Rigorous Solutions for Three-Body Rearrangement Reactions and Validity of the Distorted-Wave Born Approximation*

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In a distorted-wave type of formalism, two well-behaved integral equations have been obtained for a general three-body rearrangement reaction. The inhomogeneous terms of these equations may be considered to provide mathematically meaningful first approximations (MMFA) to the reaction amplitude. In each of the above mentioned cases, the distorted-wave Born approximation (DWBA) forms an integral part of MMFA. The extra terms in MMFA involve multiple-scattering processes and hence, at least in some cases, their matrix elements may be much smaller than those of DWBA term. This suggests that the success of DWBA may lie in the fact that DWBA is the dominating part of an MMFA. Some of the circumstances under which it can happen are discussed.

The Born series,[1] as well as the distorted-wave Born (DWB) series,[2] are based on Lippmann-Schwinger type integral equations. For the three-body rearrangement reactions the kernels of these integral equations are pathological; they have δ-function singularities over and above the center-of-mass momentum conservation δ function. As a result the solution to these problems in terms of Born series or DWB series is, in general, divergent. Apart from the divergence problem, in case of the existence of two-body bound states, the solution to the above mentioned integral equations is not unique.[3] The reasons for these pathologies and methods for curing them have been discussed and explained in a variety of ways.[3-11]

On the other hand, the distorted-wave method, and the distorted-wave Born approximation (DWBA) in particular, since the time it was first proposed by Francis and Watson[12] has worked well in a variety of nuclear reactions. Its successes include the deuteron stripping reaction which is a three-body problem. We, therefore, wish to discuss the distorted-wave equation and compare DWBA with two specific mathematically sound formalisms[13] in an attempt to see why it is so successful. Formalisms which do not involve the troublesome δ-function singularities (other than the center-of-mass momentum conservation δ function), will be referred to as mathematically sound or well behaved. A first-order approximation derived from a well behaved integral equation will be called a mathematically meaningful first approximation, abbreviated MMFA.

1. NOTATION

The complete Hamiltonian for a system of three particles can be written as

$$H = H_0 + V_1 + V_2 + V_3 + V_x = H_0 + V, \tag{1}$$

where H_0 is the free Hamiltonian or the sum of kinetic energy operators, V_1 is the interactions between particles 2 and 3 and likewise for V_2 and V_3, while V_x is the possible three-body interaction between the three particles. The Green's function for the complete Hamiltonian is denoted by

$$G = (E^+ - H)^{-1}; \quad E^+ = E + i\epsilon. \tag{2}$$

(Whenever not mentioned, it will be understood that the Green's functions we are dealing with have outgoing-wave boundary conditions.)

In the scattering theory of the three-body problem, one is concerned with reaction channels in which either all three particles propagate freely or one particle propagates freely and the other two are in a bound state. We shall label the various channels by the label of the free particle when there is only one particle that propagates freely. For the case of all three particles propagating freely, the channel shall be labeled by the subscript 0. With the definition

$$V_0 = 0, \tag{3}$$

we express the asymptotic Hamiltonian and the corresponding Green's function for any channel α, unambiguously, as follows:

$$H_\alpha = H_0 + V_\alpha; \quad G_\alpha = (E^+ - H_\alpha)^{-1}. \tag{4}$$

As is common practice, we shall use subscripts i and f for the initial and final channels, respectively. Then, for actual reactions, i can be 1, 2, or 3, while f can be any of the four channels 0, 1, 2, and 3.

The prior and post form of the transition operator can now be written as

$$U_{fi}^{-} = (1 + v_f G) v_i , \tag{5}$$

$$U_{fi}^{+} = v_f (1 + G v_i) , \tag{6}$$

where the initial and final state interactions v_i and v_f are

$$v_i = H - H_i = V - V_i , \tag{7}$$

$$v_f = H - H_f = V - V_f . \tag{8}$$

Notice the distinction between (capital) V_i and (lower case) v_i. They are not equal but are rather complementary, in that their sum equals the sum of all potentials in the problem.

