Systematic Approximations for the Single-Channel Scattering Amplitude*

F. COESTER
Argonne National Laboratory, Argonne, Illinois
(Received 4 November 1963)

The scattering amplitude for two-particle single-channel scattering may be computed by inverting a Hilbert-space operator $1-K$, where K is compleely continuous and depends on the real energy as a parameter. This inversion can always be accomplished by obtaining a finite number of eigenvalues and eigenfunctions of K together with a modified Born expansion which is guaranteed to converge. Another method consists in the inversion of a finite matrix, the elements of which are computed by a convergent perturbation series.

I. INTRODUCTION

IT is customary to distinguish between a time-independent and a time-dependent scattering theory in quantum mechanics. More important, perhaps, is the related distinction between a wave mechanical and a Hilbert space formulation of scattering theory. In the first case one solves a boundary-value problem for functions that are not square integrable. In the second case the scattering operator (S operator) is expressed as a function of known operators on Hilbert space, and the ultimate problem is to compute matrix elements $S_{ba}=(\phi_b,S\phi_a)$ for certain Hilbert space vectors ϕ_a and ϕ_b. The present paper is concerned with the Hilbert space formulation of scattering theory. The two formulations are, of course, intimately related; but a discussion of this relation is not within the scope of this paper.[1]

Recently, Weinberg[2] has given a lucid discussion of the convergence of the Born series for two-particle single-channel scattering at complex energies. Weinberg gives a necessary and sufficient condition for the convergence of the Born series and shows how a convergent modified series can always be constructed when the ordinary Born series diverges.[3] The purpose of the present paper is to modify Weinberg's treatment in such a manner that it becomes manifestly valid for real energies. Such a modification is suggested by the work of Rollnik.[4,4a]

We are concerned with the scattering of a single particle by a fixed center, or with the relative motion of two particles. The Hamiltonian of the system has the form

$$H=H_0+V, \tag{1}$$

where H_0 is the kinetic energy. The scattering amplitude may be obtained from the operator[5]

$$T(W)=V+VG(W)V, \tag{2}$$

where $G(W)$ is the resolvent of the Hamiltonian H, i.e.,

$$G(W)=(W-H)^{-1}, \tag{3}$$

and W is a complex parameter $W=E+i\epsilon$. Eventually, W must approach the real energy of the scattering system. Since

$$W-H=(W-H_0)[1-G_0(W)V]$$

with

$$G_0(W)=(W-H_0)^{-1},$$

we have the identity

$$G(W)=[1-G_0(W)V]^{-1}G_0(W). \tag{4}$$

Weinberg's treatment is based on the remark that, for reasonable potentials and W off the positive real axis, the operator

$$K_w=G_0(W)V$$

is a Hilbert-Schmidt operator $[\mathrm{Tr}(K_w^\dagger K_w)<\infty]$ and hence is completely continuous.[6] Unfortunately, the bound of K_w increases indefinitely as W approaches the positive real axis. This feature can be established easily by evaluating the expectation value of $K_w^\dagger K_w$. Let χ be defined by

$$\chi=V\psi$$

for some arbitrary vector ψ and represent these vectors by square-integrable functions of E, l, m. The norm of the vector χ is given in this representation by

$$\|\chi\|^2=\int_0^\infty dE\sum_{l=0}^{\infty}\sum_{m=-l}^{+l}|\chi(E,l,m)|^2 \tag{6}$$

---

* Work performed under the auspices of the U. S. Atomic Energy Commission.

[1] A recent paper on the wave-mechanical Born series by M. Rotenberg [Ann. Phys. (N. Y.) **21**, 599 (1963)] has many formal analogies to our treatment.

[2] S. Weinberg, Phys. Rev. **131**, 440 (1963).

[3] Weinberg's so-called quasiparticles are really irrelevant in this context.

[4] H. Rollnik, Z. Physik **145**, 639 (1956).

[4a] *Note added in proof:* See also K. Meetz, J. Math. Phys. **3**, 690 (1961). I wish to thank Dr. W. Hunziker for drawing my attention to this paper.

[5] This is a well-known result of the formal theory of scattering. See for instance M. Gell-Mann and M. L. Goldberger, Phys. Rev. **91**, 398 (1953), Eqs. (2.14) and (2.10). The precise relation of $T(W)$ to the S operator will be discussed in Sec. II.

