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Applications of Hermite–Padé approximants to water waves and the harmonic oscillator on a lattice

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Abstract. Three types of Hermite–Padé approximants are considered, known respectively as quadratic, integral and differential Padé approximants. The singularity structure of each type of approximant is described. It is more complicated than that of the standard Padé approximant, and this property may often be used to estimate the types of singularity of a function from its power series expansion, as well as evaluate it on its branch cuts.

Two applications in different fields are described which illustrate these properties of the above types of Hermite–Padé approximants. The first concerns the characteristic values of Mathieu's equation which are related to the energy eigenvalues of the harmonic oscillator on a lattice. The second concerns the investigation of the singularity structure and values of various physical quantities associated with periodic and solitary water waves.

1. Introduction

The Padé approximant has proved a useful tool in many branches of physics and applied mathematics for the summing of perturbation series which converge slowly or even diverge. The reason why Padé approximants can be used when straightforward series summation breaks down is that the former, being rational functions, have poles which can mimic the singularities of the function being approximated. However, on or close to the singularities of the original function the Padé approximants no longer converge unless these singularities are of the same type as those of the approximant, i.e. simple poles. It is therefore desirable to use generalisations of Padé approximants with more general types of singularities.

In this work we shall consider applications of three such generalisations. The first, quadratic Padé approximants, are defined by Shafer (1974) where the approximants are solutions of a quadratic equation and have square root branch cuts. The two other generalisations are defined by constructing from the original series differential equations whose solutions are taken to approximate the original function (Guttman and Joyce 1972, Gammel 1973). We will consider here two cases, the first being when the differential equation is a linear second-order homogeneous equation whose solutions are called differential Padé approximants. The second case is when the differential equation is an inhomogeneous first-order equation whose solution is called an integral Padé approximant. The singularities of these approximants are in general branch cuts. In § 2 we give precise definitions for these types of approximants, which are included in a wider class of approximants introduced originally by Hermite (1893) and Padé (1894) and termed Hermite–Padé approximants by Della Dora and Di Crescenzo (1979). We also describe briefly their singularity structure.

In this work we present applications in two fields which demonstrate the power of these approximations to continue an analytic function up to and even onto its singularities and also to determine the position and type of these singularities. The first concerns the simple harmonic oscillator in one-dimensional space when this space is latticised. It has been shown by Jurkiewicz and Woseik (1978) that the energy eigenvalues are closely related to the characteristic numbers $a_r(z)$, $b_r(z)$, $r=0, 1, \ldots,$ of Mathieu's equation (we use the same notation as Abramowitz and Stegun (1968)). Here the independent variable z is proportional to the inverse lattice spacing and the continuum limit is obtained by taking $z \to \infty$.

The above system has been used as a testing ground for methods to be used in a space–time lattice treatment of non-Abelian theories by many authors, including Carroll *et al* (1977), Jurkiewicz and Woseik (1978) and Hamer (1979). They were interested in determining from the power series for $a_r(z)$, $b_r(z)$ their limiting behaviour as $z \to \infty$. The type of limiting behaviour was assumed and ordinary Padé approximants were used to determine the strength. In § 3 we will use differential and integral Padé approximants to study the problem, and we find that in the case of $b_1(z)$ it is possible to determine the type and strength of the singular behaviour as $z \to \infty$. For other characteristic numbers it seems more difficult to determine the type of singularity, but when this is given one can often estimate the strength. Our results compare favourably with those given by the above authors.

The singularities of $a_r(z)$ and $b_r(z)$ for finite z have been studied by Hunter and Guerrieri (1981) and found to be of square root type. They show that for instance $a_0(z)$ and $a_2(z)$ have a common square root branch point at $z=z_0=-1.468\,786\mathrm{i}$, confirming earlier work of Mullholland and Goldstein (1929). We confirm these results using differential and integral Padé approximants to the power series of $a_2(z)$. Not only that, when we evaluate quadratic Padé approximants to this series, we find that one branch of the approximant gives the values for $a_2(z)$ whilst the other branch gives $a_0(z)$ for values of z in a large region of the complex plane including the cut. This demonstrates the ability of this type of approximant to continue an analytic function from one Riemann sheet to another sheet.

The second field of application which we discuss in § 4 is the study of water waves. Early work on this subject by Stokes (1847) used perturbation expansions in a parameter varying monotonically with the wave height/length ratio. However, as demonstrated by Schwartz (1974), they fail to converge for steep waves, and to compute the wave profiles in this case he used Padé approximants to sum the perturbation series.

In his original work, Stokes (1880) demonstrated that the highest water wave, assumed to be sharp crested, would have an included angle of 120° at the crest. This corresponds to a cube root singularity in the fluid velocity q as a function of the velocity potential $\chi=\phi+\mathrm{i}\psi$. However, for waves of less than maximum height, Grant (1973) has shown generally that the singularities of q must be square branch points. Schwartz (1974) studied numerically the leading singularity in q as the wave height is increased to its maximum value and obtained results in agreement with the above predictions. He used a method introduced by Domb and Sykes (1957) to determine the singular behaviour of q from its power series in χ. In § 4 we will repeat this investigation using differential Padé approximants, and we again find that they are successful in finding both the position and type of singularity of q.

