Limitations of the method of complex basis functions

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(Received 31 October 1974)

The method of complex basis functions proposed by Rescigno and Reinhardt is applied to the calculation of the amplitude in a model problem which can be treated analytically. It is found for an important class of potentials, including some of infinite range and also the square well, that the method does not provide a converging sequence of approximations. However, in some cases, approximations of relatively low order might be close to the correct result. The method is also applied to S-wave e-H elastic scattering above the ionization threshold, and spurious "convergence" to the wrong result is found. A procedure which might overcome the difficulties of the method is proposed.

INTRODUCTION

The method of complex basis functions has been suggested[1] as a means of performing scattering calculations at energies where several open channels are present. It offers the possibility of calculating the amplitude for scattering from one channel to another without the need for the explicit inclusion of any of the other channels, open or closed. An important example of a basic, nontrivial problem where such a technique would be very useful is electron–hydrogen-atom scattering.

Originally, complex basis functions were used in the framework of the Fredholm method, but the approach might just as well be applied to the direct evaluation of scattering amplitudes. This gives rise to the possibility of a new method for calculating ionization amplitudes, which so far have proved difficult to obtain.

These possibilities indicate that a study of the complex-basis-function method to determine its validity for different types of potential is worthwhile. In particular, it is of interest to atomic theorists to investigate whether or not it applies to potentials of infinite range, and this is the main object of this paper.

Unfortunately, our conclusions are largely negative. In important examples with long-range potentials that we have studied analytically and numerically, we find that the method does not converge. Moreover, there are cases where the sequence of approximations appears for a time to be converging to the wrong answer. An incautious use of numerical results could lead to incorrect conclusions.

We suggest a modification of the complex-basis-function method which overcomes the above difficulties, but is of unknown practical value. A single sequence of approximations is constructed in which the angle of rotation decreases to zero as the number of trial functions increases. It is shown in all cases studied that it is possible to find a relation between the angle and the number of trial functions that ensures that the sequence converges to the correct answer. Practical use of this result would probably depend on finding an optimum choice of the angle-number relation.

MODEL PROBLEM

We can learn much about the method of complex basis functions by applying it to a model problem in which analytic results may be obtained. Let us consider the determination of

$$I = \lim_{\epsilon \to 0^+} (f, (E + i\epsilon - H_0)^{-1} g) , \tag{1}$$

where $E = k^2$, k real, $H_0 = -d^2/dr^2$, and the scalar product of two functions $f(r)$, $g(r)$, $0 \leq r$, is defined as

$$(f, g) = \int_0^\infty dr f^*(r) g(r) . \tag{2}$$

The second term of the Born series for the amplitude for single-particle S-wave scattering could be written in this form.

To obtain an approximation to I using the method of complex basis functions, we chose a set of basis functions $u_n(r)$, $n = 0, 1, 2, \ldots$. The functions $u_n(r)$ are analytic in r, satisfy $u_n(r^*) = u_n^*(r)$, and decrease exponentially at infinity, but are not necessarily orthogonal. For a particular choice of the complex parameter $t = e^{i\alpha}$, $\alpha > 0$, we define

$$\begin{aligned} u_n^\alpha(r) &= u_n(tr) , \\ f_n &= (f, u_n^{-\alpha}) , \\ g_n &= (u_n^\alpha, g) , \\ M_{nm} &= (u_n^\alpha, (E - H_0) u_m^{-\alpha}) . \end{aligned} \tag{3}$$

The approximation I_N to I which uses the first N basis functions is

$$I_N = \sum_{m,n=0}^{N-1} f_n (M^{-1})_{nm} g_m , \tag{4}$$

where M^{-1} means the inverse of the $N\times N$ matrix M_{nm}, $n, m = 0, \ldots, N-1$.

