Neutron-deuteron scattering calculations with W-matrix representation of the two-body input

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(Received 18 June 1987)

Employing the W-matrix representation of the partial-wave T matrix introduced by Bartnik, Haberzettl, and Sandhas, we show for the example of the Malfliet-Tjon potentials I and III that the single-term separable part of the W-matrix representation, when used as input in three-nucleon neutron-deuteron scattering calculations, is fully capable of reproducing the exact results obtained by Kloet and Tjon. This approximate two-body input not only satisfies the two-body off-shell unitarity relation but, moreover, it also contains a parameter which may be used in optimizing the three-body data. We present numerical evidence that there exists a variational (minimum) principle for the determination of the three-body binding energy which allows one to choose this parameter also in the absence of an exact reference calculation. Our results for neutron-deuteron scattering show that it is precisely this choice of the parameter which provides optimal scattering data. We conclude that the W-matrix approach, despite its simplicity, is a remarkably efficient tool for high-quality three-nucleon calculations.

I. INTRODUCTION

The use of separable expansions for the two-body T matrix is one of the most successful approaches to render the three-body scattering problem practically manageable (for a recent review of existing methods to obtain such expansions, see Ref. 1). Their usefulness stems from the fact that they allow one to write the partial wave decomposed three-body equations as a coupled system of *one*-dimensional integral equations instead of the numerically much more demanding usual *two*-dimensional equations. Mostly, these approaches rely on expanding the two-body T matrix in some suitably chosen complete set of functions and, usually, one needs a number of terms in the separable expansion in order to achieve a result which is reasonably close to the corresponding exact result. The more expansion terms one needs the more the degree of coupling of the resulting system of equations increases; this is the price one has to pay for the reduced dimensionality of the integral equations. Generally, one can say, therefore, that the less expansion functions are required for any particular application, the better suited the used set of expansion functions is.

It was shown by Bartnik, Haberzettl, and Sandhas[2] that one can exactly represent the two-body partial wave T matrix by *one single* separable term plus a remainder which is real and which vanishes half on shell. This was achieved by a momentum space formulation of the two-body problem entirely in terms of only *one nonsingular inhomogeneous integral* equation which is applicable to the scattering *as well as* the bound state problem and thus provides a unified description of these problems; the solution of this integral equation is referred to as the W matrix. Also in Ref. 2, the hope was expressed that the single separable term, when used as input in three-body scattering equations, may perhaps be sufficient to provide reasonable three-body data and that the remainder of the two-body T-matrix representation can be neglected. It is the purpose of the present paper to investigate whether this approximate treatment of the two-body input in three-body calculations leads to acceptable results. From the investigations of Ref. 2 it is clear that neglecting the remainder introduces an additional free parameter into the three-body equations which concerns the definition of the W matrix at negative *two*-body energies. In the exact W-matrix representation of the T matrix the interplay of the separable part and the remainder is such that the dependence on this definition cancels, i.e., it has no bearing on the full representation. Neglecting the remainder, however, makes this dependence manifest. The corresponding free parameter may be used, therefore, to optimize the results.

The specific problem we treat here is the scattering of neutrons off deuterons. As a benchmark, we use the results of Kloet and Tjon,[3] which were obtained by solving the Faddeev equations[4] with the local Malfliet-Tjon potentials.[5] Employing the single-term separable W-matrix representation in the three-body equations by Alt, Grassberger, and Sandhas[6] (AGS), we find that, if we fully exploit the aforementioned freedom in defining the W matrix at negative two-body energies, we can reproduce *all of the results of Kloet and Tjon* to within the numerical errors[7] of their calculation.

This paper is organized as follows. In Sec. II we first present a short recapitulation of the W-matrix approach by Bartnik, Haberzettl, and Sandhas.[2] The three-body AGS equations[6] for neutron-deuteron scattering resulting from the separable part of the W-matrix representation of the two-body T matrix are given in the remainder of that section. The numerical results are summarized in Sec. III. We first deal with the bound state case and show that we can reproduce the exact triton binding energy for the Malfliet-Tjon potentials. Moreover, we

demonstrate that the freedom in defining a W matrix at negative two-body energies leads to a behavior of the three-body binding energy which is very similar to what one expects from variational approaches, namely that the exact value of the bound state energy is a lower bound on the approximate results. In the second part of Sec. III we present our scattering data: scattering lengths, phase shifts, inelasticities, and differential cross sections. We find that the only partial wave which shows any sensitivity on varying the negative-energy W matrix is the total-spin doublet channel S wave. All other partial waves exhibit no sensitivity and agree with the exact values quoted by Kloet and Tjon.[3] Varying the W-matrix input, it develops that we can also reproduce the exact doublet S-wave data if we choose *exactly the same* parameters which provided the exact triton binding energy. This remarkable finding is very important from a practical point of view because it constitutes a rule for choosing the parameters in the absence of an exact reference calculation. We conclude this section by giving a summarizing assessment of our investigation.