The above work was concerned with periodic waves, but progress has also been made recently in the understanding of solitary waves, and in particular Longuet-

Higgins and Fenton (1974) have shown that the speed, mass, momentum and energy of the wave attain maximum values for waves of less than maximum amplitude. As a consequence, there can exist for a given wave speed F near its maximum value two quite distinct solitary waves. so that when the mass M of the wave is plotted against $\gamma \equiv F^2-1$, a curve is obtained which turns back on itself. Although they had been able to construct a series for M in powers of γ, the partial sums of this series and Padé approximants to it could not give the whole curve as they only give single-valued approximations to M. We will demonstrate in § 4 that quadratic Padé approximants to M, being double valued, do approximate well both values for M.

We end this work by summarising our results in § 5 and suggesting further fields of application of the generalisations to Padé approximations considered here.

2. Hermite–Padé approximants

We introduce the three types of Hermite–Padé approximants used in this work and summarise their singularity structure.

(i) Quadratic Padé approximants to a function $f(z)$ are defined by constructing polynomials $P(z)$, $Q(z)$, $R(z)$ that formally satisfy

$$P(z)f^2(z)+Q(z)f(z)+R(z)=\mathrm{O}(z^{p+q+r+2}), \qquad P(0)=1, \qquad (2.1a,b)$$

where p, q, r are the degrees of the respective polynomials. The corresponding approximants $f_{\mathrm{A}}(z)$ to $f(z)$ are the solutions of the equation obtained from $(2.1a)$ by replacing the RHS by zero, so that

$$f_{\mathrm{A}}(z)\equiv f^{Q\pm}_{p/q/r}(z)=\{-Q(z)\pm[Q^2(z)-4P(z)R(z)]^{1/2}\}/2, \qquad (2.2)$$

and this type of approximant therefore has square root branch parts.

(ii) Integral Padé approximants are similarly defined by requiring the polynomials $P(z)$, $Q(z)$, $R(z)$ to satisfy

$$P(z)\,\mathrm{d}f(z)/\mathrm{d}z+Q(z)f(z)+R(z)=\mathrm{O}(z^{p+q+r+2}), \qquad P(0)=1. \qquad (2.3a,b)$$

Replacing the RHS of $(2.3a)$ by zero, the corresponding solution is the integral approximant (Baker and Hunter 1979)

$$f_{\mathrm{A}}(z)\equiv f_{p/q;r}(z)=\exp\left(\int_0^z \frac{Q(\xi)}{P(\xi)}\,\mathrm{d}\xi\right)\left[f(0)-\int_0^z \frac{R(\eta)}{P(\eta)}\exp\left(\int_0^\eta \frac{Q(\xi)}{P(\xi)}\,\mathrm{d}\xi\right)\mathrm{d}\eta\right]. \qquad (2.4)$$

When $f(z)$ is a real function of z as considered here,

$$\frac{Q(z)}{P(z)}=\text{polynomial}+\sum_{j=1}^{n_c}\left(\frac{\gamma_j}{z-\sigma_j}+\frac{\gamma_j^*}{z-\sigma_j^*}\right)+\sum_{j=1}^{n_r}\frac{g_j}{(z+s_j)} \qquad (2.5)$$

where n_r is the number of real roots, n_c is the number of conjugate pairs of roots and g_j, s_j are real. It is well known that $f_{p/q,r}(z)$ has singularities at the zeros of $P(z)$ and, for example, as $z\to -s_j$

$$f_{p/q;r}(z)\approx A_1(z+s_j)^{-g_j}. \qquad (2.6)$$

In our applications we shall study the behaviour of $f(z)$ as $z\to\infty$ by investigating the corresponding behaviour for $f_{\mathrm{A}}(z)$, and find it convenient to consider the approximants with $q=p-1$. We also assume that $P(z)$ has no zeros on the positive axis so that $s_j > 0$; $j = 1, \ldots, n_r$. It is straightforward to show on substituting (2.5) in (2.4) that as $z \to \infty$

$$f_{p/q;r}(z) \approx A_2 z^{-\sum_{j=1}^{n_r} g_j + 2\sum_{j=1}^{n_c} \mathrm{Re}\, \gamma_j} \tag{2.7}$$

so long as the expression in square brackets on the RHS of (2.4) tends to a finite limit, and the constant A_2 may be determined. In the example considered in § 3, $f(z) = O(z^{1/2})$ as $z \to \infty$, so that we expect

$$\sum_{j=1}^{n_r} g_j + 2\sum_{j=1}^{n_c} \mathrm{Re}\, \gamma_j \approx -\tfrac{1}{2} \tag{2.8}$$

if the asymptotic behaviour of $f_A(z)$ as given by (2.7) is to approximate closely that of $f(z)$. The integral in square brackets on the RHS of (2.4) will then tend to a finite limit as $z \to \infty$ if $p - r \geqslant 1$, and in our applications we take $p = r + 2$.

