Divergence of the Green's Function Series for Rearrangement Collisions*

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The convergence of the Born series for rearrangement collisions is investigated in a potential model. For a certain class of potentials it is shown that the iterated series for the full two particle Green's function, $(\mathbf{k}_1'\mathbf{k}_2'|G(E)|\mathbf{k}_1\mathbf{k}_2)$, in terms of either the free-particle Green's function, the initial state Green's function, or the final state Green's function, diverges for some continuous range of the variables \mathbf{k}_1 , \mathbf{k}_2 , \mathbf{k}_1' , and \mathbf{k}_2' independent of the energy, E, of the incident particle. It is suggested that the usual Born series, which is an integral over this Green's function series, therefore, also diverges for rearrangement collisions independent of the incident energy.

I. INTRODUCTION

ALCULATIONS on rearrangement collisions have been a subject for theoretical investigation since the early days of quantum mechanics. Among the more popular problems which have been treated in a nonrelativistic potential formalism are exchange scattering of an electron by an atom,¹ charge transfer between H⁺ and H,² and nuclear stripping reactions.³ For the most part, calculations have been limited to evaluation of the first and second Born approximations. While exact formal expressions for the cross sections are well established,⁴ to our knowledge the validity of the Born expansion for rearrangement collisions has never been investigated. The validity of the first Born approximation in the low-energy region has been partially explained by several authors.⁵ A natural question to ask is whether the Born expansion converges in the high-energy limit as does the Born series for the scattering of a particle by a potential.⁶ In this note we address ourselves to the question of convergence of the Born expansion for the full Green's function. We maintain that while the matrix elements calculated up to second order may well be part of a convergent scheme, the series expansion of the full Green's function in terms of the free-particle Green's function diverges; in fact, we shall prove that several of the more obvious iterative series for rearrangement collisions diverge.

In a rearrangement collision a particle, for example a neutron in a (d, p) reaction, is exchanged between the

incident particle and the target. If we examine the Born expansion of the full Green's function, $(\mathbf{n'p'}|G(E)|\mathbf{np})$, for this process we find that the convergence of the series is not necessarily determined by the incident energy E. The relevent energy involved in the Green's function expansion is not E, but a variable we call E', which is related to the magnitude of the momentum transfer to the exchanged particle. The problem of convergence of the Green's function series for rearrangement collisions then reduces to considering the three dimensional Green's function series for the scattering of the exchanged particle with incident energy E' on the target (assumed to be a potential). The variable E'is permitted to take on all possible negative values. It is proven in the text that if a bound state exists (as it must in a rearrangement collision) with energy $-E_B$ the above series will diverge for $-E_B \ge E' > 0$, and thus that the usual iterated series for the full two-particle Green's function $(\mathbf{n'p'}|G(E)|\mathbf{np})$ diverges for some continuous range of the variables n', p', n, and p. The situation in rearrangement collisions, therefore, is quite different from the case of the usual three dimensional scattering of a particle by a potential, where if the incident energy E is made large enough, the Born expansion for the Green's function $(\mathbf{k}' | G(E) | \mathbf{k})$, converges uniformly with respect to **k** and \mathbf{k}' .⁶

In the transition amplitude for the rearrangement process G(E') is integrated over a range of energies E'including negative values of E'. More precisely, the Born series, T_{fi} , for the transition amplitude may be considered as an integral over a set of subseries $T_{fi}(E')$, each subseries being obtained from the Born series for G(E'). We shall argue later in the text that the divergence of Green's function expansion in a continuous range of E' will, except for fortuitous cancellations, insure the divergence of the full Born series for T_{fi} .

In Sec. II we shall prove that for the case of an attractive potential whose Fourier transform is always negative, the three natural iterative series, the one in terms of the free-particle Green's function, the one in terms of the initial state Green's function, and the one in terms of the final state Green's function, all diverge. In Sec. III we discuss implications of our results in the formal theory of rearrangement collisions. In the Appen-

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Harrison Special Fellow. For bibliography see H. W. S. Massey, *Encyclopedia of Physics* (Springer-verlag, Berlin, 1956), Vol. 36, p. 232.

