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Observation of Padé summability in divergent L^2 complex coordinate calculations of t-matrix amplitudes in the presence of long-range forces

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The method of complex coordinates has long been known to allow L^2 calculations of t-matrix amplitudes for short-range potentials, but to yield divergent results for long-range forces. Using a spherical long-range potential as an example, it is shown here that the Padé method of summation can be used in conjunction with the diverging complex-coordinate calculations to obtain accurate values of the scattering amplitude.

We report the finding that, contrary to earlier expectations,[1,2] on-shell free-free t-matrix elements for long-range potentials may be evaluated by complex scaling techniques.[3] Considering scattering from a cut-off polarization potential,

$$V(r)=\frac{V_0(e^{-\gamma r}-1)^3}{r^4} \quad , \tag{1}$$

which was recently used in a related application of complex coordinates to the calculation of bound-free amplitudes,[4] we demonstrate the calculation of the p-wave contribution to the elastic amplitude $\langle\vec{k}|T(z)|\vec{k}\rangle$, where $|\vec{k}\rangle$ corresponds to a plane wave and $T(z)$ is the usual T operator.[5] Using only L^2 functions, results are directly obtained in the $z=E+i\epsilon$ limit as the (discretized) cut of the off-shell amplitude is rotated off the real axis.

The p-wave amplitude calculated here is $\langle\hat{j}_l|t_l|\hat{j}_l\rangle$, where $\hat{j}_l(kr)$ is a Ricatti-Bessel function[5] and $t_l(z)$, the partial-wave t operator, is given by

$$t_l(z)=V+V(z-H_l)^{-1}V \quad , \tag{2}$$

$$H_l=-\frac{1}{2}\frac{d^2}{dr^2}+\frac{l(l+1)}{2r^2}+V(r) \quad . \tag{3}$$

The Born term $\langle\hat{j}_l|V|\hat{j}_l\rangle$ is easy enough to evaluate numerically, but the integral

$$I=\langle\hat{j}_l|V(z-H_l)^{-1}V|\hat{j}_l\rangle \quad , \tag{4}$$

poses more difficulty in the limit $z\to E+i\epsilon$ if E is the spectrum of H_l. It is known that such integrals can be computed by complex scaling and finite basis (L^2 discretization) techniques provided V decays exponentially,[1] but that results diverge with increasing basis size for potentials of longer range.[2] The purpose of this Rapid Communication is to point out that these divergent results can be summed to yield the correct elastic amplitude by the technique of Padé approximants.[6]

For short-range (i.e., exponentially bounded) potentials V, the scaling $r\to re^{i\theta}$ transforms I into

$$I=\langle\hat{j}_{l\theta}|V_\theta(z-H_{l\theta})^{-1}V_\theta|\hat{j}_{l\theta}\rangle \quad , \tag{5}$$

where

$$\hat{j}_{l\theta}(kr)=e^{i\theta/2}\hat{j}_l(kre^{i\theta}) \quad , \tag{6}$$

$$V_\theta(r)=V(re^{i\theta}) \quad , \tag{7}$$

and

$$H_{l\theta}=-\tfrac{1}{2}e^{-2i\theta}\frac{d^2}{dr^2}+e^{-2i\theta}\frac{l(l+1)}{2r^2}+V_\theta(r) \quad . \tag{8}$$

Insertion of a resolution of the identity in terms of a complete discrete (L^2) set of basis function $\phi_n(r)$ then yields

$$I_N=\sum_{n,n'=0}(\langle\hat{j}_{l\theta}|V_\theta|\phi_n\rangle \times\langle\phi_n|(z-H_{l\theta})^{-1}|\phi_{n'}\rangle\langle\phi_{n'}|V_\theta|\hat{j}_{l\theta}\rangle) \quad . \tag{9}$$

The efficacy of this procedure is that, if $V_\theta(r)\hat{j}_{l\theta}(kr)$ decays exponentially as $r\to\infty$, the sums over n and n' can be truncated for practical purposes if an appropriately chosen basis is used. The intermediate matrix elements above are calculated by diagonalizing (only once for all k) the complex Hamiltonian $H_{l\theta}$ in this truncated basis. In terms of the resulting eigenvalues $E_{i\theta}$ and eigenvectors $\chi_{i\theta}$,

$$\langle\phi_n|(z-H_{l\theta})^{-1}|\phi_{n'}\rangle\simeq\sum_i\frac{\langle\phi_n|\chi_{i\theta}\rangle\langle\phi_{n'}|\chi_{i\theta}\rangle}{z-E_{i\theta}} \quad . \tag{10}$$

Numerically, the eigenvalues that lie upon the positive real axis for $\theta=0$ are swept down into the complex E plane for nonzero θ, making the $z\to E+i\epsilon$ ($E=k^2/2$) limit simple to implement. For example, Nuttall and Cohen[1] have used this method successfully for n-d s-wave scattering using short-range interaction potentials.