Throughout this paper we use natural units, with the nucleon mass being equal to unity. The conversion to the usual energy units is achieved by 41.47 MeV fm^2=1.

II. FORMALISM

In the three-body equations[4,6] one needs the off-shell two-body T matrix for all real momenta and for all energies ranging from a given three-body center-of-mass energy all the way down to $-\infty$. As explained already in the Introduction, in the present paper we want to demonstrate the usefulness of the W-matrix approach of Ref. 2 for this purpose. To this end, we first briefly recapitulate this method here.

A. W matrix

It was shown in Ref. 2 that the off-shell two-body T matrix in the partial wave l at the energy E, $T_l(p,p';E+i0)$, may be represented exactly by

$$T_l(p,p';E+i0)=W_{kl}(p,k;E)\Delta_{kl}(E+i0)W_{kl}(p',k;E)+R_{kl}(p,p';E)\ , \tag{1}$$

where

$$R_{kl}(p,p';E)=\left[W_{kl}(p,p';E)-\frac{W_{kl}(p,k;E)W_{kl}(k,p';E)}{W_{kl}(k,k;E)}\right]p'^{l} \tag{2}$$

and

$$\Delta_{kl}(E+i0)=\frac{k^l}{W_{kl}(k,k;E)\hat{F}_{kl}(E+i0)}\ , \tag{3}$$

with

$$\hat{F}_{kl}(E+i0)=1-\int_0^\infty dq\, q^2 q^l \frac{W_{kl}(q,k;E)}{E+i0-q^2}\ . \tag{4}$$

We shall refer to the ubiquitous function $W_{kl}(p,p';E)$ in this representation as the W matrix; it satisfies the integral equation

$$W_{kl}(p,p';E)=U_l(p,p')+\int_0^\infty dq\, q^2 \frac{U_l(p,q)-U_l(p,k)}{E-q^2}\times q^l W_{kl}(q,p';E)\ , \tag{5}$$

and the parameter k is subject to the constraints

$$k^2=E \quad \text{for } E\geq 0\ ,$$
$$k \text{ arbitrary} \quad \text{for } E<0\ . \tag{6}$$

The function $U_l(p,q)$ is defined by

$$U_l(p,q)=V_l(p,q)q^{-l}\ , \tag{7}$$

where $V_l(p,q)$ is the partial wave momentum space matrix element of the potential V; the factor q^{-l} in the definition (7) ensures that the q^l behavior of $V_l(p,q)$ for vanishing q is compensated and $U_l(p,q)$, therefore, does not vanish identically for $q=0$.

Clearly, for scattering energies $E\geq 0$ the integral equation (5) is *nonsingular,* because the denominator singularity at $E=q^2$ is cancelled by the zero of the difference $U_l(p,q)-U_l(p,k)$ due to the choice (6) of k, and its solutions are real. The W-matrix equation (6) thus is a much simpler equation to work with than the usual Lippmann-Schwinger (LS) equation for the T matrix,

$$T_l(p,p';E+i0)=V_l(p,p')+\int_0^\infty dq\, q^2 \frac{V_l(p,q)}{E+i0-q^2}\times T_l(q,p';E+i0)\ . \tag{8}$$

Moreover, it was proved in Ref. 2 that, at negative energies $E=-\alpha^2$, for those solutions $W_{kl}(q,k;-\alpha^2)$ which satisfy

$$\int_0^\infty dq\, q^2 q^l \frac{W_{kl}(q,k;-\alpha^2)}{-\alpha^2-q^2}=1\ , \tag{9}$$

the associated energy $-\alpha^2$ is equal to one of the binding energies $-\alpha_n^2$, i.e., $-\alpha^2=-\alpha_n^2$, and the corresponding momentum space bound state wave function $\psi_{nl}(p)$ is given by

$$\psi_{nl}(p)=\frac{W_{kl}(p,k;-\alpha_n^2)}{-\alpha_n^2-p^2}C_{nl}\ , \tag{10}$$

where C_{nl} is an arbitrary normalization constant. In other words, the *inhomogeneous* integral equation (5) not only solves the scattering problem but also the bound state problem. For the latter problem, it replaces the usually employed *homogeneous* version of the LS equation (8).

