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Analytic continuation and Green function calculations

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Abstract. Hass, Velicky and Ehrenreich have shown that Green function values can be obtained appreciably faster by performing the calculation at complex energies with large imaginary parts, and then returning to real energies by an analytic continuation algorithm. However, analytic continuation is numerically unstable and thus an error analysis is essential if one is to have confidence in the results of the continuation. In this paper, error estimates are obtained for the power series method of Hass *et al* and for a method based upon Cauchy's theorem introduced herein. These estimates can be used to select appropriate values for the parameters of the continuation algorithms.

1. Introduction

Many properties of solids can be easily expressed and calculated in terms of Green functions, and in particular, the limiting behaviour of $G(E)=(E-H)^{-1}$ on the real axis. Since this function is singular on a portion of the real axis, the traditional numerical method is to add a small imaginary part to E, thereby performing the calculation just off the axis. In a recent paper, Hass *et al* (1984) proposed an interesting alternative, one designed to increase the speed of Green function evaluations. The scheme put forth is to solve for $G(z)$ for z away from the axis, and then use an analytic continuation algorithm (based upon power series) to return to the real line. The rationale for this procedure is that $G(z)$ is given in terms of a q-space integral, q a Fourier transform variable. The singularities on the axis cause the integrand $G(q, z)$ to be a rather badly behaved function when $\mathrm{Im}(z)$ is small, and consequently obtaining the required accuracy for the integral necessitates a time-consuming evaluation of $G(q, z)$ for a great many values of q. However, off the axis $G(q, z)$ is much smoother, and thus $G(z)$ may be calculated much more easily. Using this method, Hass *et al* report being able to do a three-dimensional CPA calculation within an accuracy of 2% in one-third the time of the standard approach.

The purposes of the present paper are to describe another possible algorithm for the analytic continuation, one based upon Cauchy's theorem, and to present an error analysis of both methods. For the analytic continuation methods to be effective, an error analysis is essential because of the 'ill conditioned' nature of the problem; by this it is meant that a small change in the initial data can produce a large disturbance in the final answer (Miller 1970, Hass 1984). Consequently, the error, starting with inaccuracies in the initial data and compounded with the subsequent numerical round-off, will grow during the calculation and eventually, if the parameters are not chosen wisely, overpower the desired solution. As a result, if $G(z)$ is computed initially too far off the real line, the analytic continuation back to the axis will yield nonsense. An error analysis is therefore required in order to determine appropriate values for the parameters (the starting values of Im(z) and the discretisation variable Δ) and to have confidence in the results obtained by using an analytic continuation approach. The results of the analysis show that the Cauchy method is more stable but less accurate than the power series method. Another benefit of the error analysis is that it makes it possible to incorporate extrapolation in the algorithm, thereby improving upon the accuracy of the methods with little additional effort. This will be discussed in § 4.

2. The Cauchy method

Let $f(z)$ be a function which is analytic in the upper half plane, and assume that $f(z)$ is known at the points

$$E_{n,M} = E_0 + n\Delta + iM\Delta \tag{2.1}$$

where $-N \leqslant n \leqslant N$, N and M integers, and Δ a fixed constant. Thus, the function values are given at points which are equally spaced on a line in the upper half plane parallel to the real axis. The analytic continuation procedure will calculate $f(z)$ on the line $\mathrm{Im}(z) = (M-1)\Delta$, at the points $z_{n,M-1}$, $-N+1 \leqslant n \leqslant N-1$; repeating the process M times yields the values of f on the real axis, at the points $z_{n,0}$, $-N+M \leqslant n \leqslant N-M$. (The assumptions of equal spacing and an odd number of initial values are solely for notational convenience, and are not essential.) In Hass *et al*, the continuation method is based upon Taylor's theorem, the unknown values being computed by fitting a truncated power series through the known points. The method described in this section relies on Cauchy's theorem, which states that

$$\oint_C g(z)\,\mathrm{d}z = 0 \tag{2.2}$$

provided $g(z)$ is analytic inside the closed contour C.