The attraction of the method is that the matrix M_{nm} may be written in the form

$$M_{nm} = t^{-1}[t^2 E(u_n, u_m) - (u_n, H_0 u_m)] , \tag{5}$$

from which it follows that M_{mn} cannot be singular for $\alpha > 0$. Thus the singularity of the resolvent of H_0 which complicates the calculation of I has been rendered innocuous.

We now proceed to discuss the convergence of this method for a particular choice of basis functions. After Schwartz,[2] we take $u_n(r)$ to be obtained from the generating function $U(s, r)$ by

$$\sum_{n=0}^{\infty} u_n(r)s^n = U(s, r) = (1-s)^{-2} r \exp\left(-\frac{ra}{2}\frac{1+s}{1-s}\right) . \tag{6}$$

This means that $u_n(r)$ is a polynomial in r of degree n multiplied by $e^{-ar/2}$.

The value of I_N calculated by the procedure outlined above will be the same as that obtained from the following modified approach. We use $\bar{u}_n$ defined by

$$\sum_{n=0}^{\infty} \bar{u}_n(r)s^n = \bar{U}(s, r) = (1-s)^{-2} r \exp\left(-rb\frac{1+s}{1-s}\right) , \tag{7}$$

where $b = \frac{1}{2}ae^{-i\alpha}$. Then we set

$$\bar{f}_n = \int_0^{\infty} dr\, \bar{u}_n(r) f^*(r) ,$$

$$\bar{g}_n = \int_0^{\infty} dr\, \bar{u}_n(r) g(r) , \tag{8}$$

$$\bar{M}_{nm} = \int_0^{\infty} dr\, \bar{u}_n(r)(E - H_0)\bar{u}_m(r) ,$$

and we find

$$I_N = \sum_{n=0}^{N-1} \bar{f}_n \bar{c}_n , \tag{9}$$

where

$$\sum_{m=0}^{N-1} \bar{M}_{nm}\bar{c}_m = \bar{g}_n , \quad n = 0, \ldots, N-1 . \tag{10}$$

If we write $c_m = (m+1)\bar{c}_m$, (10) becomes, on using the results of Schwartz,

$$-Ac_{n-1} + Bc_n - Ac_{n+1} = \bar{g}_n/(n+1), \quad n = 0, 1, \ldots, N-1 , \tag{11}$$

where

$$A = \frac{1}{8b^3}(k^2 + b^2), \quad B = \frac{1}{4b^3}(k^2 - b^2) ,$$

and $c_{-1} = 0$, $c_N = 0$.

To solve (11), let us define

$$C(s) = \sum_{n=0}^{\infty} c_n s^n , \tag{12}$$

$$\bar{G}(s) = \sum_{n=0}^{\infty} \bar{g}_n s^n = \int_0^{\infty} dr\, \bar{U}(s, r) g(r) . \tag{13}$$

Then (11) gives

$$-As^2 C + BsC - A(C - c_0) = \sum_{n=0}^{\infty} \frac{\bar{g}_n s^{n+1}}{n+1} = \int_0^s ds'\, \bar{G}(s') ,$$

which may be solved to give

$$C(s) = [(s-\nu_1)(s-\nu_2)]^{-1}\left(\lambda - A^{-1}\int_{\nu_1}^{s} ds'\, \bar{G}(s')\right) . \tag{14}$$

The constant λ must be chosen to give $c_N = 0$. In (14) we have used

$$(s-\nu_1)(s-\nu_2) = s^2 - (B/A)s + 1,$$

so that

$$\nu_1 = \frac{k - ib}{k + ib}, \quad \nu_2 = \nu_1^{-1} . \tag{15}$$

Note that we have chosen the root ν_1 so that $|\nu_1| < 1$.

