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The convergence of Legendre Padé approximants to the Coulomb and other scattering amplitudes

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Abstract. The convergence of sequences of Legendre Padé approximants to scattering amplitudes arising in potential scattering is discussed. It is shown that if the amplitude for scattering by the Coulomb potential or the absorptive part of a scattering amplitude whose double spectral function obeys a certain bound are suitably modified, convergent sequences of Legendre Padé approximants may be constructed. Numerical results are presented for the Coulomb scattering amplitude.

1. Introduction

The partial-wave expansion of a scattering amplitude is most useful at low energies when only the lowest waves need be taken into account and the corresponding partial-wave amplitudes may be obtained by integrating the Schrödinger equation to get the wavefunction in the asymptotic region. As the energy of the scattered particle is increased, more waves have to be taken into account and uncertainties arise in the numerical evaluation of the corresponding amplitudes. A method for 'accelerating the convergence' of the partial-wave series is therefore desirable.

In a recent work (Common and Stacey 1978) we have discussed in detail properties and applications of 'Legendre Padé approximants'† which in the applications considered did have the above desired property of 'accelerating convergence'. The first example considered was the amplitude for scattering by repulsive inverse-square potential. The corresponding partial-wave series converges for physical values of $z=\cos\theta$ where θ is the scattering angle, but the convergence is very slow. Of the order of hundreds of terms are needed to get four-figure accuracy for the scattering amplitude in the physical region while using Legendre Padé approximants only the first ten partial waves are needed for comparable accuracy.

An even more extreme example is the amplitude for scattering by the Coulomb potential $V=e^2/r$ which has the exact form (Landau and Lifshitz 1958)

$$f_c(z)=-\frac{2^{i/k}}{k^2}(1-z)^{-1-i/k}\frac{\Gamma(1+i/k)}{\Gamma(1-i/k)}, \qquad (1.1)$$

where k is the momentum of the particles being scattered (in Coulomb units). This

† For the remainder of this work we will use the abbreviation LPA for these approximants.

has the expansion

$$f_c(z)=\sum_{l=0}^{\infty}(2l+1)\frac{(e^{2i\delta_l}-1)}{2ik}P_l(z), \tag{1.2}$$

where

$$e^{2i\delta_l}=\frac{\Gamma(l+1+i/k)}{\Gamma(l+1-i/k)}. \tag{1.3}$$

However, this series does not converge for $-1\leq z\leq 1$, and the right-hand sides of (1.1) and (1.2) are equivalent only in the sense of distributions (Taylor 1974). In this sense $f_c(z)$ also has the expansion

$$f_c(z)=\sum_{l=0}^{\infty}(2l+1)\frac{e^{2i\delta_l}}{2ik}P_l(z). \tag{1.4}$$

In the following we will present numerical results which show that the LPA to the right-hand side of (1.4) converge quickly to $f_c(z)$ except near its cut even though the series does not converge point-wise.

Although it is pleasing to have numerical convergence, it is important to prove convergence of the LPA for scattering by as wide a class of potentials as possible. The main aim of this work is to make a start on such a programme, by showing that sequences of LPA to the Coulomb scattering amplitude (suitably modified) converge in the whole complex z-plane cut from $z=1$ to ∞ which is exactly the region where $f_c(z)$ is holomorphic.

The result is extended to the absorptive part of a scattering amplitude whose double spectral function $\rho(s,t)$ for fixed s is such that if

$$\psi(1+t/2s)\equiv\rho(s,t)/\pi,$$

then

$$\psi(x)=c_1/x^{L_0+\frac{1}{2}}+\psi_2(x) \tag{1.5}$$

for all x on the support of $\psi(x)$, where

$$|\psi_2(x)|\leq c_2\frac{x^p}{(\ln x)^\alpha} \qquad p\leq L_0+\tfrac{1}{2},\ \alpha>1$$

with c_1, c_2 constants and L_0+1 is the number of subtractions in the dispersion relation satisfied by the amplitude. This class of amplitudes contains those corresponding to scattering by central potentials $V(r)$ where $V(r)$ is holomorphic in $\mathrm{Re}\, r>0$ and satisfies the bounds (Bessis 1965)

$$|V(r)|<c_3/|r|^\eta, \tag{1.6}$$

with $\eta<2$ for $|r|\leq 1$ and $\eta>\frac{7}{4}$ for $|r|\geq 1$, and c_3 is a constant.

The LPA defined by Common and Stacey (1978) have the important property that if sequences of PA to the corresponding power series converge in certain domains, then the same sequences of LPA converge in corresponding domains. It is this property which we will use to prove convergence for the particular scattering amplitudes described above. To prove convergence of the PA to the related power series, we will show that these series belong to a class of functions considered recently by Nuttall (1976).

In § 2, we introduce our LPA and give the convergence theorems mentioned above along with Nuttall's result. Then in § 3 we will show that the Coulomb scattering amplitude given by (1.1) may be suitably modified so that Nuttall's theorem may be applied to the corresponding power series and hence convergence of the LPA proved, not only in the physical domain $-1 \leq z \leq 1$ but also in the whole domain of holomorphy of $f_c(z)$. Numerical results will be presented in § 4 to illustrate rates of convergence and comparison will be made with an alternative method for summing the Coulomb series (1.2) due to Yennie *et al* (1954).

In § 5 we show how the absorptive parts of scattering amplitudes satisfying (1.5) may be modified, so that again Nuttall's theorem may be applied to the corresponding power series and convergent sequences of LPA obtained. Finally, in § 6 we give our conclusions.