The continuation algorithm is generated by choosing C to be the triangular path determined by three adjacent points on the line $\mathrm{Im}(z) = M\Delta$ together with the point just below the midpoint on the line $\mathrm{Im}(z) = (M-1)\Delta$ (see figure 1). The integral over

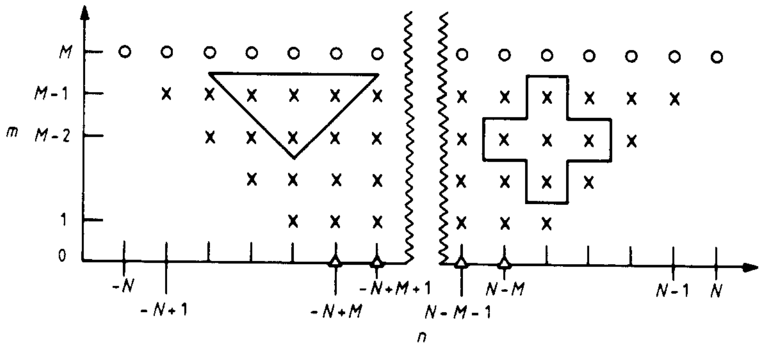

Figure 1. Schematic illustration of the Cauchy (triangle) and power series (cross) analytic continuation methods for $M = 5$. (The generation of the $\mathrm{Im}(z) = (M-1)\Delta$ line of values for the power series method is not shown.) O, given initial values of the function; ×, intermediate points where the function values are calculated; Δ, energies where the function is ultimately determined.

each of the four line segments which make up this path is approximated by the average of the function values at the endpoints times the difference of the two endpoints. Setting the integral over this triangle equal to zero yields the equation

$$f(z_{z,M-1}) = f(z_{n,M}) + \tfrac{1}{2}\mathrm{i}[f(z_{n-1,M}) - f(z_{n+1,M})] \tag{2.3}$$

for the unknown value of f. Having calculated the function values on the line $\mathrm{Im}(z) = (M-1)\Delta$, the process can now be repeated; at each step of the computation, the two endpoints are lost, and thus the initial $2N+1$ values only generate $2(N-M)+1$ values on the axis.

This is the simplest algorithm that can be constructed using the Cauchy theorem. By choosing longer paths (e.g. taking five points on the line $\mathrm{Im}(z) = m\Delta$ to generate a function value on the line $\mathrm{Im}(z) = (m-1)\Delta$), one can generate more accurate methods. In addition, one can use a more sophisticated integration scheme than the admittedly crude approach used to obtain (2.3). However, there is a trade-off between accuracy and stability, the more accurate being the more unstable (and more accurate methods may require additional initial data to generate the same number of values on the axis). The Cauchy method was deliberately designed to sacrifice accuracy for stability.

Clearly, both continuation procedures, power series and Cauchy, are trivial to implement and require little computation. Two minor advantages of the Cauchy approach are that it is much easier to implement if the initial data are not equally spaced, and that it does not require an initial step (the power series method generates the $M-1$ line of function values using a procedure different from the remainder of the algorithm). The principal disadvantage is that it is less accurate than the power series method. Consider for example the function

$$h(z) = 2[z - (z^2-1)^{1/2}] + (z + 0.1 + 0.05\mathrm{i})^{-1} + (z - 0.1 + 0.05\mathrm{i})^{-1} \tag{2.4}$$

discussed in Hass *et al.* These authors calculate $h(z)$ on the line $\mathrm{Im}(z) = 0.1$, and then use the power series method (with $M = 5$ and $\Delta = 0.02$) to obtain $h(z)$ on the axis, with excellent results. In figure 2 the results of the two methods are compared, and

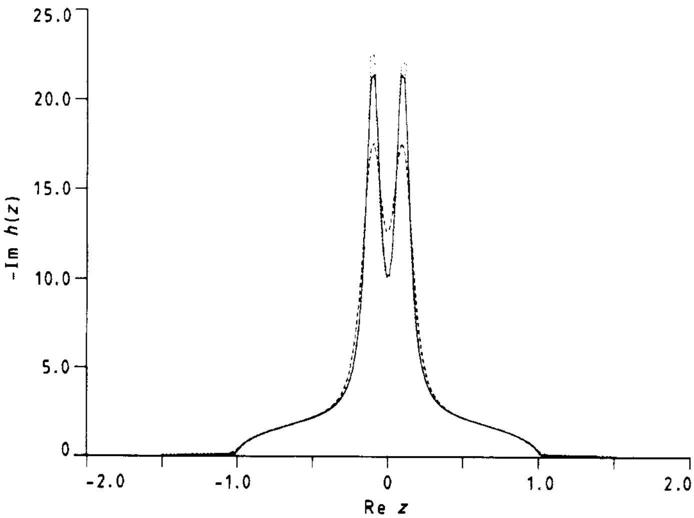

Figure 2. A comparison of the Cauchy (broken curve), power series (full curve), and exact results (dotted curve) for the function $h(z)$, with $M = 5$ and $\Delta = 0.02$.

