(Wiley, New York, 1964).

[5]H. Feshbach, Ann. Phys. (N.Y.) 5, 537 (1958); 19, 287 (1962).

[6]If P defines something other than a two-body channel the formal manipulations are the same but the interpretation of what we call the effective-potential changes. If P defines a single decaying object then the "effective potential" gives a mass renormalization (energy shift) and width to this state.

[7]M. H. Stone, *Linear Transformations in Hilbert Space* (The American Mathematical Society, New York, 1932).

[8]This phase choice $\tau|x\rangle = |x\rangle$ is conventional. For a thorough discussion of time reversal, See A. Bohr and B. Mottelson, *Nuclear Structure* (Benjamin, New York, 1969), Vol. I.

[9]This is in fact the case considered in Ref. 3.

[10]M. A. Naimark, *Linear Differential Operators, Part II* (Ungar, New York, 1968). The discussion we refer to is in Appendix II by V. E. Lyantse, p. 292.

[11]See Ref. 10 and M. Bertero and G. Dillon, Nuovo Cimento 2A, 1024 (1971).

[12]Expansions similar to this have been assumed by reaction theorists dating back to P. Kapur and R. Peierls, Proc. Roy. Soc. (London) A166, 277 (1938).

[13]This is given here in the standard form. We omit the derivation and refer the reader to Ref. 5. The effective Hamiltonian has the same form as in Eq. (2.11).

[14]The expansion parameter for which this is a first-order contribution is not V_R, which is in fact very large, but rather the square of the overlap between the inner and outer states in the inner region. This is small because the outer states do not penetrate into this region significantly.

[15]See Ref. 4, pp. 187–188.

[16]T. E. O. Ericson and F. Scheck, Nucl. Phys. B19, 450 (1970).

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Neutron-Deuteron Elastic Scattering Above the Breakup Threshold*

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Amplitudes for elastic s-wave neutron-deuteron scattering above the breakup threshold are calculated by the method of complex coordinates. The nucleon-nucleon interaction is represented by a local spin- and parity-dependent central Yukawa potential, with parameters chosen to fit low-energy two-nucleon data. Results for inelastic parameters indicate possible errors in a previous phase-shift analysis. Results for the quartet phase shift and quartet and doublet inelastic parameters are consistent with separable potential calculations, but the doublet phase shifts from the two models differ significantly.

I. INTRODUCTION

The three-nucleon scattering problem has received considerable attention in recent years.[1] The use of local nucleon-nucleon potentials has been hampered, however, by the severe numerical problems occasioned by their use in Watson-Faddeev-type integral equations; nonlocal separable potentials or separable nucleon-nucleon t matrices have been used to circumvent these problems. In the energy range below the breakup threshold the Kohn variational principle has provided an efficient technique for finding scattering amplitudes due to local interactions, but a straightforward extension to the breakup region has not so far proved useful.[2] The asymptotic behavior of the wave function necessary to describe three free particles is quite complicated,[3] and this asymptotic behavior must presumably be accurately represented in the trial function if convergence of the Kohn method is to be expected.

In this article we present calculations of s-wave elastic amplitudes in the breakup region, based on the method of complex coordinates[4] reviewed briefly in Sec. II. This method does not require the complicated asymptotic terms representing three free particles, and thus provides what appears to be a useful and productive alternative to the Kohn method. The main result of this paper is to show that for short-range local potentials which are analytic functions of the coordinates (except perhaps at the origin) calculations of elastic scattering can be performed almost as easily above the breakup threshold as below, even if substantial inelastic scattering takes place. The principle of the method also applies to the calculation of break-

up amplitudes, but as yet we have not made such a computation.

Our calculations are for a model n-d problem using a central nucleon-nucleon potential which is spin and parity dependent, with parameters chosen to fit low-energy two-nucleon data. The results, presented in Sec. III, can be compared directly with calculations using separable potentials[5] which fit the same two-nucleon data, and significant differences are apparent in the doublet phase shift. The results for inelastic parameters indicate a substantial difference in character between quartet and doublet states, suggesting inherent errors in an earlier phase-parameter analysis,[6] which assumed equal inelastic parameters in the two states. In Sec. IV we discuss the significance of our results, and comment on a recent calculation[7] with local potentials above breakup which appears to be unsuccessful, at least when there is appreciable inelastic scattering. In Sec. V we consider possible improvements and extensions of our work.

