluating $y'(0)$ gives the closed-form expression

$$y'(0) = -\epsilon^{-2/(\beta+2)}(\beta+2)^{-2/(\beta+2)}\Gamma\left(\frac{\beta+1}{\beta+2}\right)\bigg/\Gamma\left(\frac{\beta+3}{\beta+2}\right). \tag{6}$$

Now we will explain why (4) is a singular boundary-value problem. A regular perturbation problem is one for which the solution can be expanded as a series in powers of the perturbation parameter, which in this case is ϵ. However, if we attempt to represent $y(x)$ as a series in powers of ϵ, we find that all the coefficients in this series are zero. It is well known that the only way to repre-

TABLE I. The first 40 extrapolants Q_p for the cases $\beta=1$ and $\beta=2$. The convergence of these extrapolants is very different for these two cases. When $\beta=1$ the sequence Q_p is monotone increasing towards the exact answer, and when $\beta=2$ the sequence initially decreases towards the exact answer, goes below it, turns around, and crosses it again on the way up. The sequence of first Richardson extrapolants R_p for the $\beta=1$ sequence of Q_p is even more interesting, oscillating above and below the exact answer, with nearly equally spaced peaks and valleys labeled by (max) and (min) occurring about every six numbers.

Order p	Extrapolants Q_p for $\beta=1$	Richardson extrapolants R_p for Q_p at $\beta=1$	Extrapolants Q_p for $\beta=2$
1	0.693 361	0.693 361	0.707 107
2	0.693 361	0.706 614	0.687 656
3	0.697 779	0.717 416	0.679 616
4	0.702 688	0.725 459	0.675 350
5	0.707 242	0.730 848	0.672 795
6	0.711 176	0.733 691	0.671 158
7	0.714 393	0.734 234 (max)	0.670 067
8	0.716 873	0.732 998	0.669 325
9	0.718 665	0.730 772	0.668 821
10	0.719 875	0.728 441	0.668 483
11	0.720 654	0.726 722	0.668 266
12	0.721 160	0.725 980 (min)	0.668 142
13	0.721 530	0.726 212	0.668 087
14	0.721 865	0.727 159	0.668 088
15	0.722 218	0.728 443	0.668 133
16	0.722 607	0.729 686	0.668 215
17	0.723 023	0.730 586	0.668 327
18	0.723 443	0.730 964 (max)	0.668 465
19	0.723 839	0.730 787	0.668 625
20	0.724 187	0.730 165	0.668 804
21	0.724 471	0.729 311	0.669 002
22	0.724 691	0.728 474	0.669 216
23	0.724 856	0.727 868	0.669 445
24	0.724 981	0.727 616 (min)	0.669 688
25	0.725 087	0.727 732	0.669 947
26	0.725 188	0.728 140	0.670 219
27	0.725 298	0.728 704	0.670 506
28	0.725 419	0.729 274	0.670 808
29	0.725 552	0.729 716	0.671 126
30	0.725 691	0.729 941 (max)	0.671 461
31	0.725 828	0.729 923	0.671 814
32	0.725 956	0.729 691	0.672 188
33	0.726 069	0.729 327	0.672 585
34	0.726 165	0.728 930	0.673 008
35	0.726 244	0.728 600	0.673 462
36	0.726 310	0.728 405	0.673 951
37	0.726 366	0.728 372 (min)	0.674 483
38	0.726 419	0.728 488	0.675 067
39	0.726 472	0.728 706	0.675 719
40	0.726 528		0.676 457
Exact answer	0.729 011	0.729 011	0.675 978

sent the solution to (4), or more generally to (1), is by means of a WKB approximation in which terms of the form $\exp[f(x)/\epsilon]$ appear, and which does not have a smooth limit as $\epsilon \to 0$.

We claim that on the lattice (4) is converted into a regular perturbation problem. To introduce the lattice, we let

$$\begin{aligned} &x \to an\,, \\ &y(x) \to y_n\,, \\ &y'(x) \to (y_{n+1}-y_n)/a\,, \\ &y''(x) \to (y_{n+1}-2y_n+y_{n-1})/a^2\,, \end{aligned} \tag{7}$$

where a is the lattice spacing.

