# Born Approximation in a Three-Body Scattering Problem

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A one-dimensional three-body scattering problem is constructed and solved exactly. The scattering amplitudes of the exact solution are compared with those obtained by the application of the Born approximation to the problem. The latter procedure is formulated in two distinct ways, using a symmetric or asymmetric perturbation term. The results indicate that the method using symmetric perturbation is superior to that employing asymmetric perturbation, although it is more difficult mathematically. An approximation method is developed which yields results as accurate as those obtained from the symmetric perturbation and which is on the same mathematical plane of difficulty as the asymmetric perturbation scheme. Moreover, the procedure is applicable to actual physical problems and is particularly useful for the calculation of exchange scattering.

## 1. INTRODUCTION

THE application of the Born approximation to the analysis of many-body scattering phenomena gives rise to several problems.[1] Those which concern us here are the calculation of exchange scattering and the relative merits of choosing the perturbation in a symmetric or asymmetric form.

To gain some insight into these difficulties, we have constructed a one-dimensional three-body scattering problem which can be solved exactly. Such problems have recently appeared in the literature.[2] They have solutions which display all the physical characteristics, i.e., elastic, inelastic, and exchange scattering, of actual physical scattering problems. Thus, a comparison can be made between the scattering amplitudes for elastic scattering (direct and exchange) calculated by the Born approximation and the exact amplitudes. One of our results can be formulated in terms which make it applicable to real physical problems. The approximation method so obtained is particularly useful for the calculation of exchange scattering.

The following sections will include: (1) the formulation and solution of a class of one-dimensional three-body scattering problems—only elastic (direct and exchange) scattering will be treated in detail; (2) the application of the Born approximation procedure to the above problem with the perturbation taken in a symmetric form; (3) the same problem as in the preceding section but with the perturbation in an asymmetric form; and (4) the development of an approximation procedure suggested by the above material and a discussion of its applicability to actual physical problems.

## 2. EXACT SOLUTION

The Schrödinger equation for the one-dimensional three-body scattering problem is

$$\left\{-\frac{\partial^2}{\partial x_1^2}-\frac{\partial^2}{\partial x_2^2}-2B\delta(x_1)-2B\delta(x_2)+V(x_1,x_2)-E\right\}\psi(x_1,x_2)=0. \quad (1)$$

This equation represents a system composed of a particle 1, the incident particle, coming from the left with momentum $K_0$ and the struck "atom." The latter consists of a "nucleus" of infinite mass and a bound particle which is labeled with the subscript 2 and is identical to particle 1. The masses, $m_1$ and $m_2$ of particles 1 and 2, respectively, have been set equal to $\frac{1}{2}$. The choice of units is such that $\hbar=1$. The interaction of either particle with the nucleus is described by the potential function $-2B\delta(x)$, in which $B$ is a real positive constant and $\delta(x)$ is Dirac's delta function. The interaction between the identical particles is, for the present, denoted by $V(x_1,x_2)$ and its specific form will be described below. The total energy of the system is given by $E$. Finally, the time dependent part of the wave function is assumed to be $\exp(-iEt/\hbar)$.

Equation (1) is considered in momentum space. This representation is obtained by setting

$$\psi(x_1,x_2)=(1/2\pi)\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}f(k_1,k_2)\times\exp(ik_1x_1+ik_2x_2)dk_1dk_2. \quad (2)$$

Then (1) becomes

$$(k_1^2+k_2^2-E)f(k_1,k_2)-\frac{B}{\pi}\times\int f(k_1,k_2)dk_1-\frac{B}{\pi}\int f(k_1,k_2)dk_2+\frac{1}{4\pi^2}\times\int(k_1k_2|V|k_1'k_2')dk_1'dk_2'f(k_1',k_2')=0, \quad (3)$$

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[1] Bates, Fundaminsky, Leech, and Massey, Trans. Roy. Soc. (London) A243, 93 (1950).

[2] K. Wildermuth, Acta Physica Austriaca 7, 3, 299 (1953).

where the interaction kernel

$$(k_1k_2|\,V\,|k_1'k_2')=\int V(x_1,x_2)\,\exp\{i(k_1'-k_1)x_1 +i(k_2'-k_2)x_2\}dx_1dx_2. \quad (4)$$

Henceforth, as in Eqs. (3) and (4), a single integral sign will be used in the place of multiple ones. The multiplicity of integrations to be performed will be indicated by the number of variables of integration. The range of integration will always extend from $-\infty$ to $+\infty$ for all variables. Any deviation from this convention will be explicitly indicated.

