Neutron-Proton Scattering with Spin-Orbit Coupling. II. Variational Formulation and Effective Range Theory

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The variational methods of Schwinger *et al.* are used to give variationally correct expressions for the three independent real parameters in the scattering matrix ($\delta_{J\alpha}$, $\delta_{J\beta}$, and ϵ_J) for the "mixed" states, such as ${}^3S_1+{}^3D_1$, of the neutron-proton system with spin-orbit coupling. The relation between these variational principles and the effective range theory is discussed briefly. The effective range expansions are then derived nonvariationally. The two leading terms are given for $k^5\cot\delta_{1\beta}$ and for $k^{-2}\tan\epsilon_1$. The three leading terms are given for $k\cot\delta_{1\alpha}$.

1. INTRODUCTION

IN a previous paper,[1] henceforth referred to as I, we have given the scattering matrix theory of neutron-proton scattering with spin-orbit coupling. The possible triplet states of the neutron-proton system fall into two categories: single-channel states such as ${}^3P_1$, in which the spin-orbit interaction cannot admix any other state because of conservation of total angular momentum and parity; and two-channel states, such as ${}^3S_1+{}^3D_1$, in which the spin-orbit interaction admixes the other state even if the ingoing wave contains only one of the two states. The analysis of the single-channel states is simple; in particular, the scattering matrix for such a state contains only one real parameter, a phase shift, and this phase shift can be found by the usual variational methods.[2] This paper is devoted to a discussion of the two-channel states, in particular the ${}^3S_1+{}^3D_1$ state which makes the dominant contribution to (triplet) low-energy neutron-proton scattering.

The general considerations in I have shown that the scattering matrix for a two-channel state depends on three real parameters, δ_α, δ_β, and ϵ. The first two are eigenphase shifts, the last is a "mixture parameter" which specifies which particular superpositions of ${}^3S_1$ and ${}^3D_1$ wave functions are eigenfunctions of the scattering matrix. Paper I contains an explicit formula for the scattering cross section in terms of these parameters. We were also able to determine the behavior of δ_α, δ_β, and ϵ close to zero energy. Beyond that, however, the general theory is powerless; more specific assumptions must be made about the nuclear forces in order to get useful answers.

Section 2 is devoted to the variational formulation of the problem of finding the parameters δ_α, δ_β, and ϵ. Variational principles for the two eigenphase shifts have been given by Schwinger,[3] and in that respect our work represents only a slight modification of his. The variational principle for ϵ given here has not been published previously, to our knowledge.[4]

In Sec. 3 we determine the coefficients of a series expansion of the parameters $k\cot\delta_\alpha$, $k\cot\delta_\beta$, and $\tan\epsilon$. We choose to expand around zero energy, hence our zero-order trial functions are the ones appropriate to zero energy. Their asymptotic dependence for large r has been given in I. We get an effective range expansion for δ_α (we recall that the α wave is by definition predominantly of ${}^3S_1$ type at low energies), and similar expansions for δ_β and for ϵ. The trial functions can be improved systematically, using the results of calculations with lower-order trial functions, thereby yielding a step-by-step procedure for finding higher terms in the various series.

2. VARIATIONAL PRINCIPLES FOR THE SCATTERING MATRIX PARAMETERS

In order to fix our ideas, let us restrict ourselves to the ${}^3S_1+{}^3D_1$ state, and to a spin-orbit coupling of the tensor force type, i.e., the potential is

$$V=V_c(r)+V_t(r)S_{12}, \tag{2.1}$$

where S_{12} is the conventional tensor operator,

$$S_{12}=3(\boldsymbol{\sigma}_1\cdot\mathbf{r})(\boldsymbol{\sigma}_2\cdot\mathbf{r})/r^2-(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2). \tag{2.2}$$

$V_c(r)$ and $V_t(r)$ in (2.1) define the radial dependence of the central and tensor potentials, respectively. We emphasize, though, that the contents of this section are *not* restricted to tensor forces; any Hermitian operator leading to spin-orbit coupling may be substituted for $V_t(r)S_{12}$. Furthermore, only trivial modifications are

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[1] J. M. Blatt and L. C. Biedenharn, Phys. Rev. **86**, 399 (1952). General references to the literature on neutron-proton scattering with spin-orbit coupling will be found in this paper.

[2] J. Schwinger, Phys. Rev. **78**, 135 (1950); **72**, 749 (1947); L. Hulthèn, Kgl. Fysiograf. Sällskap. Lund, Förh. **14**, No. 21, 257 (1944); Skand. Mat. Kongres 1946, Copenhagen, 201 (1947); B. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950); W. Kohn, Phys. Rev. **74**, 1763 (1948); S. Huang, Phys. Rev. **76**, 1878 (1949); Toraldo di Francia, Phys. Rev. **78**, 298 (1950); T. Kato, Phys. Rev. **80**, 475 (1950); H. Feshbach and S. I. Rubinow, Phys. Rev. **88**, 484 (1952).

[3] J. Schwinger, lectures, Harvard University, 1947 (unpublished).

[4] A brief report was made at the Cambridge Meeting of the American Physical Society [Phys. Rev. **90**, 365 (1953)].

required to make the variation principles derived here applicable to other two-channel states (e.g., the ${}^3P_2+{}^3F_2$ state).

Let $u(r)$ and $w(r)$ be the radial wave functions for the ${}^3S$ and ${}^3D$ states, respectively, defined in the conventional way.[5] Let M be the nucleon mass, and E be the energy in the center-of-gravity system. Then u and w satisfy the coupled differential equations

$$-(\hbar^2/M)(d^2u/dr^2)+V_c(r)u(r) +8^{\frac{1}{2}}V_t(r)w(r)=Eu(r), \quad (2.3a)$$

$$-(\hbar^2/M)(d^2w/dr^2)+(6\hbar^2/Mr^2)w(r) +[V_c(r)-2V_t(r)]w(r)+8^{\frac{1}{2}}V_t(r)u(r)=Ew(r). \quad (2.3b)$$

We introduce a simplified notation in order to write the formulas more compactly. We define the column vector ψ by

$$\psi=\begin{pmatrix}u(r)\\ w(r)\end{pmatrix}. \quad (2.4)$$

The scalar product between two vectors ψ_1 and ψ_2 is defined by

$$(\psi_1,\psi_2)=\int_0^\infty [u_1^*(r)u_2(r)+w_1^*(r)w_2(r)]dr. \quad (2.5)$$

We also introduce the wave number k,

$$k^2=ME/\hbar^2, \quad (2.6)$$

and the kinetic energy operator T,

$$T=\begin{pmatrix}-d^2/dr^2 & 0\\ 0 & -d^2/dr^2+6/r^2\end{pmatrix}. \quad (2.7)$$

