Method of Orthogonality Constraint and Rearrangement Collisions*

A. CHEN,† S. TANI, AND S. BOROWITZ
New York University, New York, New York
(Received 13 July 1964; revised manuscript received 2 October 1964)

In treating scattering problems involving a bound state, the method of orthogonality constraint modifies the potential by projecting out the "binding" effect of the potential strong enough to support a bound state, and considers only its "scattering" effect as the perturbation on a distorted wave which is orthogonal to the bound state. The "modified" Born series obtained by iterating the relevant Lippmann-Schwinger integral equation is proved to be convergent, provided resonances not associated with the bound state are absent. The convergence proof is given for one-dimensional even waves and for a separable potential. However, the proof is also valid for the s waves. We believe, on the basis of our simplified analysis, that the method will work for a wide class of physically interesting potentials, though a rigorous proof for it is not available. The convergence of the Born expansion for rearrangement collisions is discussed in the context of a one-dimensional model for a three-body problem in which exchange scattering takes place. It is seen in the example that the kind of divergence pointed out by Aaron, Amado, and Lee may be removed by this method.

I. INTRODUCTION

THE convergence of the Born expansion for nonrelativistic potential scattering has been a subject of theoretical interest and rather extensively investigated by various authors.[1] The general conclusions are that the convergence is contingent upon the strength and certain properties of the potential and the incident energies. Usually, for a sufficiently weak potential and/or sufficiently high energy, the Born series is believed to be convergent. When the potential becomes strong enough, such features as the formation of bound states and resonances may become important. These features are considered to be nonadiabatic. In particular, the former constitutes a change in the character of the spectrum of the system. The drastic consequence of the existence of bound states and resonances is the divergence of the Born series, which makes the validity of the Born approximation doubtful. In problems dealing with scattering from compound systems or rearrangement collisions in which constituent particles can rearrange and form bound states, the Born series is believed to be divergent.[2] Some of the complexities of these problems of course lie mainly in their many-particle nature, which inevitably calls for methods of approximation[3] to carry out any numerical calculations. If one does not go beyond two-body interactions, the removal of the divergence of the Born series in the presence of bound states may restore the usefulness of perturbation theory provided the "residual interactions[4]" in the problem do not have any nonadiabatic effects. Recent theories[5] for a three-particle system also indicate that if the two-body operators corresponding to the two-body interaction can be successfully constructed, an aprrroximation scheme can be set up to make successively improved calculations for the three-particle problem. For the construction of the two-body operators for two-body interactions strong enough to support a bound state by a perturbative procedure, two methods have been proposed, namely, the method of orthogonality constraint[6] and the method of quasiparticles.[7] While the latter method has been developed rather thoroughly[8,9] and several examples using the method have been worked out,[10] a rigorous convergence proof for the former is still lacking. In this paper, such a proof is given, which, though in terms of separable potentials, is expected to be valid in general.[11]

The two methods are indeed similar, yet quite different in their details. They can be shown to be two different prescriptions for applying the distorted-wave approach of Rotenberg.[12] Though the method of quasiparticles was formulated in the spirit of the Schmidt method, its connection with Rotenberg's approach will be clarified in Sec. II. Our convergence proof is given directly with the use of a distorted wave. It is the common feature of the two methods that a separable potential is employed, but the physical pictures on which they are based are different. In the quasiparticle method the separable potential is constructed in order

* The research reported in this paper has been jointly sponsored by the U. S. Army Research Office-Durham under Grant No. DA-ARO-(D)-31-124-G276, the Office of Naval Research and the Advanced Research Projects Agency under Contract Nonr-285(49), and the National Science Foundation under Grant No. NSFG-GP-1897. This work is based on the thesis submitted by A. Chen to the New York University as a partial fulfillment of the requirements for a Ph.D. in physics.

† Present address: Physics Department, St. John's University, Jamaica, New York.

[1] See, for example: W. Kohn, Rev. Mod. Phys. **26**, 292 (1954); R. Jost and A. Pais, Phys. Rev. **82**, 840 (1951); C. Zemach and A. Klein, Nuovo Cimento **10**, 1078 (1958).

[2] R. Aaron, R. D. Amado, and B. W. Lee, Phys. Rev. **121**, 319 (1961). These authors will be referred to as AAL.

[3] See R. D. Amado, Phys. Rev. **132**, 485 (1963), for references to the approximate methods.

[4] R. D. Amado, Phys. Rev. **132**, 485 (1963).

[5] L. D. Faddeev, Zh. Eksperim. i Teor. Fiz. **39**, 1459 (1960) [English transl.: Soviet Phys.—JETP **12**, 1014 (1961)]; L. Rosenberg, Phys. Rev. **135**, B715 (1964).

[6] S. Tani, Phys. Rev. **117**, 252 (1960).

[7] S. Weinberg, Phys. Rev. **130**, 776 (1963).

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

[9] M. Scadron, S. Weinberg, and J. Wright, Phys. Rev. **135**, B202 (1964).

[10] M. Scadron and S. Weinberg, Phys. Rev. **133**, B1589 (1964).

[11] This is tantamount to showing that a particular choice of separable potentials in Weinberg's approach is sufficient to guarantee the convergence of the modified Born series.

