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Comparison of unitary and Padé sums of the perturbation series for the scattering of a spinless particle from a Yukawa potential

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Alternative methods for summing the Born series for a scattering process are derived and compared. These include Padé and unitary approximations of the scattering operator and their combinations. The various approximations are applied to an attractive Yukawa potential, and it is shown that most of the unitary and Padé approximations converge much more rapidly than the Born series. A comparison of the methods provides a practical test for convergence at a particular order of the perturbation theory.

I. INTRODUCTION

The scattering operator S maps the initial state of a scattering process into the final state. Conservation of probability is assured by the unitarity of S. The transition operator T is related to S as

$$S = 1 - 2\pi i \delta(E - H_0)T, \tag{1}$$

where H_0 is the free-particle Hamiltonian, and T is related to the interaction potential V by

$$T = V + VG_0T, \tag{2}$$

where $G_0 = (E - H_0 + i\epsilon)^{-1}$. The matrix element of T between free single-particle states with momentum $\vec{p} = \hbar\vec{k}$ is directly related to the scattering amplitude by

$$f(\theta) = -(\mu/2\pi\hbar^2)\langle\vec{k}_f|T|\vec{k}_i\rangle, \tag{3}$$

where $\vec{k}_i$ and $\vec{k}_f$ are in the incident and scattered directions, respectively, and μ is the reduced mass of the system. In solving Eq. (2) for T, it is often necessary to evaluate T approximately by iterating the equation. The result is the Born expansion in powers of the interaction strength g,

$$T = \sum_{n=1}^{\infty} g^n T_n. \tag{4}$$

There are two features of the perturbation expansion that result in a poor approximation to S. The most obvious and important is the convergence of the expansion. The second stems from the fact that the insertion of the truncated Born series into Eq. (1) does not give a unitary approximation to S, and hence the approximation does not conserve probability.

Recently, an efficient numerical technique for generating the higher-order terms in the Born series for an attractive Yukawa potential was presented.[1] However, up to seven terms in the series were needed to provide fair agreement with the numerically exact results.[2] Similar convergence problems have been noted for other potentials of current interest.[3] To accelerate convergence for the Yukawa potential, one of us (C.M.R.) in Ref. 1 resummed the Born series. An extension of Newton's variational method[4] by Rabitz and Conn[5] was used, which results in a Padé approximant for the optimum value of T.

The purpose of the present paper is to study alternative methods for expediting the convergence of the perturbation series. Padé and unitary[6] expansions of the scattering operator will be compared, and various combinations of these approximations will be derived. Such a study should lead to a better understanding of attempts for extracting the optimum amount of information from a perturbation theory.

II. UNITARY AND PADÉ APPROXIMATIONS

The scattering operator may be expressed in a manifestly unitary form as

$$S = (1 + i\kappa)/(1 - i\kappa) = e^{i\eta}. \tag{5}$$

If the Hermitian operators κ and η are expanded in powers of the interaction strength as

$$\kappa = \sum_{n=1}^{\infty} g^n \kappa_n, \quad \eta = \sum_{n=1}^{\infty} g^n \eta_n, \tag{6}$$

and the series are truncated, the resulting approximations to S are unitary. Moreover, if the two series are terminated at the same point, the results are different. The operators κ and η generate the Heitler and exponential unitary approximations, respectively.

The operator κ is related to the interaction potential V through the operator K as

$$\kappa = 2\pi\delta(E - H_0)K, \quad K = V + VG_0^P K, \tag{7}$$

where G_0^P denotes treating the singularity in the Green's function by the principal-parts method. The K operator is also related to the T operator by the on-shell Heitler equation,

$$T = K - i\pi K\delta(E - H_0)T. \tag{8}$$

Following the variational method of Rabitz and Conn,[5] an operator I, formed by

$$I = V + VG_0T_t + T_tG_0V - T_tG_0T_t + T_tG_0VG_0T_t, \tag{9}$$

is stationary for variations of T_t about the exact value of T. Writing the trial T as

$$T_t = \sum_{n=1}^{2N+1} x_n(g^n T_n), \tag{10}$$

where $g^n T_n$ is the nth term in the Born series for T, it is shown in Ref. 5 that the optimum choice of the x_n gives the $[N, N+1]$ Padé approximant[7] formed from the $2N+1$ terms of the Born series. We use the notation $T[N, N+1]$ for the optimum trial value of T.

