Configuration-Space-Faddeev Born Approximations

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Abstract

Alternative definitions of the Born approximation and the distorted-wave Born approximation within the framework of the configuration-space Faddeev equations are explored. The most natural definition does not correspond to the Born approximation derived from the Schrödinger equation, even though the exact T-matrices for both formalisms are equivalent. The Schrödinger form is optimal, although it is shown that the differences are numerically unimportant. The DWBA corresponding to the Faddeev equations is not channel symmetric, although numerically this is unimportant for the p-d (Coulomb) case. Convergence of the Born approximation partial-wave series is briefly investigated for p-d and n-d scattering below breakup threshold.
1 Introduction

Modern few-nucleon calculations are in principle a rich source of information about the nuclear force, provided that numerical results can be obtained with sufficient precision. The required level of precision depends sensitively on the observable being calculated. That level ranges from modest in the case of unpolarized observables such as the differential cross section to high in the case of some polarization observables, since the latter often depend on delicate cancellations between partial waves. One of the strengths of the few-nucleon field is that accurate calculations for realistic potentials are now routine[1, 2, 3].

One of the consequences of this numerical precision requirement is that a substantial number of partial waves may be required. This is not such a dire problem for momentum-space techniques, many of which generate a Born series for the T-matrix as the preferred method of solution. Such a series should converge faster as the angular momentum increases. That is not the case, however, in configuration space, where each partial wave is solved in its entirety. Because more and more partial waves of the potential contribute as the angular momentum increases, this significantly increasing effort is rewarded by decreasing return as the size of higher-partial-wave T-matrix elements becomes smaller and smaller. One way to increase efficiency in the process is to use the Born approximation for higher partial waves, which significantly reduces the effort[4].

We detail below several pitfalls that arise in defining the Born approximation using configuration-space Faddeev techniques[5]. While none of these difficulties are very important in practical calculations (although this is not a priori obvious), it is nevertheless worthwhile to avoid them altogether. These problems are derived in Section 2 for the Born approximation (BA) and in Section 3 for the distorted-wave Born approximation (DWBA), and a few numerical results are given and discussed in Section 4, which is followed by our summary and conclusions. We restrict ourselves to energies below the deuteron-breakup threshold, and we ignore three-nucleon forces, which are an inessential complication.

2 Faddeev Equations and the Born Approximation

The Faddeev decomposition in configuration space[6] can be pictured most easily as dividing the wave function into parts corresponding to different asymptotic processes. For three (identical) particles this leads to three equations

\[(E - T - V_i)\psi_i = V_i(\psi_j + \psi_k),\]  

(1)
where $i, j, k$ take on the values of the cyclic permutations of 1, 2, and 3, and $V_i \equiv V(x_i)$. The Schrödinger wave function is given by

$$\Psi = \psi_1(x_1, y_1) + \psi_2(x_2, y_2) + \psi_3(x_3, y_3), \quad (2)$$

with arguments fashioned from the coordinates, $r_i$, of all $i$ particles:

$$x_i \equiv r_j - r_k, \quad (3a)$$

and

$$y_i \equiv \frac{1}{2}(r_j + r_k) - r_i. \quad (3b)$$

The coordinate $x_i$ is the distance between particles $j$ and $k$, while $y_i$ is the distance between particle $i$ and the center of cluster $j+k$. Depending on the desired application a normalization factor of $1/\sqrt{3}$ may be used in the definition of $\Psi[7]$. With these definitions the sum of the three independent Eqns. (1) yields the original Schrödinger equation

$$(E - T - V_1 - V_2 - V_3)\Psi = 0. \quad (4)$$

The coordinates (3) used in the Faddeev wave functions in Eqn. (4) generate different asymptotic configurations (or channels) that facilitate the appropriate boundary conditions for this partial-differential equation. Used in this way the Faddeev equations are merely another (equivalent) form of the original Schrödinger equation.

