Adiabatic-approximation survey of breakup effects in deuteron-induced reactions

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We investigate breakup effects in a three-body model of deuteron elastic scattering and stripping reactions for a variety of potential parameters, bombarding energies, and momenturn matching conditions. The investigation is based on the adiabatic approximation with relative angular momentum $l = 0$. We test this approximation by comparisons with several available coupled-channel calculations. The adiabatic wave function is divided into elastic and breakup parts, whose contributions to stripping are discussed separately. Breakup is seen to be primarily an effect of the nuclear interior. Elastic scattering is discussed by fitting a local equivalent potential to the elastic part of the wave function. This potential shows several characteristic features which are fairly stable with respect to the potential parameters and bombarding energies. The validity and limitations of the adiabatic approximation are examined. The approximation is seen to be fairly good for elastic scattering, but of only marginal value for stripping reactions. Possible improvements of the adiabatic approximation are discussed.

NUCLEAR REACTIONS Adiabatic approximation, coupled-channel calculations, folding model, three-body wave function, local equivalent potential, deuteron stripping reactions.

I. INTRODUCTION

The large, loose structure of the deuteron easily leads to a three-body picture of deuteron-nucleus collisions, in which the relative motion of the incident proton and neutron is affected by their interactions with the target nucleus. This contrasts with the model wave function used in DWBA calculations, in which the proton-neutron relative motion is taken to be that of an unmodified deuteron. Certainly the interactions cause some excitation or "breakup" of the incident deuteron. It is of great interest to assess the modifications of DWBA calculations that are caused by such excitation effects.

Several truncated coupled channel (CC) calculations have been constructed¹⁻⁶ which omit rearrangement from the three-body model and which introduce discretized representations of the deuteron breakup continuum. However, these calculations are sufficiently lengthy so that it has not been possible to obtain a general survey of breakup effects from them, not even from the recent extensive work by the Kyushu group. 5

The three-body model has also been evaluated by adiabatic approximation,⁷ in which all the states of the breakup continuum are taken to have the same energy. This method allows fairly simple calculations from which useful results have already been obtained. 8.9 The present paper applies this simple method to develop a brief survey of breakup effects.

Our calculation specializes to relative angular momentum $l = 0$ in the proton-neutron system, as in some early CC work.^{2, 3} Although at least $l = 2$ is also known to be important, $1, 4, 5$ we feel that a survey of breakup effects for the pure $l = 0$ case is an informative first step.

The CC and adiabatic methods are outlined in Sec. II and numerical results from corresponding calculations by these two methods are compared in Sec. III. Some limitations of the adiabatic approximation are discussed there and again in later sections of the paper. The adiabatic method is rather good for elastic scattering, which is discussed in Sec. IV; useful generalities are found. The application to stripping in Sec. V is less satisfactory because breakup effects in stripping seem sensitive to the parameters of particular reactions. Section VI is a summary and a brief report of possible improvements of the adiabatic method.

II. THEORETICAL BACKGROUND

We consider the familiar three-body theoretical model in which a proton and neutron move with respect to a stationary target "nucleus," according to the Hamiltonian

$$
H = T_p + T_n + U_p(r_p) + U_n(r_n) + V(|\vec{r}_p - \vec{r}_n|) .
$$
\n(2.1)

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Relative and center of mass coordinates are introduced,

$$
\vec{r} = \vec{r}_p - \vec{r}_n , \ \vec{R} = \frac{1}{2} (\vec{r}_p + \vec{r}_n) , \qquad (2.2)
$$

and the model is truncated to relative angular momentum $l = 0$, as in previous work. Thus the reduced three-body model we study is

$$
[E - T_R - U(r, R) - T_r - V(r)]\psi(r, \vec{R}) = 0 , (2.3)
$$

$$
U(r,R) \equiv \frac{1}{4\pi} \int d\Omega_r \left[U_p \left(\left| \vec{R} + \frac{1}{2} \vec{r} \right| \right) \right. \\ \left. + U_n \left(\left| \vec{R} - \frac{1}{2} \vec{r} \right| \right) \right]. \quad (2.4)
$$

Solutions of Eq. (2.3) are obtained either in adiabatic approximation or by an (essentially exact) coupled channels method.

