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Calculating Bessel Functions with Padé Approximants*

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The solution of the two-body Schrodinger equation with a C/r^2 potential is a Bessel function. The asymptotic series in r^{-1}, which is generated from Schrodinger equation, has a zero radius of convergence. The Padé approximants to the asymptotic series in $1/z$ for $J_\nu(z)$ converge rigorously for ν real. For ν imaginary convergence appears to be the same as for ν real.

1. INTRODUCTION

The full solution of Schrodinger's equation in nonrelativistic quantum-mechanics in general involves either the solution of Schrodinger's differential equation or the equivalent integral equation. These solutions (or wave-functions) are possible, however, for only a few choices of two body interaction potentials and not possible at all for many-body interactions. An asymptotic series may generally be generated from Schrodinger's equation. This type of series solution suffers, however, in that it converges only at infinity. Padé approximants can often be used to provide a sum for such series [1] and, thus, in this case provide a numerical solution of the Schrodinger's equation.

In the case of the inverse-square potential the two-body Schrodinger equation is exactly solvable in terms of a Bessel function. The convergence of the Padé approximants may in this special case be checked. A proof is given which shows that the approximants to the asymptotic solution of the differential equation converge to the full solution, for this interaction, everywhere in many cases of physical interest. Numerical results are also given which indicate that the approximants also converge to the full solution in all

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other cases which are physically interesting. The convergence rate of the approximants to the proper solution is also discussed through the use of numerical examples.

2. Procedure

The equation for which we seek the solution is

$$\frac{d^2u}{dr^2} + \left[k^2 + \frac{l(l+1)}{r^2} - \frac{C}{r^2}\right] u(r) = 0. \tag{1}$$

We obtain, as the regular solution, the well known function

$$u(r) = r^{1/2} J_\nu(kr),$$

where $J_\nu(kr)$ is the Bessel function of the first kind of order

$$\nu = (l(l+1) + \tfrac{1}{4} + C)^{1/2}.$$

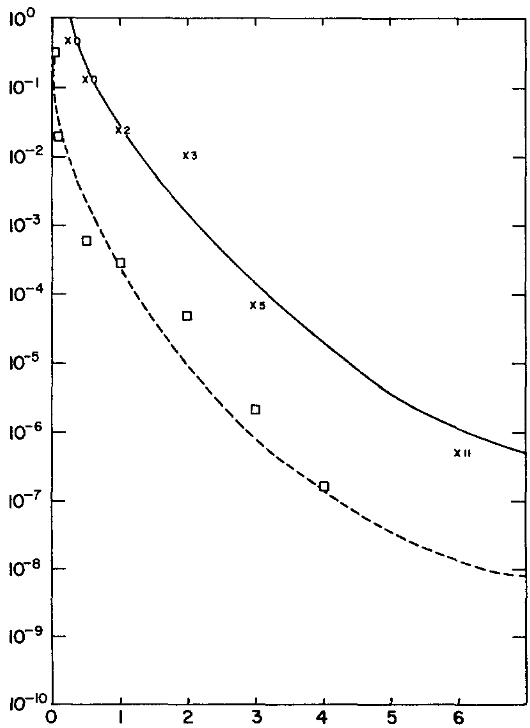

Fig. 1. Relative error in approximations to $J_0(x)$ versus x.

Rather than using the asymptotic development of $J_\nu(z)$ we choose to use the expansions of the Hankel functions of the first and second kind,

$$
\begin{aligned}
H_\nu^1(z) &= \left(\frac{2}{\pi z}\right)^{\frac{1}{2}} e^{i(z-\frac{1}{2}\pi\nu-\frac{1}{4}\pi)} \sum_{s=0}^{\infty} \frac{(\nu, s)}{(-2iz)^s} \qquad (-\pi < \arg z < 2\pi), \\
H_\nu^2(z) &= \left(\frac{2}{\pi z}\right)^{\frac{1}{2}} e^{-i(z-\frac{1}{2}\pi\nu-\frac{1}{4}\pi)} \sum_{s=0}^{\infty} \frac{(\nu, s)}{(2iz)^s} \qquad (-2\pi < \arg z < \pi),
\end{aligned} \tag{2}
$$

where (ν, s) is Hankel's symbol [2].

