Proton-Deuteron Elastic Scattering above the Deuteron Breakup

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The complex Kohn variational principle and the (correlated) hyperspherical harmonics method are applied to study the proton-deuteron elastic scattering at energies above the deuteron breakup threshold. Results for the elastic cross section and various elastic polarization observables have been obtained by taking into account the long-range effect of the Coulomb interaction and using a realistic nucleon-nucleon interaction model. Detailed comparison to the accurate and abundant elastic proton-deuteron experimental data can now be performed. [S0031-9007(99)09091-2]

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A number of nucleon-nucleon (NN) potentials are now available which can be used in a nonrelativistic approach to understand nuclear structure. Those usually referred to as realistic potentials accurately fit the data base selected by the Nijmegen group [1] with a χ^2 per datum close to 1. They produce quite reasonable values for the binding energies of different light nuclei with small deviations from the experimental values. One way of reducing these deviations is to add three-nucleon ($3N$) interaction terms determined in a semiphenomenological way.

When such potentials are used to calculate scattering states, some observables, such as the elastic N-d differential cross sections, are well predicted [2,3]. However, the situation is different for a number of observables which strongly depend on the nuclear interaction in specific waves. Examples of these are spin-dependent observables, such as the vector or the tensor analyzing powers. For these quantities there are significant differences between theoretical estimates and experimental values. This is a strong signal that there are deficiencies in the theoretical models adopted. Detailed theoretical and experimental investigations are therefore necessary in order to understand the reasons for this problem.

In this respect, the study of the p-d scattering process is of particular relevance since very accurate measurements exist for a large set of observables and kinematical regimes. The Faddeev theory has been very successfully applied to the n-d process [2,4,5] but the extension to the p-d case, taking properly into account the long-range Coulomb repulsion, presents a number of difficulties which have been the object of extensive research [6,7]. Accurate calculations of N-d scattering below the deuteron breakup threshold (DBT) have also been performed in the frame of the so-called pair-correlated hyperspherical harmonic (PHH) expansion technique [8]. The incorporation of the Coulomb potential in the PHH approach does not present particular difficulties, and p-d scattering observables have been calculated using realistic $NN + 3N$ potentials (see Refs. [3] and [8]). The technique used is variational and based on the use of the Kohn variational principle (KVP). The extension to the study of the four-body (p-^{3}He and n-^{3}H) zero energy scattering has been given in Ref. [9].

In Ref. [10] the authors used the complex form of the KVP to describe n-d and p-d scattering above the DBT, using a semiphenomenological nuclear s-wave potential, while the Coulomb interaction was included without any partial wave projection. For the n-d case, the results obtained were in close agreement with the benchmarks obtained solving the Faddeev equations in configuration and momentum space [11].

In this paper the study of N-d scattering above the DBT is extended to the case of realistic NN potentials. Cross sections as well as vector and tensor polarization observables for n-d and p-d scattering for nucleon incident energies up to 10 MeV have been calculated using the NN Argonne AV18 potential [12]. These results are compared to the available experimental data [13,14]. Some of the n-d results are compared with the values obtained by the Bochum-Cracow group [2].

The details of the variational approach used by us can be found in Refs. [8,10,15]. The applicability of the KVP above the DBT when the Coulomb interaction is taken into account deserves some attention. Here a brief discussion of its validity for the description of elastic scattering is given. A more general discussion will be reported elsewhere [16]. The scattering wave function (w.f.) Ψ is written as a sum of two terms. The first term, Ψ_C, describes the system when the three nucleons are close to each other. For large interparticle separations and energies below the DBT, it goes to zero, whereas for higher energies it must reproduce a three-outgoing-particle state. It is written as a sum of three Faddeev-like amplitudes corresponding to even permutations of the particle indices 1, 2, and 3. Each amplitude $\Psi_C(\mathbf{x}_i, \mathbf{y}_i)$, where $\mathbf{x}_i, \mathbf{y}_i$ are the Jacobi coordinates corresponding to the ith permutation, has total angular momentum JJ_z and total isospin TT_z, and it is decomposed into N_c channels using the LS coupling, namely,

