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Variational method for off-shell three-body amplitudes*

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A variational scheme of the Schwinger type, used successfully in a previous paper for calculating two-body t matrix elements of all kinds (on shell, half shell, and off shell), is here applied to the three-body collision problem. Numerical results are given for the case of the Amado model of the N-d system. These results show excellent convergence properties, even for the case of fully off-shell amplitudes in the region where the analytic structure is most troublesome. It is shown theoretically that the three-body variational method, if restricted to the case of physical on-shell amplitudes, is formally equivalent to the several variational principles given by Pieper, Schlessinger, and Wright, though the methods may differ considerably in practice. The formal equivalence is used to show that Pieper's recent perturbative calculations of N-d polarization, in which the zero-order problem was approached variationally, have a property not previously noted, namely that even the perturbed solution is fully variational. More generally, a useful degree of cooperation is shown to occur between the present variational method and the perturbation method, making it quite easy to preserve the variational property in a perturbative calculation.

[NUCLEAR REACTIONS ^{2}H(n,n), E=0–40 MeV; calculated off-shell amplitudes. Variational method, separable-potential model.]

I. INTRODUCTION

In this paper we extend to the three-body collision problem a particular variational scheme, used previously[1] with considerable success in the two-body problem, for calculating two-body t matrix elements of all kinds: on shell, half shell, and off shell.

The essence of the variational scheme, in the two-body context of paper I, is this: Let $t(z)$ be the two-body t matrix at the (complex) energy z, so that t satisfies the Lippmann-Schwinger equation

$$t = V + Vg_0t \tag{1.1}$$

$$= V + tg_0V, \tag{1.2}$$

where

$$g_0(z) = (z - h_0)^{-1}, \tag{1.3}$$

and where h_0 is the two-particle c.m. kinetic energy, and V the potential. Then it follows from the Lippmann-Schwinger equation that the expression

$$[t] = V + Vg_0t^R + t^Lg_0V - t^L(g_0 - g_0Vg_0)t^R \tag{1.4}$$

is a variational expression for t, if t^L and t^R are independent (*non*variational) approximations to t. [In other words, it is asserted that the right-hand side of (1.4) differs from t by an expression[1] that is second order in the errors in t^L and t^R.]

The procedure followed in I for using this variational principle was to express t^R and t^L (with one momentum held fixed in each case, at the initial or final momentum, respectively, of the t matrix element actually being calculated) as a linear combination of a convenient set of basis functions. Then the coefficients in the expansion were selected by the variational principle, and the final variational result was obtained by substituting again into (1.4).

An algebraically equivalent procedure is to write t^R and t^L in the form

$$t^R = \sum_{i=1}^{N} |f_i\rangle\langle\chi_i| \ , \tag{1.5}$$

$$t^L = \sum_{i=1}^{N} |\bar{\chi}_i\rangle\langle\bar{f}_i| , \tag{1.6}$$

where $|f_i\rangle$ and $\langle\bar{f}_i|$ are the chosen basis functions, and $\langle\chi_i|$ and $|\bar{\chi}_i\rangle$ are unknown functions, to be selected by the variational principle. Then it is easily seen that if the right-hand side of (1.4) is to be stationary under arbitrary variations of the $|\bar{\chi}_i\rangle$, we must choose

$$\langle\chi_i| = \sum_{i'} \Delta_{ii'}\langle\bar{f}_{i'}|g_0V , \tag{1.7}$$

and hence

$$t^{R} = \sum_{i,i'} |f_i\rangle \Delta_{ii'} \langle \bar{f}_{i'}| g_0 V , \tag{1.8}$$

where

$$(\Delta^{-1})_{i'i} = \langle \bar{f}_{i'}| (g_0 - g_0 V g_0) |f_i\rangle . \tag{1.9}$$

In a similar way we also obtain

$$t^{L} = \sum_{i,i'} V g_0 |f_i\rangle \Delta_{ii'} \langle \bar{f}_{i'}| . \tag{1.10}$$

Then by substituting (1.8) and (1.10) in (1.4) we finally obtain the variational result

$$[t] = V + \sum_{i,i'} V g_0 |f_i\rangle \Delta_{ii'} \langle \bar{f}_{i'}| g_0 V . \tag{1.11}$$

This is the expression used for the two-body variational calculations in I.

A feature of this scheme is that one obtains incidentally the two-nonvariational results (1.8) and (1.10), in addition to the variational result (1.11). We note in passing that the variational and nonvariational results are related by

$$[t] = V + V g_0 t^{R} \tag{1.12}$$

$$= V + t^{L} g_0 V , \tag{1.13}$$

if t^{R} and t^{L} are given by (1.8) and (1.10). Other formal properties of the variational scheme are discussed in I.

This variational scheme is of the type usually associated with Schwinger, but it is nevertheless not what is commonly called the Schwinger variational method. The precise relation between these and other variational schemes is discussed in I. It should be mentioned, however, that the method of I seems to be numerically much more successful than the usual Schwinger method.[2] This can perhaps be understood by noting that in the ordinary Schwinger method the trial functions are scattering wave functions,[3] which are rather singular functions in momentum space, whereas the trial functions in the method of I are t matrices, which are very smooth functions in momentum space for short-range potentials, and which are therefore easily approximated with a small number of basis functions. Another important difference is that the method of I has a much wider field of application because it can be used to calculate off-shell, half-shell, and on-shell amplitudes, whereas the conventional Schwinger method is designed only for the physical on-shell amplitudes.

The variational scheme described above is by no means restricted to the two-body problem, since it depends only on the algebraic structure of the Lippmann-Schwinger equation (1.1). In particular, it can be applied almost immediately to the three-body problem with separable two-body potentials, since in this case the scattering equations reduce, as is well known, to coupled integral equations of the Lippmann-Schwinger form (with, of course, a different potential and propagator) in a single vector variable.

This three-body separable-potential case differs from the two-body case considered in I in only one important respect, namely that the three-body amplitudes have various singularities[4] for real values of the off-shell momentum, instead of being smooth functions of momentum. In Sec. V we present numerical results for a particular three-body separable-potential case, namely the Amado model[5,6] of the nucleon-deuteron system. We show that the singularities cause no difficulties that are not easily overcome, and that excellent convergence behavior can occur in all cases, even in the case of fully off-shell amplitudes in unfavorable regions of momentum space. A preliminary account of these calculations has been given in Ref. 7.

In the present paper we also discuss in a more general way the three-body application of the variational method, beginning from the general three-body equations of Alt, Grassberger, and Sandhas[8] (AGS). This approach is developed in Sec. II. For the particular case of the on-shell physical amplitudes, the three-body variational principle so obtained turns out to be formally equivalent to the set of variational principles given by Pieper, Schlessinger, and Wright[9] (PSW).