For this choice of functions $J_\nu(z)$ is then given by the identity

$$J_\nu(z) = \tfrac{1}{2}(H_\nu^1(z) + H_\nu^2(z)).$$

The asymptotic expansions of $H_\nu^1(z)$ and $H_\nu^2(z)$ provides only an approximate solution which in fact becomes increasingly useless as one proceeds inward from infinity in z. By forming Padé approximants to $H_\nu^1(z)$ and $H_\nu^2(z)$ a sequence of functions is obtained which converge to the full solution $J_\nu(z)$ everywhere.

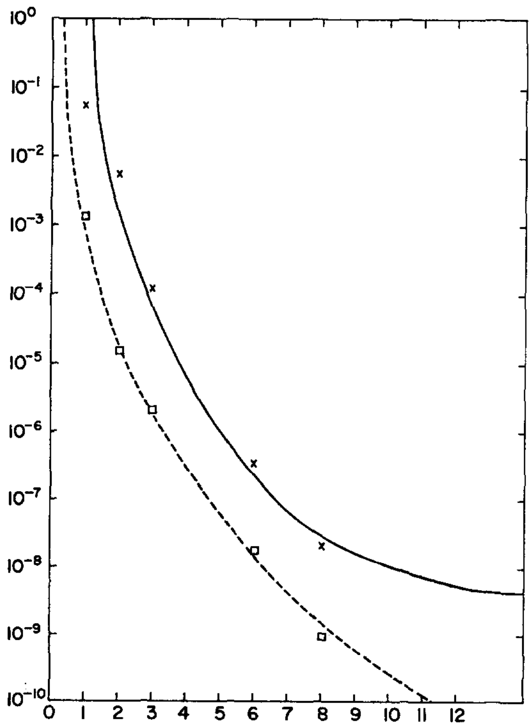

FIG. 2. Relative error in approximations to $J_1(x)$ versus x.

3. Formal Proof of Convergence

Gargantini and Henrici [3] have previously shown that the asymptotic form of the modified Bessel function of the third kind, $K_\nu(z)$, essentially forms a series of Stieltjes for ν real and $|\nu| < \frac{1}{2}$. It is evident from

$$\begin{aligned} K_\nu(z) &= \tfrac{1}{2}\pi i e^{\frac{1}{2}i\pi\nu} H_\nu{}^1(iz), \\ K_\nu(z) &= -\tfrac{1}{2}\pi i e^{-\frac{1}{2}i\pi\nu} H_\nu{}^2(-iz), \end{aligned} \tag{3}$$

that the asymptotic forms of $H_\nu{}^1(z)$ and $H_\nu{}^2(z)$ also form Stieltjes series and that Padé approximants to these series, thus, converge [4].

Essentially they begin with

$$K_\nu(z) = (2\pi z)^{1/2}\, e^{-z} \Phi_{\nu,\nu}(2z) \tag{4}$$

and write $\Phi_{\nu,-\nu}(z)$ in integral form as

$$\begin{aligned} \Phi_{\nu,-\nu}(z) &= \frac{1}{\Gamma(\frac{1}{2}+\nu)\,\Gamma(\frac{1}{2}-\nu)} \int_0^\infty \frac{e^{-t}\Phi_{\nu,\nu}(t)}{z+t}\, dt \\ &= \frac{1}{\Gamma(\frac{1}{2}+\nu)\,\Gamma(\frac{1}{2}-\nu)} \int_0^\infty \frac{e^{-t} t^{\nu-\frac{1}{2}} U(\frac{1}{2}+\nu, 1+2\nu, t)}{z+t}\, dt, \end{aligned} \tag{5}$$