The appropriate boundary conditions for elastic scattering (below breakup threshold) are easily seen from Eqn. (1). For large $|y_i|$ the scattered wave function factorizes into the product of a deuteron wave function $\phi_d(x_i)$ and an outgoing wave, $\chi(y_i)$, which guarantees that the right-hand side of Eqn. (1) vanishes in this limit. This product of $\phi_d$ and a plane wave (or a Coulomb wave in case of p-d scattering), $\chi(y_i)$, defines the “free” channel wave function, $\phi_i[7]:$

$$\phi_i(x_i, y_i) = \phi_d(x_i)\chi(y_i), \quad (5a)$$

satisfying

$$(E - T - V_i)\phi_i = 0, \quad (5b)$$

which we can use to construct the exact T-matrix and its Born approximation.

The Faddeev T-matrix is most easily developed by projecting Eqn. (1) with $\langle \phi_i |$. The resulting left-hand-side integral vanishes because of Eqn. (5b), except for surface terms that constitute the T-matrix (just like the two-body case[8])

$$t_F = \langle \phi_1|V_1|\psi_2 + \psi_3 \rangle, \quad (6)$$

and any other permutation of Eqn. (1) yields the same result. This can be converted[9] to a more recognizable form by rearranging Eqn. (5b) to $\langle \phi_1|V_1 = \langle \phi_1|(E - T)$, making use of the Hermiticity of the Hamiltonian for these wave functions below
breakup threshold, and employing Eqn. (1) to produce the Schrödinger form of the T-matrix[10]

$$t_S = \langle \phi_1 | V_2 + V_3 | \Psi \rangle . \quad (7)$$

The potential $V_2 + V_3$ is the usual “inter-cluster” potential[10] between the nucleon projectile and the deuteron target that generates the scattering T-matrix. The two forms of the T-matrix given in Eqns. (6) and (7) are exactly equivalent if the wave functions are exact.

Born approximations can be obtained from Eqns. (6) and (7) by replacing the $\psi_i$ by $\phi_i$ and $\Psi$ by $\Phi = \phi_1 + \phi_2 + \phi_3$:

$$t_{BA}^F = \langle \phi_1 | V_1 | \phi_2 + \phi_3 \rangle , \quad (8a)$$

and

$$t_{BA}^S = \langle \phi_1 | V_2 + V_3 | \Phi \rangle . \quad (8b)$$

In order to facilitate the comparison of the two Born approximations in Eqns. (8) it is convenient to introduce the compact notation

$$(ijk) \equiv \langle \phi_i | V_j | \phi_k \rangle . \quad (9)$$

Interchanging the labels of pairs of variables leads to $(132) \equiv (123)$, etc., while the trick used to convert Eqn. (6) to Eqn. (7) leads to $(122) \equiv (112)$, etc. We thus arrive at

$$t_{BA}^F = 2(112) , \quad (10a)$$

and

$$t_{BA}^S = 2(112) + 2(121) + 2(123) , \quad (10b)$$

which are distinctly different. One can also use these tricks to demonstrate that the Faddeev form of the Born-approximation T-matrix is channel symmetric:

$$t_{FA}^b = \langle \phi^a_1 | V_1 | \phi^b_2 + \phi^b_3 \rangle = \langle \phi^b_2 + \phi^b_3 | V_1 | \phi^a_1 \rangle = t_{FA}^a , \quad (10c)$$

where we have attached channel labels that were previously suppressed. In other words the “post” and “prior” forms of the Born approximation are identical, a result long known for $t_S[10]$. The numerical significance of the difference of Eqns. (10a) and (10b) will be discussed in Section (4).

An important point concerning the Born approximation has been made by Kievsky et al[4]. The Kohn variational functional can be written as[7]

$$I(\Psi) = \langle \Psi | H - E | \Psi \rangle = \langle \psi_1 | H - E | \Psi \rangle , \quad (11)$$

where the last step follows by interchange of variables and by removing the normalization factor $1/\sqrt{3}$ from each wave function. Varying $\Psi$ (and $\psi_1$) about the plane-wave limit leads to