2. Legendre Padé approximants and Nuttall's theorem

In the preceding work (Common and Stacey 1978) we discussed the convergence of sequences of LPA to

$$f(z) = \sum_{l=0}^{\infty} f_l P_l(z) \tag{2.1}$$

when the corresponding power series

$$g(w) = \sum_{l=0}^{\infty} f_l (-w)^l \tag{2.2}$$

has a rather general domain of holomorphy. In the examples considered in the following sections, $g(w)$ is holomorphic in the complex w-plane cut from $-\infty$ to $-r$ with $r \geq 1$. Then from above work, $f(z)$ is holomorphic in the complex z-plane cut from $\frac{1}{2}(r+r^{-1})$ to ∞, and has the representation

$$f(z) = \frac{1}{2\pi i} \int_\Gamma K(z, w) g(w)\, dw \tag{2.3}$$

where $K(z, w) = (1+2zw+w^2)^{-1/2}$ and the branch of the square root is chosen so that $wK(z, w) \to 1$ as $|w| \to \infty$. Γ is a contour encircling in a positive sense the cut of $K(z, w)$ which is the line joining $-z \pm (z^2-1)^{1/2}$. For z in the complex plane cut from $\frac{1}{2}(r+r^{-1})$ to ∞, Γ may be chosen to lie completely inside the holomorphy domain of $g(w)$. We now state the definition of the Legendre Padé approximants to $f(z)$ and the corresponding convergence theorem when $g(w)$ and $f(z)$ have the above domains of holomorphy.

Definition. The $[n+j/n]$ 'Legendre Padé approximant' to $f(z)$ is

$$f^{L}_{n+j/n}(z) = \frac{1}{2\pi i} \int_\Gamma K(z, w) g_{n+j/n}(w)\, dw \qquad n = 0, 1, \ldots; j = 0, \pm 1, \pm 2, \ldots, \tag{2.4}$$

where $g_{n+j/n}(w)$ is the $[n+j/n]$ Padé approximant to $g(w)$.

Theorem 2.1. If $g_{n+j/n}(w)$ converges uniformly to $g(w)$ as $n \to \infty$ for fixed $j = 0, \pm 1, \pm 2, \ldots$ in any closed bounded domain of the complex w-plane cut from $-\infty$ to

$-r$, then $f^{\mathrm{L}}_{n/n+j}(z)$ converges uniformly to $f(z)$ in any closed bounded domain of the complex z-plane cut from $\frac{1}{2}(r+r^{-1})$ to ∞.

An explicit representation for $f^{\mathrm{L}}_{n+j/n}(z)$ is given by the following theorem which was proved previously (Common and Stacey 1978).

Theorem 2.2 Let the partial fraction expansion of $g_{n+j/n}(w)$ be

$$g_{n+j/n}(w)=\sum_{p=1}^{n}\frac{\alpha_p}{1+\sigma_p w}+\sum_{q=0}^{j}\beta_q(-w)^q, \tag{2.5}$$

where the second sum on the right-hand side is absent if $j<0$. Then

$$f^{\mathrm{L}}_{n+j/n}(z)=\sum_{p=1}^{n}\frac{\alpha_p}{\sqrt{1-2\sigma_p z+\sigma_p^2}}+\sum_{q=0}^{j}\beta_q P_q(z) \tag{2.6}$$

where the branch of the square root is that which is real positive when the argument is real positive.

The partial-wave expansion of the scattering amplitude is usually written as

$$f(z)=\sum_{l=0}^{\infty}(2l+1)f_l P_l(z) \tag{2.7}$$

where the f_l have useful unitarity properties. The $[n+j/n]$ 'Legendre Padé approximants' in this case are defined by the relations

$$\begin{aligned} f^{\mathrm{L}}_{n+j/n}(z)&=\frac{1}{2\pi\mathrm{i}}\int_{\Gamma}K(z,w)\left(g_{n+j/n}(w)+2w\frac{\mathrm{d}g_{n+j/n}(w)}{\mathrm{d}w}\,\mathrm{d}w\right)\\ &=\sum_{p=1}^{n}\frac{\alpha_p(1-\sigma_p^2)}{(1-2z\sigma_p+\sigma_p^2)^{3/2}}+\sum_{q=0}^{j}(2q+1)\beta_q P_q(z), \end{aligned} \tag{2.8}$$

where $g_{n+j/n}(w)$ is the $[n+j/n]$ PA to $g(w)$ defined in (2.2) and α_p, σ_p, β_q are again the coefficients in the partial fraction expansion of $g_{n+j/n}(w)$.

We finish this section by giving an important new convergence theorem for the paradiagonal sequence of PA $g_{n-1/n}(w)$ with $n=0,1,2,\ldots$, when $g(w)$ has the representation

$$g(w)=\int_a^b\frac{\phi(v)\,\mathrm{d}v}{1-vw}. \tag{2.9}$$

If $\phi(v)$ is real non-negative and a, b real then $g(w)$ is a series of Stieltjes and it is well known that such sequences of PA converge to $g(w)$ in its domain of holomorphy. Nuttall (1976) has recently extended this result to the case when a, b are complex and $\phi(v)$ is a complex weight function by proving the following theorem.

Theorem 2.3. Let $g(w)$ have the representation (2.5) with a, b and $\phi(v)$ possibly complex and such that

$$h(\theta)\equiv\phi(\tfrac{1}{2}[(b-a)\cos\theta+a+b])|\sin\theta| \tag{2.10}$$

satisfies the following conditions for $-\pi\leqslant\theta\leqslant\pi$:

(i) $\exists$ real A, B independent of θ such that $A>|h(\theta)|>B>0$.