² Literature can be traced back from R. H. Bassel and E. Geriuoy, Phys. Rev. 117, 749 (1960).

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⁶ C. Zemach and A. Klein, Nuovo cimento 10, 1078 (1958); See also N. N. Khuri, Phys. Rev. 107, 1148 (1957); W. Kohn, Revs. Modern Phys. 26, 292 (1954); R. Jost and A. Pais, Phys. Rev. 82, 840 (1951); R. Blankenbecler, M. L. Goldberger, N. N. Khuri and S. B. Treiman Ann Phys 10 64 (1960)</sup> Khuri, and S. B. Treiman, Ann. Phys. 10, 64 (1960).

dix the case of a separable potential is treated exactly to illustrate mathematical assertions made in the text.

II. PROOF

Without loss of generality we investigate the case of two particles bound by a potential V_i incident on a fixed center of force giving rise to a potential V_f . The preceding picture may describe, for example, a deuteron incident on an infinitely heavy nucleus where V_i is the neutron-proton potential, V_f is the effective potential of the nucleus,⁷ and electromagnetic interactions have been switched off. As a further simplification let us suppose that V_f acts on only one of the incident particles, for example, the neutron. The Hamiltonian for the system is

$$H = T + V_i + V_f, \tag{1}$$

where T is the sum of the kinetic energies of the two particles. We may now define four Green's functions; the total or full Green's function G, the free-particle Green's function G_0 , the initial state Green's function G_i , and the final state Green's function G_f . They satisfy the following operator equations^{8,9}:

$$(T+V_i+V_f-E)G = -1, \quad (T+V_i-E)G_i = -1,$$

 $(T-E)G_0 = -1, \quad (T+V_f-E)G_f = -1.$ (2)

They are inter-related by

(a)
$$G = G_0 + G_0 (V_i + V_f) G$$
,
(b) $G = G_i + G_i V_f G$,
(c) $G = G_f + G_f V_i G$.
(3)

For future reference let us denote the quantity $(T+V_i)$ as the initial Hamiltonian H_i , and $(T+V_f)$ as the final Hamiltonian H_f . In the integral formulation of the scattering problem a wave function is sought which satisfies one of the following equations:

$$\Psi_i^{(\pm)} = \phi_i + G_i^{(\pm)} V_f \Psi_i^{(\pm)}$$

= $\phi_i + G^{(\pm)} V_f \phi_i,$ (4)

$$\Psi_{f}^{(\pm)} = \phi_{f} + G_{f}^{(\pm)} V_{i} \Psi_{f}^{(\pm)}$$

$$= \phi_{f} + G^{(\pm)} V_{i} \phi_{f},$$
(5)

where the superscripts (+) and (-) denote the outgoing and incoming boundary conditions. ϕ_i and ϕ_f are solutions of the initial and final Hamiltonians, respectively, and

$$\phi_i = e^{i\mathbf{k}_d \cdot (\mathbf{r}_p + \mathbf{r}_n)/2} u_d(|\mathbf{r}_p - \mathbf{r}_n|), \quad \phi_f = e^{i\mathbf{k}_p \cdot \mathbf{r}_p} v(|\mathbf{r}_n|), \quad (6)$$

where k_d and k_p are the incident deuteron and final

proton momenta, respectively;

$$E = k_{d/2}^2 - E_d = k_p^2 - E_n; \tag{7}$$

 u_d is the internal deuteron wave function, and v is the wave function of the neutron bound in the potential. The T matrix describing the transition $i \rightarrow f$ may be written¹⁰

$$T_{fi} = (\phi_f, V_i \Psi_i^{(+)}). \tag{8}$$

Substitution of Eqs. (3) and (4) in Eq. (8), and iteration according to Eq. (3a) defines the Born series:

$$(\phi_f, V_i \Psi_i^{(+)}) = (\phi_f, V_i \phi_i) + (\phi_f, V_i G_0 V_f \phi_i) + (\phi_f, V_i G_0 (V_i + V_f) G_0 \phi_i) + \cdots$$
(9)

