JOURNAL OF COMPUTATIONAL PHYSICS 21, 38–54 (1976)

Numerical Evaluation of Partial-Wave Born Approximations

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Received August 13, 1975

A method is developed for the numerical evaluation of any term in the Born series for the off-shell partial-wave T matrix. At negative energies, the integrals may be evaluated by using any appropriate quadrature formula. Numerical analytic continuation of the negative energy results to positive energies is carried out by means of Padé approximants. The method enables the rate of convergence of eigenfunction expansions for the two-body off-shell amplitude to be accelerated. Numerical results are presented for a Yukawa potential and for a neutron–proton $^3S_1$ interaction.

1. INTRODUCTION

In a previous paper [1], an eigenfunction expansion, separable in the off-shell momenta, was derived for the two-body partial-wave T matrix. It was found from calculations that the rate of convergence of this expansion was often slow. However, it was also shown that the rate of convergence could be improved by extracting the first few Born approximations and then evaluating the off-shell amplitude by employing a modified form of the eigenfunction expansion.

In this paper, a method is developed for the numerical evaluation of any term in the partial-wave Born series at either positive or negative energies. The nth Born approximation is defined recursively in terms of the $(n-1)$th Born approximation via a one-dimensional integral. At negative energies, the numerical integration may be carried out by using any appropriate quadrature formula such as a Gauss formula or a self-correcting application of Simpson's rule. A numerical analytic continuation of the negative energy results to positive energies through the upper half k^2 plane (k^2 being the energy in the center of mass frame) is then performed by means of Padé approximants satisfying the required high-energy behavior. This approach avoids the problems associated with singular integrals at positive energies.

In Section 2, a brief summary of relevant results obtained in a previous paper [1] is given, and it is shown how the separable eigenfunction expansion for the two-

body off-shell partial-wave amplitude is modified to various nonseparable forms as Born approximations of increasing order are introduced.

In Section 3, the integral defining a recurrence relation between the $(n-1)$th and nth Born approximations is transformed to a form which, at negative energies, enables the numerical integration to be carried out very easily by applying any appropriate quadrature formula. A Padé approximant, that is valid at both positive and negative energies and that satisfies a specified high energy limit, is then presented for the nth Born approximation. This approximant enables a numerical analytic continuation of the negative energy results to positive energies to be performed.

Section 4 contains numerical results for an attractive Yukawa potential that does not form any bound states or resonances and for a neutron–proton triplet S-state interaction consisting of a sum of attractive and repulsive Yukawa potentials.

2. Previous Results and the Nth Born Approximation

The off-shell partial-wave T matrix $T_l(p_1, p_2; k^2)$ satisfies the Lippmann–Schwinger equation

$$T_l(p_1, p_2; k^2) = V_l(p_1, p_2) + \int_0^\infty \frac{V_l(p_1, q)\, T_l(q, p_2; k^2)}{k^2 - q^2 + i\epsilon}\, dq, \tag{2.1}$$

at energy k^2. On the energy shell, the solution of this equation is [1]

$$T_l(k, k; k^2) = -(2k/\pi) \exp(i\delta_l) \sin \delta_l, \tag{2.2}$$

where δ_l is the phase shift with orbital angular momentum l. The two-particle interaction V_l vanishes whenever either of its momentum variables is infinite.

The off-shell amplitude can be represented by the separable eigenfunction expansion

$$T_l(p_1, p_2; k^2) = \frac{2}{\pi} \sum_N \frac{I_N(k, p_1)\, I_N(k, p_2)}{[1 - \eta_N(k^2)]\, M_N(k)}, \tag{2.3}$$

in which

$$I_N(k, p) = \int_0^\infty prj_l(pr)\, V(r)\, u_l(r)\, dr,$$

and (2.4)

$$M_N(k) = \int_0^\infty V(r)\, u_l^2(r)\, dr,$$

where $j_l(pr)$ is a spherical Bessel function of order l, $u_l(r)$ is the radial wave function, and the $\eta_N(k^2)$ are the eigenvalues of the Lippmann–Schwinger kernel. Very detailed descriptions of the methods used to compute the $I_N(k, p)$, $M_N(k)$, and $\eta_N(k^2)$ are given elsewhere [1, 2, 3]. (The methods involve the summation of various asymptotic expansions by means of Padé approximants satisfying specified high energy limits.)