[12] M. Rotenberg, Ann. Phys. **21**, 579 (1963).

to approximate the original potential insofar as it is concerned with a bound state or a resonance. In the orthogonality-constraint method we treat the bound state and the scattering problems separately. This method is recapitulated in Sec. II with the addition of remarks which have not been exhibited in Ref. 6. We start with the observation that the space orthogonal to the bound state is sufficient as far as the scattering goes. The constraint thus introduced on the kinetic energy gives rise to a distorted wave with a phase shift which is in conformity with Levinson's theorem even at the onset of a perturbative calculation; thus a separable potential appears as the cause of the distortion. While the quasiparticle method is more general in scope, the orthogonality-constraint method can cover the pathological case of a hard core[13] rather straightforwardly. As a successful version of the distorted-wave approach, the separation of binding and scattering effects of a strongly attractive potential achieved by this method may be applicable to a complicated many-body problem, since by definition it deals with only connected diagrams.

The subject of the convergence of Born expansion for rearrangement collisions will be discussed in Sec. IV in the light of the method of orthogonality constraint. The usefulness of the method in removing the kind of difficulties pointed out by Aaron, Amado, and Lee (AAL) is demonstrated by applying the method to a model one-dimensional three-body problem found in the literature.[14]

II. THE METHOD OF ORTHOGONALITY CONSTRAINT

Consider the Hamiltonian

$$H=K+V\,, \tag{II.1}$$

where K is the kinetic energy and V is the potential energy. When the potential V is strong enough to support a bound state, the Born series in terms of the free-particle Green's function and in powers of the perturbing potential V diverges at or near the bound-state energy.[15] In order to restore the usefulness of the perturbation theory in the presence of a bound state, what one can do is to split the potential V into two parts. The splitting can be effected in a number of ways.[6,7] According to the method of orthogonality constraint, we write

$$V=U+V_\perp \tag{II.2}$$

where

$$U=V-V_\perp\,. \tag{II.3}$$

It is obvious from (II.2) and (II.3) that the splitting is completely defined by the potential $V_\perp$, the orthogonalized potential given by (II.5) below. This manner of splitting, prescribed uniquely by the method of orthogonality constraint, is motivated by the dual role played by the potential under consideration, namely, the role of binding and that of scattering, with the former ascribed to U and the latter, to $V_\perp$. It is achieved by introducing the projection operator $\Lambda_{\parallel}$ which projects the Hilbert space spanned by the complete set of eigenstates of H onto a subspace of the bound state. The operator which projects the space onto the subspace orthogonal to the bound state is denoted by $\Lambda_\perp$. Clearly,

$$\Lambda_{\parallel}+\Lambda_\perp=I\,, \tag{II.4}$$

where I is the identity operator. In terms of $\Lambda_\perp$, the orthogonalized potential is given by

$$V_\perp=\Lambda_\perp V\Lambda_\perp\,. \tag{II.5}$$

The projection operators $\Lambda_{\parallel}$ and $\Lambda_\perp$ are defined by the following matrix elements:

$$(k|\Lambda_{\parallel}|k')=f(k)f(k') \tag{II.6}$$

and

$$(k|\Lambda_\perp|k')=\delta(k-k')-f(k)f(k')\,, \tag{II.7}$$

where $f(k)$ is the bound-state wave function in the momentum space, which is usually known or approximately known in practice. Throughout this paper, we assume that $f(k)$ is known exactly. If it is not, the method also provides a criterion for picking the best trial wave function.[6]

Using (II.2), we can write the Hamiltonian as

$$H=K+U+V_\perp\,. \tag{II.8}$$

The Lippmann-Schwinger integral equations corresponding to (II.1) and (II.8) are, respectively,

$$\psi=\phi+G_0V\psi \tag{II.9}$$

and

$$\psi=\phi+G_0(U+V_\perp)\psi\,, \tag{II.10}$$

where ϕ represents a plane wave and G_0 is the free-particle Green's function. It is easy to show with a little algebra that (II.10) can be written as

$$\psi=J\phi+G_\perp V_\perp\psi\,, \tag{II.11}$$

where

$$J=(I-G_0U)^{-1} \tag{II.12}$$

and

$$G_\perp=JG_0\,. \tag{II.13}$$

The formal solution of (II.11) is given by

$$\psi=(J-JG_\perp V_\perp)^{-1}\phi\,. \tag{II.14}$$

Comparing this with the formal solution

$$\psi=(I-G_0V)^{-1}\phi \tag{II.15}$$

of the integral equation (II.9), one can conclude that the splitting of the potential into two parts as shown in

[13] S. Tani and D. A. Uhlenbrock, J. Math. Phys. **3**, 1161 (1962).
[14] S. L. Schwebel, Phys. Rev. **103**, 814 (1956); A. Chen, S. Tani, and S. Borowitz, Bull. Am. Phys. Soc. **9**, 189 (1964).
[15] See, for example: N. N. Khuri, Phys. Rev. **107**, 1148 (1957); R. Blankenbecler, M. L. Goldberger, N. N. Khuri, and S. B. Treiman, Ann. Phys. (N. Y.) **10**, 62 (1960).

