The Kohn Variational Principle for Elastic Proton–Deuteron Scattering above Deuteron Breakup Threshold

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The Kohn variational principle is formulated for calculating elastic proton–deuteron scattering amplitudes at energies above the deuteron breakup threshold. The use of such a principle with an expansion of the wave function on the (correlated) hyperspherical harmonic basis is discussed.

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I. INTRODUCTION

In recent years, a series of accurate calculations of $N-d$ scattering observables below the deuteron breakup threshold (DBT) by using the Kohn variational principle (KVP) have been reported \cite{1}. The resulting elastic $n-d$ phase shifts were found to be in strict agreement with those determined via accurate solutions of the Faddeev equations (FE) \cite{3}. The interest in this reaction has been revived consequently on the observation of large disagreements between theoretical predictions and experimental data for the $p-d$ and $n-d A_y$ and $iT_{11}$ polarization observables \cite{2}. Since the solution of the $N-d$ Schrödinger equation can be obtained with high precision, the disagreements can be traced back to the current models for the nucleon–nucleon (NN) and three–nucleon (3N) interactions. Therefore, the detailed studies of this process can be used to get information on the microscopic nuclear interaction.

Above the DBT, the FE have been accurately solved for the $n-d$ reaction (see, for example, Ref. \cite{4} and references therein). For reactions where there are more than one charged particles in the final state, the proper inclusion of the Coulomb interaction is a difficult problem. On the other hand, the proton induced breakup reaction is more easily studied experimentally, and in fact, there is a large amount of high precision $p-d$ scattering data available. It should be noticed that the effect of the Coulomb potential can be rather sizeable for various polarization observables, in particular at small scattering angles. It is therefore of relevance to obtain accurate theoretical estimates of the observables of this reaction.

At present, different approaches are applied to calculating the $p-d$ elastic observables above the DBT. The method used in Refs. \cite{5,6,7} consists of separating the long–range from the short–range Coulomb effects. Then, the FE in momentum space are solved by taking into account only the short–range part of the Coulomb potential, whilst the long–range contribution is included by “renormalizing” the solutions found. This method has been pursued for applications in both atomic systems and $p-d$ scattering at $E=10$ MeV \cite{8,9}. In other approaches, the FE are solved using the Coulomb-Sturmian-space representation \cite{10}, or by directly solving the FE in configuration space \cite{11}.

The KVP was discussed in Refs. \cite{12,13} to treat breakup reactions without considering the case of two or more charged particles in the final state. In the past it has been used mainly for studying atomic processes (in particular, the scattering of electrons or positrons by hydrogen atoms). Above the ionization threshold the direct application of the KVP has however encountered various problems related to the infinite number of two–body bound states between particles of opposite charge and to the complexity of the boundary conditions to be satisfied \cite{12,13}. Various alternative formulations have then been studied and the associated difficulties analyzed \cite{14,15}.

In this paper we reconsider the direct formulation of the KVP for calculating the elastic part of the S–matrix of a $p-d$ collision above the DBT. In such a process there is no problem relating to two–body excited bound states. The long–range Coulomb interaction between the two protons introduces a distortion in the description of the asymptotic three-nucleon outgoing wave. We have proved the validity of such a principle, considering trial wave functions which satisfy “simplified” boundary conditions allowing for practical applications, even when using realistic nuclear interactions. The results for several elastic observables have been already reported in refs. \cite{20,21}.

The paper is organized as follows. Some definitions used later in the paper are given in Sect. \textsuperscript{1}. In Sect. \textsuperscript{11}, a detailed description of the asymptotic behavior of the $p-d$ scattering wave function (w.f.) is reported, while the proof of the KVP is given in Sect. \textsuperscript{11}. The use of such a principle in conjunction with the pair–correlated hyperspherical harmonic expansion technique is discussed in Sect. \textsuperscript{11}, while the conclusions are given in the last section.
II. DEFINITIONS

Let us introduce the Jacobi vectors for three equal mass particles, given by

\[
x_i = r_j - r_k, \quad y_i = \sqrt{\frac{4}{3}} \left( r_i - \frac{r_j + r_k}{2} \right),
\]

where \( i, j, k \) is a cyclic permutation of 1, 2 and 3, and \( r_i \) denotes the position of particle \( i \). The distance between the pair \( jk \) and the particle \( i \) is

\[
d_i = \kappa y_i, \quad \kappa = \sqrt{\frac{3}{4}}.
\]

For the \( p-d \) system, the non–relativistic total energy operator is written as

\[
H = -\frac{\hbar^2}{m} \sum_{i=1}^{3} \nabla_i^2 + \sum_{j<k} V_{NN}(x_i) + W_{3N} + V_C,
\]

with \( V_{NN}(x_i) \) being the pair potential between the particles \( j, k \) and \( W_{3N} \) a 3N interaction term. Both \( V_{NN} \) and \( W_{3N} \) are short–ranged. In particular, \( V_{NN}(x_i) \) and \( W_{3N} \) become vanishingly small when \( x_i > a_N \), where \( a_N \) is a distance somewhat larger than the range of the nuclear interaction. Moreover, \( V_C \) is the Coulomb interaction operator (we disregard here other electromagnetic interaction terms), namely

\[
V_C = \sum_{j<k} \frac{e^2}{x_i} \frac{1 + \tau_{jz} + 1 + \tau_{kz}}{2},
\]

where \( \tau_{mz}/2 \) is the \( z \)–component of the isospin operator of particle \( m \).

For a three–body system, the hyperradius is defined as

\[
\rho = \sqrt{x_i^2 + y_i^2},
\]

and is independent of the permutation \( i = 1, 2, 3 \). The hyperangular variables are

\[
\Omega_i \equiv (\hat{x}_i, \hat{y}_i, \theta_i),
\]

where the hyperangle \( \theta_i \) is defined by the relation

\[
\cos \theta_i = x_i / \rho.
\]

To describe a three–nucleon state with total angular momentum \( J, J_z \), the following functions are introduced

\[
\left\{ \left[ Y_{\ell \alpha}(\hat{x}_i) Y_{L \alpha}(\hat{y}_i) \right] \Lambda_\alpha \left[ (s^j s^k) s^i \right] S_\alpha \Sigma_\alpha \right\}_{J J_z} \left[ (t^j t^k) t^i \right] t^T \equiv \Upsilon_{\alpha, T, T}(i),
\]

where the variables \( s \ (t) \) specify spin (isospin) states. The quantities \( S_\alpha \ (T) \) and \( s^i \ (t^i) \) are the spin (isospin) of the pair \( j, k \) and of the third particle \( i \), respectively, and they are coupled to give \( \Sigma_\alpha \ (T) \). The index \( \alpha \) stands for the set of quantum numbers

\[
\alpha \equiv \{ \ell_\alpha, L_\alpha, \Lambda_\alpha, S_\alpha, \Sigma_\alpha \}.
\]

The indices \( \{ \alpha, T, T \} \) distinguish the various angular–spin–isospin “channels”. A generic three–body w.f. can be written as

\[
\Psi = \sum_{i=1}^{3} \psi(i), \quad \psi(i) \equiv \psi(x_i, y_i),
\]

where each amplitude \( \psi(i) \) corresponds to the \( i \)–rearrangement configuration of the three particles and it can be decomposed in channels as
\[ \psi(i) = \sum_{\alpha,T,T'} F_{\alpha,T,T'}(x_i,y_i) \mathcal{Y}_{\alpha,T,T}(i) \quad (11) \]

The antisymmetry of \( \Psi \) can be simply enforced by requiring that the amplitude \( \psi(i) \) change sign under the exchange of particles \( j \) and \( k \). This can be easily done by including only those channels having odd values of \( \ell_\alpha + S_\alpha + T \) in the sum of Eq. (11).

In the following, the projection on states with a definite value of the third component of the isospin of the three particles will be useful. Let us define

\[ \Xi_i \equiv |t_z^i = -1/2, t_z^j = 1/2, t_z^k = 1/2 \rangle \quad (12) \]

as the isospin state where particle \( i \) is the neutron. Therefore, each amplitude \( \psi(i) \) can be decomposed as

\[ \psi(i) = \sum_{\nu=1}^{3} \psi_\nu(i) \Xi_\nu \quad (13) \]

where \( \psi_\nu(i) \) is the component of the amplitude \( \psi(i) \) and particle \( \nu \) is the neutron. To expand the components \( \psi_\nu(i) \) in spherical waves, it is convenient to use

\[ \tilde{\mathcal{Y}}_\alpha(i) = \Bigl\{ [Y_{t_\alpha}(\hat{x}_i)Y_{t_\alpha}(\hat{y}_i)]_{\Lambda_\alpha} [(s^j s^k) S_\alpha s^i]_{\Sigma_\alpha} \Bigr\}_{J_J_z}, \quad (14) \]

which are a complete set of angular–spin functions. The functions \( \mathcal{Y}_{\alpha,T,T}(i) \) and \( \tilde{\mathcal{Y}}_\alpha(i) \) are related to each other by

\[ \begin{align*}
\mathcal{Y}_{\alpha,1,0}(i) &= \tilde{\mathcal{Y}}_\alpha(i) \left[ \frac{1}{\sqrt{3}} \Xi_i + \frac{1}{\sqrt{3}} \Xi_j + \frac{1}{\sqrt{3}} \Xi_k \right], \\
\mathcal{Y}_{\alpha,0,0}(i) &= \tilde{\mathcal{Y}}_\alpha(i) \left[ -\frac{1}{\sqrt{2}} \Xi_j + \frac{1}{\sqrt{2}} \Xi_k \right], \\
\mathcal{Y}_{\alpha,1,1}(i) &= \tilde{\mathcal{Y}}_\alpha(i) \left[ \frac{2}{\sqrt{6}} \Xi_i - \frac{1}{\sqrt{6}} \Xi_j - \frac{1}{\sqrt{6}} \Xi_k \right].
\end{align*} \]

The components \( \psi_\nu(i) \) can be then expanded as the sum

\[ \psi_\nu(i) = \sum_{\alpha} \tilde{F}_{\alpha,\nu}(x_i,y_i) \tilde{\mathcal{Y}}_\alpha(i), \quad (16) \]

where \( \tilde{F}_{\alpha,\nu} \) are radial amplitudes. Using Eqs. (13), it is not difficult to find the relation between the amplitude \( F_{\alpha,T,T} \) defined in Eq. (11) and the functions \( \tilde{F}_{\alpha,\nu} \).

