Neutron-Proton Scattering with Spin-Orbit Coupling. I. General Expressions

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Neutron-proton scattering in the triplet spin state is discussed under the following assumptions about the nuclear forces: (1) the forces are conservative, (2) they allow time-reversal, i.e., the reciprocity law is valid, (3) the spin vectors of the neutron and proton enter in a symmetrical way, so that the total spin of of the system is preserved during the collision, and (4) the forces have a finite range. We do not assume that the forces can be derived from a potential function (i.e., that they are velocity-independent).

General expressions are given for the scattering matrix and for the differential cross section. The matrix elements of the scattering matrix are expressed in terms of the minimum numbers of real, independent parameters. The energy dependence of these parameters near zero energy can be predicted uniquely on the basis of assumptions (1) to (4) above.

1. INTRODUCTION

THE analysis of neutron-proton scattering in the presence of spin-orbit coupling (e.g., the tensor force) is appreciably more involved than the analysis of the scattering in the absence of such coupling. There is considerable literature on this subject.[1] The purpose of the present paper is to give a general formula for the cross section in terms of the minimum number of independent real parameters and to discuss the behavior of these parameters near zero energy. We are preparing for publication a paper on low energy neutron-proton scattering with tensor forces, employing the effective range theory and giving numerical values of the relevant parameters for some representative choices of the nuclear force law. The general (but rather formal) results obtained in the present paper will be made use of in the subsequent paper.

We shall assume throughout that there are no transitions from the singlet to the triplet spin state of the neutron-proton system or vice versa. This is of course only an assumption. There is no absolute selection rule which would forbid a transition such as $^1P_1$ to $^3P_1$. However, if the spin vectors of neutron and proton enter symmetrically into the basic law of force, then such transitions would be excluded by the conservation of the spin symmetry character. In view of the unexpected difference between neutron-proton and proton-proton scattering at high energies, it is perhaps worth while to remark that transitions between the two spin states can occur in the neutron-proton scattering but are absolutely forbidden in proton-proton scattering due to the Pauli principle (e.g., in the transition cited above, the $^1P_1$ state is forbidden for two protons).

[1] J. W. Rarita and J. Schwinger, Phys. Rev. **59**, 436, 556 (1941); C. Kittel and G. Breit, Phys. Rev. **56**, 744 (1939); J. M. Jauch, Phys. Rev. **67**, 125 (1945); F. Rohrlich and J. Eisenstein, Phys. Rev. **75**, 705 (1949); J. Ashkin and T. Y. Wu, Phys. Rev. **73**, 973 (1948); Massey, Burhop, and Hu, Phys. Rev. **73**, 1402 (1948); E. H. S. Burhop and H. N. Yadav, Proc. Roy. Soc. (London) **A197**, 505 (1949); W. Hepner and R. Peierls, Proc. Roy. Soc. (London) **A44**, 712 (1951); S. A. Kushneriuk and M. A. Preston, Proc. Phys. Soc. (London) **A44**, 712 (1951).

If we neglect the possibility of such transitions, we can treat scattering in the two spin states independently. The singlet state scattering presents no difficulties since spin-orbit coupling is impossible in that state. We shall restrict ourselves to scattering in the triplet state from here on, and all formulas will refer to pure triplet state scattering. Thus they must be multiplied by the statistical factor $\frac{3}{4}$, and the singlet contribution must be added before any comparison is made with experiment.

In this paper we shall use only those arguments which are independent of the details of the force law (e.g., whether or not the force is velocity-dependent). The results are correspondingly both general and formal. Specific numerical results can be obtained only by making more definite assumptions about the neutron-proton force. Such results are deferred to a second paper, now in preparation.

2. THE SCATTERING MATRIX AND ITS EIGENSTATES

Following Rarita and Schwinger, we classify the triplet states of the neutron-proton system according to their total angular momentum J and parity Π. Instead of the actual parity $\Pi=(-)^l$ it is useful to introduce the quantum number

$$\pi=(-1)^J\Pi. \tag{2.1}$$

$\pi=+1$ if $\Pi=(-)^J$, and $\pi=-1$ if $\Pi=-(-)^J$. For each value of J, except $J=0$, there are three possible values of the orbital angular momentum l, namely $l=J$, $l=J+1$, $l=J-1$. The first of these corresponds to $\pi=1$, the last two to $\pi=-1$. If we denote by N the number of different "channels" (choices of l) consistent with a given J and π, we get

$$\begin{aligned} &N=1 \quad \text{for} \quad \pi=+1, \\ &N=2 \quad \text{for} \quad \pi=-1, \quad (\text{except } J=0,\ \pi=-1). \end{aligned} \tag{2.2}$$

The exceptional $^3P_0$ state is a single-channel state even though it has $\pi=-1$.