(II.2) is equivalent to introducing two new operators J and $G_\perp V_\perp$ to replace the operators I and G_0V. This is in line with the generalization of the Born iterative procedure proposed by Rotenberg on the basis of algebraic analogy to cope with the situation in which the Born series resulting from expanding the inverse operator in (II.15) fails to converge. The new operators are to be constructed in such a way as to make the "modified" Born series converge. It can also be shown that the splitting results in the factoring out of a factor, which is J, from the Fredholm determinant for the original integral equation (II.9) in the event that the Fredholm theory is applicable. The application of the Fredholm theory to scattering problems has been discussed by Weinberg,[8] who, in applying the Schmidt method, effects a "dissection" of the kernel by splitting the potential in such a way that quasiparticles are introduced into the problem through separable potentials constructed in a certain prescribed way and that the remainder of the potential, called the "reduced interaction," is sufficiently weak for the Born series to converge. The criterion for its convergence is discussed in a subsequent paper by Scadron *et al.*[9] The new operators introduced in this case are

$$J=(I-G_0V_1)^{-1}$$

and G_1V_s, where $G_1=JG_0$, V_1 is the reduced interaction, V_s is the separable potential and

$$V=V_1+V_s.$$

It should be noted that the method of orthogonality constraint, introduced earlier by Tani, is a distorted wave approach. This can be seen from (II.11), where J operating on the plane wave state ϕ gives rise to a distorted wave, i.e.,

$$J\phi=h\,, \tag{II.16}$$

which, by virtue of the orthogonality constraint, is orthogonal to the bound state. It is reasonable to expect that the Born series in the subspace orthogonal to the bound state will converge. The "orthogonalized" distorted wave h is an eigenfunction of the "orthogonalized" kinetic energy operator $K_\perp$ defined by

$$K_\perp=\Lambda_\perp K\Lambda_\perp. \tag{II.17}$$

That is, h can be determined from the equation

$$K_\perp h=K^2h \tag{II.18}$$

in conjunction with the constraint

$$(h,f)=0. \tag{II.19}$$

This can be done very easily since, due to the constraint (II.19), the operation (II.17) results effectively in the introduction of a nonlocal potential into $K_\perp$, the separability of which renders the equation (II.18) very tractable. The separable potential has the matrix element

$$(r|U'|r')=f(r)f(r')V(r')\,, \tag{II.20}$$

in terms of which we can set

$$K_\perp\approx K+U'\,. \tag{II.21}$$

These orthogonalized eigenfunctions, eigenfunctions of the scattering states, and the bound-state wave function form a complete set. A completeness proof is given in the Appendix. It is our aim to prove that the "modified" Born series in terms of the orthogonalized distorted wave converges in the presence of a bound state.

III. THE CONVERGENCE PROOF

(a) General Analysis

In this section, we intend to use the limited proving ground of the class of separable potentials to demonstrate the usefulness of the method of orthogonality constraint in curing the divergence of Born series when such nonadiabatic features as the formation of a bound state and the appearance of a resonance play an important role in a scattering process. The potential referred to has the form

$$V(k,k')=-u(k)u(k')\,, \tag{III.1}$$

which is strong enough to support one bound state. The function u is bounded and continuous everywhere. The proof is given for the one-dimensional even wave. It can immediately be extended to the s-wave case.[16] It is true that for separable potentials of the form (III.1) exact solutions can easily be obtained by summing a geometric series and with the artifice of analytic continuation the Born series is still a useful formal tool even when it diverges. But our aim is to explore the possibility of constructing a "modified" Born series which is convergent and which is consequently useful for obtaining approximate solutions to a given scattering problem involving a bound state. The choice (III.1) is mathematically very convenient for our purpose. On the basis of our analysis, it seems reasonable to believe that our method is useful in removing the divergence in a scattering problem involving a bound state. It can be argued that for potentials that can be expanded in to or approximated by[17]

$$V=-\sum_n^N \sigma_n\rangle\langle\sigma_n{}^\dagger\,, \tag{III.2}$$

the method will work if one of the terms in (III.2) is responsible for the bound state. The argument can be made plausible if the σ_n's are defined by

$$\sigma_n\rangle=V|\psi\rangle\,,$$
$$\langle\sigma_n{}^\dagger=\langle\psi_n|V\,,$$

[16] W. Kohn, Phys. Rev. 84, 495 (1951).
[17] F. Coester, Phys. Rev. 133, B1516 (1964).

where the ψ_n's are eigenstates corresponding to the eigenvalues η_n defined as follows[8]:

$$G_0 V\psi_n = \eta_n \psi_n \,, \qquad \text{(III.3)}$$

with the assumption that

$$|\eta_1| > 1 \quad \text{and} \quad |\eta_n| < 1,\, n \neq 1 .$$

It should be noted that the ψ_n's, and hence the σ_n's, are energy-dependent. But there exist potentials, such as the square-well potential, where the energy dependence gives rise to a minor effect and can be disregarded.

We shall now proceed to set up the machinery for the proof of convergence using a potential of the form given by (III.1).

From (II.11) and (II.16), we have

$$\psi = h + G_\perp V_\perp \psi \,, \qquad \text{(III.4)}$$

where $G_\perp$, in terms of the eigenfunction of $K_\perp$, is given explicitly by

$$G_\perp(k,k';W) = \int \frac{h(k,K)h^*(k',K)}{K^2 - W} dK. \qquad \text{(III.5)}$$