The \( N-d \) system in the asymptotic region, where a nucleon and the deuteron are far apart, is described by the following “surface” function,

\[ \Phi_{L,S}^d(i) = \left\{ [\phi_d(x_i) s^i]_S Y_{L}(\hat{y}_i) \right\}_{J_J_z} [\xi_d t^i]_{T T_z}, \quad T = \frac{1}{2}, \quad (17) \]

where \( \phi_d (\xi_d) \) is the spatial–spin (isospin) part of the deuteron w.f. The quantum number \( L \) is the relative angular momentum between the lone nucleon and the deuteron, \( S \) is the spin obtained by coupling the spin \( j = 1 \) of the deuteron with the spin 1/2 of the third nucleon. The deuteron wave function \( \psi_d = \phi_d(x_i) \times \xi_d \) satisfies the following equation

\[ \left( -\frac{\hbar^2}{m} \nabla^2_{x_i} + V_{NN}(x_i) \right) \psi_d = -B_d \psi_d. \quad (18) \]
III. THE ASYMPTOTIC BEHAVIOR

The asymptotic behavior of the w.f. describing \( N - d \) scattering has been discussed by many authors, in particular for the \( n - d \) case \(^{12,28}\). The case of the scattering of three particles, with at least two of them charged, has been considered in Refs. \(^{14,27,29}\). In this section, we rederive the asymptotic behavior of the w.f. for a \( p - d \) scattering process, in order to clarify some properties used to discuss the KVP in the following section.

The asymptotic behavior of the amplitudes \( \psi(i) \) given in Eq. (10) is analyzed by considering them as solutions of the three Faddeev–Noble equations (FNE) \(^{30}\)

\[
\left[ -\frac{\hbar^2}{m} \left( \nabla^2_i + \nabla^2_{y_i} \right) + V_C + V_{NN}(\mathbf{x}_i) - E \right] \psi(i) = -V_{NN}(\mathbf{x}_i) \left( \psi(j) + \psi(k) \right),
\]

(19)

with \( i, j, k \) cyclic. The 3N interaction \( W^{3N} \) has been disregarded since we are interested in the asymptotic solutions of Eq. (19), where at least one particle is very far from the other two. Let us consider the volume \( V(R) \) of the six–dimensional space where \( \rho \geq R \) (\( R \to \infty \)). \( V(R) \) can be divided into the following regions, corresponding to different ranges of values of the hyperangular variables \( \Omega \).

- **1+1+1 (breakup) region.** Here all the particles are well separated from each other. This breakup region is denoted as \( \mathcal{V}_b(R) \equiv \{ \rho \geq R; x_i \to \infty \text{ for } i = 1, 2, 3 \} \).

- **2+1 regions.** The part of \( V(R) \) where the particles \( j \) and \( k \) are close enough to interact through the NN potential, while particle \( i \) is very far from them, is hereafter denoted by \( \mathcal{V}_i(R) \). There are three such regions, corresponding to \( i = 1, 2, 3 \), namely \( \mathcal{V}_i(R) \equiv \{ \rho \geq R; x_i < a_N \} \). In \( \mathcal{V}_i(R) \), we have \( y_i \sim R \) but the distance \( x_i \) between particles \( j \) and \( k \) is of the order or lesser than the range \( a_N \) of the nuclear potential. As \( R \) increases, the range of the hyperangle \( \theta_i \) subtended by the region \( \mathcal{V}_i(R) \) decreases, and in the limit \( R \to \infty \) it reduces virtually only to the value \( \theta_i = \pi/2 \).

- **Transitions regions.** The regions between \( \mathcal{V}_b(R) \) and \( \mathcal{V}_i(R) \) are denoted as \( \mathcal{V}_{i,t}(R) \), \( i = 1, 2, 3 \). They can be defined as \( \mathcal{V}_{i,t}(R) \equiv \{ \rho \geq R; x_i \leq \Gamma \rho^\mu; x_i > a_N \} \), where \( \Gamma \) and \( \mu \) are suitable constants (0 < \( \mu < 1 \), as will be shown below). In this region

\[
\cos \theta_i = \frac{x_i}{\rho} \leq \Gamma \rho^{\mu-1} \to 0, \text{ for } \rho \to \infty.
\]

(20)

Therefore, for \( \rho \to \infty \) the hyperangle extension of this region reduces again to the value \( \theta_i = \pi/2 \). Such regions were considered for the first time by Merkuriev \(^{14,27}\) and should allow for a smooth transition between the solutions in the regions \( \mathcal{V}_b(R) \) and \( \mathcal{V}_i(R) \).

Let us study the asymptotic behavior of the solution of the FNE given in Eq. (19) in the above described regions.

**A. The \( \mathcal{V}_b(R) \) region**

In the breakup region \( \mathcal{V}_b(R) \) the nuclear interaction can be safely disregarded and the FNE for \( \psi(i) \) becomes

\[
\left[ -\frac{\hbar^2}{m} \left( \nabla^2_i + \nabla^2_{y_i} \right) + V_C - E \right] \psi(i) = 0.
\]

(21)

By rewriting this equation using the \( \rho, \Omega_i \) coordinates and disregarding terms vanishing faster than \( \mathcal{O}(1/\rho) \) as \( \rho \to \infty \), the solution reduces to \(^{27}\)

\[
\psi(i) = \frac{e^{iQ\rho - i\hat{\mathbf{k}} \cdot \ln 2Q\rho}}{\rho^2} \left( \sum_{\alpha, T, \mathcal{T}} A_{\alpha, T, \mathcal{T}}(\theta_i) \mathcal{Y}_{\alpha, T, \mathcal{T}}(i) \right)
+ \frac{e^{-iQ\rho + i\hat{\mathbf{k}} \cdot \ln 2Q\rho}}{\rho^2} \left( \sum_{\alpha, T, \mathcal{T}} B_{\alpha, T, \mathcal{T}}(\theta_i) \mathcal{Y}_{\alpha, T, \mathcal{T}}(i) \right), \text{ region } \mathcal{V}_b(R),
\]

(22)
where \( E = \hbar^2 Q^2 / m \) and

\[
\hat{X} = \frac{m}{2\hbar^2 Q} \sum_{i=1}^{3} \frac{e^2}{\cos \theta_i} \left( 1 + \frac{1}{2} \right) \left( 1 + \frac{1}{2} \right),
\]

(23)
is a dimensionless operator. The functions \( A_{\alpha,T,T}(\theta_i) \) and \( B_{\alpha,T,T}(\theta_i) \) are the so-called breakup amplitudes and are fixed by the dynamics of the process. For example, the cross section for the process \( p + d \rightarrow p + p + n \) is proportional to \( |A_{\alpha,T,T}(\theta_i)|^2 \).

Alternatively, \( \psi(i) \) can be decomposed as in Eq. (13), where the neutron is explicitly labelled. The corresponding components \( \psi_{\nu}(i) \) are

\[
\psi_{\nu}(i) = \frac{e^{iQ_\rho \cdot \mathbf{n}_\nu}}{\rho^2} \left( \sum_{\alpha} \tilde{A}_{\alpha,\nu}(\theta_i) \tilde{Y}_\alpha(i) \right)
\]

\[
+ \frac{e^{-iQ_\rho \cdot \mathbf{n}_\nu}}{\rho^2} \left( \sum_{\alpha} \tilde{B}_{\alpha,\nu}(\theta_i) \tilde{Y}_\alpha(i) \right), \quad \text{region } \mathcal{V}_\nu(R),
\]

(24)

where \( \eta(\theta_{\nu}) \) represents the isospin matrix elements of the operator \( \hat{X} \) and is defined as

\[
\eta(\theta_{\nu}) = \frac{me^2}{2\hbar^2 Q \cos \theta_{\nu}}, \quad \nu = 1, 2, 3.
\]

(25)
The breakup amplitudes depending on the neutron label \( \nu \) are related to the previous ones by the relations:

\[
\tilde{A}^{i}_{\alpha,1}(\theta_i) = \frac{1}{\sqrt{3}} A_{\alpha,1,1}(\theta_i) + \frac{2}{\sqrt{6}} A_{\alpha,1,\frac{1}{2}}(\theta_i),
\]

\[
\tilde{A}^{i}_{\alpha,2}(\theta_i) = \frac{1}{\sqrt{3}} A_{\alpha,1,1}(\theta_i) - \frac{1}{\sqrt{6}} A_{\alpha,1,\frac{1}{2}}(\theta_i) - \frac{1}{\sqrt{2}} A_{\alpha,0,\frac{1}{2}}(\theta_i),
\]

(26)

and analogously for \( \tilde{B}^{i}_{\alpha,1} \). The superscript \( i \) of the functions \( \tilde{A}^{i}_{\alpha,\nu} \) recalls that these amplitudes are the appropriate combinations of functions \( A_{\alpha,T,T} \) entering the expression (24) of \( \psi_{\nu}(i) \).

### B. The \( \mathcal{V}_{(i)}(R) \) region

In the following analysis we will fix our attention to the term describing outgoing breakup waves, i.e. proportional to \( \exp(iQ_\rho) \). When \( \cos \theta_{\nu} \rightarrow 0 \), namely going into the regions \( \mathcal{V}_{(i)}(R) \), the term \( \exp(-i\eta(\theta_{\nu}) \ln 2Q_\rho) \) in Eq. (24) oscillates increasingly. Moreover, it is no longer appropriate to disregard terms like \( 1/(\rho \cos \theta_{\nu})^2 \) in the construction of the solution. In this region the FNE satisfied by \( \psi(i) \) is still given by Eq. (21), since \( x_i > a_N \). We can distinguish the following cases.

1. Component \( \psi_{i}(i) \) (particle \( i \) is a neutron). The FNE satisfied by this component is

\[
\left[ -\frac{\hbar^2}{m} \left( \nabla^2_{x_i} + \nabla^2_{y_i} \right) + \frac{e^2}{x_i} - E \right] \psi_{i}(i) = 0.
\]

(27)

Since we are in a region where \( x_i \ll y_i \approx \rho \), the general solution of the above equation can be written as

\[
\psi_{i}(i) = \sum_{\alpha} \int_0^{\frac{\pi}{2}} d\varphi \ C_{\alpha,1}(\varphi) \left( \frac{me^2}{2\hbar^2 q} \right) \frac{1}{x_i} \tilde{h}_{\alpha,1}(qy_i) \tilde{Y}_{\alpha}(i).
\]

(28)

where

\[
q = Q \cos \varphi, \quad p = Q \sin \varphi,
\]

(29)
\( \hat{F}_L^+(z) = z \left(-y_L(z) + i j_L(z)\right) \), \( \hat{F}_L^+(z) \to e^{i(z-L\pi/2)} \) for \( z \to \infty \),

(30)

with \( j_L \) and \( y_L \) spherical Bessel functions. The function \( C_{\alpha,T}(\varphi) \) entering Eq. (28), whose dependence on \( Q \) is implicit, is a smooth weight function, strictly related to the breakup amplitude \( A_{\alpha,T}(\theta_i) \). It goes to zero for \( \varphi \to 0 \) or \( \pi/2 \).