We will also use forced approximants (Baker and Hunter 1979, Fisher and Au-Yang 1979). In that case the exponent of z in (2.7) is forced to have a given value by requiring the coefficients of the polynomials $P(z)$ and $Q(z)$ to satisfy a further linear relation which may be used to replace that in the defining relation (2.3a) obtained by equating coefficients of $z^{p+q+r+1}$. This further relation is obtained from (2.5) by letting $z \to \infty$, remembering that $q = p - 1$.

(iii) Finally, differential Padé approximants are defined by requiring

$$P(z)\mathrm{d}^2 f/\mathrm{d}z^2 + Q(z)\mathrm{d}f/\mathrm{d}z + R(z)f(z) = O(z^{p+q+r+2}), \qquad P(0) = 1. \tag{2.9a, b}$$

The differential approximant $f_A(z)$ is then the solution of

$$P(z)\mathrm{d}^2 f_A/\mathrm{d}z^2 + Q(z)\,\mathrm{d}f_A/\mathrm{d}z + R(z)f_A(z) = 0. \tag{2.10}$$

From standard theory, the singularities of $f_A(z)$ are at the zeros of $P(z)$ and their strength may be determined in the usual way. Forced approximants with specified singularities may again be defined (Fisher and Au-Yang 1979), and as above the extra requirements are linear relations between the coefficients of $P(z)$, $Q(z)$ and $R(z)$.

To study the behaviour of $f_A(z)$ as $z \to \infty$ one may, following any standard text (e.g. Brauer and Nohel 1967), change the variable $y = 1/z$ in (2.10) which then becomes

$$y^2\mathrm{d}^2 f_A/\mathrm{d}y^2 + yW_1(y)\,\mathrm{d}f_A/\mathrm{d}y + W_2(y)f_A(1/y) = 0, \tag{2.11}$$

where

$$W_1(y) = 2 - z\,Q(z)/P(z) \qquad W_2(y) = z^2 R(z)/P(z). \tag{2.12}$$

We require $z = \infty$ to be a regular singular point of $f_A(z)$, i.e. $W_i(y)$ to be analytic at $y = 0$. This condition is satisfied if $p \geqslant q + 1$, $p \geqslant r + 2$, and in § 3 we will use approximants where these are equalities. Then (2.11) has solutions

$$f_{A,i}(z) = z^{-\lambda_i} \sum_{k=0}^{\infty} d_{i,k}\, z^{-k}, \qquad i = 1, 2, \tag{2.13}$$

where λ_i are the roots of

$$\lambda[\lambda - 1 + W_1(0)] + W_2(0) = 0 \tag{2.14}$$

and the coefficients $d_{i,k}$ are obtained for $k > 0$ from recurrence relations involving the expansion coefficients of the $W_i(y)$ about $y = 0$. As previously, forced approximations may be defined where the λ_i have prescribed values.

3. The harmonic oscillator on a lattice

In a quantum mechanical treatment of a simple harmonic oscillator corresponding to the motion of a particle along the x axis, units may be chosen such that the Hamiltonian operator

$$H = \tfrac{1}{2}(p^2 + x^2) \tag{3.1}$$

where x is the coordinate of the particle and p its conjugate momentum. The coordinate space may be made discrete by taking the lattice of points $x = nl$ with $n = 0, \pm 1, \pm 2, \ldots$. It has been shown by Jurkiewicz and Woseik (1978) that the eigenvalues of $W = 2H/l^2$ are

$$\left.\begin{aligned} w_{i,1}(z) &= 2z + b_{2i+1}(z),\\ w_{i,2}(z) &= 2z + a_{2i+1}(z), \end{aligned}\right\} \quad i = 0, 1, 2, \ldots, \tag{3.2}$$

where $a_r(z)$, $b_r(z)$ are the characteristic values of Mathieu's equation and $z = 1/(4l^4)$. In the continuum limit $l \to 0$, i.e. $z \to \infty$, the corresponding eigenvalues of H are

$$(4z)^{-1/2} w_{i,1}(z) \to \tfrac{1}{2}(4i + 1), \tag{3.3a}$$

$$i = 0, 1, 2, \ldots,$$

$$(4z)^{-1/2} w_{i,2}(z) \to \tfrac{1}{2}(4i + 3) \tag{3.3b}$$

and this of course agrees with the continuum theory.

The analogue to z in quantum lattice field theory is used as a perturbation expansion parameter in expressions for physical quantities, so that to obtain the continuum values for these quantities one has to determine their limiting behaviour as $z \to \infty$ from their power series expansion in z. Mathematical techniques for doing this have been tested, using the above harmonic oscillator model, by seeing how well they determine the limiting behaviour (3.7) for $w_{i,1}(z)$, $w_{i,0}(z)$ from known power series expansion for these characteristic values.