The solution may be written in the form

$$C(s) = \lambda D(s) + E(s) , \tag{16}$$

where

$$D(s) = \sum_{n=0}^{\infty} d_n s^n = [(s-\nu_1)(s-\nu_2)]^{-1} , \tag{17}$$

$$E(s) = \sum_{n=0}^{\infty} e_n s^n = -A^{-1}[(s-\nu_1)(s-\nu_2)]^{-1}\int_{\nu_1}^{s} ds'\, \bar{G}(s') , \tag{18}$$

so that

$$c_n = \lambda d_n + e_n . \tag{19}$$

Thus I_N may be written

$$I_N = \lambda_N \sum_{n=0}^{N-1} \bar{f}_n d_n (n+1)^{-1} + \sum_{n=0}^{N-1} \bar{f}_n e_n (n+1)^{-1} , \tag{20}$$

with

$$\lambda_N = -e_N/d_N . \tag{21}$$

The quantities d_n, e_n, $\bar{f}_n$ are independent of N, and to study the convergence of I_N we need to know their behavior for large n. This is related to the nature of the singularities of $D(s)$, $E(s)$, and $\bar{F}(s) = \sum_{n=0}^{\infty} \bar{f}_n s^n$ that are nearest to the origin.

Suppose that $H(s)$ is an analytic function of s typical of those encountered above, and that it has a single singularity nearest to the origin at s_0. Then if

$$H(s)=\sum_{n=0}^{\infty} h_n s^n ,$$

we may write

$$h_n=\frac{1}{2\pi i}\int_{\Gamma} ds'\, s'^{-(n+1)} H(s') , \tag{22}$$

where Γ is a small circle round the origin. To estimate the form of h_n for large n, we distort Γ to Γ' in Fig. 1. The dominant contribution to the integral will come from that part of Γ' near s_0. In evaluating (22) we may approximate H by its behavior near s_0 and use the method of steepest descent or a generalization. The results for some representative choices of the functions $f(r)$ and $g(r)$ are set out below, sometimes omitting constant factors:

$$d_n \sim \nu_1^{-n} .$$

Case 1: $g_1(r)=e^{-r}$,

$$\bar{G}(s)=[(b-1)s+(b+1)]^{-2} ,$$

$$\bar{g}_n=(n+1)(1+b)^{-2-n}(1-b)^n ,$$

$$e_n \sim (b-1)^n(b+1)^{-n}+\nu_2^{-n} ,$$

$$\lambda_N \sim \nu_1^{2N} \quad [\text{if } |(b-1)/(b+1)| \leq |\nu_1|] .$$

Case 2: $g_2(r)=1, \quad r \leq R ,$

$$=0, \quad r>R ,$$

$$\bar{G}(s)=b^{-2}(1+s)^{-2}(1-\exp\{-Rb[(1+s)/(1-s)]\})$$

$$-(Rb)^{-1}(1-s^2)^{-1}\exp\{-Rb[(1+s)/(1-s)]\} ,$$

$$\bar{g}_n=n^{-1/4}\exp[2i(2Rbn)^{1/2}] ,$$

$$e_n \sim n^{-5/4}\exp[2i(2Rbn)^{1/2}]+\nu_2^{-n} ,$$

$$\lambda_N \sim N^{-5/4}\nu_1^N \exp[2i(2RbN)^{1/2}] .$$

Case 3: $g_3(r)=(r+1)^{-2}\sin kr$.

$\bar{G}(s)$ has logarithmic singularities at $s=\nu_1$, $s=\nu_2$, and an essential singularity at $s=1$.

$$\bar{g}_n \sim \nu_1^{-n}/n+\nu_2^{-n}/n+\gamma_n ,$$

where $|\gamma_n|<n^{-1}$;

$$e_n \sim \nu_1^{-n}/n+\nu_2^{-n}/n+\gamma_n' ,$$

where $|\gamma_n'|<n^{-1}$;

$$\lambda_N \sim N^{-1} .$$

CONVERGENCE

With the development of this machinery we are in a position to discuss the convergence of the complex-basis-function method in our model for six choices of the pair of functions f, g used to define I. It is straightforward to deduce that $I_N \to I$ as $N \to \infty$, provided that one of the functions f, g is chosen to be $g_1=e^{-r}$, whatever g_i, $i=1,2,3$ is chosen for the other. It also may be easily shown that the sequence I_N does not converge when both f, g are chosen from g_2 and g_3. In these cases, however, there may be apparent convergence for a range of values of N. By this we mean that $|I_N-I_{N+1}|$ decreases with increasing N and the sequence of I_N appears to be approaching a limit.