In order to analyze the asymptotic form of the solution it is convenient to decompose the Coulomb function as

\[
F_\ell(\eta, z) = \mathcal{F}_\ell(\eta, z) \sin \left(z + \beta_\ell(q, z)\right),
\]

(31)

where \( \mathcal{F}_\ell(q, z) \) and \( \beta_\ell(q, z) \) have the following asymptotic behaviors for \( z \gg \max(1, \eta^2) \),

\[
\mathcal{F}_\ell(q, z) = \begin{cases} 1, & \beta_\ell(q, z) = -\eta \ln 2z - \ell \pi/2 + \sigma_\ell(q), \\ 0, & \beta_\ell(q, z) = 0, \end{cases}
\]

(32)

(33)

\( \sigma_\ell(q) \) being the Coulomb phase–shift. For \( z \ll \min(1, 1/\eta) \) we have instead

\[
\mathcal{F}_\ell(q, z) = \frac{Q e^{-\pi n/2} |\Gamma(\ell + 1 + i\eta)| z^{\ell}}{\Gamma(2\ell + 2)},
\]

(34)

where \( \Gamma \) is the gamma function. The decomposition (31) is somewhat arbitrary. However, we require that both \( \mathcal{F} \) and \( \beta \) always be finite. Thus, \( z_n + \beta_\ell(q, z_n) = n \pi \) for \( n = 0, 1, \ldots \), where \( z_n \) are the zeros of the function \( F_\ell(\eta, z) \). An example of the decomposition is shown in Fig. (VI) for a few values of \( \eta \) and \( \ell \).

In the large \( \rho \) limit the integral in Eq. (28) can be evaluated by the saddle–point approximation. Introducing the above decomposition for the Coulomb function and the relations \( x_i = \rho \cos \theta_i \) and \( y_i = \rho \sin \theta_i \), the leading term, given by the saddle–point \( \varphi = \theta_i \), is

\[
\psi_i^t = \sum_\alpha \sqrt{\frac{2\pi}{Q}} e^{3\pi i/4} \frac{C_{\alpha,i}(\theta_i)}{2i \cos \theta_i \sin \theta_i} \mathcal{F}_{\alpha,i} \left(\eta(\theta_i), Q \rho \cos^2 \theta_i\right)
\]

\[
\times \exp \left[i \beta_{\alpha,i} \left(\eta(\theta_i), Q \rho \cos^2 \theta_i\right) - i L_{\alpha,1} \frac{\pi}{2} + i Q \rho - i \eta(\theta_i) \ln(2Q \rho \cos^2 \theta_i)\right]
\]

\[
\times \frac{1}{\rho^2} \exp \left[i Q\rho - i \eta(\theta_i) \ln(2Q \rho)\right] \hat{\mathcal{Y}}_{\alpha,i}(t),
\]

(36)

where in the last passage we have defined

\[
\hat{A}_{\alpha,i}(\theta_i) = \sqrt{\frac{2\pi}{Q}} e^{3\pi i/4} \frac{C_{\alpha,i}(\theta_i)}{2i \cos \theta_i \sin \theta_i} \times
\]

\[
\exp \left(- i \eta(\theta_i) \ln(\cos^2 \theta_i) - i (L_{\alpha,1} + L_{\alpha}) \frac{\pi}{2} + i \sigma_{\alpha}(Q \cos \theta_i)\right).
\]

(37)

The next term of the saddle–point expansion is \( \sim \rho^{-7/2} \). In the region \( \mathcal{V}_{i,i}(R) \) we have \( \cos \theta_i \to 0 \) so that \( \eta^2(\theta_i) \approx 1 \).

Therefore, if

\[
Q \rho \cos^2 \theta_i \gg \eta^2(\theta_i),
\]

(38)

or equivalently

\[
x_i \gg \rho_c \equiv \left(\frac{m^2 e^4 \rho^3}{4h^4 Q^3}\right)^{1/4},
\]

(39)

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the functions $\mathcal{F}$ and $\beta$ reach their asymptotic values given in Eqs. (32) and (33). Then, $\psi_l(i)$ reduces to the form of Eq. (24) with $\tilde{A}_{\alpha,i}$ given by Eq. (34). When Eq. (32) is not satisfied, corresponding to the situation in which the two protons approach each other, the functions $\mathcal{F}$ and $\beta$ start deviating from their asymptotic behavior and the breakup w.f. cannot be cast into the form (24) and (22). The extreme situation corresponds to the condition

$$Q\rho \cos^2 \theta_i \ll \frac{1}{\eta(\theta_i)} ,$$

or equivalently,

$$x_i \ll \rho'_c \equiv \frac{2\hbar^2}{me^2} \approx 60 \text{ fm} ,$$

and the functions $\mathcal{F}$ and $\beta$ reach the behavior given in Eqs. (34) and (35). Thus, $\mathcal{F} \rightarrow e^{-\pi me^2/h^2 Q \cos \theta_i} \rightarrow 0$ since $x_i/\rho = \cos \theta_i \rightarrow 0$. Also the successive terms in the saddle-point expansion are zero. This corresponds to the intuitive fact that the probability of finding two protons (in this case, labelled as particles $j$ and $k$) at any finite distance $x_i = r_{jk}$ is negligible in the asymptotic region $R \rightarrow \infty$. We arrive at the important result that the amplitude $\psi_l(i)$ goes smoothly from the behavior given in Eq. (24) to a vanishing value when going from the region where $x_i \gg \rho_c$ to the one where $x_i \ll \rho'_c$.

The same conclusion holds if the regular Coulomb function $F_L(i, q, z)$ is replaced by the (regular) solution of the two–body Schröedinger equation

$$\left[ \frac{d^2}{dz^2} + 1 - \frac{2\eta}{z} - \frac{\ell(\ell + 1)}{z^2} - \frac{mV_{\text{NN}}(x_i)}{\hbar^2 q^2} \right] F_L^V(i, q, x_i) = 0 , \quad z = q x_i ,$$

where, for the matter of simplicity, we have considered here a central NN potential $V_{\text{NN}}(x_i)$. Outside the range of $V_{\text{NN}}$ we have $F_L^V \rightarrow F_L + \tan \delta_l G_L$ where $G$ is the irregular Coulomb function and $\delta_l$ the phase shift induced by the NN potential. However, for $q \rightarrow 0$ or $\eta \rightarrow \infty$ it can be shown that $G \rightarrow \exp(\pi \eta)$ and $\tan \delta_l \rightarrow \exp(-2\pi \eta)$. Therefore, when $x_i \ll \rho'_c$ again $F_L^V \rightarrow 0$.

2. Component $\psi_j(i)$ (the neutron is labelled as $j$). The equation satisfied by $\psi_j(i)$ in this region is

$$\left[ -\frac{\hbar^2}{m} \left( \nabla_x^2 + \nabla_y^2 \right) \nabla_x^2 + \nabla_y^2 \right] \psi_j(i) = 0 .$$

In $\mathcal{V}_{l,i}(R)$, $x_j \approx \kappa y_i$ and therefore the solution of the above equation can be written in the form

$$\psi_j(i) = \sum_{\alpha} \int_0^{\bar{z}} d\varphi \ C_{\alpha,j}(\varphi) \frac{1}{x_j} \tilde{J}_\alpha(q x_i)$$

$$\frac{1}{y_i} \left[ G_{\alpha,i} \left( \frac{me^2}{2\hbar^2 \kappa p}, p y_i \right) + i F_{\alpha,i} \left( \frac{me^2}{2\hbar^2 \kappa p}, p y_i \right) \right] \tilde{Y}_\alpha(i) ,$$

where $G_L$ is the irregular Coulomb function and $\tilde{J}_\ell$ is a regular Riccati-Bessel function. As has been done before, this latter function can be decomposed as,

$$\tilde{J}_\ell(z) = J_\ell(z) \sin(z + \zeta_\ell(z)) ,$$

where $J_\ell(z)$ and $\zeta_\ell(z)$ have the following asymptotic behavior for $z \gg 1$,

$$J_\ell(z) = 1 ,$$

$$\zeta_\ell(z) = -\ell \pi / 2 ,$$

and for $z \ll 1$,

$$J_\ell(z) = \frac{z^\ell}{(2\ell + 1)!!} ,$$

$$\zeta_\ell(z) = 0 .$$

Note that $J_\ell(0) = J_0(0, z)$ and $\zeta_\ell(0) = \beta_\ell(0, z)$. Moreover, $J_0(z) = 1$ and $\zeta_0(z) = 0$. 




Following a procedure similar to the one adopted in point 1), the following expression for the component \( \psi_j(i) \) in \( \mathcal{V}_{\ell,i}(R) \) is found,

\[
\psi_j(i) = C(\rho) \sum_{\alpha} J_{\ell_{\alpha}}(Q \cos \theta_i x_i) \exp \left[ i \zeta_{\ell_{\alpha}}(Q \cos \theta_i x_i) + i \ell_{\alpha} \frac{\pi}{2} \right] \tilde{A}^{\ell_{\alpha},j}_{\alpha,i}(\theta_i) \tilde{\psi}_{\alpha}(i),
\]

(50)

where

\[
\tilde{A}^{\ell_{\alpha},j}_{\alpha,i}(\theta_i) = \sqrt{\frac{2\pi}{Q}} e^{3\pi i/4} \frac{C_{\alpha,j}(\theta_i)}{2i \cos \theta_i \sin \theta_i} \exp \left( -i(\ell_{\alpha} + L_{\alpha}) \frac{\pi}{2} + i \sigma_{\ell_{\alpha}}(Q \sin \theta_i) \right).
\]

(51)

In Eq. (50), we have defined

\[
C(\rho) = \frac{1}{\rho^\frac{1}{2}} \exp \left( iQ \rho - i \frac{m e^2}{2\hbar^2 Q} \ln 2Q \rho \right).
\]

(52)

Therefore, for

\[
x_i \gg \rho_n \equiv \left( \frac{\rho}{Q} \right)^{\frac{1}{2}},
\]

(53)

where the behavior given in Eqs. (46) and (47) for \( \mathcal{J}_i(x_i) \) and \( \zeta_i(x_i) \) is valid, the component \( \psi_j(i) \) coincides with Eq. (24) [note that cos \( \theta_j \approx \kappa \) in \( \mathcal{V}_{\ell,i}(R) \)].