Obviously Padé approximants to $w_{i,j}(z)$ $(j = 0, 1)$ cannot be constructed which have the limiting behaviour (3, 3), but Hamer (1979) considers the related functions

$$g(z) = \{\mathrm{d}[w_{i,j}^2(z)]/\mathrm{d}z\}^{1/2}. \tag{3.4}$$

These have the limiting behaviour

$$\begin{aligned} g(z) &\to 2(2i + 3), & j &= 1,\\ &\to 2(2i + 1), & j &= 0, \end{aligned} \tag{3.5}$$

as $z \to \infty$. He then constructed the Padé approximations $g_{N/N}(z)$ and tested whether or not they had the above limiting behaviour. He found that for the ground state (corresponding to values $i = 0, j = 1$), the asymptotic values of the approximants were in reasonable but not perfect agreement with the exact value as demonstrated in table 1, but for excited states the Padé estimates were entirely useless. For these excited states, better results were obtained by matching the Padé approximant to the asymptotic behaviour at finite values $\{z_N\}$, which approach infinity only as $N \to \infty$ (Carroll *et al* 1977, Jurkiewicz and Woseik 1978).

As described in § 2, we can estimate the asymptotic behaviour

$$f(z) = w_{i,j}(z) \approx \gamma z^{\lambda}, \tag{3.6}$$

using differential Padé approximants $f^{\mathrm{D}}_{p/q/r}(z)$, where to ensure that $z = \infty$ is a regular

Table 1. Values of Padé approximants to $g(z)=(\mathrm{d}\, w_{i,0}^2(z)/\mathrm{d}z)^{1/2}$ as $z\to\infty$.

N/N	2/2	3/3	4/4	5/5	Exact
$\lim_{z\to\infty} g_{N/N}(z)$	1.665	2.112	1.967	1.996	2.00

singular point of the corresponding differential equation (2.10), we have considered the cases when $p=q+1=r+2$. The results for the ground state are again reasonable, being presented in table 2(a), but as above for the excited states the results are useless. In a sense, our method is better than the previous one since it estimates the value $\lambda=\frac{1}{2}$ for the power behaviour whilst above this value is assumed. By using forced differential Padé approximants we can arrange for $f^{\mathrm{D}}_{p/q/r}(z)$ to have the asymptotic behaviour (3.6) with $\lambda=\frac{1}{2}$ exactly. The corresponding estimates for γ are presented in table 2(b). There is again good convergence for the ground state, but in this case we also get estimates within at least 10%–20% of the correct answer for the excited states. Remember that to determine γ, we have to determine the overall normalisation of $f^{\mathrm{D}}_{b/q/r(z)}$, and this was done by summing the series in powers of z to the original function $f(z)$ using ordinary Padé approximants, and equating the result at some intermediate value $z=z_0$ to $f_{\mathrm{A}}(z)$ computed in the same way from the series (2.14) in inverse powers of z. We were usually able to find such a value of z where both series could be summed to a good approximation. Where it was not possible, a blank entry has been left in table 2(b).

Similar results were obtained using integral Padé approximants, except that we were unable to obtain useful results for $w_{i,0}(z)$ even if we used forced integral approximants. The results are presented in tables 3(a, b) where no entry indicates that the approximant had a pole on the positive real axis, so that we could not use (2.4) to determine the behaviour of the approximant as $z\to\infty$ in a simple way.

Table 2. (a) Singular behaviour of differential approximants $f^{\mathrm{D}}_{p/q/r}(z)$ to $w_{i,0}(z)$ of the form γz^{λ} as $z\to\infty$. (b) Values of γ for forced differential approximants to $w_{i,j}(z)$ for $i,j=0,1$.

(a)

$p/q/r$	2/1/0	3/2/1	4/3/2	5/4/3	6/5/4	7/6/5	Exact
γ	49.227	2.226	1.907	2.0057	2.0082	1.9957	2.0
λ	0.6328	0.4506	0.4592	0.4960	0.4966	0.4971	0.5

(b)

$p/q/r$	b_1+2z	b_3+2z	a_1+2z	a_3+2z
2/1/0	2.002	6.093	6.239	8.847
3/2/1	3.165	8.879	6.578	—
4/3/2	1.388	10.009	5.860	4.962
5/4/3	1.977	9.888	4.982	13.576
6/5/4	2.030	—	4.080	13.144
7/6/5	1.978	9.233	5.028	15.294
Exact	2	10	6	14

Table 3.(*a*) Singular behaviour of integral approximants $f^{\mathrm{I}}_{p/q/r}$ to $w_{i,0}(z)$ of the form γz^{λ} as $z \to \infty$. (*b*) Values of γ for forced integral approximants to $w_{i,1}(z)$ for $i = 0, 1$.