Previously reported results of calculations performed with Yukawa potentials indicated that the rate of convergence of (2.3) may often be slow. However, some improvement is achieved by extracting the first Born approximation to obtain the nonseparable form

$$T_l(p_1, p_2; k^2) = T_l^{(1)B}(p_1, p_2; k^2) + \frac{2}{\pi} \sum_N \frac{\eta_N(k^2)}{1 - \eta_N(k^2)} \frac{I_N(k, p_1)\, I_N(k, p_2)}{M_N(k)}, \quad (2.5)$$

where

$$T_l^{(1)B}(p_1, p_2; k^2) = V_l(p_1, p_2). \quad (2.6)$$

The rate of convergence may be further accelerated by also extracting the second Born approximation to yield

$$T_l(p_1, p_2; k^2) = \sum_{t=1}^{2} T_l^{(t)B}(p_1, p_2; k^2) + \frac{2}{\pi} \sum_N \frac{\eta_N{}^2(k^2)}{1 - \eta_N(k^2)} \frac{I_N(k, p_1)\, I_N(k, p_2)}{M_N(k)}, \quad (2.7)$$

where

$$T_l^{(2)B}(p_1, p_2; k^2) = \int_0^\infty \frac{V_l(p_1, q)\, V_l(q, p_2)}{k^2 - q^2 + i\epsilon}\, dq, \quad (2.8)$$

which has the high-energy limit $T_l^{(2)B} \sim 1/k^2$.

The rate of convergence of the eigenfunction expansions may be continuously improved by introducing Born approximations of higher and higher order. In general, the two-body off-shell amplitude may be computed from the nonseparable series

$$T_l(p_1, p_2; k^2) = \sum_{t=1}^{n} T_l^{(t)B}(p_1, p_2; k^2) + \frac{2}{\pi} \sum_N \frac{\eta_N{}^n(k^2)}{1 - \eta_N(k^2)} \frac{I_N(k, p_1)\, I_N(k, p_2)}{M_N(k)}, \quad (2.9)$$

where, for $n \geqslant 2$,

$$T_l^{(n)B}(p_1, p_2; k^2) = \int_0^\infty \frac{V_l(p_1, q)\, T_l^{(n-1)B}(q, p_2; k^2)}{k^2 - q^2 + i\epsilon}\, dq \quad (2.10)$$

$$= \int_0^\infty \int_0^\infty \cdots \int_0^\infty \frac{V_l(p_1, q_1)\, V_l(q_1, q_2) \cdots V_l(q_{n-1}, p_2)}{(k^2 - q_1{}^2 + i\epsilon_1)(k^2 - q_2{}^2 + i\epsilon_2) \cdots (k^2 - q_{n-1}^2 + i\epsilon_{n-1})} \times dq_1\, dq_2 \cdots dq_{n-1}, \quad (2.11)$$

which has the high energy behavior

$$T_l^{(n)B} \sim 1/k^{2(n-1)}. \tag{2.12}$$

The definition (2.10) of the nth Born approximation is, of course, far more useful for computational work than Eq. (2.11).

Any bound states or resonances formed by the interaction V_l in the lth partial-wave will appear explicitly through the propagator $[1 - \eta_N(k^2)]^{-1}$ in the early terms of each of the eigenfunction expansions in Eqs. (2.3), (2.5), (2.7), and (2.9) [1, 2]. A bound state or resonance is formed whenever

$$\eta_N(0) \geqslant 1, \qquad \eta_N(k^2) = 1, \tag{2.13}$$

for a given l [4]. Thus, all the terms satisfying this condition must be included in the above eigenfunction expansions to preserve the correct analytic properties of the T matrix. Furthermore, all the terms for which

$$|\eta_N(k^2)| \geqslant 1 \tag{2.14}$$

also must be taken. For sufficiently large n in (2.9), there is obviously no need to consider any term with

$$|\eta_N(k^2)| < 1, \qquad \text{for all } k^2, \tag{2.15}$$

but several such terms usually have to be included in the separable expansion (2.3) for the latter to converge. Calculations have shown that, at high energies, the rate convergence of (2.3) is extremely slow [2].

3. Evaluation of The Nth Born Approximation

At negative definite energies, the transformation

$$q = x/(1 - x), \tag{3.1}$$

which maps the interval $0 \leqslant q \leqslant \infty$ onto the interval $0 \leqslant x \leqslant 1$, can be substituted into Eq. (2.10) to yield

$$T_l^{(n)B}(p_1, p_2; k^2) = \int_0^1 \frac{V_l(p_1, q)\, T_l^{(n-1)B}(q, p_2; k^2)}{(k^2 - q^2)(1 - x)^2}\, dx, \tag{3.2}$$

in which V_l has a zero of order at least 2 since the integral in (2.10) exists. As the integrand does not contain a singularity within the range of integration when $k^2 < 0$ this integral may be evaluated by employing any appropriate numerical

integration procedure such as a Gauss quadrature formula or a self-correcting application of Simposon's rule. It is fairly easy to program a self-correcting procedure (i.e., an adaptive quadrature method) to evaluate Eq. (3.2) for general n if use is made of the recursion facility and Jensen's device in ALGOL 60 [5]. It has been found that such a procedure requires very little computer time to perform the numerical integrations for the second and third Born approximations over a range of negative energies, but that a substantial amount of time is needed to compute higher-order negative energy Born approximations.

