Two-body bound state problem and nonsingular scattering equations

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We present a new momentum space approach to the two-body problem in partial waves. In contrast to the usual momentum space approaches, we treat the bound state case with the help of an inhomogeneous integral equation which possesses solutions for all (negative) energies. The bound state energies and corresponding wave functions are identified by an additional condition. This procedure straightforwardly leads to a nonsingular formulation of the scattering problem in terms of essentially the same equation and thus unifies the descriptions of both energy regimes. We show that the properties of our momentum-space approach can be understood in terms of the so-called regular solution of the Schrödinger equation in position space. The unified description of the bound state and scattering energy regimes in terms of one single, real, and manifestly nonsingular equation allows us to construct an exact representation of the two-body off-shell T matrix in which all the bound state pole and scattering cut information is contained in one single separable term, the remainder being real, nonsingular, and vanishing half on-shell. Such a representation may be of considerable advantage as input in three-body Faddeev-type integral equations. We demonstrate the applicability of our method by calculating bound state and scattering data for the two-nucleon system with the s-wave Malfliet–Tjon III potential.

I. INTRODUCTION

The nonrelativistic two-body problem is probably one of the best-investigated problems in quantum mechanics (see, e.g., Ref. 1 and references contained therein). Nevertheless, we want to add to the already existing approaches of solution by presenting here a formalism which in its essential aspects takes a new look at one of the two main parts of the two-body problem, namely the bound state problem.

It is the other part, the scattering problem, which is often thought to be the more difficult of the two. We do not share this point of view. Of course, we agree that the scattering problem looks *technically* more complicated than the bound state problem because of its more complex boundary conditions. However, from a *conceptual* point of view, it is the bound state problem which is more difficult. The reason is that the energy plays quite a different role in both problems. In the scattering problem, the energy is merely a continuous parameter which can be chosen arbitrarily according to the prevailing external circumstances (experiment, etc.). The problem as such, however, can be solved regardless of its precise value. This is not so in the bound state case. There the very *solvability* of the problem depends on choosing the correct value for the energy, i.e., the bound state energy. In other words, for the bound state problem one needs an additional algorithm for the determination of the bound state energy. It is this aspect of the bound state case, i.e., that it requires the *simultaneous* determination of the unique discrete binding energies and the corresponding wave functions, which makes it in our opinion so much more difficult conceptually. Of course, there exist a number of very efficient numerical algorithms for tackling this problem, and this is presumably the reason why many people do not view this conceptual difference between the bound state and the scattering problems as being essential.

The approach for solving the two-body problem we report on here is a partial wave momentum space method. It makes use of the aforementioned conceptual difference by first removing it: Instead of the usual *homogeneous* Lippmann-Schwinger (LS) equation for the bound state problem, we solve an auxiliary *inhomogeneous* equation (to which we refer as the W-matrix equation) in which the energy has the same function as in the scattering case, i.e., it is a free continuous parameter and it can be given any (negative) value. Similar to the *inhomogeneous* LS equation of the scattering problem, our new W-matrix equation possesses unique solutions for all of these energies. The desired physical solutions—the discrete bound state energies and the corresponding wave functions—are then determined by imposing an additional condition on the solution of the auxiliary W-matrix equation. This formalism is introduced in Sec. II.

As will become clear in Sec. III, this procedure has some very interesting and immediate consequences on how to proceed in the scattering case. In particular, it will turn out that the formulation of *nonsingular* scattering equations[2] is a natural consequence of such a treatment of the bound state problem. As a matter of fact, we will show that—taken at the appropriate (positive) energies and after a slight modification—the bound state W-matrix equation will also solve the scattering problem. We have thus found one single inhomogeneous integral equation which completely determines the two-body problem in the bound state as well as in the scattering energy regimes. Since our W-matrix equation is real and manifestly nonsingular even at scattering energies, we feel that it is particularly well suited for numerical applications.

It seems obvious that this unification of the bound state

and scattering problems in terms of one single momentum space integral equation cannot be accidental and must have its counterpart in the more traditional configuration space approaches found in most textbooks. This is investigated in Sec. IV and it is found that the properties of our W-matrix equation are intimately connected to the so-called "regular" solution of the Schrödinger equation.[1] Among other things, this connection will allow us to conclude that the W-matrix equation can be solved by iteration under only very global constraints on the potential. Furthermore, it will become clear that with the W matrix one can find a very simple integral representation of the Jost function. This representation (which has also been given in Ref. 3) in terms of but momentum space quantities is also immediately seen to be easily applicable in practical calculations.

In Sec. V we present an off-shell generalization of the W-matrix equation analogous to the off-shell Lippmann-Schwinger equation for the T matrix. With its help, we then write a representation of the off-shell T matrix entirely in terms of the W matrix. Its structure is very similar to the Noyes-Kowalski representation.[4] However, owing to the fact that the W matrix, by construction, is free of any singularities at negative energies, our representation remains well defined in this energy regime, quite in contrast to the Noyes-Kowalski representation. This feature of our representation makes it particularly well suited as an input in Faddeev-type formulations of the three-body problem, where the negative energy domain of the two-body T matrix forms an important part of the required input.[5]

In Sec. VI of this paper we report on some numerical test calculations performed with the local Malfliet-Tjon potential.[6] In particular, we show that for this potential the W-matrix equation can be solved by iteration with a very rapid rate of convergence. We conclude this section by giving a summarizing assessment of our approach. Furthermore, in the Appendix we prove the existence of a certain integral necessary for the derivation of our bound state W-matrix equation.

Throughout this paper we use natural units, with the nucleon mass being equal to unity.