(ii) $\exists\ L, \lambda > 0$ independent of θ such that

$$|\{h(\theta+\delta)\}^{-1} - \{h(\theta)\}^{-1}| < B^{-2}L|\ln \delta|^{-1-\lambda}.$$

Then the $[n-1/n]$ Padé approximant to $g(w)$ converges uniformly to $g(w)$ as $n \to \infty$ in any closed, bounded region of the w-plane cut along the arc $w = +1/v$ with $v = \frac{1}{2}[(b-a)t + a + b]$, $-1 \leq t \leq 1$.

The domain of convergence is therefore the holomorphy domain of $g(w)$. We will show in the following sections how the scattering amplitudes we wish to consider may be manipulated so that the corresponding power series has the representation (2.9) with $\phi(v)$ satisfying the conditions of theorem 2.3. Using this theorem, we will then prove convergence of the corresponding sequence of LPA.

3. The Coulomb scattering amplitude

In this section we will obtain sequences of approximants from the partial-wave expansion (1.4) of $f_c(z)$ and show that they converge to $f_c(z)$ in the complex z-plane cut from 1 to ∞. These approximants are a further modification of the LPA defined in (2.6) and (2.8). However, the techniques involved show how one should proceed in the case of the more general class of potentials considered in § 5, when an approximant similar to (2.8) will be used.

The power series corresponding to the Legendre series (1.4) is

$$g(w) = \sum_{l=0}^{\infty} \frac{(2l+1)}{2\mathrm{i}k} \frac{\Gamma(l+1+\mathrm{i}/k)}{\Gamma(l+1-\mathrm{i}/k)}(-w)^l = \frac{(2w\mathrm{D}+1)(w\mathrm{D}+1-\mathrm{i}/k)}{2\mathrm{i}k\Gamma(1-2\mathrm{i}/k)} G(w) \tag{3.1}$$

where $\mathrm{D} \equiv \mathrm{d}/\mathrm{d}w$ and

$$G(w) = \sum_{l=0}^{\infty} B(l+1+\mathrm{i}/k, 1-2\mathrm{i}/k)(-w)^l = \int_0^1 \frac{\phi(v)\,\mathrm{d}v}{1+vw} \tag{3.2}$$

with $\phi(v) = v^{\mathrm{i}/k}(1-v)^{-2\mathrm{i}/k}$, using the standard integral representation of the beta function (Abramowitz and Stegun 1968).

As it stands, the weight function $\phi(v)$ does not satisfy condition (i) of theorem (2.3). To rectify this we write

$$G(w) = \int_0^1 \frac{\phi_1(v)\,\mathrm{d}v}{1+vw} - \frac{C}{2}\int_0^1 \frac{\mathrm{d}v}{(v-v)^{1/2}(1+vw)} \equiv N(w) - CS(w) \tag{3.3}$$

where C is a complex constant to be chosen, and

$$\phi_1(v) = \phi(v) + \tfrac{1}{2}C(v-v^2)^{1/2}. \tag{3.4}$$

Explicitly $S(w)$ is

$$\frac{\pi}{2}\frac{1}{(1+w)^{1/2}} \equiv \sum_{l=0}^{\infty} a_l(-w)^l$$

where $a_l = (\pi/2)(2l-1)!!/(l!2^l)$, and the corresponding Legendre series is

$$\sum_{l=0}^{\infty} (2l+1)a_l P_l(z)$$

$$= \frac{1}{2}\int_0^{\pi} \frac{dv}{[1+z+(z^2-1)^{1/2}\cos v]^{3/2}}$$

$$= \frac{E[\![\{2(z^2-1)^{1/2}/[1+z+(z^2-1)^{1/2}]\}^{1/2}]\!]}{[1+z-(z^2-1)^{1/2}][1+z+(z^2-1)^{1/2}]^{1/2}}$$

where E is an elliptic integral of the second kind. This could have been evaluated directly, but in the following we use our LPA to evaluate it.

The following lemma will allow us to apply Nuttall's theorem to $G(w)$.

Lemma 3.1. If $|C|>1$, then $h(\theta)\equiv\phi_1[\frac{1}{2}(\cos\theta+1)]|\sin\theta|$ satisfies conditions (i) and (ii) of theorem 2.3.

Proof. From (3.4), and the expression for $\phi(v)$,

$$h(\theta)=|\sin\theta|(\cos\tfrac{1}{2}\theta)^{2i/k}(\sin\tfrac{1}{2}\theta)^{-4i/k}+C. \tag{3.5}$$

Now, the first term on the right-hand side of (3.5) has modulus $|\sin\theta|$. Therefore for $-\pi\leqslant\theta\leqslant\pi$,

$$0<|C|-1\leqslant|h(\theta)|\leqslant 1+|C| \tag{3.6}$$

when $|C|>1$, so that $h(\theta)$ satisfies condition (i) of theorem 2.3. It is straightforward to show that for $-\pi\leqslant\theta\leqslant\pi-\delta$, there exists M independent of θ such that

$$|h(\theta+\delta)-h(\theta)|<M\delta. \tag{3.7}$$

This follows from the existence and boundedness of the derivative of $h(\theta)$ for $-\pi\leqslant\theta\leqslant\pi$ except at $\theta=-\pi$, 0, π and the existence at these exceptional points of right-hand and left-hand derivatives of $h(\theta)$ which are different but finite. That condition (ii) is satisfied is an immediate consequence of (3.6) and (3.7).

Let the $[n-1/n]$ Padé approximants to the functions $N(w)$ and $S(w)$ defined by (3.3) have the partial fraction expansions

$$N_n(w)=\sum_{p=1}^{n}\frac{\alpha_p}{1+\sigma_p w} \tag{3.8}$$

$$S_n(w)=-\frac{1}{C}\sum_{p=n+1}^{2n}\frac{\alpha_p}{1+\sigma_p w}. \tag{3.9}$$

We can define from (3.3) the corresponding approximant

$$G_n(w)=N_n(w)-CS_n(w)=\sum_{p=1}^{2n}\frac{\alpha_p}{1+\sigma_p w} \tag{3.10}$$

to $G(w)$ and from (3.1) the approximant

$$g_n(w)=\frac{(2wD+1)(wD+1-i/k)}{2ik\Gamma(1-2i/k)}G_n(w) \tag{3.11}$$

to $g(w)$.