For a more detailed account of the W-matrix approach, we refer to Ref. 2, where also references to related approaches may be found. Here we only want to stress those features of the representation (1) that are important for the three-body applications we have in mind here. First and foremost, we note that the first term on the right-hand side of Eq. (1) is *separable* in the momenta p and p' and it contains *all* the scattering cut informa-

tion via $\hat{F}_{kl}(E+i0)$ of Eq. (4). The latter entity was shown in Ref. 2 to be a generalization of the well-known Jost function, the decisive difference being the treatment of the negative energy domain [if the constraint (6) for $E<0$ were the same as for positive energies, the function (4) would be a representation of the usual Jost function for the entire energy range from $-\infty$ to $+\infty$]. This generalization is constructed such that it has no left-hand cut but the same one-to-one correspondence between the zeros of (4) and the bound state energies as the true Jost function [cf. Eq. (9)]: As is obvious from (1), the zeros of (4) provide the bound state poles of the T matrix, with the residual functions of these poles being related to the bound state wave functions according to (10). Second, the remaining term $R_{kl}(p,p';E)$ on the right-hand side of (1) is real for all energies and it is easily seen to vanish if p, or p', is equal to the parameter momentum k, which means, in particular, that $R_{kl}(p,p';E)$ vanishes half on shell for scattering energies $E\geq 0$.

As explained in the Introduction, we want to investigate here whether the *single* separable term in the representation (1) suffices to reproduce acceptable results in three-body calculations. As the underlying two-body interactions we use here the S-wave projections of the Malfliet-Tjon (MT) I and III potentials.[5] The exact solutions for this input for the scattering of neutrons off deuterons were obtained by Kloet and Tjon[3] employing a Padé technique[8] for the multiple scattering series resulting from iterating the three-body Faddeev equations.[4] We shall use these theoretical data as a benchmark to assess the usefulness of replacing the full off-shell two-body T matrix $T(p,p';E+i0)$ resulting from the MT I and III potentials by

$$T(p,p';E+i0)\rightarrow T^{s}(p,p';E+i0) = W(p,k;E)\Delta(E+i0)W(p',k;E) , \quad (11)$$

where the index s stands for "separable." Since, for this separable part of the representation (1), we need only the half-on-shell solutions of (5), we have omitted the redundant index k here on the W matrices, because it is specified already by the argument k. Moreover, since the MT I and MT III potentials act only in $l=0$, we have suppressed the partial wave index l.

The separable approximation (11) will be used as input in the three-body equations by AGS.[6] In this context, it should be noted that *the approximation (11) satisfies the full two-body off-shell unitarity;* the neglected remainder (2) does not contribute to the unitarity relation because—as emphasized already—it is real and it vanishes half on shell.

B. Three-body AGS equations

We shall not give any details of the formalism behind the AGS equations; for these, we refer to Ref. 6. Here, we only give the final effective two-body equations for neutron-deuteron scattering which result from a single-term separable approximation of the two-body T matrix as in Eq. (11). Denoting the total angular momentum of the three nucleons by L, the AGS equations for the total-spin doublet ($S=\frac{1}{2}$) channel are given by

$$\begin{aligned}{}^{2}T_{L}^{\mu\nu}(q,q';E+i0) &= {}^{2}V_{L}^{\mu\nu}(q,q';E+i0) \\ &\quad + \sum_{\kappa}\int_{0}^{\infty} dq''q''^{2}\,{}^{2}V_{L}^{\mu\kappa}(q,q'';E+i0) \\ &\quad \times\Delta^{\kappa}(E-\tfrac{3}{4}q''^{2}+i0) \\ &\quad \times{}^{2}T_{L}^{\kappa\nu}(q'',q';E+i0) .\end{aligned} \quad (12)$$

Here, the energy E is now the three-body center-of-mass energy and the left index 2 on the partial wave matrix elements T and V denotes the total-spin doublet channel. The summation runs over the two possible two-body subsystem configurations, the two-body spin triplet (described by the MT III potential; denoted by $\kappa=\mathrm{d}$) and the spin singlet (MT I; $\kappa=\mathrm{s}$) states. Since we are only interested in physically observable reactions, we need to consider only the coupled set of equations with a deuteron in the entrance channel, i.e., $\nu=\mathrm{d}$. In the total-spin quartet ($S=\frac{3}{2}$) channel we have a single, uncoupled equation with the only possible two-body subsystem being a deuteron:

$$\begin{aligned}{}^{4}T_{L}^{\mathrm{dd}}(q,q';E+i0) &= {}^{4}V_{L}^{\mathrm{dd}}(q,q';E+i0) \\ &\quad + \int_{0}^{\infty} dq''q''^{2}\,{}^{4}V_{L}^{\mathrm{dd}}(q,q'';E+i0) \\ &\quad \times\Delta^{\mathrm{d}}(E-\tfrac{3}{4}q''^{2}+i0) \\ &\quad \times{}^{4}T_{L}^{\mathrm{dd}}(q'',q';E+i0) .\end{aligned} \quad (13)$$