[6] A definition of completely continuous operators is given in the appendix. Other equivalent definitions and properties can be found in standard textbooks on functional analysis, for instance F. Riesz and B. Sz.-Nagy, *Functional Analysis* (Frederick Ungar Publishing Company, New York, 1955), p. 206; and N. I. Akhiezer and I. M. Glazman, *Theory of Linear Operators in Hilbert Space* (Frederick Ungar Publishing Company, New York, 1961), pp. 56 ff.

and the vector $H_0\chi$ is represented by the function $E\chi(E,l,m)$. We have then

$$\|K_w\psi\|^2=\int_0^\infty dE'\sum_{l,m}|\chi(E',l,m)|^2[(E'-E)^2+\epsilon^2]^{-1}; \quad (7)$$

and since

$$\lim_{\epsilon\to 0}\epsilon\int_0^\infty dE'F(E')[(E-E)^2+\epsilon^2]^{-1}=\pi F(E_0),$$

the inequality

$$\|K_w\psi\|^2>\frac{\pi}{2\epsilon}\sum_{lm}|\chi(E,l,m)|^2 \quad (8)$$

holds for all ϵ that are smaller than some $\epsilon_0(\psi)$. One should not conclude that the eigenvalues of K_w increase in the same manner. They are continuous functions of W which have limits as W approaches the real axis.[2,7] But these limits are not eigenvalues of the unbounded operator $K_w(E)$. The eigenfunctions cease to be square integrable as ϵ tends to zero.

In Sec. II, the relation between $T(W)$ and the S operator will be examined. The result is that the operator limit

$$T(E)=\lim_{\epsilon\to 0}T(E+i\epsilon)$$

exists and is related to the scattering amplitude in the usual fashion. The operator $T(E)$ is obtained as a function of a known completely continuous operator $K(E)$, and the problem of computing the scattering amplitude is reduced to inverting 1-K. Systematic approximations are discussed in Sec. III.

II. PROPERTIES OF THE SCATTERING OPERATOR

The scattering operator S is defined in terms of the Møller operators $\Omega^{(\pm)}$ by

$$S=\Omega^{(+)\dagger}\Omega^{(-)}, \quad (9)$$

where

$$\Omega^{(\pm)}=\lim_{t\to\pm\infty}\Omega(t),$$

$$\Omega(t)\equiv e^{iHt}e^{-iH_0t}. \quad (10)$$

The limits are strong operator limits.[8] All operator limits in the following are understood to be strong limits unless otherwise specified. From Eq. (10) follows that

$$\lim_{t\to\pm\infty}\frac{d\Omega(t)}{dt}=H\Omega^{(\pm)}-\Omega^{(\pm)}H_0=0 \quad (11)$$

and

$$\Omega^{(\pm)\dagger}\Omega^{(\pm)}=1.$$

For the S operator, we may write

$$S=\lim_{t\to+\infty}\Omega(t)^\dagger\Omega^{(-)}$$

$$=\lim_{t\to-\infty}\Omega(t)^\dagger\Omega^{(-)}+\int_{-\infty}^{+\infty}dt\frac{d\Omega^\dagger(t)}{dt}\Omega^{(-)} \quad (12)$$

and therefore,

$$S=1-i\int_{-\infty}^{+\infty}dte^{iH_0t}V\Omega^{(-)}e^{-iH_0t}. \quad (13)$$

For any integrable function $g(t)$ for which the limit $g(-\infty)$ exists, that limit satisfies the relation

$$g(-\infty)=\lim_{\epsilon\to 0}\epsilon\int_{-\infty}^0 dte^{\epsilon t}g(t). \quad (14)$$

Similarly, if an operator $A(t)$ is integrable and the strong limit

$$\lim_{t\to-\infty}A(t)=A^{(-)} \quad (15)$$

exists, then[9,10]

$$A^{(-)}=\lim_{\epsilon\to 0}\epsilon\int_{-\infty}^0 dtA(t)e^{\epsilon t}. \quad (16)$$

The Møller operator $\Omega^{(-)}$ may therefore be obtained from

$$\Omega^{(-)}=\lim_{\epsilon\to 0}\int[1+G(E+i\epsilon)V]dP_0(E), \quad (17)$$

where $dP_0(E)$ is the spectral projection of H_0.[11] We have thus the result

$$V\Omega^{(-)}=\lim_{\epsilon\to 0}\int T(E+i\epsilon)dP_0(E), \quad (18)$$

with $T(W)$ defined by Eq. (2). Equations (13) and (18) give us the desired relation between $T(W)$ and the S operator. The limit $\epsilon\to 0$ must be taken after the integration over E unless the interchange can be justified. The practical advantages of such an interchange are manifest.