If, as is the case here, one is interested in calculating elastic amplitudes in the presence of long-range forces, there appears to be an immediate problem. The function $\hat{j}_l$ is a

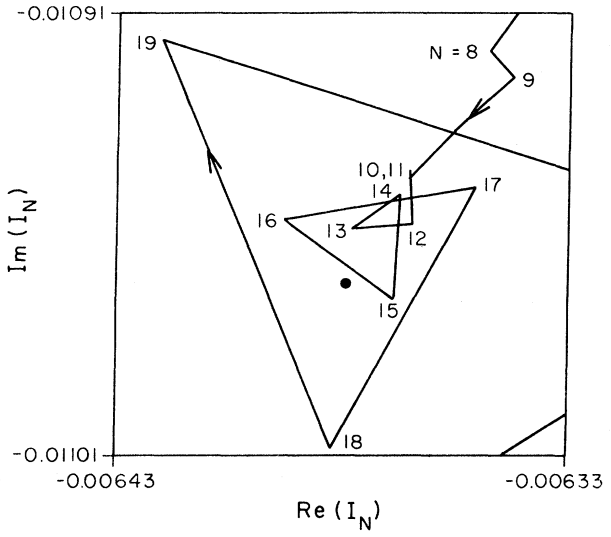

FIG. 1. Behavior of amplitudes I_N for $V_0=1$, $\gamma=1$, and $k=1$. The numbers indicate the size of the Laguerre-type basis of order 4 and scale factor 3 (see Ref. 4). The angle of rotation is $\theta=25°$. Note the approximate stationarity near the accurate amplitude (represented by the dot) for a limited range of N.

TABLE I. Diagonal $[N,N]$ Padé approximants for I_N formed from calculations using up to 40 basis functions. Parameters correspond to those in Fig. 1.

N	$[N,N]$	
0	−0.006 229 388	$-i$0.009 092 146
1	−0.005 705 158	$-i$0.010 671 417
2	−0.006 252 684	$-i$0.010 955 857
3	−0.006 332 018	$-i$0.010 954 464
4	−0.006 363 595	$-i$0.010 951 759
5	−0.006 371 141	$-i$0.010 962 266
6	−0.006 378 530	$-i$0.010 963 081
7	−0.006 377 443	$-i$0.010 968 467
8	−0.006 377 228	$-i$0.010 968 465
9	−0.006 378 699	$-i$0.010 970 399
10	−0.006 378 950	$-i$0.010 970 626
11	−0.006 379 050	$-i$0.010 970 911
12	−0.006 379 415	$-i$0.010 971 433
13	−0.006 379 203	$-i$0.010 971 326
14	−0.006 379 166	$-i$0.010 971 423
15	−0.006 379 279	$-i$0.010 971 503
16	−0.006 379 281	$-i$0.010 971 571
17	−0.006 379 275	$-i$0.010 971 557
18	−0.006 379 297	$-i$0.010 971 577
19	−0.006 379 305	$-i$0.010 971 533

linear combination of incoming and outgoing spherical waves (Ricatti-Hankel functions), and, upon rotation, one of the latter diverges asymptotically as $e^{kr\sin\theta}$. Thus, unless the potential decays exponentially, the t-matrix elements are expressed in terms of a seemingly divergent integral. This is a serious handicap to what would otherwise be a clean and logical answer to the problem[7] associated with using real finite-basis t-matrix methods in the $E+i\epsilon$ limit in the presence of long-range forces appropriate to e^--atom scattering.

In the calculations, of course, the component matrix elements $\langle\phi_n|V_\theta|\hat{j}_{l\theta}\rangle$ in Eq. (9) can all be made finite by proper choice of the L^2 functions $\phi_n(r)$ (here a Laguerre-type basis as described in Ref. 4). It is intuitively reasonable, however, that the amplitudes calculated for long-range potentials as in (1) will not converge. This was indicated by the results of Baumel, Crocker, and Nuttall,[2] who found that such expansions in the long-range case may hover or spiral around the correct answer, but will eventually diverge for large enough basis size. This has prevented the use of complex coordinates in the calculation of elastic and inelastic electron-atom amplitudes via t-matrix methods.

Precisely as in Ref. 2, the results for the present example do indeed diverge as a function of N. Figure 1 shows a representative sequence of amplitudes for I_N. The calculated amplitudes slow down in the neighborhood of the exact one for a limited range of basis size, then spiral away with increasing N. This behavior resembles that of an asymptotic expansion. Our treatment of a similarly spiralling amplitude for bound-free transitions in Ref. 4 suggested that Padé approximants formed from the present divergent sequence might be well behaved. Given the calculated quantities I_N one uses Wynn's identity[6] to form the corresponding Padé approximants, or Shanks' extrapolants, of the sequence. The diagonal approximants $[N,N]$, which are ratios of polynomials of order N, are listed in Table I for a particular momentum magnitude k.