II. COMPLEX-COORDINATE METHOD

The method of complex coordinates for three-particle scattering was proposed by Nuttall and Cohen,[4] who also showed that it could be used successfully in a two-body problem. The idea of the method is that, for analytic potentials such as a superposition of Yukawa potentials, the outgoing wave function χ is an analytic function of the coordinates which will fall off exponentially for rotated $r = |r|e^{i\alpha}$, $\alpha > 0$ no matter how many open channels there are. By χ we mean the difference between the complete scattering wave function ψ and the wave function ϕ describing the incident state. In addition, it is possible to write the physical scattering amplitude as an integral involving χ defined for the rotated coordinates, so that the whole calculation can be performed using a wave function which decreases exponentially.

The basic equation that we use for the elastic n-d scattering calculation is a variational expression for the elastic amplitude:

$$\begin{aligned}[T_{el}] = {} & \langle \vec{p}', \phi_0 | (V_2 + V_3) | \vec{p}, \phi_0 \rangle \\ & + \theta^{-6} \langle \vec{p}'\theta, \phi_0(\theta \vec{Y}) | (V_2 + V_3)_\theta | \chi \rangle \\ & + \theta^{-6} \langle \chi' | (V_2 + V_3)_\theta | \vec{p}\theta^*, \phi_0(\theta^* \vec{Y}) \rangle \\ & - \theta^{-6} \langle \chi' | [E - \theta^2 T - (V_1 + V_2 + V_3)_\theta] | \chi \rangle . \end{aligned} \tag{1}$$

The initial state, consisting of a plane wave for particle 1 and bound-state function ϕ_0 for particles 2 and 3, is the s-wave part of

$$|\vec{p}, \phi_0\rangle = (2\pi)^{-3/2} e^{i\vec{p}\cdot\vec{X}_1} \phi_0(\vec{Y}_1) \sigma_{Q,D} , \tag{2}$$

where $\sigma_{Q,D}$ represents a quartet or doublet spin function symmetric in the spins of particles 2 and 3. (In our model calculation, states and amplitudes are antisymmetrized in all coordinates of particles 1 and 2, the two neutrons.) The coordinates are defined as

$$\vec{Y}_1 = (\vec{r}_2 - \vec{r}_3)/\sqrt{2} , \quad \vec{X}_1 = \sqrt{\tfrac{2}{3}} [\vec{r}_1 - (\vec{r}_2 + \vec{r}_3)/2] ,$$

with cyclic permutations. The phase factors θ or θ^* ($\theta = e^{-i\alpha}$) multiply each coordinate where they appear in incident or final states and in kinetic and potential operators [in particular $V_{i\theta} = V_i(\vec{Y}\theta^*)$]. The phase factors have the effect of rotating the coordinates into the complex plane.

The function χ (or χ') satisfies the inhomogeneous equation

$$[E - \theta^2 T - (V_1 + V_2 + V_3)_\theta]\chi = (V_2 + V_3)_\theta |\vec{p}\theta^*, \phi_0(\theta^* \vec{Y})\rangle . \tag{3}$$

The right-hand side is exponentially decreasing at large interparticle separation, provided the rotation parameter α is within the limits $0 < \tan\alpha < \sqrt{3B_d}/p$, where B_d is the deuteron binding energy (with $\hbar^2/2m = 1$). Then χ will also be exponentially decreasing and can be represented by a suitable set of finite-range trial functions. For s-wave scattering we use, with r_{ij} the interparticle distances:

$$\chi_Q = e^{-(a/2)(r_{23}+r_{13})} \sum_{i,k>j}^{i+j+k=M} C^Q_{ijk} r^i_{12} (r^j_{23} r^k_{13} - r^k_{23} r^j_{13}) \sigma_Q \tag{4}$$

in the quartet state and

$$\begin{aligned} \chi_D = e^{-(a/2)(r_{23}+r_{13})} \Bigg[& \sum_{i,k>j}^{i+j+k=M} C^D_{ijk} r^i_{12} (r^j_{23} r^k_{13} - r^k_{23} r^j_{13}) \sigma'_D \\ & + \sum_{i,k\geq j}^{i+j+k} D^D_{ijk} r^i_{12} (r^j_{23} r^k_{13} + r^k_{23} r^j_{13}) \sigma''_D \Bigg] \end{aligned} \tag{5}$$

in the doublet state, with σ_Q and σ'_D being spin functions symmetric in the spins of particles 1 and 2 (the two neutrons), and σ''_D being antisymmetric in those spins.

It should be emphasized that Eq. (1) is a valid variational expression for the physical amplitude for any choice of the rotation parameter within the limits specified [after Eq. (3)]; this contrasts with the complex-energy method,[8] which appears somewhat similar in actual use, in which results must be obtained at several complex energies, and then numerically continued to the physical (real) energy. Also, only the incident (and final) state is formally required in the asymptotic region, whereas use of the standard Kohn technique requires a very complicated asymptotic form[3] in the trial function.