To complete the mathematical description of the problem the interaction kernel of Eq. (4) was chosen to be

$$(k_1k_2|\,V\,|k_1'k_2')=2ATi\left\{\frac{k_1-k_1'}{(k_1^2+T^2)(k_1'^2+T^2)} +\frac{k_2-k_2'}{(k_2^2+T^2)(k_2'^2+T^2)}\right\}, \quad (5)$$

where $A$ and $T$ are real positive constants. This interaction kernel is obviously Hermitian and symmetric in the interchange of particles 1 and 2. In coordinate space, the interaction $V(x_1,x_2)$ is given by an integral operator which has for its kernel the expression

$$A[K(x_1,x_2)K(x_1',x_2')-K(-x_1,x_2)K(-x_1',x_2') +K(x_2,x_1)K(x_2',x_1')-K(-x_2,x_1)K(-x_2',x_1')],$$

where

$$K(x_1,x_2)=\delta(x_2)\eta(-x_1)\exp(Tx_1)$$

and

$$\eta(x)=\begin{cases}0 & (x<0)\\ 1 & (x>0)\end{cases}.$$

This explicit representation of the interaction exhibits its short-range character.

Simpler forms for (5) can be chosen as we will see below, but such obvious choices as a product of Dirac delta functions or the delta function $\delta(x_1-x_2)$ for $V(x_1,x_2)$ are not satisfactory. The first leads to divergent integrals[2] and the second does not give an equation which is readily solved.[3]

Much of the work that follows is developed for an interaction kernel of which (5) is a special case. However, where the results of specific calculations are mentioned, they were obtained with the use of (5).

The unperturbed equation obtained from (3) by setting $(k_1k_2|\,V\,|k_1'k_2')=0$ is separable. For this reason, it is relatively simple to obtain the Green's function associated with it. In terms of this Green's function, $G(k_1k_2;k_1'k_2')$, the solution of (3) can be represented by the integral equation

$$f(k_1,k_2)=f_0(k_1,k_2)-(1/4\pi^2) \times\int G(k_1k_2;k_1'k_2')dk_1'dk_2' \times(k_1'k_2'|\,V\,|k_1''k_2'')dk_1''dk_2''f(k_1'',k_2''), \quad (6)$$

where $f_0(k_1,k_2)$ is the solution of the unperturbed wave equation which describes the initial state of the system and the Green's function is the one which describes outgoing waves in coordinate space.

If the interaction between particles 1 and 2 can be written

$$(k_1k_2|\,V\,|k_1'k_2')=\sum_{l=1}^{n} g_l(k_1,k_2)h_l(k_1',k_2'), \quad (7)$$

where $g_l$ and $h_l$ are arbitrary functions of $k_1$ and $k_2$, then (6) yields the exact solution of the problem. For, substituting (7) into (6), we obtain

$$f(k_1,k_2)=f_0(k_1,k_2)+\sum_{l-1}^{n} C_lJ_l(k_1,k_2), \quad (8)$$

where

$$J_l(k_1,k_2)=(-1/4\pi^2) \times\int G(k_1k_2;k_1'k_2')dk_1'dk_2'g_l(k_1',k_2') \quad (9)$$

and

$$C_l=\int h_l(k_1,k_2)dk_1dk_2f(k_1,k_2). \quad (10)$$

These constants are determined by substituting Eq. (8) into (10) and solving the resulting linear inhomogeneous equations. Thus (8), coupled with (9) and (10), is the exact solution.

### 3. SYMMETRIC PERTURBATION—FIRST BORN APPROXIMATION AND EXPANSION

Equation (6) is the starting point in the Born procedure. Since the interaction between the identical particles 1 and 2, e.g., (5), is taken as the perturbation, we have designated it by the term, "symmetric." The first Born approximation to the wave function is obtained by replacing $f(k_1,k_2)$ with $f_0(k_1,k_2)$ in (6). It is evident from the way in which the exact solution was found that the effect of this replacement is merely the determination of different values, $C_l{}^b$ for the exact $C_l$. Thus, the functional dependence of the Born result on $k_1$ and $k_2$ is precisely that of the exact solution. In particular, the Born result contains exchange-scattered amplitudes. This remark, though it applies only to the specific problems that were formulated above, is important for what follows.

[3] K. Wildermuth, Z. Physik **127**, 92 (1949).

TABLE I. Symmetric perturbation—symmetric solution.[a]

| $z$ | Exact $Q_{es}$ | Radius $\rho_s$ | Born approximation $Q_{eB}$ |
|---|---|---|---|
| −0.9 | 0.853805 | 1.06744 | 1.47820 |
| −0.5 | 1.05210 | 0.903667 | 2.27123 |
| −0.1 | 1.10402 | 0.925606 | 2.32585 |
| −0.05 | 1.10477 | 0.930891 | 2.31255 |
| −0.01 | 1.10476 | 0.935332 | 2.30006 |
| −0.005 | 1.10473 | 0.935894 | 2.29841 |
| −0.001 | 1.10468 | 0.936347 | 2.29703 |
| +0.001 | 1.10467 | 0.936573 | 2.29633 |
| +0.005 | 1.10464 | 0.937026 | 2.29500 |
| 0.01 | 1.10459 | 0.937594 | 2.29326 |
| 0.05 | 1.10364 | 0.942112 | 2.27868 |
| 0.1 | 1.10154 | 0.947773 | 2.25885 |
| 0.5 | 1.06137 | 0.990463 | 2.06239 |
| 0.9 | 1.00185 | 1.03888 | 1.84770 |
| 5. | 0.518503 | 1.47143 | 0.651187 |
| 10. | 0.284078 | 1.91763 | 0.289203 |
| 100. | 0.015933 | 6.01935 | 0.013138 |
| 1000. | 0.001053 | 20.0416 | 0.001033 |

[a] $z$ = total energy $E$ in units of the bound state energy $B^2$; $Q_{es}$ = elastic scattering cross section for symmetrical wave function; $Q_{eB}$ = elastic scattering cross section for first Born approximation to symmetrical wave function; $\rho_s = |A/4\pi|$ = radius of convergence of Born expansion for symmetric wave function.