W in (III.5) is the complex energy. In order to prove the convergence of the Neumann series, or the modified Born series, which resulted from iterating (III.4), it is sufficient to show that the resolvent of the kernel exists, i.e., the series

$$G_\perp + G_\perp V_\perp G_\perp + G_\perp V_\perp G_\perp V_\perp G_\perp + \cdots \qquad \text{(III.6)}$$

converges. We recognize that (III.6) is the series solution of the integral equation for the resolvent

$$G = G_\perp + G_\perp V_\perp G. \qquad \text{(III.7)}$$

Substituting (III.5) into (III.6), we obtain

$$G(k,k';W) - G_\perp(k,k';W) = \int \frac{h(k,K)h^*(k',K')}{(K^2 - W)(K'^2 - W)} dK dK' S(K,K';W) \,, \qquad \text{(III.8)}$$

where

$$S(K,K';W) = M(K,K') + \int \frac{M(K,K'')M(K'',K')}{K''^2 - W} dK'' + \int \frac{M(K,K'')M(K'',K''')M(K''',K')}{(K''^2 - W)(K'''^2 - W)} \times dK'' dK''' + \cdots \qquad \text{(III.9)}$$

with the matrix element $M(K,K')$ defined by

$$M(K,K') = \int h^*(k,K) V(k,k') h(k',K') dk dk' \,, \qquad \text{(III.10)}$$

since

$$V_\perp = \Lambda_\perp V \Lambda_\perp$$

and

$$\Lambda_\perp |h\rangle = |h\rangle \,,$$
$$\langle h| \Lambda_\perp = \langle h| \,.$$

Using (III.1) and the solution to (II.18) given by

$$h(k,K) = \delta(k-K) + \chi(K) f(k) [1/(k^2 - K^2 - i\epsilon)] \,, \qquad \text{(III.11)}$$

we obtain from (III.10)

$$M(K,K') = -(1/C^2) \chi^*(K) \chi(K) \,, \qquad \text{(III.12)}$$

which follows from

$$(1/C)\chi(K) = \int h(k,K) u(k) dk \,, \qquad \text{(III.13)}$$

and

$$\chi(K) = -f(K)/D(K). \qquad \text{(III.13')}$$

In terms of (III.12), the series (III.9) now becomes

$$S(K,K';E+i\epsilon) = -(1/C^2)\chi^*(K)\chi(K') \times [1 + r_\perp(E+i\epsilon) + r_\perp^2(E+i\epsilon) + \cdots] \,, \qquad \text{(III.14)}$$

where $r_\perp(E+i\epsilon)$, the ratio of the geometric series, is given by

$$r_\perp(E+i\epsilon) = \frac{1}{C^2} \int \frac{|\chi(K)|^2}{K^2 - E - i\epsilon} dK. \qquad \text{(III.15)}$$

Note that the small positive imaginary part of the energy is explicitly shown in (III.11), (III.14), and (III.15) as required by the outgoing wave boundary condition. Since

$$D(K) = \int \frac{f^2(k)}{k^2 - K^2 - i\epsilon} dk \,, \qquad \text{(III.16)}$$

and

$$1/(x - i\delta) = P(1/x) + i\pi\delta(x) \,,$$

we have

$$D(K) = R(K) + iI(K) \,, \qquad \text{(III.17)}$$

where

$$R(K) = \int \frac{f^2(k)}{k^2 - K^2} dk \,, \qquad \text{(III.18)}$$

and

$$I(K) = (\pi/K) f^2(K). \qquad \text{(III.19)}$$

Letting $K^2 = z'$, and $E + i\epsilon = z$, we obtain from (III.15)

$$r_\perp(z) = \frac{1}{C^2 \pi} \int_0^\infty \frac{I(z')}{R^2(z') + I^2(z')} \frac{dz'}{z' - z}. \qquad \text{(III.20)}$$

According to (A5) and (A10),

$$\frac{1}{\pi} \int_0^\infty \frac{I(z')}{R^2(z') + I^2(z')} \frac{dz'}{z' - z} = -\gamma(z) \,, \qquad \text{(III.21)}$$

where

$$\gamma(z) = [1/D(z)] + z - \alpha. \qquad \text{(III.22)}$$

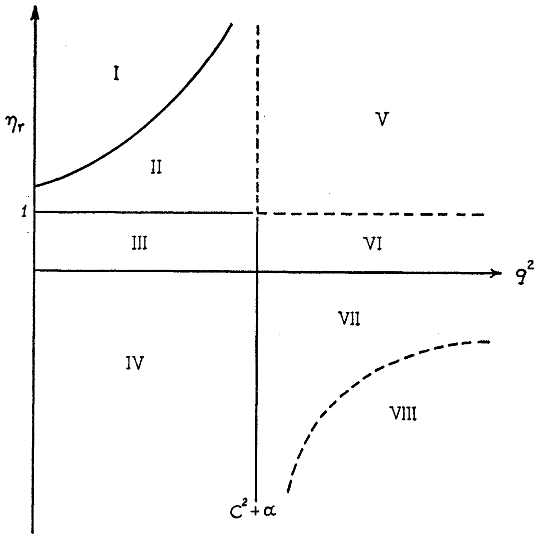

FIG. 1. The eight regions for the classification of potentials. I, III, and IV are regions of unconditional convergence. II, VI, and VII are regions of conditional convergence. V and VIII are regions where convergence is not possible. The dashed lines are boundaries included in the impossible regions.

The constant α in (III.22) is

$$\alpha=\int f^2(k)k^2dk\,, \tag{III.23}$$

which is the kinetic energy of the bound state. α can be shown to be related to the normalization constant C and the bound state energy $-B^2$ by the simple equation

$$\alpha-C^2=-B^2.$$

In terms of the above, it is of interest to point out that C^2 can be interpreted as the magnitude of the "potential energy" associated with the bound state.