A faster alternative to the use of an automatically self-correcting numerical integration procedure is to evaluate the negative energy $T_l^{(n)B}$ by employing a quadrature formula of the form

$$T_l^{(n)B}(q_t, p; k^2) = \sum_{m=0}^{M} w_m \frac{V_l(q_t, q_m)\, T_l^{(n-1)B}(q_m, p; k^2)}{(k^2 - q_m^2)(1 - x_m)^2}, \tag{3.3}$$

for $t = 0, 1, 2, \ldots, M$, particularly when $n \geqslant 4$. The weights w_m and pivotal points $x_m (m = 0, 1, 2, \ldots, M)$ are determined by the chosen quadrature formula.

In view of the high energy limit (2.12), the nth Born approximation can be represented at both positive and negative energies by an $[m + 2n - 2, m]$ Padé approximant [6, 7, 8]

$$T_l^{(n)B}(p_1, p_2; k^2) \approx P_m(K)/Q_{m+2n-2}(K) = \left(\sum_{t=0}^{m} a_t K^t\right) \Big/ \left(\sum_{t=0}^{m+2n-2} b_t K^t\right), \tag{3.4}$$

in which $K = ik$, and where the coefficients a_t and b_t are functions of p_1 and p_2. If the recurrence relation (3.2) is employed to compute the nth Born approximation at $(2m + 2n - 1)$ negative energy values for a given pair of off-shell momenta, the curve passing through these points can be fitted by means of the approximant (3.4) by using the method described in a previous paper [3]. After the polynomial coefficients a_t and b_t have been determined, this Padé approximant can be employed to perform a numerical analytic continuation of the nth Born approximation (for the same pair of off-shell momenta) from negative energies to positive energies through the upper half k^2-plane because such approximants preserve analytic properties of functions such as poles and zeros.

It should be noted that the sum of all the terms in any of the series (2.3), (2.5), (2.7), or (2.9) for the two-particle off-shell amplitude may be represented by an $[m, m]$ Padé approximant [9, 10, 11]. The positions of the zeros of the denominator polynomial $Q_m(K)$ will determine whether the T matrix has any bound state or resonance poles.

4. Applications of the Method

Computer calculations have been performed with interactions of the form

$$V_l(p_1, p_2) = \sum_t \frac{A_t}{\pi} Q_l\left(\frac{p_1^2 + p_2^2 + \mu_t^2}{2p_1 p_2}\right), \tag{4.1}$$

where $Q_l(...)$ is a Legendre function of order l of the second kind. In the coordinate representation, this potential has the well-known form

$$V(r) = \sum_t A_t \exp(-\mu_t r)/r. \tag{4.2}$$

The method of evaluating the nth Born approximation, described in the previous section, was first tested on the attractive Yukawa potential $V(r) = -\exp(-r)/r$ for which results concerning the phase shift δ_l, the eigenvalues $\eta_N(k^2)$, and the $I_N(k, p)$ and $M_N(k)$ are already available [1, 2, 3].

Table I contains values of the first five S-wave Born approximations at negative energies, with $p_1 = p_2 = 1$, computed from Eq. (3.2) (via a self-correcting procedure for $T_0^{(2)B}$ and $T_0^{(3)B}$, and via Eq. (3.3) for $T_0^{(4)B}$ and $T_0^{(5)B}$). These results were fitted by the $[m + 2n - 2, m]$ Padé approximant (3.4) in the variable $K = ik$, for $n = (2, 3, 4, 5)$, in order to perform numerical analytic continuations of the various Born approximations from negative energies to positive energies; positive and negative energy results obtained from the fits are presented in Tables II and III.

The rate of convergence of the Padé approximants for the second and third Born approximations is displayed in Tables IV and V. It can be clearly seen that the $[m + 2, m]$ approximant for $T_0^{(2)B}$ converges extremely rapidly as m increases, while the rate of convergence of the $[m + 4, m]$ approximant for $T_0^{(3)B}$ is a little less rapid. Further calculations have shown that the rate of convergence of the $[m + 2n - 2, m]$ Padé approximant (3.4) becomes slower as the order n of the Born approximation $T_l^{(n)B}$ increases. This deterioration in the rate of convergence is probably due to the increasing complexity of the high-energy limit (2.12), which is a property of approximant (3.4).

A simple check can be carried out to determine the accuracy of the imaginary part of the second S-wave Born approximation computed at positive energies from the $[m + 2, m]$ approximant. By extracting the principal value integral, Eq. (2.8) may be rewritten in the form

$$T_l^{(2)B}(p_1, p_2; k^2) = P\int_0^\infty \frac{V_l(p_1, q)\, V_l(q, p_2)}{k^2 - q^2}\, dq - \frac{i\pi}{2k} V_l(p_1, k)\, V_l(k, p_2), \tag{4.3}$$

TABLE I

The First Five S-wave Born Approximations at Negative Energies[a]