In a similar manner, an operator J defined as

$$J = V + VG_0^PK_t + K_tG_0^PV - K_tG_0^PK_t + K_tG_0^PVG_0^PK_t \tag{11}$$

is stationary for variations of K_t about the exact value. Writing the trial K as

$$K_t = \sum_{n=1}^{2N+1} x_n(g^n K_n), \tag{12}$$

where $g^n K_n$ is the nth term in the Born series for K, one finds that the optimum choice for the variational parameters x_n leads to the $[N, N+1]$ Padé approximant to K formed from the $2N+1$ terms of the Born series, and this value is denoted $K[N, N+1]$.

III. VARIOUS APPROXIMATIONS FROM A PARTIAL-WAVE DECOMPOSITION

The approximations to the scattering operator are easily defined and compared in the context of a partial-wave decomposition. This decomposition is effected by using the closure condition

$$(2\pi)^{-3}\int d^3k\,|\vec{k}\rangle\langle\vec{k}| = 1$$

and the following representations in terms of the eigenvectors $|klm\rangle$ of H_0, $\vec{L}^2$, and L_z:

$$\delta(E - H_0) = \frac{1}{\pi}\sum_{l,m}|klm\rangle\langle klm|,$$

$$|\vec{k}\rangle = \frac{4\pi\hbar}{(2\mu k)^{1/2}}\sum_{l,m}|klm\rangle Y_l^{m*}(\theta_k, \phi_k),$$

where $E = \hbar^2k^2/2\mu$, and θ_k and ϕ_k are the spherical angles for $\vec{k}$. With these relationships, the matrix element of Eq. (8) between the initial and final free-particle states reduces to the algebraic relation

$$T_l = K_l + iK_lT_l, \tag{13}$$

where, by rotational invariance for a spherically-symmetrical potential,

$$\begin{aligned}\langle kl'm'|T|klm\rangle &\equiv -T_l\,\delta_{ll'}\,\delta_{mm'},\\ \langle kl'm'|K|klm\rangle &\equiv -K_l\,\delta_{ll'}\,\delta_{mm'}.\end{aligned} \tag{14}$$

The scattering amplitude, Eq. (3), likewise reduces to

$$f(\theta) = \frac{1}{k}\sum_l T_l(2l+1)P_l(\cos\theta), \tag{15}$$

where θ is the scattering angle. We now formulate the various approximations.

A. Born and Born-Padé approximations

The Born series approximation to T_l is

$$\begin{aligned}T_l^B &\equiv \sum_{n=1}^{2N+1} g^n T_l^n,\\ T_l^n &\equiv -\langle klm|T_n|klm\rangle.\end{aligned} \tag{16}$$

Substitution of T_l^B for T_l in Eq. (15) gives the Born approximation $f_B(\theta)$.

The approximation to $f(\theta)$ that gives a stationary value of $\langle kl'm'|I|klm\rangle$ is

$$f_{\rm BP}^{(1)}(\theta) = \frac{1}{k}\sum_l (2l+1)T_l[N, N+1]P_l(\cos\theta). \tag{17}$$

Here, $T_l[N, N+1]$ is the $[N, N+1]$ Padé approximant formed from the $2N+1$ terms $g^n T_l^n$.

There is yet another way to construct a Padé approximation to the scattering amplitude based on a variational principle. If we first perform the partial-wave sum

$$T_n(\theta) \equiv \langle\vec{k}_f|T_n|\vec{k}_i\rangle = \frac{-2\pi\hbar^2}{k\mu}\sum_l (2l+1)T_l^nP_l(\cos\theta), \tag{18}$$

the Padé approximant $T_\theta[N, N+1]$ formed from the $2N+1$ terms $g^n T_n(\theta)$ yields a stationary value of the matrix element $\langle\vec{k}_f|I|\vec{k}_i\rangle$. The corresponding Padé approximation to the amplitude is

$$f_{\rm BP}^{(2)}(\theta) = -(\mu/2\pi\hbar^2)T_\theta[N, N+1]. \tag{19}$$

This is a different approximation than Eq. (17), since a stationary value of $\langle \vec{k}_f | I | \vec{k}_i \rangle$ does not imply that $\langle klm | I | klm \rangle$ is stationary, although the converse is true.