$$\Psi_C(\mathbf{x}_i,\mathbf{y}_i) = \sum_{\alpha}^{N_c} \phi_\alpha(x_i,y_i)\mathcal{Y}_\alpha(jk,i), \tag{1}$$

$$\mathcal{Y}_\alpha(jk,i) = \{[Y_{\ell_\alpha}(\hat{x}_i)Y_{L_\alpha}(\hat{y}_i)]_{\Lambda_\alpha}[s_\alpha^{jk}s_\alpha^{i}]_{S_\alpha}\}_{JJ_z} \times [t_\alpha^{jk}t_\alpha^{i}]_{TT_z}, \tag{2}$$

where x_i, y_i are the moduli of the Jacobi coordinates and $\mathcal{Y}_\alpha$ is the angular spin-isospin function for each channel. The two-dimensional amplitude ϕ_α is expanded in terms of the PHH basis

$$\phi_\alpha(x_i,y_i) = \rho^{\ell_\alpha+L_\alpha-5/2} f_\alpha(x_i) \times \left[\sum_K u_K^\alpha(\rho)\,{}^{(2)}P_K^{\ell_\alpha,L_\alpha}(\phi_i)\right], \tag{3}$$

where the hyperspherical variables are defined by the relations $x_i = \rho\cos\phi_i$ and $y_i = \rho\sin\phi_i$, $f_\alpha(x_i)$ is a pair correlation function, and ${}^{(2)}P_K^{\ell,L}(\phi)$ is a hyperspherical polynomial.

The second term in the variational scattering w.f. describes the asymptotic motion of a deuteron relative to the third nucleon. It can also be written as a sum of three amplitudes in terms of the ingoing and outgoing solutions of the asymptotic N-d Schrödinger equation,

$$\Omega^+_{LSJ}(\mathbf{x}_i,\mathbf{y}_i) = \Omega^{\rm in}_{LSJ}(\mathbf{x}_i,\mathbf{y}_i) - \sum_{L'S'} {}^J S^{SS'}_{LL'}\Omega^{\rm out}_{L'S'J}(\mathbf{x}_i,\mathbf{y}_i), \tag{4}$$

where ${}^J S^{SS'}_{LL'}$ are the elastic S-matrix elements.

The three-nucleon scattering w.f. for an incident state with relative angular momentum L, spin S, and total angular momentum J is

$$\Psi^+_{LSJ} = \sum_{i=1,3}[\Psi_C(\mathbf{x}_i,\mathbf{y}_i) + \Omega^+_{LSJ}(\mathbf{x}_i,\mathbf{y}_i)], \tag{5}$$

and its complex conjugate is Ψ^-_{LSJ}. A variational estimate of the trial parameters in the w.f. Ψ^+_{LSJ} can be obtained by requiring that, in accordance with the complex KVP, the functional

$$[{}^J S^{SS'}_{LL'}] = {}^J S^{SS'}_{LL'} + i\langle\Psi^-_{LSJ}|H - E|\Psi^+_{L'S'J}\rangle, \tag{6}$$

be stationary.

The validity of the KVP above the DBT, and with charged particles for the elastic S-matrix elements, is briefly discussed below. Let us consider the w.f. $\overline{\Psi}^+_{LSJ}$ describing the p-d process for an energy E, and a trial approximation of it, Ψ^+_{LSJ}. Both wave functions can be written in the form given in Eq. (5), with the assumption that, for the exact one, the sum in Eq. (3) is not truncated at any level. The hyperradial functions and S-matrix coefficients entering the w.f. $\overline{\Psi}^+_{LSJ}$ will be specified by an overline to distinguish them from the corresponding trial quantities. In the asymptotic region $\rho\to\infty$, the hyperradial functions are superpositions of ingoing and outgoing waves