TABLE II. Symmetric perturbation—antisymmetric solution.[a]

| $z$ | Exact solution $Q_{ea}$ | Radius $\rho_a$ | Born approximation $Q_{eB}$ |
|---|---|---|---|
| −0.9 | 0.948379 | 1.75739 | 0.922751 |
| −0.5 | 0.786795 | 1.78538 | 0.730850 |
| −0.1 | 0.678528 | 1.82632 | 0.630407 |
| −0.05 | 0.667623 | 1.83194 | 0.621099 |
| −0.01 | 0.659256 | 1.83644 | 0.614017 |
| −0.005 | 0.658233 | 1.83700 | 0.613154 |
| −0.001 | 0.657397 | 1.83757 | 0.612465 |
| +0.001 | 0.657011 | 1.83766 | 0.612121 |
| 0.005 | 0.656205 | 1.83810 | 0.611440 |
| 0.01 | 0.655196 | 1.83866 | 0.610589 |
| 0.05 | 0.647282 | 1.84295 | 0.603945 |
| 0.1 | 0.637722 | 1.84820 | 0.596012 |
| 0.5 | 0.576029 | 1.87063 | 0.543805 |
| 0.9 | 0.520376 | 1.92261 | 0.504394 |
| 5. | 0.259111 | 2.28234 | 0.290243 |
| 10. | 0.147364 | 2.67852 | 0.174831 |
| 100. | 0.012500 | 6.46166 | 0.0127781 |
| 1000. | 0.001016 | 20.2075 | 0.00103251 |

[a] $z$ = total energy $E$ in units of the bound state energy $B^2$; $Q_{ea}$ = elastic scattering cross section for antisymmetric wave function; $Q_{eB}$ = elastic scattering cross section for first Born approximation to antisymmetric wave function; $\rho_a = |A/4\pi|$ = radius of convergence of Born expansion for antisymmetric wave function.

The Born expansion,[4] the series that results by iteration of the procedure given above, can be shown to converge to the exact solution. The proof is to be found in Appendix I. Here again we note that each term in the expansion contains exchange scattered waves.

For purposes of reference, the first Born approximation to the direct and exchange scattered amplitudes of the exact wave function is given:

$$2^{-\frac{1}{2}}\left\{\frac{B}{\pi}\frac{K_0}{K_0-Bi}-\frac{lN\pi}{B}\left[\frac{Ck_1}{K_0^2+T^2}-\frac{D}{T(T+B)}\frac{K_0}{K_0-Bi}\times\left(\frac{T^2-B^2}{K_0^2+T^2}\pm 1\right)\right]\right\}. \quad (11)$$

Here $l=(2ATi/4\pi^2)$, $K_0^2=B^2+E$, where $K_0$ is the momentum of the incident particle, $N=(2/\pi)^{\frac{1}{2}}B^{\frac{3}{2}}$,

$$C=\frac{N\pi}{BT(T+B)}\frac{K_0}{K_0-Bi}\left[\frac{T^2-B^2}{K_0^2+T^2}\pm 1\right], \quad (12)$$

and

$$D=\frac{N\pi}{B}\left(\frac{K_0}{K_0^2+T^2}\right). \quad (13)$$

The plus in the ambiguous $\pm$ sign in these equations is associated with the symmetric solution and the minus with the antisymmetric solution. Equation (11) differs from the exact value only in the values for the constants $C$ and $D$. No purpose is served in giving their exact values.

Tables I and II contain the computed values of the exact elastic scattering cross sections and those obtained from the first Born approximation. Each table contains the radius of convergence $\rho$ of the Born expansion for each type of solution. This quantity represents that value of the interaction parameter $(A/4\pi)$ within which $(0\leq|A/4\pi|<\rho)$ the series converges. The values tabulated are for $T=2B$ and $(A/4\pi)=1$. It is to be noted that where $(A/4\pi)=1$ falls within the radius of convergence, the first Born approximation gives good results.

## 4. ASYMMETRIC PERTURBATION

The Schrödinger Eq. (3) may be written

$$(k_1^2+k_2^2-E)f(k_1k_2)-(B/\pi)\int f(k_1k_2)dk_2 = (B/\pi)\int f(k_1k_2)dk_1-(1/4\pi^2)\times\int(k_1k_2|V|k_1'k_2')dk_1'dk_2'f(k_1'k_2'). \quad (14)$$

This arrangement is analogous to the one used in actual physical problems.[5] The perturbation terms on the right-hand side of (14) consist of the interaction between the incident particle and the center of force in addition to the interaction between the incident and bound particles. Hence the designation of "asymmetric" perturbation.