A. Adiabatic approximation

The model Schrödinger equation (2.3) is rewritten

$$
[E - T_R - U(r, R) - \epsilon_d] \psi(r, \vec{R})
$$

=
$$
[T_r + V(r) - \epsilon_d] \psi(r, \vec{R}) , \quad (2.5)
$$

where

$$
[T_r + V(r)]\phi_d(r) = \epsilon_d \phi_d(r) \tag{2.6}
$$

and $\phi_d(r)$ is the deuteron wave function. If we imagine $\psi(r,\vec{R})$ to be expanded in the set of eigenstates

$$
\{\phi_d(r), \phi(k,r)\},\tag{2.7}
$$

$$
\psi(r,\vec{\mathbf{R}})=\sum_{LM_L}a_{LM_L}[Y_{LM_L}(\hat{R})/rR]\{\phi_d(r)f_L(R)+\int_0^\infty dk\phi(k,r)g_L(k,R)\}\ ,
$$

in which a_{LM_L} are coefficients determined by the incident plane wave part of ψ . The continuum integral is replaced by a finite sum over bins. Substitution in the model Schrödinger equation (2.3) then gives coupled equations for the undetermined functions $f_L(R)$, $g_L(k, R)$; these equations are solved by straightforward numerical means. Use of outgoing boundary conditions for $f_L(R)$, $g_L(k,R)$ produces appropriate asymptotic behavior for $\psi(r, \vec{R})$, with both the proton and neutron outgoing. Each term of $\psi(r,\mathbf{R})$ reduces asymptotically to the correct total energy, independent of the value of k.

Solutions of the coupled equations are obtained in Refs. 2 and 3 for the case $E = 22.9$ MeV, with

$$
U_p(r_p) = U_n(r_p)
$$

= -(50 MeV)(1+0.1*i*) $e^{-\alpha^2 r_p^2}$ (2.12)

with

$$
[T_r + V(r)]\phi(k,r) = (\hbar^2 k^2 / M)\phi(k,r) , \qquad (2.8)
$$

then it is plausible that the higher-energy terms of the set (2.7) occur in ψ with low probability and therefore the right hand side (RHS) of (2.5) tends to be small.

In the adiabatic approximation we omit the RHS of (2.5), to get

with
$$
[E - T_R - U(r, R) - \epsilon_d] \psi^{\text{AD}}(r, \vec{R}) = 0.
$$
 (2.9)

This is now an elastic scattering problem for the coordinate \overline{R} , in which r appears only as a parameter. We solve this problem separately for each value of r, using partial waves in the vector \hat{R} and outgoing wave boundary conditions. Evidently the r dependence of ψ^{AD} defines a rather complicate wave packet composed of the states (2.7) . The r dependence of the asymptotic wave function implies a mixture of these states, having an unphysical mixture of energies. Such a wave function cannot be used at asymptotically large values of r.

In applications the incident wave part of ψ^{AD} contains a single relative state, say ϕ_d , which we emphasize by introducing a partially factored form

$$
\psi^{\text{AD}}(r,\vec{R}) = \phi_d(r)\chi^{\text{AD}}(r,\vec{R})\ . \tag{2.10}
$$

In this form it is understood that the incident wave part of χ^{AD} is a normalized plane wave.

B. Coupled channels

In the CC method ψ is expanded immediately in the set of eigenstates (2.7), to give

and
$$
\alpha = 0.25
$$
 fm⁻¹. The Coulomb potential is not included. Solutions are obtained again in Ref. 10 with the imaginary part of (2.12) omitted. These two sets of solutions are available for comparison with corresponding adiabatic calculations.