$$\rho^{\ell_\alpha+L_\alpha}u_K^\alpha(\rho) \to \sum_{\alpha' K'}(e^{+i\chi\log 2Q\rho})^{KK'}_{\alpha\alpha'}B^{\alpha'}_{K'}e^{-iQ\rho} - \sum_{\alpha' K'}(e^{-i\chi\log 2Q\rho})^{KK'}_{\alpha\alpha'}A^{\alpha'}_{K'}e^{iQ\rho}, \tag{7}$$

where $Q^2 = M_N E/\hbar^2$ and the χ matrix originates from the Coulomb potential. Since we are interested in the process $p + d \to (p + d) + (p + p + n)$, the boundary conditions to be imposed are

$$B_K^\alpha = 0, \qquad \text{for all } K,\alpha. \tag{8}$$

For $\rho\to\infty$ we can specify four regions, characterized by different ranges of values of the hyperangular variables $[\Omega = \phi,\hat{x},\hat{y}]$. The $[\Omega_b]$ region is the breakup region, where all of the particles are well separated. The region where the particles j and k are close to each other, while particle i is very far from them, is hereafter denoted by $[\Omega_i]$. There are three such regions, corresponding to the cases $i = 1,2,3$. Let us consider the integral

$$I = \langle\overline{\Psi}^-_{LSJ}|(H - E)|\Psi^+_{L'S'J}\rangle_R - \langle\Psi^-_{L'S'J}|(H - E)|\overline{\Psi}^+_{LSJ}\rangle_R, \tag{9}$$

where $\langle\rangle_R$ stands for the integration in the six-dimensional volume with $\rho \le R$ (and $R\to\infty$). Only the differential operators present in H contribute to I. After integrating by parts, the contributions come from the hypersurface at $\rho = R$, where the trial and exact wave functions have reached their asymptotic behavior.

Let us write $I = I_b + \sum_{i=1}^3 I_i$, where I_b (I_i) is the contribution coming from the region $[\Omega_b]$ ($[\Omega_i]$). In $[\Omega_b]$, the asymptotic functions Ω^+_{LSJ} are vanishingly small and I_b reduces to

$$I_b \propto \sum_{K\alpha}\left\{\bar{u}_K^\alpha(\rho)\frac{d}{d\rho}u_K^\alpha(\rho) - u_K^\alpha(\rho)\frac{d}{d\rho}\bar{u}_K^\alpha(\rho)\right\}_R. \tag{10}$$

The above form has been obtained after orthonormalizing the PHH basis elements at $\rho = \infty$. Using the asymptotic behavior given in Eqs. (7) and (8) for both the exact and trial hyperradial functions, $I_b \to 0$ as $R\to\infty$. In the three regions $[\Omega_i]$, the breakup part of the w.f. can be neglected since it gives contributions which go to zero as $R^{-3/2}$, therefore $\sum_{i=1}^3 I_i \propto {}^J\overline{S}^{SS'}_{LL'} - {}^J S^{SS'}_{LL'}$. Finally, using the fact that $(H - E)\overline{\Psi}^+_{LSJ} = 0$, it is possible to show that the functional $[{}^J S^{SS'}_{LL'}]$ differs from ${}^J\overline{S}^{SS'}_{LL'}$ only quadratically in the difference $\epsilon = \overline{\Psi} - \Psi$.

The crucial points of the proof are (i) the outgoing boundary conditions satisfied by Ψ_C and (ii) the null contribution to I_i of the breakup part. The presence of the Coulomb potential introduces a distortion in the outgoing waves which, essentially, does not change the main points of the demonstration of the KVP given for the elastic part of the S matrix in the n-d case [17].