The spin and angle dependence of a wave function with total angular momentum J, z component thereof

equal to M, orbital angular momentum l, and spin angular momentum s ($s=1$ for triplet states) is given by

$$\mathcal{Y}_{Jls}{}^{M}(\theta,\phi,\sigma)=\sum_{m_l+m_s=M}(lsm_lm_s|lsJM)\times Y_{lm_l}(\theta,\phi)\,\chi_{sm_s}(\sigma), \quad (2.3)$$

where $(lsm_lm_s|lsJM)$ is a Clebsch-Gordon coefficient in the notation of Condon and Shortley,[2] the Y's are spherical harmonics defined as in Condon and Shortley, and χ_{sm_s} is a spin function for spin s and z component of the spin equal to m_s.

Now consider a typical single-channel state with $\pi=+1$ and hence $l=J$. The wave function for this state can be written in the form

$$\psi=r^{-1}v_J(r)\mathcal{Y}_{JJ1}{}^{M}(\theta,\phi,\sigma). \quad (2.4)$$

No other state can be "mixed in" because of the selection rules. The radial function $v_J(r)$ has a complicated behavior as long as r is less than the range of the forces. For large values of r, however, $v_J(r)$ can be written as a linear superposition of an ingoing and an outgoing wave

$$v_J(r)=A\exp[-i(kr-\tfrac{1}{2}J\pi)]-B\exp[+i(kr-\tfrac{1}{2}J\pi)]. \quad (2.5)$$

If the incoming wave has a given amplitude A, the amplitude of the outgoing wave B is determined (mathematically the ratio of B to A is determined by the condition that v be that solution of the radial wave equation which vanishes at $r=0$). The scattering matrix, which in this case becomes just an ordinary number, is defined by

$$B=SA. \quad (2.6)$$

Since in pure elastic scattering the flux of the outgoing wave is equal to that of the ingoing wave, we get $|S|^2=1$ and hence S can be written in the form

$$S=\exp(2i\delta_{J,0}), \quad (2.7)$$

where the real quantity $\delta_{J,0}$ is called the phase shift. The asymptotic behavior of $v_J(r)$ is found by substituting (2.6) and (2.7) into (2.5), giving (C=constant)

$$v_J(r)=C\sin(kr-\tfrac{1}{2}J\pi+\delta_{J,0}). \quad (2.8)$$

We now apply the same method to the states with $\pi=-1$, where the orbital angular momentum can assume two values, $l=J-1$ and $l=J+1$. Corresponding to these two values of l there are two radial functions. The wave function as a whole for a state with total angular momentum J and $\pi=-1$ [parity$=(-1)^{J+1}$] can be written as

$$\psi=r^{-1}u_J(r)\mathcal{Y}_{J,J-1,1}{}^{M}(\theta,\phi,\sigma)+r^{-1}w_J(r)\mathcal{Y}_{J,J+1,1}{}^{M}(\theta,\phi,\sigma). \quad (2.9)$$

[2] E. U. Condon and G. H. Shortley, *Theory of Atomic Spectra* (Cambridge University Press, London, 1935).

For large values of r each radial wave function is a linear superposition of an ingoing and an outgoing wave, i.e.,

$$\begin{aligned}u_J(r)&=A_1\exp\{-i[kr-\tfrac{1}{2}(J-1)\pi]\}-B_1\exp\{+i[kr-\tfrac{1}{2}(J-1)\pi]\},\\ w_J(r)&=A_2\exp\{-i[kr-\tfrac{1}{2}(J+1)\pi]\}-B_2\exp\{+i[kr-\tfrac{1}{2}(J+1)\pi]\}.\end{aligned} \quad (2.10)$$

If the amplitudes of the incoming waves (A_1 and A_2) are given, the amplitudes of the outgoing waves (B_1 and B_2) are determined by the wave equation. The scattering matrix is now a 2-by-2 matrix, defined by

$$\begin{aligned}B_1&=S_{11}A_1+S_{12}A_2,\\ B_2&=S_{21}A_1+S_{22}A_2,\end{aligned} \quad (2.11)$$

or, in matrix notation[3]

$$b=Sa. \quad (2.11a)$$

According to general theorems the scattering matrix S must be unitary (conservation of probability) and symmetric (reciprocity). The most general unitary and symmetric 2-by-2 matrix contains 3 real independent parameters and can be written in the form

$$S=U^{-1}\exp(2i\Delta)\,U, \quad (2.12)$$

where U is an orthogonal matrix depending on only one real parameter which we shall call ϵ_J or just ϵ, when the value of J is understood.