If \( x_i \ll \rho_n \), the amplitudes of the channels having \( \ell_{\alpha} > 0 \) become vanishing small since \( \mathcal{J}_{\ell_{\alpha}} \propto (x_i/\rho_n)^{2\ell_{\alpha}} \). This corresponds to the intuitive fact that the probability of finding two nucleons (in this case, labelled as particles \( j \) and \( k \)) with a vanishing relative velocity and relative orbital angular momentum greater than zero is negligible in the asymptotic region \( R \to \infty \). Therefore,

\[
\psi_j(i) \to C(\rho) \sum_{\alpha} \delta_{\ell_{\alpha},0} \tilde{A}^{\ell_{\alpha},j}_{0,i}(\frac{\pi}{2}) \tilde{\psi}_{\alpha}(i), \quad x_i \ll \rho_n.
\]

(54)

3. Component \( \psi_k(i) \) (the neutron is labelled as \( k \)). The solution for this case coincides with that discussed in point 2.

Finally, we can estimate of the value of the constant \( \mu \) defining the region \( \mathcal{V}_{\ell,i}(R) \). In the \( n - d \) case, the appropriate value is \( \mu \approx 1/2 \) [see Eq. (55)]. In the \( p - d \) case, a value of \( \mu \approx 3/4 \) can be chosen in accordance with Eq. (56). As shown in Ref. [14], the presence of those regions does not alter the validity of the KVP for the \( n - d \) case. Therefore, it can be expected that such regions do not play any important role also in the \( p - d \) case, as will become evident in the next section.

C. The \( \mathcal{V}_i(R) \) region

In this region the nuclear interaction between particles \( j \) and \( k \) cannot be disregarded, whereas particle \( i \) is far from the other two. The solution consists of an elastic \( p - d \) amplitude \( \psi^{(e)}(i) \) plus a breakup amplitude \( \psi^{(b)}(i) \), namely

\[
\psi(i) = \psi^{(e)}(i) + \psi^{(b)}(i).
\]

The amplitude \( \psi^{(e)} \) has the form

\[
\psi^{(e)}(i) = \sum_{LS} \Phi^{LS}_{\ell_{\alpha}}(i) \left[ a_{LS} \mathcal{H}^{+}_{L}(\eta_0, q_0 d_i) + b_{LS} \mathcal{H}^{-}_{L}(\eta_0, q_0 d_i) \right],
\]

(55)

where \( \Phi^{LS}_{\ell_{\alpha}}(i) \) is given in Eq. (17), the distance \( d_i \) in Eq. (2), and

\[
\mathcal{H}^{\pm}_{L}(\eta_0, q_0 d_i) = \frac{G_{L}(\eta_0, q_0 d_i) \pm iF_{L}(\eta_0, q_0 d_i)}{q_0 d_i}.
\]

(56)

The functions \( F \) and \( G \) are the regular and irregular Coulomb functions and

\[
\eta_0 = \frac{m e^2}{2\hbar^2 q_0},
\]

(57)

is the usual Coulomb parameter, with the wave number \( q_0 \) satisfying the relation
\[ -B_d + \frac{1}{(k^2)} \frac{\hbar^2}{m} \rho_0^2 = E . \]  

The coefficients \( a_{LS} \) (\( b_{LS} \)) are the amplitudes of the corresponding incoming (outgoing) waves. In fact, \( H^\pm \approx \exp(\pm iQ\rho + \ldots) \) in the limit of large \( q_0d_1 \) values. 

The amplitude \( \psi^{(o)}(i) \), when particles \( j \) and \( k \) are protons, again vanishes for \( \rho \rightarrow \infty \) due to the Coulomb repulsion, namely \( \psi^{(o)}_i = 0 \). When one of the particles is a neutron, it takes the form 

\[ \psi^{(o)}_i = \sum_\alpha \delta_{\alpha,0} \phi^0_\alpha(x_i) A^i_{\alpha,\nu}(\frac{\pi}{2}) C(\rho) \tilde{Y}_\alpha(i) , \quad \nu = j \text{ or } k , \]  

where \( \phi^0_\alpha \) is the s–wave solution of an inhomogeneous zero energy two–body Schroedinger–like equation \([29, 26]\) derived from Eq. \((19)\) by taking into account the coupling between \( \psi(i) \) and \( \psi(j) + \psi(k) \) induced by the NN potential. The amplitude \( \psi^{(o)}_{j, k}(i) \) vanishes for \( \ell_\alpha > 0 \) due to the centrifugal repulsion. For the present discussion of the KVP the precise form of the functions \( \phi^0_\alpha \) is not important. They are normalized so that \( \phi^0_\alpha \rightarrow 1 \) outside \( \mathcal{V}_1(R) \), namely when \( x_i \gg a_N \), in order to match the result obtained in the transition region. The derivation of the equation satisfied by \( \phi^0_\alpha \) is reported in the Appendix. 

**D. The \( \mathcal{V}_1(R) + \mathcal{V}_{i,j}(R) \) regions** 

In these regions \( y_j \rightarrow \infty \) and \( x_j/y_j \rightarrow 0 \) and therefore we can approximate \( x_i \sim \kappa y_j \) and \( y_i \sim y_j/2 \). Then, the component \( \psi_i \) satisfies again the uncoupled FNE given in Eq. \((21)\). Moreover, \( \cos \theta_i \sim \kappa \) or \( \theta_i \sim \pi/6 \) and from Eq. \((30)\) 

\[ \psi(i) \rightarrow C(\rho) \sum_\alpha \tilde{A}_{\alpha,i}(\frac{\pi}{6}) \tilde{Y}_\alpha(i) , \quad \text{region } \mathcal{V}_1(R) . \]  

In fact, here (for \( \rho \rightarrow \infty \)) we always have \( Q\rho \cos^2 \theta_i \gg \eta^2(\theta_i) \). The same conclusion is reached for \( \psi_k \). Both components can be obtained directly by taking the limit \( \theta_i \rightarrow \pi/6 \) in Eq. \((24)\). 

The component \( \psi_j \) is more difficult to obtain. In fact, since here \( x_j \) can become very small, we have to fully take into account the distortion due to the Coulomb potential. This component can be calculated by expressing it in terms of the coordinates \( x_j \) and \( y_j \) and by rewriting Eq. \((21)\) as 

\[ \left[ -\frac{\hbar^2}{m} \left( \nabla^2_{x_j} + \nabla^2_{y_j} \right) + \frac{e^2}{x_j} - E \right] \psi_j(i; x_j, y_j) = 0 . \]  

Now \( \psi_j(i; x_j, y_j) \) can be determined by following the same procedure as in Sect. \( \text{III} \text{H} \). In particular, it has been shown there that for \( x_j \ll \rho^*_\ell \), \( \psi_j(i) \) vanishes due to the Coulomb repulsion between the protons. 

The behavior of \( \psi(i) \) in \( \mathcal{V}_k(R) \) and \( \mathcal{V}_{i,k}(R) \) can be analyzed in the same manner. Here the components \( \psi_i(i) \) and \( \psi_j(i) \) are given by Eq. \((21)\) and can be obtained directly as the limit of the solution valid in \( \mathcal{V}_b(R) \). The component \( \psi_k(i) \) will be distorted by the Coulomb repulsion and will vanish inside \( \mathcal{V}_k(R) \). 

**E. Summary** 

It is straightforward to show that the behavior of the incoming wave \( \propto \exp(-iQ\rho + \ldots) \) has similar properties. Therefore, the behavior of the amplitudes \( \psi(i) \) in the asymptotic regions can be put in the form, 

\[ \psi(i) = \sum_{LS} \Phi^d_L(i) \left[ a_{LS} \mathcal{H}^+_L(\eta_0, q_0d_i) + b_{LS} \mathcal{H}^-_L(\eta_0, q_0d_i) \right] 
\]  

\[ + \frac{e^{-iQ\rho - i\kappa \ln(2Q\rho)}}{\rho^*_L} \left( \sum_{\alpha,T,T} A_{\alpha,T,T}(\rho, \Omega_i) \mathcal{Y}_{\alpha,T,T}(i) \right) 
\]  

\[ + \frac{e^{-iQ\rho + i\kappa \ln(2Q\rho)}}{\rho^*_L} \left( \sum_{\alpha,T,T} \mathcal{B}_{\alpha,T,T}(\rho, \Omega_i) \mathcal{Y}_{\alpha,T,T}(i) \right) . \]  

\[(62)\]
The “distorted” breakup amplitudes \( \mathcal{A}_{\alpha,T,T} \) and \( \mathcal{B}_{\alpha,T,T} \) have been written as functions of \( (\rho, \Omega_i) \) taking into account the modifications induced by the Coulomb, centrifugal and NN potentials. In \( \mathcal{V}_b(R) \), clearly \( \mathcal{A}_{\alpha,T,T}(\rho, \Omega_i) \rightarrow \mathcal{A}_{\alpha,T,T}(\theta_i) \) and \( \mathcal{B}_{\alpha,T,T}(\rho, \Omega_i) \rightarrow \mathcal{B}_{\alpha,T,T}(\theta_i) \). Moreover, as discussed in Sect. \( \text{III B} \) and \( \text{III C} \), in the region \( \mathcal{V}_i(R) \) and \( \mathcal{V}_{i,i}(R) \), a good approximation for the (isospin-projected components of) \( \mathcal{A}_{\alpha,T,T}(\rho, \Omega_i) \) should be

\[
\begin{align*}
\tilde{\mathcal{A}}_{\alpha,i}(\rho, \Omega_i) & \rightarrow \mathcal{F}^{(c)}_{\ell\alpha}(x_i, \theta_i) \tilde{\mathcal{A}}_{\alpha,i}(\theta_i), \\
\tilde{\mathcal{A}}_{\alpha,j}(\rho, \Omega_i) & \rightarrow \mathcal{F}^{(n)}_{\ell\alpha}(x_i, \theta_i) \tilde{\mathcal{A}}_{\alpha,j}(\theta_i), \\
\tilde{\mathcal{A}}_{\alpha,k}(\rho, \Omega_i) & \rightarrow \mathcal{F}^{(n)}_{\ell\alpha}(x_i, \theta_i) \tilde{\mathcal{A}}_{\alpha,k}(\theta_i),
\end{align*}
\]

where the following functions have been introduced,

\[
\mathcal{F}^{(c)}_{\ell\alpha}(x_i, \theta_i) = \mathcal{F}_{\ell\alpha} \left( \eta(\theta_i), Q_\rho \cos^2 \theta_i \right) \exp \left[ i \delta_{\ell\alpha} \left( \eta(\theta_i), Q_\rho \cos^2 \theta_i \right) + i \eta(\theta_i) \ln(2Q_\rho \cos^2 \theta_i) + i \ell \pi \frac{\alpha}{2} - i \sigma_{\ell\alpha} (Q_\rho \cos \theta_i) \right],
\]

\[
\mathcal{F}^{(n)}_{\ell\alpha}(x_i, \theta_i) = \left( \delta_{\ell\alpha,0} (\phi_{\eta}^0(x_i) - 1) + 1 \right) \mathcal{J}_{\ell\alpha} (Q_\rho \cos^2 \theta_i) \times \exp \left[ i \delta_{\ell\alpha} \left( Q_\rho \cos^2 \theta_i \right) + i \ell \pi \frac{\alpha}{2} \right].
\]