From (III.20), (III.21), and (III.22), we have

$$r_\perp(z)=-(1/C^2)[(1/D(z))+z-\alpha]. \tag{III.24}$$

$D(z)$, according to (A7), is given by

$$D(z)=-[z+\alpha-F(z)]/z^2\,, \tag{III.25}$$

where

$$F(z)=\int\frac{f^2(k)k^4}{k^2-z}dk. \tag{III.26}$$

Evaluation of the integral in (III.26) gives

$$F(z)=\frac{\alpha(z+B^2)B^2+C^2z[B^2+z\eta_r(E)]+iC^2z^2\eta_i(E)}{(z+B^2)^2}, \tag{III.27}$$

where η_r and η_i are the real and imaginary parts of the eigenvalue defined in (III.3):

$$\eta(E+i\epsilon)=\int\frac{u^2(k)}{k^2-E-i\epsilon}dk=\eta_r(E)+i\eta_i(E). \tag{III.28}$$

From (III.24), (III.25), and (III.27) and after some extensive algebraic manipulations, we obtain

$$r_\perp(z)=-\frac{C^2+(z-\alpha)\eta_r(E)+i(z-\alpha)\eta_i(E)}{z+C^2+B^2-C^2\eta_r(E)-iC^2\eta_i(E)}, \tag{III.29}$$

By letting $\epsilon\rightarrow 0$, z becomes $E=q^2$, and the ratio now becomes

$$r_\perp(q^2)=-\frac{X(q^2)+iY(q^2)}{W(q^2)+iZ(q^2)}, \tag{III.30}$$

where

$$X(q^2)=C^2+(q^2-\alpha)\eta_r(q^2),$$
$$Y(q^2)=(q^2-\alpha)\eta_i(q^2)\,,$$
$$W(q^2)=q^2+C^2+B^2-C^2\eta_r(q^2)\,,$$
$$Z(q^2)=-C^2\eta_i(q^2)\,.$$

If we can show that

$$|r_\perp(q^2)|<1 \tag{III.31}$$

for all values of q^2, then we have succeeded in proving the absolute and uniform convergence of (III.13). This means that we must show that

$$\frac{X^2(q^2)+Y^2(q^2)}{W^2(q^2)+Z^2(q^2)}<1\,,$$

or

$$\eta_i^2(C^2+\alpha-q^2)>[(q^2-C^2-\alpha)\eta_r(q^2)+q^2+B^2+2C^2]\times[\eta_r(q^2)-1], \tag{III.32}$$

which is the condition that has to be satisfied for convergence.

(b) Classification of Potentials

To draw useful conclusions from (III.32), we find it helpful to classify potentials into different categories by plotting $\eta_r(q^2)$ against q^2 as shown in Fig. 1. It will be seen, as concluded at the end of this subsection, that the case where a resonance or an antiresonance[18] exists above a certain energy has to be excluded since we have not done anything to cope with the divergence of Born series caused by such a phenomenon.

It is evident from the inequality (III.32) that the convergence depends upon the behavior of $\eta_r(q^2)$ and $\eta_i(q^2)$ as a function of the energy variable q^2, which in turn depends upon the properties of the potential function $u(k)$. Referring to the graph, we divide the $q^2\geq 0$ energy domain into eight regions as suggested by the inequality (III.32) itself. To simplify the analysis further, we also consider the different possible cases

[18] When η_r crosses unity, we shall state that there is a resonance (an antiresonance) if the phase shift is rising (falling) through $\pi/2$ (mod π).

with respect to energy and the sign of η_r as follows:

(1) Case 1: $q^2<C^2+\alpha$, $\eta_r\geq 0$. Includes regions I, II, and III.

(a) $\eta_i(0)\neq 0$,
(b) $\eta_i(0)=0$.

(2) Case 2: $q^2<C^2+\alpha$, $\eta_r<0$. Includes region IV.

(3) Case 3: $q^2=C^2+\alpha$.

(4) Case 4: $q^2>C^2+\alpha$, $\eta_r\geq 0$. Includes regions V and VI.

(5) Case 5: $q^2>C^2+\alpha$, $\eta_r<0$. Includes regions VII and VIII.

Let us now proceed with the analysis.

Consider Case 1(a). In this case, $\eta_i\neq 0$ is always satisfied in one-dimensional problems. In fact, $\eta_i(0)=\infty$.

Region I: $\eta_r(q^2)\geq(q^2+2C^2+B^2)/(C^2+\alpha-q^2)$.

The right-hand side (rhs) of the inequality is negative definite or zero while the left-hand side (lhs) is positive definite and nonvanishing on account of $\eta_i(0)\neq 0$. Hence, the inequality is always satisfied and convergence is unconditionally guaranteed.

Region II: $1<\eta_r(q^2)<(q^2+2C^2+B^2)/(C^2+\alpha-q^2)$.

In this region, both the lhs and the rhs are positive definite. Therefore, (III.32) provides a functional relationship between $\eta_r(q^2)$ and $\eta_i(q^2)$ that has to be satisfied within the energy range within which the $\eta_r(q^2)$ lies in this region. This requirement imposes certain restrictions on the potential and can be met by a variety of appropriate potentials, such as those we consider as examples towards the end of this section.

Region III: $0\leq\eta_r\leq 1$.

Same as for region I.