We shall denote by R_{fi} the difference of T_{fi} and its first Born approximation $T_{fi}{}^{B} = (\phi_{f}, V_{i}\phi_{i}).$

$$R_{fi} = (\phi_f, V_i G V_f \phi_i). \tag{10}$$

Upon substituting complete sets of plane waves of neutrons and protons, we obtain

$$R_{fi} = \sum_{\mathbf{n},\mathbf{p}} \sum_{\mathbf{n}',\mathbf{p}'} (f | V_i | \mathbf{n}\mathbf{p}) (\mathbf{n}\mathbf{p} | G | \mathbf{n}'\mathbf{p}') (\mathbf{n}'\mathbf{p}' | V_f | i).$$
(11)

It is important to note that in a rearrangement collision, since ϕ_i and ϕ_f describe at least one particle in a bound state, neither of the matrix elements $(f|V_i|\mathbf{np})$ nor $(\mathbf{n'p'}|V_f|i)$ contains any delta functions on energy or momentum,10 and thus the intermediate momenta \mathbf{n} , \mathbf{p} , \mathbf{n}' , \mathbf{p}' can assume all possible values. We now consider the iterated series for the full Green's function in Eq. (10):

$$(\mathbf{np} | G(E) | \mathbf{n'p'}) = (2\pi)^{6} \delta(\mathbf{n} - \mathbf{n'}) \delta(\mathbf{p} - \mathbf{p'}) G^{(0)}(\mathbf{n}, \mathbf{p}; E) + G^{(0)}(\mathbf{n}, \mathbf{p}; E) v(\mathbf{n} - \mathbf{n'}; \mathbf{p} - \mathbf{p'}) G^{(0)}(\mathbf{n}, \mathbf{p}; E) + \frac{1}{(2\pi)^{6}} \int dn'' \int dp'' G^{(0)}(\mathbf{n}, \mathbf{p}; E) v(\mathbf{n} - \mathbf{n''}; \mathbf{p} - \mathbf{p''}) \times G^{(0)}(\mathbf{n''}, \mathbf{p''}; E) v(\mathbf{n''} - \mathbf{n'}; \mathbf{p''} - \mathbf{p'}) \times G^{(0)}(\mathbf{n'}, \mathbf{p''}; E) + \cdots, \quad (12)$$

where

$$G^{(0)}(\mathbf{n},\mathbf{p}; E) = \frac{1}{E + i\eta - n^2 - p^2},$$
 (13)

and

$$\eta(\mathbf{k};\mathbf{q}) = \int d\mathbf{r}_n \int d\mathbf{r}_p \, e^{i(\mathbf{k}\cdot\mathbf{r}_n+\mathbf{q}\cdot\mathbf{r}_p)} \\ \times [V_i(|\mathbf{r}_n-\mathbf{r}_p|) + V_f(|\mathbf{r}_n|)]. \quad (14)$$

In order to prove the divergence of the Born series, Eq. (12), it is sufficient to consider the following subseries I_f of terms containing only the Fourier

⁷ The nucleus is assumed to have infinite mass and the spins of

The nucleons are ignored. ⁸ The boundary conditions associated with these equations are well understood. See E. Gerjuoy, Ann. Phys. 5, 58 (1958); and E. Gerjuoy, Phys. Rev. 109, 1806 (1958). ⁹ We take units in which $\hbar = 2m = 1$.

¹⁰ B. A. Lippmann (see reference 4).

5)

transform of V_f :