Theorem 3.1. The approximants

$$f_n^{\mathrm{L}}(z)=\frac{1}{2\pi \mathrm{i}}\int_\Gamma K(z,w)g_n(w)\,\mathrm{d}w=\frac{1}{\pi}\int_0^\pi g_n[-z-(z^2-1)^{1/2}\cos\psi]\,\mathrm{d}\psi \tag{3.12}$$

converge uniformly to

$$\frac{1}{2\pi \mathrm{i}}\int_\Gamma K(z,w)g(w)\,\mathrm{d}w$$

as $n\to\infty$ in any closed bounded domain of the complex z-plane cut from 1 to ∞, and this limit is the Coulomb scattering amplitude $f_c(z)$ defined in (1.1).

Proof. From the lemma, $N(w)$ and $S(w)$ have weight functions satisfying the conditions of Nuttall's theorem. ($S(w)$ is also a series of Stieltjes.) Therefore, $N_n(w)$ and $S_n(w)$ converge uniformly to $N(w)$ and $S(w)$ respectively and hence $G_n(w)$ converges to $G(w)$. It immediately follows that $g_n(w)$ given by (3.11) converges uniformly to $g(w)$ in any closed bounded domain of the w-plane cut from 1 to ∞. Proceeding as in theorem 3.2 of the work of Common and Stacey (1978), it follows finally that $f_n^{\mathrm{L}}(z)$ defined by (3.12) converges as in the statement of the theorem.

To prove that this limit equals $f_c(z)$, we note that, from (3.1) and (3.2)

$$g(w)=\frac{1}{2\mathrm{i}k\Gamma(1-2\mathrm{i}/k)}\int_0^1 v^{\mathrm{i}/k}(1-v)^{-2\mathrm{i}/k}\,\mathrm{d}v\left(\frac{4}{(1+vw)^3}-\frac{3+2\mathrm{i}/k}{(1+vw)^2}+\frac{\mathrm{i}/k}{1+vw}\right). \tag{3.13}$$

Using the relation (Gradshteyn and Ryzhik 1965)

$$\frac{1}{\pi}\int_0^\pi\frac{\mathrm{d}\psi}{\{1-v[z+(z^2-1)^{1/2}\cos\psi]\}^m}=\frac{P_{m-1}[(1-vz)/(1-2vz+v^2)^{1/2}]}{(1-2vz+v^2)^{m/2}}, \tag{3.14}$$

the limiting integral is

$$\begin{aligned}\frac{1}{2\pi \mathrm{i}}&\int_\Gamma K(z,w)g(w)\,\mathrm{d}w\\ &=\frac{1}{\pi}\int_0^\pi g[-z-(z^2-1)^{1/2}\cos\psi]\,\mathrm{d}\psi\\ &=\frac{1}{2\mathrm{i}k\Gamma(1-2\mathrm{i}/k)}\int_0^1 v^{\mathrm{i}/k}(1-v)^{-2\mathrm{i}/k}\,\mathrm{d}v\left(\frac{\frac{3}{2}(1-v^2)^2}{(1-2vz+v^2)^{5/2}}\right.\\ &\qquad\left.+\frac{\frac{1}{2}(3-2\mathrm{i}/k)(1-v^2)-2}{(1-2vz+v^2)^{3/2}}\right)\end{aligned} \tag{3.15}$$

for all z in the plane cut from 1 to ∞. To complete the proof we have to show that the right-hand side of (3.15) is

$$f_c(z)=-\frac{2\mathrm{i}/k}{k^2}\frac{\Gamma(1+\mathrm{i}/k)}{\Gamma(1-\mathrm{i}/k)}(1-z)^{-1-\mathrm{i}/k}. \tag{1.1}$$

This is accomplished by showing that the nth derivatives of each expression at $z=1$ are equal to

$$-\frac{2^{-1-n}}{k^2 n!}\frac{\Gamma(n+1+\mathrm{i}/k)}{\Gamma(1-\mathrm{i}/k)}.$$

In the latter case, the result follows from straightforward differentiation, and in the former from differentiation under the integral sign and application of standard formulas (Abramowitz and Stegun 1968) involving the hypergeometric functions so obtained.

An explicit expression may be obtained for the approximant $f_n^{\mathrm{L}}(z)$. It is given by the following theorem.

Theorem 3.2. Let $\{\alpha_p, \sigma_p: p=1,\ldots,2n\}$ be the coefficients of the partial fraction expansions of $N_n(w)$ and $S_n(w)$ given in (3.8) and (3.9). Then

$$f_n^{\mathrm{L}}(z)=\frac{1}{2ik\Gamma(1-2i/k)}\sum_{p=1}^{2n}\alpha_p\left(\frac{\frac{3}{2}(1-\sigma_p^2)^2}{(1-2\sigma_p z+\sigma_p^2)^{5/2}}+\frac{\frac{1}{2}(3-2i/k)(1-\sigma_p^2)-2}{(1-2\sigma_p z+\sigma_p^2)^{3/2}}\right). \tag{3.16}$$

Proof. Substituting from (3.10) for $G_n(w)$ in (3.11) we find that

$$g_n(w)=\frac{1}{2ik\Gamma(1-2i/k)}\sum_{p=1}^{2n}\alpha_p\left(\frac{4}{(1+\sigma_p w)^3}-\frac{(3+2i/k)}{(1+\sigma_p w)^2}+\frac{i/k}{1+\sigma_p w}\right). \tag{3.17}$$

Using this expression for $g_n(w)$ in (3.12), the representation (3.16) follows.