Case 1(b) is important in three-dimensional cases or when odd waves in a one-dimensional problem are considered. In this case, the lhs vanishes at zero energy and the inequality can be satisfied only if

$$\eta_r(0)>1+[2B^2/(C^2+\alpha)]. \tag{III.33}$$

This means that η_r must enter the positive energy domain through region I. This requirement is not entirely impossible and can most likely be met in all cases. Because it is known that

$$\eta(-B^2)=1, \tag{III.34}$$

and $\eta(q^2)$ is a monotonically increasing function for negative energies as energy increases from $-B^2$ to zero. It can be shown that

$$\eta(0)>1+(B^2/C^2). \tag{III.35}$$

But

$$\eta(0)=[\eta_r^2(0)+\eta_i^2(0)]^{1/2}=\eta_r(0), \tag{III.36}$$

since $\eta_i(0)=0$ in this case. From (III.35) and (III.36) we obtain

$$\eta_r(0)>1+(B^2/C^2) \tag{III.37}$$

as a lower bound for $\eta_r(0)$. The actual value of $\eta_r(0)$ for any potential might be much larger and still satisfy (III.33).

Region IV: $\eta_r<0$.

This region is under Case 2. For negative values of η_r, the inequality (III.32) can be rewritten as

$$\eta_i^2(C^2+\alpha-q^2)>-(1+|\eta_r|)\times[q^2+B^2+2C^2+(C^2+\alpha-q^2)|\eta_r|]. \tag{III.38}$$

From (III.38), it is evident that unconditional convergence is guaranteed in this region even if $\eta_i(0)=0$.

Case 3, where $q^2=C^2+\alpha$ is a borderline case. Since the lhs vanishes, the rhs must be positive definite in order to satisfy the inequality. This is met if

$$\eta_r(C^2+\alpha)<1. \tag{III.39}$$

Region V: $\eta_r\geq 1$.

This is a region in which the inequality is never satisfied. Hence, convergence is impossible if $\eta_r\geq 1$ for $p^2>C^2+\alpha$.

Region VI: $0\leq\eta_r<1$.

It can be shown that in this region the convergence is contingent upon the condition

$$\eta_i^2(q^2)<(1-\eta_r)\left(\eta_r+\frac{q^2+B^2+2C^2}{q^2-C^2-\alpha}\right). \tag{III.40}$$

Region VII: $(q^2+B^2+2C^2)/(C^2+\alpha-q^2)<\eta_r<0$.

Referring to (III.40), we obtain the condition for negative values of η_r as follows:

$$\eta_i^2(q^2)<(1+|\eta_r|)\left(\frac{q^2+B^2+2C^2}{q^2-C^2-\alpha}-|\eta_r|\right). \tag{III.41}$$

Region VIII: $\eta_r\leq(q^2+B^2+2C^2)/(C^2+\alpha-q^2)$.

This is again a region where convergence is impossible to achieve.

We note that when $|\eta|\geq 1$ for some positive energy, there is, roughly speaking, a resonance or an antiresonance. In regions V and VIII, it is impossible to have convergence because $|\eta|\geq 1$. Therefore, for potentials which produce resonances or antiresonances at energies greater than or equal to $C^2+\alpha$, the method of orthogonality constraint cannot cure the divergence of the Born series. The divergence due to an antiresonance at low energies can be cured by our method once the bound-state effect is removed. This is what happens when in certain regions convergence of the modified Born series is guaranteed even for values of η_r greater than unity. The problem of removing the effect of resonances or antiresonances at high energies is not within the scope of our investigation and therefore will not be discussed.

We now investigate the behavior of $r_\perp(q^2)$ for $q^2<0$. From (III.24), (III.25) and (III.26), since $q^2=E$ and $z=q^2+i\epsilon$, $r_\perp(0)$ can be obtained by evaluating (III.24) for $q^2=0$ and then letting ϵ go to zero. In so doing, we find that

$$r_\perp(0)=\alpha/C^2<1. \qquad \text{(III.42)}$$

We note that $r_\perp(-|q^2|)$ is a monotonically increasing function of $|q^2|$, i.e., $r_\perp(-|q^2|)$ increases as q^2 decreases. In view of (III.42), therefore, $r_\perp(-|q^2|)$ is less than unity for all negative values of q^2.

(c) Examples

We shall now make use of the results of the above analysis to test the convergence for a number of separable potentials.

(1) Delta-function potential:

$$u(k)=(B/\pi)^{1/2}=\text{constant},$$
$$\eta_r(q^2)=0,$$
$$\eta_i(q^2)=B/q.$$

$\eta_r(q^2)$ is on the positive q^2 axis and runs through region III, the point $q^2=C^2+\alpha$ and region VI. In region III, convergence is unconditional. At $q^2=C^2+\alpha$, since $\eta_r=0<1$, the condition (III.39) is satisfied. In region VI, the inequality (III.40) leads to

$$-B^2(C^2+\alpha)<p^2(p^2+2C^2)$$

which is certainly true. Therefore, convergence is guaranteed by the method.

(2) Square-well separable potential (in configuration space):

$$u(k)=2V_0\sin ka/k$$
$$\eta_r(q^2)=-(4\pi V_0^2a/q^2)[1-(\sin 2aq/2aq)]$$
$$\eta_i(q^2)=4\pi V_0^2\sin^2 aq/q^3.$$

Since η_r is negative, it goes through region IV where convergence is unconditional. It is easy to see by choosing appropriate value for the product V_0a, η_r can be made to pass through region VII and the inequality (III.41) be satisfied.

It is also instructive to see that by making $a\to 0$ and $V_0\to\infty$ such that the product V_0a remains constant and letting $2V_0a=B/\pi$, one obtains

$$\eta_r\to 0,\quad \eta_i\to B/q.$$

In other words, in the limit, the square-well potential approaches the delta-function potential.