$$I_{f}(\mathbf{n},\mathbf{n}'; E-p^{2}) = V_{f}(\mathbf{n}-\mathbf{n}') + \frac{1}{(2\pi)^{3}} \int d\mathbf{n}'' V_{f}(\mathbf{n}-\mathbf{n}'') \\ \times G^{(0)}(\mathbf{n}'',\mathbf{p}; E) V_{f}(\mathbf{n}''-\mathbf{n}') + \cdots \\ = V_{f}(\mathbf{n}-\mathbf{n}') + \frac{1}{(2\pi)^{3}} \int d\mathbf{n}'' V_{f}(\mathbf{n}-\mathbf{n}'') \\ \times \frac{1}{(E-p^{2}+i\eta)-n''^{2}} V_{f}(\mathbf{n}''-\mathbf{n}') \\ + \frac{1}{(2\pi)^{6}} \int dn'' \int dn''' V_{f}(\mathbf{n}-\mathbf{n}'') \\ \times \frac{1}{(E-p^{2}+i\eta)-n''^{2}} V_{f}(\mathbf{n}''-\mathbf{n}'') \\ \times \frac{1}{(E-p^{2}+i\eta)-n''^{2}} V_{f}(\mathbf{n}''-\mathbf{n}') + \cdots$$
(1)

Equation (15) may be interpreted as the formal expansion of the final state interaction operator, defined by

$$(\mathbf{n},\mathbf{p}|G_{f}(E)|\mathbf{n}'\mathbf{p}') = (2\pi)^{3}\delta(\mathbf{p}-\mathbf{p}')[(2\pi)^{3}\delta(\mathbf{n}-\mathbf{n}')G^{(0)}(\mathbf{n}\mathbf{p};E) + G^{(0)}(\mathbf{n},\mathbf{p};E)I_{f}(\mathbf{n},\mathbf{n}';E-p^{2})G^{(0)}(\mathbf{n}',\mathbf{p}';E)].$$
(16)

The interaction operator $I_f(\mathbf{q},\mathbf{q}'; E)$ satisfies the integral equation

$$I_{f}(\mathbf{q},\mathbf{q}'; E) = V_{f}(\mathbf{q} - \mathbf{q}') + \frac{1}{(2\pi)^{3}} \int dq'' V_{f}(\mathbf{q} - \mathbf{q}'') \\ \times \frac{1}{E + i\eta - q''^{2}} I_{f}(\mathbf{q}'',\mathbf{q}'; E). \quad (17)$$

We now proceed with the machinery set up in the last paragraph to prove divergence of Born series for a somewhat restricted class of potentials. We insist upon an attractive potential whose Fourier transform is always negative for all real values of momentum. This class, however, includes all the more common potentials such as the Gaussian, the exponential, the Yukawa, and the Hulthén potentials, and one would indeed be surprised if the result were not true in general for attractive potentials. The instructive case of a separable potential is treated in detail separately in the Appendix. We again emphasize that, in the final expressions for the transition amplitude, such as Eq. (11), **p** is integrated over all momentum space, and therefore the argument $E - p^2$ of I_f in Eq. (15) can take on negative

and positive values.¹¹ If we let

$$V_f(\mathbf{q}) = -\lambda_f M(\mathbf{q}), \quad \lambda_f > 0, \quad M(\mathbf{q}) \ge 0, \quad (18)$$

and consider only those values of **p** for which $\alpha^2 = p^2 - E$ >0, then the $i\eta$ in Eq. (15) is superfluous, and Eq. (15) can be rewritten in the form

$$I_{f}(\mathbf{q},\mathbf{q}'; -\alpha^{2}) = \lambda_{f} M(\mathbf{q} - \mathbf{q}') + \frac{\lambda_{f}^{2}}{(2\pi)^{3}} \int \mathbf{d}q'' M(\mathbf{q} - \mathbf{q}'') \frac{1}{q''^{2} + \alpha^{2}} M(\mathbf{q}'' - \mathbf{q}') + \frac{\lambda_{f}^{3}}{(2\pi)^{6}} \int \mathbf{d}q'' \int \mathbf{d}q''' M(\mathbf{q} - \mathbf{q}'') \frac{1}{q''^{2} + \alpha^{2}} M(\mathbf{q}'' - \mathbf{q}''') \times \frac{1}{q'''^{2} + \alpha^{2}} M(\mathbf{q}''' - \mathbf{q}') + \cdots$$
(15')

This clearly is the Neumann series solution of the integral equation, Eq. (17). Note that each term on the right-hand side of Eq. (15') is positive and its derivative with respect to α^2 is negative. Thus $I_f(\mathbf{q},\mathbf{q}'; -\alpha^2)$ is motonically increasing as $\alpha^2 > 0$ decreases. From the study of the three dimensional potential scattering problem it is well known that if a bound state exists with binding energy $-E_B$, the series I_f will converge for α^2 sufficiently greater than E_B ,¹² and diverge at E_B where the Green's function has a pole. Thus the series must diverge at some $\alpha^2 = E_0$ such that $E_0 \ge E_B$. Since each term in the series I_f is positive and increasing as α^2 decreases, the series will certainly diverge for all values of $\alpha^2 \le E_0$, and thus I_f is absolutely divergent for $0 < \alpha^2 \le E_B$.