$$U=\begin{pmatrix}\cos\epsilon & \sin\epsilon\\ -\sin\epsilon & \cos\epsilon\end{pmatrix}, \quad (2.13)$$

and Δ is a diagonal matrix whose diagonal elements are real and are the "eigen-phaseshifts" for the state J, $\pi=-1$:[4]

$$\Delta=\begin{pmatrix}\delta_{J\alpha} & 0\\ 0 & \delta_{J\beta}\end{pmatrix}=\begin{pmatrix}\delta_\alpha & 0\\ 0 & \delta_\beta\end{pmatrix}. \quad (2.14)$$

These parameters have the following interpretation: We can construct an incoming wave with a ratio $A_2:A_1$ such that the outgoing wave is a mixture of the two states $l=J-1$ and $l=J+1$ in the same proportion, i.e., such that $B_2:B_1=A_2:A_1$. Such a state is an eigenstate of the scattering matrix, in the sense that the scattering matrix produces merely a change of the phase of the outgoing wave with respect to that of the incoming wave, without admixing new states. There are two such eigenstates, which we shall call α and β, given by

$$A_{2\alpha}/A_{1\alpha}=\tan\epsilon, \quad A_{2\beta}/A_{1\beta}=-\cot\epsilon. \quad (2.15)$$

The equations connecting the amplitudes of the outgoing waves to those of the incoming waves then are

$$B_{1\alpha}=\exp(2i\delta_\alpha)\,A_{1\alpha}, \quad B_{1\beta}=\exp(2i\delta_\beta)\,A_{1\beta}. \quad (2.16)$$

[3] We use small letters, a, b for vectors (column matrices) and capital letters S, U, etc., for linear operators (square matrices).

[4] The use of the eigenstates of the scattering matrix is due to J. Schwinger (unpublished lectures, Harvard, 1947).

In each case B_2 is determined by (2.15) coupled with the condition that the ratio B_2/B_1 is identical with A_2/A_1.

It hardly needs to be emphasized that the eigenphaseshifts δ_α and δ_β are not to be thought of as phaseshifts for the states $l=J-1$ and $l=J+1$, respectively. There are no such phaseshifts, since neither of these two states is an eigenstate of the scattering matrix. The "mixture parameter" ϵ which determines the "correct" mixtures of these two states is an essential parameter in the scattering matrix and enters explicitly into the differential cross section.

It remains to identify the parameters δ_α, δ_β, and ϵ, which enter into the scattering matrix, in terms of the behavior of the radial wave functions $u_J(r)$ and $w_J(r)$ for large values of r. We substitute (2.15) and (2.16) into (2.10) and get, apart from constant factors,

$$\begin{aligned} u_{J\alpha}(r)&=\cos(\epsilon_J)\,\sin[kr-\tfrac{1}{2}(J-1)\pi+\delta_{J\alpha}],\\ w_{J\alpha}(r)&=\sin(\epsilon_J)\,\sin[kr-\tfrac{1}{2}(J+1)\pi+\delta_{J\alpha}], \end{aligned} \tag{2.17}$$

and

$$\begin{aligned} u_{J\beta}(r)&=-\sin(\epsilon_J)\,\sin[kr-\tfrac{1}{2}(J-1)\pi+\delta_{J\beta}],\\ w_{J\beta}(r)&=\cos(\epsilon_J)\,\sin[kr-\tfrac{1}{2}(J+1)\pi+\delta_{J\beta}]. \end{aligned} \tag{2.18}$$

Equations (2.17) and (2.18) show that the radial wave functions for the eigenstates of the scattering matrix are distinguished by having the same phaseshift δ appearing in the asymptotic formulas for both $u_J(r)$ and $w_J(r)$.

It is apparent from (2.17) and (2.18) that there is a relation between the ratio of the amplitudes of w to u in the "α" state and in the "β" state, namely

$$(w/u)_\alpha=-(u/w)_\beta \quad (\text{for } r\to\infty). \tag{2.19}$$

This relation is a consequence of (2.15) and is an expression of the fact that the eigenvectors of a unitary matrix (such as the scattering matrix S) are orthogonal to each other. The orthogonality relation reads

$$A_{1\alpha}{}^*A_{1\beta}+A_{2\alpha}{}^*A_{2\beta}=0. \tag{2.20}$$

Equation (2.19) follows from (2.20) together with the additional observation that the eigenvectors are real; the latter observation follows from the reciprocity law (from the time reversal symmetry). We emphasize that these considerations do not depend on the particular force law (e.g., on the assumption that the force can be written as the gradient of a potential function), even though the usual proof depends on such assumptions.[5]