The matrix elements of S are to be taken between states ϕ_a and ϕ_b which are almost sharp in the energy, i.e.,

$$\int_{E_a-\Delta}^{E_a+\Delta}dP_0(E)\phi_a=\phi_a \quad (19)$$

[7] A proof is given at the end of Sec. II.

[8] The definitions of various operator limits are listed in the Appendix. See also N. I. Akhiezer and I. M. Glazman, *Theory of Linear Operators in Hilbert Space* (Frederick Ungar Publishing Company, New York, 1961), p. 61.

[9] J. M. Jauch, Helv. Phys. Acta **31**, 127 (1958).

[10] A. Galindo Tixaire, Helv. Phys. Acta **32**, 412 (1959).

[11] In Dirac's notation one would write $dP_0(E)=|E\rangle\langle E|dE$.

for some "small" Δ. The limit $\epsilon \to 0$ and the integration over E may therefore be interchanged in Eq. (18) if the operator $T(E+i\epsilon)$ converges to a limit $T(E)$ uniformly in E for finite intervals. We prove the existence of this limit by expressing T as a strongly continuous function of an operator $K(E+i\epsilon)$ that has the desired limit.

The resolvent $G_0(E+i\epsilon)$ may be represented by an integral kernel in the $\mathbf{x}$ representation

$$(\mathbf{x}|G_0(W)|\mathbf{x}')=\frac{M}{2\pi}\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}, \tag{20}$$

where $k=(2MW)^{1/2}$. It is therefore possible to factor any reasonable interaction operator V according to

$$V=V^{(+)}V^{(-)} \tag{21}$$

such that the operator

$$K(E+i\epsilon)=V^{(-)}G_0(E+i\epsilon)V^{(+)} \tag{22}$$

remains bounded as ϵ tends to zero. The precise choice of $V^{(+)}$ and $V^{(-)}$ is arbitrary to a large extent. The trace of $K^\dagger K$ may be computed from the expression

$$\mathrm{Tr}(K^\dagger K)=\left(\frac{M}{2\pi}\right)^2\int d\mathbf{x}\int d\mathbf{x}'\int d\mathbf{y}\int d\mathbf{y}'(\mathbf{y}'|V^{(-)\dagger}V^{(-)}|\mathbf{x})$$
$$\times(\mathbf{x}'|V^{(+)}V^{(+)\dagger}|\mathbf{y})\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}\frac{e^{-ik^*|\mathbf{y}-\mathbf{y}'|}}{|\mathbf{y}-\mathbf{y}'|}. \tag{23}$$

For local potentials and $\epsilon=0$, this expression reduces to

$$\mathrm{Tr}(K^\dagger K)=\left(\frac{M}{2\pi}\right)^2\int d\mathbf{x}\int d\mathbf{x}'\frac{|V^{(-)}(\mathbf{x})|^2|V^{(+)}(\mathbf{x}')|^2}{|\mathbf{x}'-\mathbf{x}|^2}. \tag{24}$$

The operator $K(E)$ is therefore a Hilbert-Schmidt operator provided the interaction potential decreases sufficiently rapidly for large $|\mathbf{x}|$.

From the identity (4) we get

$$V^{(-)}G(W)V^{(+)}=(1-K)^{-1}K, \tag{25}$$

and therefore,

$$T(E)=V+V^{(+)}[1-K(E)]^{-1}K(E)V^{(-)}$$
$$=V^{(+)}[1-K(E)]^{-1}V^{(-)}. \tag{26}$$

With Eq. (26) we have reached the objective of this section.