In attempting to improve the convergence of the variational results (as more terms are added to the trial function) we have added a term to the trial function which would represent the asymptotic form of an n-d scattered wave in the limit of $\alpha \to 0$. This term is

$$\chi_S = \frac{[e^{ipX_1\theta^*} - e^{-bX_1\theta^*} f(X_1\theta^*)]}{pX_1\theta^*} \phi_0(\vec{Y}_1\theta^*)\sigma_{Q,D} \tag{6}$$

[cf. Eq. (2)], where the function f is chosen in the same way as by Humberston[9] to ensure satisfactory behavior of the origin. This term is particularly helpful in the quartet calculations, and in fact represents a fair trial function by itself. This is because of the symmetry of the quartet state (antisymmetric to neutron space exchange): the wave function is excluded from the region in which the two neutrons would interact. Use of this term makes little difference in the doublet calculations where the "internal" region dominates the wave function.

III. RESULTS FOR A MODEL n-d PROBLEM

s-wave doublet and quartet amplitudes have been calculated[10] with the nucleon-nucleon interaction represented as a charge-independent local spin- and parity-dependent central potential. In order to be closely comparable to separable-potential calculations of Sloan and Aaron, Amado, and Yam,[5] even-parity potentials are taken as single Yukawa terms, with parameters (Table I) chosen to fit the same low-energy two-nucleon data (Table II), and the odd-parity interactions are taken as zero. Results with the odd-parity interaction not zero show little change from those presented here.

Estimates from the variational method for both amplitudes at a laboratory energy of 24 MeV with $\alpha = 20°$ are shown in Fig. 1 for a number of values of a and M. The method appears to converge very satisfactorily. If we set $\alpha = 0$, there is no sign of convergence in the doublet state where there is substantial inelastic scattering, but apparent convergence persists in the quartet state, especially at lower energies, no doubt because there is little inelasticity in this state. In the doublet state with $\alpha = 20°$, the rate of convergence decreases somewhat as the energy is reduced towards the breakup threshold.

TABLE I. Two-nucleon potential parameters (even-parity states). Each Yukawa term is written: $V_0 e^{-X}/X$, with $X = r/\lambda$.

Spin state	Potential depth (MeV)	Potential range λ (F)
Triplet	−50.036	1.41
Singlet	−48.95	1.155

TABLE II. Low-energy two-nucleon data used to fix the potential parameters of Table I.

Deuteron binding energy	2.226 MeV
Triplet-s scattering length	5.41 F
Singlet-s scattering length	−23.78 F
Singlet-s effective range	2.70 F

The results are presented in Figs. 2 and 3 in a notation in which the complex phase shift is written $\delta = \delta_R + i\epsilon$ with the "inelastic parameter" being $y = e^{-2\epsilon}$. Results from Sloan and from a phase analysis[6] are shown for comparison. For completeness we show phase shifts calculated below threshold as well as above.

The real parts of the quartet phase shifts from the various calculations are all quite similar, corroborating previous findings that quartet results are only slightly model dependent, especially at lower energies.[11] The quartet inelastic parameters from the present work and from Sloan's are nearly unity, and differ significantly in that respect from the phase-analysis values where the quartet and doublet inelastic parameters were forced to be the the same.

The present results give a much smaller (in modulus) doublet phase shift than either Sloan or the phase analysis. The inelastic parameters from the phase analysis are larger than those giv-

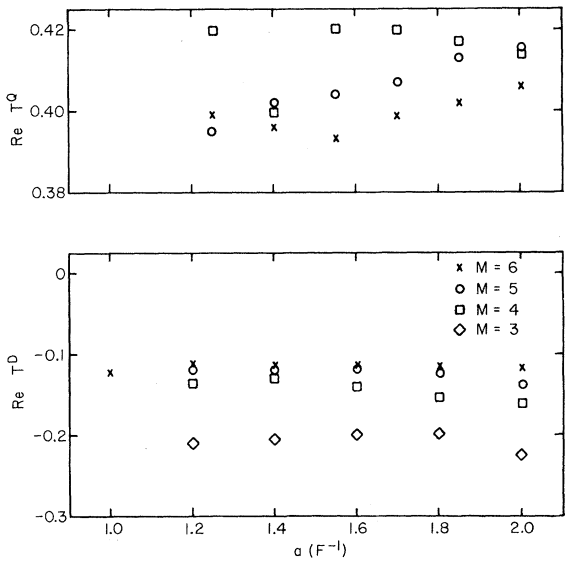

FIG. 1. Estimates of the real parts of the quartet and doublet amplitudes calculated with $\alpha = 20°$ for a number of values of a and M [see Eqs. (4) and (5)].

en by either potential model, again reflecting the restriction imposed on the phase-analysis values.