To illustrate how this apparent convergence can come about, consider the case of $f=g=g_2$. If the factor $\exp[2i(2Rbn)^{1/2}]$ were not present in the expressions for λ_n, $\bar{f}_n$, e_n, then I_N as given by (20) would converge to

$$\sum_{n=0}^{\infty} \bar{f}_n e_n (n+1)^{-1} \tag{23}$$

as the first term in (20) would approach zero. However, because of the exponential factor, (23) does not converge and the first term in (20) does not approach zero. For small α the exponential factor will not begin to dominate and cause divergence until $N>O(\alpha^{-2})$. Thus the divergence will not appear in calculations for small values of α until N has a value larger than that reached in many numerical calculations. The value to which I_N appears to converge in such a case may be wrong, although if α is small it may be close to I.

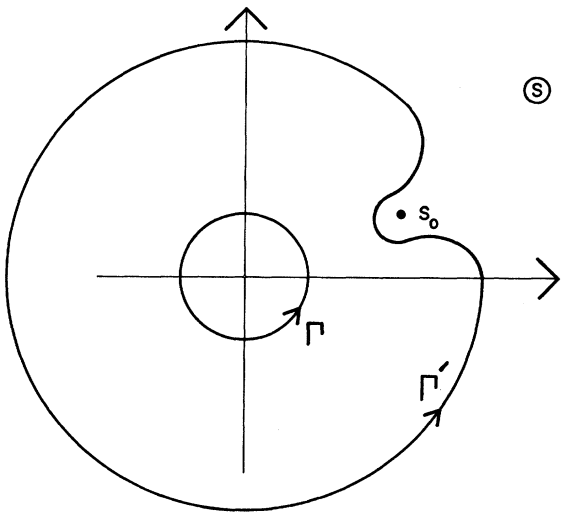

Fig. 1. Contour Γ used to write h_n in terms of $H(s)$ and contour Γ' used to evaluate h_n for large n.

This behavior is illustrated by the results shown in Figs. 2 and 3, where we plot sequences of values of I_N for $f=g=g_2$ with different values of α. For $\sin\alpha=0.1$, I_N appears to be converging to a value close to the correct answer $I=2.825\,159 - i2.081\,998$ (shown by a star) for N up to 56, and this trend continues at least until $N\approx 200$ (not shown in Fig. 2). However, for $\sin\alpha=0.175$, apparent convergence occurs at $N\approx 45$ and then a steady divergence appears. In each case results of sufficient accuracy for many practical purposes could be obtained.

In Figs. 4 and 5 we give some typical results for the case $f=g=g_3$, which have a similar behavior to the previous case. (We have not calculated I in this case.)

With this background, it is interesting to consider the results of a more realistic calculation. We have applied the method of complex basis functions to S-wave elastic electron–hydrogen-atom scattering in the singlet spin state at a kinetic energy of 1.69 Ry, which is 0.69 Ry above the ionization threshold. We augmented a set of Hylleraas trial functions (using the notation of Ref. 3)

$$u_{lmn}(r_1r_2r_3)=(r_1^l r_2^m + r_1^m r_2^l)r_3^n e^{-(r_1+r_2)}$$

by the function

$$\theta = r_2^{-1}e^{-r_1}e^{ikr_2}(1-e^{-r_2})+(r_1 \rightleftharpoons r_2),\quad k^2=E-1\ .$$

The coordinates in the functions u_{lmn} were transformed by $r\rightarrow re^{i\alpha}$, but this was not done to the function θ. The amplitude was calculated in a manner similar to that of Ref. 3. The results