The effective potentials ${}^{i}V_{L}^{\nu\mu}$ in these equations are given by

$${}^{i}V_{L}^{\nu\mu}(q,q';E+i0) = {}^{i}\Lambda_{\nu\mu}V_{L}^{\nu\mu}(q,q';E+i0) , \quad (14)$$

where the ${}^{i}\Lambda_{\nu\mu}$ are the usual spin-isospin recoupling coefficients,

$${}^{2}\Lambda_{\mathrm{dd}}={}^{2}\Lambda_{\mathrm{ss}}=\tfrac{1}{4},\quad {}^{2}\Lambda_{\mathrm{ds}}={}^{2}\Lambda_{\mathrm{sd}}=-\tfrac{3}{4},\quad {}^{4}\Lambda_{\mathrm{dd}}=-\tfrac{1}{2} ,$$

and

$$V_{L}^{\nu\mu}(q,q';E+i0) = \int_{-1}^{+1} d\xi\, P_{L}(\xi)\frac{W^{\nu}(x,k;E-\frac{3}{4}q^{2})W^{\mu}(y,k';E-\frac{3}{4}q'^{2})}{E-q^{2}-q'^{2}-qq'\xi+i0} . \quad (15)$$

Here, $P_{L}(\xi)$ is a Legendre polynomial of the first kind and x and y are abbreviations defined by

$$x^{2}=\tfrac{1}{4}q^{2}+q'^{2}+qq'\xi \quad\text{and}\quad y^{2}=\tfrac{1}{4}q'^{2}+q^{2}+qq'\xi . \quad (16)$$

To simplify the notation in Eqs. (12) and (13), we have not explicitly expressed the dependence of the effective potential $V_{L}^{\nu\mu}$ and the two-body propagator Δ^{κ} on the parameter momenta k or k'. We want to make it quite clear, however, that according to (6) the solutions of the three-body equations (12) and (13) will depend on our

choice for these parameters at negative *two-body energies,* i.e., when $E=-\frac{3}{4}q^2<0$ (similarly for q' and q''). This dependence originates from the approximation (11), of course; had we taken into account the full T-matrix representation (1) no such dependence would occur. In our approximate treatment of the two-body input for three-body equations we thus have an additional free parameter to optimize the results.

III. NUMERICAL RESULTS AND DISCUSSION

The various methods for the numerical solution of three-body integral equations have become standard by now. We, therefore, will only make a few remarks here. We have solved the integral equations (12) and (13) on the real axis by expanding the solutions in cubic B splines[9] and solving a system of linear equations for the unknown expansion coefficients. The technically most difficult part of such a procedure concerns the treatment of the logarithmic singularities of the effective potentials arising from the partial wave integration in Eq. (15).[10] We have tackled this problem by explicitly extracting the singularity through a subtraction procedure and subsequent employment of a special quadrature routine for the resulting integral containing the singular logarithm.[11] (A detailed account of these technical points may be found in Ref. 12.)

In contrast to most separable approximations of the two-body T matrix,[1] the representation (11) works with *energy dependent* functions $W(p,k;E)$. This, however, introduces only slight difficulties for the numerical solutions of the three-body equations because these functions are real and very well behaved. As can be seen from Fig. 1, the dependence of the half-on-shell W matrix on the energy is very smooth. We have found that it is sufficient to solve the W matrix equation (5) for $W(p,k;E)$ *once* on a grid of 48 mesh points for the momentum p and 50 energies ranging from a given three-body c.m. energy down to $-\infty$; the necessary matrix elements in (15) and (3) at intermediate values of p and E are then very easily—and very accurately—obtained by a two-dimensional spline interpolation. From the computational point of view, the energy dependence of $W(p,k;E)$, therefore, results in only a slight increase in computing time as compared to an energy-independent single-term separable approximation (i.e., spline interpolation versus simple function evaluation), but it requires a somewhat larger memory space to store the grid for the W matrix. However, storage capacity is usually no problem in modern computing facilities.

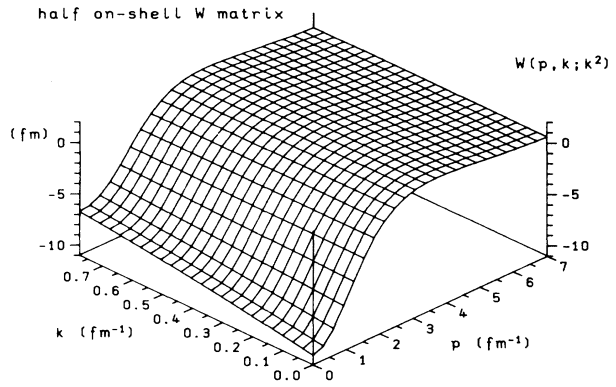

FIG. 1. Two-dimensional plot of the half-on-shell W matrix at positive energies.