(*a*)

$p/q/r$	2/1/0	3/2/1	4/3/2	5/4/3	6/5/4	7/6/5	Exact
γ	1.241	1.895	1.804	—	1.862	—	2.0
λ	0.6254	0.5100	0.5207	0.2666	0.5126	0.5127	0.500

(*b*)

$p/q/r$	b_1+2z	b_3+2z
2/1/0	1.849	10.14
3/2/1	1.978	—
4/3/2	1.978	8.707
5/4/3	1.980	9.537
6/5/4	1.992	10.17
7/6/5	—	10.06
Exact	2.0	10.0

As stated in the introduction, we have constructed differential and integral approximants to $a_2(z)$ from its power series in z^2 (McLachlan 1947). As we vary the degrees of the polynomials $P(z)$, $Q(z)$ and $R(z)$ the number, position and type of the singularities of each approximant will vary. However, we find that all have singularity close to $z^2 = z_0^2 = -1.468\,7686^2$ and of approximately square root type, the results being presented in table 4.

Since the branch point is of square root type, we would expect quadratic approximants to work well in this case. We have therefore computed these approximants to $a_2(z)/4$ from its power series in z^2. The results for $z_0^2 \leq z^2 < 0$ are given in table 5(*a*) and for $z^2 < z_0^2$ table 5(*b*) where they compared with the values

Table 4. The most stable singularity of differential and integral approximants to $a_2(z)$ of type $(z^2 - z_1^2)^{\lambda}$.

$p/q/r$	Differential approximant z_1^2	λ	Integral approximant z_1^2	λ
1/0/0	−2.153 9047	0.498 86	−2.384 8084	0.368 19
1/1/1	−2.158 3777	0.496 51	−2.166 4156	0.479 101
1/2/2	−2.157 3141	0.499 80	−2.156 7378	0.502 52
1/3/3	−2.157 2786	0.500 03	−2.157 2335	0.500 39
2/1/1	−2.157 3288	0.499 57	−2.158 5665	0.495 97
2/2/2	−2.157 2849	0.499 98	−2.157 3802	0.499 40
2/3/3	−2.157 2827	0.499 98	−2.157 2782	0.500 03
3/1/1	−2.157 3352	0.499 67	−2.157 5632	0.498 65
3/2/2	−2.157 2806	0.500 00	−2.157 2839	0.499 98
4/1/1	−2.157 2738	0.500 05	−2.157 3606	0.499 54
4/2/2	−2.157 2810	0.500 00	−2.157 2800	0.500 01
Exact	−2.157 2812			

Table 5. (a) Quadratic Padé approximants to $f(z^2) \equiv a_2(z)$ compared when $z_0^2 < z^2 \leq 0$ with values for $a_2(z)$ and $a_0(z)$ computed by Mullholland and Goldstein (1929). (b) Quadratic Padé approximants to $f(z^2) \equiv a_2(z)$ compared when $z^2 < z_0^2$ with values for $a_2(z)$ computed by Mullholland and Goldstein (1929).

(a)

z^2	$f^{Q-}_{1/1/1}(z)$ $f^{Q+}_{1/1/1}(z)$	$f^{Q-}_{2/2/2}(z)$ $f^{Q+}_{2/2/2}(z)$	$f^{Q-}_{3/3/3}(z)$ $f^{Q+}_{3/3/3}(z)$	$a_0(z)/4$ $a_2(z)/4$
−0.0256	0.044 030 0.997 324	0.003 565 0.997 324	0.003 218 0.997 324	0.003 209 0.997 324
−0.1024	0.052 756 0.989 185	0.013 285 0.989 185	0.012 955 0.989 185	0.012 947 0.989 185
−0.2304	0.067 696 0.975 226	0.029 877 0.975 226	0.029 574 0.975 226	0.029 567 0.975 226
−0.4096	0.089 530 0.954 772	0.054 011 0.954 772	0.053 746 0.954 772	0.053 740 0.954 772
−0.6400	0.119 426 0.926 663	0.086 844 0.926 663	0.086 623 0.926 663	0.086 618 0.926 663
−0.9216	0.159 423 0.888 867	0.130 399 0.888 869	0.130 226 0.888 869	0.130 223 0.888 869
−1.12544	0.213 441 0.837 477	0.188 569 0.837 489	0.188 446 0.837 489	0.188 444 0.837 489
−1.6384	0.290 933 0.763 052	0.270 712 0.763 155	0.270 637 0.763 155	0.270 636 0.763 155
−2.0736	0.439 797 0.617 711	0.422 324 0.620 329	0.422 321 0.620 331	0.422 320 0.620 331