In the regions \( \mathcal{V}_i(R) + \mathcal{V}_{i,i}(R) \) the divergent behavior of \( \dot{\chi} \) for \( \cos \theta_i \rightarrow 0 \) is completely canceled by terms in \( \mathcal{A}_{\alpha,T,T} \). It can be checked that outside of the region \( \mathcal{V}_i(R) + \mathcal{V}_{i,i}(R) \) the functions \( \mathcal{A} \) reduce to the breakup amplitude \( A \), since in \( \mathcal{V}_b(R) \) \( \mathcal{F}^{(c)}(x_i, \theta_i) \rightarrow 1 \) \((z = c, n)\). The factor \( \mathcal{F}^{(c)} \) takes into account the effect of the Coulomb and centrifugal potential in \( \mathcal{V}_{i,i}(R) \) and goes to zero in \( \mathcal{V}_i(R) \). Conversely the factor \( \mathcal{F}^{(n)} \) takes into account the effects of the NN potential and the centrifugal barrier. Since for \( \ell_\alpha > 0 \) \( \mathcal{J}_{\ell\alpha} \) vanishes in \( \mathcal{V}_i(R) \), the influence of the NN potential has been taken into account only in the \( \ell_\alpha = 0 \) wave.

**IV. THE KOHN VARIATIONAL PRINCIPLE**

The process we are interested in is a collision between a proton and a deuteron, namely, the reaction

\[(p + d) \rightarrow (p + d) + (n + p + p).\]

If the incident state of the \( p - d \) system has quantum numbers \( L_0, S_0 \) and \( J \), the elastic amplitude in Eq. \( (62) \) is characterized by

\[b_{LS} = \delta_{LL_0} \delta_{SS_0}.\]

The coefficient \( a_{LS} \) is usually renamed as \(-\mathcal{S}_{L_0 S_0 L, S, \mathcal{S}_L S_0 L, S} \) being the elements of the elastic S–matrix. Since the breakup part should not include incoming waves, we must have

\[\mathcal{B}_{\alpha,T,T}(x_i, \theta_i) = 0.\]

The Eqs. \( (59) \)\( (70) \) give the boundary conditions to be satisfied by the w.f. describing the process \( (58) \). Explicitly, the asymptotic amplitude is

\[
\psi(i) = \sum_{LS} \Phi_{LS}^i \left[ -\mathcal{S}_{L_0 S_0 L, S, \mathcal{S}_L S_0 L, S} \mathcal{H}_L^+(\eta_0, q_0 d_i) + \delta_{LL_0} \delta_{SS_0} \mathcal{H}_L^-(\eta_0, q_0 d_i) \right] + \frac{e^{i Q_\rho - i \pi \ln(2Q_\rho)}}{\rho^2} \left( \sum_{\alpha,T,T} \mathcal{A}_{\alpha,T,T}(\rho, \Omega_i) \mathcal{V}_{\alpha,T,T}(i) \right), \quad \rho \geq R.
\]

Let us now consider the integral

\[
I = \langle \Psi_{L_0 S_0}^{(c)} \rangle (H - E) \langle \Psi_{L_0 S_0} \rangle_R - \langle \mathcal{V}_{L_0 S_0}^{(c)} \rangle (H - E) \langle \Psi_{L_0 S_0} \rangle_R.
\]
where \( \langle \rangle_R \) stands for the integration over \( d^3x_i\) \( d^3y_i \) of the six–dimensional volume with \( \rho \leq R \) (\( R \to \infty \)) and \( \Psi^{(-)} \) is the time–reversal w.f. In the end the limit \( R \to \infty \) is taken. The function \( \overline{\Psi} \) is a trial w.f. which will be chosen to satisfy the boundary conditions. Without loss of generality, the trial w.f. can be decomposed into three amplitudes, \( \overline{\Psi} = \sum_i^{3} \overline{\Psi}(i) \). The asymptotic behavior of \( \overline{\Psi}(i) \) can be written as

\[
\overline{\Psi}(i) = \sum_{LS} \Phi^i_{LS}(i) \left[ -S_{L_{0}S_{0},L_{0}S_{0},L_{0}S_{0}}(\eta_0, q_0 d_i) + \delta_{L_{0},L_{0}} \delta_{S_{0},S_{0}} S_{L_{0}S_{0}}(\eta_0, q_0 d_i) \right] + \frac{e^{iQ \rho - \pi \log \nu}}{\rho^2} \left( \sum_{\alpha, T, T} \overline{A}_{\alpha,T,T}(\rho, \Omega_i) \overline{V}_{\alpha,T,T}(i) \right), \quad \rho \geq R.
\] (73)

The overlined quantities are free parameters which represent approximations to the exact values. It should be noticed that an approximate expression \( \overline{\Psi} \) of the operator \( \overline{\chi} \) has been introduced in the above equation.

The important point is that the validity of the KVP for the elastic part of the \( S \)-matrix can be proved also in this case. However, the “choice” of \( \overline{\Psi} \) is not completely arbitrary, since the matrix element \( \langle \Psi|(H-E)|\overline{\Psi} \rangle \) has to be finite. Moreover, in a practical calculation the convergence of the elastic \( S \)-matrix should be checked whenever an improvement is made to \( \overline{\Psi} \).

For example, in the case considered in Sect. \( \overline{\Psi} \) the operator \( \overline{\chi} \) is represented as an expansion over the Hyperspherical Harmonic functions and therefore has not any singular behavior for \( \theta_i \to \pi/2, \quad i = 1, 2, 3 \). Moreover, \( \overline{\Psi} \to \overline{\chi} \) as the number of terms included in the expansion basis is increased. Such a procedure may result in a slow convergence of \( \overline{A} \) towards the exact \( A \), in particular for \( \theta_i \to \pi/2, \quad i = 1, 2, 3 \). However, this problem has no practical consequences for the calculation of the elastic \( S \)-matrix, as will be shown in Sect. \( \overline{\Psi} \).

Contributions to the integral \( I \) come only from the differential operators present in \( H \). By integrating by parts, \( I \) takes contribution only from the hypersurface \( \Omega \) at \( \rho = R \). Let us denote with \( \Omega \) the parts of \( \Omega \) corresponding to a particular asymptotic region \( \nu_x(R) \). Therefore,

\[
I = \sum_{i=1}^{3} (I_i + I_{i,i}) + I_b,
\] (74)

where \( I_i, I_{i,i} \) and \( I_b \) are the contributions coming from \( \Omega \), \( \Omega_{i,i} \) and \( \Omega_b \), respectively. On the hypersurface \( \Omega \), the trial \( T \) and exact wave functions have reached the asymptotic behavior given in Eqs. (71) and (72). In \( \Omega \), only the elastic part contributes, with the result

\[
I_i = \frac{2i \bar{\kappa}}{q_0} \frac{\hbar^2}{m} \left( S_{L_0S_0,L_0S_0} - S_{L_0S_0,L_0S_0} \right).
\] (75)

In fact, the breakup part goes like \( \rho^{-5/2} \) and gives a contribution \( \propto R^{-3/2} \) which vanishes in the limit \( R \to \infty \). The contribution \( I_{i,i} \) coming from the region \( \Omega_{i,i} \) is also zero. First of all, only breakup waves can contribute since the elastic wave vanishes outside \( \nu_x(R) \). Moreover, the “dimension” of the surface \( \Omega_{i,i} \) is proportional to \( R^{2+\nu} \), whereas the integrand is proportional to \( 1/R^6 \). Thus, for \( R \to \infty \) the integral in \( \Omega_{i,i} \) behaves \( \propto R^{3(\nu-1)} \to 0 \). Finally, in the case in which only outgoing breakup waves are present in both the trial and exact w.f. the contributions of the two terms in Eq. (72) cancel each other.

In \( \Omega_b \), \( I_b \) reduces to

\[
I_b = - \frac{\hbar^2}{m} \int_{\Omega_b} d\Omega \left[ \rho^2 \overline{\Psi}_{L_0S_0} \frac{d}{d\rho} \rho^2 \overline{\Psi}_{L_0S_0} - \rho^2 \overline{\Psi}_{L_0S_0} \frac{d}{d\rho} \rho^2 \overline{\Psi}_{L_0S_0} \right] \bigg|_{\rho=R},
\] (76)

and, using the asymptotic behaviors given in Eqs. (72) and (73), \( I_b \propto 1/R \to 0 \) for \( R \to \infty \).