How does one choose the parameter k in (5) at negative energies? We, at first, made the simplest possible choice which provides for a smooth transition from the positive to the negative energy domain; namely, we took $k=0$ for all negative (two-body) energies. Clearly, any continuous functional dependence $k=f(E)$ with $f(0)=0$ will yield a W matrix which is continuous at all energies. However, for the physically relevant three-nucleon scattering solutions to be continuous functions of the energy, the function $f(E)$ only needs to be *piecewise continuous,* i.e., it may have finite discontinuities.

A. Bound state results

We first calculated the triton binding energy E_t. This was done in the standard fashion by determining the zero of the Fredholm determinant of the homogeneous version of the doublet equation (12). Our result obtained with the choice $k=0$ at negative energies in (5) is $E_t=-7.88$ MeV. This value has to be compared with the result of Kloet and Tjon[3] (KT). They quote $E_t=-8.3$ MeV; however, the numerical error of their result is rather large.[7] In a later, more accurate calculation,[13] it was found that the MT I and MT III potentials yield a triton binding energy of $E_t=-8.58$ MeV, the error[7] being roughly ± 0.1 MeV. In view of this, our result, which is off by 0.7 MeV, seems rather disappointing.

It must be noted, however, that the choice of the parameter k is of decisive importance in three-body binding energy calculations because *only W matrices at negative two-body energies* appear in the homogeneous bound state version of (12). In order to assess the dependence of E_t on k, we have varied k. Rather than assuming some wild functional forms for k, we always chose k to be constant, but different from zero; the resulting function $E_t=E_t(k)$ is plotted in Fig. 2. We find that $E_t(k)$ has a minimum at $k_t=0.655$ fm^{-1}. It is remarkable that *the corresponding minimal energy $E_t(k_t)=-8.595$ MeV is equal to the exact binding energy.* The fact that for all possible values of k the energy is always bounded below by the exact value is very reminiscent of variational methods for the determination of binding energies.[14] We conjecture, therefore, that there exists an underlying variational principle which actually explains our finding. We have not been able to prove this conjecture, however. In the absence of any proof, we can only emphasize once again that we have not found any choice of k which yielded any energy below the exact value.

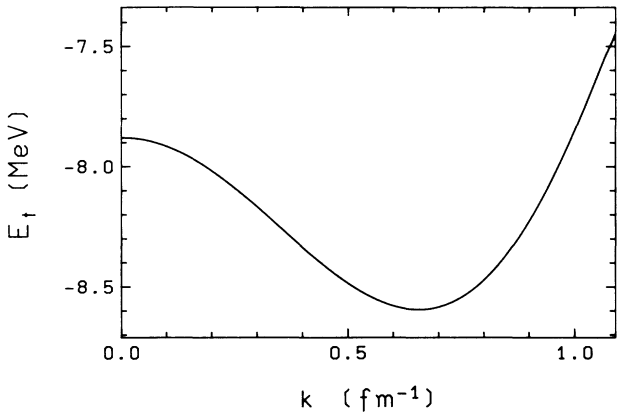

FIG. 2. Variation of the triton binding energy E_t with the negative-energy W-matrix parameter k [cf. Eqs. (5) and (6)].

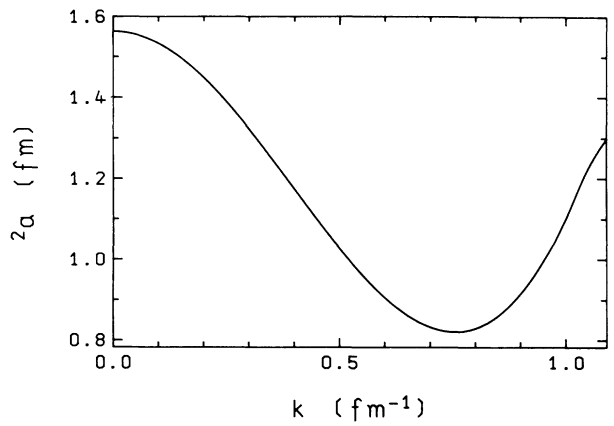

FIG. 3. Variation of the doublet scattering length ^2a with the negative-energy W-matrix parameter k [cf. Eqs. (5) and (6)].

B. Scattering results

The quartet and doublet scattering lengths given by KT (Ref. 3) are $^4a=6.35$ fm and $^2a=0.9$ fm, respectively. Our values are

$$^4a=6.39 \text{ fm} \quad \text{and} \quad ^2a=1.56 \text{ fm} \quad \text{for } k=0$$

and

$$^4a=6.41 \text{ fm} \quad \text{and} \quad ^2a=0.86 \text{ fm}$$

$$\text{for } k=k_t=0.655 \text{ fm}^{-1} .$$

As can be seen, the values for the quartet scattering length ^4a are not very sensitive to the variation of the negative-energy W-matrix parameter k. Moreover, within the numerical errors[7] of their calculation, our results agree with those of KT. The situation is very much different for the doublet scattering length. In Fig. 3 we have plotted ^2a as a function of k, similar to the binding energy plot in Fig. 2. As in the latter case, we find that $^2a(k)$ exhibits a minimum at a position $k_a=0.755$ fm^{-1}, which is larger than the minimum position k_t of the triton binding energy; the corresponding scattering length is $^2a(k_a)=0.82$ fm. However, in view of the conjectured underlying variational principle for the binding energy calculation, we feel that in order to be consistent we have to choose the same value of k which minimizes the energy, i.e., $k=k_t$.