$$t_{Kohn} = \langle \phi_1 | V_2 + V_3 | \Phi \rangle + O(V^2) , \quad (12)$$
since any change in $\Psi$ beyond the plane-wave part must be proportional to the potential, and the Kohn error is proportional to the square of that change in $\Psi$. For this reason $t_{\text{BA}}^F$ in Eqn. (8b) gives the optimal Born approximation. The two terms missing in $t_{\text{BA}}^F$ are “hidden” in $\psi_2 + \psi_3$. Even though $t_{\text{BA}}^F$ is linear in the potential $V_1$, that potential serves partly to drive the dynamics (since Eqn. (6) is exact) and partly to bind the deuteron; the latter terms do not directly contribute to the T-matrix, and serve to “hide” $V_2$ and $V_3$ terms residing in $\psi_2$ and $\psi_3$. Thus the Faddeev Born approximation has first-order (in $V$) errors, unlike the Schrödinger result.

3 Faddeev Equations and the DWBA

The remaining task is to compare distorted-wave Born approximations from the Faddeev and the Schrödinger equations. This is complicated by the fact that long-range forces (such as Coulomb) have been treated in the Faddeev formalism in a variety of ways, reflecting the non-unique character of the Faddeev equations themselves. A powerful formal device is the introduction of Faddeev distortion potentials, $X_i$. We can replace Eqn. (1) by

$$\left[E - T - V_1 - X_j - X_k\right]\psi_i = (V_i - X_i)(\psi_j + \psi_k).$$

If one sums the three independent (cyclic-permutation) members of this set, one obtains the original Schrödinger equation in Eqn. (4) (i.e., the $X_i$ cancel), and $\Psi$ is free of the arbitrary $X_i$, as well, although individual $\psi_i$ are not free. It is effective to choose the $X_i$ so that long-range distortions are built into the wave functions $\psi_i$. As a specific example we treat the important case of long-range Coulomb distortions, and write $V_i = V_{i}^{\text{st}} + V_{i}^{\text{C}}$, where $V_{i}^{\text{st}}$ and $V_{i}^{\text{C}}$ are the strong-interaction and Coulomb parts of the nuclear force. In this case we have found it most efficient numerically to choose $X_i = V_{i}^{\text{C}}$, which places all of the Coulomb interaction on the left-hand side of Eqn. (13). Other choices are possible and have been used by others[11, 12].

We begin our treatment of DWBA by noting that if a long-range force modifies the asymptotic form of the inter-cluster scattering wave function, $\chi(y_i)$, our basis wave functions (i.e., the “free” scattering wave functions) are modified and correspond to

$$\left(E - T - V_1 - U_1\right)\phi_1 = 0,$$

where $U_1$ is an appropriate long-range interaction potential (e.g., $Z\alpha/y$ for p-d Coulomb scattering). We next rearrange Eqn. (13) (choosing $i = 1$) by moving all $X$-terms to the right-hand side, and then adding and subtracting a potential $U_1$:

$$\left(E - T - V_1 - U_1\right)\psi_1 = (X_2 + X_3 - U_1)\psi_1 + (V_1 - X_1)(\psi_2 + \psi_3).$$

Projecting this equation on the left with $\langle \phi_1 |$ gives a left-hand-side that vanishes because of Eqn. (14) except for surface terms (that comprise the T-matrix, as before)

$$\bar{t}_F = \langle \phi_1 | X_2 + X_3 - U_1 | \psi_1 \rangle + \langle \phi_1 | V_1 - X_1 | \psi_2 + \psi_3 \rangle,$$
where we ignore here (and hereafter) the T-matrix coming solely from the potential $U_1$ (e.g., the point-Coulomb T-matrix), which is important but peripheral to our discussion. The barred-$t$ indicates asymptotic states modified by $U_1$. Choosing $X_i = V^C_i$ in the Coulomb case leads to our preferred form of the Coulomb-distorted-wave Faddeev T-matrix, $\tilde{t}_F^C$:

$$\tilde{t}_F^C = \langle \phi_1 | V_1^{st} | \psi_2 + \psi_3 \rangle + \langle \phi_1 | V^C - U_1 | \psi_1 \rangle,$$

(17)

where $V^C$ is $V_2^C + V_3^C$, and we have used the fact that $V_1^C$ vanishes. If we again use $\langle \phi_1 | V_1 = \langle \phi_1 | (E - T)$ in Eqn. (16), we obtain after some algebra

$$\tilde{t}_S = \langle \phi_1 | V_2 + V_3 - U_1 | \Psi \rangle,$$

(18)

a remarkably different-looking, but equivalent, result. Equation (18) is the usual Schrödinger form of the distorted-wave T-matrix, and differs from Eqn. (7) only by the $U_1$ term[10].