Finally, we observe that there is the following ambiguity inherent in the developments so far: There are two eigenstates of the scattering matrix, but so far no prescription has been given for calling one of them the "α" state and the other the "β" state. Indeed, all formulas so far are invariant under the interchange of δ_α and δ_β, provided that ϵ is simultaneously changed into $\epsilon'=\epsilon+\frac{1}{2}\pi$. We can make the assignments α and β unique in the following way: In the limit as the collision energy approaches zero, the difference between the centrifugal barrier effects for $l=J-1$ and $l=J+1$ is so pronounced that these two states become eigenstates. According to (2.17) and (2.18) this means that ϵ approaches either 0 or $\frac{1}{2}\pi$ in that limit. We now define the assignments α and β so that in that limit the α-wave corresponds to the state $l=J-1$ and the β-wave to the state $l=J+1$. That is, we require

$$\lim_{E\to 0}\epsilon_J=0 \quad (\text{every } J). \tag{2.21}$$

Near zero energy the α-wave is then predominantly $l=J-1$, the β-wave is predominantly $l=J+1$. Of course, this is true only fairly close to zero energy, since ϵ_J is in general quite energy-dependent.

In addition to the above ambiguity which is now taken care of, there is the usual ambiguity inherent in all phaseshifts which is that we can add any integral multiple of π to δ_α or δ_β or both, as well as to ϵ, without changing the scattering matrix.

Finally, we have to include the exceptional ${}^3P_0$ state ($J=0$, $\pi=-1$) into the formalism. This can be done most simply by including it with the $\pi=+1$ states, since it is a one-channel state. However, for purely formal reasons involving convenience of writing the formulas later on, it is advantageous to use a somewhat different procedure. We define, for $J=0$ and $\pi=-1$,

$$\epsilon_J=\epsilon_0\equiv 0, \quad \delta_{0\alpha}\equiv 0, \quad \delta_{0\beta}\equiv\delta({}^3P_0). \tag{2.22}$$

This is equivalent to the introduction of a formal state with $l=-1$ and associated phaseshift equal to 0. Of course, this formal state has no physical reality and drops out of the final formulas.

3. GENERAL FORMULA FOR THE CROSS SECTION

We are now in a position to write down the general formula for the differential scattering cross section for neutron-proton scattering in the triplet spin state. We use methods developed before.[6] The cross section can be written as a sum of Legendre polynomials of type

$$d\sigma=\frac{\lambda\!\!\!^{-2}}{3}\sum_{L=0}^{\infty}B_L P_L(\cos\theta)d\Omega, \tag{3.1}$$

where B_L is given by formulas (4.25) and (4.26) of reference 6. We can simplify the appearance of the final formula somewhat by a notation which allows us to treat states of the same J but opposite parity together. We introduce an index ρ which can assume the three values $\rho=\alpha$, $\rho=\beta$, and $\rho=0$. The phaseshift δ_J is then equal to $\delta_{J\alpha}$, $\delta_{J\beta}$, and δ_{J0}, respectively. We also introduce the eigenvectors x_J corresponding to these three

[5] The usual proof employs the constancy of the Wronskian of the pair of coupled second-order differential equations for $u(r)$ and $w(r)$. We need not assume that u and w satisfy any differential equations.

[6] J. M. Blatt and L. C. Biedenharn (to be published).

values of ρ

$$x_{J\alpha}=(\cos\epsilon_J, 0, \sin\epsilon_J),$$
$$x_{J\beta}=(-\sin\epsilon_J, 0, \cos\epsilon_J), \quad (3.2)$$
$$x_{J0}=(0, 1, 0).$$

In each bracket the first symbol is the component of x_J belonging to $l=J-1$, the second is the component belonging to $l=J$, the third is the component for $l=J+1$.

We now introduce the quantity $X(J_1\rho_1 J_2\rho_2, L)$ defined by

$$X(J_1\rho_1 J_2\rho_2, L)=\sum_{l_1=J_1-1}^{J_1+1}\sum_{l_2=J_2-1}^{J_2+1} Z(l_1 J_1 l_2 J_2, 1L) \times(x_{J_1\rho_1})_{l_1}(x_{J_2\rho_2})_{l_2}, \quad (3.3)$$

where the components $(x_{J\rho})_l$ are given explicitly in (3.2), and the Z coefficients for $s=1$ are tabulated in reference 6. The coefficient B_L in (3.1) is then given by

$$B_L=\sum_{J_1=0}^{\infty}\sum_{J_2=|J_1-L|}^{J_1+L}\sum_{\rho_1}\sum_{\rho_2}[X(J_1\rho_1 J_2\rho_2, L)]^2 \times\sin\delta_{J_1\rho_1}\sin\delta_{J_2\rho_2}\cos(\delta_{J_1\rho_1}-\delta_{J_2\rho_2}). \quad (3.4)$$