II. THE BOUND STATE FORMALISM

In momentum space, the partial wave bound state functions $\psi_{nl}(p)$ may be written as

$$\psi_{nl}(p)=\frac{g_{nl}(p)}{-\alpha_n^2-p^2}\ , \tag{1}$$

where the α_n^2 are the binding energies enumerated by the index n. The form factors $g_{nl}(p)$ are determined as the nontrivial solutions of the homogeneous LS equation,

$$g_{nl}(p)=\int_0^\infty dq\, q^2 V_l(p,q)\frac{g_{nl}(q)}{-\alpha_n^2-q^2}\ , \tag{2}$$

which is completely equivalent to the Schrödinger equation for the bound state case. In the context of the LS equation (2), the usual algorithm for the determination of the binding energies α_n^2 is to search for the zeros in energy of the Fredholm determinant of Eq. (2). For any other energy Eq. (2) has, of course, no solutions, and this is a direct consequence of the fact that it is a *homogeneous* integral equation.

For reasons which will become apparent below, we propose now to replace Eq. (2) by an *inhomogeneous* integral equation. To this end, we first note that, for reasonable potentials V, the momentum space partial wave matrix elements $V_l(p,q)$ behave as q^l for vanishing q (similarly for p). The (unsymmetric) function $U_l(p,q)$, defined by

$$U_l(p,q)=V_l(p,q)q^{-l}\ , \tag{3}$$

therefore, does not vanish for $q=0$. With this technical detail, we now define $W_{kl}(p,k;-\alpha^2)$ by the integral equation

$$W_{kl}(p,k;-\alpha^2)=U_l(p,k)+\int_0^\infty dq\, q^2\frac{U_l(p,q)-U_l(p,k)}{-\alpha^2-q^2}q^l\times W_{kl}(q,k;-\alpha^2)\ , \tag{4}$$

where k is a free parameter momentum. The definition (3) ensures that the inhomogeneity of this equation does not vanish identically even if k is chosen as $k=0$. [The double occurrence of k in the notation $W_{kl}(p,k;-\alpha^2)$ is necessary in order to have notational consistency with the generalizations given in Sec. V.]

Equation (4) is the desired inhomogeneous integral equation; we shall refer to its solution as the bound state W matrix. Its relevance in the bound state problem is established by the following.

Theorem: If and only if the energy $E=-\alpha^2$ is chosen such that the corresponding solution of Eq. (4) satisfies

$$\int_0^\infty dq\, q^2 q^l\frac{W_{kl}(q,k;-\alpha^2)}{-\alpha^2-q^2}=1\ , \tag{5}$$

then $\alpha^2=\alpha_n^2$, i.e., it is equal to one of the binding energies, and the corresponding bound state wave function is given by

$$\psi_{nl}(p)=\frac{W_{kl}(p,k;-\alpha_n^2)}{-\alpha_n^2-p^2}C_{nl}\ , \tag{6}$$

where C_{nl} is an arbitrary normalization constant.

The proof is straightforward and will only be sketched here. In one direction, one simply notes that, with condition (5) satisfied, Eq. (4) reduces to Eq. (2), and since the latter has unique solutions, $\alpha^2=\alpha_n^2$ and Eq. (6) follow immediately. The constant C_{nl} takes into account the fact that Eq. (2) leaves the normalization of $g_{nl}(p)$ free, whereas the inhomogeneous equation (4) fixes the normalization of $W_{kl}(p,k;-\alpha_n^2)$. For the other direction of the proof, we start from Eq. (2) and replace $V_l(p,q)$ in its kernel by the identity

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

which yields

$$g_{nl}(p)=U_l(p,k)\int_0^\infty dq\,q^2q^l\frac{g_{nl}(q)}{-\alpha_n^2-q^2}+\int_0^\infty dq\,q^2\frac{U_l(p,q)-U_l(p,k)}{-\alpha_n^2-q^2}q^l g_{nl}(q)\ . \quad (8)$$

By comparing this with Eq. (4), we then find that $W_{kl}(p,k;-\alpha_n^2)$ is related to $g_{nl}(p)$ by

$$g_{nl}(p)=W_{kl}(p,k;-\alpha_n^2)\int_0^\infty dq\,q^2q^l\frac{g_{nl}(q)}{-\alpha_n^2-q^2}\ . \quad (9)$$

Note that this result shows explicitly that the bound state solutions $W_{kl}(p,k;-\alpha_n^2)$ of Eq. (4) are independent of the choice of k, as they must be, of course. The condition (5), for $\alpha^2=\alpha_n^2$, is now obtained by simply integrating the relation (9). From Eq. (9) it also follows [cf. Eqs. (1) and (6)] that the normalization C_{nl} in Eq. (6) is represented by

$$C_{nl}=\int_0^\infty dq\,q^2q^l\frac{g_{nl}(q)}{-\alpha_n^2-q^2}=\int_0^\infty dq\,q^2q^l\psi_{nl}(q)\ . \quad (10)$$

This completes the proof.

The relation (9) shows explicitly that solving Eq. (4) for energies for which the condition (5) holds is equivalent to solving the homogeneous LS equation (2). Both solutions differ only by the constant C_{nl}, but since the normalization of $g_{nl}(p)$ is not determined by Eq. (2), it can be adjusted to give C_{nl} any desired value. However, in writing Eq. (9) or Eq. (8) we have made the basic assumption that the integral (10) exists. In view of the factor q^l in the integrand, this seems to be nontrivial, especially for higher partial waves, but in the Appendix it is shown that this is indeed the case. In fact, it is proved there that the existence of the integral (10) is the momentum space equivalent of the usual coordinate space regularity condition at the origin, satisfied, of course, by the corresponding transform of $\psi_{nl}(q)$.

Clearly, in contrast to Eq. (2), the inhomogeneous integral equation (4) possesses solutions for any (negative) value of the energy $E=-\alpha^2$. Among these solutions the bound state solutions corresponding to Eq. (2) are identified by the condition (5), which allows one to determine the binding energies α_n^2 within the context of Eq. (4). The relations (4)–(6), therefore, establish a complete, self-contained alternative to the usual approach to the bound state problem. In Sec. IV we shall point out some properties of our method which are of importance in practical applications.

III. THE SCATTERING FORMALISM

In contrast to the usual approaches, we have treated in the preceding section the negative energy domain by an *inhomogeneous* integral equation. Such a treatment is usually associated only with the scattering problem at positive energies. Since, by construction, we may continuously vary the energy parameter $E=-\alpha^2$ in Eq. (4) for all energies $E\le 0$, it seems natural to expect that Eq. (4) remains of significance if we allow E to become positive.