It is seen that straightforward convergence with increasing N is obtained. In Table II we compare the resulting matrix elements with those obtained by stopping at the point of

TABLE II. Comparison of phase shifts calculated from t-matrix extrapolants of present paper, wave-operator methods of Ref. 4, and exact answers.

						Phase shifts (modulo π)			
k	$\langle\hat{j}_1\|V\|\hat{j}_1\rangle$ [a]	I_N [b]		I_N [c]		δ_I [d]	δ_{II} [e]	δ_{III} [f]	δ_{exact} [a]
0.5	−0.014 914 36	−0.001 373 8	$-i$ 0.001 064 9	−0.001 375 39	$-i$ 0.001 065 94	0.065 343	0.065 344	0.065 344	0.065 344 3
1.0	−0.066 870 2	−0.006 366	$-i$ 0.010 948	−0.006 379 3	$-i$ 0.010 971 5	0.148 677	0.148 679	0.148 680	0.148 680
1.5	−0.134 983 5	−0.009 18	$-i$ 0.028 62	−0.009 241 7	$-i$ 0.028 843 0	0.197 382	0.197 385	0.197 385	0.197 387
2.0	−0.204 881	−0.008 90	$-i$ 0.047 36	−0.008 936	$-i$ 0.048 022	0.220 928	0.220 932	0.220 931	0.220 937
2.5	−0.271 28	−0.006 97	$-i$ 0.062 78	−0.006 99	$-i$ 0.065 35	0.230 66	0.230 69	0.230 70	0.230 711

[a] From numerical integration.
[b] From truncation before smallest term.
[c] From extrapolants using up to 40 basis functions.
[d] From $\arg(\langle\hat{j}_1|t_l|\hat{j}_1\rangle)$, calculated via Padé extrapolation.
[e] From $\mathrm{Im}(\langle\hat{j}_1|t_l|\hat{j}_1\rangle) = (-k/2)\sin^2\delta$, via Padé extrapolation.
[f] From methods of Ref. 2.

slowest change with increasing basis size (as for asymptotic expansions where one truncates just before the smallest term in the expansion). The results from the approximants, coupled with the numerically integrated results for the Born terms, allow evaluation of the p-wave t-matrix elements through Eq. (2). These are related to the phase shift δ by

$$\langle \hat{j}_l | t_l | \hat{j}_l \rangle = \frac{k}{2} e^{-i\delta} \sin\delta \ . \tag{11}$$

Conservation of unitarity is determined by comparison of the phase shift calculated from the argument of the t matrix to that calculated from the imaginary part alone. For further comparison, the phase shifts calculated by the wave operator methods of Ref. 4 are presented. All three of these determinations are in excellent agreement with the results of numerical integration.

We have demonstrated that apparent divergences in long-range complex coordinate scattering calculations are not as crippling as at first supposed. The approximants calculated have been shown capable of bringing the divergence with increasing basis dimensionality N under control and of yielding quantitative results. While the current method of calculation may not be the most economical, we feel that an extension of the present results may eventually lead to development of techniques for direct calculation of free-free matrix elements for more complicated systems, and in particular for calculation of *inelastic* electron-atom scattering amplitudes at intermediate energies where t matrix and Fredholm L^2 methods have failed.[8] Finally, it is to be noted that we do not, as yet, fully understand the relationship of the present results to the usual analyticity arguments used to justify use of complex coordinate techniques.[9]

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[8]F. A. McDonald and J. Nuttall, Phys. Rev. Lett. 23, 361 (1969); F. A. McDonald and J. Nuttall, Phys. Rev. A 4, 1821 (1971); and T. N. Rescigno and W. P. Reinhardt, *ibid.* 10, 158 (1974), report successful calculations of elastic e^--atom amplitudes at intermediate energies: however, none of these techniques has been able to produce, say, the $e^- + H(1s) \rightarrow e^- + H(2p)$ amplitude, due either to analyticity constraints as discussed in Ref. 7, or to the divergence discussed in Ref. 2.

[9]It is important to note that the Padé summations were only found to succeed when the t-matrix elements were taken between the regular Ricatti-Bessel functions $\hat{j}_l(kr)$. If these functions are decomposed into spherically incoming and outgoing waves, the amplitude I in Eq. (5) becomes the sum of four terms, each of which may be treated by the method described above. However, when they were examined (for $k=1$), none of the resulting series of approximants was found to converge, and the component integrals which were (formally) exponentially growing and decaying exhibited very similar behavior.