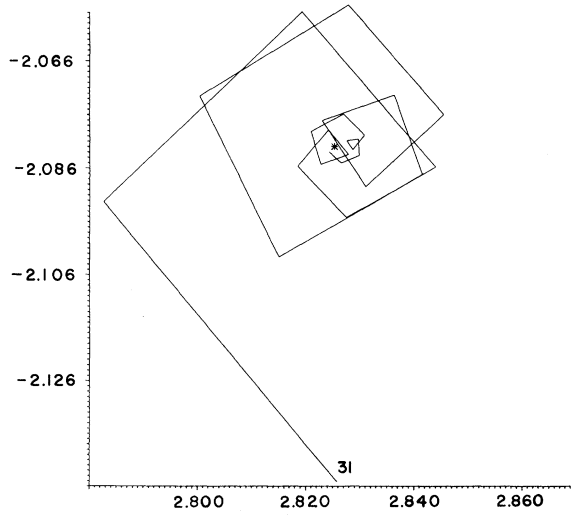

Fig. 2. Plot in the complex plane showing values of I_N for $N=31-56$ in the case $f=g=g_2$, $R=3$, $a=1$, $k=1$, $\sin\alpha=0.1$. Successive values are joined by straight lines.

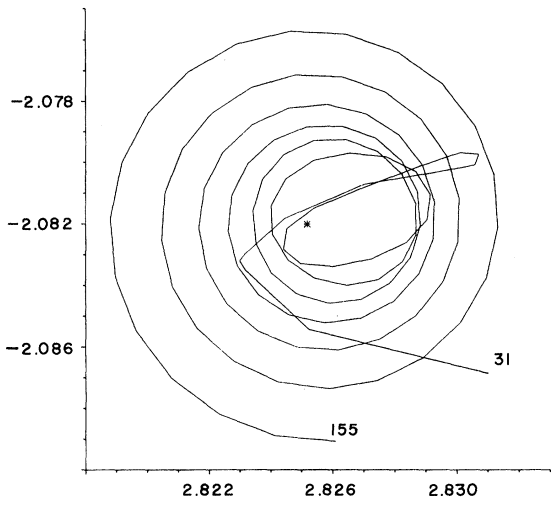

Fig. 3. Plot in the complex plane showing values of I_N for $N=31-155$ in the case $f=g=g_2$, $R=3$, $k=1$, $a=1$, $\sin\alpha=0.175$. Successive values are joined by straight lines.

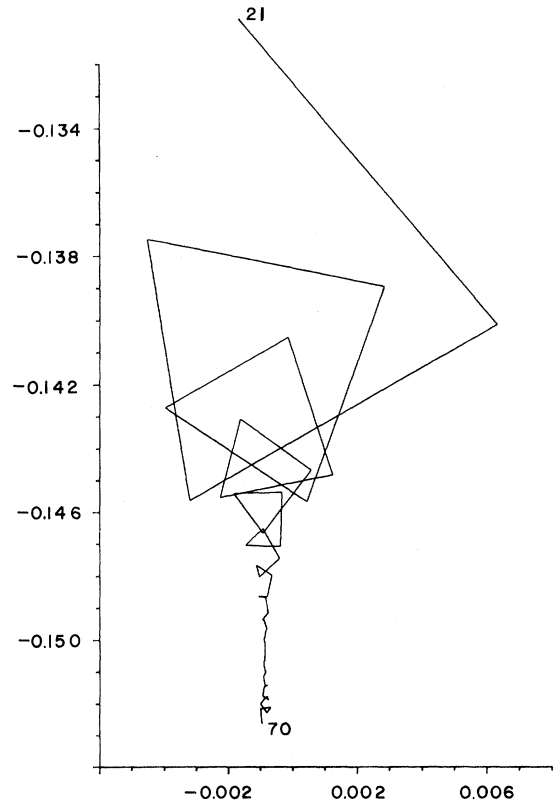

Fig. 4. Plot in the complex plane showing values of I_N for $N=21-70$ in the case $f=g=g_3$, $k=1$, $a=1$, $\sin\alpha=0.1$. Successive values are joined by straight lines.