In doing so, however, we find that the kernel of Eq. (4) acquires a singularity at $q^2=E\ (>0)$. The simplest way of removing this singularity now is to choose the previously free parameter k as $k^2=E$. The singularity is then cancelled by the zero of the difference $U_l(p,q)-U_l(p,k)$ at $q=k$, and Eq. (4) becomes well defined also for positive energies:

$$W_{kl}(p,k;k^2)=U_l(p,k)+\int_0^\infty dq\,q^2\frac{U_l(p,q)-U_l(p,k)}{k^2-q^2}q^l\times W_{kl}(q,k;k^2)\ . \quad (11)$$

It develops now that this result represents a special case of a *nonsingular scattering equation*.[2] Its solution, referred to here as the W matrix, is real and completely determines the partial wave half on-shell T matrix.

This is easily seen by starting from the LS equation for the T matrix at the energy $E=k^2$,

$$T_l(p,k;k^2+i0)=V_l(p,k)+\int_0^\infty dq\,q^2\frac{V_l(p,q)}{k^2+i0-q^2}\times T_l(q,k;k^2+i0)\ , \quad (12)$$

and replacing the potential matrix element $V_l(p,q)$ by the splitting (7). With the definition (3), one then obtains

$$T_l(p,k;k^2+i0)=U_l(p,k)\frac{k^l}{F_l(k)}+\int_0^\infty dq\,q^2\frac{U_l(p,q)-U_l(p,k)}{k^2-q^2}q^l\times T_l(q,k;k^2+i0)\ , \quad (13)$$

where the function $F_l(k)$ is defined by

$$\frac{1}{F_l(k)}=1+k^{-l}\int_0^\infty dq\,q^2q^l\frac{T_l(q,k;k^2+i0)}{k^2+i0-q^2}\ . \quad (14)$$

Note here the great structural similarity between Eqs. (8) and (13) (see also the Appendix). And just as Eqs. (8) and (4) led to the representation (9) for the bound state form factor, we find now, by comparing Eq. (13) with (11), that the half on-shell T matrix may be written as

$$T_l(p,k;k^2+i0)=W_{kl}(p,k;k^2)\frac{k^l}{F_l(k)}\ . \quad (15)$$

Using this result in Eq. (14), this then allows one to recast $F_l(k)$ in a representation in terms of $W_{kl}(q,k;k^2)$,

$$F_l(k)=1-\int_0^\infty dq\,q^2q^l\frac{W_{kl}(q,k;k^2)}{k^2+i0-q^2}\ . \quad (16)$$

This completes the demonstration that the partial wave half on-shell T matrix is completely determined by the solution of the nonsingular W-matrix equation (11).

Equation (11) is not new. As noted above, it is a special example of a wide class of nonsingular formulations of

the two-body scattering problem in momentum space.[2] These investigations were initiated by the works of Noyes and Kowalski,[4] and it was later realized[2] that all of these momentum space approaches are closely related to a coordinate space method by Sasakawa.[7] Within the context of nonsingular scattering equations, Eq. (11) has been investigated by Blasczak and Fuda.[3] The equation as such, however, had been given already in 1963 by Brown *et al.* [Ref. 8, Eq. (17)]. These authors were interested in applications to complex angular momenta and do not seem to have realized the significance of their formulation in terms of a nonsingular momentum space equation for the scattering problem. Nevertheless, to our knowledge, they were the first to write down such an equation.

What is new, as far as we know, about our approach described here is the finding that the nonsingular formulation of the scattering problem is obtained as the natural extension of our particular way of treating the bound state problem in terms of an inhomogeneous integral equation. The W-matrix equations for the bound state problem, Eq. (4), and the scattering problem, Eq. (11), provide a very convenient unified description of these two problems. This unification was arrived at here in a constructive way; in the next section we shall investigate the mathematical reason behind it.

Of course, the unified description of the bound state and scattering energy regimes as given here is not unique. The essential step in deriving Eqs. (4) and (11) was the replacement of the potential matrix element $V_l(p,q)$ by the splitting (7), but it is clear that any splitting of the general form[2]

$$V_l(p,q)=V_l(p,k)\gamma_l(k,q) + [V_l(p,q)-V_l(p,k)\gamma_l(k,q)] \tag{17}$$

will produce similar results provided the function $\gamma_l(k,q)$ is chosen such that all integrals involved converge and it satisfies the constraint

$$\gamma_l(k,k)=1 . \tag{18}$$

In our particular case [cf. Eq. (7)], we have

$$\gamma_l(k,q)=(q/k)^l . \tag{19}$$

This choice is distinguished by the following properties: It cancels the k^l threshold behavior of the potentials $V_l(p,k)$ [cf. Eq. (3) and discussion there], and provides the q^l factor that allows one to relate the existence of all relevant momentum space integrals to the coordinate space regularity condition at the origin (see Appendix). Obviously, Eq. (19) is the simplest choice with these two features. Furthermore, and most important, it is the only choice which allows one to make contact—in a direct way—with well-established results of the traditional coordinate space treatment of the two-body problem. This will be the subject of the next section. As an example, we mention already here that, if the underlying interaction is local, the function $F_l(k)$ of Eqs. (14) and (16) is the Jost function (see also Ref. 3).

IV. THE COORDINATE SPACE APPROACH

In this section we want to relate the momentum space formulations of the preceding sections to the more traditional configuration space approach found in most textbooks. Since most mathematically rigorous results in the nonrelativistic two-body problem have been derived under the assumption of a local potential $V(r)$ that is the same in all partial waves, we shall also adopt this assumption for the purpose of the following comparison. Without going into details here, we shall further assume that this potential is such that all of the formal manipulations performed below are meaningful. Details, and more background information on the textbook results quoted below, may be found, e.g., in Ref. 1.