We have also calculated quartet and doublet scattering lengths using standard variational techniques.[12] The results are

$$a_Q = 6.3 \pm 0.1 \text{ F}, \quad a_D = -8.0 \pm 0.5 \text{ F}.$$

Finally, we have found a lower bound to the triton binding energy of 13.3 ± 0.1 MeV. Note that this combination of doublet scattering length and triton energy would not fall on the linear plot originated by Phillips for separable potentials.[13]

IV. DISCUSSION

There are two features of our results which seem particularly interesting over and above the demonstration of the success of the complex-coordinate method. The first is the great difference in quartet and doublet inelastic parameters, especially as it may bear on the validity of the phase analysis which assumed equal inelastic parameters.[14] There seems substantial reason to expect quite different inelasticities in the two states. Antisymmetry to neutron space exchange in the quartet state forces the wave function to be small when the interneutron separation is small and effectively prevents a strong short-range interaction of incident neutron and deuteron. There is thus little chance of inelastic scattering (breakup). The opposite is true in the doublet state where part of the wave function is symmetric in neutron space exchange [cf. second sum in Eq. (5)]. The results are consistent with these ideas, and it would be interesting to repeat the phase analysis with the inelastic parameters allowed to be independent. A strong possibility exists that the real phases would be significantly altered as well, especially at the higher energies.

The difference in doublet real phase shifts from the two potentials is more evidence that three-body results depend on more than the low-energy two-body data used to fix the parameters of the interactions. Part of this effect may lie in the difference between local and nonlocal potentials, and part certainly depends on the choice of a single Yukawa term to represent each two-body spin- and parity-state interaction.[15] In the present work the short range of the singlet-even potential probably acts to force the doublet wave function to be concentrated toward small interparticle separations, leading to a very strong effective interaction. The large triton binding energy and large negative doublet scattering length indicate that this is the case. To test this supposition we can introduce a "soft core" (repulsive, short-range Yukawa term) in the singlet potential, readjusting the potential parameters to fit the same singlet scattering length and effective range. Preliminary results give a real phase shift at $E_{\text{lab}} = 24$ MeV of about 135°, evidencing a substantial shift toward the Sloan result. The doublet scattering length becomes -4.3 ± 0.2 F and the triton binding energy (lower bound) about 12.1 ± 0.3 MeV. A range of core potentials can be used, and we are continuing to investigate this point. Sloan has also found[16] that simulating repulsion in the singlet state (with

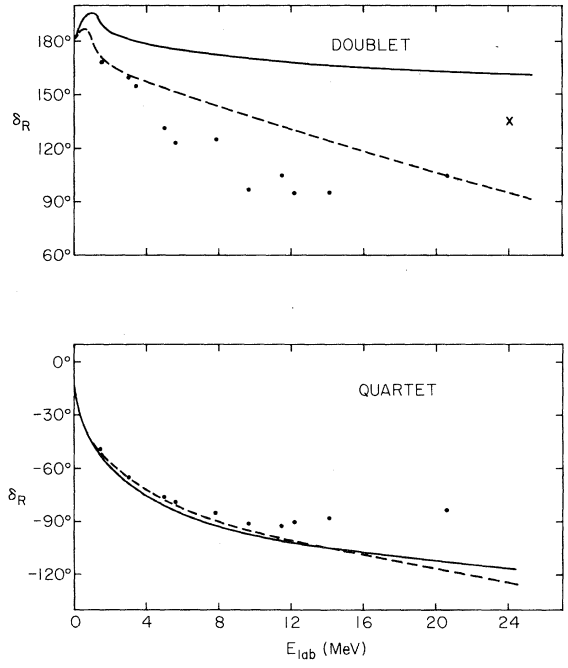

FIG. 2. Real phase shifts δ_R for elastic s-wave n-d scattering. Solid curves are from present work, dashed curves from Sloan (Ref. 5), and the solid points are from the phase analysis (Ref. 6). The cross (×) results from use of a singlet potential with soft core; see text discussion, Sec. IV.