It is true that we have proven divergence for a particular subset of the Green's function series, and one might be tempted to argue that divergences may cancel if one considers the entire series. However, the iteration in terms of G_0 is a double power series in the two potential strengths $\lambda_i(V_i)$ and $\lambda_f(V_f)$. Since the usual theorems about absolute convergence and rearrangement of single power series are easily extended to double series,¹³ the absolute divergence of the series in a particular arrangement, namely, taking first the terms involving λ_i to the zero power, cannot in general be avoided by a rearrangement of the series. Thus the iteration series for the total Green's function in terms of the free particle Green's function diverges at least in a continuous range of p such that $0 < p^2 - E \leq E_B$.

Finally we prove that iteration in terms of either the initial state Green's function or the final state Green's

 $^{^{11}}E-p^2$ is the variable E' defined in Sec. I as a variable related to the magnitude of the momentum transfer to the exchanged particle.

particle. ¹² See references cited in footnote 6; it can be easily seen that the Fredholm determinant for Eq. (17) is identical with that appearing in the Green's function.

¹¹³ See, for example, E. T. Whittaker and G. N. Watson, *Modern Analysis* (Cambridge University Press, Cambridge, 1958), pp. 26-32,

function also produces divergent results. Let us deal specifically with the expansion in terms of G_i . The

mutandis. Consider the formal expansion for G in terms of G_f and V_f :

proof for the expansion in terms of G_f follows mutatis

$$G = G_i + G_i V_f G_i + G_i V_f G_i + \cdots$$
(19)

We may further write

$$G_i = G_0 + G_0 V_i G_i.$$
 (20)

After substituting Eq. (20) in Eq. (19), we group the result as follows:

$$G = F(V_i) + G_0 + G_0 V_j G_0 + G_0 V_j G_0 V_j G_0 + \cdots, \quad (21)$$

where $F(V_i)$ contains an infinite number of terms, all of which are explicitly dependent on V_i .¹⁴ We have proven above the divergence of $G-F(V_i)$ in a certain region of momentum space. Since the potentials V_i and V_f are independent, in general divergences in $F(V_i)$ cannot cancel the divergences in the remaining series of Eq. (21). Hence the divergence of Eq. (15) implies the divergence of Eq. (19).

III. CONCLUSIONS

We would like to be able to prove that the Born series for the transition amplitude diverges. However, even though the Green's function series is a divergent sum of positive terms in a finite measure of the integration, this is not enough to insure the divergence of the transition amplitude which is an integral over this series. If in Eq. (11) the function $(f|V_i|\mathbf{np})$ and $(\mathbf{n'p'}|V_f|i)$ can change sign in the integration interval then a cancellation is possible and one cannot conclude that the integral diverges. But for the class of potentials used in our proof, at least for the first S-wave bound state, the matrix elements $(f|V_i|\mathbf{np})$ and $(\mathbf{n'p'}|V_f|i)$ never change sign. For these restrictive cases the cancellation cannot occur, and we would be surprised if it did in more general examples. A more difficult point concerns the interval of convergence of the Green's function expansion. The series for G probably diverges in other integration ranges than those concentrated on in the text (for example, for small positive values of $E - p^2$), and divergent contributions from these ranges might be of opposite sign and cancel the divergences arising from $E < p^2 \leq E_B$. This cancellation would, of course, depend delicately on the functions $(f|V_i|\mathbf{np})$ and $(\mathbf{n'p'}|V_f|i)$ and seems highly unlikely to occur. Thus we believe that the Born series for the scattering amplitude in a rearrangement collision diverges, and we have pointed out the origins of this divergence, but a rigorous proof involves very difficult mathematical questions which we cannot as yet resolve.