In order to illustrate the use of these formulas, we calculate explicitly the differential cross section for neutron-proton scattering in the triplet spin state at low energies. For low energies we can make the assumption that all phaseshifts vanish with the exception of the α-wave phaseshift $\delta_{1\alpha}$ associated with the ${}^3S_1+{}^3D_1$ state ($J=1$, $\pi=-1$). The β-wave phaseshift can be neglected at low energies, since the β-wave is a mixture of ${}^3S$ and ${}^3D$ with a predominant ${}^3D$ component, and we shall show in Sec. 4 that $\delta_{1\beta}$ behaves like a typical D wave phaseshift as far as its dependence on energy is concerned. Thus there are only two parameters necessary to describe the scattering, the phaseshift $\delta_{1\alpha}$ and the mixture parameter ϵ_1.[7] Equation (3.4) then becomes

$$B_L=[X(1\alpha 1\alpha, L)]^2\sin^2(\delta_{1\alpha}). \quad (3.5)$$

We now use the tables in reference 6 to compute the relevant values of X

$$X(1\alpha 1\alpha, 0)=\sqrt{3}(\cos^2\epsilon_1+\sin^2\epsilon_1)=\sqrt{3}, \quad (3.6)$$

$$X(1\alpha 1\alpha, 2)=0\times\cos^2\epsilon_1+\sqrt{3}\cos\epsilon_1\sin\epsilon_1 +\sqrt{3}\sin\epsilon_1\cos\epsilon_1+\sqrt{\tfrac{3}{2}}\sin^2\epsilon_1 =\sqrt{3}\sin\epsilon_1(2\cos\epsilon_1+2^{-\frac{1}{2}}\sin\epsilon_1). \quad (3.7)$$

All other X vanish because of selection rules for the Z coefficients. Thus we get from (3.1)

$$d\sigma=\lambda^2\sin^2(\delta_{1\alpha})[1 +\sin^2\epsilon_1(2\cos\epsilon_1+2^{-\frac{1}{2}}\sin\epsilon_1)^2P_2(\cos\theta)]d\Omega. \quad (3.8)$$

We see that the α-wave scattering is not equivalent to pure S wave scattering. It reduces to pure S wave scattering only if $\epsilon_1=0$.

The first few terms of the series (3.4) have been written by Rohrlich and Eisenstein (reference 1) and also by Biedenharn.[8] The quantity ζ_J used there is equal to $\tan\epsilon_J$ in the present notation.

4. THE BEHAVIOR OF THE SCATTERING MATRIX NEAR ZERO ENERGY

We now investigate the behavior of the parameters entering the scattering matrix (the phaseshifts $\delta_{J\alpha}$, $\delta_{J\beta}$, δ_{J0}, and the mixture parameter ϵ_J) at very low energies. One of the results of this section has been stated already in formula (2.21).

We shall make the assumption that the forces have a limited (even though perhaps a large) range, i.e., that there exists an inter-particle distance R such that, for $r\geqslant R$, the particles do not exert any forces on each other. We emphasize that this assumption does not mean that the forces must be derivable from a potential function. Velocity-dependent forces are permitted, provided that they have a finite range.

We use the derivative matrix of Wigner and Eisenbud.[9] Consider first the single-channel states, i.e., $\pi=+1$, $l=J$. The wave function is given by (2.4). But instead of the decomposition (2.5), we now decompose the radial wave function $v_J(r)$ in a different manner. Following Wigner and Eisenbud, we define two functions $\mathcal{S}_l(r)$ and $\mathcal{C}_l(r)$ by the requirements that both satisfy the radial equation for orbital angular momentum l in the absence of forces between the particles and furthermore that they satisfy the following boundary conditions at $r=R$:[10]

$$\mathcal{S}_l(R)=0, \quad \mathcal{C}_l(R)=(M/2\hbar)^{\frac{1}{2}},$$
$$\mathcal{S}_l'(R)=(M/2\hbar)^{\frac{1}{2}}, \quad \mathcal{C}_l'(R)=-(l/R)(M/2\hbar)^{\frac{1}{2}}. \quad (4.1)$$

Since $\mathcal{S}_l(r)$ and $\mathcal{C}_l(r)$ both satisfy the force-free radial equation for orbital angular momentum l, both of them can be written as linear combinations of the standard

[7] Actually this argument is oversimplified. We shall derive the energy dependences of all the relevant parameters in Sec. 4 of this paper. When these energy dependences are substituted into the formula for the cross section at low energies, it can be seen that the approximations made here (neglecting all parameters other than $\delta_{1\alpha}$ and ϵ_1) are not really consistent, i.e., there are other terms in the cross section which are of the same order, or even lower order, in the energy than the terms we have kept in (3.8). Some of these other terms are connected with scattering in the P state ($l=1$); the present experimental data indicate that the P state scattering is very much smaller than expected and may even be altogether absent. However, the interference terms between the α-wave and the β-wave, as well as the interference terms between the α-wave and other waves involving D states, are of the same order in the energy as the angle-dependent term in (3.8), and they should be taken into account. Thus (3.8) should be considered an illustrative example rather than a consistent approximation formula.