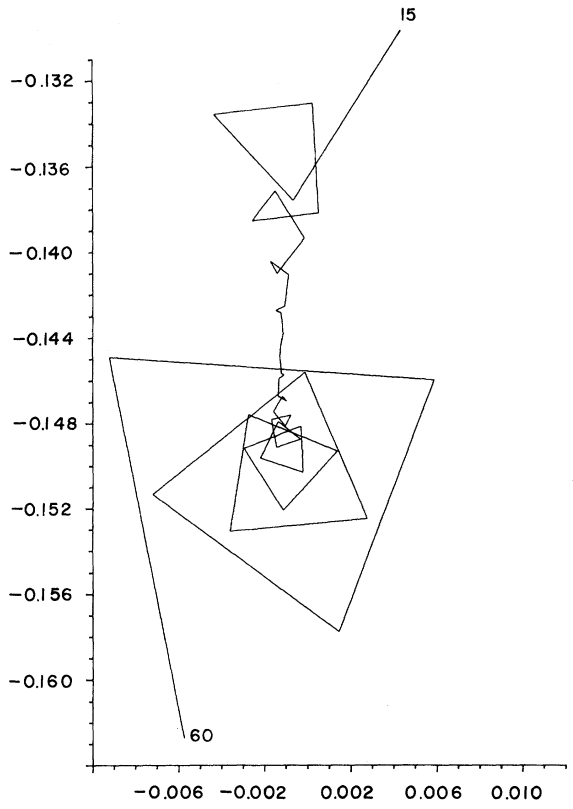

Fig. 5. Plot in the complex plane showing values of I_N for $N=15$–60 in the case $f=g=g_3$, $k=1$, $a=1$, $\sin\alpha=0.15$. Successive values are joined by straight lines.

are shown in Table I for several values of α and $N=\max(l+m+n)$. There appears to be convergence to within an accuracy of ± 0.01 for the real part of the amplitude for each value of α, but the results differ significantly. In each case the result differs from the value of 0.34, which was found by the energy-extrapolation method, and a similar value obtained by Rescigno and Reinhardt[4] using a different extrapolation procedure. Note that extrapolation in α would yield a value close to 0.34. The differences between imaginary parts for different α and previous calculations are less significant.

These results demonstrate that apparent convergence for a particular value of α does not imply that the correct result has been obtained.

DISCUSSION

The method of complex basis functions was originally suggested in the context of the Fredholm method,[1] whereas we have applied it to the calculation of amplitudes. We expect that problems similar to those we have found will also appear in the Fredholm method. In some cases the Fredholm method with complex basis functions can be justified because it is equivalent to using a rotated Hamiltonian with real basis functions. Thus we believe that the Fredholm method with complex basis functions will be valid for scattering of a particle in an analytic potential, even one of infinite range. It should also apply to a many-body problem with Coulomb potentials in the region where only one channel is open.

We presume that difficulties with the Fredholm method using complex basis functions will appear in any problem containing potentials with a local, infinite-range part, and also some of short range, when we are working at an energy at which two or more channels are open. In the method as described by Rescigno and Reinhardt[1] it is necessary to calculate substituted determinants in order to obtain physical scattering amplitudes. One of the terms that arises in the expansion of such a determinant for a two-channel problem such as that treated as an example by Rescigno and Reinhardt[1] is

$$J=\lim_{\epsilon\to 0+}\mathrm{Tr}\left[(E+i\epsilon-H_0)^{-1}V_{12}(E+B-i\epsilon-H_0)^{-1}V_{21}\right] .$$

Here V_{12} and V_{21} are potentials and $B>0$. The method of complex basis functions approximates J by

$$J^N=\sum_{jlmn}^{N-1}(M^{-1})_{mn}\,V_{12}^{nj}(M_B^{-1})_{jl}\,V_{21}^{lm} ,$$

where

TABLE I. Real and imaginary parts of approximations to the S-wave singlet e^--H scattering amplitude at $k=1.3$ a.u. for differing values of rotation angle α and $N=\max(l+m+n)$.