C. Wave function at coincidence

It is of particular interest to examine $\psi(r,\mathbf{R})$ at the coordinate value $r = 0$, both because the theoretical expressions simplify at $r=0$ and because $r\approx 0$ tends to dominate stripping calculations. At $r = 0$ the radial part of Eq. (2.11) takes the form

$$
f_L(R) + h_L(R) = F_L(R) , \qquad (2.13)
$$

with

$$
h_L(R) \equiv \lim_{r \to 0} \int_0^\infty dk \left[\phi(k,r) / \phi_d(r) \right] g_L(k,R) \tag{2.14}
$$

(2.11)

ding radial functions $f_L^{AD}(R)$ and $h_L^{AD}(R)$ are obtained in the adiabatic approximation by ap plying the p

$$
|\phi_d\rangle\langle\phi_d| \ , \ 1-|\phi_d\rangle\langle\phi_d| \ , \qquad (2.15)
$$

to the partial wave components of $\psi^{AD}(r, \vec{R})$, to select the elastic and nonelastic parts of the adiabatic wave function.

III. COMPARISON OF ADIABATIC WITH CC

It is much easier to derive the adiabatic solution of the model Schrödinger equation than the CC solution. It is therefore important to compare correding solutions, wherever possible how reasonable it may be to use the adiabatic approximation as a substitute for CC calculations. We now compare the adiabatic with the CC calculations arrell, Vincent, and Austern $(FVA)^3$ referred to in connection with Eq. (2.12) .

Previous comparisons¹¹ of adiabatic and FVA results showed that the elastic cross sections and S matrix elements are in very good agreement, and the energy-integrated breakup cross sections are in good agreement. However, it was found that for low angular momenta L the adiabatic calculation of the distribution of the breakup cross section with respect to relative momentum k is excessively weighted toward high k .

We now compare the adiabatic projected radial f_I^{AD} , h_I^{AD} sponding FVA wave functions.³ Figure 1 shows a typical set of comparisons. One difference is seen immediately; h_L^{AD} lacks the strong decrease at large R that is typical of h_L from the CC calculation. This is understandable: We see in Eq. (2.14) that combination of channel functions that have mbination of channel func
relative energies ϵ_k —as R k as R increases these functions drift out of phase and they begin fere destructively. Although the same channel funcent implicitly in the adiabatic wa function, they all have the same relative energy and therefore they maintain the same relative phase at all R. It is not too surprising that h_L^{AD} actually resembles in detail the lowest energy bin function $g_L(k, R)$ of FVA.

Comparisons at small values of R or for single e relative energy are n ases in the fashion described above. In conse quence it is gratifying to see that the wave function e elastic radia s f_L , f_L^{AD} of the two calculations are

FIG. 1. Moduli of radial wave functions at coincidenc $_{L}(R)$ and the breakup part $h_{L}(R)$, respectively. Solid line represents total coincident wave function $F_{L} = f_{L} + h_{L}$. Left and right portions are, respectively, coupled channel wave functions and adiabatic wave functions.

in excellent agreement, and that h_L and h_L^{AD} have very similar behavior in the nuclear interior. Certainly h_L and h_L^{AD} have approximately the same magnitudes at small R.

We conclude that the adiabatic method gives a useful approximation to the more accurate CC results, except for the summed breakup function $h_L(R)$ at large R, where relative phases matter. Therefore it seems appropriate to apply the adiabatic method under a variety of conditions, to assess the importance of three-body effects in deuteron reactions. Of course, as we note again in Sec. V, $h_L(R)$ in the nuclear exterior region is needed for stripping.

Since the adiabatic and CC calculations of the elastic wave function are in good agreement, we can apply the adiabatic method with confidence to survey the infiuence of breakup on elastic scattering. We discuss the elastic radial wave functions $f_I^{AD}(\overline{R})$ in terms of trivially equivalent local optical potentials that exactly fit these wave functions:

$$
U_L^{\rm TE}(R)\!\equiv\![E-\epsilon_d\!-\!T_L(R)]f_L^{\rm AD}/f_L^{\rm AD}\;, \eqno(4.1)
$$

in which

$$
T_L(R) = -\frac{\hbar^2}{4M} \left[\frac{d^2}{dR^2} - \frac{L(L+1)}{R^2} \right].
$$
 (4.2)

Although such trivially equivalent potentials have a pole at every zero of the wave function, in a calculation with complex potentials or with multichannel coupling these poles are displaced into the complex R plane and are not disturbing. [Even so, whenever there is nonlocality in the derivation of a wave function, the associated U_L^{TE} tends to have some oscillations. These oscillations arise because nonlocality displaces the zeros of the numerator in Eq. (4.1) from those of the denominator; they provide an indication of the range of nonlocality.]