As in the previous section we may now proceed to apply the Born approximation and obtain the Born expansion. It has been conjectured[6] that such a program would not yield exchange-scattered waves. The results of the present problem indicate that such is the case. The procedure is straightforward and has been carried

[4] R. Jost and A. Pais, Phys. Rev. 82, 840 (1951).

[5] S. Borowitz and B. Friedman, Phys. Rev. 89, 441 (1953).

[6] W. Kohn (private communication).

out elsewhere.[7] This result is in contrast with that obtained for the symmetric perturbation.

A procedure used to circumvent the above difficulty is discussed quite thoroughly by Mott and Massey.[8] Its principal feature is the expansion of the wave function in terms of two separate and distinct complete sets of eigenfunctions, one which spans the $k_1$ space and the other the $k_2$ space. Thus

$$f(k_1,k_2)=f_1(k_1)(2/k_2)+\int f_2(k_1,K_2)dK_2(K_2/k_2), \quad (15)$$

or

$$=g_1(k_2)(1/k_1)+\int g_2(k_2,K_1)dK_1(K_1/k_1). \quad (16)$$

The functions $(2/k_2)$ and $(K_2/k_2)$ are the complete set of eigenfunctions which span $k_2$ space. The first is a bound state—there is only one[7]—and the second represents the continuum states with $K_2$ representing the momentum of these states. Explicitly, these functions are

$$(2/k_2)=N/(k_2^2+B^2), \quad (17)$$

where

$$N=(2/\pi)^{\frac{1}{2}}B^{\frac{3}{2}}, \quad E=-2B^2,$$

and

$$(K_2/k_2)=\delta(k_2-K_2)+\frac{B}{\pi}\frac{|K_2|}{|K_2|-Bi}\frac{1}{k_2^2-K_2^2} \quad (E>0). \quad (18)$$

These eigenfunctions form a complete orthonormal set, as can be easily verified.

The functions $(1/k_1)$ and $(K_1/k_1)$ which appear in (16) are the symmetric counterparts of $(2/k_2)$ and $(K_2/k_2)$. This is a consequence of the symmetry of the problem and the fact that particles 1 and 2 are identical. The functions $f_1(k_1)$ and $f_2(k_1,K_2)$ are the "Fourier" expansion coefficients to be determined. A similar statement about $g_1(k_2)$ and $g_2(K_1,k_2)$ can be made. In particular, we are concerned with the calculation of $f_1(k_1)$ and $g_1(k_2)$, for these represent the amplitudes of the elastically scattered waves. We find that

$$f_1(k_1)=\delta(k_1-K_0)+\frac{1}{k_1^2-K_0^2}\int(2/k_2)^* \times dk_2 w(k_1k_2;k_1'k_2')dk_1'dk_2'f(k_1',k_2') \quad (19)$$

and

$$g_1(k_2)=\frac{1}{k_2^2-K_0^2}\int(1/k_1)^* \times dk_1 v(k_1k_2;k_1'k_2')dk_1'dk_2'f(k_1',k_2'), \quad (20)$$

where

$$w(k_1k_2;k_1'k_2')=(B/\pi)\delta(k_2-k_2') -(1/4\pi^2)(k_1k_2|V|k_1'k_2'), \quad (21)$$

and

$$v(k_1k_2;k_1'k_2')=w(k_2k_1;k_2'k_1'). \quad (22)$$

The functions (21) and (22) are the asymmetric perturbations which result when the Schrödinger equation is cast in the form given by (14).

Equations (19) and (20) are exact. To obtain an approximate solution, the exact wave function in these equations is replaced by the solution of the unperturbed system, i.e., the first Born approximation. When this is done, the amplitude of the elastically scattered wave is given by

$$2^{-\frac{1}{2}}\left\{\frac{B}{\pi}\pm\frac{N^2}{K_0^2+B^2}-i\left(\frac{N\pi}{B}\right)^2 \times\left[\frac{k_1}{K_0^2+T^2}\frac{1}{T(T+B)}\left(\frac{T(T+B)}{K_0^2+T^2}\pm1\right) -\frac{K_0}{K_0^2+T^2}\frac{1}{T(T+B)}\left(\frac{T(T+B)}{K_0^2+T^2}\pm1\right)\right]\right\}. \quad (23)$$

This result, when compared with (11), obtained from a consideration of the symmetric perturbation is, except for the term $N^2/(K_0^2+B^2)$, as accurate as (11) up to the first order in $B$. The method which yielded (23) seems preferable to that giving (11) since it is far less complex mathematically and appears to lead to equally reliable results. However, $N^2/(K_0^2+B^2)$ is a spurious term and the appearance of such terms in the procedure we are considering is well known.[8] They imply the existence of exchange scattering even when the interaction between incident and bound particles vanishes. This is physically inadmissible.

If we assume that the interaction between incident and bound particles vanishes, we can show that the spurious terms approach zero as the number of iterations increases. Thus, the above procedure is theoretically sound but certainly unsatisfactory as an approximation procedure.