Summing up all the contributions and remembering that \( (H-E)\overline{\Psi}_{L_0S_0} = 0 \) the exact expression is obtained:

\[
S_{L_0S_0,L_0S_0} = S_{L_0S_0,L_0S_0} - \frac{mq_0}{6i\kappa R^2} \left( \overline{\Psi}^{(-)}_{L_0S_0}(H-E)(\overline{\Psi}_{L_0S_0}) + \frac{mq_0}{6i\kappa R^2} \epsilon^{(-)}_{L_0S_0}(H-E)\epsilon_{L_0S_0} \right),
\] (77)

where \( \epsilon_{L_0S_0} = \overline{\Psi}_{L_0S_0} - \Psi_{L_0S_0} \) is the “error” introduced in the trial w.f. It can be noticed that Eq. (77) is variational in character, since the last term is quadratic in the error function \( \epsilon_{L_0S_0} \). Therefore, the functional

\[
[S_{L_0S_0,L_0S_0}] = S_{L_0S_0,L_0S_0} - \frac{mq}{6i\kappa R^2} \overline{\Psi}^{(-)}_{L_0S_0}(H-E)(\overline{\Psi}_{L_0S_0}),
\] (78)
represents a second order estimate for the exact diagonal element \( S_{L_0S_0,L_0S_0} \). The search of stationary solutions through the equation
\[
\delta [S_{L_0S_0,L_0S_0}] = 0 ,
\] (79)
provides the optimum estimate. Here \( \delta \) denotes the variation with respect to all the trial parameters entering \( \mathbf{\Psi}_{L_0S_0} \), including \( S \) and \( \mathbf{A} \). Moreover, the KVP can be readily generalized to obtain variational relations for the non–diagonal matrix elements \( S_{L_1S_1,L_2S_2} \) of the elastic collisional matrix.

Clearly, the principle is meaningful only if the two matrix elements entering Eq. (77) are both finite. This is not evident since for \( p > R \) both \( \mathbf{\Psi} \) and \( \mathbf{e} \) have oscillatory behaviors. However, since Eq. (74) is exact and \( S \) and \( \mathbf{A} \) are finite, it is sufficient to check that one of the matrix elements is finite, in particular \( \langle \mathbf{\Psi} | (H - E) | \mathbf{\Psi} \rangle \). This imposes some constraints on \( \mathbf{\chi} \), which usually has to be chosen coherently with the expansion basis used to construct \( \mathbf{\Psi} \) (see Sect. \( \mathbf{V} \) for a practical example).

Applications of the KVP usually start with the expansion of the w.f. in a certain basis which is truncated at some level. The stability of the functional (74) is studied in terms of the dimension of the basis and in terms of the nonlinear parameters (if any). Spurious resonances or spurious solutions in the convergence procedure could appear due to a zero eigenvalue present in the operator \( H - E \) \( \mathbf{[31]} \). These spurious solutions have been studied for a long time and it was shown that the KVP in its complex form, as presented here, is well-behaved \( \mathbf{[32]} \). Spurious solutions could appear in this case too, but these occur for unrealistic values of the nonlinear parameters, which are in general present in the form of a regularizing factor or inside some exponent \( \mathbf{[33]} \). Below the DBT, a practical rule to verify the presence of spuriousities is to apply the principle to the reactance matrix \( K \) and its inverse \( K^{-1} \) (inverse KVP) and verify the relation \( K K^{-1} = I \). Similarly, for energies above the DBT, one could apply the variation principle for the T-matrix (which can be derived by following an analogous procedure to the one described here). With two independent estimates of (the elastic part of) the S– and T–matrices one can test, for example, the relation \( (\mathbf{S} \mathbf{S}) \). With two independent estimates of (the elastic part of) the S– and T–matrices one can test, for example, the relation \( \mathbf{S} \mathbf{T} \).

In this Section, the application of the pair–correlated hyperspherical harmonic (PHH) technique to describe \( p – d \) scattering for energies above the DBT is discussed. In the PHH approach, the trial w.f. is written as
\[
\mathbf{\Psi}_{L_0S_0} = \Psi_A + \Psi_C , \quad \Psi_A = \sum_{i=1}^{3} \overline{\psi}_A(i) , \quad \Psi_C = \sum_{i=1}^{3} \overline{\psi}_C(i) .
\] (80)
The first term \( \Psi_A \) describes the system when the two incident clusters are well separated and it is written in the form
\[
\psi_A(i) = \sum_{L,S} \Phi_{LS}(i) \left[ -S_{L_0S_0,L_S} \mathcal{H}_L^-(\eta_0,q_0d_i) + \delta_{LL_0} \delta_{SS_0} \mathcal{H}_L^+(\eta_0,q_0d_i) \right] ,
\] (81)
where
\[
\mathcal{H}_L^\pm(\eta_0,q_0d_i) = \frac{(1 - e^{-\gamma d_i})^{2L+1}}{q_0d_i} G_L(\eta_0,q_0d_i) \pm i F_L(\eta_0,q_0d_i) .
\] (82)
The factor \( (1 - e^{-\gamma d_i})^{2L+1} \) has been introduced to regularize the function \( G \) at the origin, and \( \gamma \) is taken as a nonlinear variational parameter. Its choice is not a critical problem due to the large flexibility of the trial w.f. in the internal
region. The range of values $\gamma = 0.3 - 0.5 \text{ fm}^{-1}$ has been found to be adequate in all the cases studied. For $d_i \gg 1/\gamma$, $\psi_A(i)$ coincides with the first term of the asymptotic form \cite{73}.

The second term $\Psi_C$ of the trial w.f. must describe those configurations of the system where the particles are close to each other. For large interparticle separations and energies below the DBT, $\Psi_C$ goes to zero, whereas for higher energies it must reproduce an outgoing three particle state. Each amplitude $\psi_C(i)$ is expanded in terms of the PHH basis \cite{24,21},

$$\psi_C(i) = \rho^{-5/2} \sum_{\alpha,T,T,K} u_{\alpha,T,T,K}(\rho)f_\alpha(x_i)^{(2)}P^{\ell_\alpha,L_\alpha}_K(\theta_i)Y_{\alpha,T,T}(i) , \quad (83)$$

where $(2)P^{\ell_\alpha,L_\alpha}_K$ is a hyperspherical polynomial, defined for example in Ref. \cite{74}, $u_{\alpha,T,T,K}(\rho)$ are the hyperradial functions to be determined by the variational procedure and $f_\alpha(x_i)$ is a correlation function. In the “uncorrelated” hyperspherical harmonic expansion (HH) one has $f_\alpha(x_i) = 1$, whereas in the PHH approach it is included in order to better take into account those correlations introduced by the repulsion of the potential at short distances. The correlation function is calculated by solving a two-body Schroedinger–like equation and it goes to one for large values of the interparticle distance $x_i$. In Eq. \cite{74}, the sum over $\alpha, T, T$ is truncated after the inclusion of $N_c$ channels. Usually all the channels with $\ell_\alpha + L_\alpha \leq L_{\text{max}}$, where $L_{\text{max}} = 6$ or 7, are included in the expansion. For each channel, the sum over the index $K$ of the hyperspherical polynomial runs from $K = 0, 1, 2, \ldots$ up to a maximum value $K_{\alpha,T,T}$. The latter values are chosen in order to achieve the required convergence in the quantities of interest. The total number of basis functions is therefore

$$M = \sum_{\alpha,T,T} (K_{\alpha,T,T} + 1) . \quad (84)$$

To simplify the notation let us label the basis elements with the index $\mu \equiv [\alpha, T, T, K]$, and introduce the following completely antisymmetric correlated spin-isospin-hyperspherical basis elements

$$\mathcal{P}_\mu(\rho, \Omega) = \sum_{i=1}^{3} f_\alpha(x_i)^{(2)}P^{\ell_\alpha,L_\alpha}_K(\theta_i)Y_{\alpha,T,T}(i) , \quad (85)$$

which depends on $\rho$ through the correlation factor and form a non–orthogonal basis. In terms of $\mathcal{P}_\mu(\rho, \Omega)$ the internal part is written as

$$\Psi_C = \rho^{-5/2} \sum_{\mu=1}^{M} u_\mu(\rho)\mathcal{P}_\mu(\rho, \Omega) . \quad (86)$$

The “uncorrelated” basis elements $\mathcal{P}_\mu^0(\Omega)$ are obtained from Eq. \cite{74} in which all the correlation functions are $f_\alpha(x_i) = 1$. It is important to note that also the elements $\mathcal{P}_\mu^0(\Omega)$ do not form an orthogonal basis, as has been discussed in Ref. \cite{74}. In particular, those elements having the same grand–angular quantum number $G = \ell_\alpha + L_\alpha + 2K$ but belonging to different channels are not orthogonal among themselves. Moreover, some $\mathcal{P}_\mu^0(\Omega)$ with the same $G, \Lambda_\alpha, \Sigma_\alpha, T$ quantum numbers are linearly dependent. In Ref. \cite{74} these states have been identified and eliminated from the expansion.

In the present case, the basis elements $\mathcal{P}_\mu(\rho \to \infty, \Omega)$ reduce to the uncorrelated ones $\mathcal{P}_\mu^0(\Omega)$ in the asymptotic region $V_b(R)$. Therefore, it will be useful to combine the correlated basis \cite{74} in order to define a new basis with the property of being orthonormal for $\rho = \infty$. This can be readily accomplished by noting that

$$n_{\mu\mu'}(\rho) = \int d\Omega \mathcal{P}_\mu(\rho, \Omega)^\dagger \mathcal{P}_{\mu'}(\rho, \Omega) \to N_{\mu\mu'}^{(0)} + \frac{N_{\mu\mu'}^{(3)}}{\rho^2} + \mathcal{O}(1/\rho^5) , \quad \text{for } \rho \to \infty , \quad (87)$$

where, in particular,

$$N_{\mu\mu'}^{(0)} = \int d\Omega \mathcal{P}_\mu^0(\Omega)^\dagger \mathcal{P}_{\mu'}^0(\Omega) . \quad (88)$$

Let us define a matrix $U$ such that $U N^{(0)} U^\dagger = \mathcal{D}$ is a diagonal matrix with diagonal elements $\mathcal{D}_\mu$ either 1 or 0. The $\mathcal{D}_\mu = 0$ correspond to the states $\mathcal{P}_\mu^0(\Omega)$ linearly dependent on the others. New uncorrelated and correlated bases are defined as:

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In practice, the functions are identically zero. Therefore, some correlated elements have the property:

\[ \text{have the following behavior} \]

where the matrix \( c \). Due to the fact that some of the uncorrelated elements \( P^0(\Omega) \) are linearly dependent, some elements \( Q^0(\Omega) \) are identically zero. Therefore, some correlated elements have the property: \( Q_\mu(\rho, \Omega) \to 0 \) as \( \rho \to \infty \).

In terms of the new basis, the internal part \( \Psi_C \) is simply

\[ \Psi_C = \rho^{-5/2} \sum_{\mu=1}^M \omega_\mu(\rho) Q_\mu(\rho, \Omega) , \] (90)

where \( \omega_\mu = \sum_{\mu'} (U^{-1})_{\mu\mu'} u_{\mu'} \).