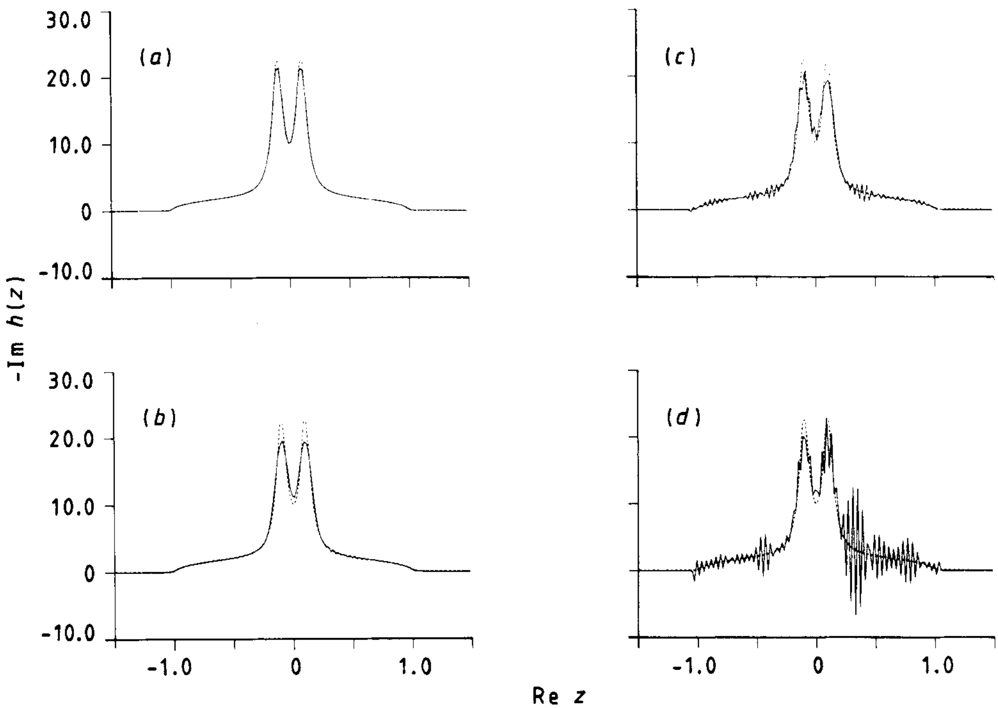

Figure 3. The breakdown of the power series method for the function $h(z)$, with $\Delta = 0.02$ and (*a*) $M = 5$, (*b*) $M = 20$, (*c*) $M = 21$ and (*d*) $M = 22$. The broken curve is the exact result.

clearly the power series is superior. If, however, the initial values are moved further from the real axis, then the results deteriorate until there is no resemblance between the computed and actual values. This is demonstrated in figure 3 (power series) and figure 4 (Cauchy). In these figures, the initial data have been moved away from the real axis, increasing the number of steps M needed to reach the axis. Note that the power series calculation disintegrates much sooner than the Cauchy. In the remainder of the paper, an error analysis is performed to explain this behaviour, and to provide guidelines for choosing M and Δ so as to obtain meaningful results.

3. Error analysis

One source of error in any numerical continuation procedure is the discretisation of the function and the enforcement of analyticity in only an approximate manner. In the power series method, the power series representing the function is truncated, whereas the Cauchy method only computes an approximation to the contour integral over the triangle. For both of these methods, however, the magnitude of this error is relatively easy to compute as a function of Δ; this is accomplished in theorems 1 and 2. On the other hand, the numerical round off error is much harder to analyse, and the results below only present a crude upper bound. Nevertheless, these estimates can be effectively used to determine values for M and Δ which will lead to reasonable results.

The first result describes the discretisation error for the Cauchy method.