In order to be able to relate the solutions $^iT_L^{dd}$ of Eqs. (12) and (13) for elastic neutron-deuteron scattering to the physical data, they have to be normalized according to

$$^i\hat{T}_L^{dd}=N_d^2\,{}^iT_L^{dd} , \tag{17}$$

where N_d^2 is the residue of the deuteron propagator at the deuteron pole,

$$N_d^2=\mathrm{Res}\Delta^d(E_d)=\left\{\int_0^\infty dp\,p^2\left[\frac{W^d(p,k;E_d)}{E_d-p^2}\right]^2\right\}^{-1} . \tag{18}$$

This is (not surprisingly) just the normalization of the deuteron wave function; cf. Eq. (10). [$E_d=-2.272$ MeV is the deuteon binding energy of the MT III potential; it was determined by searching for the zero of $\hat{F}_{kl}$; cf. Eqs. (4) and (9).] With these renormalized amplitudes, the elastic neutron-deuteron phase shifts are obtained through [$q^2=\frac{4}{3}(E-E_d)$]

$$\tan{}^i\delta_L(E)=\frac{\mathrm{Im}\,{}^i\hat{T}_L^{dd}(q,q;E+i0)}{\mathrm{Re}\,{}^i\hat{T}_L^{dd}(q,q;E+i0)}-\frac{{}^i\eta_L(E)-1}{(4\pi q/3)\mathrm{Re}\,{}^i\hat{T}_L^{dd}(q,q;E+i0)} , \tag{19}$$

where the inelasticities $^i\eta_L$ are given by

$${}^i\eta_L(E)=\left[\frac{16\pi^2q^2}{9}\left|{}^i\hat{T}_L^{dd}(q,q;E+i0)\right|^2+\frac{8\pi q}{3}\mathrm{Im}\,{}^i\hat{T}_L^{dd}(q,q;E+i0)+1\right]^{1/2} . \tag{20}$$

For the spin-averaged differential cross section it then follows that

$$\frac{d\sigma}{d\Omega}=\frac{1}{4q^2}\left\{\frac{1}{3}\left|\sum_L(2L+1)P_L(\cos\theta)[{}^2\eta_L\exp(2i\,{}^2\delta_L)-1]\right|^2+\frac{2}{3}\left|\sum_L(2L+1)P_L(\cos\theta)[{}^4\eta_L\exp(2i\,{}^4\delta_L)-1]\right|^2\right\} . \tag{21}$$

(Although these formulas may be found also in the literature, we have given them here in order to make the present paper self-contained.)

In Fig. 4 we present our results for the quartet phase shifts for the S and P waves. The crosses are some representative values taken from Ref. 3. As can be seen, our data are in complete agreement with these reference solutions (according to Tjon[7] the numerical errors of the

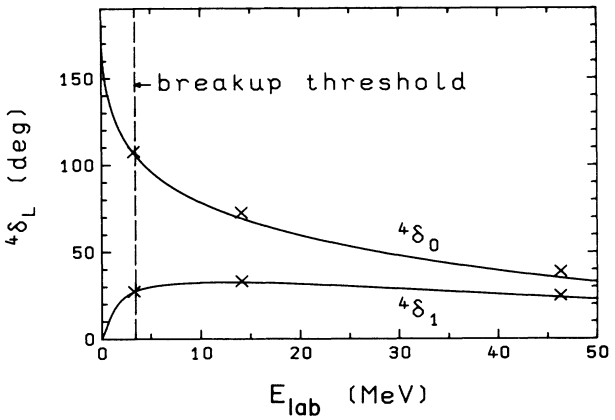

FIG. 4. Quartet S- and P-wave phase shifts; crosses are from Ref. 3.