[8] L. C. Biedenharn, M.I.T. thesis (1949).

[9] E. P. Wigner and L. Eisenbud, Phys. Rev. **72**, 29 (1947); E. P. Wigner, Phys. Rev. **73**, 1002 (1948). The developments of this section are a straightforward application of the methods of the second reference. We give the details of the derivation merely because the simple problem discussed here allows the use of an appreciably simpler notation.

[10] These are identical with the definitions of reference 8, if one observes that the "M" of that reference is the reduced mass in the channel, i.e., in our case equal to $\frac{1}{2}M$.

regular and irregular solutions of that equation, $F_l(r)$ and $G_l(r)$, where $F_l(r)$ and $G_l(r)$ are defined by their asymptotic behavior

$$F_l(r)\cong\sin(kr-\tfrac{1}{2}l\pi),\ G_l(r)\cong\cos(kr-\tfrac{1}{2}l\pi),\ (r\to\infty). \quad (4.2)$$

Indeed, simple substitution gives the relations[11]

$$\mathcal{S}_l(r)=k^{-1}(M/2\hbar)^{\frac{1}{2}}[G_l(R)F_l(r)-F_l(R)G_l(r)], \quad (4.3)$$

$$\mathcal{C}_l(r)=k^{-1}(M/2\hbar)^{\frac{1}{2}}\{[F_l'(R)+(l/R)F_l(R)]G_l(r) -[G_l'(R)+(l/R)G_l(R)]F_l(r)\}. \quad (4.4)$$

We now write the radial function $v_J(r)$ in (2.4) as a linear combination of $\mathcal{S}_J(r)$ and $\mathcal{C}_J(r)$

$$v_J(r)=A'\mathcal{S}_J(r)+B'\mathcal{C}_J(r) \quad (4.5)$$

and define the derivative matrix (which is a simple number here) by

$$B'=\mathcal{R}A'. \quad (4.6)$$

The coefficients A' and B' in (4.5) are of course related to the coefficients A and B in (2.5), and this relation can be determined by straightforward use of Eqs. (4.2), (4.3), and (4.4). We then get a relation between the derivative matrix and the scattering matrix $S=\exp(2i\delta_{J0})$ which can be stated as follows:

$$\tan\delta_{J0}=-\frac{F_J(R)-\mathcal{R}[F_J'(R)+(J/R)F_J(R)]}{G_J(R)-\mathcal{R}[G_J'(R)+(J/R)G_J(R)]}. \quad (4.7)$$

We now use the asymptotic forms of F and G for small values of kr

$$F_l(r)\cong(kr)^{l+1}/(2l+1)!!,\quad G_l(r)\cong(2l-1)!!/(kr)^l, \quad (\text{for } kr\ll l) \quad (4.8)$$

where $(2l+1)!!\equiv1\times3\times5\times\cdots\times(2l+1)$. In addition we use the fact that *the derivative matrix $\mathcal{R}$ approaches a constant value as the energy approaches zero.* This can be seen from the fact that the derivative matrix can be defined in terms of "interior" quantities only, i.e., in terms of a boundary value problem for the domain $0\leqslant r\leqslant R$.[9] Substitution of (4.8) into (4.7) then gives the following relation which is valid near zero energy:

$$k\cot\delta_{J0}\cong\frac{[(2J-1)!!]^2}{(kR)^{2J}[\mathcal{R}-R/(2J+1)]} \quad (\text{for } kR\ll J). \quad (4.9)$$

Thus the phaseshift δ_{J0} is, in general, proportional to k^{2J+1}, which is the usual result for scattering with orbital angular momentum $l=J$. An exception occurs when the asymptotic value of the derivative matrix $\mathcal{R}$ at zero energy is equal to $R/(2J+1)$. This corresponds to a scattering resonance at exactly zero energy. We shall ignore this possibility in the remainder of the discussion.