(b)

z^2	Re $f^{Q+}_{1/1/1}(z)$ Im $f^{Q+}_{1/1/1}(z)$	Re $f^{Q+}_{2/2/2}(z)$ Im $f^{Q+}_{2/2/2}(z)$	Re $f^{Q+}_{3/3/3}(z)$ Im $f^{Q+}_{3/3/3}(z)$	Re $a_2(z)/4$ Im $a_2(z)/4$
−2.56	0.530 753 −0.215 243	0.526 247 −0.217 455	0.526 248 −0.217 463	0.526 248 −0.217 463
−10.24	0.567 197 −1.016 848	0.600 202 −0.992 528	0.599 822 −0.992 7926	0.599 837 −0.992 788
−23.04	0.659 073 −1.874 056	0.704 205 −1.633 420	0.705 638 −1.641 590	0.705 302 −1.640 667
−40.96	0.967 051 −3.419 906	0.795 126 −2.261 885	0.833 487 −2.317 690	0.821 211 −2.306 374
−64.00	—	0.805 949 −2.226 812	1.046 511 −3.073 079	0.931 317 −2.995 455

given by Mullholland and Goldstein (1929). It is interesting to see that they not only converge well for points right up to the branch point but also converge on the branch cut itself. However, it is even more interesting, when we consider the other branch of the quadratic approximant, to see that it gives very good estimates for $a_0(z)/4$ for these same values of z^2, demonstrating that $a_0(z)$ and $a_2(z)$ are two branches of the same analytic function.

4. Singularities of water waves

We first of all consider periodic waves and use the same notation as Longuet-Higgins (1978), so that we consider waves in water of infinite depth moving with velocity c and wavelength L. The motion is two dimensional and we take the coordinate frame $0xy$ with $0y$ vertically upwards and $0x$ horizontal such that the waves are moving in the positive x direction. The frame is assumed to be moving with the waves such that the peak of a particular wave is always at $x=0$. Units are chosen such that the acceleration due to gravity $g=1$ and $L=2\pi$. The velocity potential w is a function of $z=x+\mathrm{i}y$ and is such that the velocity of the fluid at (x, y) is $q \equiv \mathrm{d}w/\mathrm{d}z$.

If $w(z)=\phi+\mathrm{i}\psi$ where ϕ and ψ are real functions of (x, y), then we may make the expansions

$$\begin{aligned} x &= \phi/c + H_1 \mathrm{e}^{\psi/c} \sin\phi/c + H_2 \mathrm{e}^{2\psi/c} \sin 2\phi/c + \ldots, \\ y &= \psi/c + \tfrac{1}{2}H_0 + H_1 \mathrm{e}^{\psi/c} \cos\phi/c + H_2 \mathrm{e}^{2\psi/c} \cos 2\phi/c + \ldots. \end{aligned} \tag{4.1}$$

The H_i are constants which have been determined by Longuet-Higgins (1978) from cubic relations corresponding to the condition of constant pressure at the surface of the water ($\psi=0$). He has kindly provided us with copies of his computer programs to determine these constants for waves of differing height.

If we define $\zeta=\mathrm{e}^{w/\mathrm{i}c}$, then from (4.1)

$$\frac{c}{q}=\frac{\mathrm{d}z}{\mathrm{d}w}=c\,\frac{\mathrm{d}z/\mathrm{d}\zeta}{\mathrm{d}w/\mathrm{d}\zeta}=1+H_1\zeta+2H_2\zeta^2+\ldots. \tag{4.2}$$

From the power series on the right we can construct differential Padé approximants and so estimate the singularities of q. As mentioned in the introduction, Stokes (1880) showed that the highest wave has a sharp crest with included angle of 120°, and this corresponds to a cube root singularity in q at the crest. For waves of less than maximum height all singularities of q are of square root type, and are outside the water, as proved by Grant (1973) and shown explicitly through numerical evaluation by Schwartz (1974). In particular, from figure 10 of this latter work, it can be seen that the leading singularity for waves of roughly $\frac{2}{3}$ maximum height is indeed of square root type, but as the wave height is increased still further, the square root branch points combine to give an effective leading singularity which tends to cube root type as the maximum height is reached.

We present our estimates for the behaviour

$$q=\mathrm{O}[(\zeta-\zeta_0)^{\lambda}]$$

of this effective singularity using a sequence of differential Padé approximants in table 6, for wave heights up to the maximum value of 0.886. We have compared them where applicable with the corresponding values given in figure 10 of Schwartz (1974), where the abscissa A/L is $(1/2\pi)\times$wave height. These latter values were obtained using the method introduced by Domb and Sykes (1957) to analyse the singular behaviour of an analytic function from its power series.

It will be seen that the differential Padé approximants predict the leading singularity to be of the square root type almost up to the maximum height. The predicted positions of the singularity are stable and agree with the results of Schwartz quoted in table 6, when inherent inaccuracies in taking them from a figure in his paper are taken into account.

Table 6. Leading singularity $\zeta = \zeta_0$ of q and corresponding exponent λ for waves of various heights as estimated using differential Padé approximants and compared with the predictions of Schwartz (1974).