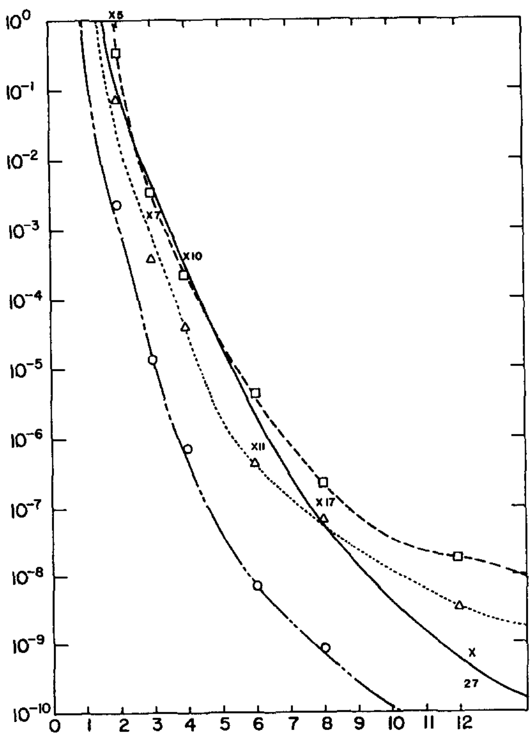

Fig. 3. Relative error in approximations to $J_4(x)$ versus x.

where $U(z, b, z)$ is Kummer's function [5]. $\Phi_{\nu,-\nu}(z)$ will then be the integral form of a series of Stieltjes if

$$\frac{d}{dt} G(t) = e^{-t} t^{\nu - \frac{1}{2}} U(\tfrac{1}{2} + \nu, 1 + 2\nu, t)$$

is the derivative of a bounded nondecreasing function $G(t)$. Essentially the only problem occurs at the origin where $(d/dt)\, G(t)$ diverges like

$$\lim_{t \to 0} \frac{d}{dt} G(t) \to t^{-\nu - \frac{1}{2}}.$$

A divergence at the origin no stronger than t^{-1} is allowed so that if $\Phi_{\nu,-\nu}(z)$ is to be a series of Stieltjes it is required that $\nu < \frac{1}{2}$. Likewise as

$$U(\tfrac{1}{2} - \nu, 1 - 2\nu, t) = t^{2\nu} U(\tfrac{1}{2} + \nu, 1 + 2\nu, t),$$

it is necessary that $\nu > -\frac{1}{2}$ which makes $\Phi_{\nu,-\nu}(z)$ a series of Stieltjes for $|\nu| < \frac{1}{2}$.

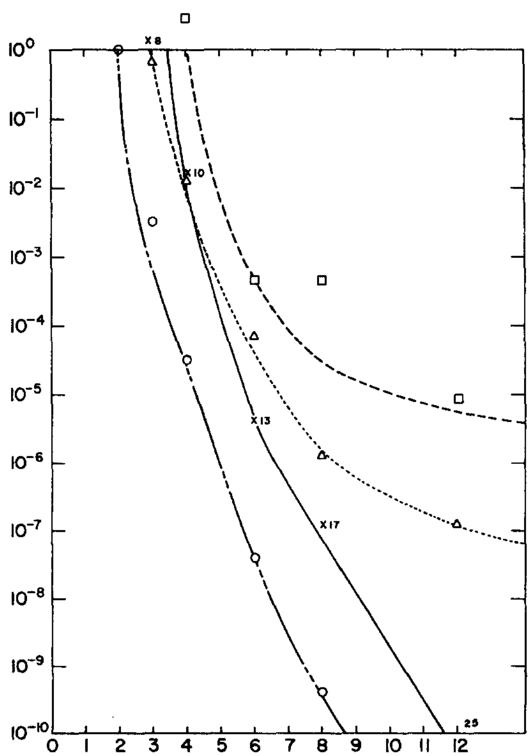

FIG. 4. Relative error in approximations to $J_6(x)$ versus x.