For complex W the operators K_w and K have the same eigenvalues. Let η be an eigenvalue of K_w. Since

$$V^{(-)}K_w=KV^{(-)}, \tag{27}$$

it follows from

$$K_w\phi=\phi\eta \tag{28}$$

that

$$KV^{(-)}\phi=V^{(-)}\phi\eta. \tag{29}$$

As ϵ tends to zero, the vectors $V^{(-)}\phi$ converge to a strong limit while the vectors ϕ do not.

III. APPROXIMATION PROCEDURES

A completely continuous operator K has essentially the properties of a finite matrix because it may be approximated uniformly by a sequence $\{K_N\}$ of operators of finite rank N.[12] Therefore the sequence $\{(1-K_N)^{-1}K_N\}$ converges uniformly to $(1-K)^{-1}K$.[13]

The Neumann series

$$(1-K)^{-1}=\sum_m K^m \tag{30}$$

converges uniformly if and only if

$$\lim_{m\to\infty}\|K^m\|=0, \tag{31}$$

since

$$(1-K)^{-1}-\sum_{n=0}^{m-1}K^n=(1-K)^{-1}K^m. \tag{32}$$

If η_1 is the largest eigenvalue of K, then

$$\|K\|\geqslant|\eta_1|. \tag{33}$$

For completely continuous operators[14]

$$\lim_{m\to\infty}\|K^m\|^{1/m}=\eta_1. \tag{34}$$

Therefore Eq. (31) holds and the Neumann series (30) converges[2] if and only if $|\eta_1|<1$. But $|\eta_1|\ll 1$ does not guarantee rapid convergence. An example would be a large Jordan box[12] with zero eigenvalues.

Instead of expanding $(1-K)^{-1}$ in a Neumann series, one might simply select a suitable K_N and invert the corresponding matrix. The following scheme combines both procedures. Let P_N be a projection operator that projects into an N-dimensional subspace of the Hilbert space, and define

$$K_N=P_NKP_N \tag{35}$$

such that

$$\|K-K_N\|<1. \tag{36}$$

A useful expression for the operator

$$P_N(1-K)^{-1}KP_N=P_N(1-K)^{-1}P_N-P_N \tag{37}$$

is easily derived from the identity

$$(1-K)^{-1}=(1-K_N-K'')^{-1}[1+K'(1-K)^{-1}], \tag{38}$$

where

$$K'=P_NK(1-P_N)+(1-P_N)KP_N \tag{39}$$

and

$$K''=(1-P_N)K(1-P_N)$$
$$=(1-P_N)(K-K_N)(1-P_N). \tag{40}$$

From Eqs. (36) and (40) it follows that

$$\|K''\|\leqslant\|K-K_N\|<1.$$

[12] For the properties of operators of finite rank, see for instance F. R. Gantmacher, *The Theory of Matrices* (Chelsea Publishing Company, New York, 1959), Chap. 7.

[13] M. A. Naimark, *Normed Rings* (P. Noordhoff Ltd., Groningen, The Netherlands, 1959), Chap. II, Sec. 9, No. 3, Theorem I.

[14] F. Riesz and B. Sz.-Nagy, *Functional Analysis* (Frederick Ungar Publishing Company, New York, 1955), p. 425.

From Eq. (38) it follows that

$$P_N(1-K)^{-1}P_N = (1-K_N)^{-1}[P_N+K'(1-P_N)(1-K)^{-1}P_N] \quad (41)$$

and

$$(1-P_N)(1-K)^{-1}P_N = (1-K'')^{-1}K'P_N(1-K)^{-1}P_N. \quad (42)$$

Substituting (42) into (41) yields

$$P_N(1-K)^{-1}KP_N=(1-K_N-K_N')^{-1}(K_N+K_N'), \quad (43)$$

where

$$K_N'=P_NK'(1-K'')^{-1}K'P_N. \quad (44)$$

The matrix representing $(1-K_N-K_N')$ may be inverted by standard numerical methods. The operator K_N' should be computed as a perturbation series, i.e., from

$$K_N'=P_NK'\textstyle\sum_m(K'')^mK'P_N. \quad (45)$$

The larger the value of N, the smaller is the number of terms needed in the series (45) since $\|K''\|$ decreases as N increases. In practice one must compromise between the competing desires for a small N and for rapid convergence of the series (45).