In the following, we shall deal with U_{fi}^{+} alone [Eq. (6)]. The corresponding equations for U_{fi}^{-} can easily be derived in an analogous manner or even written down by comparison.

2. DISTORTED-WAVE TREATMENT

The essence of the distorted-wave method is to take into account parts of v_i and v_f in such a way that one obtains for the on-shell matrix elements of the transition operator an expression given by the following equation

$$\langle f(E) | U_{fi}^{+} | i(E) \rangle = \langle f(E) | W_f^{-\dagger} \hat{U}_{fi}^{+} W_i^{+} | i(E) \rangle = \langle \chi_f^{-} | \hat{U}_{fi}^{+} | \chi_i^{+} \rangle , \tag{9a}$$

where the new transition operator $\hat{U}_{fi}^{+}$ is

$$\hat{U}_{fi}^{+} = (v_f - w_f)[1 + G(v_i - w_i)] . \tag{9b}$$

In short the initial and final waves are replaced by some distorted waves and the new transition operator as compared to the original transition operator [Eq. (6)] has v_f replaced by $(v_f - w_f)$ and v_i replaced by $(v_i - w_i)$. Here w_i and w_f are the initial- and final-state distortion potentials and are now taken care of through the wave operators

$$W_f^{-\dagger} = 1 + w_f g_f , \quad g_f = (E^{+} - H_f - w_f)^{-1} , \tag{10}$$

and

$$W_i^{+} = 1 + g_i w_i , \quad g_i = (E^{+} - H_i - w_i)^{-1} . \tag{11}$$

Thus the distorted waves χ_f^{-} and χ_i^{+} are scattering-state solutions to $H_f + w_f$ and $H_i + w_i$, respectively.

Equation (9) follows from the operator identity,[2]

$$U_{fi}^{+} = W_f^{-\dagger}(v_f - w_f) W_i^{+} + W_f^{-\dagger}(v_f - w_f) G (v_i - w_i) W_i^{+} + w_f g_f G_i^{-1} , \tag{12}$$

provided that

$$\lim_{\epsilon \to 0} i\epsilon \langle f(E) | w_f g_f | i(E) \rangle = 0 . \tag{13a}$$

In case of rearrangement collisions (such as deuteron stripping and breakup), i and f are distinct channels. Therefore, the overlap $\langle f(E) | i(E) \rangle$ is identically zero. The above condition can then be written as

$$\langle f(E) | W_f^{-\dagger} | i(E) \rangle = \text{finite} . \tag{13b}$$

The condition (13b) is usually satisfied by choosing for w_f a pseudopotential which produces only elastic scattering in the final channel and hence cannot lead to rearrangements, although other choices are also possible. Note, however, that there is no restriction, whatsoever, on the choice of initial-state distorting potential w_i. In the corresponding equations for U_{fi}^{-} the roles of w_i and w_f are interchanged.

Once w_f has been properly chosen, we need consider only the first two terms in Eq. (12). The second term involves the full Green's function G and is difficult to evaluate with the present day techniques. The DWBA completely neglects the second term. Thus

$$U_{fi}^{+}(\text{DWBA}) = W_f^{-\dagger}(v_f - w_f) W_i^{+} , \tag{14}$$

which approaches exact result when $w_i \to v_i$ [cf. Eq. (12)]. However, the choice $w_i = v_i$ is not practical as we are lead back to the same problem of having to evaluate the full Green's function G. The hope of DWBA being a good approximation, heuristically, lies in the possibility that one can choose a w_i close to v_i and yet practical enough for efficient numerical calculations.

3. VALIDITY OF DWBA AND INTEGRAL EQUATIONS WITH DWBA AS INHOMOGENEOUS TERM

From another point of view, based on a comparison of Eq. (14) with Eq. (12), it is clear that the validity of DWBA depends on the relative magnitudes of the matrix elements of the two terms of Eq. (12) between energy conserving states of H_i and H_f. One way to answer this question is to set Eq. (12) in the form of an integral equation of which DWBA will be the inhomogeneous term and to check if an iterative solution to such an equation is possible. If the iterative solution exists then the rate of convergence of such a solution will be a direct measure of the validity of the DWBA. However, the nonexistence of the iterative solution to an integral equation which one may obtain *does not* constitute a conclusive proof that the DWBA is not a good approximation. We therefore proceed to obtain integral equations with com-

pact kernels and therefrom infer about the validity of DWBA.