We expand $(z+t)^{-1}$ as

$$\frac{1}{z+t} = \frac{1}{z} - \frac{t}{z(z+t)} \tag{6}$$

and insert this expansion into Eq. (5) to obtain

$$\Phi_{\nu,-\nu}(z) = \frac{1}{\Gamma(\nu+\frac{1}{2})\,\Gamma(\nu-\frac{1}{2})}\left[\frac{1}{z}\int_0^\infty e^{-t}t^{\nu-\frac{1}{2}}U(\tfrac{1}{2}+\nu, 1+2\nu, t)\right.$$
$$\left. + \frac{1}{z}\int_0^\infty \frac{e^{-t}t^{\nu+\frac{1}{2}}U(\frac{1}{2}+\nu, 1+2\nu, t)\,dt}{z+t}\right].$$

The second integral appears to have the form of a series of Stieltjes and when the divergence requirement at the origin is applied it is seen to be such for $|\nu| < \frac{3}{2}$.

In general then we choose n such that

$$n + \tfrac{1}{2} < |\nu| < n + \tfrac{3}{2},$$

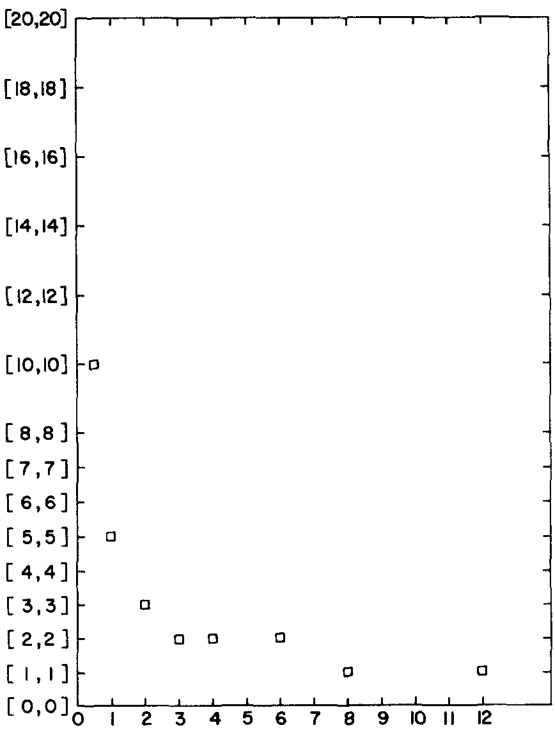

FIG. 5. Order of the approximant which approximates $J_0(x)$ to a relative error less than 10^{-4} versus x.

and expand $(z + t)^{-1}$ $n + 1$ times as in Eq. (6). The final result of this will be an integral of the form

$$\frac{1}{\Gamma(\nu + \frac{1}{2})\,\Gamma(\nu - \frac{1}{2})} \frac{(-1)^{n+1}}{z^{n+1}} \int_0^\infty \frac{e^{-t} t^{\nu - \frac{1}{2} + n + 1} U(\frac{1}{2} + \nu, 1 + 2\nu, t)\, dt}{z + t}, \tag{7a}$$

which is a series of Stieltjes. There will also be $n + 1$ terms to be added to this integral which will be given by

$$\frac{1}{\Gamma(\nu + \frac{1}{2})\,\Gamma(\nu - \frac{1}{2})} \sum_{j=0}^{n} \frac{(-1)^j}{z^{j+1}} \int_0^\infty e^{-t} t^{\nu - \frac{1}{2} + j} U(\tfrac{1}{2} + \nu, 1 + 2\nu, t)\, dt. \tag{7b}$$

As this result will be seen to yield the same results for $|\nu| > \frac{1}{2}$ we have analytically continued $\Phi_{\nu,-\nu}(z)$ to $|\nu| > \frac{1}{2}$. It is seen then that the asymptotic expansion of $H_\nu^1(z)$ and $H_\nu^2(z)$ may be reduced to a finite power expansion plus a series of Stieltjes for all real ordered Hankel functions, and so we are assured that the sum of approximants to these functions converges to $J_\nu(z)$.