If we examine Eq. (19) and replace $f(k_1,k_2)$ which appears in the integrand on the right-hand side with Eq. (15), we find that

$$f_1(k_1)=\delta(k_1-K_0)+\frac{B}{\pi}\frac{1}{k_1^2-K_0^2} \times\int f_1(k_1)dk_1-\frac{1}{4\pi^2}\frac{1}{k_1^2-K_0^2}\int(2/k_2)^* \times dk_2(k_1k_2|V|k_1'k_2')dk_1'dk_2'f(k_1',k_2'). \quad (24)$$

The first two terms in the right have the form of $(K_0/k_1)$ of (18) which represents a continuum eigenfunction.

[7] S. L. Schwebel, thesis, New York University, 1954 (unpublished).

[8] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Clarendon Press, Oxford, 1949), second edition.

This suggests that we use as a trial function $(K_0/k_1)(2/k_2)$. This function represents the product of a continuum eigenfunction of particle 1 and the bound state of particle 2. When this is done, we find that

$$g_1(k_2)=-\frac{1}{4\pi}\frac{1}{k_2^2-K_0^2}\int(1/k_1)^*dk_1(k_1k_2|\,V\,|k_1'k_2') \times dk_1'dk_2'(K_0/k_1')(2/k_2'). \quad (25)$$

The exchange-scattered amplitude that this equation yields clearly vanishes with the interaction between incident and bound particles.

This result can be taken over directly to actual physical problems, and it is a simple matter to verify that such a trial function does not lead to spurious terms in the calculation of exchange scattering (see Appendix II). Furthermore, this trial function represents a more detailed and accurate picture of the initial state than does the usual Born trial function.

A detailed calculation using the trial function $(K_0/k_1)(2/k_2)$ gives the following for the elastic scattering coefficient:

$$2^{-\frac{1}{2}}\left\{\frac{B}{\pi}\frac{K_0}{K_0-Bi}-l\left(\frac{N\pi}{B}\right)^2 \times\left[\frac{k_1}{K_0^2+T^2}\frac{1}{T(T+B)}\frac{K_0}{K_0-Bi}\left(\frac{T^2-B^2}{K_0^2+T^2}\pm1\right) -\frac{K_0}{K_0^2+T^2}\frac{1}{T(T+B)}\left(\frac{T(T+B)}{K_0^2+T^2}\pm1\right)\right]\right\}. \quad (26)$$

Comparison of this result with our previous calculations indicates not only an improved approximation but one which does not contain spurious terms.

### 5. ALTERED INITIAL STATE PROCEDURE

The trial function previously considered may be incorporated into a procedure developed by Borowitz and Friedman.[5] In its altered form, this method retains the mathematical advantages of the asymmetric perturbation formulation. It does not yield spurious terms in the calculation of exchange scattering and it can be iterated to obtain higher order approximations. We will apply it to the problem considered here. However, what follows is applicable to actual physical problems.

We assume that the wave function can be expressed as

$$f(k_1,k_2)=f_0(k_1,k_2)+h(k_1,k_2), \quad (27)$$

where $f_0(k_1,k_2)$ is the solution of the unperturbed Schrödinger equation obtained from (3) by setting the interaction between incident and bound particle equal to zero. Then $h(k_1,k_2)$ represents the outgoing flux of incident and/or formerly bound particles. In addition, $h(k_1,k_2)$ must vanish with the interaction between the identical particles. Substituting (27) into (3), we obtain an inhomogeneous equation for $h(k_1,k_2)$. This equation is handled in the manner described for the asymmetric perturbation.

The calculations lead to equations which are analogous to (19) and (20):

$$h_1(k_1)=-\frac{1}{(4\pi^2)(k_1^2-K_0^2)}\int(2/k_2)^* \times dk_2(k_1k_2|\,V\,|k_1'k_2')dk_1'dk_2'f_0(k_1',k_2') +\frac{1}{k_1^2-K_0^2}\int(2/k_2)^* \times dk_2w(k_1k_2;\,k_1'k_2')dk_1'dk_2'h(k_1',k_2'), \quad (28)$$

$$g_1(k_2)=-\frac{1}{(4\pi^2)(k_2^2-K_0^2)}\int(1/k_1)^* \times dk_1(k_1k_2|\,V\,|k_1'k_2')dk_1'dk_2'f_0(k_1',k_2') +\frac{1}{k_2^2-K_0^2}\int(1/k_1)^* \times dk_1v(k_1k_2;\,k_1'k_2')dk_1'dk_2'h(k_1',k_2'). \quad (29)$$

These equations differ from (19) and (20) in several important respects. First, both of these equations contain an inhomogeneous term which not only vanishes with the interaction between the identical particles but also represents outgoing waves. Thus (28) and (29), when inserted in (15) and (16), determine in a systematic way a trial function for $h(k_1,k_2)$ (the inhomogeneous term) which satisfies the boundary conditions. Secondly, we have placed no restriction on the form of $f_0(k_1,k_2)$ in (27). Therefore, this procedure can treat equally well initial states, whether symmetric or not. In a certain sense, we have achieved a simpler treatment in that, since symmetric or antisymmetric solutions are to be considered, only one of the Eqs. (28) or (29) has to be evaluated.