B. Heitler and Heitler-Padé approximations

The Born approximation to K_l, denoted K_l^B, is

$$K_l^B = \sum_{n=1}^{2N+1} g^n K_l^n , \quad K_l^n \equiv -\langle klm | K_n | klm \rangle , \tag{20}$$

where K_n is the nth term in the Born series for K. The matrix elements K_l^n are real as the operators K_n are Hermitian, and they are related to the complex matrix elements T_l^n by Eq. (13). The result is

$$T_l^n = K_l^n + i \sum_{n'=1}^{n-1} K_l^{n'} T_l^{n-n'} . \tag{21}$$

The Heitler unitary approximation to the scattering amplitude follows from Eqs. (13), (15), and (20),

$$f_H(\theta) = \frac{1}{k} \sum_l (2l+1) \left(\frac{K_l^B}{1 - iK_l^B} \right) P_l(\cos\theta) . \tag{22}$$

The approximation to $f(\theta)$ that yields a stationary value of the matrix element $\langle kl'm' | J | klm \rangle$ is

$$f_{\mathrm{HP}}^{(1)}(\theta) = \frac{1}{k} \sum_l (2l+1) \left(\frac{K_l^{(1)}[N, N+1]}{1 - iK_l^{(1)}[N, N+1]} \right) P_l(\cos\theta) . \tag{23}$$

Here, $K_l^{(1)}[N, N+1]$ is the $[N, N+1]$ Padé approximant formed from the $2N+1$ terms $g^n K_l^n$. Note that this is also a unitary approximation to S.

As in the case of the Born-Padé approximations, another Heitler-Padé unitary approximation is constructed by first summing over the partial-wave terms as

$$K_n(\theta) \equiv \langle \vec{k}_f | K_n | \vec{k}_i \rangle = -\frac{2\pi\hbar^2}{k\mu} \sum_l (2l+1) K_l^n P_l(\cos\theta) . \tag{24}$$

The Padé approximant $K_\theta[N, N+1]$ is formed from the $2N+1$ terms $g^n K_n(\theta)$, and this gives a stationary value of the matrix element $\langle \vec{k}_f | J | \vec{k}_i \rangle$. The approximant $K_\theta[N, N+1]$ is decomposed as

$$K_l^{(2)}[N, N+1] = \frac{-k\mu}{4\pi\hbar^2} \int_{-1}^{1} K_\theta[N, N+1] P_l(\cos\theta)\, d\cos\theta ,$$

and this gives the second unitary Heitler-Padé approximation

$$f_{\mathrm{HP}}^{(2)}(\theta) = \frac{1}{k} \sum_l (2l+1) \left(\frac{K_l^{(2)}[N, N+1]}{1 - iK_l^{(2)}[N, N+1]} \right) P_l(\cos\theta) . \tag{25}$$

C. Exponential approximation

The exponential unitary approximation to the scattering operator is given in Eq. (5). If the operator N is introduced by

$$\eta = -\pi \delta(E - H_0) N , \tag{26}$$

which by rotational invariance satisfies

$$\langle kl'm' | N | klm \rangle \equiv -\delta_{ll'} \delta_{mm'} N_l , \tag{27}$$

the matrix element

$$\langle kl'm' | e^{i\eta} | klm \rangle = \langle kl'm' | [1 - 2\pi i \delta(E - H_0) T] | klm \rangle \tag{28}$$

reduces to

$$e^{iN_l} = 1 + 2iT_l = (1 + iK_l)/(1 - iK_l) . \tag{29}$$

The Born series for the operator η is given in Eq. (6), and the corresponding Born approximation to N_l is

$$N_l^B = \sum_{n=1}^{N} g^n N_l^n , \quad N_l^n \equiv \langle klm | \eta_n | klm \rangle . \tag{30}$$

The substitution of the expansions in Eqs. (30) and (20) into Eq. (29) gives, upon equating like powers of g through the fifth,

$$\begin{aligned} &N_l^1 = 2K_l^1 , \quad N_l^2 = 2K_l^2 , \quad N_l^3 = 2K_l^3 - \tfrac{2}{3}(K_l^1)^3 , \\ &N_l^4 = 2K_l^4 - 2K_l^2 (K_l^1)^2 , \\ &N_l^5 = 2K_l^5 - 2K_l^3 (K_l^1)^2 - 2K_l^1 (K_l^2)^2 + \tfrac{2}{5}(K_l^1)^5 . \end{aligned} \tag{31}$$