The relation between the present variational method and the PSW methods is discussed in Sec. IV. In spite of the formal equivalence, there are substantial differences between the methods, both in principle and in practice. One difference is in the quantities that are used as trial functions in the two cases: In the PSW method they are wave functions, whereas in the present method they are three-body amplitudes, which in general are fully off shell. This leads to a more important difference: In the present work we are able to use the variational principle for calculating three-body amplitudes of all kinds, including the fully off-shell amplitudes, whereas the PSW methods are only designed for calculating the on-shell physical amplitudes. The fully off-shell amplitudes are needed for studying any system containing more than three particles, and therefore the ability to handle fully off-shell amplitudes is considered a major advantage of the present approach.

In three-body calculations with complicated two-body interactions, one might reasonably want to treat some parts of the two-body force by a per-

turbation method,[10-12] and use the variational method only for the zero-order problem. In this situation, one would naturally prefer the variational property to hold for the perturbed amplitudes, not just for the amplitudes from the zero-order problem. It is therefore interesting to consider the interaction between the variational and perturbation methods. This is done in Sec. III. This question proves to be easy to discuss in the present formulation, and it turns out that there is no difficulty at all in obtaining a final perturbed result that is fully variational.

One previous calculation that combines variational and perturbation methods has been made by Pieper[13,14] in a rather successful calculation of polarization observables in elastic N-d scattering. In Pieper's calculations the zero-order problem (corresponding to separable S-wave N-N interactions) was solved[13] using the PSW variational principle. However, the variational principle was only used for selecting the coefficients in a linear expansion of the zero-order wave function, and no claim was made that the final perturbed result was variational; indeed, a variational final result would hardly be expected, since the zero-order wave functions that are fed into the perturbation calculation are certainly *not* variational.

In spite of this, we are able to show with the present formulation that Pieper's final results[14] *are* in fact fully variational, even though not designed to be so. This property follows from the connection with the PSW method established in Sec. IV, and is discussed at the end of that section. It undoubtedly contributes in an important way to the numerical stability of Pieper's results. The fact that the variational property is clear within the present formulation demonstrates, in our view, the conceptual advantages of the present approach.

To summarize the structure of this paper, in Sec. II the variational method is developed for the three-body problem. Then in Sec. III the joint use of the perturbation and variational methods is explored. The relation between the present formulation and the PSW variational principles is discussed in Sec. IV, and so too are Pieper's perturbation calculations.[13,14] Finally, in Sec. V we discuss in detail the application of the variational method to the particular case of the Amado model, and present numerical results for three-body amplitudes in a variety of situations.

II. THREE-BODY VARIATIONAL PRINCIPLE

As basic three-body scattering equations, we use the AGS equations[8]

$$U_{\beta\alpha} = (1-\delta_{\beta\alpha})G_0^{-1} + \sum_{\gamma\neq\beta} T_\gamma G_0 U_{\gamma\alpha}\,, \tag{2.1}$$

where α, β, γ take the values 1, 2, 3, and where

$$G_0 = (s - H_0)^{-1}\,, \tag{2.2}$$

$$T_\gamma = V_\gamma + V_\gamma G_0 T_\gamma\,. \tag{2.3}$$

Here V_γ is the interaction between the pair γ, with $\gamma = 1$ denoting the pair (2, 3), etc. The operator H_0 is the three-particle kinetic energy in the c.m. system, and s is the complex energy parameter, which for the physical three-body problem is given by $s = E + i\epsilon$, E being the c.m. energy.

Formally, all that needs to be done before we can use the variational principle (1.4) is to write the equations in the form of the Lippmann-Schwinger equation (1.1). That is easily achieved through the definition of 3×3 matrices Y, $\overline{G}_0$, and T, with matrix elements

$$Y_{\beta\alpha} = G_0 U_{\beta\alpha} G_0\,, \tag{2.4}$$

$$(\overline{G}_0)_{\beta\alpha} = (1-\delta_{\beta\alpha})G_0\,, \tag{2.5}$$

$$T_{\beta\alpha} = \delta_{\beta\alpha} T_\beta\,. \tag{2.6}$$

Then Eq. (2.1) is equivalent to the matrix equation of Lippmann-Schwinger form

$$Y = \overline{G}_0 + \overline{G}_0 T Y. \tag{2.7}$$

Similarly, the transposed equation

$$Y = \overline{G}_0 + Y T \overline{G}_0 \tag{2.8}$$

is equivalent to the transposed form[8] of Eq. (2.1).

Then by immediate analogy with Eq. (1.4) we can write down a variational expression for Y,

$$[Y] = \overline{G}_0 + \overline{G}_0 T Y^R + Y^L T \overline{G}_0 - Y^L (T - T\overline{G}_0 T) Y^R\,, \tag{2.9}$$

where Y^L and Y^R are independent approximations to Y. This is the fundamental statement of our three-body variational principle.

In practice one is usually interested in particular transition amplitudes rather than complete operators $Y_{\beta\alpha}$ or $U_{\beta\alpha}$. For example, if one is concerned with a rearrangement from the bound state ϕ_α of the pair α to the bound state ϕ'_β of the pair β, then the appropriate transition amplitude is the matrix element

$$\langle \phi'_\beta \vec{k}'_\beta | U_{\beta\alpha} | \phi_\alpha \vec{k}_\alpha \rangle = \langle \phi'_\beta \vec{k}'_\beta | G_0^{-1} Y_{\beta\alpha} G_0^{-1} | \phi_\alpha \vec{k}_\alpha \rangle\,, \tag{2.10}$$

where $\vec{k}_\alpha$ and $\vec{k}'_\beta$ are the c.m. momenta of the free particle in the initial and final state, respectively. An explicit variational expression for this matrix element follows immediately from Eq. (2.9), on sandwiching the β, α component of that equation between $\langle \phi'_\beta \vec{k}'_\beta | G_0^{-1}$ and $G_0^{-1} | \phi_\alpha \vec{k}_\alpha \rangle$. This discussion also includes the case of elastic or inelastic collisions in the direct channel α by setting β equal to α.

So far we have excluded breakup processes from

our considerations. The easiest way to obtain a suitable variational principle for breakup is to make use of the relation

$$U_{0\alpha} = \sum_{\beta} T_\beta G_0 U_{\beta\alpha}$$

$$= \sum_{\beta} T_\beta Y_{\beta\alpha} G_0^{-1}, \tag{2.11}$$

which expresses the transition operator for breakup in terms of the operators for elastic and rearrangement processes.[15] An explicit variational expression for breakup can be obtained, if desired, by substituting the variational expression for $Y_{\beta\alpha}$ [Eq. (2.9)] into the right-hand side of (2.11).