4. INTEGRAL EQUATIONS WITH COMPACT KERNELS

The process of obtaining an integral equation corresponding to Eq. (12) for the transition amplitude, consists of expressing the second term involving the full Green's function G in the form $U_{fi}^{+}K+I$. The operator K will then be the kernel of the integral equation. The simplest way to achieve this is to use the identity

$$G=(1+Gv_i)G_i \tag{15}$$

for the Green's function. We then use the following result which is a special case of Eq. (12) for the transition amplitude, when one chooses the arbitrary initial-state distortion potential w_i to be zero

$$U_{fi}^{+}=W_f^{-\dagger}(v_f-w_f)(1+Gv_i)+w_f g_f G_i^{-1} \tag{16}$$

to set the second term of Eq. (12) in the proper form mentioned above. However, in general, this leads to an integral equation with a noncompact kernel involving a δ-function singularity. One way to overcome this difficulty is to use a "subtraction" (the meaning of this terminology will soon become clear) and thereby change the term which is to be cast in the form of homogeneous term $(U_{fi}^{+}K)$ plus an extra term (I). For this purpose, we use an arbitrary Hamiltonian H_c, corresponding Green's function G_c and $v_c=H-H_c$. Then using the identity $G=G_c+Gv_cG_c$, the second term of Eq. (12) becomes,

$$W_f^{-\dagger}(v_f-w_f)G_c(v_i-w_i)W_i^{+} +W_f^{-\dagger}(v_f-w_f)Gv_cG_c(v_i-w_i)W_i^{+}. \tag{17}$$

The new term [second term of Eq. (17)] to be set in the desired form is just the same old term but with G replaced by $G-G_c=Gv_cG_c$. This is what we mean by subtraction.

Once again, substituting Eq. (15) for G into Eq. (17) and making use of Eq. (16) to recognize the homogeneous term, we obtain the following integral equation corresponding to Eq. (12) for the transition amplitude:

$$U_{fi}^{+}=W_f^{-\dagger}(v_f-w_f)W_i^{+}+W_f^{-\dagger}(v_f-w_f)G_c(v_i-w_i)W_i^{+} +w_f g_f G_i^{-1}[1-G_i v_c G_c(v_i-w_i)W_i^{+}] +U_{fi}^{+}G_i v_c G_c(v_i-w_i)W_i^{+}. \tag{18}$$

The obvious choice of a v_c that does not involve any of the two-body potentials in (v_i-w_i), insures that there are no troublesome δ-function singularities in the kernel of Eq. (18). As a result it has a chance of being a Hilbert-Schmidt integral equation.

In Eq. (18) both the initial- and final-state distortion potentials are completely arbitrary. If one restricts the choice of w_f to satisfy condition (13), then the term $w_f g_f G_i^{-1}$ can be completely dropped from Eq. (12) . The modified transition operator then satisfies the equation

$$\tilde{U}_{fi}^{+}=W_f^{-\dagger}(v_f-w_f)W_i^{+}+W_f^{-\dagger}(v_f-w_f)G_c(v_i-w_i)W_i^{+} +\tilde{U}_{fi}^{+}G_i v_c G_c(v_i-w_i)W_i^{+}, \tag{19}$$

which is identical with Eq. (40) of Ref. 11.

Although Eqs. (18) and (19) appear to be rather complex, yet a judicious choice of w_i, w_f, and v_c, in many cases, can considerably simplify the final integral equation. In Ref. 11, Dodd and Greider discuss several applications of an equation for U_{fi}^{-} which is analogous to our Eq. (19). The present authors[14, 15] have used Eqs. (18) and (19) to obtain simple integral equations for deuteron elastic scattering, stripping, and breakup reactions on recoilless targets.