The variation of the functional \( \omega_\mu(\rho) \) with respect to the hyperradial functions \( \omega_\mu(\rho) \), which are the unknown quantities entering in the description of the internal part of the w.f. \( \Psi_C \), leads to the set of inhomogeneous second order differential equations given in Ref. [20], where the method of solution has been discussed. For \( \rho \to \infty \), neglecting terms going to zero faster than \( \rho^{-1} \), the asymptotic expression of such a set of differential equations reduces to the form

\[ \sum_{\mu'} \left\{ -\frac{h^2}{m} \left( \frac{d^2}{d\rho^2} + Q^2 \right) D_\mu c_{\mu,\mu'} + \frac{2Q c_{\mu,\mu'}}{\rho} + O\left( \frac{1}{\rho^2} \right) \right\} \omega_\mu(\rho) = 0 , \] (91)

where the matrix \( c \) is defined as

\[ c_{\mu,\mu'} = \int d\Omega Q^0_\mu(\Omega) \bar{x} Q^0_{\mu'}(\Omega) . \] (92)

From the above equation it is clear that an enlargement of the PHH basis by increasing \( N_c \) and \( K_{\alpha,T,\tau} \) improves the trial w.f. both in the internal and in the asymptotic regions. The choice in Eqs. (93) and (96) is natural in the calculation scheme outlined here and ensures that the matrix element \( \langle \Psi_{L_0 S_0}(\rho) | (H - E) | \Psi_{L_0 S_0} \rangle \) be finite. In fact

\[ < \Psi_{L_0 S_0}(-) | H - E | \Psi_{L_0 S_0} > = \int_0^\infty d\rho I(\rho) , \] (97)

and for \( \rho \to \infty \) one has
\[ I(\rho) \rightarrow \frac{k^2}{m} \sum_{\mu=1}^{M} \sum_{\mu'=1}^{M} \left\{ -\omega_\mu(\rho) \left( \frac{d^2}{d\rho^2} + Q^2 \right) D_{\mu,\mu'} B_{\mu,\mu'}(\rho) + \omega_\mu(\rho) \frac{2Qc_{\mu,\mu'}}{\rho} \omega_{\mu'}(\rho) + O(\rho^2) \right\} \rightarrow O(\rho^2). \] (98)

In conclusion, the procedure appears to be well founded and in the (hypothetical) limit of an infinite expansion it leads to the exact results. The breakup amplitudes \( \mathcal{A}_\alpha(\rho, \Omega_i) \) are obtained in first order approximation in terms of the PHH basis elements \( Q_{\mu}(\rho, \omega) \), via Eq. (95). The convergence of \( \mathcal{A}_\alpha(\rho, \Omega_i) \) as a function of \( N_c \) and \( K_{\alpha,T,T} \) has been found to be very slow when \( \theta_1 \rightarrow \pi/2 \). This is related to the difficulties for the expansion \( \sum_{\mu=1}^{M} B_{\mu,\mu'}(\rho) \) of reproducing the \( x_i \) dependence of the breakup amplitudes in the region \( \mathcal{N}_i(\rho) + \mathcal{N}_i(\rho) \) specified in Eqs. (63–65). However, this problem has no consequences on the calculation of the elastic S-matrix elements \( [S] \), since the regions \( [\Omega_i] \) and \( [\Omega_{i,a}] \) do not give any contribution to the error term \( \langle \epsilon H - E \rangle \cdot \).

Once proved that the procedure can lead to the correct solution of the problem, there are two main questions to be taken care of in practical applications, namely:

1. The boundary conditions given in Eq. (63) are valid only at \( \rho = \infty \). However, such a problem can be overcome by using the procedure proposed in Ref. [21]. First of all, a set of \( M \) coupled differential equations are derived from the variational condition \( \delta \omega_\mu[S] = 0 \). The functions \( \omega_\mu(\rho) \) are determined in the region \( \rho > \rho_0 \) by expanding in powers of \( 1/\rho \) and verifying the boundary conditions of Eq. (63). Values of \( \rho_0 \approx 100 \text{ fm} \) have been found to be appropriate.

2. The convergence of the functional \( [S] \) with \( N_c \) and \( K_{\alpha,T,T} \). In all the calculations performed [21], the convergence pattern of \( [S] \) above the DBT was found to be rather similar to that observed below the threshold [19]. To give an idea of the convergence, the calculated S-matrix elements for \( p - d \) scattering at \( E_{lab} = (3/2)E = 5 \text{ MeV} \) and 10 MeV are reported in Table VI. The state considered is \( J^P = 1^{+} \), which is in general the most structured one since it must satisfy the orthogonality condition with respect to the three-nucleon bound state. In this case the S-matrix is a \( 2 \times 2 \) (complex) matrix corresponding to the \( p - d \) asymptotic states \( L = 0 \), \( S = 1/2 \) and \( L = 2, S = 3/2 \). The NN interaction considered is the AV18 potential [22].

In Table VI, the real and complex part of the two phase-shifts \( 2S_{1/2}, 4D_{1/2} \) and the mixing parameter \( m_{1/2+} \) are given for different values of the number of channels \( N_c = 8, 18, 26 \). In the first case \( N_c = 8 \) only the 8 channels given in Table II have been considered since they give the major contribution to the bound state. The cases 18 and 26 correspond to including all the \( T = 1/2 \) channels with \( \ell_\alpha + L_\alpha \leq 4 \) and 6, respectively. In all the cases, the number of hyperspherical states for each channel has been increased until the convergence was reached. It has been found that a number of states similar to the one used for energies below the DBT is sufficient to get converged results, i.e. 8 basis elements for the first 4 channels, 6 basis elements for channels 5–14 and 4 basis elements for the successive channels.

Also the convergence with \( N_c \) is analogous to that obtained for energies below the deuteron breakup, as can be seen in Table VI. The first 8 channels give the most important contribution to the S-matrix, with results accurate up to three digits. Higher order channels give minor contributions, of the order of a few percent. The contribution of the channels with \( T = 3/2 \) has been found to be very small and it has been disregarded in the calculation presented here.

VI. CONCLUSIONS

The purpose of this paper is to demonstrate the validity of the KVP to describe \( p - d \) elastic scattering above the DBT. The practical application of the principle has been analyzed, with particular reference to the use of the PHH expansion technique. It was shown that the principle remains formally unchanged when the breakup channels are open. In this case, the asymptotic behavior of the w.f. has been extensively discussed with special care in the treatment of the long range Coulomb potential. Different asymptotic regions has been introduced for different values of the hyperspherical variables \( (\rho, \theta, \phi) \) and the solution of the Faddeev-Noble equations has been studied in each case. It was found that certain asymptotic configurations in the \( p + p + n \) system have negligible probability. For example, the breakup w.f. vanishes in region \( \mathcal{V}_i \) when particles \( j, k \) are protons or when they are in a relative state with angular momentum \( \ell_\alpha > 0 \), independently of the fact that they form a \( p - p \) or an \( n - p \) pair. The transition from the solution in region \( \mathcal{V}_b \) to these vanishing solutions has been studied.
Moreover, it was explicitly shown that the use of “approximate” terms in the asymptotic logarithmic distortion of the breakup wave function does not influence the formal derivation and the practical application of the principle. This is due to the fact that exp(−i ln(2Qρ)) × A_{α,T,T} is in any region a smooth function (as discussed in Sect. II B). Thus it is not very critical to try to reproduce it with some approximate method like an expansion over HH functions.

The hyperspherical basis has been found to be a rather natural one to describe the asymptotic behavior of the wave function describing scattering above the DBT, including also the long-range Coulomb interaction. In fact, the equations to be solved have a very simple structure in terms of ρ in the asymptotic region and, accordingly, analytical solutions can be obtained. In practical applications it is not difficult to reduce the problem to the determination of the hyperradial functions in the range 0 ≤ ρ ≤ ρ₀ with the application of specific boundary conditions at ρ₀. Appropriate values of the matching radius ρ₀ have been found to be in the range of 80 ÷ 200 fm.

The convergence of the quantities of interest is the usual problem which one has to face when applying a variational procedure. In two preceding papers [20,21], it has been shown that the convergence of the elastic observables can be achieved with the same precision as below DBT. Realistic NN and 3N interactions can be used to calculate the quantities of interest is the usual problem which one has to face when applying a variational procedure. In two preceding papers [20,21], it has been shown that the convergence of the elastic observables can be achieved with the same precision as below DBT. Realistic NN and 3N interactions can be used to calculate the elastic part of the S–matrix at energies above the DBT even with the inclusion of the long range Coulomb interaction. Applications of the method described here were already reported in Refs. [21,38] where the description of the outgoing breakup waves was presented, including a numerical example.

In conclusion, the KVP provide a formalism from which it is possible to obtain reliable and fully–converged results for the elastic part of the p – d S–matrix at energies above the DBT even with the inclusion of the long range Coulomb interaction. Applications of the method described here were already reported in Refs. [21,38] where the elastic differential cross section and the vector and tensor analyzing powers were studied at E_{lab} = 5 MeV and 10 MeV. The further problem related to a precise determination of the breakup amplitudes A_{α,T,T} is currently under progress and it will be discussed elsewhere [37].

APPENDIX:

In this appendix, the asymptotic behavior of the (outgoing) breakup wave of ψ(i) in V_{i}(R) is given. As discussed in Sect. II B, only the ℓα = 0 channels of the components ψ_j(i) and ψ_k(i) do not vanish in V_{i}(R) and we have

ψ_i(i) = 0 ,
ψ_j(i) = C(ρ) \sum_{AS\Sigma} (-)^S f_{AS\Sigma}(x_i) \sqrt{2} x_j \tilde{Y}_{0AS\Sigma}(i) , \quad \text{region } V_{i}(R) ,
\psi_k(i) = C(ρ) \sum_{AS\Sigma} g_{AS\Sigma}(x_i) \sqrt{2} x_k \tilde{Y}_{0AS\Sigma}(i) ,

where C(ρ) and \tilde{Y}_{k,L,A,S,Σ}(i) are defined in Eqs. (22) and (4), respectively. The sum over the channels has been restricted to those with ℓ = 0 as stated previously. The factors (-)^S and 1/√2 have been introduced for convenience. The functions f and g are determined as explained in the following. First of all, g_{AS\Sigma} = f_{AS\Sigma} since ψ(i) must be antisymmetric under the exchange j ↔ k. Therefore, the amplitude ψ(i) = ψ_i(i) Ξ_i + ψ_j(i) Ξ_j + ψ_k(i) Ξ_k can be cast in the form

ψ(i) = C(ρ) \sum_{AS\Sigma} \frac{f_{AS\Sigma}(x_i)}{x_i} \sqrt{2} x_j \tilde{Y}_{AS\Sigma}(i) ,
(A2)

where

\tilde{Y}_{AS\Sigma}(i) = \tilde{Y}_{0AS\Sigma}(i)((t^1\tilde{t}^k)_T,0(t^i)_{T,S} \pm \frac{1}{2} T ) , \quad T = 1 – S .
(A3)

The amplitude ψ(i) given in Eq. (A2) is easily seen to be antisymmetric with respect to the exchange j ↔ k.