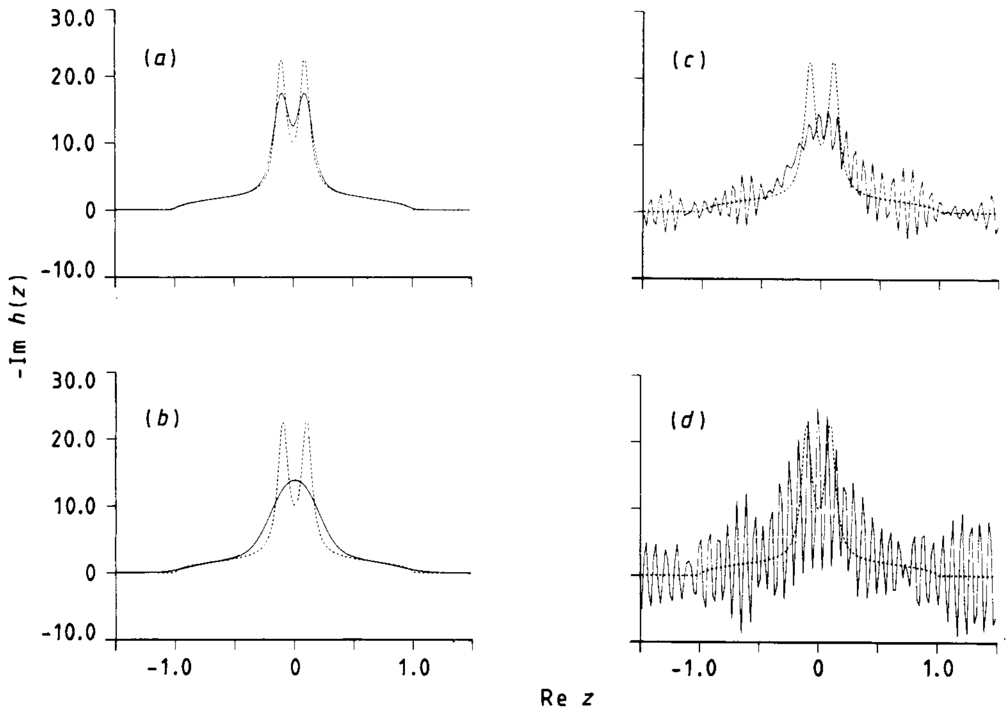

Figure 4. The breakdown of the Cauchy method for the function $h(z)$, with $\Delta = 0.02$ and (a) $M = 5$, (b) $M = 40$, (c) $M = 56$ and (d) $M = 57$. The broken curve is the exact result.

Theorem 1. Let $g(z)$ be analytic in the upper half plane, and assume $g(z)$ is known for $z_{n,M} = E_0 + n\Delta + \mathrm{i}M\Delta$, where $-N \leqslant n \leqslant N$, M and n are integers, $0 < M < N$, and Δ is a positive constant. If $\hat{g}(z_{n,M-m})$, $1 \leqslant m \leqslant M$, denotes the result of the Cauchy continuation, then for $-N + m \leqslant n \leqslant N - m$

$$\hat{g}(z_{n,M-m}) = g(z_{n,M-m}) + \tfrac{1}{2}m\Delta^2 g''(z_{n,M-m+1}) + \mathrm{o}(\Delta^2). \tag{3.1}$$

Proof. Consider the four points z_0, $z_0 \pm \Delta$, $z_0 - \mathrm{i}\Delta$, as shown in figure 1. Define $f_l(z) = (z - z_0)^l$, and apply (2.3) to f_l to obtain for $l \geqslant 1$,

$$\hat{f}_l(z_0 - \mathrm{i}\Delta) = -\tfrac{1}{2}\mathrm{i}[\Delta^l - (-\Delta)^l]. \tag{3.2}$$

Thus, the error E_l arising from the continuation is

$$\begin{aligned} E_l &= f_l(z_0 - \mathrm{i}\Delta) - \hat{f}_l(z_0 - \mathrm{i}\Delta) \\ &= (-\mathrm{i}\Delta)^l + \tfrac{1}{2}\mathrm{i}[\Delta^l - (-\Delta)^l] \\ &= \begin{cases} 0 & l = 0, 1 \\ \mathrm{i}^l\Delta^l & l \text{ even } \geqslant 2 \\ \mathrm{i}\Delta^l - \mathrm{i}^l\Delta^l & l \text{ odd } \geqslant 3. \end{cases} \end{aligned} \tag{3.3}$$