Following closely the conventions and notations of Ref. 1, let us first recapitulate some well-known definitions of the two-body scattering theory. In terms of a local potential $V(r)$, the momentum space partial wave potential matrix elements read

$$V_l(p,q)=\frac{2}{\pi}\int_0^\infty dr\, r^2 j_l(pr)V(r)j_l(qr) , \tag{20}$$

where the $j_l(\rho)$ are the spherical Bessel functions. The half on-shell T-matrix elements at the energy $E=k^2$ are given as

$$T_l(p,k;k^2+i0)=\frac{2}{\pi}\int_0^\infty dr\, r^2 j_l(pr)V(r)\tilde{\psi}_{l,k}^{(+)}(r) , \tag{21}$$

with $\tilde{\psi}_{l,k}^{(+)}(r)$ being the partial wave scattering wave function. This physical solution of the Schrödinger equation is, of course, regular at the origin, and its normalization is determined at infinity by the usual boundary condition. However, for the sake of a more concise presentation, both of these conditions may be cast formally into one single expression by requiring that the physical solution behave as

$$\tilde{\psi}_{l,k}^{(+)}(r)\underset{r\to 0}{\to}\frac{j_l(kr)}{F_l(k)} \tag{22}$$

at the origin, where $F_l(k)$ is the Jost function. This assumes, of course, knowledge of the latter, and that is why this is only a formal way of writing the boundary conditions for the physical solution, because to know the Jost function means that one has practically solved the scattering problem.

Now, in addition to the physical solution, one often considers the so-called "regular" solution $\tilde{\phi}_{l,k}(r)$ of the Schrödinger equation which is related to $\tilde{\psi}_{l,k}^{(+)}(r)$ by separating out the Jost function, viz.,

$$\tilde{\psi}_{l,k}^{(+)}(r)=\frac{\tilde{\phi}_{l,k}(r)}{F_l(k)} . \tag{23}$$

Of course, both $\tilde{\psi}_{l,k}^{(+)}$ and $\tilde{\phi}_{l,k}$ are regular at the origin, but the latter derives its name from the fact that its normalization is also fixed at the origin by relating it to $j_l(kr)$ only, i.e.,

$$\tilde{\phi}_{l,k}(r)\underset{r\to 0}{\to} j_l(kr) . \tag{24}$$

The regular solution $\tilde{\phi}_{l,k}(r)$ is real and is, in general, as we

shall see, a much simpler function to work with than $\tilde{\psi}_{l,k}^{(+)}(r)$. Its knowledge completely determines the right-hand side of (23) because also the Jost function is given via $\tilde{\phi}_{l,k}$ as

$$F_l(k)=1+k\int_0^\infty dr\, r^2 h_l^{(+)}(kr)V(r)\tilde{\phi}_{l,k}(r)\ , \tag{25}$$

where $h_l^{(+)}(\rho)$ is the Hankel function with outgoing wave asymptotic behavior. In other words, if one knows $\tilde{\phi}_{l,k}(r)$, one has solved the scattering problem.

A. The scattering W matrix

We claim now that the W matrix of Eq. (11) is related to this regular solution by

$$W_{kl}(p,k;k^2)k^l=\frac{2}{\pi}\int_0^\infty dr\, r^2 j_l(pr)V(r)\tilde{\phi}_{l,k}(r)\ ; \tag{26}$$

that is, in much the same way in which the T matrix is related to the physical scattering solution. [The factor k^l on the left-hand side of (26) occurs here because W_{kl} of Eq. (11) is determined not in terms of the potential V_l, as the T matrix in the LS equation (12), but in terms of the reduced quantity U_l.] The proof of (26) is relatively straightforward; all we have to show is that, with (26) as the basic definition, we can reproduce Eq. (11): Using the completeness of the spherical Bessel functions and the formula

$$k\int_0^\infty dr\, r^2 h_l^{(+)}(kr)j_l(qr)=-\left[\frac{q}{k}\right]^l\frac{1}{k^2+i0-q^2}\ , \tag{27}$$

one first immediately verifies that the Jost function (25) may indeed be cast into the momentum space representation (16) if one uses Eq. (26). We had already anticipated this finding by using the same notation $F_l(k)$ in both Eqs. (16) and (25). [Within the context of their investigation of Eq. (11), the Jost function representation (16) has also been given in Ref. 3.] In the next step, employing Eq. (23) in the T-matrix definition (21) then yields Eq. (15); and using the latter representation to replace the T matrices in the LS equation (12), this obviously leads finally to the W-matrix equation (11) if one multiplies the LS equation by $F_l(k)$ in the form (16).

The result (26) means, of course, that many of the established features of the regular solution $\tilde{\phi}_{l,k}(r)$ may be used in investigating properties of the W-matrix equation (11). For example, it is well known that the (inhomogeneous) coordinate space integral equation solved by $\tilde{\phi}_{l,k}(r)$ is of the Volterra type and one can show (see, e.g., Ref. 1) that the series for $\tilde{\phi}_{l,k}(r)$ obtained by iterating this integral equation converges for a local potential of arbitrary strength, provided only it satisfies

$$\int_0^\infty dr\,|rV(r)|<\infty\ . \tag{28}$$

Clearly, this implies that, if (28) holds true, then also the W-matrix equation (11) can be solved by iteration, since the integration over $\tilde{\phi}_{l,k}$ according to (26) does not alter the convergence proof in any essential way. The numerical examples presented in Sec. VI show that the rate of convergence of the iterative solution of Eq. (11) may indeed be very fast.

The condition (28) for the convergence of the iterative solution of the W-matrix equation (11) was arrived at here by simply looking up well-known results quoted in textbooks for the regular solution. It was shown by Coester[9] that, if the underlying interaction is local, the condition (28) is sufficient for the convergence of the iterative series for *any* nonsingular equation obtained from a splitting of the potential matrix elements of the general form (7). As was pointed out by Coester, the reason behind it is that in coordinate space all of these equations correspond to Volterra-type integral equations, similar to the one for the regular solution. Unfortunately, no general convergence criteria are known for nonlocal potentials.