For the remainder of this section we restrict ourselves to finite-rank two-body potentials, deferring any discussion of the local potential case until Sec. IV, when we can make use of the discussion in PSW. For the finite-rank case the variational method turns out to be particularly straightforward, and the analogy with the two-body case particularly direct.

In the finite-rank case the operator T_γ of Eq. (2.3) can be written in the form

$$T_\gamma = \sum_{n'n} |\gamma n'\rangle \tau_{\gamma n' n} \langle \bar{\gamma n}|, \tag{2.12}$$

where the "form factors" $|\gamma n\rangle$ and $\langle \bar{\gamma n}|$ are vectors in the momentum space of the pair γ, and where $\tau_{\gamma n' n}$ is a diagonal operator in the momentum space of the third particle relative to the pair. The latter has matrix elements of the form

$$\langle \vec{p}'_\gamma | \tau_{\gamma n' n} | \vec{p}_\gamma \rangle = \delta(\vec{p}'_\gamma - \vec{p}_\gamma) F_{\gamma n' n}(s - p_\gamma^2/2M_\gamma), \tag{2.13}$$

where M_γ is given in terms of the individual masses $m_\alpha, m_\beta, m_\gamma$ by

$$M_\gamma^{-1} = m_\gamma^{-1} + (m_\alpha + m_\beta)^{-1}, \tag{2.14}$$

α, β, γ being a permutation of 1, 2, 3.

If we now define

$$X_{\beta n', \alpha n} = \langle \bar{\beta n'} | Y_{\beta\alpha} | \alpha n \rangle$$

$$= \langle \bar{\beta n'} | G_0 U_{\beta\alpha} G_0 | \alpha n \rangle, \tag{2.15}$$

$$Z_{\beta n', \alpha n} = (1 - \delta_{\beta\alpha}) \langle \bar{\beta n'} | G_0 | \alpha n \rangle, \tag{2.16}$$

then from the AGS equations (2.1) we obtain immediately the coupled equations

$$X_{\beta n', \alpha n} = Z_{\beta n', \alpha n} + \sum_{\gamma m' m} Z_{\beta n', \gamma m'} \tau_{\gamma m' m} X_{\gamma m, \alpha n}, \tag{2.17}$$

which we write in the obvious way as a matrix equation of Lippmann-Schwinger form,

$$X = Z + Z\tau X. \tag{2.18}$$

The corresponding variational principle

$$[X] = Z + Z\tau X^R + X^L \tau Z - X^L(\tau - \tau Z \tau) X^R \tag{2.19}$$

follows immediately from the two-body analogy, or directly from Eq. (2.9).

We suppose for simplicity that there is at most one bound state ϕ_α between each pair α, and that the form factors $|\alpha n'\rangle$ and $\langle \bar{\alpha n}|$ in the expansion (2.12) for T_α are chosen so that the $n' = n = 0$ term corresponds to the bound state, with

$$|\alpha 0\rangle = V_\alpha |\phi_\alpha\rangle, \quad \langle \bar{\alpha 0}| = \langle \phi_\alpha | V_\alpha. \tag{2.20}$$

It then follows from the Schrödinger equation that

$$|\alpha 0\rangle\, |\vec{k}_\alpha\rangle = G_0(E + i\epsilon)^{-1} |\phi_\alpha \vec{k}_\alpha\rangle \tag{2.21}$$

in the limit $\epsilon \to 0^+$, if $\vec{k}_\alpha$ is the on-shell c.m. momentum of particle α. It follows in turn from Eq. (2.10) that the physical amplitudes for elastic scattering and rearrangement collisions are just the on-shell matrix elements $\langle \vec{k}'_\beta | X_{\beta 0, \alpha 0}(E + i\epsilon) | \vec{k}_\alpha \rangle$.

The amplitudes for breakup on the other hand are given according to Eqs. (2.11), (2.12), (2.13), and (2.15) by

$$\langle \vec{p}_1 \vec{p}_2 \vec{p}_3 | U_{0\alpha} | \phi_\alpha \vec{k}_\alpha \rangle = \sum_{\beta n' n} \langle \vec{q}_\beta | \beta n' \rangle F_{\beta n' n}(E + i\epsilon - p_\beta^2/2M_\beta)$$

$$\times \langle \vec{p}_\beta | X_{\beta n, \alpha 0} | \vec{k}_\alpha \rangle, \tag{2.22}$$

where

$$\vec{q}_1 = (m_2 + m_3)^{-1}(m_3 \vec{p}_2 - m_2 \vec{p}_3), \text{ etc.}$$

Thus the breakup amplitudes are expressed in terms of half-shell matrix elements of the matrix X. Obviously, the variational expression (2.19) is just as useful for these half-shell matrix elements as it is for the on-shell elastic amplitudes, so that there is no need to write out the variational expression for breakup explicitly.

More generally, the three-body amplitudes that are required in the N-body problem involve the fully off-shell matrix elements $\langle \vec{p}'_\beta | X_{\beta n', \alpha n} | \vec{p}_\alpha \rangle$, and these too are included in the variational expression (2.19). In Sec. V we shall use (2.19) to calculate matrix elements of all types (on shell, half shell, and off shell, for a simple separable-potential model of N-d scattering.

III. COMBINED PERTURBATION AND VARIATIONAL METHODS

We briefly describe here the three-body perturbation method of Sloan[10,12] and Kowalski and Pieper,[11] and then point out that there is a useful

degree of cooperation between the variational and perturbation methods if the zero-order problem in the perturbation method is solved variationally. Since the perturbation method is expected to be most useful in the context of finite-rank potentials we restrict ourselves to this case, and use the formalism of Ref. 12. However, the argument is easily generalized to arbitrary potentials.[11]