Since g is analytic, there is a convergent power series representation, $g(z) = \sum_{l=0}^{\infty} a_l(z - z_0)^l$, with radius of convergence greater or equal to $\mathrm{Im}(z_0)$. Using the linearity of the continuation and (3.3), one finds

$$\hat{g}(z_0 - i\Delta) = \sum_{l=0}^{\infty} a_l \hat{f}_l(z_0 - i\Delta) = \sum_{l=0}^{\infty} a_l f_l(z_0 - i\Delta) - \sum_{l=0}^{\infty} a_l E_l$$
$$= g(z_0 - i\Delta) + a_2\Delta^2 + o(\Delta^2)$$
$$= g(z_0 - i\Delta) + \tfrac{1}{2}\Delta^2 g''(z_0) + o(\Delta^2). \qquad (3.4)$$

Since g'' is itself analytic, (3.4) can be applied to itself to obtain $\hat{g}(z_0 - 2i\Delta)$:

$$\hat{g}(z_0 - 2i\Delta) = g(z_0 - 2i\Delta) + \tfrac{1}{2}\Delta^2 g''(z_0 - i\Delta) + o(\Delta^2)$$
$$+ \tfrac{1}{2}\Delta^2[g''(z_0 - i\Delta) + \tfrac{1}{2}\Delta^2 g^{(4)}(z_0) + o(\Delta^2)] + o(\Delta^2)$$
$$= g(z_0 - 2i\Delta) + \Delta^2 g''(z_0 - i\Delta) + o(\Delta^2). \qquad (3.5)$$

A simple induction argument now yields (3.1).

The leading term in the discretisation error is thus of order Δ^2, and should be largest where the second derivative is large. In figures 5 and 6 the imaginary part of the calculated error, $\hat{g} - g$, and the leading order term, $\frac{1}{2}M\Delta^2 g''(z_{n,1})$, are plotted against the number of steps M to the real axis (for $\Delta = 0.02$) and the step size Δ (for $M = 5$);

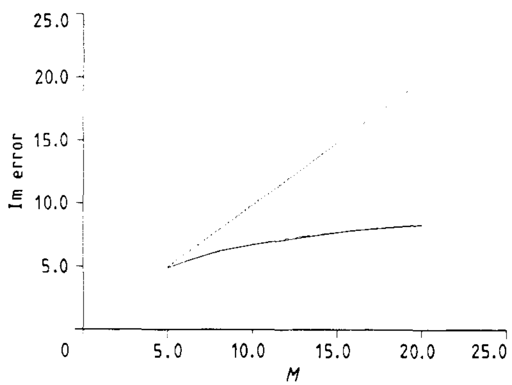

Figure 5. The imaginary part of the error $\hat{g} - g$ (full curve) and the imaginary part of the leading error term (broken curve) on the real axis as a function M, with $\Delta = 0.02$. This is for the Cauchy method acting on the function $h(z)$ at the point $z = -0.09$.

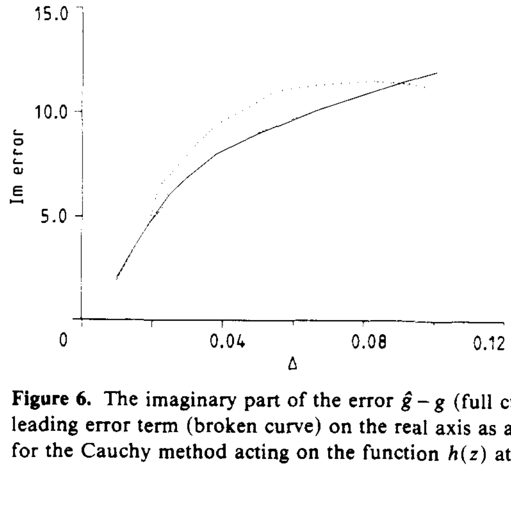

Figure 6. The imaginary part of the error $\hat{g} - g$ (full curve) and the imaginary part of the leading error term (broken curve) on the real axis as a function of Δ, with $M = 5$. This is for the Cauchy method acting on the function $h(z)$ at the point $z = -0.09$.

this is for the function $h(z)$ at $z=-0.09$. This point is one of the peaks of $h(z)$, and thus a place where the error is likely to be largest. In both cases, the Δ^2 term gives a reasonably good estimate of the actual error, especially as one should expect, for the smaller values of M and Δ likely to be used in practice. These error estimates can therefore be used to determine appropriate values for M and Δ. Note that when Δ is varied, the point at which the second derivative is evaluated also changes, which explains the downturn of the curve in figure 6.

In the power series method, the procedure for generating the second line, i.e. the function values at $z_{n,M-1}$, is different from the basic algorithm employed to compute the remaining $M-1$ lines. However, for the purposes of the error analysis, it is convenient to ignore this minor technicality and assume that the function values $f(z_{n,M-1})$ are also known exactly.