N \ α	0.1	0.2	0.3	0.4
3	(0.394, 0.355)	(0.405, 0.393)	(0.424, 0.401)	(0.449, 0.394)
4	(0.339, 0.452)	(0.371, 0.428)	(0.384, 0.425)	(0.392, 0.443)
5	(0.360, 0.394)	(0.376, 0.422)	(0.390, 0.430)	(0.407, 0.428)
6	(0.360, 0.456)	(0.372, 0.436)	(0.386, 0.442)	(0.402, 0.453)
7	(0.351, 0.426)	(0.370, 0.441)	(0.384, 0.447)	(0.390, 0.455)
8	(0.365, 0.442)	(0.373, 0.445)	(0.389, 0.449)	(0.415, 0.445)

$$(M_B)_{nm} = (u_n^{-\alpha},\ (E + B - H_0)u_m^{\alpha}) ,$$

$$V_{lm}^{nj} = (u_n^{\alpha},\ V_{12}u_j^{\alpha}) ,$$

$$V_{21}^{lm} = (u_l^{-\alpha},\ V_{21}u_j^{-\alpha}) .$$

We have calculated J^N for the case of a square-well potential used by Rescigno and Reinhardt[1] and find a result similar to that of our previous calculations. The sequence of approximations appears to be converging but then diverges (Fig. 6). When a potential of the form $(r+1)^{-2}$ was used, no sign of convergence was found, and for larger angles of rotation there was a rapid divergence.

A calculation using complex basis functions of the first term in the Fredholm determinant expansion $\mathrm{Tr}(G_0V)$ is also instructive. With a square-well potential we could not see convergence, which indicates that the Fredholm method with complex basis functions might not work even for one-channel scattering in this case. Presumably, the singularity in the potential is to blame. For a long-range potential without real singularity, $(r+1)^{-2}$, the same method gave results for $\mathrm{Tr}(G_0V)$ that may be very slowly converging.

The difficulties we have raised here about using the Fredholm method with complex basis functions to perform calculations with several open channels appear to call into question the results of Rescigno and Reinhardt[4] on e-H elastic scattering above the ionization threshold. However, in spite of the way in which these authors describe their calculation, referring to the many-channel part of Ref. 1, it may be thought of as a one-channel calculation using an optical potential obtained by a different method (extrapolation), and therefore it could well be legitimate. Indeed, it agrees with previous results.[3]

The main advantage of the method of complex basis functions (when it works) is that, in addition to the elimination of the need for open-channel descriptions, the amplitude is obtained as the result of a single sequence of approximations. In the alternative method of extrapolation from complex energies[3] a double limit must be taken. It is therefore of interest to point out that, in the model problems we have discussed, a single limiting procedure can be devised which gives a sequence of approximations converging to I. In the Appendix we sketch a proof of the result that, if $N(\alpha) = (\epsilon/\alpha)\ln(\epsilon/\alpha)$, when ϵ is a suitably chosen constant, then $I_{N(\alpha)} \to I$ as $\alpha \to 0$ for any of the six possible forms of I discussed previously. For the case of $f = g = g_2$, it is possible to choose $N(\alpha)$ to have the form $N(\alpha) = \epsilon/\alpha^2$.

It is likely that this result generalizes to cases of more practical interest. If so, it would be helpful to know which form of $N(\alpha)$ leads to the highest rate of convergence.

ACKNOWLEDGMENTS

The authors are grateful to Dr. G. D. Doolen and Dr. R. W. Stagat for helpful discussions and for much assistance with the computer program used to calculate e-H scattering.