	$T_0^{(n)B}$				$\sum_{n=1}^{5} T_0^{(n)B}$
$-ik$	$(n = 2)$	$(n = 3)$	$(n = 4)$	$(n = 5)$	
0.2	−0.111968	−0.052230	−0.024534	−0.011548	−0.456430
0.4	−0.091023	−0.034875	−0.013560	−0.005296	−0.400904
0.6	−0.075039	−0.024270	−0.008050	−0.002696	−0.366203
0.8	−0.062685	−0.017457	−0.005044	−0.001476	−0.342812
1.0	−0.053007	−0.012903	−0.003300	−0.000861	−0.326221
1.2	−0.045321	−0.009760	−0.002236	−0.000523	−0.313990
1.4	−0.039137	−0.007531	−0.001561	−0.000332	−0.304711
1.6	−0.034102	−0.005912	−0.001118	−0.000219	−0.297501
1.8	−0.029954	−0.004712	−0.000819	−0.000147	−0.291782
2.0	−0.026504	−0.003806	−0.000613	−0.000102	−0.287175
2.2	−0.023605	−0.003111	−0.000464	−0.000072	−0.283402
2.4	−0.021149	−0.002570	−0.000357	−0.000052	−0.280278
2.6	−0.019051	−0.002144	−0.000279	−0.000038	−0.277662
2.8	−0.017246	−0.001804	−0.000221	−0.000028	−0.275449
3.0	−0.015682	−0.001530	−0.000176	−0.000022	−0.273560
3.2	−0.014320	−0.001307	−0.000142	−0.000017	−0.271936
3.4	−0.013126	−0.001124	−0.000116	−0.000013	−0.270529
3.6	−0.012074	−0.000972	−0.000095	−0.000010	−0.269301
3.8	−0.011142	−0.000846	−0.000079	−0.000008	−0.268225
4.0	−0.010313	−0.000740	−0.000066	−0.000006	−0.267275

[a] With $p_1 = p_2 = 1$, computed from Eq. (3.2) for the potential $V(r) = -\exp(-r)/r$. The value of leading Born approximation is $V_0(1, 1) = -0.256150$.

from which we obtain [for $V(r) = -\exp(-r)/r$]

$$\text{Im } T_0^{(2)B}(1, 1; 0.25) = -\frac{1}{0.5 \times 8\pi}\left[\log\left(\frac{3.25}{1.25}\right)\right]^2 = -0.072654,$$

$$\text{Im } T_0^{(2)B}(1, 1; 1) = -\frac{1}{8\pi}(\log 5)^2 = -0.103065,$$

$$\text{Im } T_0^{(2)B}(1, 1; 2.25) = -\frac{1}{1.5 \times 8\pi}\left[\log\left(\frac{7.25}{1.25}\right)\right]^2 = -0.081961,$$

$$\text{Im } T_0^{(2)B}(1, 1; 4) = -\frac{1}{16\pi}(\log 5)^2 = -0.051532.$$

TABLE II

The Second and Third S-wave Born Approximations[a]

	$T_0^{(2)B}(1,1;k^2)$			$T_0^{(3)B}(1,1;k^2)$		
k	(Re $T(k^2)$)	(Im $T(k^2)$)	($T(-k^2)$)	(Re $T(k^2)$)	(Im $T(k^2)$)	($T(-k^2)$)
0.0	−0.1397	0	−0.1397	−0.0826	0	−0.0826
0.1	−0.1386	−0.0159	−0.1248	−0.0794	−0.0199	−0.0652
0.2	−0.1352	−0.0314	−0.1120	−0.0702	−0.0373	−0.0522
0.3	−0.1296	−0.0463	−0.1008	−0.0571	−0.0502	−0.0424
0.4	−0.1219	−0.0602	−0.0910	−0.0419	−0.0582	−0.0349
0.5	−0.1122	−0.0726	−0.0825	−0.0267	−0.0615	−0.0290
0.7	−0.0879	−0.0920	−0.0685	−0.0004	−0.0572	−0.0205
1.0	−0.0458	−0.1030	−0.0530	0.0222	−0.0369	−0.0129
1.5	0.0060	−0.0819	−0.0365	0.0232	−0.0065	−0.0067
2.0	0.0229	−0.0516	−0.0265	0.0125	0.0033	−0.0038
2.5	0.0238	−0.0315	−0.0201	0.0058	0.0042	−0.0023
3.0	0.0205	−0.0198	−0.0157	0.0027	0.0033	−0.0015
4.0	0.0140	−0.0091	−0.0103	0.0006	0.0017	−0.0007
5.0	0.0097	−0.0048	−0.0073	0.0001	0.0009	−0.0004

[a] With $p_1 = p_2 = 1$, computed respectively from [10,8] and [10,6] Padé approximants in the variable $K = ik$ fitted to the results of Table I for the potential $V(r) = -\exp(-r)/r$.

It can be seen from Tables II and IV that the results for $k = 0.5$, 1.0, 1.5, and 2.0 are in very close agreement with the above exact results. Thus, we may be confident that the Padé approximant (3.4) provides a simple reliable representation and numerical analytic continuation of at least the second Born approximation, and also probably of high-order Born approximations too. However, the zero energy value of the fifth S-wave Born approximation obtained from the [10, 2] approximant appears to be incorrect because its magnitude should be smaller than that of the fourth Born approximation at that energy.