Theorem 2. Let $g(z)$ be analytic in the upper half plane, and assume that $g(z)$ is known for $z_{n,M}$ and $z_{n,M-1}$, where $z_{n,m}=E_0+n\Delta+\mathrm{i}m\Delta$, $-N\leqslant n\leqslant N$, Δ a positive constant. If $g(z_{n,M-m})$, $1\leqslant m\leqslant M$ denotes the result of the power series continuation algorithm, then for $-N+m\leqslant n\leqslant N-m$

$$\tilde{g}(z_{n,M-m})=g(z_{n,M-m})-\tfrac{1}{6}m\Delta^4 g^{(4)}(z_{n,M-m+1})+\mathrm{o}(\Delta^4).$$

Proof. As in theorem 1, the effect of the continuation procedure on the functions $f_l(z)=(z-z_0)^l$ will first be examined. Using the points z_0, $z_0\pm\Delta$, $z_0+\mathrm{i}\Delta$ as shown in figure 1, the method of Hass *et al* sets

$$\tilde{f}(z_0-\mathrm{i}\Delta)=4f(z_0)-f(z_0+\mathrm{i}\Delta)-f(z_0-\Delta)-f(z_0+\Delta) \tag{3.6}$$

for any analytic function f. Note that this equation simply expresses the fact that the value of an analytic function at the centre of a circle is the average of its values along the circle.

For $f(z)=f_l(z)=(z-z_0)^l$, the error E_l is found to be

$$E_l=f_l(z_0-\mathrm{i}\Delta)-\tilde{f}_l(z_0-\mathrm{i}\Delta)=\begin{cases}4\Delta^l & l\equiv 0 \bmod 4\ l>0\\ 0 & \text{otherwise.}\end{cases} \tag{3.7}$$

Thus, for $g(z)=\Sigma_{l=0}^{\infty}a_l(z-z_0)^l$,

$$\begin{aligned}\tilde{g}(z_0-\mathrm{i}\Delta)&=g(z_0-\mathrm{i}\Delta)-\sum_{l=4}^{\infty}a_lE_l\\&=g(z_0-\mathrm{i}\Delta)-\tfrac{1}{6}g^{(4)}(z_0)\Delta^4+\mathrm{o}(\Delta^4).\end{aligned} \tag{3.8}$$

The same reasoning employed in theorem 1 now yields

$$\tilde{g}(z_0-m\mathrm{i}\Delta)=g(z_0-m\mathrm{i}\Delta)-\tfrac{1}{6}m\Delta^4g^{(4)}[z_0-(m-1)\mathrm{i}\Delta)]+\mathrm{o}(\Delta^4) \tag{3.9}$$

and this completes the proof.

It is easy to check that the initial procedure used to generate the function values at $z_{n,M-1}$ (see Hass *et al* 1984) is also a fourth-order accurate process; thus, the leading error term for the power series method is of order Δ^4. The function $h(z)$ at the point $z=-0.09$ will again be used to test this result. In figures 7 and 8, the calculated error, $g-\tilde{g}$, and the error predicted by the leading term in (3.9) are plotted against M (for $\Delta=0.02$) and Δ (for $M=5$). It is seen that, as with the Cauchy method, the predictions serve as adequate estimates of the error.

Theorems 1 and 2 indicate that the power series method is more accurate than the Cauchy method; this is not surprising, since the latter only uses three values to generate

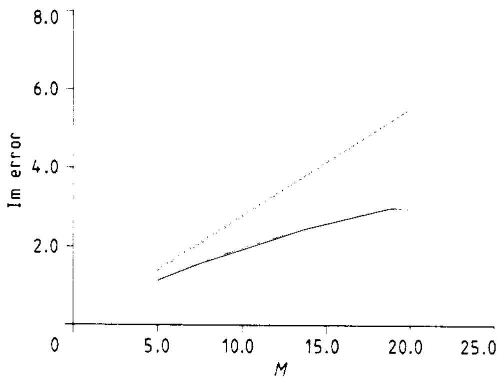

Figure 7. The imaginary part of the error $g - \tilde{g}$ (full curve) and the imaginary part of the leading error term (broken curve) on the real axis as a function of M, with $\Delta = 0.02$. This is for the power series method acting on the fucntion $h(z)$ at the point $z = -0.09$.