The separable terms in the expansion (2.12) are supposed to be split into two sets, one to be treated exactly, the other perturbatively. Correspondingly, the matrix τ of Eq. (2.12) is split into two parts $\tau^{(0)}$ and τ',

$$\tau = \tau^{(0)} + \tau', \tag{3.1}$$

where $\tau^{(0)}$ connects only the terms to be treated exactly and τ' is supposed to be a small perturbation. Then the zero-order problem corresponding to Eq. (2.18) is

$$X^{(0)} = Z + Z\tau^{(0)}X^{(0)}, \tag{3.2}$$

or

$$X^{(0)} = Z + X^{(0)}\tau^{(0)}Z,$$

and the exact solution of (2.18) satisfies the equation

$$X = X^{(0)} + X^{(0)}\tau' X. \tag{3.3}$$

The perturbation method uses the leading terms in the iterative solution of this equation,

$$X = X^{(0)} + X^{(0)}\tau' X^{(0)} + \cdots. \tag{3.4}$$

Let us now consider how the first-order perturbation term in Eq. (3.4) is to be calculated in practice for the particular case of elastic scattering. Obviously the perturbation term is essentially a sum of integrals with the integrands involving certain half-shell matrix elements of $X^{(0)}$. If the zero-order equations have been solved conventionally, i.e., by an explicit numerical solution of the coupled integral equations (3.2), then some half-shell matrix elements $\langle \vec{p}_\beta | X^{(0)}{}_{\beta n,\alpha 0} | \vec{k}_\alpha \rangle$ are already available, but these are not the ones that are needed in the perturbation calculation since the values of n that occur are those corresponding to $\tau^{(0)}$ rather than τ'. However, the desired matrix elements of $X^{(0)}$ can be obtained easily by using the integral equation for $X^{(0)}$ once more. Thus in practice one uses not (3.4) but rather

$$X = X^{(0)} + (Z + X^{(0)}\tau^{(0)}Z)\tau'(Z + Z\tau^{(0)}X^{(0)}) + \cdots, \tag{3.5}$$

since this involves only the matrix elements of $X^{(0)}$ that are already available from the solution of the zero-order problem.

Suppose now that the zero-order problem has instead been solved by the variational method of the previous sections. If each $X^{(0)}$ on the right-hand side of Eq. (3.5) is obtained variationally, then it is obvious that the entire right-hand side will be variational in the same sense—i.e., the errors will be second order in the errors in the trial operators $X^{(0)L}$ and $X^{(0)R}$. What is perhaps not immediately obvious is that the right-hand side of (3.5) can be variational even if *non*variational approximations to $X^{(0)}$ are used in calculating the perturbation.

Specifically, let us approximate the first term of Eq. (3.5) by $[X^{(0)}]$ (the variational solution of the zero-order problem) but approximate the $X^{(0)}$ on the left and right, respectively, of the second term by the nonvariational quantities $X^{(0)L}$ and $X^{(0)R}$. Since the nonvariational and variational results from the zero-order problem are related by analogs of Eqs. (1.12) and (1.13), specifically

$$[X^{(0)}] = Z + Z\tau^{(0)}X^{(0)R} \tag{3.6}$$

$$= Z + X^{(0)L}\tau^{(0)}Z, \tag{3.7}$$

the right-hand side of (3.5) can then be written

$$[X^{(0)}] + [X^{(0)}]\tau'[X^{(0)}] + \cdots, \tag{3.8}$$

which is just the variational form of (3.4). [Equations (3.6) and (3.7), which in effect assert that an iteration of the solution makes the nonvariational results variational, are only valid if the variational principle is used in the way described in Sec. I. In particular, the trial functions must be a linear combination of some basis set with *all* coefficients being selected by the variational principle itself.]

In summary, if the variational method is used for the zero-order problem a variational final result can be achieved *either* by using the variational values of $X^{(0)}$ directly in Eq. (3.4), *or* by using the nonvariational approximations in Eq. (3.5), in the manner described in the preceding paragraph. In the following section the latter result is used to establish that Pieper's perturbative calculations,[14] which use the PSW variational method for the zero-order problem, are in fact finally variational, even though the zero-order wave functions that are used in the perturbation calculation are not—a fortunate circumstance that seems not to have been previously recognized.

IV. PSW VARIATIONAL METHODS

In this section we show how the variational principles of Sec. II are related to the separate variational principles for elastic scattering, rearrangement, and breakup, given by PSW.[9] We shall show that the variational principles are essentially equivalent, provided that we restrict ourselves to the on-shell versions of the varia-

tional principles in Sec. II. However, the variational principles of Sec. II have a wider range of application, since they apply equally to off-shell three-body amplitudes. And even in the on-shell case the way in which the variational principles are used in the two cases is not always the same.

According to Sec. II, the variational principle for the physical elastic scattering or rearrangement amplitudes is obtained in the present work by substituting the variational expression (2.9) for $Y_{\beta\alpha}$ into Eq. (2.10). To establish the connection with PSW for the elastic scattering case, we set $\beta = \alpha = 1$, and relate our trial functions to those of PSW by the equations

$$Y^{R}_{\gamma 1} G_0^{-1} | \phi_1 \vec{k}_1 \rangle = | \psi^{\delta} + \psi^{\epsilon} \rangle , \tag{4.1}$$

$$\langle \phi_1 \vec{k}_1' | G_0^{-1} Y^{L}_{1\gamma} = \langle \tilde{\psi}^{\delta} + \tilde{\psi}^{\epsilon} | , \tag{4.2}$$

where the quantities on the right are the Faddeev[16] components of the wave function, defined explicitly by PSW, and where γ, δ, ϵ is a permutation of 1, 2, 3. Then on writing out the summations in Eq. (2.9) explicitly we immediately obtain the PSW variational principle [their Eq. (4.6)]. Similarly, for the rearrangement case we set $\beta = 2$, $\alpha = 1$, and use

$$\langle \phi_2 \vec{k}'_2 | G_0^{-1} Y^{L}_{2\gamma} = \langle \tilde{\chi}^{\delta} + \tilde{\chi}^{\epsilon} | , \tag{4.3}$$

together with Eq. (4.1), and once again obtain the corresponding PSW variational principle [their Eq. (4.11)].

The present variational principle for the physical breakup amplitude is obtained, according to the discussion in Sec. II, by substituting the variational expression for $Y_{\beta\alpha}$ [Eq. (2.9)] into the on-shell version of Eq. (2.11), i.e., into

$$\langle \phi_0 | U_{0\alpha} | \phi_\alpha \vec{k}_\alpha \rangle = \sum_{\beta} \langle \phi_0 | T_\beta Y_{\beta\alpha} G_0^{-1} | \phi_\alpha \vec{k}_\alpha \rangle , \tag{4.4}$$

where ϕ_0 is an on-shell eigenstate of the free-particle Hamiltonian. The resulting variational principle becomes equivalent to the PSW variational principle for breakup [their Eq. (4.16)] if our trial functions (with $\alpha = 1$) are related to theirs by Eq. (4.1), together with

$$\sum_{\beta} \langle \phi_0 | T_\beta Y^{L}_{\beta\gamma} = \langle \tilde{\xi}^{\delta} + \tilde{\xi}^{\epsilon} | , \tag{4.5}$$

where the PSW trial functions on the right are the Faddeev components of the wave function appropriate to the final state. [The relations

$$\langle \phi_0 | T_3 = \langle \tilde{\Phi}^{12} | V_3 ,$$

and

$$\langle \phi_0 | T_3 G_0 = \langle \tilde{\Phi}^{12} | - \langle \phi_0 | ,$$

which follow from the definition of $\langle \tilde{\Phi}^{12} |$ in PSW, are needed for completing the proof of the equivalence for the breakup case.]