Finally, we introduce an operator W which corresponds to $-(M/\hbar^2)$ times the potential energy (the negative sign is chosen so that W is positive for attractive potentials, and the factor $M/\hbar^2$ ensures that W has the dimension cm^{-2}),

$$W=-(M/\hbar^2)\begin{pmatrix}V_c(r) & 8^{\frac{1}{2}}V_t(r)\\ 8^{\frac{1}{2}}V_t(r) & V_c(r)-2V_t(r)\end{pmatrix}. \quad (2.8)$$

With this notation, Eqs. (2.3) can be rewritten as

$$(T-k^2)\psi=W\psi. \quad (2.9)$$

The operator $T-k^2$ can be inverted. We look for standing-wave solutions (i.e., solutions of type $\Psi_a^{(1)}$ in the notation of Lippmann and Schwinger[2]). The Green's function operator then is

$$\mathcal{G}=\text{principal value of}\left(\frac{1}{T-k^2}\right) =k^{-1}\begin{pmatrix}F_0(r_<)G_0(r_>) & 0\\ 0 & F_2(r_<)G_2(r_>)\end{pmatrix}, \quad (2.10)$$

where $F_l(r)$ and $G_l(r)$ are the regular and irregular solutions of the radial wave equation for a free particle of orbital angular momentum l and wave number k (as defined in I, for example), and $r_<$ is the smaller one of r, r'; $r_>$ is the larger one of r, r'. To avoid misunderstanding, we write out explicitly the effect of the operation $\mathcal{G}$ on the state vector ψ,

$$\mathcal{G}\psi=\begin{bmatrix}k^{-1}G_0(r)\int_0^r F_0(r')u(r')dr' \\ \qquad +k^{-1}F_0(r)\int_r^\infty G_0(r')u(r')dr' \\ k^{-1}G_2(r)\int_0^r F_2(r')w(r')dr' \\ \qquad +k^{-1}F_2(r)\int_r^\infty G_2(r')w(r')dr'\end{bmatrix}. \quad (2.11)$$

Let ϕ_a be any solution of the force-free radial wave equation regular at the origin; i.e.,

$$\phi_a=\begin{pmatrix}A_0k^{-1}F_0(r)\\ A_2k^{-1}F_2(r)\end{pmatrix}, \quad (T-k^2)\phi_a=0, \quad (2.12)$$

where A_0 and A_2 are arbitrary constants. Then the standing wave solution ψ_a of the complete problem associated with the free state ϕ_a satisfies the integral equation,

$$\psi_a=\phi_a+\mathcal{G}W\psi_a. \quad (2.13)$$

It will prove convenient to introduce an explicit notation for the free-state solutions ϕ associated with pure S waves and pure D waves. We define

$$\phi_0=\begin{pmatrix}k^{-1}F_0(r)\\ 0\end{pmatrix}, \quad \phi_2=\begin{pmatrix}0\\ k^{-1}F_2(r)\end{pmatrix}. \quad (2.14)$$

In this notation (2.12) becomes

$$\phi_a=A_0\phi_0+A_2\phi_2. \quad (2.12a)$$

We now determine the asymptotic form of ψ_a for large values of r. We use the asymptotic forms of $F(r)$ and $G(r)$ given in I as well as formulas (2.11) and (2.13) to get

$$\psi_a(r)=\begin{pmatrix}A_0k^{-1}\sin(kr)\\ A_2k^{-1}\sin(kr-\pi)\end{pmatrix} +\begin{pmatrix}(\phi_0, W\psi_a)\cos(kr)\\ (\phi_2, W\psi_a)\cos(kr-\pi)\end{pmatrix}, \quad (2.15)$$

where the scalar products $(\phi_0,W\psi_a)$ and $(\phi_2,W\psi_a)$ are defined by (2.5), (2.8), and (2.14).

We now look for eigenstates of the scattering matrix. The eigenstates can be characterized by the requirement

[5] J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley and Sons, Inc., New York, 1952), Chap. II, Sec. 5D.

that the asymptotic form for large r is

$$\psi_a(r)\sim\begin{pmatrix} B_0k^{-1}\sin(kr+\delta) \\ B_2k^{-1}\sin(kr-\pi+\delta)\end{pmatrix}, \tag{2.16}$$

where the eigenphase shift δ is the *same* for both components of ψ_a. The two eigenphase shifts δ_α and δ_β are associated with different ratios of B_2 to B_0. Comparing (2.15) and (2.16), we get

$$A_0=k\cot\delta(\phi_0,W\psi_a),\qquad A_2=k\cot\delta(\phi_2,W\psi_a), \tag{2.17}$$

and hence (2.13) can be rewritten, for the special case of eigenstates of the scattering matrix, as

$$\psi_a=k\cot\delta[(\phi_0,W\psi_a)\phi_0+(\phi_2,W\psi_a)\phi_2]+\mathcal{G}W\psi_a. \tag{2.18}$$

This equation has the tremendous advantage that it is homogeneous in ψ_a and may therefore be considered an eigenvalue problem with $k\cot\delta$ as the eigenvalue. We simplify the notation by introducing the projection operator $\mathcal{F}$,

$$\mathcal{F}\psi=(\phi_0,\psi)\phi_0+(\phi_2,\psi)\phi_2. \tag{2.19}$$

The matrix form of the operator $\mathcal{F}$ is

$$\mathcal{F}=\begin{pmatrix} k^{-2}F_0(r)F_0(r') & 0 \\ 0 & k^{-2}F_2(r)F_2(r')\end{pmatrix}. \tag{2.19a}$$

This operator satisfies the operator equation $(T-k^2)\mathcal{F}=0$, whereas the Green's function operator $\mathcal{G}$ (2.10) satisfies the operator equation $(T-k^2)\mathcal{G}=\mathbf{1}$ where $\mathbf{1}$ is the unit operator. We can now rewrite (2.18) as an eigenvalue equation for $k\cot\delta$,

$$(1-\mathcal{G}W)\psi=k\cot\delta\,\mathcal{F}W\psi. \tag{2.10}$$

This equation still suffers from one defect: the operators $1-\mathcal{G}W$ and $\mathcal{F}W$ are not Hermitian. We can remedy this defect by premultiplying both sides of (2.20) by the operator W. We therefore define the two Hermitian operators,

$$Z=W-W\mathcal{G}W\quad\text{and}\quad Y=W\mathcal{F}W, \tag{2.21}$$

to get

$$Z\psi=(k\cot\delta)Y\psi. \tag{2.20a}$$

From this it follows immediately that a variationally correct form for the eigenvalue $k\cot\delta$ is

$$k\cot\delta=\frac{(\psi,Z\psi)}{(\psi,Y\psi)}=\frac{(\psi,W\psi)-(\psi,W\mathcal{G}W\psi)}{(\psi,W\mathcal{F}W\psi)}. \tag{2.22}$$

Writing out the denominator explicitly, we find that (2.22) becomes

$$k\cot\delta=\frac{(\psi,W\psi)-(\psi,W\mathcal{G}W\psi)}{|(\phi_0,W\psi)|^2+|(\phi_2,W\psi)|^2}. \tag{2.22a}$$

This variational expression for the eigenphase shifts was first given by Schwinger[3] and the derivation presented here is identical with his except for notation.