Our adiabatic calculations were performed at three energies, $E=10$, 22.9, 80 MeV, using the FVA Gaussian potential of Eq. (2.12), with three values of the imaginary well depth, $W_0=0$, 5, 10 MeV at each energy. A typical U_L^{TE} graph is shown in Fig. 2.

It is instructive to compare U_L^{TE} with the Watanabe folded potential

$$
U^{\text{fold}}(R) \equiv \int d^3r \phi_d{}^2(r) U(r, R) \;, \tag{4.3}
$$

as in Fig. 2, and with the elementary Johnson-Soper

FIG. 2. Trivially equivalent local optical potential U_L^{TE} FIG. 2. Trivially equivalent local optical potential U_L (solid lines) and folding potential U_L^{fold} (dotted lines) for $L = 0$ at $E = 22.9$ MeV. FVA Gaussian potential (Ref. 2) with $V_0 = 50$ MeV and $W_0 = 5$ MeV are used for V_p and V_n .

potential

ential

$$
U^{JS}(R) \equiv U(0,R) = U_p(R) + U_n(R) , \qquad (4.4)
$$

that generates the entire adiabatic wave function $\psi^{AD}(r,\vec{R})$ at $r=0$. In our numerical calculations the relations among these potentials are found to be extremeley stable with respect to variations of E and W_0 . In summary, the comparisons show that: (1) W_0 . In summary, the comparisons show that: (1) U_L^{TE} and U^{fold} are essentially equal at large R, where they decrease a little more slowly than U^{IS} ; (2) in the nuclear interior the real part of U_L^{TE} for low partial waves is approximately 5 MeV stronger than that of U^{fold} , but it is about 10 MeV weaker than the real part of U^{JS} ; (3) the imaginary part of U_L^{TE} for low partial waves is about 10 MeV stronger than in the other potentials; (4) for high partial waves, which do not penetrate to the nuclear interior, we obtain $U_L^{TE} \approx U^{\text{fold}}$. Thus the elastic adiabatic calculation provides several significant corrections to the simple folding model of elastic scattering. Calculations with Woods-Saxon potentials give similar results.

It is noteworthy that modifications due to breakup seem to be localized in the nuclear interior, where they cause increased attraction and increased absorption. The absorption is easy to understand. The presence of breakup in the nuclear interior (independent motion of the proton and neutron) implies loss

of flux from the elastic projected part of ψ^{AD} . As to the real potential, retention of the nonelastic part of ψ^{AD} seems to avoid the averaging effect of Eq. (4.3), which causes the Watanabe potential to be weaker than the sum of short range potentials $U_n(R) + U_n(R)$. Subsequent projection on the elastic channel gives a real potential that more nearly resembles that of Eq. $(4.4).^{12}$ Another indication that breakup tends to emphasize the nuclear interior was seen in the previous CC work,^{2,3} where the total CC radial wave function $F_L(R)$ at low L is a little larger in the interior than the wave function from the corresponding folded potential calculation. An interesting speculation about these effects is that breakup may tend to trap the separated particles in the nuclear interior, as if a mini compound nucleus were being formed.

V. COINCIDENCE WAVE FUNCTIONS: STRIPPING

Figure ¹ shows a typical set of radial wave functions $f_L(R)$, $h_L(R)$, $F_L(R)$, which describe the makeup of $\psi(r, \vec{R})$ at $r = 0$. It has already been remarked that h_L^{AD} is misleading at large R, where the absence of phase averaging prevents it from decreasing appropriately. It is now of interest to examine the radial wave functions in greater detail. We recall that zero-range reaction calculations, as for stripping, tend to be determined by $F_L(R)$, the radial part of the total coincidence wave function $\psi(0,\mathbf{R})$. Since $F_L(R)$ contains $h_L(R)$, this breakup function affects the stripping.