The exponential unitary approximation to the scattering amplitude is therefore given by

$$f_E(\theta) = \frac{1}{k} \sum_l (2l+1) \left(\frac{e^{iN_l^B} - 1}{2i} \right) P_l(\cos\theta) . \tag{32}$$

IV. APPLICATION TO A YUKAWA POTENTIAL

These techniques are applied to the attractive Yukawa potential

$$V(r) = g e^{-s_0 r}/r . \tag{33}$$

The terms in the Born series for the transition operator T are obtained in Ref. 1 in terms of one-dimensional integrals,

$$\langle \vec{k}_f | T_n | \vec{k}_i \rangle = F_{n-1}(k_0, s_0) , \tag{34}$$

where

$$\begin{aligned} &F_n(k, s) = -\frac{1}{k} \int_0^k \frac{F_{n-1}(\tau, s_0 + s')}{s'} \, d\tau , \\ &s'^2 = \sigma\tau - \tau^2 - k_0^2 , \quad \sigma = (s^2 + k^2 + k_0^2)/k . \end{aligned} \tag{35}$$

The details of the evaluation of these integrals is given in Ref. 1, and the numerical values of $\langle \vec{k}_f | T_n | \vec{k}_i \rangle$ are given in Table I of Ref. 1(b) for

TABLE I. Low-energy scattering amplitude for the various approximations. The real and imaginary parts are given, and $k_0=0.663$.

Scattering angle	$\theta=0°$	$\theta=90°$	$\theta=180°$
Walters's exact result	1.116, 1.671	−0.142, 1.5041	−0.651, 1.3584
Rosenthal's [2,3] Padé	1.1589, 1.6818	−0.1106, 1.5123	−0.6424, 1.3606
Results for three terms in the Born series			
Born series	3.1617, 2.9623	1.8971, 2.8107	1.3729, 2.6817
Exponential	0.7754, 1.5730	−0.4806, 1.4084	−0.9962, 1.2665
Heitler	1.7299, 1.3828	0.4781, 1.2197	−0.0334, 1.0795
Born-Padé (1)	1.3367, 1.7489	0.0725, 1.2197	−0.4511, 1.4391
Born-Padé (2)	1.2770, 1.9862	0.0718, 1.5701	−0.3404, 1.2341
Heitler-Padé (1)	1.1192, 1.6717	−0.1454, 1.5038	−0.6694, 1.3586
Results for five terms in the Born series			
Born series	1.5948, 4.0997	−1.1072, 3.9328	−1.6332, 3.7888
Exponential	0.7382, 1.5483	−0.5271, 1.3801	−1.0518, 1.2347
Heitler	1.5765, 1.5419	0.3119, 1.3740	−0.2121, 1.2288
Born-Padé (1)	1.1463, 1.6729	−0.1197, 1.5045	−0.6450, 1.3589
Born-Padé (2)	1.1517, 1.6818	−0.1101, 1.5122	−0.6382, 1.3606
Heitler-Padé (1)	1.1463, 1.6729	−0.1197, 1.5045	−0.6450, 1.3589

$g=-1.1825$, $s_0=1$. A comparison is made with the numerical results of Ref. 2.

The Rosenthal technique is used to obtain T, and the matrix elements T_l^n, defined in Eq. (16) are extracted. These determine the matrix elements K_l^n and N_l^n as described in Sec. III.

V. DISCUSSION OF RESULTS AND CONCLUSIONS

The scattering amplitude at c.m.-system scattering angles of 0°, 90°, and 180° are shown in Tables I and II at the energies $k_0=0.663$ and 1.816 in atomic units. These values of k_0 are chosen to

TABLE II. High-energy scattering amplitude for the various approximations. The real and imaginary parts are given, and $k_0=1.816$.