In order to put the calculation of the scattering matrix on a completely variational basis, we still need a variation principle for the mixture parameter ϵ defined in I. Two *nonvariational* expressions for $\tan\epsilon$ follow from (2.17). Let δ be the α-wave eigenphase shift δ_α and ψ_a be the corresponding eigensolution ψ_α. Then according to Eq. (2.17) of I, the ratio of A_2/A_0 is equal to $\tan\epsilon$; i.e.,

$$\tan\epsilon=(\phi_2,W\psi_\alpha)/(\phi_0,W\psi_\alpha). \tag{2.23}$$

Now let δ be the other eigenphase shift δ_β and compare with Eq. (2.18) of I. The ratio of A_2/A_0 is now $-\cot\epsilon$, so that

$$\tan\epsilon=-(\phi_0,W\psi_\beta)/(\phi_2,W\psi_\beta). \tag{2.24}$$

Expressions (2.23) and (2.24) are homogeneous in ψ, so that both are independent of the normalization of ψ. We now search for a variational expression for $\tan\epsilon$ which preserves this property.

It is well known that two eigenfunctions of the usual eigenvalue problem $H\psi=\lambda\psi$, belonging to two different eigenvalues λ_1 and λ_2, are orthogonal to each other; i.e., $(\psi_1,\psi_2)=0$ and also $(\psi_1,H\psi_2)=\lambda_2(\psi_1,\psi_2)=0$. By an obvious extension of the usual proof to the modified eigenvalue problem $Z\psi=\lambda Y\psi$, we find that eigenfunctions ψ_α and ψ_β of (2.21) belonging to two different eigenvalues $k\cot\delta_\alpha$ and $k\cot\delta_\beta$, respectively, satisfy the relations

$$(\psi_\alpha,Y\psi_\beta)=0,\quad(\psi_\alpha,Z\psi_\beta)=0. \tag{2.25}$$

Let us now consider trial wave functions ψ_a and ψ_b which are close to the eigenfunctions ψ_α and ψ_β, respectively. That is, we assume

$$\psi_a=\psi_\alpha+\eta E_a,\quad\psi_b=\psi_\beta+\eta E_b, \tag{2.26}$$

where E_a and E_b are arbitrary vectors and η is a small parameter. If we compute $(\psi_a,Z\psi_b)$ we find, using (2.22) and (2.25),

$$\begin{aligned}(\psi_a,Z\psi_b)&=(\psi_b,Z\psi_a)\\&=\eta(\psi_\alpha,ZE_b)+\eta(\psi_\beta,ZE_a)+O(\eta^2)\\&=\eta k\cot\delta_\alpha(\psi_\alpha,YE_b)+\eta k\cot\delta_\beta(\psi_\beta,YE_a)+O(\eta^2),\end{aligned}$$

so that

$$\begin{aligned}(\psi_a,Z\psi_b)=k\cot\delta_\alpha&(\psi_\alpha,Y\psi_b)\\&+k\cot\delta_\beta(\psi_\beta,Y\psi_a)+O(\eta^2).\end{aligned} \tag{2.27}$$

We now use the definition of the operator Y and Eq. (2.23) in order to get an explicit form for $(\psi_\alpha,Y\psi_b)$; that is,

$$\begin{aligned}(\psi_\alpha,Y\psi_b)&=(\phi_0,W\psi_\alpha)(\phi_0,W\psi_b)+(\phi_2,W\psi_\alpha)(\phi_2,W\psi_b)\\&=(\phi_0,W\psi_\alpha)(\phi_2,W\psi_b)\left[\frac{(\phi_0,W\psi_b)}{(\phi_2,W\psi_b)}+\tan\epsilon\right].\end{aligned} \tag{2.28a}$$

Similarly, using (2.21) and (2.24), we get

$$\begin{aligned}&(\psi_\beta,Y\psi_a)\\&\quad=(\phi_0,W\psi_\beta)(\phi_0,W\psi_a)+(\phi_2,W\psi_\beta)(\phi_2,W\psi_a)\\&\quad=(\phi_0,W\psi_a)(\phi_2,W\psi_\beta)\left[-\tan\epsilon+\frac{(\phi_2,W\psi_a)}{(\phi_0,W\psi_a)}\right].\end{aligned} \tag{2.28b}$$

According to Eq. (2.23) the expression $(\phi_2,W\psi_a)/(\phi_0,W\psi_a)$ is an approximation to $\tan\epsilon$ homogeneous in the trial function ψ_a with an error of first order. We use the symbol t for this expression, i.e.,

$$t\equiv(\phi_2,W\psi_a)/(\phi_0,W\psi_a)=\tan\epsilon+O(\eta). \quad (2.29a)$$

We also introduce the symbol t' for

$$t'\equiv-(\phi_0,W\psi_b)/(\phi_2,W\psi_b)=\tan\epsilon+O(\eta). \quad (2.29b)$$

Thus to an error of second order, we may write for (2.28)

$$\begin{aligned}(\psi_\alpha,Y\psi_b)&=(\phi_0,W\psi_a)(\phi_2,W\psi_b)[-t'+\tan\epsilon]+O(\eta^2)\\(\psi_\beta,Y\psi_a)&=(\phi_0,W\psi_a)(\phi_2,W\psi_b)[t-\tan\epsilon]+O(\eta^2).\end{aligned} \quad (2.30)$$

Substituting this into Eq. (2.27) and solving for $\tan\epsilon$, we find an expression for $\tan\epsilon$ accurate to an error of second order in η, i.e., *a variational expression for $\tan\epsilon$ homogeneous in the trial wave functions*

$$\tan\epsilon=(k\cot\delta_\beta-k\cot\delta_\alpha)^{-1}\left[tk\cot\delta_\beta-t'k\cot\delta_\alpha-\frac{(\psi_a,Z\psi_b)}{(\phi_0,W\psi_a)(\phi_2,W\psi_b)}\right]. \quad (2.31)$$

In this expression ψ_a must be chosen close to ψ_α, ψ_b close to ψ_β, t and t' are defined by (2.29), and $k\cot\delta_\alpha$ and $k\cot\delta_\beta$ are defined by (2.22) with ψ_a and ψ_b, respectively. Since (2.22) is itself a variational form, the error introduced by its use is also of the order of the square of the errors in ψ_a and ψ_b.