B. The bound state W matrix

The connection (26) between the regular solution $\tilde{\phi}_{l,k}(r)$ and the W matrix, which was established here for scattering energies $E=k^2\geq 0$, now also provides an alternative derivation of our bound state method. It is well known[1] that the coordinate space bound state wave function $\tilde{\psi}_{nl}(r)$ [cf. Eq. (A1) in the Appendix] is obtained, up to some constant, from $\tilde{\phi}_{l,k}(r)$ by analytically continuing the latter in the on-shell momentum k to the pure imaginary value $k=i\alpha_n$ $(\alpha_n>0)$:

$$\tilde{\phi}_{l,i\alpha_n}(r)=i^l D_{nl}\tilde{\psi}_{nl}(r)\ . \tag{29}$$

Here, we have used the fact[1] that the proportionality constant may be written as a factor i^l times a real constant D_{nl}. With this relation, and Eqs. (A1) and (20), we then find from (26) that

$$W_{i\alpha_n l}(p,i\alpha_n;-\alpha_n^2)(\alpha_n)^l=D_{nl}\int_0^\infty dq\, q^2 V_l(p,q)\psi_{nl}(q)\ , \tag{30}$$

whence

$$\frac{W_{i\alpha_n l}(p,i\alpha_n;-\alpha_n^2)}{-\alpha_n^2-p^2}\frac{(\alpha_n)^l}{D_{nl}}=\psi_{nl}(p)\ . \tag{31}$$

This result is very similar to Eq. (6); it differs only inasmuch as the free parameter k of our bound state W-matrix equation (4) is now fixed at $k=i\alpha_n$, in accordance with the consequent analytic continuation of Eqs. (26) and (11). However, as was pointed out in Sec. II after Eq. (9), the bound state solutions $W_{kl}(p,k;-\alpha_n^2)$ of Eq. (4) do not depend on the choice of k; what matters is only the correct choice of the bound state energy $E=-\alpha_n^2$. Therefore, the W matrices of Eqs. (6) and (31) are identical and we find that

$$D_{nl}=\frac{(\alpha_n)^l}{C_{nl}}\ , \tag{32}$$

which relates the constant D_{nl} of Eq. (29) with the integral (10).

In order to obtain the bound state function $\psi_{nl}(p)$, Eq. (31) suggests that the parameter k in Eq. (4) ought to be chosen as $k=i\alpha$. However, as mentioned above, we know from the findings of Sec. II that this is not necessary. It is quite instructive to investigate in a little more detail in the context of the relation (26) why this is not the case. To this end, let us regroup the terms in Eq. (4) and write it as

$$W_{kl}(p,k;-\alpha^2)=U_l(p,k)\left[1-\int_0^\infty dq\,q^2q^l\frac{W_{kl}(q,k;-\alpha^2)}{-\alpha^2-q^2}\right]+\int_0^\infty dq\,q^2\frac{U_l(p,q)}{-\alpha^2-q^2}q^lW_{kl}(q,k;-\alpha^2)\ . \tag{33}$$

The only place where k enters this equation *as input* is in the function $U_l(p,k)$, which multiplies the expression in the large square brackets. If we now set $k=i\alpha$, this equation is the consequent analytic continuation of Eq. (11), and of Eq. (26). The important point to note then is that (for $k=i\alpha$) the term in the large square brackets is the value of the Jost function [cf. Eq. (16)] at $i\alpha$, $F_l(i\alpha)$. Hence, because of the well-known one-to-one correspondence between the positions of the bound states and of the roots of the Jost function,[1] we know then that the large square brackets (for $k=i\alpha$) vanish if and only if $\alpha^2=\alpha_n^2$. However, if $\alpha^2=\alpha_n^2$, and if therefore the expression in the large square brackets vanishes, then the function $U_l(p,k=i\alpha_n)$, which multiplies it, may be replaced by any (nonpathological) function, since the product is zero anyway. In particular, we may relax the requirement that $k=i\alpha_n$ in $U_l(p,k)$ and allow k to become a free parameter. As long as we do not change the energy $\alpha^2=\alpha_n^2$ in the denominators of Eq. (33), we obviously will not change its solution, and therefore the relation (31), by this procedure. But this is precisely the way in which Eq. (4) differs from a consequent analytic continuation of Eq. (11). We thus have arrived here independently at the results of Sec. II, starting from Eq. (26) as the basic definition. Moreover, we see that the eigenvalue condition (5) is very closely related to the properties of the Jost function.

The fact that, in order to treat the bound state case according to Eqs. (4)—(6) we are not required to consider pure imaginary values of k, is of obvious practical advantage: the functions $U_l(p,k)$ are much more readily available for real k. [It is worth noting in this context, however, that even for pure imaginary $k=i\alpha$, the functions $U_l(p,k)$ are real, which was one of the reasons for introducing them.] A further convenient feature in numerical applications is that for real k the bound state equation (4) may be solved by the same computer code as the scattering equation (11) by changing only a few parameters.

However, the most important advantage of being allowed to choose k real in Eq. (4) will only become apparent in the considerations of the next section: As we shall see, this feature will help us avoid the so-called dynamical singularities originating from the analytic continuation of the potential matrix elements $V_l(p,q)$ to pure imaginary momenta.

To conclude this section, let us finally emphasize that the results of Secs. II and III are, of course, valid irrespective of whether the potential is local or not. As stated at the beginning of this section, the local potential $V(r)$ was chosen here solely for the purpose of comparison.

V. THE OFF-SHELL GENERALIZATION

Since the half on-shell T matrix completely determines the physical scattering wave function [cf. Eq. (A5)], the W matrix of Eq. (11) provides, of course, a complete solution of the scattering problem via Eqs. (15) and (16). However, for those applications in which the fully off-shell two-body T matrix is required, it will be advantageous to work with an off-shell generalization of Eq. (11). The specific application we have in mind concerns the use of the two-body T matrix as input in Faddeev-type formulations of the three-body problem.[5] The particular kinematical situation in which the two-body T matrix enters the three-body equations requires the knowledge of the off-shell T-matrix elements $T_l(p,p';E+i0)$ for all real momenta p and p' and for all energies E ranging from a given three-body center-of-mass energy all the way down to minus infinity.[5] As we shall see, the smooth transition from the positive to the negative energy domain as afforded by our approach makes the W matrix particularly well suited in dealing with such a situation.