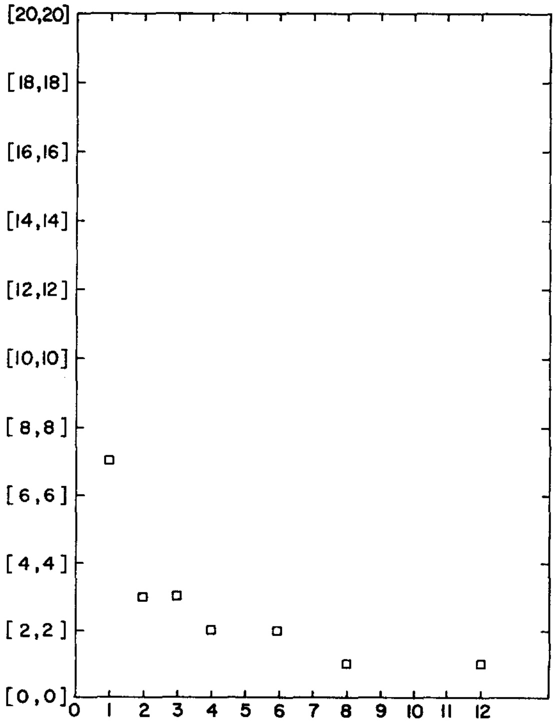

FIG. 6. Order of the approximant which approximates $J_1(x)$ to a relative error less than 10^{-4} versus x.

Following the same arguments as those above complex ordered Bessel functions may be considered. Looking again at

$$\lim_{t\to 0} e^{-t} t^{\nu-\frac{1}{2}} U(\tfrac{1}{2}+\nu, 1+2\nu, t) \to t^{-\frac{1}{2}-\nu},$$

it is seen that, for ν complex, oscillation in sign occurs, which rules out the possibility that $\Phi_{\nu,-\nu}(z)$ forms a series of Stieltjes.

4. Numerical Results

Even having proved that for real ν the approximants converge to the proper wave-function it is still of interest to give numerical results relating to the rate at which this convergence takes place. As the wave-functions under consideration are Bessel functions of real order, considering for the time being only those cases for which $(l(l+1)+C+\frac{1}{4})>0$, we shall consider

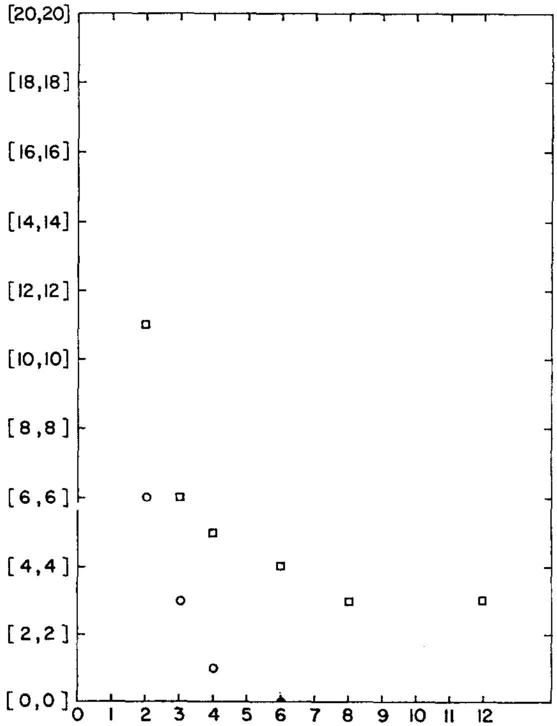

FIG. 7. Order of the approximant which approximates $J_4(x)$ to a relative error less than 10^{-4} versus x.