The amplitudes ψ(j) and ψ(k) in the region V_{j}(R) and V_{k}(R) can be obtained in the same way as in Sect. II B, where the behavior of ψ(i) in V_{j}(R) and V_{k}(R) is discussed. In this region the following relations hold

x_j \rightarrow -κy_i , \quad y_j \rightarrow -\frac{1}{2} y_i , \quad θ_j \rightarrow -\frac{π}{6} ,
(A4)

and

x_k \rightarrow κy_i , \quad y_k \rightarrow -\frac{1}{2} y_i , \quad θ_k \rightarrow \frac{π}{6} .
(A5)
where \( \alpha = \{ \ell, L, A, S, \Sigma \} \).

Since, under the exchange \( j \leftrightarrow k \), it must be verified that \( \psi(j) \rightarrow -\psi(k) \) and vice versa, the amplitudes \( \tilde{A}_{\alpha,j} \) or \( \tilde{A}_{\alpha,k}^{\prime}(\pi/6) \) are not independent. Using the previous relations for the Jacobi coordinates, then

\[
\tilde{\gamma}_{\alpha}(j) \rightarrow \sum_{S'}(-)^{S}D_{\alpha,S'}\tilde{\gamma}_{0\alpha\Lambda\Lambda\Sigma}(i),
\]

\[
\tilde{\gamma}_{\alpha}(k) \rightarrow \sum_{S'}(-)^{\ell+S}D_{\alpha,S'}\tilde{\gamma}_{0\alpha\Lambda\Lambda\Sigma}(i),
\]

where

\[
D_{\alpha,S'} = (-)^{S+S'}\ell\hat{L}\hat{S}\hat{S'}\left( \begin{array}{ccc} \ell & L & \Lambda \\
\Sigma & \frac{1}{2} & S \\
& & \end{array} \right),
\]

and \( \ell = \sqrt{2\ell + 1} \), etc. Note that only states with orbital angular momentum \( \ell = 0 \) enter the r.h.s of Eqs. (A8) and (A9). Finally, we can write

\[
\psi(j) + \psi(k) = C(\rho) \sum_{\Lambda,S^2,\Sigma} K_{\Lambda S^2,\Sigma} \gamma_{\Lambda S^2,\Sigma}(i), \quad \text{region } \mathcal{V}_{i}(R),
\]

where \( \gamma_{\Lambda S^2,\Sigma}(i) \) is given in Eq. (A3) and

\[
K_{\Lambda S^2,\Sigma} = \sum_{\ell\hat{L}\hat{S}} \left( \tilde{A}_{\alpha,j}^{\prime}(\pi/6) + (-)^{S}\tilde{A}_{\alpha,k}^{\prime}(\pi/6) \right)D_{\alpha,S'}\sqrt{2}.
\]

Inserting the expressions (A2) and (A11) in the FNE and disregarding all terms \( \mathcal{O}(1/y_i) \) or \( \mathcal{O}(1/\rho) \), the following equation is obtained

\[
-\frac{\hbar^2}{m}f''_{\Lambda S^2\Sigma}(x_i) + V_{2S+1}(x_i)f_{\Lambda S^2\Sigma}(x_i) = -x_iV_{2S+1}(x_i)K_{\Lambda S^2\Sigma},
\]

where

\[
\int d\hat{x}_i d\hat{y}_i \left( \gamma_{\Lambda S^2,\Sigma}(i) \right)' V_{\text{NN}}(x_i)\gamma_{\Lambda S^2,\Sigma}(i) = V_{2S+1}(x_i)\delta_{SS'}\delta_{\Lambda\Lambda'}\delta_{\Sigma\Sigma'}.
\]

\( V_{2S+1}(x_i) \) is the projection of the NN potential acting in a state with orbital angular momentum zero, spin \( S \) and isospin \( T = 1 - S \).

The general solution of Eq. (A13) can be written as the sum of the solution of the homogeneous part and a particular solution of the complete equation. The solution of the homogeneous part will be denoted as \( \gamma_{\Lambda S^2\Sigma}f_{2S+1}^{h}(x_1) \), where \( \gamma_{\Lambda S^2\Sigma} \) is an arbitrary coefficient; \( f_{2S+1}^{h} \) coincides with the (regular) solution of the zero–energy Schroedinger equation of a two–nucleon system in the \( 2S + 1 \) s-wave state. For large \( x_i \) values it goes like \( x_i - a_{2S+1} \), where \( a_1 \) (or \( a_3 \)) is the singlet (triplet) scattering length.

A particular solution is simply

\[
\hat{f}_{\Lambda S^2\Sigma}^{p} = -x_i K_{\Lambda S^2\Sigma}.
\]

Note that the particular solution exactly cancels the amplitudes \( \psi(j) + \psi(k) \) in \( \mathcal{V}_{i}(R) \). In fact,

\[
\Psi = \psi(i) + \psi(j) + \psi(k),
\]

\[
\approx C(\rho) \sum_{\Lambda S^2,\Sigma} \gamma_{\Lambda S^2\Sigma} \hat{f}_{\Lambda S^2\Sigma}^{p}(x_i)\gamma_{\Lambda S^2\Sigma}(i).
\]
Namely, in $\mathcal{V}_i(R)$ the pair $jk$ is in a relative s–wave state with vanishing relative velocity, whereas the motion of the third particle $i$ is governed by the distorted wave $C(\rho) \approx C(y_i)$.

For large values of $x_i$, $f_{\text{ASS}}(x_i)/x_i \to \text{const}$. In the region $\mathcal{V}_i(R)$, the amplitude given in Eq. (A11) should smoothly match the behavior of $\psi_j(i)$ and $\psi_k(i)$. Therefore, the constants $\gamma_{\text{ASS}}$ are related to the breakup amplitudes $\tilde{A}_{n,j}$ via the relations

$$\left(\frac{-S}{\sqrt{2}}\right)(\gamma_{\text{ASS}} - K_{\text{ASS}}) = \tilde{A}_{0\text{ASS},j}(\pi/2) .$$ (A17)

Finally, the functions $\phi_{\alpha}(x_i)$ introduced in Eq. (59) have been defined to be

$$\phi_{0\text{ASS}}(x_i) = \left(\frac{-S}{\sqrt{2}}\right) \frac{1}{\tilde{A}_{0\text{ASS},j}(\pi/2)} x_i.$$ (A18)
A. Kievsky, Phys. Rev. C60, 034001(1999)

M. Viviani, A. Kievsky and S. Rosati, in preparation

\[ E_{\text{lab}} = 5 \text{ MeV} \]

\[ \begin{array}{ccc}
\text{State} & N_c = 8 & N_c = 18 & N_c = 26 \\
\hline
4D_{1/2} & (-5.45,0.004) & (-5.43,0.004) & (-5.43,0.004) \\
2S_{1/2} & (-42.0,1.74) & (-41.8,1.74) & (-41.8,1.74) \\
\eta_{1/2^+} & (1.06,-0.03) & (1.06,-0.03) & (1.05,-0.03) \\
\end{array} \]

\[ E_{\text{lab}} = 10 \text{ MeV} \]

\[ \begin{array}{ccc}
\text{State} & N_c = 8 & N_c = 18 & N_c = 26 \\
\hline
4D_{1/2} & (-7.41,0.23) & (-7.31,0.24) & (-7.30,0.24) \\
2S_{1/2} & (-60.8,11.7) & (-60.6,11.7) & (-60.6,11.7) \\
\eta_{1/2^+} & (1.04,0.06) & (1.02, 0.06) & (1.01,0.06) \\
\end{array} \]

**TABLE I.** Convergence of the eigenphase shift and mixing angle parameters of elastic \( p - d \) scattering as a function of the number of channels included in the PHH expansion of the internal part of the w.f. The state considered has quantum number \( J^\Pi = 1/2^+ \). The nuclear potential model considered is the AV18 interaction. \( E_{\text{lab}} \) is the laboratory energy of the incident proton (the center of mass energy is \( E = 2/3E_{\text{lab}} \)).

\[ \begin{array}{cccccccc}
\alpha & \ell_\alpha & L_\alpha & \Lambda_\alpha & S_\alpha & T & \Sigma_\alpha & J \\
\hline
1 & 0 & 0 & 0 & 1 & 0 & 1/2 & 1/2 \\
2 & 0 & 0 & 0 & 0 & 1 & 1/2 & 1/2 \\
3 & 0 & 2 & 2 & 1 & 0 & 3/2 & 1/2 \\
4 & 2 & 0 & 2 & 1 & 0 & 3/2 & 1/2 \\
5 & 2 & 2 & 0 & 1 & 0 & 1/2 & 1/2 \\
6 & 2 & 2 & 2 & 1 & 0 & 3/2 & 1/2 \\
7 & 2 & 2 & 1 & 1 & 0 & 1/2 & 1/2 \\
8 & 2 & 2 & 1 & 1 & 0 & 3/2 & 1/2 \\
\end{array} \]

**TABLE II.** Quantum numbers for the first 8 channels considered in the expansion of the internal part of the three–nucleon scattering w.f.
FIG. 1. Decomposition of the regular Coulomb function $F_{\ell}(\eta, z) = \mathcal{F}_{\ell}(\eta, z) \sin[z + \beta_{\ell}(\eta, z)]$ for a few values of $\eta$ and $\ell$. Case (a): $\ell = 0$ and $\eta = 1$; Case (b): $\ell = 2$ and $\eta = 1$; Case (c): $\ell = 0$ and $\eta = 10$. The thick solid, thin solid and the dashed lines show the functions $F_{\ell}(\eta, z)$, $\mathcal{F}_{\ell}(\eta, z)$ and $\beta_{\ell}(\eta, z)$, respectively.