IV. REARRANGEMENT COLLISIONS

The model problem we consider here was formulated by Schwebel.[14] It is a one-dimensional problem with the Hamiltonian of the form

$$H=K_1+K_2+V_1+V_2+V_{12}, \qquad \text{(IV.1)}$$

where the K's and V's have the same meaning as defined before. The subscripts denote the two particles, 1 and 2, which are assumed to have the same mass m. The third particle, the "nucleus," is assumed to have an infinite mass. The initial state of the system is that particle 1 is incident with momentum K_0 while particle 2 is bound to the nucleus by the potential V_2, the bound-state energy being $-B^2$ ($\hbar=2m=1$). The potentials V_1 and V_2 in the model problem are delta-function potentials having, respectively, the following matrix elements in momentum space:

$$V_1(k_2,k_2')=-(B/\pi)\delta(k_2-k_2'); \qquad \text{(IV.2)}$$

$$V_2(k_1,k_1')=-(B/\pi)\delta(k_1-k_1'). \qquad \text{(IV.3)}$$

The matrix element of V_{12} is separable. The exact solution to the problem has been obtained by Schwebel; therefore, the elastic, inelastic and exchange scattering amplitudes are known. It has also been demonstrated that the asymmetric-perturbation approach, i.e., considering V_1 and V_{12} as perturbation, gives rise to a Born series containing a geometric subseries with ratio

$$r=iB/(K_0^2-B^2-k_2^2)^{1/2}. \qquad \text{(IV.4)}$$

The ratio becomes unity, and consequently the Born series diverges as no cancellation of the divergent subseries is possible at the singularity $k_2=K_0$, the singularity needed for exchange scattering. Besides, the asymmetric perturbation approach fails to yield the exchange scattering amplitude to any order of the Born approximation. In what follows we shall show that the divergence in the subseries is cured by the method of orthogonality constraint and that the "modified" asymmetric approach yields its first Born approximation to the exchange scattering amplitude in good agreement with the exact solution.

Corresponding to the bound state in the original channel and that in the rearranged channel, we introduce two sets of projection operators defined by the following matrix elements:

$$(k_i|\Lambda_{i\parallel}|k_i')=f(k_i)f(k_i') \qquad \text{(IV.5)}$$

and

$$(k_i|\Lambda_{i\perp}|k_i')=\delta(k_i-k_i')-f(k_i)f(k_i'), \qquad \text{(IV.6)}$$
$$i=1,2,$$

where $f(k)$ is the bound-state wave function in momentum space. With the use of these operators, the Hamiltonian in (IV.1) can be transformed into

$$H=-B^2(\Lambda_{1\parallel}+\Lambda_{2\parallel})+K_{1\perp}+V_{1\perp}+K_{2\perp}+V_{2\perp}+V_{12}. \qquad \text{(IV.7)}$$

The binding effect of V_1 and V_2 is taken care of by the operators $\Lambda_{i\parallel}$ ($i=1,2$). On the other hand, the scattering effect or the initial (final) state interaction is described by $V_{1\perp}(V_{2\perp})$.

Our modified asymmetric-perturbation approach considers either $V_{1\perp}+V_{12}$ or $V_{2\perp}+V_{12}$ as perturbation and the resulting integral equations are

$$\psi=\psi_{1\perp}+G_{1\perp}(V_{1\perp}+V_{12})\psi \tag{IV.8}$$

and

$$\psi=\psi_{2\perp}+G_{2\perp}(V_{2\perp}+V_{12})\psi, \tag{IV.9}$$

where

$$\psi_{1\perp}=h_1f_2, \tag{IV.10}$$

$$\psi_{2\perp}=\xi_1f_2, \tag{IV.11}$$

$$G_{1\perp}=[E+B^2(\Lambda_{1\|}+\Lambda_{2\|})-K_{1\perp}-K_{2\perp}-V_{2\perp}]^{-1}, \tag{IV.12}$$

and

$$G_{2\perp}=[E+B^2(\Lambda_{1\|}+\Lambda_{2\|})-K_{1\perp}-K_{2\perp}-V_{1\perp}]^{-1}. \tag{IV.13}$$

The modified Born series can be obtained by iterating (IV.8) or (IV.9), which will contain a subseries in $V_{1\perp}$ or $V_{2\perp}$. Either one is a geometric series. By dropping the subscript, the ratio of these geometric series is given by

$$r_\perp(K_2)=iB/[(E-K_2^2)^{1/2}+2iB]. \tag{IV.14}$$

It is evident from (IV.14) that the ratio remains less than unity for all values of its argument. Hence, the subseries is absolutely and uniformly convergent. A comparison between (IV.14) and (IV.4) indicates that the method of orthogonality constraint applied to the problem with a rearrangement of particles greatly improves the convergence property of the Born series. With the bound particle 2 outgoing with momentum K_0, the ratios are

$$r=1$$

and

$$r_\perp=1/3.$$

Therefore, the kind of divergence pointed out by AAL is removed and, if V_{12} does not have any nonadiabatic effects on the scattering, the modified Born series may very well be convergent. The investigation of the effect of V_{12} on the convergence properties of the Born series is outside the scope of the paper. Let us instead evaluate the first Born approximation from (IV.8) and (IV.9).