Expressions (2.22) and (2.31) put the calculation of the scattering matrix on a completely variational basis, in terms of the minimum number of parameters.[6] Just as the Schwinger variational principle for the diagonal elements of the scattering matrix (the eigenphase shifts essentially) is not confined to a two-channel system, so the variational principle in (2.31) can be generalized for determining the $N(N-1)/2$ remaining independent parameters of the scattering matrix for an N-channel problem. This will be treated in a separate paper.

3. THE EFFECTIVE RANGE EXPANSION AND THE VARIATION PRINCIPLE

The general considerations of Sec. 4 of I have determined the behavior of the parameters δ_α, δ_β, and ϵ near zero energy. The same considerations moreover fixed the asymptotic behavior of the zero energy eigenfunctions.[7] Restricting our attention to $J=1$ ($^3S_1+^3D_1$ state), we find the following asymptotic forms for the zero energy wave functions:

$$\psi_{0\alpha}\sim\psi_{0\alpha}{}^{(\infty)}=\begin{pmatrix}u_{0\alpha}{}^{(\infty)}\\ w_{0\alpha}{}^{(\infty)}\end{pmatrix}=\begin{pmatrix}r-a_\alpha\\ -3qa_\alpha/r^2\end{pmatrix}, \quad (3.1a)$$

$$\psi_{0\beta}\sim\psi_{0\beta}{}^{(\infty)}=\begin{pmatrix}u_{0\beta}{}^{(\infty)}\\ w_{0\beta}{}^{(\infty)}\end{pmatrix}=\begin{pmatrix}-15qr\\ r^3-a_\beta{}^5/5r^2\end{pmatrix}. \quad (3.1b)$$

Utilizing the above as a boundary condition on the two independent zero energy solutions of the wave equation (2.9) leads to the desired zero energy eigenfunctions. With these as trial functions in the variational expressions (2.22) and (2.31) we can determine $k\cot\delta$ and $\tan\epsilon$ to an error of order k^4—the square of the error in the trial functions. Greater accuracy can be obtained with iterated solutions (see below) of the Schrödinger equation (2.9) accurate to an error of order k^4, and we can thus systematically improve our results.

The variational approach leads in a natural fashion to expressions of the form

$$k\cot\delta=\frac{a_0+a_1k^2+a_2k^4+\cdots}{b_0+b_1k^2+b_2k^4+\cdots}, \quad (3.2)$$

where a_0, a_1, b_0, b_1 can be found from the zero energy trial functions. Trial functions correct to order k^2 can be used to obtain expressions for a_2, a_3, b_2, b_3, and so on.

The effective range theory is obtained by rewriting (3.2) as a power series in k^2; i.e.,

$$k\cot\delta_\alpha=c_0+c_1k^2+c_2k^4+\cdots. \quad (3.2a)$$

It should be emphasized, perhaps, that (3.2a) is equivalent to (3.2) only within the radius of convergence (in the k^2 plane) of (3.2a). In general, this radius of convergence is very much smaller than the radii of convergence of the series in the numerator and denominator of (3.2). Thus, the reduction of (3.2) to (3.2a) gives rise to an appreciable reduction in the range of validity of the expression for $k\cot\delta_\alpha$.

The nonvariational derivations current in the literature[8] all lead to expressions of the form (3.2a). To the extent that the variational form (3.2) is reduced to (3.2a), the nonvariational formulations of the theory are equivalent to the variational formulation. However, this reduction need not be made in the variational formulation, whereas it is made automatically [i.e., (3.2) is never obtained] in the nonvariational formulation. Thus, the two formulations of the effective range theory are not equivalent, the variational one being rather more powerful.

For example, the series (3.2a) breaks down if the scattering length is zero, i.e., if the coefficient c_0 in (3.2a) becomes infinite. This can happen when there

[6] The calculation of Rohrlich and Eisenstein (see reference 1) was variational only to the extent that the eigenphase shifts were computed variationally. The mixture parameters found by them are correct only to a first-order error.

[7] Note the misprint in Eq. 4.22 of I. The superscript $2J+l$ should be $2J+3$.

[8] H. A. Bethe, Phys. Rev. **76**, 38 (1949); R. E. Peierls and M. A. Preston, Phys. Rev. **72**, 250 (1947); Hatcher, Arfken, and Breit, Phys. Rev. **75**, 1389 (1949); G. F. Chew and M. L. Goldberger, Phys. Rev. **75**, 250 (1947); see also G. Breit, Revs. Modern Phys. **23**, 238 (1951).

is a repulsive core and an attractive outside region. Expression (3.2), however, retains its usefulness even when the scattering length vanishes.

Since wells with hard repulsive cores are becoming increasingly fashionable, we may be forced to use expressions of type (3.2) rather than (3.2a), in spite of their more awkward form. In this paper, however, we shall reduce all results to the power series form (3.2a).

We write these expansions in the form

$$k\cot\delta_\alpha = -1/a_\alpha + r_\alpha k^2/2 - P r_\alpha^3 k^4 + \cdots, \tag{3.3}$$

$$k^5\cot\delta_\beta = (225/a_\beta^4)[-1/a_\beta + r_\beta k^2/2 + \cdots], \tag{3.4}$$

$$\tan\epsilon = qk^2 + q_1 k^4 + \cdots. \tag{3.5}$$

The lowest-order terms are known from Sec. 4 of I. The coefficient a_α is the usual triplet scattering length, while r_α is the triplet effective range. $\tan\epsilon$ is a measure of the mixing of the S and D states in the deuteron problem, and to a first approximation, q is proportional to the quadrupole moment of the deuteron. The coefficients a_β and r_β are the analogs of the a_α and r_α, respectively.