4. Numerical results for the Coulomb amplitude

In table 1 we illustrate the numerical convergence of the approximants $f_n^{\mathrm{L}}(z)$ given in (3.16) when $k=1$, at a selection of points on the real axis. It will be seen that for physical scattering angles the convergence is very quick except near the forward direction where the amplitude is singular. Even far out on the negative real axis convergence is still reasonable and this is true in the whole complex z-plane except near the cut of $f_c(z)$ from $z=1$ to ∞.

Table 1. Values of the approximants $f^{\mathrm{L}}_{n(z)}$ to $f_c(z)$ at momentum $k=1$.

z	$f_2^{\mathrm{L}}(z)$	$f_4^{\mathrm{L}}(z)$	$f_6^{\mathrm{L}}(z)$	$f_c(z)$
0·951	32·1	20·2	20·44	20·42
	−10·0 i	−0·4 i	−0·72 i	−0·71 i
0·0	−0·95	−0·995 965 i	−0·995 965 1	−0·995 964 7
	0·15 i	−0·089 83 i	−0·089 745 8 i	−0·089 745 6 i
−1·0	−0·43	−0·411 67	−0·411 739 40	−0·411 739 39
	+0·31	+0·283 68 i	+0·283 673 59 i	+0·283 673 53 i
−6·213	0·02	0·065	0·046	0·043
	0·15 i	0·135 i	0·131 i	0·132 i

In table 2 we compare various methods for summing the Coulomb series. Each approximant is constructed from the set of phase shifts $\{\delta_l; l=0,1,\ldots,9\}$ with δ_l given by (1.3). The approximant $f_5^{\mathrm{L}}(z)$ is given in the second column, while the third column contains values of the LPA $f_{4/5}^{\mathrm{L}}(z)$ to the series (1.14).

We compare these results with those obtained from an alternative method for summing the Coulomb series due to Yennie *et al* (1954). Their method involves

Table 2. Comparison of the values of approximants to $f_c(z)$ constructed from the first ten partial waves ($k = 1$).

z	$f_5^L(z)$	$f_{4/5}^L(z)$	$f_{3,6}^{YRW}(z)$	$f_c(z)$
0·951	20·21 −1·11 i	22·3 −5·4 i	27·8 +4·0 i	20·42 −0·71 i
0·0	−0·995 966 −0·089 759 i	−0·995 99 −0·089 76 i	−0·996 4 −0·089 74 i	−0·995 965 −0·089 746 i
−1·0	−0·411 736 +0·283 677 i	−0·411 738 +0·283 671 i	−0·411 4 +0·283 5 i	−0·411 739 +0·283 674 i
−6·213	+0·055 +0·133 i	0·034 +0·136 i	12·5 −6·4 i	0·043 +0·132 i

replacing the series (1.2) by the mth 'reduced' series, defined by

$$(1-z)^m f_c(z) \equiv \sum_{l=0}^{\infty} a_l^{(m)} P_l(z). \tag{4.1}$$

The resulting function has a 'softer' singularity at $z = 1$, and except close to this singularity the series on the right-hand side of (4.1) converges quite quickly for physical values of z when $m \geq 3$. Each coefficient $a_l^{(m)}$ may be obtained from a finite number of partial waves of the original series (1.2), e.g. given the set $\{\delta_l; l = 0, 1, \ldots, 9\}$, the set of coefficients $\{a_l^{(3)}; l = 0, \ldots, 6\}$ may be evaluated. From these coefficients we can calculate the sum of the first seven terms of the third 'reduced' series which we denote by

$$f_{3,6}^{YRW}(z) = \sum_{l=0}^{6} a_l^{(3)} P_l(z), \tag{4.2}$$

and we give its values in the fourth column of table 2. Finally, in the fifth column we give the exact values of $f_c(z)$.

These results presented in table 2 may be summarised as follows. The three types of approximants all converge quickly for physical values of z except near the singularity at $z = 1$. Near $z = 1$, the approximants $f_n^L(z)$ are better than the other two types of approximants when $k = 1$, although for other values of k this is not always the case.

Away from the physical region $-1 \leq z \leq 1$, the approximants of Yennie *et al* fail to converge, whereas the approximants $f_n^L(z)$ and $f_{n-1/n}^L(z)$ converge quite quickly except near the cut of $f_c(z)$ running from $z = 1$ to ∞.

5. Absorptive part of general scattering amplitude

In this section we shall define a sequence of LPA to the absorptive part of an amplitude, and make use of the Froissart–Gribov representatation of its partial waves to prove convergence when the double spectral function satisfies a certain bound.

The fixed s dispersion relation for the absorptive part is

$$\operatorname{Im} f(s, t) = \frac{t^{L_0+1}}{\pi} \int_{4\mu^2}^{\infty} \frac{dt' \rho(s, t')}{t'^{L_0+1}(t'-t)} + \sum_{l=0}^{L_0} \frac{t^l}{l!} g_l(s) \tag{5.1}$$

where L_0+1 is the number of subtractions. In forming approximants to $\operatorname{Im} f(s, t)$ we shall ignore the polynomial part of (5.1). Writing $\operatorname{Im} f(s, t)$ as a partial-wave series

$$\operatorname{Im} f(s, t)=\sum_{l=0}^{\infty}(2l+1)f_l(s)P_l\left(1+\frac{2t}{s-4\mu^2}\right), \tag{5.2}$$

the partial-wave amplitudes $\{f_l : l \geqslant L_0+1\}$ have the Froissart–Gribnov representation

$$f_l=\int_{x_0}^{\infty} Q_l(\chi)\psi(\chi)\,\mathrm{d}\chi \qquad (l \geqslant L_0+1) \tag{5.3}$$

where

$$\chi_0=\frac{4\mu^2+s}{4\mu^2-s} \qquad \text{and} \qquad \psi\left(\frac{2t'}{s-4\mu^2}+1\right)=\rho(s, t').$$