Since $V_{1\perp}$, being orthogonal to the bound state of particle 1, will not effect the binding of that particles to result in an exchange and

$$(V_{2\perp},f_2)=0,$$

the first Born approximations of (IV.8) and (IV.9) are given, respectively, by

$$\psi^{(1)}=G_{1\perp}V_{12}\psi_{1\perp} \tag{IV.15}$$

and

$$\psi^{(1)}=G_{2\perp}V_{12}\psi_{2\perp}. \tag{IV.16}$$

Two different results are obtained by evaluating the integrals, the latter being in better agreement with the exact exchange scattering amplitude. The difference between the two results is not the well-known post-prior discrepancy. The two values correspond to the two extremes of the first Born approximation to the exchange scattering amplitude that can be obtained by applying the method of orthogonality constraint to the problem. For, by comparing the initial states (IV.10) and (IV.11), we note that the particle-1 states, h_1 and ξ_1, are different, being related by

$$\xi_1=h_1+G_\perp^{(1)}V_{1\perp}\xi_1, \tag{IV.17}$$

where

$$G_\perp^{(1)}=1/(E_1-K_{1\perp}).$$

(IV.17) has series solution

$$\xi_1=h_1+G_\perp^{(1)}V_{1\perp}h_1+G_\perp^{(1)}V_{1\perp}G_\perp^{(1)}V_{1\perp}h_1+\cdots, \tag{IV.18}$$

which can be shown to be an absolutely and uniformly convergent geometric series with a ratio of the form given in (IV.14). Therefore, the state ξ_1 has accounted completely for the influence of the potential V_1. In other words, the initial state interaction on particle **1** is fully taken into account, and consequently the use of ξ_1 should give a better result. It is reasonable to expect that the inclusion of higher order terms of (IV.18) in $\psi_{1\perp}$ of (IV.10) will improve the Born approximation (IV.15). In the example of our model problem, we have seen that the method of orthogonality constraint applied to rearrangement collisions not only guarantees the convergence but also provides a prescription for improving approximate calculations.

ACKNOWLEDGMENT

The authors wish to thank Professor L. Rosenberg for a number of helpful discussions.

APPENDIX

We shall prove that the orthogonalized distorted wave $h(k,K)$ and the bound state wave function $f(k)$ form a complete set.[19] That is,

$$\int h(k,K)h^*(k',K)dK+f(k)f^*(k')=\delta(k-k'). \tag{A1}$$

The normalized solution of $h(k,K)$ under outgoing wave boundary conditions is given by

$$h(k,K)=\delta(k-K)+\chi(K)f(k)\frac{1}{k^2-K^2-i\epsilon}. \tag{A2}$$

Evaluating the integral in (A1), we obtain

$$\int h(k,K)h^*(k',K)dK =\delta(k-k')+\frac{\chi^*(k)f^*(k')}{k'^2-k^2+i\epsilon}+\frac{\chi(k')f(k)}{k^2-k'^2-i\epsilon} +\mathcal{J}(k,k')f(k)f^*(k'), \tag{A3}$$

[19] One of the authors (S.T.) would like to express his gratitude to Professor K. W. Symanzik for useful suggestions to the proof given here.

where

$$\mathcal{G}(k,k')=\int\frac{\chi(K)\chi^*(K)}{(K^2-k^2+i\epsilon)(K^2-k'^2-i\epsilon)}dK. \quad \text{(A4)}$$

According to (III.13), (III.17), and (III.19),

$$\chi(K)\chi^*(K)=\frac{2}{\pi}\frac{KI(K)}{R^2(K)+I^2(K)}=\frac{2K}{\pi}\,\mathrm{Im}D^{-1}(K), \quad \text{(A5)}$$

where Im denotes the imaginary part of the function. Now consider the function

$$D(z)=\int\frac{f^2(E)}{E-z}dE \quad \text{(A6)}$$

of a complex variable z, which for large values of $|z|$ can also be written as

$$D(z)=-\frac{1}{z}-\frac{\alpha}{z^2}+\frac{1}{z^2}\int\frac{f^2(k)k^4}{k^2-z}dk. \quad \text{(A7)}$$

Let

$$\gamma(z)=D^{-1}(z)+z-\alpha, \quad \text{(A8)}$$

where

$$\alpha=\int f^2(k)k^2dk.$$

From (A7) and (A8), it is obvious that for $|z|\to\infty$, $|\gamma(z)|\to 0$. Therefore, according to the Cauchy integral formula,

$$\frac{1}{2\pi i}\oint\frac{dz'}{z'-z}\gamma(z')=\gamma(z). \quad \text{(A9)}$$

Since $\gamma(z)$ has a discontinuity across the real axis, evaluating the contour integral, we obtain from (A9)

$$\gamma(z)=-\frac{1}{\pi}\int\mathrm{Im}D^{-1}(z')\frac{dz'}{z'-z}. \quad \text{(A10)}$$

Let $E=K^2$, $z^*=k^2-i\epsilon$, and $z'=k'^2+i\epsilon$. Then the integral (A4) becomes

$$\mathcal{G}(z,z'^*)=-\frac{1}{\pi}\frac{1}{z^*-z'}\int\mathrm{Im}D^{-1}(E)\left(\frac{1}{E-z^*}-\frac{1}{E-z'}\right)dE. \quad \text{(A11)}$$

Using (A10) and (A8), we have

$$\mathcal{G}(k,k')=\frac{1}{k^2-k'^2-2i\epsilon}[-D^{-1}(k')^*+D^{-1}(k')]-1, \quad \text{(A12)}$$

since, according to definition,

$$D(z^*)=D^*(z).$$

With the use of the reality of $f(k)$ and (III.13), substitution of (A12) into (A3) establishes immediately the completeness condition (A1).