We now proceed to the two-channel states, $\pi=-1$, $l=J\pm1$. The wave function is given by (2.9), and we introduce the derivative matrix as before by a decomposition of the radial functions $u_J(r)$ and $w_J(r)$ in terms of $\mathcal{S}(r)$ and $\mathcal{C}(r)$

$$u_J(r)=A_1'\mathcal{S}_{J-1}(r)+B_1'\mathcal{C}_{J-1}(r),\quad w_J(r)=A_2'\mathcal{S}_{J+1}(r)+B_2'\mathcal{C}_{J+1}(r), \quad (4.10)$$

with the relations

$$B_1'=\mathcal{R}_{11}A_1'+\mathcal{R}_{12}A_2',\quad B_2'=R_{21}A_1'+\mathcal{R}_{22}A_2'. \quad (4.11)$$

Again the constants A', B' in (4.10) are related to the constants A, B in (2.10) through (4.2) and (4.3). The derivative matrix $\mathcal{R}_{ij}$ is real and symmetric and approaches a constant matrix as the energy approaches zero. Given the derivative matrix, the computation of the scattering matrix S is a straightforward procedure; the necessary relation is given in reference 8 but can be derived here directly without trouble. We then express the scattering matrix in the form (2.12), (2.13), (2.14), and approximate the radial functions by (4.8). We omit details. The results are[12]

$$\epsilon_J\cong\frac{(kR)^2}{2J+1}\frac{\mathcal{R}_{12}}{(2J-1)\mathcal{R}_{11}-R}, \quad (4.12)$$

$$k\cot\delta_{J\alpha}\cong\frac{[(2J-3)!!]^2}{(kR)^{2J-2}}\left[\mathcal{R}_{11}-\frac{R}{2J-1}\right]^{-1}, \quad (4.13)$$

$$k\cot\delta_{J\beta}\cong\frac{[(2J+1)!!]^2}{(kR)^{2J+2}}\times\left[\mathcal{R}_{22}-\frac{R}{2J+3}-\frac{(\mathcal{R}_{12})^2}{\mathcal{R}_{11}-R/(2J-1)}\right]^{-1}. \quad (4.14)$$

These expressions, valid near zero energy, show that the mixture parameter ϵ_J vanishes near zero energy; for low energies ϵ_J is proportional to k^2, i.e., to the energy. The mixture parameter is proportional also to the off-diagonal matrix element $\mathcal{R}_{12}$ of the derivative matrix, as should be expected. The α-wave phaseshift $\delta_{J\alpha}$ is proportional to k^{2J-1}, i.e., it behaves like a phaseshift for a pure $l=J-1$ state. Similarly the β-wave phaseshift $\delta_{J\beta}$ is proportional to k^{2J+3} just like a phaseshift for a pure $l=J+1$ state. This is to be expected, of course, because the fact that $\epsilon_J\to0$ as the energy approaches zero means that the eigenstates of the scattering matrix become pure $l=J-1$ and $l=J+1$ states, respectively.

Expressions (4.12), (4.13), and (4.14) suffer from the defect that the quantity R, the radius of the "interior" region, appears explicitly. Unlike resonance reactions, in neutron-proton scattering we can hardly expect to be able to give a good physical definition of R which is

[11] We use the Wronskian relation $F_l'(r)G_l(r)-F_l(r)G_l'(r)=k$.

[12] Equation (4.12) really contains $\frac{1}{2}\tan(2\epsilon_J)$ on the left-hand side. Hence ϵ_J approaches either 0 or $\frac{1}{2}\pi$ as the energy approaches zero. We then make the choice (2.21), i.e., $\epsilon_J\to0$ and replace $\frac{1}{2}\tan(2\epsilon_J)$ by ϵ_J.

free from ambiguities; the mathematical definition of R is quite indefinite. If $R=R_1$ satisfies the conditions of the derivative matrix theory, then any $R_2>R_1$ is also an acceptable value of R. Thus we need to define parameters which are invariant under the choice of R, i.e., parameters which are directly related to the scattering matrix. We define two scattering lengths, $a_{J\alpha}$ and $a_{J\beta}$, and a parameter q_J by the following relations, valid near zero energy:

$$\epsilon_J \cong q_J k^2, \tag{4.15}$$

$$\delta_{J\alpha} \cong -(ka_{J\alpha})^{2J-1}/[(2J-1)!!]^2, \tag{4.16}$$

$$\delta_{J\beta} \cong -(ka_{J\beta})^{2J+3}/[(2J+3)!!]^2. \tag{4.17}$$

In the special case of $J=1$, the ${}^3S_1+{}^3D_1$ state, $a_{J\alpha}=a_{1\alpha}$ is just the usual triplet scattering length, and we shall show in a subsequent paper that the quantity q_1 is to a first approximation proportional to the quadrupole moment of the deuteron.