It is implied in the arguments above that each of the relations (4.1), (4.2), (4.3), and (4.5) becomes an identity if the trial functions are replaced by the corresponding exact functions. This is easily verified, by showing that the left-hand side of each equation satisfies the same equation as the right-hand side. The latter follow immediately from the Faddeev equations[16] for the various wave function components, which are given by PSW.

The particular case of local two-body potentials received considerable attention in PSW, and numerical results were given there for elastic scattering in a simple local-potential model. It is a straightforward task to translate the observations and methods of PSW for the local-potential case into the present notation with the aid of Eqs. (4.1) and (4.2), but we shall not do so here as we have nothing to add to their discussion of the on-shell local-potential case.

In the case of finite-rank potentials, however, there is an interesting practical difference between the PSW method and that developed in Sec. II, even in the on-shell situation. The difference is that whereas in the present work we use as trial functions the matrices X^{L} and X^{R} [see Eq. (2.19)], the corresponding PSW trial functions [which can be identified through Eqs. (4.1), (4.2), and (4.3), and the appropriate definitions in PSW] are essentially $X^{L}\tau$ and τX^{R}. The latter are more singular because of the bound-state pole in τ, but since the basis functions used in PSW explicitly include this pole singularity the existence of this singularity is not necessarily a reason for preferring the present method. However, a more serious problem with the PSW choice of trial functions occurs with the N-N interaction, in that the antibound state in the ^1S channel corresponds to a pole in τ which is located on the second sheet of the two-body energy plane, but lying very close to the branch point. This nearby singularity turned out to have a very large effect on the numerical calculations of Ref. 13, and it was found necessary there to include an approximate representation of this singularity in the basis set. No such problem arises in the present method.

But the main difference between the present variational method and that of PSW lies in the different scope of the methods: The present approach applies to amplitudes of all kinds, including half-shell and off-shell amplitudes, whereas the PSW approach is designed only for the physical on-shell amplitudes.

The advantage of the wider point of view is clear-

ly seen in the following discussion, in which we reconsider the method used by Pieper[14] in his recent interesting calculations of N-d polarization observables. Those calculations used the perturbation method described in Sec. III, with the zero-order problem including only S-wave N-N interactions, and the noncentral parts of the N-N interaction being included as perturbations. The point of present interest is that the zero-order problem was solved[13] by the PSW variational method, i.e., by taking the zero-order wave function to be a linear combination of a suitable set of basic functions and then using the variational principle for the elastic amplitude to select the coefficients in the expansion. These zero-order wave functions, which are themselves *not* variational, were then used[14] to calculate the perturbation term with the aid of a formula equivalent to Eq. (3.5). But, from the discussion in this section and the last we recognize that this procedure is equivalent to using the nonvariational approximations $X^{(0)L}$ and $X^{(0)R}$ on the left and right of the perturbation term of Eq. (3.5). And, as we have already observed in Sec. III, that in fact makes the final result fully variational.

We therefore conclude that Pieper's N-d polarization calculations[14] are in fact fully variational (i.e., the errors are second order in the errors in the zero-order trial wave functions), even though they are apparently not designed to be so. It is very likely that this hidden variational property plays an important part in the numerical stability of the calculations, since the finally calculated polarization observables apparently converge quite well[14] as the number of basis functions is increased, whereas the convergence of the zero-order wave functions themselves is not particularly impressive.[13]

V. NUMERICAL RESULTS FOR THE AMADO MODEL

In this final section we apply the variational method to a simple model of the three-nucleon system, with the two-nucleon interaction taken to be of spin-dependent, S-wave, separable form. This model, first studied by Aaron, Amado, and Yam[5] and Aaron and Amado,[6] has been used rather successfully in a number of calculations of N-d scattering and breakup.[5,6,17-19]

The operator T_γ [Eq. (2.12)] for this particular case has momentum-space matrix elements of the form

$$\langle \vec{p}_\gamma \vec{q}_\gamma | T_\gamma(s) | \vec{p}'_\gamma \vec{q}'_\gamma \rangle = \sum_{n=0,1} P_{\gamma n} g_n(\vec{q}_\gamma) \delta(\vec{p}_\gamma - \vec{p}'_\gamma) \times F_n(s - \tfrac{3}{4} p_\gamma^2) g_n(\vec{q}'_\gamma), \tag{5.1}$$

where $\vec{q}_\gamma$ is the relative momentum of the pair γ, and where the units are such that m (nucleon mass) $= \hbar = 1$. The $P_{\gamma n}$ are spin-isospin projectors onto the spin triplet ($n=0$) and spin singlet ($n=1$) states of the pair γ. Also, the form factors have the familiar Yamaguchi form

$$g_n(\vec{q}) = N_n(q^2 + \beta_n^2)^{-1}, \tag{5.2}$$

and F_n is given by

$$F_n^{-1}(z) = -\frac{1}{\lambda_n} + 4\pi \int_0^\infty q^2 dq \, \frac{g_n^2(q)}{q^2 - z}. \tag{5.3}$$

The numerical parameters for the two states (^3S and ^1S) are those of Ref. 5.

The integral equations (2.17) for this case, after antisymmetrization and partial-wave analysis, take the explicit form

$$\langle p | X_{nn'}^{(L,S)} | p' \rangle = \langle p | Z_{nn'}^{(L,S)} | p' \rangle - \frac{3}{2\pi} \sum_{n''} \int_0^\infty p''^2 dp'' \langle p | Z_{nn''}^{(L,S)} | p'' \rangle F_{n''}(s - \tfrac{3}{4} p''^2) \langle p'' | X_{n''n'}^{(L,S)} | p' \rangle, \tag{5.4}$$

where

$$\langle p | Z_{nn'}^{(L,S)} | p' \rangle = \frac{8\pi^2}{3} J_{nn'}^S \int_{-1}^{1} \frac{P_L(x) g_n(\tfrac{1}{2}\vec{p} + \vec{p}') g_{n'}(\tfrac{1}{2}\vec{p}' + \vec{p})}{p^2 + p'^2 + pp'x - s} dx, \tag{5.5}$$

with $x = \hat{p} \cdot \hat{p}'$. Here $J_{nn'}^S$ is the spin-isospin overlap factor; in the isospin $\frac{1}{2}$ case (which is the appropriate isospin for the N-d system) its values are $J_{00}^{3/2} = -\frac{1}{2}$, $J_{01}^{3/2} = J_{10}^{3/2} = J_{11}^{3/2} = 0$; $J_{00}^{1/2} = J_{11}^{1/2} = \frac{1}{4}$, $J_{01}^{1/2} = J_{10}^{1/2} = -\frac{3}{4}$. The total orbital angular momentum L and spin S are conserved separately, because the assumed nucleon-nucleon force is central. In the doublet ($S = \frac{1}{2}$) case there are two coupled equations, in the quartet ($S = \frac{3}{2}$) case only one.