The proportionality of Q and q can be seen in the following way.[3] The quadrupole moment is given by the expression

$$Q = (\sqrt{2}/10)\int_0^\infty r^2(uw - 8^{-\frac{1}{2}}w^2)dr.$$

Because of the smallness of the percentage D state in the deuteron problem, it is a good approximation to neglect the w^2 term in this expression. Furthermore the factor r^2 insures the major contribution (~90 percent in actual cases) will come from large distances, outside the nuclear interaction, but still in the region where the centrifugal well dominates the behavior of the D state. Thus it is sufficient to use the asymptotic forms:

$$u = Ae^{-\gamma r}, \qquad w = A\times C\times e^{-\gamma r}(1+3/\gamma r+3/\gamma^2 r^2),$$

$$\gamma = (M|E_d|)^{\frac{1}{2}}/\hbar, \quad E_d = \text{deuteron binding energy}.$$

The normalization can be determined approximately from the effective range by neglecting the effects of the D state (this procedure compensates slightly for the neglect of w^2 in Q). Thus we take

$$A^{-2}\cong(1-\gamma r_\alpha)/2\gamma,$$

and then find that

$$C\cong(1-\gamma r_\alpha)^2\times\sqrt{2}\times Q\gamma^2.$$

But the constant C is the asymptotic ratio of D to S state, i.e., just the quantity denoted by $\tan\epsilon$ for positive energy states. Hence C is $\tan\epsilon$ for the negative energy given by $k=-i\gamma$, $k^2=-\gamma^2$.[9] We therefore get

$$(\tan\epsilon)_{k^2=-\gamma^2} = -q\gamma^2 + q_1\gamma^4 - \cdots \cong (1-\gamma r_\alpha)^2\sqrt{2}Q\gamma^2.$$

To the rather moderate (perhaps 10 percent) accuracy of the approximations made already, we can ignore the term in q_1 and obtain

$$q\cong -(1-\gamma r_\alpha)^2\times\sqrt{2}Q. \tag{3.5a}$$

[9] This extension of positive-energy relations to include ground-state properties is valid only for a restricted class of potentials V; see R. Jost and W. Kohn, Kgl. Danske Videnskab. Selskab Mat.-fys. Medd. **27**, No. 9, 1-19 (1953), and other papers referred to there. For central forces, a sufficient (but not necessary) condition upon V is that V must decrease, for large r, faster than the probability density $u^2(r)$ in the ground state; i.e.,

$$\lim_{r\to\infty}[e^{2\gamma r}V(r)] = 0.$$

Presumably a similar condition exists for tensor forces. Whatever it is, we shall presume it to be satisfied for our present purpose.

The coefficients r_α, r_β, and q_1 can be obtained explicitly in terms of the wave functions $\psi_{0\alpha}$ and $\psi_{0\beta}$ by means of (2.22) and (2.31). Some care in carrying out this reduction must be exercised in order not to misuse the variational principle.[10] Let us denote by $\mathcal{V}_\alpha(k^2;\psi_\alpha)$ the variational principle for $k\cot\delta_\alpha$ given by (2.22). Then, according to (3.3) we have

$$\begin{aligned}\tfrac{1}{2}r_\alpha &= \lim_{k^2\to 0}\left(\frac{d\mathcal{V}_\alpha}{dk^2}\right)\\ &= \lim_{k^2\to 0}\left(\frac{\partial\mathcal{V}_\alpha}{\partial k^2}+\frac{\delta\mathcal{V}_\alpha}{\delta\psi_\alpha}\cdot\frac{\partial\psi_\alpha}{\partial k^2}\right)\\ &= \lim_{k^2\to 0}\left(\frac{\partial\mathcal{V}_\alpha}{\partial k^2}\right).\end{aligned} \tag{3.6}$$

The last equation results from the fact that $\delta\mathcal{V}_\alpha/\delta\psi_\alpha = 0$ for all values of k^2 by the stationary property of (2.22). The limit $k^2\to 0$ was taken in order to determine a value for $\frac{1}{2}r_\alpha$. If we do *not* take this limit, however, Eq. (3.6) yields an *exact* expression for $d(k\cot\delta_\alpha)/dk^2$ in terms of ψ_α alone, which is, to be sure, no longer a variationally stationary result. The expression obtained is, in fact, the precise equivalent to the usual starting point for the nonvariational approach to the effective range expansion.[8]

We do not give this derivation in this paper, however, for the following reason: if the effective range expansion (3.2a) is all that is desired, it is simpler and more straightforward to derive it directly from the differential equations satisfied by the wave functions u and w, along the lines of Bethe.[8] We therefore do so in the following section, and we would like to thank Professor Bethe for permission to publish this material.[11] All results have been checked independently by rederiving them directly from the variational expressions given in Sec. 2; however, since this derivation is much more lengthy, we do not give it here.

4. THE EFFECTIVE RANGE EXPANSION: NONVARIATIONAL DERIVATION

We shall normalize the α-wave functions ψ_α so that in the limit of zero energy, the normalization agrees with (3.1a); that is, for large values of r ($r>b$), we have

$$u_\alpha^{(\infty)} = -a_\alpha\cos\epsilon(\cot\delta_\alpha F_0 + G_0), \tag{4.1a}$$

$$w_\alpha^{(\infty)} = -a_\alpha\sin\epsilon(\cot\delta_\alpha F_2 + G_2). \tag{4.1b}$$

[10] The point at issue here is that $k\cot\delta$ and $\tan\epsilon$, as defined by (2.22) and (2.31), are both *explicit* functions of k^2, through the operators $\mathcal{F}$ and $\mathcal{G}$, and *implicit* functions of k^2, through the wave functions ψ. The stationary property asserts only that the first-order variations in ψ cancel out. If one labels this variation by k^2, it is clear that confusion with the explicit dependence on k^2 might arise.

[11] Professor Bethe has obtained Eq. (4.11) and its consequences independently. We believe that Eqs. (4.19) and (4.26) represent new contributions.

Denote by $\psi_{\alpha 1}$ the α-wave function, normalized in this way, at energy E_1, and by $\psi_{\alpha 2}$ the α-wave function at energy E_2. They satisfy the differential equations

$$(T-k_1^2)\psi_{\alpha 1}=W\psi_{\alpha 1}, \tag{4.2a}$$

$$(T-k_2^2)\psi_{\alpha 2}=W\psi_{\alpha 2}, \tag{4.2b}$$

each set of two differential equations being written in abbreviated form. We multiply the u part of (4.2a) by $u_{\alpha 2}$, the w part by $w_{\alpha 2}$; we multiply the u part of (4.2b) by $u_{\alpha 1}$, the w part by $w_{\alpha 1}$. Subtraction then gives

$$\begin{aligned} &u_{\alpha 2}d^2u_{\alpha 1}/dr^2+w_{\alpha 2}d^2w_{\alpha 1}/dr^2-u_{\alpha 1}d^2u_{\alpha 2}/dr^2-w_{\alpha 1}d^2w_{\alpha 2}/dr^2 \\ &\quad=(d/dr)(u_{\alpha 2}u'_{\alpha 1}+w_{\alpha 2}w'_{\alpha 1}-u_{\alpha 1}u'_{\alpha 2}-w_{\alpha 1}w'_{\alpha 2}) \\ &\quad=(k_2^2-k_1^2)(u_{\alpha 1}u_{\alpha 2}+w_{\alpha 1}w_{\alpha 2}). \end{aligned} \tag{4.3}$$