Scattering angle	$\theta=0°$	$\theta=90°$	$\theta=180°$
Walters's exact result	2.182, 0.739	0.079, 0.3478	−0.05, 0.2134
Rosenthal's [2,3] Padé	2.1865, 0.7387	0.0796, 0.3474	−0.0482, 0.2123
Results for three terms in the Born series			
Born series	2.2443, 0.9223	0.1526, 0.5270	−0.0013, 0.3869
Exponential	2.1489, 0.7523	0.0757, 0.3612	−0.0645, 0.2267
Heitler	2.1644, 0.6790	0.0993, 0.2948	−0.0353, 0.1664
Born-Padé (1)	2.1832, 0.7237	0.1096, 0.3370	−0.0307, 0.2053
Born-Padé (2)	2.1605, 0.7659	0.1168, 0.3273	−0.0019, 0.1936
Heitler-Padé (1)	2.0533, 0.4014	−0.0290, 0.0019	−0.1764, −0.1401
Heitler-Padé (2)	1.4666, 2.2286	0.2341, −0.0851	−0.8642, −0.0904
Results for five terms in the Born series			
Born series	2.0936, 0.7218	0.0206, 0.3304	−0.1189, 0.1947
Exponential	2.1564, 0.7364	0.0804, 0.3452	−0.0570, 0.2108
Heitler	2.1624, 0.7180	0.0898, 0.3275	−0.0496, 0.1938
Born-Padé (1)	2.1557, 0.7375	0.0832, 0.3471	−0.0565, 0.2123
Born-Padé (2)	2.1555, 0.7359	0.0814, 0.3471	−0.0562, 0.2111
Heitier-Padé (1)	2.1556, 0.7381	0.0823, 0.3470	−0.0577, 0.2127
Heitler-Padé (2)	2.1338, 0.7256	0.0892, 0.3482	−0.0465, 0.2251

allow a comparison with the results of Walters.[2] The amplitudes calculated by Rosenthal in Ref. 1(b) are also included, as they are the direct [2,3] Padé approximation to the T matrix element which avoids the partial-wave expansions.

We will pay closest attention to the convergence of the various approximations and the correspondence of these approximations at the same order. The second point is stressed, as it provides a practical test of convergence without going to a higher order.

At the lower energy (see Table I) we see that the Born series is a poor representation of $f(\theta)$, even after five terms are taken. For easy reference, the remaining approximations are denoted as follows: $f_E(\theta)$, exponential unitary as given in Eq. (32); $f_H(\theta)$, Heitler unitary as given in Eq. (22); $f_{\rm HP}^{(1)}(\theta)$, Heitler-Padé as given in Eq. (23); $f_{\rm HP}^{(2)}(\theta)$, Heitler-Padé as given in Eq. (25); $f_{\rm BP}^{(1)}(\theta)$, Born-Padé as given in Eq. (17); and $f_{\rm BP}^{(2)}(\theta)$, Born-Padé as given in Eq. (19).

The Heitler-Padé (2) approximation $[f_{\rm HP}^{(2)}(\theta)]$ was found to converge slowly at both energies, and it is not shown in Table I. The unitary approximations $f_H(\theta)$ and $f_E(\theta)$ are both superior to the Born series, and $f_E(\theta)$ gives reasonably good results even after three terms. The consistency among the Padé approximations is striking at five terms, at which point the Born series is still quite poor.

At the higher energy, Table II, the Born series converges reasonably well by five terms, but it is not so good at three terms. At three terms, however, both unitary approximations $f_E(\theta)$ and $f_H(\theta)$ are much better than the Born series. The exponential form is an especially good representation of $f(\theta)$. The Born-Padé approximations are equally good, but they are not as good as $f_E(\theta)$ at three terms. The Heitler-Padé approximations are poor representations of $f(\theta)$ at three terms. At five terms, all of the methods except the Born and Heitler-Padé (2) have converged to values quite close to the exact results.

For the Yukawa potential at the energies selected, the following summary can be made:

(1) The unitary approximations $f_H(\theta)$ and $f_E(\theta)$ are superior to the Born series, and $f_E(\theta)$ is better than $f_H(\theta)$. In fact, the exponential unitary approximation is an excellent approximation at the higher energy.

(2) The Born-Padé approximations $f_{\rm BP}^{(1)}(\theta)$ and $f_{\rm BP}^{(2)}(\theta)$ are closely matched, although not the same, and they converge rapidly to values in excellent agreement with the exact results. These are the most consistently good approximations.

(3) The Heitler-Padé approximation $f_{\rm HP}^{(1)}(\theta)$ converges faster than any other at the low energy, but it does not do as well at the high energy. The approximation $f_{\rm HP}^{(2)}(\theta)$ does not do well at all.

We have given the derivation of unitary and Padé approximations for the scattering of a spinless particle by a central potential. Each method is well justified, and most are superior to the Born series for the example chosen. This variety of techniques provides a self-consistent scheme for testing convergence at a particular order of the perturbation theory. Such a test has not been proposed before, and it could be valuable when the calculation of higher Born terms is prohibitively difficult.

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