The physical elastic scattering amplitude, according to Sec. II, is the on-shell matrix element $\langle k | X_{00}^{(L,S)} | k \rangle$, where $k^2 = \frac{4}{3}(E + \alpha^2)$, and where E is the total c.m. energy and α^2 the binding energy of the deuteron. [The normalization of the elastic amplitude implied by (5.4) is $\exp(i\delta_{L,S}) \sin\delta_{L,S}/k$, where $\delta_{L,S}$ is the phase shift.] On the other hand, we recall that the breakup amplitude [see Eq. (2.22)] is constructed from the half-shell amplitudes $\langle p | X_{n0}^{(L,S)} | k \rangle$, with $p \leq (\frac{4}{3}E)^{1/2} < k$, and that the

fully off-shell amplitudes $\langle p|X^{(L,S)}_{nn'}|p'\rangle$ are needed in the N-body problem. In the numerical calculations we therefore consider amplitudes of each of these kinds.

To apply the variational method we write the integral equations (5.4) as

$$X = Z + Z\tau X \tag{5.6}$$

so that we can make immediate use of the variational principle (2.19). By analogy with the two-body case in Sec. I, we expand the trial operators X^R and X^L in the form

$$X^R = \sum_{i=1}^{N} |f_i\rangle\langle\chi_i|, \tag{5.7}$$

$$X^L = \sum_{i=1}^{N} |\bar{\chi}_i\rangle\langle\bar{f}_i|, \tag{5.8}$$

where the $|f_i\rangle$ and $\langle\bar{f}_i|$ are basis functions chosen for convenience, and the $\langle\chi_i|$ and $|\bar{\chi}_i\rangle$ are unknown functions, to be selected by the variational principle, i.e., by requiring that the right-hand side of Eq. (2.19) be stationary under arbitrary variations of the $\langle\chi_i|$ and $|\bar{\chi}_i\rangle$.

For the quartet case these considerations are identical with the two-body case discussed in Sec. I, but for the doublet case a slight extension is needed to cope with the fact that Eq. (5.6) actually represents a pair of coupled equations labeled by the two values of n. The appropriate extension is that the basis functions $|f_i\rangle$ and $\langle\bar{f}_i|$ become diagonal 2×2 matrices with diagonal elements, say, $|f_{i,n}\rangle$ and $\langle\bar{f}_{i,n}|$, while the $|\chi_i\rangle$ and $\langle\bar{\chi}_i|$ become general 2×2 matrices to be selected by the variational principle. With this understanding we can retain the notation of (5.7) and (5.8) for both cases.

Then an argument analogous to that in Sec. I gives

$$X^R = \sum_{i,i'} |f_i\rangle\Delta_{i,i'}\langle\bar{f}_{i'}|\tau Z, \tag{5.9}$$

$$X^L = \sum_{i,i'} Z\tau|f_i\rangle\Delta_{i,i'}\langle\bar{f}_{i'}|, \tag{5.10}$$

and then from Eq. (2.19)

$$[X] = Z + \sum_{i,i'} Z\tau|f_i\rangle\Delta_{i,i'}\langle\bar{f}_{i'}|\tau Z, \tag{5.11}$$

where Δ is defined though its inverse in the direct product space

$$(\Delta^{-1})_{i'n',in} = \langle\bar{f}_{i',n'}|(\tau - \tau Z\tau)_{n'n}|f_{i,n}\rangle. \tag{5.12}$$

(Thus Δ is found in the doublet case by inverting a $2N\times 2N$ matrix, and in the quartet case an $N\times N$ matrix.)

Written out explicitly the variational result (5.11) becomes

$$[\langle p|X_{nn'}|p'\rangle] = \langle p|Z_{nn'}|p'\rangle + \sum_{imi'm'} \langle p|Z_{nm}\tau_m|f_{i,m}\rangle\Delta_{im,i'm'}\langle\bar{f}_{i',m'}|\tau_{m'}Z_{m'n'}|p'\rangle, \tag{5.13}$$

where

$$\langle p|Z_{nm}\tau_m|f_{i,m}\rangle = -\frac{3}{2\pi}\int_0^\infty p'^2dp'\langle p|Z_{nm}|p'\rangle F_m(E+i\epsilon-\tfrac{3}{4}p'^2)\langle p'|f_{i,m}\rangle, \tag{5.14}$$

with the labels L and S suppressed. The explicit form of (5.12) is

$$(\Delta^{-1})_{i'n',in} = -\frac{3}{2\pi}\delta_{n'n}\int_0^\infty p^2dp\langle\bar{f}_{i',n}|p\rangle F_n(E+i\epsilon-\tfrac{3}{4}p^2)\langle p|f_{i,n}\rangle$$

$$-\left(-\frac{3}{2\pi}\right)^2\int_0^\infty p'^2dp'\int_0^\infty p^2dp\langle\bar{f}_{i',n'}|p'\rangle F_{n'}(E+i\epsilon-\tfrac{3}{4}p'^2)\langle p'|Z_{n'n}|p\rangle F_n(E+i\epsilon-\tfrac{3}{4}p^2)\langle p|f_{i,n}\rangle. \tag{5.15}$$

Before specifying the basis functions, it is useful to consider the analytic structure of the amplitudes one wishes to approximate. Firstly, the half-shell amplitude $\langle p|X_{n0}|k\rangle$ is known[4] to be an analytic function of p on the whole real axis, except for a square-root branch point at

$$p_0 \equiv [\tfrac{4}{3}(E+i\epsilon)]^{1/2}, \tag{5.16}$$

coming from the integral term in Eq. (5.4). (Note that the Born term $\langle p|Z_{n0}|k\rangle$ does not contain this singularity.) The discontinuity acrosss the cut is proportional to $(p_0-p)^{1/2}$ for p near the branch point.[20] In the numerical results to be presented later, this branch point turns out to be an extremely important feature.