The variation of the functional with respect to the hyperradial functions leads to the following set of coupled equations:

$$\sum_{\alpha',k'}\left[A^{\alpha\alpha'}_{kk'}(\rho)\,\frac{d^2}{d\rho^2}+B^{\alpha\alpha'}_{kk'}(\rho)\,\frac{d}{d\rho}+C^{\alpha\alpha'}_{kk'}(\rho)+\frac{M_N}{\hbar^2}\,EN^{\alpha\alpha'}_{kk'}(\rho)\right]u^{\alpha'}_{k'}(\rho)=D^{\lambda}_{\alpha k}(\rho)\,. \quad (11)$$

For each asymptotic state $^{(2S+1)}L_J$, two different inhomogeneous terms can be constructed corresponding to the asymptotic Ω^{λ}_{LSJ} functions with $\lambda \equiv \text{in, out}$. The numerical technique used to solve the above set of equations imposing outgoing boundary conditions at a finite value of the hyperradius $\rho = \rho_0$ is given in Ref. [10]. Essentially, the solutions of Eq. (11) for $\rho > \rho_0$ are obtained as a series in $1/\rho$, imposing the outgoing boundary conditions of Eqs. (7) and (8). In the case of n-d scattering such solutions evolve as outgoing Hankel functions $H^{(1)}(Q\rho)$. In the region $\rho \le \rho_0$ the hyperradial functions have been expanded as

$$\rho^{-5/2}u^{\alpha}_{K}(\rho)=\sum_{m=0}^{M}A^{m}_{\alpha,K}L^{(5)}_{m}(z)\exp(-z)+A^{M+1}_{\alpha,K}\tilde{u}_{\alpha,K}(\rho)\,, \quad (12)$$

where $z = \gamma\rho$ and γ is a nonlinear parameter. The functions $L^{(5)}_m(z)$ are Laguerre polynomials. The parameters A^m and γ are determined by the variational procedure. The functions defined above are matched to the outgoing solutions at ρ_0. The value of the matching radius ρ_0 is not critical and a value of $\rho_0 \approx 100$ fm has been found to be satisfactory.

The functions $\tilde{u}_{\alpha,k}(\rho)$ are the solutions of Eq. (11), where all of the couplings between the differential equations have been neglected (and applying outgoing boundary conditions). Their inclusion is necessary since the functions $u^{\alpha}_{K}(\rho)$ already show an oscillatory behavior for $\rho > 30$ fm. To reproduce such a behavior would require a rather large value for M in Eq. (12). However, the inclusion of the terms $\tilde{u}_{\alpha,K}$ allows values of M similar to those needed for describing N-d scattering below the DBT [15].

In order to check the convergence properties of the PHH expansion for energies above the DBT, we first solved the same problem treated in Ref. [10] using the present technique. All phase-shift and inelasticity parameters were reproduced with the same previous accuracy, i.e., with a precision of four figures. As compared with Ref. [10], the dimensions of the matrices involved in the eigenvalue problem came out reduced by 1 order of magnitude.

Let us start studying N-d scattering above the DBT using the AV18 interaction. The nuclear elastic S matrix has been calculated up to total angular momentum states $J = 11/2^+$. This includes all partial waves with relative angular momentum $L \le 4$. Higher partial waves (up to $L = 8$) were included in the calculation of the observables using the Born approximation [3]. For each J^{π} state all channels with $\ell_\alpha + L_\alpha \le K_0$ have been included. The number of hyperradial functions has been increased until convergence was reached. The maximum value $K_0 = 6$ was found appropriate to obtain the elastic scattering observables within an accuracy of 1%. The pattern of convergence in terms of K_0 was studied in Ref. [18] for energies below the DBT and a similar behavior has been observed here.