A similar expression can be derived for the asymptotic forms (4.1). However, this is not very useful because $w_\alpha^{(\infty)}$ diverges at $r=0$. It is more useful to define a set of functions, related to (4.1), with the property that they are finite both as r approaches zero and as r approaches infinity. These functions will be distinguished by bars, and are defined as follows:

$$\begin{aligned} &\bar{u}_\alpha=u_\alpha^{(\infty)}, \\ &\bar{w}_\alpha=w_\alpha^{(\infty)}+3a_\alpha\sin\epsilon(kr)^{-2} \\ &\qquad=-a_\alpha\sin\epsilon[\cot\delta_\alpha F_2+G_2-3(kr)^{-2}]. \end{aligned} \tag{4.4}$$

The differential equations satisfied by $\bar{\psi}_\alpha$ are, again in the abbreviated notation,

$$(T-k^2)\bar{\psi}_\alpha=\begin{pmatrix}0\\-3a_\alpha\sin\epsilon\, r^{-2}\end{pmatrix}. \tag{4.5}$$

By a procedure analogous to the one followed to derive (4.3), we get

$$\begin{aligned} &(d/dr)[\bar{u}_{\alpha 1}\bar{u}'_{\alpha 2}+\bar{w}_{\alpha 1}\bar{w}'_{\alpha 2}-\bar{u}'_{\alpha 1}\bar{u}_{\alpha 2}-\bar{w}'_{\alpha 1}\bar{w}_{\alpha 2}] \\ &\qquad=(k_1^2-k_2^2)(\bar{u}_{\alpha 1}\bar{u}_{\alpha 2}+\bar{w}_{\alpha 1}\bar{w}_{\alpha 2}) \\ &\qquad\quad+3a_\alpha r^{-2}(\sin\epsilon_2\,\bar{w}_{\alpha 1}-\sin\epsilon_1\,\bar{w}_{\alpha 2}), \end{aligned} \tag{4.6}$$

where ϵ_1 stands for the value of the mixture parameter ϵ at energy E_1. In spite of appearances, the last term of (4.6) is finite as r approaches zero. This can be seen by using the series expansions of F_2 and G_2 in the second equation (4.4).

Following Bethe, we now combine (4.3) and (4.6) and integrate the resulting expression from zero to infinity. This yields

$$\begin{aligned} &[\bar{u}_{\alpha 1}\bar{u}'_{\alpha 2}+\bar{w}_{\alpha 1}\bar{w}'_{\alpha 2}-\bar{u}'_{\alpha 1}\bar{u}_{\alpha 2}-\bar{w}'_{\alpha 1}\bar{w}_{\alpha 2} \\ &\quad-u_{\alpha 1}u'_{\alpha 2}-w_{\alpha 1}w'_{\alpha 2}+u'_{\alpha 1}u_{\alpha 2}+w'_{\alpha 1}w_{\alpha 2}]_0^\infty \\ &\qquad=(k_1^2-k_2^2)[(\bar{\psi}_{\alpha 1},\bar{\psi}_{\alpha 2})-(\psi_{\alpha 1},\psi_{\alpha 2})] \\ &\qquad\quad+3a_\alpha\int_0^\infty dr\, r^{-2}(\sin\epsilon_2\,\bar{w}_{\alpha 1}-\sin\epsilon_1\,\bar{w}_{\alpha 2}). \end{aligned} \tag{4.7}$$

The terms on the left side of (4.7) all vanish at infinity, and only the barred functions contribute at $r=0$. By using (4.4) and (4.1), we get

left side of (4.7)

$$=a_\alpha^2\cos\epsilon_1\cos\epsilon_2(k_1\cot\delta_{\alpha 1}-k_2\cot\delta_{\alpha 2}). \tag{4.8}$$

It remains to evaluate the integral on the right side of (4.7). We use the identities

$$\begin{aligned} &\int_a^\infty dr\, r^{-2}F_2(r)=F_1(a)/ka^2, \\ &\int_a^\infty dr\, r^{-2}G_2(r)=G_1(a)/ka^2, \end{aligned} \tag{4.9}$$

in order to get

$$\begin{aligned} &3a_\alpha\int_0^\infty dr\, r^{-2}(\sin\epsilon_2\,\bar{w}_{\alpha 1}-\sin\epsilon_1\,\bar{w}_{\alpha 2}) \\ &\qquad=-a_\alpha^2\sin\epsilon_1\sin\epsilon_2(k_1\cot\delta_{\alpha 1}-k_2\cot\delta_{\alpha 2}). \end{aligned} \tag{4.10}$$

We combine (4.7), (4.8), and (4.10), divide both sides by $k_1^2-k_2^2$, and take the limit as k_1 approaches k_2. The final result is

$$\begin{aligned} \frac{d(k\cot\delta_\alpha)}{d(k^2)}=a_\alpha^{-2}\int_0^\infty &[(\bar{u}_\alpha)^2+(\bar{w}_\alpha)^2 \\ &-(u_\alpha)^2-(w_\alpha)^2]dr. \end{aligned} \tag{4.11}$$

This identity forms the basis for the nonvariational approach to the effective range theory. As remarked before, the same identity can be derived from the explicit derivative of the variational expression (2.22), after a fair amount of manipulation.

The determination of the effective range r_α from (4.11) is immediate. All we have to do is to take the limit as the energy approaches zero. The left side is then equal to $\frac{1}{2}r_\alpha$, as can be seen from (3.3). On the right side, the function $\bar{w}_\alpha$ vanishes in this limit, and $\bar{u}_\alpha=u_\alpha^{(\infty)}$ becomes equal to $u_{0\alpha}=r-a_\alpha$, according to (3.1a). We therefore get (denoting zero energy functions by the subscript 0)

$$r_\alpha=2(a_\alpha)^{-2}\int_0^\infty[(u_{0\alpha}^{(\infty)})^2-(u_{0\alpha})^2-(w_{0\alpha})^2]dr. \tag{4.12}$$