Although the two forms of the T-matrix in Eqns. (16) and (18) are formally identical, they lead to very different DWBAs. Replacing $\psi_i$ by $\phi_i$ and $\Psi$ by $\Phi$ in Eqn. (16) leads to a formally unacceptable DWBA, because it would depend on the unphysical (i.e., artificial) $X_i$

$$\tilde{t}_F^{DWBA} = \langle \phi_1 | X_2 + X_3 - U_1 | \phi_1 \rangle + \langle \phi_1 | V_1 - X_1 | \phi_2 + \phi_3 \rangle,$$

(19)

although the choice of $X_i$ leading to Eqn. (17) obscures this fact. The DWBA obtained from Eqn. (18)

$$\tilde{t}_S^{DWBA} = \langle \phi_1 | V_2 + V_3 - U_1 | \Phi \rangle,$$

(20)

is free of that disease because Eqn. (18) depends only on $\Psi$, and not the individual $\psi_i$. The Schrödinger DWBA is the optimal one in the sense that corrections to it are second order in the potential. The techniques that led to Eqn. (10c) also demonstrate that the distorted-wave T-matrix in Eqn. (19) is not symmetric under interchange of incoming and outgoing channels (post and prior forms), because of terms involving $X_1$ and $U_1$. This is a serious disease, since it violates a symmetry, although we shall see in the next section that the effect is sufficiently small that it is not a significant practical problem. Equation (20) can be shown by the same techniques to be channel symmetric.

In summary the “Faddeev” form of the DWBA has three formally serious problems: (1) it leads to a non-symmetric T-matrix; (2) it leads to manifestly non-unique results (viz., the $X$-terms); (3) it leads to errors linear in the potential. How important these flaws are in a numerical sense is discussed next.
4 Numerical Results

We briefly report two numerical results on: (1) differences between the Faddeev and Schrödinger forms of the Born approximation, together with the magnitude of the lack of symmetry of the post and prior forms of the T-matrix; (2) the fractional errors in the difference of the exact Faddeev and Born approximation results for both p-d and n-d scattering below deuteron-breakup threshold.

The form of the Born approximations given by Eqns. (10a) and (10b) suggests that numerical differences should be small. Below the threshold for deuteron breakup the region of configuration space where scattering can occur is very limited. The deuteron bound-state wave function has a finite extent, $R_d$, while the nuclear force has a significantly smaller range, $R_V$. For this reason the integrand of the configuration (123), for example, is important only in the very small region where the nuclear potential in variable $x_2$ overlaps with a deuteron wave function in variable $x_1$ and another in variable $x_3$. This occurs only for very small $|y_1|$, where the wave function is suppressed for large values of the angular momentum. By far the largest configuration will be (112), since $V_1$ overlaps easily with $\phi_d(x_1)$, and this result has a much larger overlap with the deuteron wave function in variable $x_2$. Numerical results bear this out; the (112) matrix element completely dominates. This immediately suggests that the lack of symmetry between (off-diagonal) T-matrix elements is also numerically small.

The importance of the Born amplitudes for higher partial waves (in $J$, the total angular momentum of the channel states) is indicated in Table I, where both the differential cross section, $d\sigma/d\Omega$, and analyzing power, $A_y$, have been computed using the AV18 potential[13]. These observables were computed in two ways: exact calculations through $J = 11/2$ (supplemented by Born approximation results for higher waves where needed) and various comparison calculations described below. The maximum value of the magnitude of the fractional difference between the exact and comparison calculations was computed for the angular range $\theta = 30^\circ - 150^\circ$. The restricted angular range was used because the analyzing power gets small outside that range, and relatively large fractional errors in that regime would be meaningless. In the small table labelled Truncation the comparison calculation had its partial-wave series truncated at the labelled $J$ (i.e., that $J$-wave and all higher ones were omitted), leading to some very large errors. If one adopts the criterion that observables should be calculated to 1% accuracy, one needs to keep all matrix elements through $J = 9/2$ for the differential cross section, and through $J = 15/2$ for the analyzing power for 3 MeV p-d scattering.