the rate at which the sum of approximants to the asymptotic form of $H_\nu^1(z)$ and $H_\nu^2(z)$ converge to $J_\nu(z)$. Though results given so far apply to any point in the complex plane (with appropriate phase restrictions), only convergence along the real axis will be considered since we are interested in a physical problem. On the positive real axis there, of course, exist error bounds as we are dealing with a series of Stieltjes. These bounds are

$$[N, N](x) \geqslant f(x) \geqslant [N, N-1](x).$$

Bounds also exist for the approximants throughout the cut complex plane though these are generally moie difficult to use [4].

Various sequences of $[n, n \pm j]$ approximants, generated by the epsilon algorithm [6], were studied, but none appeared to converge generally more rapidly than the $[n, n]$ and so all results will be referred to this sequence of approximants. Convergence was viewed in two manners, first by the relative error which a given order approximant would give to $J_\nu(x)$ as x varied and

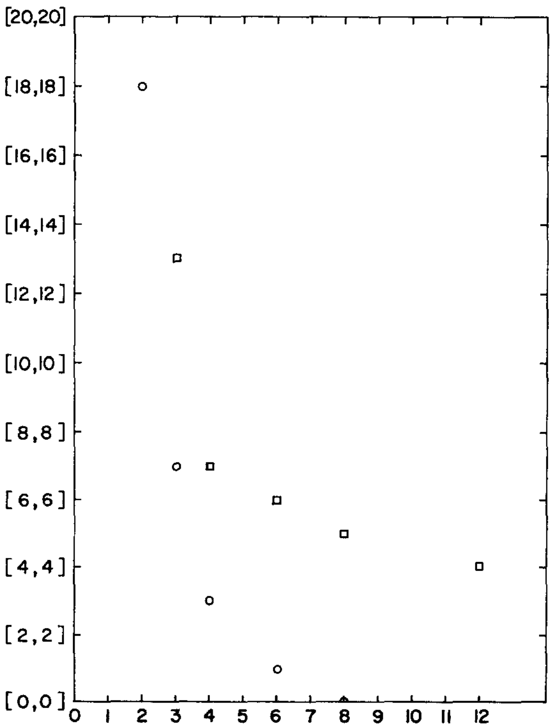

FIG. 8. Order of the approximant which approximates $J_8(x)$ to a relative error less than 10^{-4} versus x.

second by the order of the approximant required to approximate $J_\nu(x)$ to within a given relative error as x increased. The correct answer in these comparisons was considered to be that given by the Computation Laboratory of Harvard University [7] in a series of volumes containing $J_\nu(x)$ for various ν and x.

In all figures of the first kind, Figs. 1–4, we plot the relative error in the best answer to $J_\nu(x)$ which the asymptotic series provides (solid line through the x's—note also that the exponent of the last term used is given also) and also the relative error in the [4, 4] approximate to $J_\nu(x)$ (dotted line through the boxes). For those cases considered here the error in truncating the asymptotic series at some point will be bounded by the absolute value of the first neglected term. We consider the best answers which the series provides to be that sum for which the next term would have the smallest absolute value. In addition to those curves just mentioned the figures containing $J_4(x)$ and $J_6(x)$ will be seen to have two additional curves plotted. These curves are plots of the relative error ensued in computing the approximant by splitting up the asymptotic series into a finite power series and a series of Stieltjes as done