An alternative procedure consists in reducing K by computing first a finite number of eigenvalues and eigenfunctions. Let $\eta_1, \eta_2, \cdots, \eta_n$ be the n largest eigenvalues of K, with

$$|\eta_1| \geqslant |\eta_2| \geqslant |\eta_2| \geqslant \cdots.$$

We assume that there is a linearly independent eigenvector ψ_ν for each eigenvalue η_ν. This is certainly the case if the eigenvalues are all different or if the degeneracies are due to symmetries (such as rotational symmetry). The case of accidental degeneracies, which may involve nonlinear elementary divisors, is not of physical interest. The method described here could, however, be easily adapted to include that case. If η_ν is an eigenvalue of K, then η_ν^* is an eigenvalue of $K^\dagger$. Let χ_ν be the corresponding eigenvector. Then

$$K\psi_\nu=\eta_\nu\psi_\nu, \quad (46)$$

$$K^\dagger\chi_\nu=\eta_\nu^*\chi_\nu. \quad (47)$$

The sets $\{\psi_\nu\}$ and $\{\chi_\nu\}$ are bi-orthogonal, i.e.,

$$(\chi_\mu,\psi_\nu)=\delta_{\mu\nu}; \quad (48)$$

and the reduced operator K_n', defined by

$$K_n'f=Kf-\sum_{\nu=1}^{n}\psi_\nu\eta_\nu(\chi_\nu,f), \quad (49)$$

has the properties

$$K_n'\psi_\nu=0 \quad (50)$$

and

$$K_n'^\dagger\chi_\nu=0 \quad (51)$$

for $\nu=1,\cdots,n$. The largest eigenvalue of K_n' is η_{n+1}.

From Eqs. (49), (50), and (51), it follows that

$$(1-K)^{-1}Kf=\sum_{\nu=1}^{n}\psi_\nu\frac{1}{1-\eta_\nu}\eta_\nu(\chi_\nu,f)+(1-K_n')^{-1}K_n'f. \quad (52)$$

An eigenvalue η_μ can be equal to unity only if there is a true bound state of the Hamiltonian H at the energy E. In that case Eq. (52) remains valid for all f which are orthogonal to χ_μ. The term $\nu=\mu$ should be omitted from the sum.

For a completely continuous operator K, the eigenvalue η_{n+1} can be made arbitrarily small by choosing n sufficiently large. The convergence of the Neumann series for $(1-K_n')^{-1}$ is therefore assured. But there is no assurance that $\|K_n'\|$ will become small. Inspection of the eigenvalues alone does not give sufficient information about the number of terms needed in the Neumann series to achieve a given accuracy. Nevertheless, it seems plausible that a few eigenvalues of K and the first term in the series may give an adequate approximation in practice.

The preceding developments allow a trivial generalization to two-particle many-channel scattering if all particles are elementary. Rearrangement collisions require special consideration. They will be dealt with in a subsequent paper.

APPENDIX

For the convenience of the reader, the definitions of three modes of convergence of a sequence of bounded linear operators $\{A_n\}$ on a Hilbert space $\mathfrak{H}$ are listed.

Definition 1. The sequence $\{A_n\}$ *converges weakly* to A if for each pair of vectors $f\epsilon\mathfrak{H}$ and $g\epsilon\mathfrak{H}$

$$\lim_{n\to\infty}(g,A_nf)=(g,Af).$$

Definition 2. The sequence $\{A_n\}$ *converges strongly* to A if for each $f\epsilon\mathfrak{H}$

$$\lim_{n\to\infty}\|(A-A_n)f\|=0.$$

Definition 3. The sequence $\{A_n\}$ *converges uniformly* if for every $\epsilon>0$ there exists an N such that

$$\|(A-A_n)f\|<\epsilon\|f\|$$

for all $n>N$ and all $f\epsilon\mathfrak{H}$.

Complete continuity of an operator may be defined in many different but equivalent ways.[6] The following definition is the one most convenient for our purposes.

Definition. A linear operator K is *completely continuous* if there exists a sequence of operators K_N of finite rank N that converges uniformly to K.

ACKNOWLEDGMENTS

I wish to thank Dr. J. M. Cook and Dr. H. Ekstein for many helpful comments and criticisms.