To solve the asymmetric problem in the first Born approximation, $h(k_1,k_2)$ is set equal to zero on the right-hand side of (28). This yields the same results as those obtained by using the new trial function of the preceding section. However, we now have a systematic method by which this trial function can be improved and the latter has become an integral part of a procedure of general scope.

We have carried out a partial evaluation of the second integral on the right-hand side of (28) and found the first Born results given by Eq. (11) for the symmetric perturbation. These results are much better than those obtained from the usual first Born approximation in the asymmetric perturbation calculation, i.e., Eq. (23), or from the use of the new trial function suggested there, i.e., Eq. (26).

There is a further conclusion which can be drawn

from the details of the above calculation but which is also true in actual problems. The usual formulation in terms of the asymmetric perturbation treats two of the potential terms on different levels. Thus, the interaction of one of the particles with the source of the field, with the nucleus for example, is considered a significant part of the Hamiltonian, whereas the equivalent term for the second particle is considered as a perturbation. This is unreasonable on physical grounds. The altered initial-state procedure minimizes this difference in treatment by using as an initial state a function obtained by including both interactions with the center of force in its computation. Furthermore, as Eqs. (28) and (29) show, the altered procedure leads to integral equations having inhomogeneous terms which depend on the interaction between the particles. Iteration of such equations results in terms having this interaction to the same or higher order of magnitude. Thus, the disparity in the treatment of the interactions with the nucleus is further reduced. This last observation also indicates the desirability of iterating at least once when applying this method. It also explains the improvement in the results noted above when a partial integration of the integral term in (28) was effected (see Appendix II).

## 6. SUMMARY

The solution of a fictitious three-body scattering problem has enabled us to study elastic scattering in detail. Some results of interest are:

1. Exchange-scattering contributions are present when the Born approximation method is applied to a symmetric perturbation formulation of the problem.
2. When the perturbation is asymmetric, such contributions are not present even though the Born expansion does converge to the exact solution. Mathematically, this implies that the series does not converge uniformly.

These results are negative in character since they were shown to be valid only for the specific problems studied. However, a positive result is obtained. An approximation method which falls between the symmetric and asymmetric perturbation formulation of the Born approximation procedure is developed. This method is of general applicability and its value resides in the following properties which it displays:

1. Spurious terms which appear in the calculation of exchange scattering by the usual Born approximation method are eliminated.
2. The particular symmetry of the initial state of the system does not present any difficulty since all states can be handled equally well.
3. A systematic method of improving the trial function is a direct consequence of the method.
4. The "smallness" of the perturbation function is consistently treated.

We may further remark that the second property named has the feature that the maximum knowledge of the initial state of the system can be included *ab initio* and need not be restricted by the mathematical formulation of the problem.

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## APPENDIX I. CONVERGENCE OF THE BORN EXPANSION—SYMMETRIC PERTURBATION

Let $f^{(n)}(k_1,k_2)$ represent the $n$th-order approximation obtained from the $n$th iteration. Thus

$$f^{(0)}(k_1,k_2)=f_0(k_1,k_2)$$

and

$$f^{(1)}(k_1,k_2)=f_0(k_1,k_2)+\sum_{\alpha=1}^{n} C_\alpha{}^{(1)}J_\alpha(k_1,k_2). \tag{A.1}$$

This equation corresponds to Eq. (8) except that

$$C_\alpha{}^{(1)}=\int h_\alpha(k_1,k_2)dk_1dk_2f_0(k_1,k_2).$$

It is easily shown that

$$f^{(2)}(k_1,k_2)=f_0(k_1,k_2)+\sum_{\alpha=1}^{n} J_\alpha[C_\alpha{}^{(1)}+\sum_{\beta=1}^{n} D_{\alpha\beta}C_\beta{}^{(1)}], \tag{A.2}$$

where

$$D_{\alpha\beta}=\int h_\alpha(k_1,k_2)dk_1dk_2J_\beta(k_1,k_2).$$

This equation, written in matrix notation, becomes

$$f^{(2)}(k_1,k_2)=f_0(k_1,k_2)+J[I+D]C^{(1)},$$

where

$J=(J_\alpha)$, $\alpha=1, \cdots, n$, and is a row matrix,

$D=(D_{\alpha\beta})$, $\alpha, \beta=1, \cdots, n$,

$C^{(1)}=(C_\alpha{}^{(1)})$ is a column matrix,

and $I$ represents the identity matrix.

In a straightforward manner, we can prove by mathematical induction that

$$f^{(n)}(k_1,k_2)=f_0(k_1,k_2)+J(I+D+\cdots+D^{n-1})C^{(1)}. \tag{A.3}$$

Let $n\to\infty$; then

$$f(k_1,k_2)=f_0(k_1,k_2)+J(I-D)^{-1}C^{(1)}. \tag{A.4}$$

The radius of convergence $\rho$ is determined by the validity of the representation $(I-D)^{-1}=I+D+D^2+\cdots$.