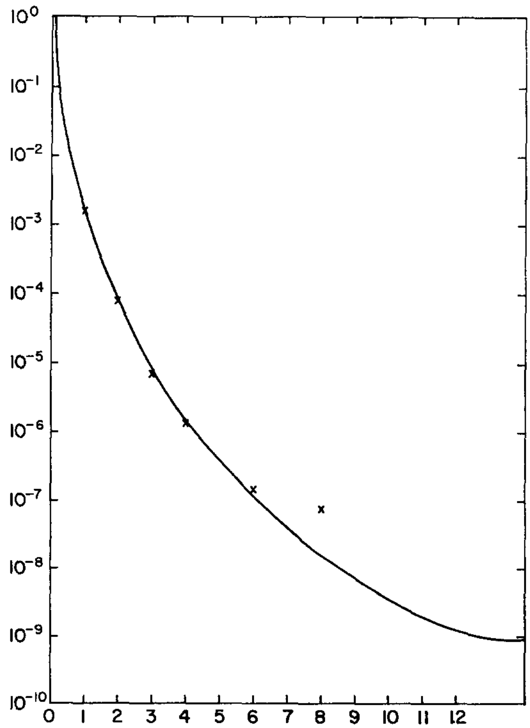

FIG. 9. Relative error in the [4, 4] approximant to $J_i(x)$ versus x.

in the proof. Following the expansion of Eq. (7) the value of the approximant will be given by the value of a finite power series plus and $[n, n]$ approximant to the remaining series of Stieltjes. The solid-dashed curve through circles represents the foregoing process where a [4, 4] approximant is used. It is essentially just as simple to approximate the series in this manner as it is with a [4, 4] to the entire series, as much more effort is required to form the approximate than to simply add terms of a power series. Nonetheless, the answer provided by the finite sum and a [4, 4] approximate to a series of Stieltjes must provide the best answer as more terms of the original series are included. To this extent the other curve (dashed line through triangles) represents that answer provided by a finite sum plus an $[n, n]$ approximate so that only those coefficients used to form the [4, 4] to the whole series will be included. For $J_4(x)$ we then use a [2, 2] approximate and for $J_6(x)$ a [1, 1] approximant.

In the graphs of comparisons of the second kind, Figs. 5–8, two sets of points are plotted; first (shown by squares) the $[n, n]$ approximant which provides a relative error smaller than one part in 10^{-4} to $J_\nu(x)$ and second (shown by

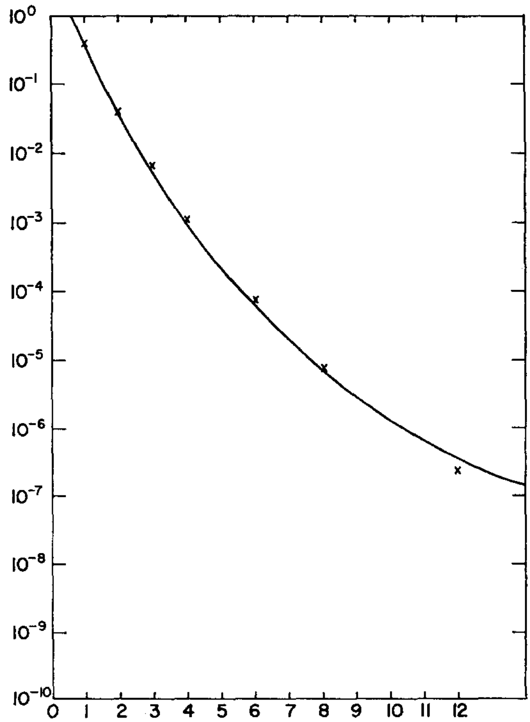

FIG. 10. Relative error in the [4, 4] approximant to $J_{4i}(x)$ versus x.

circles) that answer provided by a finite power series and an $[n, n]$ approximant to a series of Stieltjes which also gives $J_\nu(x)$ to less than one part in 10^{-4}. With these conventions in mind the utility of forming an answer for $|\nu| > \frac{1}{2}$ by the sum of a finite power expansion and an approximant to a series of Stieltjes can obviously be seen. It can readily be observed also that even a relatively small order approximant, [4, 4] can provide a fairly accurate value for the wave-function everywhere—though perhaps questionably as the origin is approached. Though certain that the sequence of $[n, n]$ approximants as n approaches infinity will converge arbitrarily close to the origin it might at first appear that a small order approximant simply does not approximate $J_\nu(x)$ will in this region—though it does provide a much better answer than the asymptotic series. It must be remembered, however, that $J_\nu(x)$ $(\nu \neq 0)$ are zero at the origin and are slowly increasing away from this point, especially in the sense as ν increases. This is to say that though the [4, 4] may give an appreciable relative error in this region the absolute error is quite small. Thus, as we generally consider the wave-function only in an integral of some