5. COMMENT ON COMPARISON BETWEEN EQUATIONS FOR $\tilde{U}_{fi}^{+}$ AND U_{fi}^{+}

Perhaps it is worthwhile to remark that even when the condition (13) is satisfied, so that

$$\langle f(E)|\tilde{U}_{fi}^{+}|i(E)\rangle=\langle f(E)|U_{fi}^{+}|i(E)\rangle, \tag{20}$$

nevertheless, the first-order approximations [the inhomogeneous terms of Eqs. (18) and (19)] differ by the quantity

$$\langle f(E)|w_f g_f v_c G_c(v_i-w_i)W_i^{+}|i(E)\rangle \tag{21}$$

which is not always zero. Thus the iterative solutions to Eqs. (18) and (19) will have different convergence properties. In particular, one of the series may converge while the other does not.

Under the circumstances being considered (when U and $\tilde{U}$ equations both have the same w_i, w_f, and v_c), we know the equality between the complete matrix elements of U_{fi}^{+} and $\tilde{U}_{fi}^{+}$ to be a fact. Therefore, we conclude that in the iterative series solution, the sum of extra subseries generated by the extra inhomogeneous term of Eq. (18) must vanish identically. Thus the convergence of the iterative solution to Eq. (18) as compared to that of Eq. (19) will further depend on the rate at which the above mentioned subseries converges to zero. However, it is conceivable that these subseries may cancel out the oscillatory character of the rest of the iterative solution and thereby improve the convergence of the over-all iterative solution.

In general, since Eq. (19) is a well behaved integral equation, its iterative solution will not be oscillatory and hence it should be preferable to use Eq. (19).

6. ON THE VALIDITY OF DWBA

If the iterative solution to, say Eq. (19), were convergent then the inhomogeneous terms give a mathematically meaningful first approximation to the full transition amplitude. It is interesting to note that the first inhomogeneous term is the DWBA operator. The second inhomogeneous term involves one extra scattering process and hence, at least in some cases, its matrix elements may be much smaller than those of the DWBA operator. Thus, even though on the basis of pathological integral equations which have DWBA as their inhomogeneous term, DWBA has been written off by some authors[2] as mathematically unsound, yet in some cases it may not differ much from the mathematically meaningful first approximation which Eq. (19) provides. Therefore, so long as physicists remain content with first-order approximations, the objection to DWBA on the grounds that the DWB series diverges is purely academic when the relevant matrix elements of correction terms are negligible compared to DWBA. For example, in the context of Eq. (19), the correction to DWBA can be written as $(|c\rangle \equiv$ eigenstate of $H_c)$ $S_c\langle\chi_f^-|v_f-w_f|c\rangle\langle c|v_i-w_i|\chi_i^+\rangle/(E^+-E_c)$. This is negligible compared to DWBA under any one of the following conditions:

(a) Initial-state distortion potential w_i simulates v_i very closely such that (v_i-w_i) is a very weak potential.

(b) A less stringent condition is to require that (v_i-w_i) connects the initial distorted wave to eigenstates of H_c very weakly, i.e., $\langle c|v_i-w_i|\chi_i^+\rangle \ll (E^+-E_c)$.

(c) $\langle\chi_f^-|v_f-w_f|c\rangle$ and $\langle c|v_i-w_i|\chi_f^+\rangle$ are peaked functions of E_c with peaks in different parts of the spectrum away from $E_c=E$.

(d) A condition similar to (b) for (v_f-w_f). However, unlike w_i the choice of w_f is restricted by Eq. (13). This condition (d), therefore, is less likely to be satisfied.

In conclusion we would like to add a note of caution. Although this paper may appear to be building a case in favor of DWBA, yet the best we have been able to demonstrate is that DWBA is closely related to some mathematically meaningful first-order approximations. One must check to see that it dominates the mathematically meanginful first approximation one constructs, in order to have a good level of confidence in its validity.

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