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APPENDIX: SEPARABLE POTENTIAL

For a separable potential $-\lambda v(\mathbf{p})v(\mathbf{q})$, the Schrödinger equation in momentum space may be written

$$(p^2-k_0^2)h(\mathbf{p},k_0)-\lambda v(\mathbf{p})\int \mathbf{d}q \ v(\mathbf{q})h(\mathbf{q},k_0)=0, \quad (A.1)$$

where $h(\mathbf{p}, k_0)$ is the wave function and k_0^2 is the energy eigenvalue. If a bound state exists at energy $k_0^2 = -E_B$, the solution of Eq. (A.1) becomes

$$h(\mathbf{p}, E_B) = \frac{\lambda v(\mathbf{p})}{p^2 + E_B} \int \mathbf{dq} \ v(\mathbf{q}) h(\mathbf{q}, E_B).$$
(A.2)

One can readily verify that the condition for the existence of a bound state, $h(\mathbf{p}, E_B)$, is

$$\lambda \int \mathbf{d}q \frac{v(\mathbf{q})}{E_B + q^2} = 1, \qquad (A.3)$$

and also that there exists only one such solution.

The interaction operator of Eq. (15), for a separable potential, becomes

$$I_{f} = \lambda v(\mathbf{p}) v(\mathbf{q}) \begin{pmatrix} 1 + \lambda \int \mathbf{d}q \frac{v^{2}(\mathbf{q})}{q^{2} - k_{0}^{2} - i\eta} \\ + \lambda^{2} \left(\int \mathbf{d}q \frac{v^{2}(\mathbf{q})}{q^{2} - k_{0}^{2} - i\eta} \right)^{2} + \cdots \end{pmatrix}.$$
(A.4)

In terms of the ratio test, the condition for convergence is given by

$$\lambda \left| \int \mathbf{d}q \frac{v^2(\mathbf{q})}{q^2 - k_0^2 - i\eta} \right| < 1. \tag{A.5}$$



FIG. 1. The shaded area represents that region in which the Born series converges in the complex k plane.

 $^{^{14}}$ While this point is suspect, the authors strongly believe it to be valid.

Equation (A.3) insures the divergence of the series of Eq. (A.4) at the bound state energy E_B , while the series will diverge for $-E_B \leq k_0^2 < 0$ for the same reason as discussed in the text in Sec. II. (The potential must of course satisfy the same conditions.) In general it is extremely difficult to investigate the region of convergence of the above series in the complex $k \ (=k_0+i\eta)$



FIG. 2. The region of convergence of the Born series in Fig. 1 maps into the above shaded region in the complex energy plane.

plane. However, if we choose $v(\mathbf{q})$ as a Yukawa-like potential,

$$v(\mathbf{q}) = 1/(q^2 + \mu^2),$$
 (A.6)

where μ is the range of the potential, all the integrals can be evaluated, and Eq. (A.5) can be written as

$$\left| \int_{0}^{\infty} \frac{q^{2} dq}{(q^{2} + \mu^{2})(q^{2} - k_{0}^{2} - i\epsilon)} \right| < \frac{1}{4\pi\lambda}.$$
 (A.7)

Upon performing the integration, the above condition becomes

$$k_0^2 + (\eta + \mu)^2 > \pi^2 \lambda / \mu.$$
 (A.8)

For the particular potential under consideration the bound state energy is given by solving Eq. (A.3) and we obtain

$$E_B = \pi^2 \lambda / \mu - \mu. \tag{A.9}$$

From Eq. (A.8) the region of convergence in the k plane is seen to be the region outside the circle of radius $R = \pi^2 \lambda/\mu$ surrounding the point $k = -i\mu$, as illustrated in Fig. (1). The region of convergence in the energy plane is shown in Fig. (2). It is interesting to note that the Born series diverges everywhere within a circle (in the k plane) of radius $|k| = \sqrt{E_B}$ surrounding the origin.