We now wish to determine the asymptotic forms of the radial functions $u_J(r)$ and $w_J(r)$ for the α-wave and β-wave solutions in the limit of zero energy. The asymptotic forms in question are given by (2.17) and (2.18) for values of r such that $kr \gg J$. This condition cannot be fulfilled when k approaches zero. Hence we must first rewrite these asymptotic expressions in a form valid for all $r \geqslant R$. Using (4.2), we get

$$\begin{aligned} u_{J\alpha}(r) &= \cos(\epsilon_J)[\cos(\delta_{J\alpha})F_{J-1}(r)+\sin(\delta_{J\alpha})G_{J-1}(r)], \\ w_{J\alpha}(r) &= \sin(\epsilon_J)[\cos(\delta_{J\alpha})F_{J+1}(r)+\sin(\delta_{J\alpha})G_{J+1}(r)]. \end{aligned} \tag{4.18}$$

This equation reduces to (2.17) for $kr \gg J$ but is valid for all $r \geqslant R$. We now use the asymptotic forms (4.8) which are valid for very small k (more precisely, for $kr \ll J$) together with (4.15) and (4.16). We omit a common factor $k^J/(2J-1)!!$ in both $u_{J\alpha}$ and $w_{J\alpha}$ to get the result

$$\begin{aligned} u_{J\alpha}(r) &= r^J - (a_{J\alpha})^{2J-1}/[(2J-1)r^{J-1}], \\ w_{J\alpha}(r) &= -(2J+1)q_J(a_{J\alpha})^{2J-1}/r^{J+1}. \end{aligned} \qquad (k=0, r \geqslant R) \tag{4.19}$$

Thus *the α-wave solution at zero energy is recognizable by the fact that $w_{J\alpha}(r)$ does not contain a component proportional to r^{J+2}*. This condition leads to an eigenvalue problem for $a_{J\alpha}$ and q_J. Fortunately, this eigenvalue problem is of a very simple type and can be solved immediately if any two linearly independent pairs of solutions (u, w) are known at zero energy. Call them (u_1, w_1) and (u_2, w_2). For $r \geqslant R$, they assume the form (g_1, g_2, h_1, h_2, etc., are constants)

$$\begin{aligned} u_i(r) &= g_i r^J + h_i r^{-J+1}, \\ w_i(r) &= g_i' r^{J+2} + h_i' r^{-J-1}. \end{aligned} \qquad (i=1, 2) \tag{4.20}$$

The solution (u_α, w_α) is that particular linear superposition of (u_1, w_1) and (u_2, w_2) for which the coefficient of r^J in $u(r)$ is unity and the coefficient of r^{J+2} in $w(r)$ is zero. That is

$$\begin{aligned} u_\alpha(r) &= [g_2' u_1(r) - g_1' u_2(r)]/[g_1 g_2' - g_2 g_1'], \\ w_\alpha(r) &= [g_2' w_1(r) - g_1' w_2(r)]/[g_1 g_2' - g_2 g_1']. \end{aligned} \tag{4.21}$$

By comparing (4.20) and (4.21) with (4.19), we can express the quantities $a_{J\alpha}$ and q_J in terms of the g's and h's. This illustrates the advantage of starting the numerical solution of problems of this type at some energy $E \geqslant 0$ ($E=0$ is most convenient practically but any non-negative E could be treated by a similar method) rather than trying to start with numerical solutions for the energy of the bound state of the deuteron.

An entirely similar development for the β-wave leads to the following expressions valid at zero energy [we have omitted a common factor $k^{J+2}/(2J+3)!!$ in both $u_{J\beta}(r)$ and $w_{J\beta}(r)$]:

$$\begin{aligned} u_{J\beta}(r) &= -(2J+1)(2J+3)q_J r^J, \\ w_{J\beta}(r) &= r^{J+2} - (a_{J\beta})^{2J+1}/[(2J+3)r^{J+1}]. \end{aligned} \qquad (k=0, r \geqslant R) \tag{4.22}$$

Thus *the β-wave solution at zero energy is recognizable by the fact that $u_{J\beta}(r)$ does not contain a component proportional to r^{-J+1}*. Notice that the *decreasing* (with r) component is absent in $u_{J\beta}(r)$, whereas the *increasing* component was absent in $w_{J\alpha}(r)$. Given the numerical solutions (u_1, w_1) and (u_2, w_2), we can construct the solution (u_β, w_β) by a linear superposition analogous to (4.21), namely,

$$\begin{aligned} u_\beta(r) &= [h_2 u_1(r) - h_1 u_2(r)]/[h_2 g_1' - h_1 g_2'], \\ w_\beta(r) &= [h_2 w_1(r) - h_1 w_2(r)]/[h_2 g_1' - h_1 g_2']. \end{aligned} \tag{4.23}$$

By evaluating the quantity q_J first by the use of (4.21) and (4.19), then again by the use of (4.23) and (4.22), we obtain the following identity between the coefficients in the numerical solution (4.20):

$$(g_1 h_2 - g_2 h_1)/(g_1' h_2' - g_2' h_1') = -(2J+3)/(2J-1). \tag{4.24}$$

This (Wronskian) identity serves as a useful check on the accuracy of the numerical solutions (4.20).