The exact solution given by (8) is

$$f(k_1,k_2)=f_0(k_1,k_2)+JC, \tag{A.5}$$

where in matrix notation $C=(C_\alpha)$ is a column matrix. From the definition of $C_\alpha$ given by (10), we find that

$$C=C^{(1)}+DC,$$

whence

$$C=(I-D)^{-1}C^{(1)}. \tag{A.6}$$

This relation establishes the equivalence of (A.4) and (A.5).

## APPENDIX II

The Schrödinger equation for the collision between an electron and hydrogen atom is

$$\left\{\frac{h^2}{8\pi^2m}(\nabla_1^2+\nabla_2^2)+E+\frac{e^2}{r_1}+\frac{e^2}{r_2}-\frac{e^2}{r_{12}}\right\}\psi=0. \tag{A.7}$$

The wave function is expanded into the form

$$\psi=\left(\sum_n+\int\right)F_n(\mathbf{r}_1)\psi_n(\mathbf{r}_2) \tag{A.8}$$

for the calculation of the direct scattering, and into the alternative expression

$$\psi=\left(\sum_n+\int\right)G_n(\mathbf{r}_2)\psi_n(\mathbf{r}_1) \tag{A.9}$$

for the calculation of the exchange scattering. We are following the notation and development given in Mott and Massey.[8]

The $\psi_n(r)$ is an orthonormal set of hydrogen wave functions, i.e., the $\psi_n$, for either particle satisfies the equation

$$\left(\frac{h^2}{8\pi^2m}\nabla^2+E_n+\frac{e^2}{r}\right)\psi_n=0 \tag{A.10}$$

and appropriate initial conditions.

Substituting (8) and (9) into (7), we obtain the following equations:

$$(\nabla^2+k_n^2)F_n(\mathbf{r}_1)=\frac{8\pi^2m}{h^2}\int\left(\frac{e^2}{r_{12}}-\frac{e^2}{r_1}\right)\psi\psi_n^*(\mathbf{r}_2)d\tau_2, \tag{A.11}$$

and

$$(\nabla^2+k_n^2)G(\mathbf{r}_2)=\frac{8\pi^2m}{h^2}\int\left(\frac{e^2}{r_{12}}-\frac{e^2}{r_2}\right)\psi\psi_n^*(\mathbf{r}_1)d\tau_1, \tag{A.12}$$

with

$$k_n^2=8\pi^2m(E-E_n)/h^2.$$

Substitute Eq. (8) for $\psi$ in (11). Then this equation becomes

$$\left(\nabla^2+k_n^2+\frac{8\pi^2me^2}{h^2}\frac{1}{r_1}\right)F_n=\frac{8\pi^2m}{h^2}\int\frac{e^2}{r_{12}}\psi\psi_n^*(\mathbf{r}_2)d\tau_2. \tag{A.13}$$

A similar procedure followed for Eqs. (9) and (12) yields

$$\left(\nabla^2+k_n^2+\frac{8\pi^2me^2}{h^2}\frac{1}{r_2}\right)G_n=\frac{8\pi^2m}{h^2}\int\frac{e^2}{r_{12}}\psi\psi_n^*(\mathbf{r}_1)d\tau_1. \tag{A.14}$$

These equations are exact. For the purpose of formulating an approximating procedure, these equations can be used to give the first order approximations for $F_n$ and $G_n$. Thus, if $e^2/r_{12}$ is considered small, the solutions of the homogeneous equations obtained from (13) and (14), by setting their right-hand sides equal to zero, are the first order approximations to the exact wave function. These solutions must satisfy the initial conditions of the problem. It should be noted that for these approximate solutions, expansions (8) and (9) are identical. This is expected because with $e^2/r_{12}$ set equal to zero, Eqs. (13) and (14) yield the exact functions which combined with associated expansions (8) and (9), respectively, give the solution of (7) under the same condition.

Thus, let us write the solution of (7) as follows:

$$\psi=\phi_0+\phi, \tag{A.15}$$

where $\phi_0$ is the solution of the equation

$$\left\{\frac{h^2}{8\pi^2m}(\nabla_1^2+\nabla_2^2)+E+\frac{e^2}{r_1}+\frac{e^2}{r_2}\right\}\phi_0=0. \tag{A.16}$$

We find that $\phi$ must satisfy the equation

$$\left[\frac{h^2}{8\pi^2m}(\nabla_1^2+\nabla_2^2)+E+\frac{e^2}{r_1}+\frac{e^2}{r_2}-\frac{\lambda e^2}{r_{12}}\right]\phi=\frac{\lambda e^2}{r_{12}}\phi_0. \tag{A.17}$$

The parameter $\lambda$ has been inserted for purposes of exposition. Its value in (17) is one.