To this end, we need an off-shell generalization of Eqs. (4) and (11). In analogy to the off-shell T matrix [cf. Eq. (38)], we therefore define the off-shell W matrix at the energy E by

$$W_{kl}(p,p';E)=U_l(p,p')+\int_0^\infty dq\,q^2\frac{U_l(p,q)-U_l(p,k)}{E-q^2}q^l\times W_{kl}(q,p';E)\ , \tag{34}$$

where the parameter k is subject to the following constraints:

$$k^2=E \quad \text{for } E\geq 0\ ,\qquad k \text{ arbitrary for } E<0\ . \tag{35}$$

With these choices, the off-shell generalization (34) is real and nonsingular at all energies; obviously, for $p'=k$ we recover the bound state equation (4) for $E<0$ and the scattering equation (11) for $E\geq 0$.

Furthermore, in order to be able to choose k different from $k^2=E$ at negative energies, we also need an appropriate generalization of the Jost function (16). If we define

$$\hat{F}_{kl}(E+i0)=1-\int_0^\infty dq\,q^2q^l\frac{W_{kl}(q,k;E)}{E+i0-q^2}\ , \tag{36}$$

this function obviously is identical with the Jost function at positive energies,

$$\hat{F}_{kl}(k^2+i0)\equiv F_l(k)\ , \tag{37}$$

and at negative energies, where $k^2\neq E$, this function is real and it is zero if and only if $E=-\alpha_n^2$. In other words, its inverse $1/\hat{F}_{kl}(E+i0)$ contains all the information on the scattering cut and possible resonances, and it contains all bound state poles.

The relevance of Eqs. (34) and (36) for the off-shell T matrix is established by noting that the off-shell LS equation,

$$T_l(p,p';E+i0)=V_l(p,p') + \int_0^\infty dq\, q^2 \frac{V_l(p,q)}{E+i0-q^2} T_l(q,p';E+i0), \tag{38}$$

is solved in terms of the W matrix of Eq. (34) by

$$T_l(p,p';E+i0)=W_{kl}(p,p';E)p'^l + \frac{W_{kl}(p,k;E)}{\hat{F}_{kl}(E+i0)} \times \int_0^\infty dq\, q^2 q^l \frac{W_{kl}(q,p';E)}{E+i0-q^2} p'^l . \tag{39}$$

This equation is obtained from (38) after some algebra with the help of the splitting (7). It implies, in particular, that

$$T_l(p,k;E+i0)=W_{kl}(p,k;E)\frac{k^l}{\hat{F}_{kl}(E+i0)} . \tag{40}$$

At positive energies $E=k^2$, this relation is identical to the half on-shell result (15), of course. At negative energies, however, it is different because k may be chosen real and $\hat{F}_{kl}$ is then no longer the Jost function. Now using Eq. (40), we find, after some more algebra, from Eqs. (34) and (38), that the integral in (39) may be expressed as

$$\int_0^\infty dq\, q^2 q^l \frac{W_{kl}(q,p';E)}{E+i0-q^2} p'^l = \frac{W_{kl}(p',k;E)}{W_{kl}(k,k;E)} k^l - \hat{F}_{kl}(E+i0)\frac{W_{kl}(k,p';E)}{W_{kl}(k,k;E)} p'^l , \tag{41}$$

where we have used $V_l(p,p')=V_l(p',p)$.

Now inserting (41) into (39), this finally leads to

$$T_l(p,p';E+i0)=W_{kl}(p,k;E)\Delta_{kl}(E+i0)W_{kl}(p',k;E) + R_{kl}(p,p';E) , \tag{42}$$

where

$$\Delta_{kl}(E+i0)=\frac{k^l}{W_{kl}(k,k;E)\hat{F}_{kl}(E+i0)} \tag{43}$$

and

$$R_{kl}(p,p';E)=\left[W_{kl}(p,p';E) - \frac{W_{kl}(p,k;E)W_{kl}(k,p';E)}{W_{kl}(k,k;E)} \right] p'^l . \tag{44}$$

Equation (42) is the central result of this section; it provides a representation of the off-shell T matrix which is well defined at all energies and has several attractive additional features: The first term on the right-hand side of (42), which is separable in the momenta p and p', contains all the scattering cut information via $\hat{F}_{kl}(E+i0)$ in Eq. (43). Furthermore, with the help of the bound state formalism of Sec. II, it is very easy to extract the behavior of the T matrix around the bound state poles because it is already given explicitly in terms of the zeros of $\hat{F}_{kl}$ and the corresponding bound state form factors $W_{kl}(p,k;-\alpha_n^2)$ [cf. Eqs. (5) and (6)]. The second term on the right-hand side of (42) is real and nonsingular for all energies and it vanishes if either p or p' is equal to k, which means, in particular, that it vanishes half on-shell for scattering energies $E \geq 0$.

For positive energies, the representation (42) is very similar to the one obtained by Noyes and Kowalski[4] in their nonsingular formulations of the scattering problem. The main difference, in our notation, lies in the way in which the function Δ_{kl} of (43) is written. Whereas we write it essentially in terms of the function $\hat{F}_{kl}$ (which, at positive energies, is identical to the Jost function), Noyes and Kowalski write it as ($E=k^2 \geq 0$)

$$\Delta_{kl}(k^2+i0)=\frac{T_l(k,k;k^2+i0)}{[W_{kl}(k,k;k^2)]^2} , \tag{45}$$

i.e., in terms of the on-shell T matrix $T_l(k,k;k^2+i0)$ [cf. Eq. (15)]. Of course, this is only a technical difference at positive energies. At negative energies, however, the analytic continuation of the on-shell T matrix acquires the so-called dynamical singularities (i.e., the left-hand cut familiar from dispersion relations),[1] which originate from the corresponding analytic continuation of the potential matrix element $V_l(k,k)$ to pure imaginary momenta $k=i\alpha$ ($\alpha>0$). This fact makes the Noyes-Kowalski representation of the T matrix impractical as an input to the three-body problem, because there the negative energy domain of the two-body T matrix constitutes an important and indispensable part of the required two-body input.[5]

Obviously, this shortcoming does not arise for our representation (42) because at negative energies, as we have shown, we no longer need to impose the on-shell condition $k^2=E$, but rather allow k to be chosen freely. As emphasized above already, our representation of the off-shell T matrix is free of any unwanted singularities at all energies; it only possesses the scattering cut and the bound state poles. In other words, it has, for all energies, only those singularities which are present already in $T_l(p,p';E+i0)$, and no additional artificial ones.