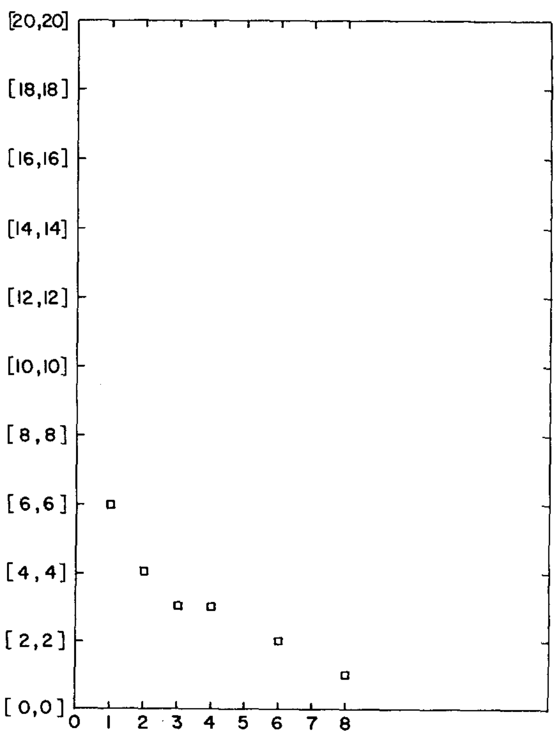

FIG. 11. Order of the approximant which approximates $J_i(x)$ to a relative error less than 10^{-4} versus x.

type it is seen that little error will arise in the numerical evaluation of this integral through the use of a small order Padé approximant as the wave-function.

Finally we move to solution corresponding to $(l(l+1) + C + \frac{1}{4}) < 0$ for which we have complex ordered Bessel functions. Numerical comparisons made for these solutions follow the same pattern as those described previously and are presented in Figs. 9–12. It is apparent from the graphs that the approximants in this case also converge to the proper answer. The rate of this convergence seems to be roughly equivalent for $J_\nu(x)$ and $J_{i\nu}(x)$.

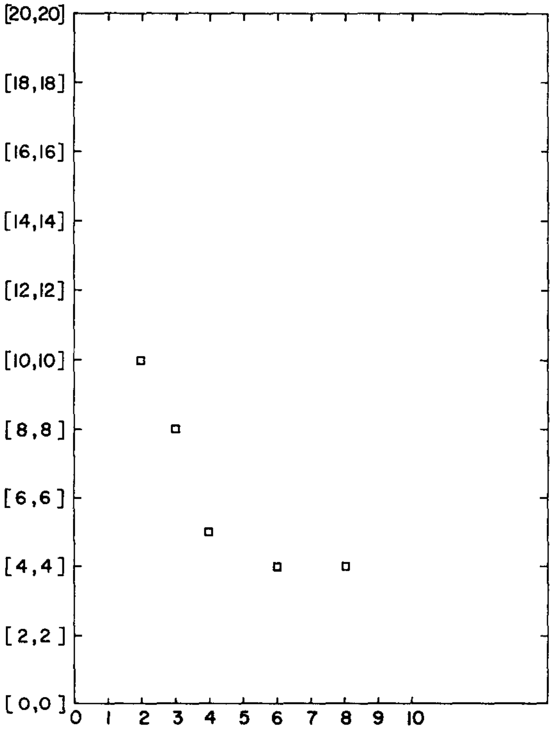

FIG. 12. Order of the approximant which approximates $J_{4i}(x)$ to a relative error less than 10^{-4} versus x.

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