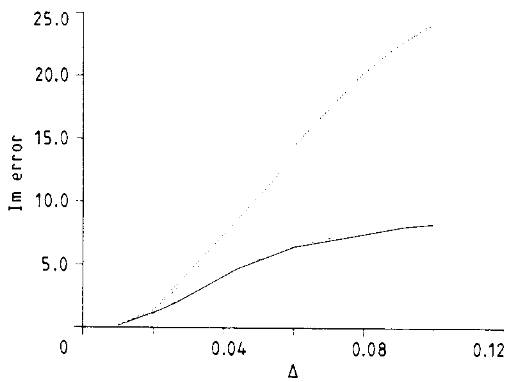

Figure 8. The imaginary part of the error $g - \tilde{g}$ (full curve) and the imaginary part of the leading error term (broken curve) on the real axis as a function of Δ, with $M = 5$. This is for the power series method acting on the function $h(z)$ at the point $z = -0.09$.

a new point, whereas the former uses four. However, this cannot be the complete picture of the error in the computation. Even though this leading term increases with M, the above error analysis does not explain the rapid breakdown of the calculations as M increases, or the greater 'stability' of the Cauchy method. The above theorems have assumed an exact computation, ignoring numerical errors, whereas the ill posed nature of the problem indicates that numerical error will grow during the computation. As the power series method more accurately represents the continuation process, it will naturally be more susceptible to the inherent numerical instabilities. A very crude, but nevertheless useful, analysis of the numerical errors will now be performed.

For the Cauchy method, represent the given data, $g(z_{n,M})$, as a vector in C^{2N+1}

$$g_o = \begin{pmatrix} g(z_{-N,M}) \\ \vdots \\ g(z_{N,M}) \end{pmatrix} + E_0 \tag{3.10}$$

where $E_0 \in C^{2N+1}$ represents the error vector. In the example discussed above, the function $h(z)$, this error vector is a consequence of numerical errors in calculating the function values at the points $z_{n,M}$ caused by the finite computer precision, and is consequently very small. However, for practical applications, the initial data (the Green function values) are themselves calculated only in an approximate fashion, and thus E_0 will be significantly larger. A convenient measure for the size of E is the ∞-norm

$$\|E\|_\infty = \|(e_j)\|_\infty = \max_j |e_j|. \tag{3.11}$$

Denote by $\hat{g}_m + E_m$, $1 \leqslant m \leqslant M$, the result of applying the Cauchy continuation to $g(z)$ m times. From (2.3), it is obvious that

$$\|E_m\|_\infty \leqslant 2\|E_{m-1}\|_\infty \tag{3.12}$$

and thus

$$\|E_m\|_\infty \leqslant 2^m \|E_0\|_\infty . \tag{3.13}$$

A similar analysis for the power series method yields

$$\|E_m\|_\infty \leqslant 7^m \|E_0\|_\infty . \tag{3.14}$$

Although (3.13) and (3.14) are rather crude estimates, they do give an indication of the quick deterioration of both methods as the initial data are moved further from the real axis. These estimates, together with theorem 1 or 2, can be used to obtain effective values for M and Δ.

As a demonstration of the predictive capabilities of (3.13) and (3.14), the breakdown of both methods will be examined, with the function $h(z)$ again used as a test case. The following analysis is rather imprecise, but nevertheless illustrates the usefulness of these estimates. Since the initial values of $h(z)$ off the axis are computed directly from the definition (equation (2.4)), the initial error norm is of order 10^{-15}. Since 7^{18} is of the order 1.6×10^{15}, the above analysis predicts that the numerical error will dominate the power series continuation for $M \geqslant 18$. Since (3.14) is an upper bound this is of course a conservative estimate; calculations indicate that for this example the power series method becomes unreliable at $M = 22$. Similarly, for the Cauchy method, (3.13) predicts breakdown at M about 52, while the calculations fall apart for M approximately 56.

For practical problems, $M = 17$ and $M = 51$ are unrealistically large, as the error in the initial data is much larger than 10^{-15}. To simulate this situation, a sequence of random numbers ε_n were generated from the interval $[10^{-4}, 10^4]$; the initial values $h(z_{n,M})$ were then replaced by $(1+\varepsilon_n)h(z_{n,M})$. For the power series method (resp Cauchy method), the error analysis now estimates numerical instability setting in at about $M = 4$ (resp $M = 11$) and the calculations show $M = 6$ (resp $M = 15$). Thus, the above estimates work reasonably well in setting an upper bound on the value of M.