An indirect check can be carried out to estimate the accuracy of the third, fourth, and fifth S-wave Born approximations computed from both Eqs. (3.2) and (3.4). Table VI compares two methods of evaluating the sum of the first five S-wave Born approximations at positive and negative energies. In one of the methods a [9, 9] Padé approximant in the variable $K = ik$ was fitted to the negative energy sums of the first five Born approximations displayed in the final column of Table I. In the other method, the sum was determined directly from the results

in Tables II and III. It can be seen that both methods yield identical results at almost every point at negative energies, while at positive energies, there is fairly good agreement at most points. We shall now compare the on-shell results of Table VI, i.e., the sums at $k = 1$, against the value of the on-shell S-wave T matrix obtained from Eq. (2.2). As the S-wave phase shift of $V(r) = -\exp(-r)/r$ at $k = 1$ is $\delta_0 = 27.51°$ [1], we find that

$$T_0(1, 1; 1) = -0.261 - 0.136i.$$

The on-shell sum computed from the [9, 9] approximant is closer to this result than the sum determined directly from the on-shell values in Tables II and III. In the first method of summation the errors in the numerical analytic continuation arise only from the [9, 9] approximant, while in the second method each of the four Padé approximants employed to yield the results of Tables II and III contributes to the errors in the analytic continuation.

TABLE III

The Fourth and Fifth S-wave Born Approximations[a]

	$T_0^{(4)B}(1,1;k^2)$			$T_0^{(5)}(1,1;k^2)$		
k	(Re $T(k^2)$)	(Im $T(k^2)$)	($T(-k^2)$)	(Re $T(k^2)$)	(Im $T(k^2)$)	($T(-k^2)$)
0.0	−0.04948	0	−0.04948	−0.078788	0	−0.078788
0.1	−0.04468	−0.01820	−0.03423	−0.009841	−0.020409	−0.019863
0.2	−0.03293	−0.03087	−0.02453	−0.006461	−0.011668	−0.011548
0.3	−0.01900	−0.03660	−0.01805	−0.007628	−0.008642	−0.007665
0.4	−0.00599	−0.03681	−0.01356	−0.012064	−0.004800	−0.005296
0.5	0.00483	−0.03314	−0.01037	−0.009770	0.007510	−0.003741
0.7	0.01743	−0.01912	−0.00633	0.000769	0.002906	−0.001977
1.0	0.01506	−0.00103	−0.00330	0.000626	0.000528	−0.000861
1.5	0.00472	0.00391	−0.00132	0.000199	−0.000050	−0.000270
2.0	0.00121	0.00320	−0.00061	0.000026	−0.000048	−0.000102
2.5	−0.00077	0.00221	−0.00032	−0.000001	−0.000016	−0.000044
3.0	−0.00107	0.00037	−0.00018	−0.000002	−0.000005	−0.000024
4.0	−0.00016	−0.00007	−0.00007	−0.000001	−0.000001	−0.000006
5.0	−0.00004	−0.00003	−0.00003	−0.000000	−0.000000	−0.000002

[a] With $p_1 = p_2 = 1$, computed respectively from [10,4] and [10,2] Padé approximants in the variable $K = ik$ fitted to the results of Table I for the potential $V(r) = -\exp(-r)/r$.

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TABLE IV

Rate of Convergence of the $[m + 2, m]$ Padé Approximant at Positive Energies for $T_0^{(2)B}(1, 1; k^2)$[a]

k	[10,8]		[9,7], [8,6], [7, 5]		[6,4]		[5,3], [4,2]		[3,1]		[2,0]	
	(Re T)	(Im T)	(Re T)	(Im T)	(Re T)	(Im T)	(Re T)	(Im T)	(Re T)	(Im T)	(Re T)	(Im T)
0.0	−0.13969	0	−0.13969	0	−0.13969	0	−0.13970	0	−0.13970	0	−0.13965	0
0.5	−0.11219	−0.07265	−0.11221	−0.07264	−0.11221	−0.07264	−0.11224	−0.07264	−0.11224	−0.07264	−0.11222	−0.07283
1.0	−0.04580	−0.10305	−0.04578	−0.10306	−0.04578	−0.10306	−0.04572	−0.10306	−0.04571	−0.10306	−0.04545	−0.10279
1.5	0.00602	−0.08194	0.00600	−0.08191	0.00601	−0.08192	0.00597	−0.08185	0.00597	−0.08184	0.00572	−0.08152
2.0	0.02292	−0.05160	0.02290	−0.05161	0.02290	−0.05161	0.02284	−0.05163	0.02283	−0.05163	0.02250	−0.05164

[a] For the potential $V(r) = -\exp(-r)/r$.