Rewriting (17), we obtain

$$\left[\frac{h^2}{8\pi^2m}(\nabla_1^2+\nabla_2^2)+E+\frac{e^2}{r_2}\right]\phi=\frac{\lambda e^2}{r_{12}}\phi_0-\left(\frac{e^2}{r_1}-\frac{\lambda e^2}{r_{12}}\right)\phi. \tag{A.18}$$

This equation can be represented by an integral equation:

$$\phi=\lambda e^2\int G(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2')\frac{1}{r_{12}'}\phi_0(\mathbf{r}_1',\mathbf{r}_2')d\tau_1'd\tau_2'$$
$$-e^2\int G(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2')\times\left(\frac{1}{r_1'}-\frac{\lambda}{r_{12}'}\right)\phi(\mathbf{r}_1',\mathbf{r}_2')d\tau_1'd\tau_2', \tag{A.19}$$

where the Green's function, $G(\mathbf{r}_1\mathbf{r}_2; \mathbf{r}_1'\mathbf{r}_2')$ is obtained for the operator on the left-hand side of Eq. (18) under the condition that it represents outgoing waves.

If $\lambda$ is set equal to zero, (19) reduces to a homogeneous integral equation which has the solution zero under the given initial conditions. For from (15), if the interaction vanishes, so must the function $\phi$. This property has the further consequence that exchange terms cannot appear when the interaction between the electrons is not taken into account.

The inhomogeneous term in (19) vanishes with the interaction between incident and bound electrons. Therefore, this equation is in a suitable form for carrying out an iterative procedure.

Using the parameter $\lambda$ to indicate orders of magnitude, the desirability of carrying out a partial integration of the second integral in (19) becomes apparent. In this way, the contribution of the $1/r_1$ term, of the same order of magnitude as the inhomogeneous term, can be obtained.

In the course of the derivation of Eq. (19), we have verified most of the statements listed in the summary of the text. The others are consequences which readily follow from our definitions and equations.

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# Reduction of Relativistic Wave Equations and the "Contact Interaction"

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A new formulation of the large-component reduction method for one- and two-particle relativistic wave equations is presented and compared with the reduction procedure by the method of successive canonical transformations. Sufficient conditions are given for the identity, to the order $(1/c)^2$, of the energy spectra obtained by the two methods. The "contact interaction" term resulting from the latter procedure is shown to arise in the former as well, contrary to a statement by Wu and Tauber.

## INTRODUCTION

TO reduce the number of components of a relativistic wave equation, two methods are in general use: one method is based on the fact that some of the components of $\Psi$ are larger than others[1]; and the other applies successive canonical transformations (also known as the Foldy-Wouthuysen method).[2] The latter has some distinct advantages. Moreover, as Becker[3] has shown, it is the method to which one is led when one attempts consistently to meet the basic requirements that the reduced wave equation have (to within an approximation) an energy spectrum identical with that of the full equation. Since in the past the older large-component method has enjoyed wide use, the question may be raised whether its application does not in some way impair the results. This question has become of interest recently, as Wu and Tauber have stated[4] that it was impossible to obtain the so-called "contact interaction" term in a two-particle problem by means of the large-component method. This is our motivation for presenting in this note some considerations, hitherto unpublished,[5] on the two methods.

We first formulate the large-component method in a way that will facilitate a comparison with the method of successive canonical transformations, both for the one-particle and the two-particle case. Then we establish sufficient conditions for their equivalence, and finally we show that the term in question is obtained by either method.

## ONE-PARTICLE CASE

A one-particle relativistic wave equation of the Dirac type may be written as

$$\mathcal{H}\Psi \equiv \{\beta mc^2 + \mathcal{E} + \mathcal{O}\}\Psi = i\hbar \frac{\partial}{\partial t}\Psi. \tag{1}$$

The even[6] part $\mathcal{E}$ and the odd part $\mathcal{O}$ of the Hamiltonian can be written as follows:

$$\mathcal{E} = \begin{pmatrix} \mathcal{E}' & 0 \\ 0 & \mathcal{E}'' \end{pmatrix}; \quad \mathcal{O} = \begin{pmatrix} 0 & \mathcal{O}' \\ \mathcal{O}'' & 0 \end{pmatrix}, \tag{2}$$

where $\mathcal{E}'$, $\mathcal{E}''$, $\mathcal{O}'$, $\mathcal{O}''$ are $2\times 2$ matrix operators. We shall assume that $\mathcal{O}$ (and $\mathcal{O}'$, $\mathcal{O}''$) is of the order of $c$, and $\mathcal{E}$ (with $\mathcal{E}'$, $\mathcal{E}''$) of order $c^0$. We consider here only the case of a time-independent $\mathcal{H}$. The usual substitution

$$\Psi = \exp\left\{\frac{W+mc^2}{i\hbar}t\right\}\begin{vmatrix} \psi \\ \psi'' \end{vmatrix}, \tag{3}$$

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[1] See, for example, W. Pauli, *Die Allgemeinen Prinzipien der Wellenmechanik* (Edwards Brothers, Inc., Ann Arbor, 1950), p. 237.

[2] L. L. Foldy and S. A. Wouthuysen, Phys. Rev. **78**, 29 (1950).

[3] R. Becker, Göttinger Nachr., p. 39 (1945).

[4] Ta-You Wu and G. E. Tauber, Phys. Rev. **100**, 1767 (1955).

[5] Technical report issued Aug. 16, 1955, under a U. S. Air Force contract (unpublished).

[6] We follow the terminology and notation of Z. V. Chraplyvy, Phys. Rev. **91**, 388 (1953); **92**, 1310 (1953), referred to as I and II.