As usual, we consider the power series corresponding to the Legendre series (5.2), i.e.

$$g(w)=\sum_{l=0}^{\infty} f_{l+L_0+1}(-w)^l \tag{5.4}$$

$$=\frac{1}{(-w)^{L_0+1}}\int_{x_0}^{\infty}\left(L(-w, x)-\sum_{l=0}^{L_0}(-w)^l Q_l(x)\right)\psi(x)\,\mathrm{d}x \tag{5.5}$$

where

$$L(w, x)=\sum_{l=0}^{\infty}(+w)^l Q_l(x). \tag{5.6}$$

This series converges for $|w|<r=x_0+(x_0^2-1)^{1/2}$ and x not in $[-1, 1]$. In order to apply Nuttall's theorem to $g(w)$ we need the following two lemmas.

Lemma 5.1. The function $g(w)$ defined in (5.4) has the representation

$$g(w)=\int_0^{1/r}\frac{\phi(v)\,\mathrm{d}v}{1+vw} \tag{5.7}$$

where $r=x_0+(x_0^2-1)^{1/2}$ is the radius of convergence of (5.4) and

$$\phi(v)=v^{L_0+1}\int_{x_0}^{\frac{1}{2}(v+1/v)}\frac{\psi(x)\,\mathrm{d}x}{(1-2vx+v^2)^{1/2}}. \tag{5.8}$$

Proof. $L(w, x)$ defined in (5.6) has the representation (Kinoshita *et al* 1964)

$$L(w, x)=\int_{x+(x^2-1)^{1/2}}^{\infty}\frac{\mathrm{d}u}{(u-w)(1-2ux+u^2)^{1/2}}.$$

Therefore

$$\frac{1}{(-w)^{L_0+1}}\left(L(-w, x)-\sum_{l=0}^{L_0}(-w)^l Q_l(w)\right)$$

$$=\int_{x+(x^2-1)^{1/2}}^{\infty}\frac{\mathrm{d}u}{u^{L_0+1}(u+w)(1-2ux+u^2)^{1/2}}. \tag{5.9}$$

Suppose w has a fixed value in the complex plane cut from $-r$ to ∞. We may substitute from (5.9) into (5.5) and interchange the order of integration over u and x (which is then allowable since the behaviour at infinity of $\psi(x)$ is such that the integrals on the right-hand side of (5.3) exist) and find

$$g(w)=\int_r^\infty \frac{1}{u^{L_0+1}(u+w)}\left(\int_{x_0}^{\frac{1}{2}(u+1/u)} \frac{\psi(x)\,\mathrm{d}x}{(1-2ux+u^2)^{1/2}}\right)\mathrm{d}u$$

$$=\int_0^{1/r} \frac{v^{L_0+1}}{(1+vw)}\left(\int_{x_0}^{\frac{1}{2}(v+1/v)} \frac{\psi(x)\,\mathrm{d}x}{(1-2vx+v^2)^{1/2}}\right)\mathrm{d}v=\int_0^{1/r}\frac{\phi(v)\,\mathrm{d}v}{(1+vw)}.$$

Lemma 5.2. Let

$$\phi_3(v)=\phi(v)+\frac{\mathrm{i}c}{2}(rv-r^2v^2)^{-1/2} \tag{5.10}$$

where c is a real non-zero constant and $\phi(v)$ is defined in (5.8). Then if for all $x \geqslant x_0$,

$$\psi(x)=c_1\psi_1(x)+c_2\psi_2(x) \tag{5.11}$$

where

$$\psi_1(x)=x^{L_0+1/2}$$

$$|\psi_2(x)|\leqslant\frac{x^p}{(\ln x)^\alpha},\qquad p\leqslant L_0+\tfrac{1}{2},\ \alpha>1 \tag{5.12}$$

then $h(\theta)=|\sin\theta|\phi_3-\frac{1}{2}r(1+\cos\theta)]$ satisfies conditions (i) and (ii) of Nuttall's theorem.

Proof. From (2.10) and (5.8) the contribution from ψ_1 to $h(\theta)$ is

$$h_1(\theta)=2(rv-r^2v^2)^{1/2}v^{L_0+1}\int_{x_0}^{\frac{1}{2}(v+1/v)}\frac{x^{L_0+1/2}\,\mathrm{d}x}{(1-2vx+v^2)^{1/2}},$$

where $v=(1+\cos\theta)2r$. Making the substitution $y=[1-2x/(v+v^{-1})]^{1/2}$,

$$h_1(\theta)=(2\surd 2)(r-r^2v)^{1/2}[\tfrac{1}{2}(v^2+1)]^{L_0+1}\int_0^{y_0}(1-y^2)^{L_0+1/2}\,\mathrm{d}y \tag{5.13}$$

where $y_0=[1-2x_0/(v+1/v)]^{1/2}$, it follows immediately that

$$0\leqslant h_1(\theta)\leqslant M_1 \qquad -\pi\leqslant\theta\leqslant\pi$$

and similarly if $h_2(\theta)$ is the contribution to $h(\theta)$ from $\psi_2(x)$, then

$$|h_2(\theta)|\leqslant M_2 \qquad -\pi\leqslant\theta\leqslant\pi$$

where M_i are constants.