We now turn to the beta-wave solution, and the expansion (3.4). We again normalize the function ψ_β at arbitrary energy E so that it reduces to the standard zero energy solution (3.1b) at $E=0$. That means

$$u_\beta^{(\infty)}=(1/15)k^2a_\beta^5\sin\epsilon(\cot\delta_\beta F_0+G_0), \tag{4.13a}$$

$$w_\beta^{(\infty)}=-(1/15)k^2a_\beta^5\cos\epsilon(\cot\delta_\beta F_2+G_2), \tag{4.13b}$$

and we define the barred functions, which are regular at zero, by

$$\bar{u}_\beta=u_\beta^{(\infty)}, \tag{4.14a}$$

$$\bar{w}_\beta=w_\beta^{(\infty)}+a_\beta^5\cos\epsilon/(5r^2). \tag{4.14b}$$

By using the same methods as before, we obtain an equation entirely analogous to (4.11), namely,

$$k^4\frac{d(k\cot\delta_\beta)}{d(k^2)}=\frac{225}{a_\beta{}^{10}}\int_0^\infty[(\bar{u}_\beta)^2+(\bar{w}_\beta)^2-(u_\beta)^2-(w_\beta)^2]dr. \quad (4.15)$$

Equation (4.15) is valid for all positive energies. However, difficulties arise when we try to go to the limit as the energy approaches zero, in order to obtain the quantity r_β in (3.4).

Looking back at Eq. (3.4), the quantity

$$k^4\frac{d}{d(k^2)}(k\cot\delta_\beta)=\frac{225}{a_\beta{}^4}\left[\frac{2}{a_\beta k^2}-\frac{1}{2}r_\beta+\cdots\right],$$

and hence diverges as $k^2\to 0$. The quantity of interest to us is not this, but rather

$$\frac{d}{dk^2}(k^5\cot\delta_\beta)=k^4\frac{d}{d(k^2)}(k\cot\delta_\beta)+2k^3\cot\delta_\beta. \quad (4.16)$$

In order to obtain an equation involving this quantity, we examine the integral on the right side of (4.15) in the limit as $k^2\to 0$. In that limit, the integrand is

$$(\bar{u}_{0\beta})^2-(u_{0\beta})^2+(\bar{w}_{0\beta})^2-(w_{0\beta})^2=(-15qr)^2-(u_{0\beta})^2+r^6-(w_{0\beta})^2. \quad (4.17)$$

For large values of r, (4.17) becomes

$$0+r^6-(w_{0\beta}{}^{(\infty)})^2=r^6-[r^3-(a_\beta{}^5/5r^2)]^2,$$

and this contains a term proportional to r. In order to avoid this difficulty, we add and subtract in the integrand the term

$$2(\bar{w}_\beta-w_\beta{}^{(\infty)})\left(-\frac{a_\beta{}^5\cos\epsilon}{15}k^2\cot\delta_\beta F_2\right),$$

which is that part of the cross term causing the trouble. (The complete cross term is $2(\bar{w}_\beta-w_\beta{}^{(\infty)})\bar{w}_\beta$, but using this would introduce a divergence at the origin.) The integral of this added term can be evaluated from (4.9) and is

$$\int_0^\infty 2(\bar{w}_\beta-w_\beta{}^{(\infty)})\left(-\frac{k^2a_\beta{}^5\cos\epsilon}{15}\cot\delta_\beta F_2\right)dr=-2\frac{a_\beta{}^{10}}{225}\cos^2\epsilon\,k^3\cot\delta_\beta. \quad (4.18)$$

By combining (4.15), (4.16), and (4.18) we obtain the equation

$$\frac{d(k^5\cot\delta_\beta)}{d(k^2)}=2k^3\sin^2\epsilon\cot\delta_\beta+\frac{225}{a_\beta{}^{10}}\int_0^\infty[(\bar{u}_\beta)^2+(\bar{w}_\beta)^2+(2/15)(\bar{w}_\beta-w_\beta{}^{(\infty)})\times(a_\beta{}^5\cos\epsilon\,k^2\cot\delta_\beta F_2)-(u_\beta)^2-(w_\beta)^2]dr, \quad (4.19)$$

or, equivalently (using 4.14)

$$\frac{d(k^5\cot\delta_\beta)}{d(k^2)}=2k^3\sin^2\epsilon\cot\delta_\beta+\frac{225}{a_\beta{}^{10}}\int_0^\infty\left[(u_\beta{}^{(\infty)})^2+(w_\beta{}^{(\infty)})^2-(u_\beta)^2-(w_\beta)^2+\frac{a_\beta{}^{10}\cos^2\epsilon}{75}\left(\frac{3}{r^4}-\frac{2k^2G_2}{r^2}\right)\right]dr. \quad (4.19')$$

Unlike (4.15), this equation is also valid in the limit as the energy (k^2) approaches zero. In this limit the first term on the right of (4.19) vanishes, and we get the following expression for r_β in (3.4):

$$r_\beta=2a_\beta{}^{-6}\int_0^\infty[(u_{0\beta}{}^{(\infty)})^2+r^3(2w_{0\beta}{}^{(\infty)}-r^3)-(u_{0\beta})^2-(w_{0\beta})^2]dr. \quad (4.20)$$

It remains now to determine the coefficient q_1 in the expansion for $\tan\epsilon$, Eq. (3.5). Again the nonvariational derivation of such a limited result is more straightforward than the derivation starting from the variational expression (2.31). By methods entirely analogous to the ones used so far, we derive

$$k_2{}^2\frac{a_\alpha a_\beta{}^5}{15}\cos\epsilon_1\cos\epsilon_2(k_2\cot\delta_{\beta 2}-k_1\cot\delta_{\alpha 1})(\tan\epsilon_2-\tan\epsilon_1)=(k_1{}^2-k_2{}^2)\int_0^\infty(\bar{u}_{\alpha 1}\bar{u}_{\beta 2}+\bar{w}_{\alpha 1}\bar{w}_{\beta 2}-u_{\alpha 1}u_{\beta 2}-w_{\alpha 1}w_{\beta 2})dr. \quad (4.21)$$

Dividing (4.21) by $(k_1{}^2-k_2{}^2)$ and going to the limit $k_1\to k_2$ yields

$$k^{-2}\frac{d}{dk^2}(\tan\epsilon)=15[a_\alpha a_\beta{}^5\cos^2\epsilon(k^5\cot\delta_\alpha-k^5\cot\delta_\beta)]^{-1}\times\int_0^\infty(\bar{u}_\alpha\bar{u}_\beta+\bar{w}_\alpha\bar{w}_\beta-u_\alpha u_\beta-w_\alpha w_\beta)dr. \quad (4.22)$$

Again we encounter difficulties in going to the limit $k^2\to 0$. We really need

$$\frac{d}{d(k^2)}\left(\frac{\tan\epsilon}{k^2}\right)=k^{-2}\frac{d}{d(k^2)}(\tan\epsilon)-k^{-4}\tan\epsilon. \quad (4.23)$$