Wave height \ Approximant		2/2/2	3/3/3	4/4/4	5/5/5	6/6/6	7/7/7	Schwartz
0.6283	λ	0.502 92	0.499 97	0.499 94	0.500 0	0.500 0	0.500 0	0.489
	ζ_0	1.280 64	1.280 47	1.280 47	1.280 47	1.280 47	1.280 47	1.25
0.8168	λ	0.464 35	0.493 58	0.499 06	0.499 73	0.499 82	0.499 95	0.42
	ζ_0	1.048 36	1.048 96	1.0490 4	1.049 07	1.049 07	1.049 07	1.05
0.84	λ	0.455 75	0.485 726	0.501 90	0.499 42	0.499 05	0.499 40	
	ζ_0	1.028 67	1.029 30	1.029 49	1.029 45	1.029 45	1.029 45	
0.85	λ	0.448 32	0.396 89	0.511 38	0.501 62	0.497 24	0.501 77	
	ζ_0	1.020 66	1.020 23	1.021 75	1.021 55	1.021 50	1.021 54	
0.86	λ	0.436 12	0.436 49	0.432 46	0.514 24	0.487 69	0.488 63	
	ζ_0	1.013 02	1.013 17	1.013 30	1.014 14	1.013 87	1.013 88	
0.87	λ	0.415 04	0.406 25	—	0.439 07	0.438 89	0.458 64	
	ζ_0	1.005 89	1.005 53	—	1.006 39	1.006 39	1.006 66	
0.88	λ	0.338 97	0.392 32	0.334 06	0.347 88	—	0.344 30	
	ζ_0	0.999 18	1.111 20	0.999 12	0.999 72	—	1.000 01	
0.886	λ	0.325 83	0.350 02	0.310 50	0.343 78	0.336 96	0.319 74	0.3333
	ζ_0	0.998 86	1.003 10	0.994 34	1.002 09	1.001 37	0.999 35	1.0000
0.886	λ	0.332 10	0.333 13	0.326 70	0.324 55	0.334 41	0.325 63	
Forced	ζ_0	1.000 0	1.000 0	1.000 0	1.000 0	1.000 0	1.000 0	

However, it is interesting to see that the transition from a square root to a cube root singularity as the wave height reaches its maximum is much more abrupt when differential approximants are used compared with when the Domb–Sykes method is used. The estimates for the degree λ of the singularity do tend to become unstable close to the highest wave, but this is probably due to the fact that the accuracy of determination of the coefficients $\{H_i\}$ deteriorates in this situation. In the final two rows of table 6 we give estimates for the values of λ for the highest wave using forced differential approximants, and we find that they are more stable than in the unforced case.

Important advances have also been made recently in the understanding of solitary water waves. For instance, it has been shown by Longuet-Higgins and Fenton (1974) that for a given wave speed c, there can exist when c is near its maximum two quite distinct solitary waves. In the notation of the above authors, we consider a solitary water wave of arbitrary amplitude a, propagating with velocity c in water of undisturbed depth h. Units are chosen so that $g = h = 1$, and then the Froude number of the wave $F \equiv c/\sqrt{gh} = c$. Power series expansions for quantities of physical interest were derived in terms of $\gamma \equiv F^2 - 1$. For example,

$$M = \frac{4}{\sqrt{3}} \gamma^{1/2} \sum_{n=0}^{\infty} c_n \gamma^n, \qquad \varepsilon = \gamma \sum_{n=0}^{\infty} a_n \gamma^n, \tag{4.3}$$

where M is the excess mass of the wave and $\varepsilon = a/h$. The coefficients $\{a_n\}$, $\{c_n\}$ are given in table 2 of their paper for $0 \leqslant n \leqslant 14$. It was not found possible to compute completely M and ε as functions of γ from the above expansions for reasons we will see shortly. However, M, ε and γ can be computed as functions of $w \equiv 1-u^2/gh$ where u is the velocity of the water at the wave crest (in the frame of reference moving with the wave speed). The authors plotted for example M against γ in their figure 2 which we reproduce in our figure 1. It is then obvious why the partial sums of the series (4.3) for M or even Padé approximants to this series (we plot the 5/5 and 6/6 Padé approximant on our figure 1) cannot give M completely since it becomes a double-valued function of γ for $\gamma \geqslant 0.653$.

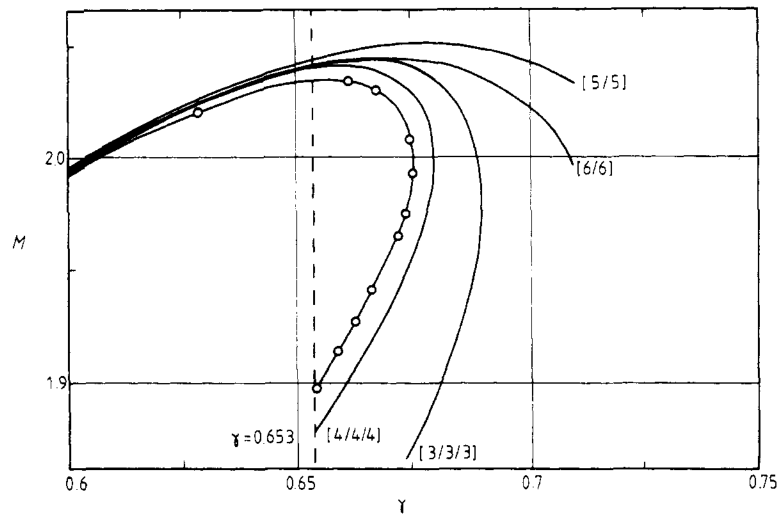

Figure 1. Estimates for M as a function of γ given by quadratic Padé approximants and Padé approximants compared with the exact values computed by Longuet-Higgins and Fenton (1974), and indicated by open circles.