Using these bounds with (5.10),

$$|h(\theta)|=|\sin\theta|\,|\phi_3[(1+\cos\theta)/2r]|\leqslant M_1+M_2+|c|. \tag{5.14}$$

Also, since $\phi(v)$ is real,

$$|h(\theta)|\geqslant|c|>0.$$

Therefore $h(\theta)$ satisfies condition (i) of Nuttall's theorem. To show that the continuity condition is also satisfied, first suppose that $\theta \neq -\pi$, i.e. $v \neq 0$. Then from (5.8) for small $\delta\theta > 0$,

$$|h(\theta-\delta\theta)-h(\theta)| = 2[(1-rv)vr]^{1/2}v^{L_0+1}(I_1+I_2)+\mathrm{O}(\delta v) \tag{5.15}$$

where δv is the corresponding increment in v and

$$I_1 = \int_{\frac{1}{2}(v+1/v)}^{\frac{1}{2}(v+1/v)+\frac{1}{2}\delta v(v2-1)} \frac{\psi(x)\,dx}{[1-2vx+v^2+2\delta v(v-x)]^{1/2}}$$

$$I_2 = \int_{x_0}^{\frac{1}{2}(v+1/v)} \left(\frac{1}{[1-2vx+v^2+2\delta v(v-x)]^{1/2}} - \frac{1}{(1-2vx+v^2)^{1/2}}\right)\psi(x)\,dx. \tag{5.16}$$

From the boundness of $|\psi(x)|$, it follows that for $v \neq 0$,

$$I_1 \simeq \mathrm{O}(\delta v^{1/2}), \qquad I_2 \simeq \mathrm{O}(\delta v).$$

Hence for $v \neq 0$, i.e. $\theta \neq -\pi$

$$|h(\theta-\delta\theta)-h(\theta)| \leq |\delta\theta|^{1/2} \times \text{constant} \tag{5.17}$$

Suppose now $\theta = -\pi$, i.e. $v = 0$. Then $\delta v = (\delta\theta)^2/4r$ and from (5.13)

$$|h_1(\delta\theta)-h_1(-\pi)| \leq \delta v \times \text{constant} = (\delta\theta)^2 \times \text{constant}. \tag{5.18}$$

Finally,

$$h_2(\theta) = 2(rv-r^2v^2)^{1/2}v^{L_0+1}\int_{x_0}^{\frac{1}{2}(v+1/v)} \frac{\psi_2(x)\,dx}{(1-2vx-v^2)^{1/2}}. \tag{5.19}$$

Using the bound (5.12) on $\psi_2(x)$ it follows that $h_2(-\pi) = 0$ and

$$|h_2(\delta\theta)| \leq 2(2r)^{1/2}\int_0^{1-x_0\delta v} \frac{(1-y^2)^p\,dy}{[\ln(1-y^2)-\ln(2\delta v)]^\alpha} + \mathrm{O}(\delta v)$$

where, as previously, we have made the substitution $y = [1-2x/(v+1/v)]^{1/2}$ in (5.19). Therefore

$$|h_2(\delta\theta)| \leq 2(2r)^{1/2}\left(\int_{1-x_0(\delta v)^{1/2}}^{1-x_0\delta v} \frac{(1-y^2)^p\,dy}{\ln x_0} + \int_0^{1-x_0(\delta v)^{1/2}} \frac{(1-y^2)^p\,dy}{[\ln(x_0\delta v)]^\alpha}\right) + \mathrm{O}(\delta v). \tag{5.20}$$

The first integrand is $\mathrm{O}[(\delta v)^{1/2}]$ and the second $\mathrm{O}[(\ln\delta v)^{-\alpha}]$. Therefore

$$|h_2(\delta\theta)-h_2(-\pi)| \leq \mathrm{O}[(\ln\delta v)^{-\alpha}] \simeq \mathrm{O}[(\ln\delta\theta)^{-\alpha}]. \tag{5.21}$$

Combining (5.21) and (5.18),

$$|h(\delta\theta)-h(\theta)| \leq c_1|\ln\delta\theta|^{-\alpha} \tag{5.22}$$

when $\theta = -\pi$. From (5.17) and (5.22) it follows that $h(\theta)$ defined in (5.10) satisfies condition (ii) of Nuttall's theorem when $\alpha > 1$ so the lemma is proved.

We are now ready to prove the main result of this section which is the following theorem.

Theorem 5.1. Let

$$\mathrm{Im}\, f(s,t) = \sum_{l=0}^{\infty}(2l+1)f_l(s)P_l\left(1+\frac{2t}{s-4\mu^2}\right) \tag{5.2}$$

where the partial-wave amplitudes $\{f_l; l \geq L_0+1\}$ have the Froissart–Gribov representation

$$f_l = \int_{x_0}^{\infty} Q_l(x)\psi(x)\,dx \qquad (l \geq L_0+1) \tag{5.3}$$

where $\psi(x)$ satisfies the conditions (5.11), (5.12).

If

$$g_n(w) \equiv \sum_{p=1}^{2n} \frac{\alpha_p}{1+\sigma_p w}$$

is the approximant to

$$g(w) \equiv \sum_{l=0}^{\infty} f_{l+L_0+1}(-w)^l$$

$$\equiv \int_0^{1/r} \frac{\phi_3(v)\,dv}{1+vw} - \frac{ic}{2}\int_0^{1/r} \frac{dv}{(rv-r^2v^2)^{1/2}(1+vw)} \equiv N(w) - CS(w) \tag{5.4}$$

formed by taking the $[n-1/n]$ Padé approximants to $N(w)$ and $S(w)$, then the sequence of approximants

$$f_n^{\rm L}(z) = \sum_{p=1}^{2n} \frac{\alpha'_p(1-\sigma_p^2)}{(1-2\sigma_p z+\sigma_p^2)^{3/2}} + \sum_{l=0}^{L_0} (2l+1)\Big(f_l - \sum_{p=1}^{2n} \alpha'_p\sigma_p^l\Big)P_l(z) \tag{5.23}$$

where $\alpha'_p = \alpha_p\sigma_p^{-L_0-1}$ and $z = 1+[2t/(s-4\mu^2)]$, converge uniformly to $f(z) \equiv \operatorname{Im} f(s,t)$ as $n \to \infty$ (for fixed $s > 4\mu^2$), for all t in any closed bounded domain of the complex t-plane cut from $4\mu^2$ to ∞.