The fully off-shell amplitude $\langle p|X_{nn'}|p'\rangle$ also has

this square-root branch point[4] at $p=p_0$, and in addition has logarithmic singularities[6] at

$$p=\pm\tfrac{1}{2}p'\pm(E-\tfrac{3}{4}p'^2)^{1/2} \tag{5.17}$$

if $p'<p_0$, corresponding to the fact that all three particles can be asymptotically free if $p'<p_0$. The logarithmic singularities come from the Born term in Eq. (5.4), and are therefore automatically included correctly in the variational expression (5.11). However, to the extent that these logarithmic singularities are not correctly included in the trial functions X^R and X^L, as of course they cannot be in the finite-rank expressions (5.7) and (5.8), the variational method has to work harder than, for example, in the two-body case. The square-root branch point, on the other hand, is easily included in X^R and X^L by including it in the basis functions, and this was done in the present calculations.

The specific basis functions used in the numerical calculations were

$$\langle p|f_{i,n}\rangle=\langle\bar{f}_{i,n}|p\rangle=\frac{p^L}{(p^2+a^2)^2(p^2+i^2b^2)},$$

$$i=1,\ 3,\ 5,\ \ldots,\ N-1$$

$$=(p_0^2-p^2)^{1/2}\langle p|f_{i-1,n}\rangle,$$

$$i=2,\ 4,\ \ldots,\ N,$$

with no distinction being made between the trial functions for the triplet ($n=0$) and singlet ($n=1$) cases. These trial functions ensured the correct p dependence of $\langle p|X^R_{nn'}|p'\rangle$ and $\langle p'|X^L_{n'n}|p\rangle$ at small values of p, but not necessarily at large values of p; the precise behavior at large values of p turned out to be of little practical importance. The numerical values of the parameters were chosen, after a small amount of experimentation, to be $a^2=0.5\ \text{fm}^{-2}$, $b=0.5\ \text{fm}^{-1}$.

In the direct solution of the integral equation (5.4), the main difficulties[6] come from the singularities in the kernel and inhomogeneous term. Related singularities occur in the integrals in (5.14) and (5.15), with the important difference, however, that here we are dealing with integrals with explicit integrands, rather than with integral equations. The integrals were evaluated by the contour deformation method,[6,18] i.e., by rotating the integration contours by a suitable angle ϕ into the lower half plane. In the case of (5.14), a more complicated contour is necessary[6] when $p<p_0$; we used the contour of Ref. 6 in the way described in Ref. 18.

Now the numerical results: We have established that the convergence is generally slowest for $L=0$ (a result to be expected, because of the increasing importance of the Born term in higher partial waves), and therefore we show explicit numerical results only for this case. Furthermore, because the convergence in the ^2S and ^4S cases turned out to be similar, we discuss explicitly only the more difficult one, the ^2S case. The amplitude in this case is a 2×2 matrix, but we show only the $n=n'=0$ component in each case, in order to restrict the number of figures. The amplitude plotted in the first four figures is the dimensionless quantity

$$\langle p|T_{00}|p'\rangle=k\langle p|X_{00}|p'\rangle.$$

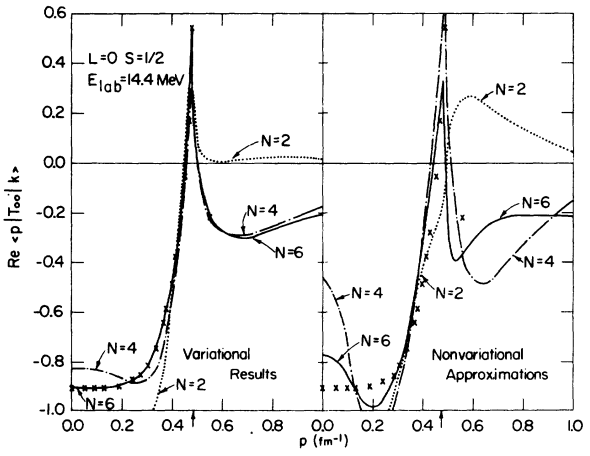

FIG. 1. Variational and nonvariational results for the real part of the ^2S half-shell amplitude $\langle p|T_{00}|k\rangle$, at a nucleon lab energy of 14.4 MeV. The label N is the number of basis functions in Eqs. (5.7) and (5.8). The crosses are results obtained (Ref. 18) by explicit solution of the integral equations, using contour rotation techniques. The arrows indicate the square-root branch point at $(\frac{4}{3}E)^{1/2}$.

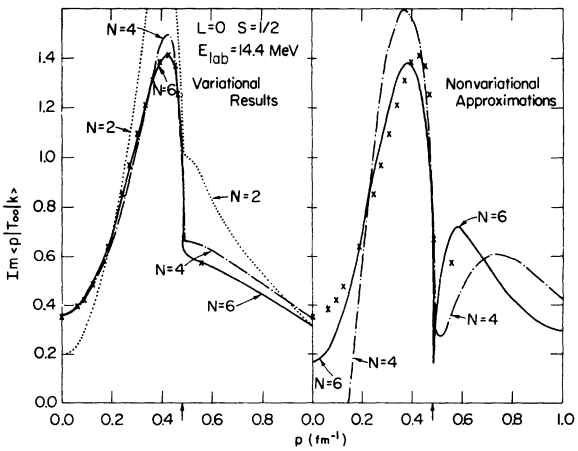

FIG. 2. Variational and nonvariational results for the imaginary part of the ^2S half-shell amplitude $\langle p|T_{00}|k\rangle$, at 14.4 MeV. The meaning of the curves and symbols is the same as in Fig. 1.

Figures 1 and 2 show the real and imaginary parts of the half-shell ^2S amplitude, at a nucleon lab energy of 14.4 MeV. The left-hand side of each figure shows the variational amplitude [Eq. (5.11)], and the right-hand side the nonvariational result from the trial function X^R [Eq. (5.9)]. The crosses are unpublished amplitudes from the breakup calculations of Ref. 18, obtained by direct solution of the integral equation (5.4), using the contour rotation techinque. The momentum p in these physical breakup amplitudes ranges from $p=0$ up to the branch point at $p=p_0$, which is indicated by an arrow on the p axis. The single cross to the right of the branch point is the elastic amplitude at the on-shell momentum $p=k$.

It is clear from Figs. 1 and 2 that the convergence of the variational results is excellent, since accurate results are apparently obtained with only six trial functions. And in fact a further increase in N from 6 to 10 changes the variational results by only about 1%.