High quality measurements of p-d scattering have been presented in Ref. [13]. Cross sections and proton analyzing powers have been measured up to $E_{\text{lab}} = 18$ MeV, and deuteron analyzing powers and tensor analyzing powers up to $E_{\text{lab}} = 9$ MeV ($E_d = 18$ MeV). In Fig. 1 our theoretical predictions for these observables are compared to the data at $E_{\text{lab}} = 5$ MeV. In Fig. 2 the same set of observables at $E_{\text{lab}} = 10$ MeV are compared to the data of Ref. [14]. In addition to the p-d calculations (solid line), the n-d results (dashed line) are also shown for the sake of comparison. A good agreement between theory and experiment is observed for the differential cross section. The already known puzzle has been found again for the vector analyzing powers A_y and iT_{11} which are underpredicted by about 30%. The tensor analyzing powers are rather well described, with small underpredictions at the second minimum in T_{20}, the second maximum in T_{21}, and the minimum in T_{22}. These differences increase with energy. The origin of these discrepancies can be analyzed in terms of phase-shift and mixing parameters. For example, in Ref. [3] phase-shift analyses were performed at $E_{\text{lab}} = 2.5$ and 3.0 MeV with the conclusion that small differences in the P-wave phase-shift and mixing parameters were responsible for the discrepancy in the A_y and iT_{11} observables. This problem with the P-wave parameters seems to also persist at higher energies. The small discrepancies in the tensor observables could originate

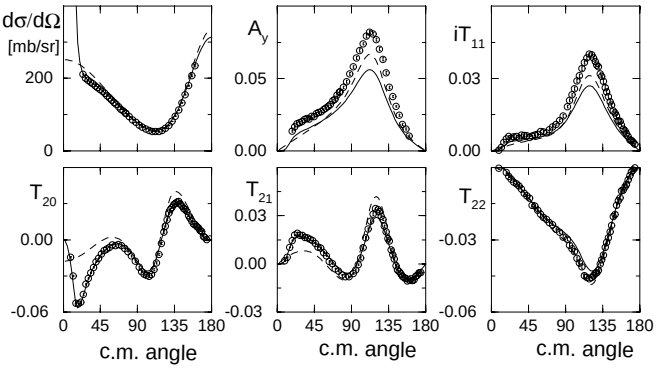

FIG. 1. Differential cross section $d\sigma/d\Omega$, proton analyzing power A_y, deuteron analyzing power iT_{11}, and tensor analyzing powers T_{20}, T_{21}, and T_{22} calculated at $E_{\text{lab}} = 5$ MeV and compared with the data of Ref. [13] (circles with error bars). The solid (dashed) lines are the p-d (n-d) results.

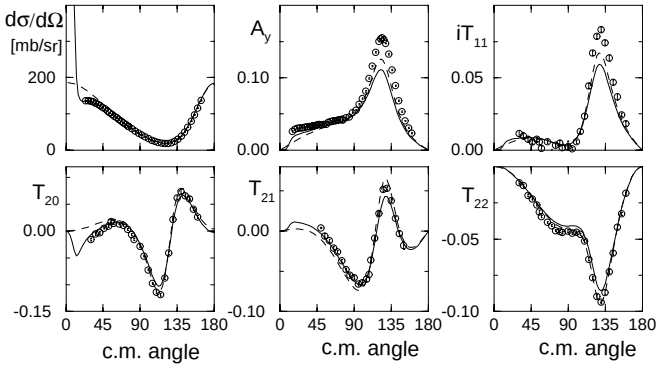

FIG. 2. The same as in Fig. 1, but for $E_{\text{lab}} = 10$ MeV. The data reported here are from Ref. [14].

from higher partial waves. In fact, the tensor observables are particularly sensitive to phase-shift and mixing parameters for $L \geq 2$. At $E_{\text{lab}} \leq 3.0$ MeV, just below the DBT, these parameters are small due to centrifugal barrier effects, but at the energies considered here their contribution becomes appreciable.

Faddeev calculations in momentum space for n-d elastic scattering at $E_{\text{lab}} = 5$ and 10 MeV have been presented in Ref. [2] for several potential models including the AV18 potential. Our corresponding results are in complete agreement with those reference calculations.

In conclusion, p-d elastic cross sections and polarization observables have been calculated with a realistic interaction for energies above the DBT up to $E_{\text{lab}} = 10$ MeV and taking into account Coulomb interaction effects. Accurate calculations of p-d observables and their comparison with the available experimental data may give stringent tests of the existing models of NN and $3N$ interactions. The extension of the present technique to higher energies and to the breakup cross sections will be the subject of a forthcoming paper.

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