TABLE V

Rate of Convergence of the $[m + 4, m]$ Padé Approximant at Positive Energies for $T_0^{(3)B}(1, 1; k^2)$[a]

k	[10,6]		[9,5]		[8,4]		[7,3]	
	(Re T)	(Im T)	(Re T)	(Im T)	(Re T)	(Im T)	(Re T)	(Im T)
0.0	−0.08265	0	−0.08265	0	−0.08268	0	−0.08268	0
0.5	−0.02667	−0.06148	−0.02667	−0.06148	−0.02674	−0.06139	−0.02673	−0.06140
1.0	0.02217	−0.03690	0.02215	−0.03688	0.02228	−0.03709	0.02227	−0.03707
1.5	0.02325	−0.00652	0.02325	−0.00634	0.02335	−0.00631	0.02333	−0.00633
2.0	0.01246	0.00333	0.01248	0.00333	0.01231	0.00342	0.01232	0.00341

	[6,2]		[5,1]		[4,0]	
	(Re T)	(Im T)	(Re T)	(Im T)	(Re T)	(Im T)
0.0	−0.08270	0	−0.08275	0	−0.08260	0
0.5	−0.02677	−0.06134	−0.02684	−0.06118	−0.02649	−0.06161
1.0	0.02231	−0.03720	0.02241	−0.03751	0.02173	−0.03648
1.5	0.02343	−0.00623	0.02363	−0.00598	0.02299	−0.00598
2.0	0.01226	0.00348	0.01210	0.00365	0.01298	0.00365

[a] For the potential $V(r) = -\exp(-r)/r$.

Hence, if only the sum of the first n Born approximations is required at positive energies rather than the individual Born approximations, then the analytic continuation obtained from a single $[m, m]$ Padé approximant (in the variable $K = ik$) fitted to the negative energy sum of the first n Born approximations is likely to be more accurate than the analytic continuation determined by direct summation of the leading Born approximation plus $(n - 1)$ approximants of the form (3.4).

Table VII presents a comparison of the rates of convergence of the eigenfunction expansions (2.3), (2.5), and (2.7) for $T_0(1, 1; \pm 1)$ for the Yukawa potential $V(r) = -\exp(-r)/r$. (In evaluating these expansions use has been made of values of $\eta_N(k^2)$, $I_N(k, p)$, and $M_N(k)$ presented elsewhere [1, 2].) It is clearly observed that the convergence of the separable expansion (2.3) is rather poor but that considerable improvement is achieved with the nonseparable series (2.5) in which the first Born approximation has been extracted. In fact, the use of only the leading

TABLE VI

The Sums of the First Five S-wave Born. Approximations for the Potential $V(r) = \exp(-r)/r^a$

k	$\sum_{n=1}^{5} T_0^{(n)B}$ [b]			$\sum_{n=1}^{5} T_0^{(n)B}$ [c]		
	(Re $\Sigma_n(k^2)$)	(Im $\Sigma_n(k^2)$)	($\Sigma_n(-k^2)$)	(Re $\Sigma_n(k^2)$)	(Im $\Sigma_n(k^2)$)	($\Sigma_n(-k^2)$)
0.0	−0.5576	0	−0.5576	−0.6067	0	−0.6067
0.1	−0.5435	−0.0684	−0.4984	−0.5287	−0.0744	−0.5002
0.2	−0.5078	−0.1218	−0.4564	−0.5009	−0.1112	−0.4564
0.3	−0.4635	−0.1554	−0.4251	−0.4695	−0.1417	−0.4251
0.4	−0.4197	−0.1726	−0.4009	−0.4380	−0.1600	−0.4009
0.5	−0.3803	−0.1786	−0.3817	−0.4000	−0.1597	−0.3818
0.7	−0.3174	−0.1710	−0.3534	−0.3262	−0.1654	−0.3535
1.0	−0.2585	−0.1380	−0.3262	−0.2641	−0.1404	−0.3262
1.5	−0.2235	−0.0807	−0.3009	−0.2220	−0.0845	−0.3009
2.0	−0.2218	−0.0454	−0.2872	−0.2195	−0.0452	−0.2872
2.5	−0.2274	−0.0266	−0.2789	−0.2273	−0.0251	−0.2789
3.0	−0.2332	−0.0165	−0.2736	−0.2337	−0.0161	−0.2736
4.0	−0.2414	−0.0074	−0.2673	−0.2417	−0.0075	−0.2672
5.0	−0.2462	−0.0038	−0.2639	−0.2464	−0.0039	−0.2639

[a] With $p_1 = p_2 = 1$, computed from [9,9] Padé approximants in the variable $K = ik$ fitted to the results of Table I, and determined directly from the results in Tables II and III. The first Born approximation is $V_0(1, 1) = -0.25615$.

[b] From [9,9] Padé approximants.

[c] From Tables II and III.