In contrast, the nonvariational results shown in Figs. 1 and 2 are converging rather slowly (though the behavior near the branch point is greatly helped, it may be noted, by the square-root contribution in the basis functions). Even more extreme is the *other* nonvariational approximation [Eq. (5.10)], which is not shown in the figures: This turns out to show almost no sign of convergence for $p<p_0$. This is easily understood from the fact that the trial function $\langle p|X^L|p'\rangle$ for this case must try to represent the logarithmic singularities at $p'=\pm\frac{1}{2}p\pm(E-\frac{3}{4}p^2)^{1/2}$, as discussed above. Nevertheless, it makes the observed excellent convergence of the variational result all the more impressive, since one is finally obtaining an accurate variational result with quite inaccurate nonvariational input.

An interesting feature of the variational method is that the variational amplitude automatically contains the important singularities (including the logarithmic singularities and the square-root branch point), even when the trial X^L and X^R that go into it do not. This might be the reason why the convergence of the variational method can remain good, even when the nonvariational approximations are seriously affected by singularities. From now on we ignore the nonvariational approximations, and concentrate on the variational results.

The next case we consider (Fig. 3) is a fully off-shell calculation at the same energy (14.4 MeV), with $p'=0.3$ fm^{-1}, and with p ranging from 0 to 1.0 fm^{-1}. (For comparison, the on-shell momentum at this energy is $k=0.556$ fm^{-1}, and the square-root branch point occurs at $p_0=0.487$ fm^{-1}.) Since this value of p' is less than p_0, the situation faced by the variational method is particularly challenging in this case, especially when $p<p_0$ also, since then *both* of the trial functions X^L and X^R have to try to represent logarithmic singularities. Yet we see from the results in Fig. 3 that even in this case the convergence of the variational method is excellent. The quantities actually plotted in Fig. 3 are the real and imaginary parts (on the left and right, respectively) of the amplitudes *minus* the corresponding Born terms, so that we do not have to draw the logarithmic singularities from the Born term. The convergence behavior for the variational amplitude itself (which of course includes the logarithmic singularity exactly) is similar to that shown in Fig. 3.

To demonstrate that the method also works at other energies, we show first in Fig. 4 the half-

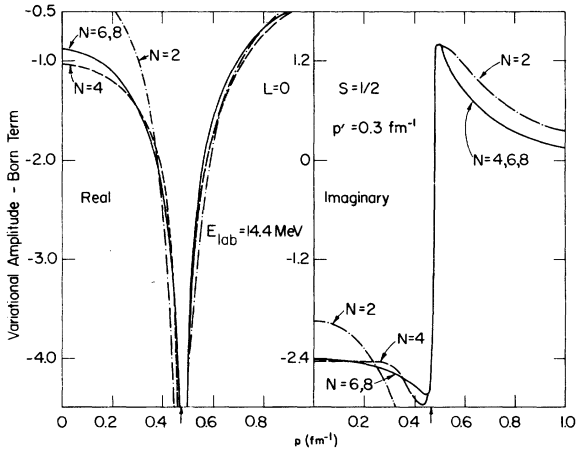

FIG. 3. Variational results for the real and imaginary parts of the off-shell ^2S amplitude *minus* the corresponding Born term, at 14.4 MeV, and with $p'=0.3$ fm^{-1}.

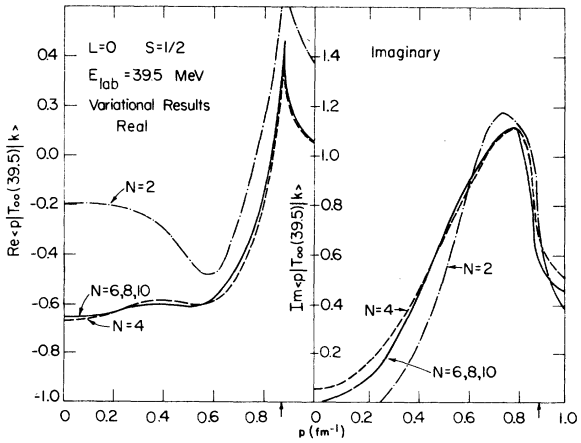

FIG. 4. Variational results for the real and imaginary parts of the half-shell amplitude $\langle p|T_{00}|k\rangle$ at 39.5 MeV.

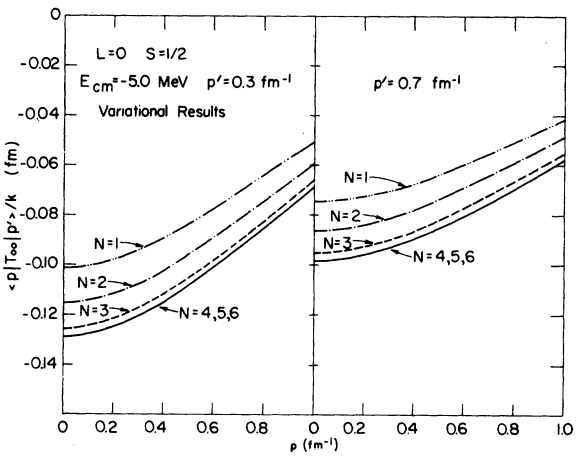

FIG. 5. Variational results for the fully off-shell amplitude at $E_{c.m.} = -5.0$ MeV, with $p' = 0.3$ fm^{-1} in the left-hand figure and $p' = 0.7$ fm^{-1} in the right-hand figure.

shell amplitude (real and imaginary parts) at a higher energy, 39.5 MeV. Evidently the convergence behavior is similar to that shown in Figs. 1 and 2. Finally, in Fig. 5 we show some fully off-shell amplitudes at a *negative* c.m. energy, −5.0 MeV. (Here the plotted quantity is the real amplitude $\langle p|X_{00}|p'\rangle \equiv \langle p|T_{00}|p'\rangle/k$.) The singularity structure is of course simpler at negative energies. In particular, there is no square-root branch point, so that the basis functions containing square roots in (5.18) were deleted. The observed convergence is then very rapid, with only four basis functions being needed to give an accuracy of 1%.

In summary, our numerical calculations for the Amado model, some of which have been presented above, show that the variational method is a numerically successful way of solving the integral equations (5.4). It is computationally quite simple, and it has the virtue of treating on-shell, half-shell, and off-shell amplitudes in a unified way, and with comparable success. We note finally that the method can easily be extended to separable potentials of higher rank, and that, as shown in Sec. III, it can be combined in a rather natural way with a perturbative treatment of small parts of the potential.

Note added in proof: Some related results on three-body variational principles, and in particular on the off-shell extension of the PSW variational principle, have been obtained previously by Grassberger, Alt, and Sandhas.[21] The authors are indebted to Dr. P. Grassberger for drawing attention to this reference.

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in the approximate $Y^L_{0\gamma}$, even when calculating a physical breakup amplitude. It seems simpler to use instead the alternative definition of $U_{0\alpha}$ given in Eq. (2.11).

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