The properties of $h_L(R)$ and $h_L^{AD}(R)$ can be classified both by radius—in which we distinguish regions of R that are *inside* or *outside* the nucleusand by angular momentum L . Partial waves of low L penetrate to the inside and are affected by all parts of the interaction $U(r, R)$. Partial waves of high L do not penetrate and are only affected by the long range tails of $U(r, R)$.

We find that at low L the wave functions $h_L^{AD}(R)$ always have an abrupt change of shape at the nuclear surface, as if there were independent breakup processes in the inside and outside regions which meet and interfere at the surface.¹³ This effect is also visible to some extent in the $g_L(k, R)$ channel functions of the CC calculation; it is obscured by phase averaging when $h_L(R)$ is constructed. Both in the adiabatic and CC calculations, in the inside region h_L^{AD} and h_L oscillate in phase with the elastic function $f_L(R)$, however, in the outside region the breakup functions have maxima where $f_L(R)$ has minima. The existence of distinct inside and outside

FIG. 3. Stripping amplitudes for ${}^{40}Ca(d,p)^{41}Ca(d_{3/2})$ at $E=22.9$ MeV as a function of deuteron center-of-mass angular momentum L. The form factor of Ref. 2 is used, with $Q = 4.4$ MeV.

breakup processes is certainly related to the interference minimum at the $L = 9$ grazing angular momentum, found in the FVA calculation.

We find that at low L the $h_L(R)$ are very sensitive to the imaginary well depth W_0 . With an average dimensionless elastic magnitude $f_L(R)$ at the nuclear surface of about 0.5, and with $W_0=0$, 5, 10 MeV, respectively, the corresponding breakup magnitudes at the nuclear surface are found to be about 0.3, 0.1, 0.03. This sensitivity to W_0 affects the inside and outside regions to about the same extent. Of course absorption also affects the elastic wave function. It is remarkable that for all values of W_0 and E , and also with Woods-Saxon single-partic potentials, the magnitude of h_L^{AD} in the deep interior remains approximately half that of f_I^t

A possible explanation for the uniform influence of W_0 throughout the inner and outer regions, and for the constant ratio of h_L to f_L , is that breakup is dominated by the interior. Therefore the entire function h_L is generated from f_L in the interior, and the absorption that reduces f_L in the interior affects h_L to the same extent.

Breakup at high L is nearly independent of the absorption. Moreover, although the large statistical weights of high partial waves produce substantial contributions to the breakup cross section, the associated wave functions $h_L(R)$ are never large.

In applications to zero-range calculations of stripping, we distinguish contributions from the elastic

wave functions $f_L(R)$ and from the breakup wave functions $h_L(R)$. The elastic contributions can be understood in terms of the discussion of the $f_L^{AD}(R)$ functions by means of equivalent potentials $\overline{U}_L^{\text{TE}}$ in Sec. IV, where it was found that breakup causes significant changes from folding model calculations. Figure 3 shows the resulting modifications of a typical stripping amplitude, obtained from the $f_L^{AD}(\tilde{R})$, and Fig. 4(b) shows the associated modification of the cross section. Evidently the modifications of the elastic radial wave functions only affect the (d,p) amplitude in low partial waves, and therefore they

FIG. 4. Stripping cross sections for ⁴⁰Ca(d,p)⁴¹Ca(d_{3/2}) at $E=22.9$ MeV for various matching conditions; case (a) $Q = 14.4$ MeV, $k_d = 1.49$ fm⁻¹, and $k_p = 1.33$ fm⁻¹; case (b) $Q = 4.4$ MeV, $k_d = 1.49$
fm⁻¹, and $k_p = 1.13$ fm⁻¹; case (c) $Q = -5.6$ MeV, $k_d = 1.49$ fm⁻¹, and $k_p = 0.90$ fm

do not change the cross section very much.