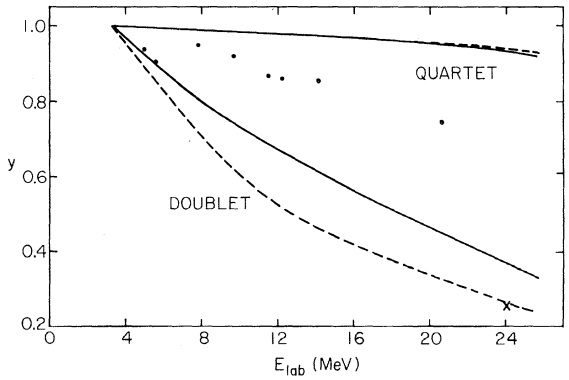

FIG. 3. Inelastic parameters y for elastic s-wave n-d scattering. Notation is that of Fig. 2.

the Tabakin potential[17]) produced doublet results closer to experimental values.

Another calculation of three-nucleon elastic amplitudes with local potentials has appeared recently.[7] Amplitudes were calculated below the elastic threshold and analytically continued above the breakup threshold. Difficulties connected to continuation past this breakup threshold introduce substantial errors in the results and the authors state that errors are of the same magnitude as the inelastic scattering, so that one is not even able to determine inelastic parameters. We have modified our calculation to use the model of Ref. 7 (especially with respect to symmetry character) and find results consistent within errors quoted. This provides a useful partial check on our computer program. Our results do not have such substantial errors; note that such errors would be disastrous in our doublet amplitude in which there is considerable inelasticity. It is interesting to note that one advantage of this method of Pieper, Wright, and Schlessinger[7] is that one needs only the initial state [Eq. (2)] in the asymptotic region. As a practical matter we have also found that in our doublet calculation, only this term is required; this saves considerable computer time required for numerical integrations of matrix elements with the term of Eq. (6). However, introduction of other terms requiring numerical integration may improve convergence, as discussed in Sec. V.

V. FUTURE WORK

We are pursuing several facets of the application of the complex-coordinate method to the three-nucleon problem. One is to introduce into the trial function a term (or terms) representing the longest-range behavior of the variational results, perhaps giving an improvement in their convergence.

We are already investigating the use of more complicated nucleon-nucleon interactions in our elastic-amplitude calculations. Repulsive cores and tensor potentials are features of realistic internucleon interactions which can be introduced, especially if convergence can be improved as indicated above.

Nuttall and Cohen have already indicated the outline for calculations of inelastic amplitudes by this method. Efficient representation of their "subtraction" terms will be required in order to make this calculation tractable within present computing capabilities.

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[1]Extensive references can be found in *Three-Body Problem in Nuclear and Particle Physics,* edited by J. S. C. McKee and P. M. Rolph (North-Holland, Amsterdam, 1970); also in *Three-Particle Scattering in Quantum Mechanics,* edited by J. Gillespie and J. Nuttall, (Benjamin, New York, 1968).

[2]J. Nuttall and J. G. Webb (unpublished).

[3]J. Nuttall, Phys. Rev. Letters 19, 473 (1967); J. Nuttall and J. G. Webb, Phys. Rev. 178, 2226 (1969).

[4]J. Nuttall and H. L. Cohen, Phys. Rev. 188, 1542 (1969).

[5]I. H. Sloan, Nucl. Phys. A168, 211 (1971). Also see R. Aaron, R. D. Amado, and Y. Y. Yam, Phys. Rev. 140, B1291 (1965); R. Aaron and R. D. Amado, Phys. Rev. 150, 857 (1966).

[6]W. T. H. van Oers and K. W. Brockman, Jr., Nucl. Phys. A92, 561 (1967).

[7]S. C. Pieper, J. Wright, and L. Schlessinger, Phys. Rev. D 3, 2419 (1971).

[8]F. A. McDonald and J. Nuttall, Phys. Rev. Letters 23, 361 (1969); Phys. Rev. A 4, 1821 (1971).

[9]J. W. Humberston, Nucl. Phys. 69, 291 (1964).

[10]Quartet results have been previously reported: F. A. McDonald and J. Nuttall, Bull. Am. Phys. Soc. 15, 1588 (1970).

[11]Cf. H. P. Noyes, p. 10 of the first item in Ref. 1.

[12]L. Rosenberg, L. Spruch, and T. F. O'Malley, Phys. Rev. 118, 184 (1960).

[13]A. C. Phillips, Nucl. Phys. A107, 209 (1968).

[14]Sloan has previously noted this discrepancy (Ref. 5).

[15]We note that the square-well model of Brayshaw and Buck [Phys. Rev. Letters 24, 733 (1970)] gives good agreement with the phase-analysis real phase shifts.

[16]I. H. Sloan, Phys. Letters 31B, 353 (1970).

[17]F. Tabakin, Phys. Rev. 174, 1208 (1968).