These replacements convert the boundary-value problem (4) into its discrete lattice analog:

$$\delta(y_{n+1}-2y_n+y_{n-1})=n^\beta y_n\,,\qquad y_0=1\,,\ y_n\to 0 \text{ as } n\to\infty \tag{8}$$

with

$$\delta=\epsilon^2/a^{\beta+2}\,. \tag{9}$$

On the lattice, we regard the lattice spacing a as being fixed and ϵ as small, and therefore we think of δ as a new small expansion parameter.

We solve (8) by expanding y_n at the nth lattice point as a regular perturbation series in the parameter δ. The trick is to recognize that at the nth lattice point the perturbation series begins with a δ^n term:

$$y_n=\sum_{j=n}^{\infty}A_{n,j}\delta^j\,,\quad n>0\,. \tag{10}$$

Substituting (10) into (8) and equating coefficients of like powers of δ then gives the following recursion relation for the coefficients $A_{n,j}$:

$$A_{n,j}=\begin{cases}0 \quad (j<n)\,,\\ 0 \quad (n=0,\ j>0)\,,\\ 1/(n!)^\beta \quad (j=n)\,,\\ (1/n^\beta)(A_{n-1,n}-2A_{n,n}) \quad (j=n+1)\,,\\ (1/n^\beta)(A_{n+1,j-1}-2A_{n,j-1}+A_{n-1,j-1})\\ (n>0,\ j>n+1)\,.\end{cases} \tag{11}$$

Our objective is to compute $y'(0)$. Using (7) we represent $y'(0)$ as the limit

$$\begin{aligned} y'(0)&=\lim_{a\to 0}(y_1-y_0)/a\\ &=-\lim_{a\to 0}(1/a)\left(1-\sum_{j=1}^{\infty}A_{1,j}\delta^j\right)\\ &=-\epsilon^{-2/(\beta+2)}\lim_{\delta\to\infty}\delta^{1/(\beta+2)}\left(1-\sum_{j=1}^{\infty}A_{1,j}\delta^j\right), \end{aligned} \tag{12}$$

where we have used (9) to eliminate the lattice spacing a in favor of the dimensionless parameter δ.

Observe that the lattice limit in (12) is extremely singular; keeping only a finite number of terms in the series leads to a divergent result for the limit. Thus, to perform the limit in (12), one must use an extrapolation technique. It is through this extrapolation technique that the singular nature of the boundary-value problem in (4) is restored.

The extrapolation method used here was first proposed in Ref. 2, and some of its properties were studied in subsequent papers.[3]

Briefly, the procedure consists of (a) raising the series $(1-\sum_{j=1}^{\infty}A_{1,j}\delta^j)$ in (12) to the power $-p(\beta+2)$ $(p=1,2,3,\ldots)$ and then (b) raising the coefficient of δ^p in the resulting series to the power $-1/(p\beta+2p)$. This produces the pth extrapolant, Q_p. The hope is that the sequence $-\epsilon^{-2/(\beta+2)}Q_p$ converges to, or at least closely approximates, the exact answer in (6) as $p\to\infty$. This extrapolation procedure is more fully discussed in Refs. 1 and 2.

In Table I, we give the first 40 extrapolants for the cases $\beta=1$ and $\beta=2$. Observe that in the case $\beta=1$ (this is the most common case and one for which the exact solution is given in terms of Airy functions) the extrapolants Q_p are monotonically increasing and appear to be converging slowly to the exact answer. The convergence can be accelerated using Richardson extrapolation.[4] In Table I, we list the first 39 Richardson extrapolants R_p defined by

$$R_p=(p+1)Q_{p+1}-pQ_p\,. \tag{13}$$

It is interesting that these extrapolants oscillate slowly above and below the exact answer, and that averaging the peaks and valleys of the Richardson extrapolants using a Shanks transformation[4] gives an approximation to the exact answer which is accurate to a relative error of about 0.01%.

We also list in Table I the first 40 extrapolants Q_p for the case $\beta=2$. These extrapolants decrease monotonically until they reach a minimum in 13th order which falls about 1% below the exact answer. Then they increase at an accelerating rate. This kind of behavior is strongly reminiscent of the behavior exhibited by asymptotic series, in which partial sums first approach the exact answer, and then rapidly deviate from it.

Finally, we note that for more complicated choices than monomials for $s(x)$, (4) is not in general soluble in terms of known special functions. However, it is trivial to generalize the recursion relation in (11) to cover such cases.

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