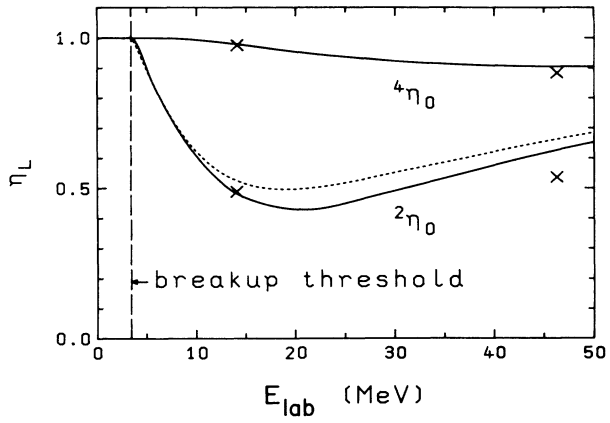

FIG. 6. Doublet and quartet S-wave inelasticities, crosses are from Ref. 3. The solid-line doublet inelasticity results from the optimized choice $k=k_t=0.655$ fm^{-1}, whereas the dashed line corresponds to $k=0$ (see text).

phase-shift calculation of KT are in the range of a few degrees). The same quality in reproducing the phase shifts by KT (Ref. 3) is also found at higher partial waves; we have omitted plotting these because nothing new can be learned from them. Furthermore, varying the W-matrix parameter k produces only changes which are of the order of the numerical errors of our calculation (which we estimate to be below 1 deg for the phase shifts). In the doublet case, we find the same kind of agreement with the data of KT for all partial waves except the S wave. Consistent with the finding for the doublet scattering length, the latter phase shift turns out to be quite sensitive on the negative-energy W matrix. In Fig. 5 we have plotted the S-wave doublet phase shift $^2\delta_0$ for two values of k; namely, for $k=0$ (dashed line) and for $k=k_t=0.655$ fm^{-1} (solid line). Again, we find that the latter choice leads to almost perfect agreement with the values of KT.[3] As a typical representative of how well the higher partial waves are reproduced within the W-matrix approach, we have also drawn the doublet P wave in Fig. 5. Our results for the inelasticity parameters are given in Fig. 6. Again, the quartet S-wave case is insensitive to k and very well reproduced, while the doublet S-wave values require that k be chosen as $k=k_t$. Also here, higher partial waves are indistinguishable from the results of KT and, consequently, have not been plotted.

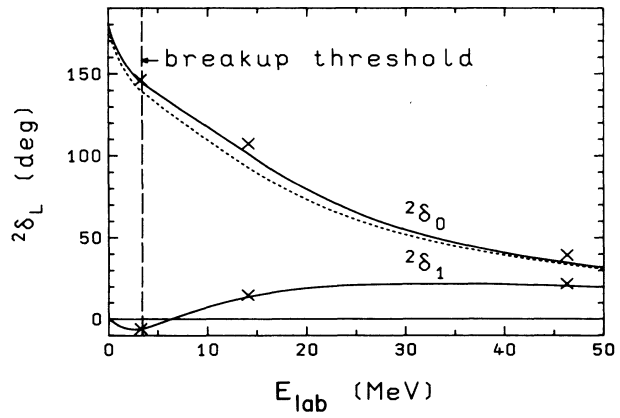

FIG. 5. Doublet S- and P-wave phase shifts; crosses are from Ref. 3. The solid-line S-wave phase shifts have been obtained with the optimized choice $k=k_t=0.655$ fm^{-1}, whereas the dashed line corresponds to $k=0$ (see text).

In order to give a complete picture of the utility of the approach adopted here, we, in addition, give in Figs. 7 and 8 differential cross sections at laboratory energies of 2.45 and 46.3 MeV, respectively. (Some care must be exercised in interpreting here the agreement with the results of KT, because the crosses in Figs. 7 and 8 have not been drawn from numbers given by KT, as was the case with the phase shifts and inelasticities, but were taken directly from the figures plotted in Ref. 3. In drawing the crosses for Figs. 7 and 8, the numerical errors of the calculation of KT were folded, therefore, with our errors in reading their figures.) Nevertheless, even with this caveat in mind, we feel safe in assessing our results as being in excellent agreement with KT if we choose the W-matrix parameter k according to the triton binding energy results as $k=k_t$. Comparing the latter two figures, one sees, moreover, that the influence of the doublet S-wave phase shifts and inelasticities, which exhibited the strongest influence of k, becomes considerably less at higher energies.

C. Conclusions

We have shown here for the example of elastic neutron-deuteron scattering that the W-matrix representation of the two-body T matrix by Bartnik, Haberzettl, and Sandhas[2] is an extremely useful method for simplifying the two-body input for three-body calculations. Employing the three-body AGS equations[6] and using as input the W-matrix representation's *single*-term separable part only, we obtained almost perfect agreement with