In the limit $k^2\to 0$, the integrand in (4.22) becomes, for large values of r,

$$\bar{w}_{0\alpha}\bar{w}_{0\beta}-w_{0\alpha}{}^{(\infty)}w_{0\beta}{}^{(\infty)}=0-\left(\frac{-3qa_\alpha}{r^2}\right)\left(r^3-\frac{a_\beta{}^5}{5r^2}\right). \quad (4.24)$$

This contains a term proportional to r, which can be considered as the limit of a cross term between F_2 and

$1/r^2$, just as in (4.17). If we add in, and subtract from, the integrand the terms,

$$(-a_\alpha \sin\epsilon \cot\delta_\alpha F_2)(w_\beta^{(\infty)}-\bar{w}_\beta) + \left(\frac{-a_\beta^5}{15}\cos\epsilon\, k^2 \cot\delta_\beta F_2\right)(w_\alpha^{(\infty)}-\bar{w}_\alpha),$$

then these troublesome cross terms are cancelled, and the integrals still remain well behaved at the origin. Using (4.9), the integral of these added terms is found to be

$$\int_0^\infty \Big[-a_\alpha \sin\epsilon \cot\delta_\alpha F_2(w_\beta^{(\infty)}-\bar{w}_\beta) - \frac{a_\beta^5}{15}\cos\epsilon\cdot k^2 \cot\delta_\beta F_2(w_\alpha^{(\infty)}-\bar{w}_\alpha)\Big]dr = \frac{a_\alpha a_\beta^5 \sin\epsilon\cos\epsilon}{15}(k\cot\delta_\alpha + k\cot\delta_\beta). \quad (4.25)$$

Combining (4.22), (4.23), and (4.25), we get

$$\frac{d}{d(k^2)}\left(\frac{\tan\epsilon}{k^2}\right) = 15[a_\alpha a_\beta^5 \cos^2\epsilon(k^5\cot\delta_\alpha - k^5\cot\delta_\beta)]^{-1} \times\Big\{-\frac{2}{15}a_\alpha a_\beta^5 \cos\epsilon \sin\epsilon\cdot k\cot\delta_\alpha + \int_0^\infty\Big[\bar{u}_\alpha\bar{u}_\beta+\bar{w}_\alpha\bar{w}_\beta-u_\alpha u_\beta-w_\alpha w_\beta - a_\alpha \sin\epsilon\cdot\cot\delta_\alpha\cdot F_2(w_\beta^{(\infty)}-\bar{w}_\beta) - \frac{a_\beta^5}{15}\cos\epsilon\cdot k^2\cot\delta_\beta\cdot F_2(w_\alpha^{(\infty)}-\bar{w}_\alpha)\Big]dr\Big\}. \quad (4.26)$$

We can now go to the limit $k^2\to 0$, to obtain the coefficient q_1 in Eq. (3.5):

$$q_1 = (15a_\alpha)^{-1}\int_0^\infty [u_{0\alpha}^{(\infty)}u_{0\beta}^{(\infty)} - 3qa_\alpha r - u_{0\alpha}u_{0\beta} - w_{0\alpha}w_{0\beta}]dr. \quad (4.27)$$

Equations (4.12), (4.20), and (4.27) give the first two terms in the power series (3.3) to (3.5). For purposes of estimating the error in this approximation higher terms are needed. We shall confine our attention to the "P" term in (3.3), the so-called "well shape parameter." According to the stationary property of (2.22), both P and the term of order k^6 can be determined exactly from trial functions accurate through order k^2. It is probably simplest to proceed directly from the differential equation (2.9). Define

$$\psi_\alpha \equiv \psi_{0\alpha} + k^2\psi_{2\alpha} + k^4\psi_{4\alpha} + \cdots. \quad (4.28)$$

Then from (2.9) we have

$$(T-W)\psi_{2\alpha} = \psi_{0\alpha}. \quad (4.29)$$

The boundary conditions on $\psi_{2\alpha}$ are first that it vanish at the origin, and second that it have the asymptotic behavior specified by (4.1). Expanding (4.1) in powers of k^2 and using (3.3), (3.5) we get

$$\psi_{2\alpha}\sim\begin{pmatrix} -r^3/6 + a_\alpha r^2/2 - r_\alpha a_\alpha r/2 \\ -a_\alpha q/2 - 3a_\alpha q_1 r^{-2}\end{pmatrix}. \quad (4.30)$$

Any solution to (4.29), vanishing properly at the origin, is equal to the desired solution $\psi_{2\alpha}$ plus undetermined amounts of the two independent solutions $\psi_{0\alpha}$ and $\psi_{0\beta}$ of the homogeneous equations. Let a solution of (4.29) be denoted by $\chi_{2\alpha}$. According to the differential equation (4.29), the asymptotic behavior for large r of the solution $\chi_{2\alpha}$ must be

$$\chi_{2\alpha}^{(\infty)} = \begin{pmatrix} A + Br + a_\alpha r^2/2 - r^3/6 \\ Cr^{-2} - a_\alpha q/2 + Dr^3\end{pmatrix}, \quad (4.31)$$

where A, B, C, and D are constants which can be determined by a numerical integration. By comparing (3.1), (4.30), and (4.31), we see that

$$\psi_{2\alpha} = \chi_{2\alpha} + (A/a_\alpha)\psi_{C\alpha} - D\psi_{0\beta}. \quad (4.32)$$

Furthermore, comparing the coefficients of r and r^{-2} on both sides of (4.32), we get the identities

$$-r_\alpha a_\alpha/2 = A/a_\alpha + 15qD + B, \quad (4.33)$$

$$-3a_\alpha q_1 = C - 3qA + a_\beta^5 D/5. \quad (4.34)$$

In other words, a given solution to (4.29), $\chi_{2\alpha}$ (numerically determined for example) automatically yields a value for both r_α and q_1—quantities known already from the zero energy solutions $\psi_{0\alpha}$ and $\psi_{0\beta}$. This feature of the calculations affords a useful check on the numerical accuracy of the work.

An explicit formula for P utilizing $\psi_{2\alpha}$ is readily determined from (4.11). Differentiating this equation, and taking the limit for $k^2\to 0$, one finds

$$P = -a_\alpha^{-2}r_\alpha^{-3}\int_0^\infty [u_{0\alpha}^{(\infty)}u_{2\alpha}^{(\infty)} - u_{0\alpha}u_{2\alpha} - w_{0\alpha}w_{2\alpha}]dr. \quad (4.35)$$

Similar coefficients can be determined for $k\cot\delta_\beta$ and $\tan\epsilon$, by using (4.19) and (4.26), respectively, but we shall not consider them in this paper.