The specific contributions to the (d,p) amplitudes from the breakup functions $h_L(R)$ are sensitive to the matching between entrance channel and exit channel momenta. We recall that in the accurate CC calculation the $h_L(R)$ are small outside the nucleus and they are expected to become especially small if physically-plausible absorption strengths are used. Since good momentum matching emphasizes the exterior region, it ought to minimize effects from the $h_L(R)$. Figure 3 shows an example in which the $h_L(R)$ cause small but interesting modifications of the stripping amplitude at low L, which help to enhance L localization of the (d,p) reaction. Unfortunately the modifications due to $h_L(R)$ do not seem very systematic. In calculations with poor momentum matching or with form factors that emphasize the interior, a considerable variety of effects can be obtained. This effect of momentum matching is illustrated in Fig. 4 by stripping calculations with three different values of the exit channel energy.

VI. SUMMARY AND IMPROVEMENTS

Because our adiabatic calculations are limited to relative $l = 0$, the numerical results in this paper are essentially qualitative. Other work^{1,4,5} has already shown the importance of $l\neq0$ states and especially of states with $l = 2$. Antisymmetrization is also significant. On the other hand, the present work should at least indicate what kind of results are available from an adiabatic survey of three-body effects.

Comparison with CC calculations indicates that the elastic projection of the adiabatic wave function, onto an unmodified deuteron internal wave function, is rather accurate. We studied the elastic adiabati radial wave functions $f_L^{AD}(R)$ for individual partia waves, in terms of the trivially-equivalent local potentials $U_L^{\text{TE}}(R)$ that fit the $f_L^{\text{AD}}(R)$ exactly. Comparison with the corresponding folded potential for elastic scattering indicates that for partial waves that penetrate to the nuclear interior the U_L^{TE} differ consistently from the folded potential in two respects: (a) the imaginary part of U_L^{TE} shows a substantial short range enhancement, because of flux loss to breakup in the interior; and (b) the real part of U_L^{TE} also has some short range enhancement, because breakup enables the particles to overlap better with the individiual nuclear potentials U_p and U_n . These enhancements seem independent of bombarding energy and of the detailed properties of U_p and U_n . Long range three-body modifications of deuteron scattering¹⁴ are much weaker than the effects just discussed, and they are not seen very distinctl in \boldsymbol{U}

We also examined three-body effects in a zerorange calculation of deuteron stripping. Such a calculation depends on the summed radial wave functions

 $F_L(R) = f_L(R) + h_L(R)$

introduced in Sec. II C in which $h_L (R)$ are the nonelastic parts of the three-body wave functions, evaluated at $r = 0$. In first approximation $f_L \gg h_L$, therefore three-body effects in stripping are determined by properties of $f_L(R)$, already discussed in the preceding paragraph. The breakup functions $h_L(R)$ are only appreciable for low partial waves in the deep nuclear interior, where their magnitudes are about half those of the $f_L(R)$, whether the latter are strongly or weakly absorbed. On the other hand, in the nuclear surface region and the exterior the $h_L (R)$ are weakened by absorption and phase averaging. The adiabatic calculation gives a clear indication of the absorptive weakening of the $h_I(R)$, but it loses the phase averaging effect. We can conclude that stripping reactions that have good matching of entrance and exit channel momenta, so that they are dominated by large R , must be dominated by the well-understood $f_L(R)$ functions.

If momentum matching is not as good, or if the stripping form factor forces large contributions from the interior region, the $h_L(R)$ can substantially change the results for low partial waves. Unfortunately, there does not appear to be a consistent pattern in the changes that occur. It is also unfor-

tunate that the adiabatic approximation does not seem adequate for an actual calculation of these effects of the $h_L(R)$, because although it gives a reasonable description of $h_L(R)$ in the deep interior, the lack of phase averaging confuses the competing contributions from large R. The adiabatic calculation of the wave functions does tend to become more accurate at higher bombarding energies, 3 however, this is not likely to improve the accuracy of adiabatic (d,p) calculations, because as the bombarding energy increases the momentum transfer also increases.

Another effect that has been discussed in adiabatic approximation is the cross section for deuteron breakup. The energy-integrated breakup cross sec-
tion is given accurately.¹¹ This is possible despite tion is given accurately.¹¹ This is possible despit the problems with the $h_L (R)$, because the phase errors that affect the $h_L(R)$ are not relevant to the integrated cross sections.