It would therefore seem appropriate to try to evaluate M from the series (4.3) by using double-valued approximants. We have a particular example at hand which is of course quadratic Padé approximants. In figure 1 we compare the 3/3/3 and 4/4/4 quadratic Padé approximants to M as a function of γ with the exact value and the values of the 5/5 and 6/6 Padé approximants. For $\gamma \geqslant 0.653$ the positive branch of each quadratic approximant gives the greater of the two estimates for M, whilst the negative branch gives the smaller value. Also in table 7 we compare our estimates for M at various values of γ with those of table 5 of the above paper. The values in the upper half of our table correspond to the larger value of M for a given γ, and in the lower half to the smaller value of M. We see that the quadratic approximants are converging very well for the upper branch, but also quite well for the lower branch.

For $\gamma \geqslant 0.674$ our quadratic approximants become complex conjugates of one another, and this would suggest that M has a square root branch point at $\gamma \approx 0.674$ in conflict with the conclusions of the above authors who, using the Domb–Sykes method, estimate that the singularity is of the form $M \approx M_0 + K(0.662-\gamma)^p$ with $p \approx 1$, so that it is weak and possibly logarithmic. However, the nature of the singularity near the crest of steep water waves has been investigated further by Longuet-Higgins and Fox (1977, 1978) and Williams (1981). In particular, Fox (1977) has shown that

Table 7. Quadratic approximants to the excess mass M as a function of γ compared with the exact values as computed by Longuet-Higgins and Fenton (1974).

γ	3/3/3	4/4/4	M
0.60166	1.993	1.992	1.992
0.6286	2.021	2.020	2.020
0.6506	2.036	2.034	2.033
0.6665	2.039	2.035	2.030
0.6742	2.036	2.026	2.008
0.6711	1.854	1.938	1.964
0.6530	1.784	1.878	1.897

for almost highest waves,

$$\begin{aligned} \gamma &= \gamma_0 - 2.21\varepsilon_F^{\frac{3}{2}} \cos(2.143 \log \varepsilon_F + 1.33) + o(\varepsilon_F^{\frac{3}{2}}) \\ M &= M_0 - 3.96\varepsilon_F^{\frac{3}{2}} \cos(2.143 \log \varepsilon_F - 0.516) + o(\varepsilon_F^{\frac{3}{2}}) \end{aligned} \tag{4.4}$$

where ε_F is the ration of the crest particle velocity in the frame of reference moving with the wave to $\sqrt{2}$ times the wave speed. Also $M_0 = 1.968$ and $\gamma_0 = 0.6664$, being the values of M, γ for the highest wave. As demonstrated by Fox in a private communication subsequent to our work, γ has a stationary value 0.676 when $\varepsilon_F = 0.1933$ if higher-order terms are neglected in (4.4). Then for ε_F close to this value

$$\gamma \approx 0.676 - \kappa_1(\varepsilon_F - 0.1933)^2, \quad M \approx 1.985 + \kappa_2(\varepsilon_F - 0.1933) \approx 1.985 + \kappa_3(0.676 - \gamma)^{1/2} \tag{4.5}$$

where κ_i are constants. These estimates would therefore support our suggestion that, as the quadratic Padé approximants are appearing to converge to both branches of M as a function of γ, then M has a square root branch rather than a logarithmic branch point as a function of γ.

5. Conclusions

We have considered here three types of generalisations to Padé approximants which are all contained in the wider class known as Hermite–Padé approximants. The singularity structure of each type of approximant was described and it was shown how this structure could be forced to be of a given form. It is interesting to note that forcing approximants allows higher orders to be evaluated from a given number of coefficients of the original power series, compared with the standard case.

In our application to the harmonic oscillator on a lattice, we have shown that the forced approximants give at least rough estimates to the limit of the energy levels as the lattice spacing tends to zero. This would suggest that our methods could be used to study the continuum limit of more realistic field theories, but the number of coefficients required to ensure convergence of corresponding approximants may be prohibitively difficult to evaluate.

In our application to water waves, we have again demonstrated that the approximants used here can give good estimates of the singularity structure of functions of physical interest, and that multivalued functions may be approximated even if only a single power series for the function is provided. We are encouraged by this and other work (Gammel 1976, Reddall 1978, Nuttall 1980 and Baumel *et al* 1981) to suggest that there are other situations in fluid mechanics where the above approximants could prove useful. Possibilities that come to mind are the study of breaking waves and shock waves.

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