TABLE VII

Comparison of the Rates of Convergence of the Eigenfunction Expansions (2.3), (2.5), and (2.7) for $T_0(1, 1; \pm 1)$ for the Potential $V(r) = -\exp(-r)/r^a$

	Expansion (2.3)			Expansion (2.5)			Expansion (2.7)		
N	(Re $T_0(1)$)	(Im $T_0(1)$)	($T_0(1-)$)	(Re $T_0(1)$)	(Im $T_0(1)$)	($T_0(-1)$)	(Re $T_0(1)$)	(Im $T_0(1)$)	($T_0(-1)$)
1	−0.315	−0.294	−0.246	−0.248	−0.154	−0.320	−0.261	−0.136	−0.326
2	−0.372	−0.117	−0.302	−0.266	−0.139	−0.326	−0.261	−0.136	−0.326
3	−0.290	−0.061	−0.318	−0.263	−0.134	−0.327	−0.261	−0.136	−0.326

[a] N is the number of eigenfunction terms used in these expansions. The S-wave phase shift at $k = 1$ yields the on-shell value $T_0(1,1; 1) = -0.261 - 0.136i$.

eigenfunction term in (2.5) yields a more accurate result than summation over the first three terms in (2.3), particularly at positive energies. It also can be seen that the inclusion of the first three eigenfunction terms in (2.5) leads to a result that differs only slightly from the on-shell S-wave amplitude calculated from Eq. (2.2). However, when using the nonseparable expansion (2.7), in which the first two Born approximations have been extracted, the inclusion of the leading eigenfunction term alone is sufficient to yield the correct value of the on-shell T-matrix. It should also be noted that the use of (2.5) with the first three eigenfunction terms, and of (2.7) with the leading eigenfunction term, has produced results of higher accuracy than the sums of the first five Born approximations presented in Table VI.

The method of Section 3 was also applied to the neutron–proton triplet S-state potential [12]

$$V(r) = 4A \exp(-2\mu r)/r - \mathrm{A} \exp(-\mu r)/r, \tag{4.4}$$

with $A = 42.48$ and $\mu = 2.307$ [13]. This interaction has a repulsive core and an attractive outer region. With the values of A and μ just quoted, $k^2 = 1$ represents an energy of 41.5 MeV in the center of mass frame. Table VIII displays the first four Born approximations, with $p_1 = p_2 = 1$, computed at negative energies from Eq. (3.2). The resulting $[m + 2n - 2, m]$ Padé approximant fits in the variable $K = ik$, evaluated at both positive and negative energies, are presented in Table IX. It can be clearly seen that in this case, the Born series diverges as predicted by Weinberg [4] for interactions that have any eigenvalues $\eta_N(k^2)$ satisfying the inequality (2.14). The $^3S_1$ potential (4.4) has four such eigenvalues [2, 3, 13]. Thus, in this case, the sum of the first n Born approximations cannot, by itself, provide an estimate of the off-shell T matrix. It must be used in the nonseparable series (2.9) only in conjunction with at least all the eigenfunction terms whose $\eta_N(k^2)$ satisfy (2.14).

The imaginary part of the second Born approximation computed at positive energies from the [10, 8] approximant for the $^3S_1$ interaction (4.4) may also be compared against the exact values calculated from Eq. (4.3), which yields

$$\begin{aligned}
\mathrm{Im}\ T_0^{(2)B}(1, 1; 0.25) &= -0.338, \\
\mathrm{Im}\ T_0^{(2)B}(1, 1; 1) &= -1.180, \\
\mathrm{Im}\ T_0^{(2)B}(1, 1; 2.25) &= -3.043, \\
\mathrm{Im}\ T_0^{(2)B}(1, 1; 4) &= -6.006.
\end{aligned}$$

Thus, we find that the Table IX values of $\mathrm{Im}\ T_0^{(2)B}(1, 1; k^2)$ contain errors of about three units in the third significant figure.

TABLE VIII

The First Four Born Approximations at Negative Energies[a]

	$T_0^{(n)B}(1,1;k^2)$		
$-ik$	$(n=2)$	$(n=3)$	$(n=4)$
0.2	−15.6968	178.64	−2139.7
0.4	−15.4438	170.70	−1978.4
0.6	−15.1213	162.02	−1816.2
0.8	−14.7495	153.03	−1659.2
1.0	−14.3443	144.03	−1510.9
1.2	−13.9183	135.23	−1373.1
1.4	−13.4813	126.75	−1246.4
1.6	−13.0408	118.68	−1130.9
1.8	−12.6023	111.05	−1026.2
2.0	−12.1699	103.88	−931.5
2.2	−11.7466	97.17	−846.1
2.4	−11.3345	90.91	−769.1
2.6	−10.9351	85.09	−699.9
2.8	−10.5492	79.67	−637.6
3.0	−10.1773	74.64	−581.5
3.2	−9.8197	69.98	−531.0
3.4	−9.4764	65.65	−485.5
3.6	−9.1472	61.64	−444.5
3.8	−8.8317	57.91	−407.8
4.0	−8.5296	54.45	−374.0

[a] With $p_1 = p_2 = 1$, computed from Eq. (3.2) for the $^3S_1$ potential (4.4). The value of the leading Born approximation is $V_0(1, 1) = 0.866803$.