4. Extrapolation

In addition to assisting in the choice of parameter values, the error estimates of the previous section can also be used as the basis of extrapolation procedures. Thus, with only a small amount of additional computation, one can improve upon the accuracy of the continuation methods. We will illustrate this idea for the Cauchy method, the analogous steps for the power series method being obvious.

If, in addition to computing $\hat{g}(z_{n,0})$, $-N+M \leqslant n \leqslant N-M$ using the discretisation Δ, one also uses every other initial point to define two discretisations of size 2Δ, then, with obvious notation, theorem 1 implies

$$\begin{aligned}\hat{g}_{\Delta}(z_{n,0}) &= g(z_{n,0}) + \tfrac{1}{2}M\Delta^2 g''(z_{n,0}) + o(\Delta^2)\\ \hat{g}_{2\Delta}(z_{n,0}) &= g(z_{n,0}) + \tfrac{1}{4}M(2\Delta)^2 g''(z_{n,0}) + o(\Delta^2).\end{aligned} \tag{4.1}$$

The algorithm must be done twice with step size 2Δ in order to generate an approximation to $g(z_{n,0})$, $-N+M+1 \leqslant n \leqslant N-M-1$. Thus, eliminating the second-order term in Δ from (4.1), and defining

$$\hat{g}_e(z_{n,0}) \equiv 2\hat{g}_{\Delta}(z_{n,0}) - \hat{g}_{2\Delta}(z_{j,0}) \tag{4.2}$$

one has

$$\hat{g}_e(z_{n,0}) - g(z_{n,0}) = o(\Delta^2). \tag{4.3}$$

The extrapolated value is therefore a better estimate of $g(z)$. Figure 9 shows a comparison of the Cauchy method with the extrapolated Cauchy for the function $h(z)$, with $M=6$ and $\Delta=0.02$. As the error analysis would indicate, there is a significant improvement, but it is still not as accurate as the power series method.

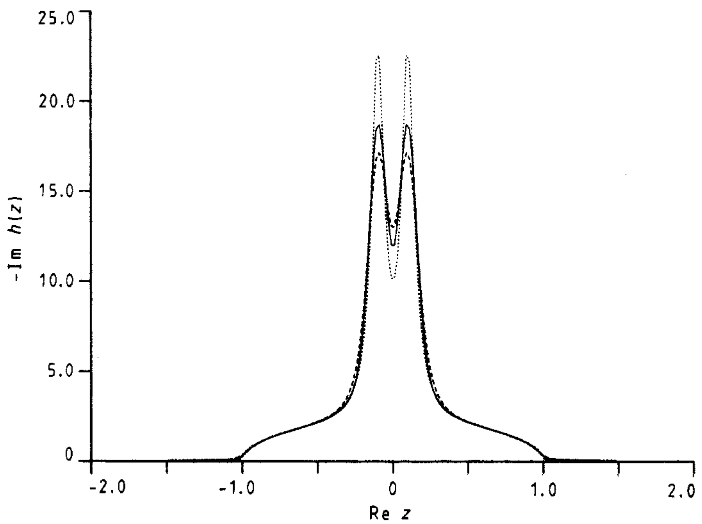

Figure 9. A comparison of the Cauchy (broken curve), extrapolated Cauchy (full curve) and the exact (dotted curve) results for $h(z)$ with $M=6$ and $\Delta=0.02$.

5. Conclusion

Hass *et al* have demonstrated that analytic continuation can be effectively used to speed up Green function calculations. An alternative algorithm for the continuation has been described herein, and the errors arising from both methods have been examined. Although using this approach for calculating Green functions will always entail a loss of accuracy, these error estimates can be used to determine values for M and Δ for which the error is sufficiently small. Analytic continuation can be especially useful in locating model parameters to fit experimental data; in this situation, a great many calculations must be done, and until one gets close to a good set of values, a few per cent in accuracy is not important.

The analysis has shown that the power series method is more accurate, and consequently more susceptible to numerical instability. If one knows what the errors are in the initial data, then the power series method should be used. However, if these errors are unknown, then it would be safer to use the Cauchy method with extrapolation. (Because of the higher accuracy of the power series algorithm, extrapolation is not likely to change the final result significantly, and is therefore not worth the effort.) Using the results developed in this paper, it is possible to choose the method and the parameters that are best suited to a particular calculation.

Acknowledgments

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