APPENDIX

We consider the expression (20) for I_N and assume that positive constants A, β, c may be found such that

$$|\bar{f}_n|\ ,\ |\bar{g}_n| \leq An^{-\beta}e^{c\alpha n} ,$$

$$|e_n| \leq A(n^{-\beta}e^{c\alpha n} + |\nu_2^{-n}|) .$$

These properties hold for all the cases of the model discussed above.

We may prove that a positive constant ϵ may be found so that, with

$$N(\alpha) = (\epsilon/\alpha)\ln(\epsilon/\alpha) ,$$

$$I_{N(\alpha)} \to I .$$

The basic elements of the proof are the following observations, which are not difficult to verify:

(i) As $\alpha \to 0$, $\bar{f}_n \to \bar{f}_n^0$, $e_n \to e_n^0$ for fixed n, where the quantities $\bar{f}_n^0$, e_n^0 are related to I by the convergent series

$$I = \sum_{n=0}^{\infty} \bar{f}_n^0 e_n^0 (n+1)^{-1} .$$

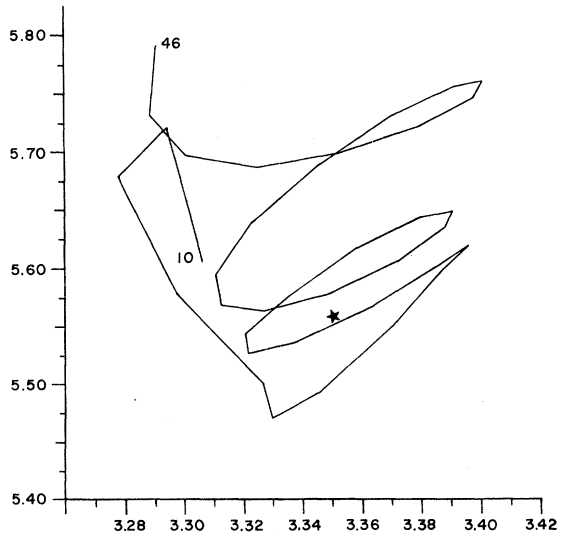

Fig. 6. Plot in the complex plane showing values of J^N for $N = 10$–46 in the case $E = 1.0$, $B = 0.375$, $\alpha = 0.3$, $a = 1$, with potential $V_{21}(r) = V_{12}(r) = 1$, $r \leq 3$, and $V_{21} = V_{12} = 0$, $r \geq 3$. The correct result is shown by a star.

(ii) If $\epsilon < \beta/c$, then $\lambda_{N(\alpha)} \to 0$ as $\alpha \to 0$. This follows because constants A' and c' independent of α may be found so that $|d_n| \geq A' e^{c'\alpha n}$.

(iii) Define

$$\gamma_n(\alpha) = (\lambda_{N(\alpha)} d_n + e_n)\bar{f}_n(n+1)^{-1}, \quad n < N(\alpha)$$
$$= 0, \quad n \geq N(\alpha) ,$$

so that

$$I_{N(\alpha)} = \sum_{n=0}^{\infty} \gamma_{n(\alpha)} .$$

Then as $\alpha \to 0$, $\gamma_n(\alpha) \to \gamma_n = \bar{f}_n^0 e_n^0 (n+1)^{-1}$.

(iv) For $\alpha < \alpha'$, $n > n'$, where α' and n' depend on ϵ, there is a constant C such that

$$|\gamma_n(\alpha)| \leq C n^{-1-\beta+c\epsilon} .$$

Thus, provided $\epsilon < \beta/c$, the dominated convergence theorem shows that, as $\alpha \to 0$,

$$I_{N(\alpha)} = \sum_{n=0}^{\infty} \gamma_n(\alpha) \to \sum_{n=0}^{\infty} \gamma_n = I .$$

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*Supported in part by the National Research Council of Canada and in part by the Centre for Interdisciplinary Studies in Chemical Physics, University of Western Ontario.

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