In view of all these properties of Eq. (42), we feel that it provides a practical representation of the required two-body input for three-body calculations. In this context, one of the most attractive features of (42) is that *all* of the dominant scattering and bound state information is contained in one single, *separable* term, which, if used as the lowest order two-body input in three-body calculations, would greatly simplify such calculations. The remainder R_{kl} may be taken into account perturbatively, or perhaps, it may even be neglected.

VI. NUMERICAL EXAMPLES AND CONCLUSIONS

Before we give a summarizing assessment of our approach, let us present briefly the results of some numerical test calculations.

A. Numerical results

In order to test the practical applicability of our method, we have used the s-wave projection of version III of the local Malfliet-Tjon potential[6] (MT III) as an input to our W-matrix equations.

In the bound state case, we have solved Eq. (4) for a wide range of negative energies $E=-\alpha^2$ and various choices of the parameter k. We found that the bound state condition (5), which corresponds, of course, to a zero of the function $\hat{F}_{kl}(-\alpha^2)$ of (36), allows one a very accurate determination of the binding energy, which is at least as reliable as the usual search for the zero of the Fredholm determinant of Eq. (2). In general, our experience is that the inhomogeneous integral equation (4) allows for a more stable numerical solution by standard inversion routines than the homogeneous equation (2).

Since the local MT III potential satisfies the condition (28), Eq. (4) may be solved by iteration for this case. Figure 1 shows the rapid convergence of Eq. (4) for the bound state wave function according to Eq. (6). These calculations were done with $k=0$, and our numerical investigations suggest that this is generally the best choice in order to achieve rapid convergence when iterating Eq. (4). Without going into details here, we mention that this finding is intimately connected to the fact that the bound state wave function $\psi_{nl}(p)$ has a pole for pure imaginary $p=i\alpha_n$ [cf. Eq. (1)], and $k=0$ is the real value closest to this pole position.

For scattering energies, the W-matrix equation (11)—being nonsingular and real—is obviously much easier to solve numerically than the LS equation (12). As a matter of fact, changing a few parameters, Eq. (11) can be solved by the same computer code, and with equal ease, as the bound state equation (4). In terms of the solution of Eq. (11), the scattering length a and the phase shifts for s waves are given by (index kl omitted)

$$\frac{1}{a}=\frac{2}{\pi}\frac{1}{W(0,0;0)}\left[1+\int_0^\infty dq\, W(q,0;0)\right] \tag{46}$$

and

$$\tan\delta(k)=\frac{-\frac{\pi}{2}kW(k,k;k^2)}{1-\int_0^\infty dq\frac{q^2W(q,k;k^2)-k^2W(k,k;k^2)}{k^2-q^2}}, \tag{47}$$

respectively. The numerical results for the MT III potential obtained in this way were found to be in perfect agreement with those of a variable phase method[1] calculation.

Furthermore, we present in Fig. 2 the plots of the iterative solution of Eq. (11) for the MT III potential. Again, as in the bound state case of Fig. 1, the third order iteration of Eq. (11) is already indistinguishable from the exact result. [A point worth noting in this context is that, since the W matrix is real, the T matrix remains unitary even if W_{kl} in Eq. (15), or also in Eq. (42), is replaced by an approximation.] This particular calculation was done at an energy of 25 MeV; in Fig. 3 we compare the bound state solution of Eq. (4) at the deuteron energy of -2.27 MeV with two solutions of the scattering equation (11) at 25 and 50 MeV. As can be seen, these plots look very similar in structure and seem to differ essentially only by an overall (energy dependent) normalization factor. We believe that this finding actually explains—at least partially—the success of separable approximations of the two-body T matrix, because in the dominant first (separable) term on the right-hand side of the T-matrix representation (42) these overall factors largely cancel.

Summarizing the numerical aspects of our approach, we think that it indeed provides a reliable and practical alternative to the traditional methods of solving the two-body problem. We have demonstrated here that with our approach the scattering case is technically not more difficult than the bound state case.

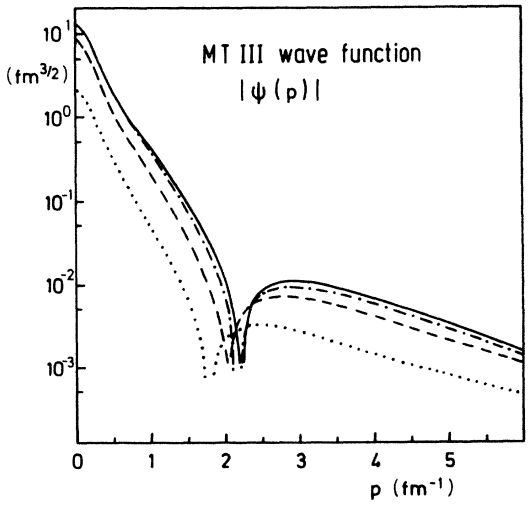

FIG. 1. The bound state wave function according to Eq. (6) using iterations of Eq. (4): exact result (solid line), zeroth (dotted), first (dashed), and second (dashed-dotted) order iterations. Higher orders are indistinguishable from the exact result.