As the phase shift of the potential (4.4) at $k = 1$ is $\delta_0 = 47.6°$, the value of the on-shell amplitude obtained from (2.2) is

$$T_0(1, 1; 1) = -0.317 - 0.347i.$$

The use of the separable expansion (2.3) with the four eigenfunction terms whose $\eta_N(k^2)$ satisfy the inequality (2.14) does not provide an adequate approximation

TABLE IX

The Second, Third, and Fourth Born Approximations[a]

k	$T_0^{(2)B}(1, 1; k^2)$			$T_0^{(3)B}(1, 1; k^2)$			$T_0^{(4)B}(1, 1; k^2)$		
	(Re $T(k^2)$)	(Im $T(k^2)$)	($T(-k^2)$)	(Re $T(k^2)$)	(Im $T(k^2)$)	($T(-k^2)$)	(Re $T(k^2)$)	(Im $T(k^2)$)	($T(-k^2)$)
0.0	−15.855	0	−15.855	185.26	0	185.26	−22.91.9	0	−2291.9
0.1	−15.871	−0.051	−15.790	185.51	2.88	182.16	−2294.6	−72.0	−2217.8
0.2	−15.918	−0.106	−15.697	186.28	5.86	178.64	−2302.6	−145.7	−2139.7
0.3	−15.995	−0.170	−15.580	187.53	9.05	174.80	−2315.5	−222.9	−2059.7
0.4	−16.102	−0.247	−15.444	189.26	12.55	170.70	−2332.9	−305.5	−1978.4
0.5	−16.237	−0.341	−15.290	191.42	16.47	166.42	−2353.9	−395.4	−1897.0
0.7	−16.583	−0.597	−14.940	196.80	26.06	157.54	−2401.3	−605.2	−1736.8
1.0	−17.247	−1.207	−14.344	205.96	46.55	144.03	−2448.4	−1022.9	−1510.9
1.5	−18.459	−3.010	−13.261	210.59	100.85	122.66	−2155.5	−1977.9	−1187.2
2.0	−19.194	−5.863	−12.170	177.73	161.31	103.88	−1144.6	−2574.1	−931.5
2.5	−18.764	−9.378	−11.133	121.03	189.32	87.95	−281.8	−2385.1	−735.5
3.0	−16.896	−12.749	−10.177	77.02	189.80	74.64	31.5	−2104.7	−581.5
4.0	−10.550	−16.442	−8.530	38.97	197.04	54.45	−824.2	−2659.2	−374.0
5.0	−4.615	−16.021	−7.208	−10.36	364.68	40.86	−814.0	775.2	−247.8

[a] With $p_1 = p_2 = 1$, computed respectively from [10,8], [10,6], and [10,4] Padé approximants in the variable $K = ik$ fitted to the results of Table VIII for the $^3S_1$ potential (4.4).

to this result. The application of (2.5) with the four leading eigenfunction terms leads to an improved estimate for $T_0(1, 1; 1)$, while (2.7) yields a far more accurate result for this amplitude.

5. Conclusion

In this paper, a simple method has been presented for the numerical evaluation at positive and negative energies of any term in the Born series for the two-particle off-shell partial-wave T matrix. It has been found that a self-correcting procedure requires very little computer time to perform the numerical integrations for the second and third Born approximations over a range of negative energies, but that higher-order negative energy Born approximations should be computed from the recursive quadrature formula (3.3). After having determined $T_l^{n(B)}$ at an adequate number of negative energy points for a given pair of off-shell momenta, only a few seconds are required on an ICL 1907 computer to construct a Padé approximant fit of the form (3.4) and to evaluate it at many positive and negative energies for the specified value of n. (All the approximants that were employed to compute the various results presented in Section 4 were found to be stable at all energies with the single exception of the [10, 2] approximant of Table III for $T_0^{(5)B}$ when evaluated at zero energy.)

Furthermore, if only the sum of first n Born approximations is required at positive energies rather than the individual Born approximations, then a single $[m, m]$ Padé approximant fitted to the negative energy sum of the first n Born approximations (for a given pair of off-shell momenta) is likely to yield the most accurate numerical analytic continuation to positive energies. This practical method of summing the leading terms in the Born series enables the rate of convergence of eigenfunction expansions for the two-body off-shell partial-wave amplitude to be accelerated by using the nonseparable series (2.9).

It is, of course, well known that the most convenient form of the two-particle T matrix to use in the three-particle Faddeev equations is a separable eigenfunction expansion such as (2.3). Unfortunately, its rate of convergence for interactions of the form (4.2) is frequently not rapid enough to provide a useful approximation to the two-body amplitude, and so a modified accelerated form of the series, such as (2.9), may have to be employed instead. The numerical method developed in this paper, when used in conjunction with previous published results concerning techniques for computing the $I_N(k, p)$, $M_N(k)$, and $\eta(k^2{}_N)$ [defined in Section 2], provides a practical tool for evaluating the nonseparable series (2.9) at positive and negative energies.

Acknowledgment

The author wishes to thank the referees for their comments.

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