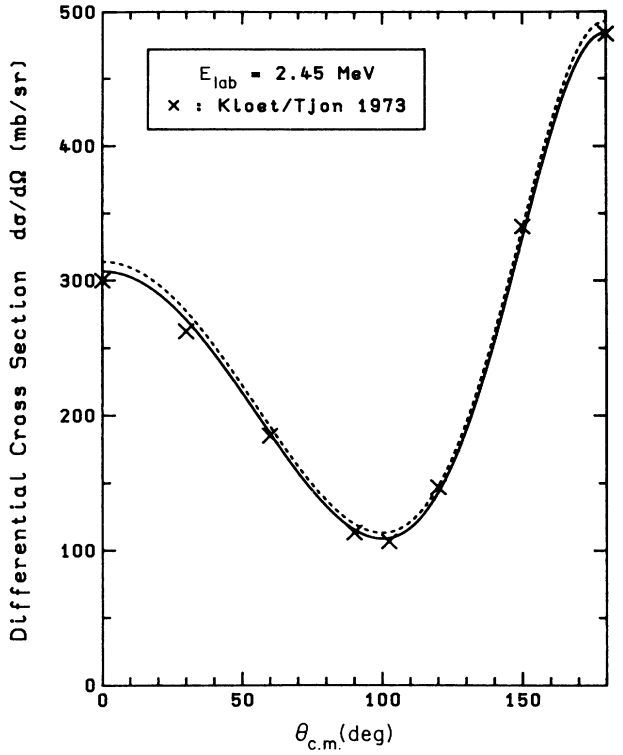

FIG. 7. Differential cross section at $E_{lab}=2.45$ MeV; crosses are from Ref. 3 (see text). The solid line corresponds to the optimized choice $k=k_t=0.655$ fm^{-1}, whereas the dashed line corresponds to $k=0$ (see text).

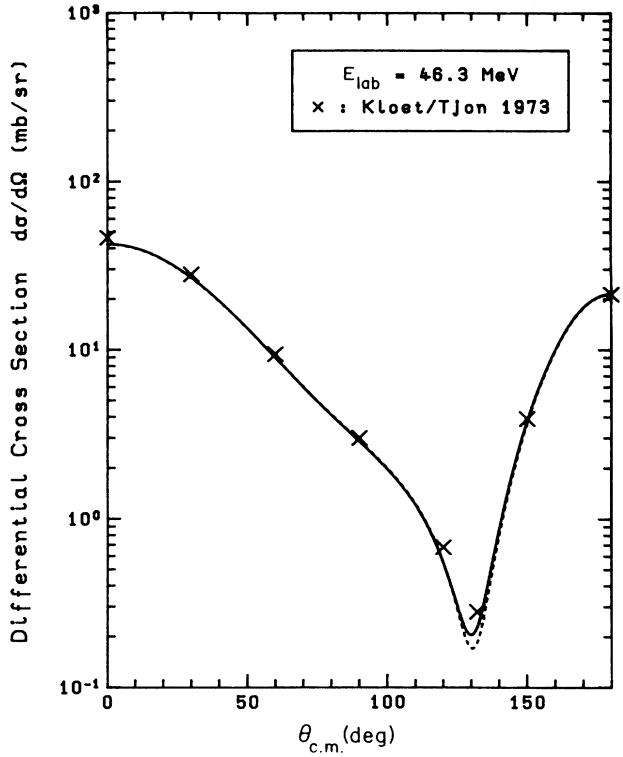

FIG. 8. Differential cross section at $E_{lab}=46.3$ MeV. Notation as in Fig. 7.

the results of the exact calculation by Kloet and Tjon[3] obtained for the semirealistic Malfliet-Tjon potentials I and III.[5]

In our opinion, one of the most important findings from a practical point of view is the fact that the free parameter k of the negative-energy W matrix [cf. Eqs. (5) and (6)] may be determined by minimizing the three-body binding energy. This feature of the W-matrix approach reminds one of variational procedures for binding energy calculations and, as already mentioned above, although we could not prove it, we actually conjecture that there exists an underlying variational principle in the present case also. (The finding that here the minimal three-nucleon binding energy turned out to be just the exact binding energy of the problem may be just an accident, but nevertheless makes a proof of our conjecture all the more desirable.) This feature allows one to choose a parameter k also in the absence of an exact reference solution and is therefore of extreme practical importance. It is remarkable that the value of k determined in this way proved to be just the right value to yield the correct scattering data.

The test calculations were performed here for the semirealistic S-wave Malfliet-Tjon potentials, because these are relatively easy to handle and, moreover, because there exists an exact reference calculation by Kloet and Tjon.[3] We are convinced, however, that the W-matrix representation of the two-body T matrix will also be helpful in simplifying three-body calculations with more realistic potentials; the corresponding investigations are in progress.

Summarizing, the single-term separable W-matrix representation of the two-body T matrix is an extremely powerful method for drastically reducing the inherent complexity of three-body calculations. We conclude that it is not only superior to any other single-term separable approximation known to us but actually reaches the quality usually achieved only with expansions of high rank. Our investigations show that the W-matrix approach, despite its simplicity, is a remarkably efficient tool for high-quality three-nucleon calculations.

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