Proof. The power series corresponding to the Legendre series (5.2) is

$$G(w) \equiv \sum_{l=0}^{\infty} f_l(-w)^l = \sum_{l=0}^{L_0} f_l(-w)^l + (-w)^{L_0+1}g(w) \tag{5.24}$$

and with the usual notation

$$\operatorname{Im} f(s,t) = \int_{\Gamma} K(z,w)(2wG'(w)+G(w))\,dw. \tag{5.25}$$

The approximants to $G(w)$ are

$$G_n(w) \equiv \sum_{l=0}^{L_0} f_l(-w)^l + (-w)^{L_0+1}g_n(w) = \sum_{p=1}^{2n} \frac{\alpha'_p}{1+\sigma_p w} + \sum_{l=0}^{L_0}\Big(f_l - \sum_{p=1}^{2n} \alpha'_p\sigma_p^l\Big)(-w)^l \tag{5.26}$$

where $\alpha'_p = \alpha_p\sigma_p^{-L_0-1}$.

From the assumed properties of $\psi(x)$ and hence of $\phi_3(v)$, Nuttall's theorem may be used to prove that $g_n(w) \to g(w)$ as $n \to \infty$ uniformly for w in any closed bounded domain of the w-plane cut from $-r$ to $-\infty$. Similarly $G_n(w) \to G(w)$ and $G'_n(w) \to G'(w)$. Therefore from (5.26)

$$f_n^{\rm L}(z) = \int_{\Gamma} K(z,w)(2wG'_n(w)+G_n(w))\,dw$$

$$= \sum_{p=1}^{2n} \frac{\alpha'_p(1-\sigma_p^2)}{(1-2\sigma_p z+\sigma_p^2)^{3/2}} + \sum_{l=0}^{L_0} (2l+1)\Big(f_l - \sum_{p=1}^{2n} \alpha'_p\sigma_p^l\Big)P_l(z) \tag{5.27}$$

and $f_n^{\rm L}(z)$ converges to $f(z)$.

We have shown that the conditions (5.11), (5.12) on

$$\psi(x)=\psi\left(\frac{2t'}{s-4\mu^2}+1\right)=\frac{\rho(s,t')}{\pi}$$

are sufficient for the sequence of approximants $f_n^L\{1+[2t/(s-4\mu^2)]\}$ to converge to $\operatorname{Im} f(s,t)$ for fixed s in the whole complex t-plane cut from $4\mu^2$ to ∞. As mentioned in the introduction, these conditions are satisfied in the case of scattering by a potential $V(r)$ which is holomorphic in $\operatorname{Re} r>0$ and satisfies the bounds

$$|V(r)|<c_3/|r|^\eta \tag{1.6}$$

with $\eta<2$ for $|r|\leq 1$ and $\eta>\frac{7}{4}$ for $|r|\geq 1$, and c_3 is a constant.

This follows from the fact that for this class of potentials it may be proved that (Bessis 1965),

$$|\rho(s,t')|\leq c[(st')^{-1/4}+(2+t')^{L_0}s^{-1/2}] \tag{5.28}$$

for fixed $s>4\mu^2$ and all $t'>4\mu^2$. So that for fixed $s>4\mu^2$,

$$|\psi(x)|\leq B_1x^{-1/4}+B_2x^{L_0} \tag{5.29}$$

when $x=[2t'/(s-4\mu^2)]+1$, and where B_i are constants.

Therefore, for $L_0=0,1,\ldots,\psi(x)$ satisfies the conditions (5.12).

To widen the class of potentials from that given by (1.6) to the case when $\eta<\frac{7}{4}$, one could proceed in the manner suggested by Bessis (1965). For these values of η one expects to find a finite number of distributions in $\rho(s,t)$. These distributions correspond to the lowest-order terms in the Born approximation and hopefully can be removed from $\rho(s,t)$ to leave a part which is bounded in the manner above.

6. Conclusions

We have shown that our 'Legendre Padé approximants' may be used to construct sequences of approximants from the partial-wave expansion (1.4) to the Coulomb scattering amplitude $f_c(z)$, and we have proved that such sequences converge to $f_c(z)$ in its whole domain of holomorphy.

Numerical examples show that sequences of LPA constructed from the partial-wave series of other scattering amplitudes corresponding to, for instance, the inverse-square and Yukawa potentials, do seem to converge to the exact amplitude in similar domains. However, it is important to construct sequences of approximants which can be *proved* to converge. As a start we have done this in § 5 for the absorptive part of scattering amplitudes corresponding to a certain class of potentials. An important objective in the future will be to extend these results to the real part of the amplitude and for a wider class of potentials.

The procedure of Yennie *et al* (1954) which essentially weakens the singularity of $f_c(z)$ at $z=1$, has also been used in the case of scattering by Yukawa and exponential potentials, the idea in the cases being to remove the nearest singularities, and thus accelerate the convergence of the 'reduced' partial-wave series. However, the 'reduced' series will still not converge in the whole domain of holomorphy of the amplitude. The procedure also requires precise knowledge of the nature of the nearby singularities.

In comparison our approximants converge in the holomorphy domain of the amplitude and do not use such details of the amplitudes singularities.

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