Finally, it is interesting to ask whether the simple adiabatic approximation can be used as a starting point for more accurate three-body calculations. A principal failing of the adiabatic wave function $\psi^{AD}(r,\vec{R})$ is that it misrepresents the phase relations among the different breakup components $\phi(k, r)$ of Eq. (2.11}. It is straightforward to remedy this defect by resolving $\psi^{AD}(r,\vec{R})$ into components and then giving each component a propagator with the correct energy. The improved solution obtained by this procedure is

$$
\psi^{\text{imp}}(r,\vec{R}) = \phi_d(r)(\phi_d(r'),\psi^{\text{AD}}) + \int_0^\infty dk \ \phi(k,r)(E^+ - \epsilon_k - T_R)^{-1}(E - \epsilon_d - T_R)(\phi(k,r'),\psi^{\text{AD}}) \ , \tag{6.1}
$$

in which the component $(\phi(k,r'), \psi^{AD})$ is multiplied first by the inverse of the free propagator for the adiabatic choice of relative energy ϵ_d , and then by the free propagator for the energy ϵ_k . Since these propagators commute with $\phi(k, r')$, we can use Eq. (2.9) to get

$$
\psi^{\text{imp}}(r,\vec{R}) = \phi_d(r)(\phi_d(r'),\psi^{\text{AD}}) + \int_0^\infty dk \, \phi(k,r)(E^+ - \epsilon_k - T_R)^{-1}(\phi(k,r'),U(r',R')\psi^{\text{AD}}(r',R')) \,. \tag{6.2}
$$

I

The elastic component of Eq. (6.2) is the same as that of ψ^{AD} , already known to be rather accurate. Modifications develop gradually as ϵ_k increases, until for $\epsilon_k > E$ we obtain bound admixtures in ψ ^{imp}, where ψ^{AD} has spurious outgoing waves. Thus the properties of ψ ^{imp} seem very reasonable. Unfor tunately, Eq. (6.2) is not an easy expression to apply. It requires three numerical integrations: over r' , over R' in the Green's function, and finally over k . This is comparable in difficulty to a calculation by the exact CC method in the first place.

The good physical properties of Eq. (6.2) are understandable. Performing the k integration first would produce the free three-body configuration space Green's function. Thus Eq. (6.2) is a one-step

iteration of Eq. (2.3), based on the zero-order solution ψ^{AD} . The new properties of Eq. (6.2) are properties of the three-body Green's function. The complication of Eq. (6.2) is also a property of the Green's function.

In an attempt to find a simpler iterative approach, we insert ψ^{AD} on the RHS of Eq. (2.5) and use

$$
\psi(r,\vec{\mathbf{R}}) = \phi_d(r)\chi(r,\vec{\mathbf{R}})
$$
\n(6.3)

on the LHS. The differential equation for $\chi(r,\vec{R})$ then is

$$
[E - \epsilon_d - T_R - U(r, R)]\chi = S\chi^{AD}, \qquad (6.4)
$$

with

$$
S\chi^{AD} \equiv -\frac{\hbar^2}{M} \nabla_r^2 \chi^{AD} - \frac{\hbar^2}{M} (\vec{\tau} \cdot \nabla_r) \chi^{AD} , \qquad (6.5)
$$

in which

$$
\vec{\tau}(r) \equiv 2(\nabla_r \phi_d / \phi_d) \tag{6.6}
$$

It would be convenient if $S\chi^{AD}$ were a short-ranged function of R , because Eq. (6.4) would then resemble the original adiabatic equation (2.9), and it could be solved in the same fashion. However, χ^{AD} remains a function of r even for asymptotically large values of R, therefore the RHS of Eq. (6.4) has infinite range. As before, this long range correction term

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expresses the incorrect asymptotic distribution of energies in ψ^{AD} .

We conclude that the adiabatic approximation is not a helpful starting point for more accurate calculations. However, it is a simple source of useful information, as discussed in the remainder of this paper.

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