In the tables labelled Born Substitution the comparison case involved substituting the (Schrödinger) Born amplitude for the labelled wave and all higher ones through the maximum value of $J = 15/2$. The differential cross sections are accu-
Table I. Maximum absolute values of the fractional differences between exact and comparison calculations for differential cross sections and analyzing powers versus partial wave. The comparison labelled Truncation deletes the labelled partial wave and all higher ones. The comparison labelled Born Substitution substitutes the Born approximation for the exact T-matrix elements for the labelled partial wave and all higher ones. Results are presented in the format $x.x[n] \equiv x.x \times 10^n$.

| Partial Wave | $\frac{5}{2}$ | $\frac{7}{2}$ | $\frac{9}{2}$ | $\frac{11}{2}$ | $\frac{13}{2}$ | $\frac{15}{2}$ |
|--------------|-------------|-------------|-------------|-------------|-------------|-------------|
| **Truncation – 3 MeV p-d** | | | | | | |
| $\Delta (d\sigma/d\Omega)/(d\sigma/d\Omega)$ | 4.9[-1] | 1.1[-1] | 2.8[-2] | 7.8[-3] | 2.0[-3] | 3.9[-4] |
| $\Delta (A_y)/A_y$ | 3.1[ 1] | 4.4[ 0] | 1.5[ 0] | 3.9[-1] | 8.6[-2] | 1.8[-2] |
| **Born Substitution – 3 MeV n-d** | | | | | | |
| $\Delta (d\sigma/d\Omega)/(d\sigma/d\Omega)$ | 1.4[-1] | 2.2[-3] | 1.2[-4] | 8.9[-6] | | |
| $\Delta (A_y)/A_y$ | 4.1[ 0] | 2.2[-1] | 1.9[-2] | 1.9[-3] | | |
| **Born Substitution – 1 MeV p-d** | | | | | | |
| $\Delta (d\sigma/d\Omega)/(d\sigma/d\Omega)$ | 7.0[-2] | 7.1[-4] | 1.3[-5] | 4.3[-6] | | |
| $\Delta (A_y)/A_y$ | 8.6[ 0] | 1.3[-1] | 1.1[-2] | 2.7[-3] | | |
| **Born Substitution – 3 MeV p-d** | | | | | | |
| $\Delta (d\sigma/d\Omega)/(d\sigma/d\Omega)$ | 8.5[-2] | 2.1[-3] | 9.7[-5] | 5.8[-6] | | |
| $\Delta (A_y)/A_y$ | 4.2[ 0] | 1.4[-1] | 1.3[-2] | 1.1[-3] | | |

Rately computed (using the 1% criterion) by keeping exact matrix elements through $J = 5/2$, while the analyzing power requires exact $J = 9/2$ matrix elements. Exact configuration-space Faddeev calculations for large values of $J$ (such as 11/2) require significant computational resources, and should be avoided if possible.

The difference between the Faddeev Born approximation and the Schrödinger Born approximation depends on the particular matrix element, but typically is only a few per cent, and this is not likely to be very important. The Schrödinger form of the BA and DWBA is nevertheless demonstrably closer to the exact matrix elements for higher partial waves than is the Faddeev form of those matrix elements. The channel asymmetry in p-d scattering matrix elements at 3 MeV is typically a few times $10^{-3}$, and hence is numerically unimportant for the Coulomb DWBA problem.

In summary, we have shown that the most natural Born approximation for the Faddeev T-matrix differs from that of the Schrödinger equation. We have shown
that the Faddeev DWBA has three formally serious properties: (1) it leads to a non-symmetric T-matrix; (2) it leads to manifestly non-unique results; (3) it leads to errors linear in the potential. In practical (i.e., numerical) terms these defects are not very important. Our analysis demonstrates that the dominant part of the Born approximation is contained in both approaches, and they differ only in much smaller contributions.

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