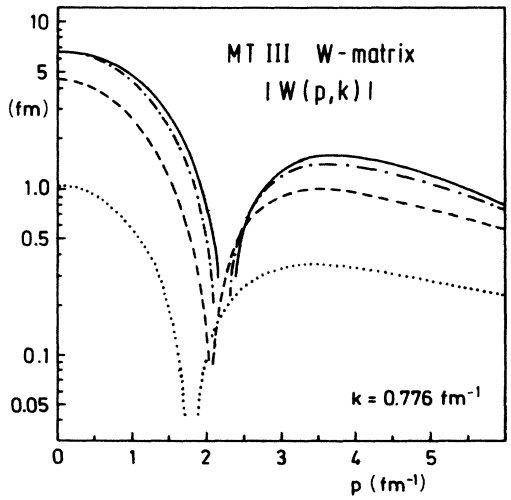

FIG. 2. The iterative solution of the scattering W-matrix equation (11). The notation is the same as in Fig. 1.

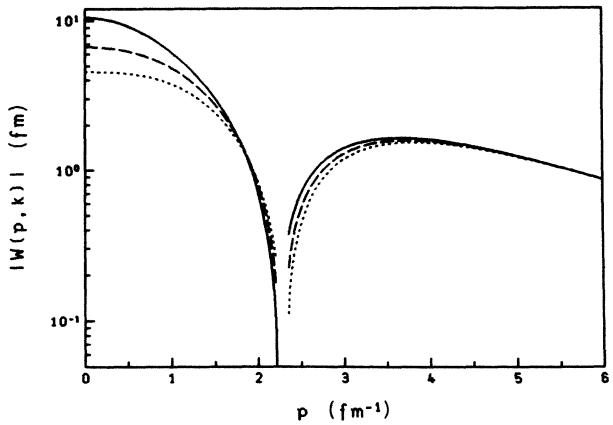

FIG. 3. Comparison of the bound state W matrix [Eq. (4)] at -2.27 MeV (solid line) with two solutions of the scattering equation (11) at 25 MeV (dashed line) and 50 MeV (dotted line).

B. Conclusions

We have treated here the bound state problem by a method which is usually associated only with the scattering problem, i.e., by an *inhomogeneous* integral equation. This allowed us to make a smooth transition between the bound state and scattering regimes and enabled us to show that nonsingular scattering equations arise naturally in the context of such a formulation. This is the new unifying aspect brought about by our treatment of the two-body problem. The finding that both of these regimes can be handled with the same equation, the W-matrix equation (34) (or its variants as given in Secs. II and III), is interesting not only from a purely formal point of view, but has also some very practical consequences, most of which have already been discussed in the course of the presentation of our method.

Let us emphasize here once again that in our opinion the most important of these practical consequences is the fact that the representation (42) of the off-shell T matrix is also applicable at negative energies (in contrast to the similar Noyes-Kowalski representation) and that it may therefore be used as an input in three-body calculations. Preliminary test calculations in the three-nucleon problem indicate that the first (separable) term of Eq. (42) is indeed an excellent approximation to the T matrix over a wide range of off-shell momenta.

Again on the more formal side, let us add that our formalism is, of course, particularly well suited for the investigation of resonance phenomena: these are intermediate between bound and scattering states and are therefore best treated by a method which does not distinguish formally between these two regimes.

In summary, we think that the method presented here is both formally appealing and practical. Moreover, our whole approach suggests that, for many investigations which traditionally are done in configuration space, the momentum space is actually to be preferred. As a case in point, we recall the integral representation (16) for one of the most important tools of the potential scattering theory, the Jost function $F_l(k)$. This representation is not only simple, but also practical, because the integral equation (11) can be solved very easily numerically.

Note added in proof. There exists an approach to the bound state problem by Adhikari and Tomio (Ref. 10) which is similar to the one presented in Sec. II. These authors employ the splitting (17) to arrive at their equations, however, with a $\gamma_l(k,q)$ rather different from the present choice (19). We emphasize that it is just this choice which provides the connection with the well-known coordinate space results (cf. Sec. IV and Appendix) and which, in particular, leads to the important generalization (36) of the Jost function.

APPENDIX

For the proof that the integral (10) exists, we note that the coordinate space transform of the partial wave bound state function $\psi_{nl}(q)$,

$$\tilde{\psi}_{nl}(r)=\int_0^\infty dq\, q^2 j_l(qr)\psi_{nl}(q)\ , \tag{A1}$$

is, of course, regular at the origin; in other words,

$$\lim_{r\to 0} r^{-l}\tilde{\psi}_{nl}(r) \text{ exists}\ . \tag{A2}$$

Also, the spherical Bessel functions $j_l(qr)$ are regular at the origin, and one has

$$\lim_{r\to 0} r^{-l} j_l(qr)=\frac{q^l}{(2l+1)!!}\ . \tag{A3}$$

Hence,

$$\lim_{r\to 0} r^{-l}\tilde{\psi}_{nl}(r)=\lim_{r\to 0} r^{-l}\int_0^\infty dq\, q^2 j_l(qr)\psi_{nl}(q)=\int_0^\infty dq\, q^2[\lim_{r\to 0} r^{-l} j_l(qr)]\psi_{nl}(q)=\frac{1}{(2l+1)!!}\int_0^\infty dq\, q^2 q^l\psi_{nl}(q) \text{ exists}\ . \tag{A4}$$

The interchange of the limit and the integration here is permitted because the Fourier transform (A1) is well defined for all r and the limit (A3) is valid for all q.

We thus see that the existence of the momentum space integral (10) is equivalent to the coordinate space regularity condition at the origin of the partial wave bound state function.

In fact, the existence of momentum space integrals of the type given in Eq. (10) is not restricted to the bound state case, but also holds true for the scattering wave function.

In terms of the partial wave T matrix the momentum space scattering wave function at the energy $E=k^2$ is given as

$$\psi_{l,k}^{(+)}(q)=\frac{\delta(q-k)}{k^2}+\frac{T_l(q,k;k^2+i0)}{k^2+i0-q^2}\ , \tag{A5}$$

whence

$$\int_0^\infty dq\, q^2 q^l \psi_{l,k}^{(+)}(q) = k^l\left[1-k^{-l}\int_0^\infty dq\, q^2 q^l \frac{T_l(q,k;k^2+i0)}{k^2+i0-q^2}\right]\ . \tag{A6}$$

According to Eqs. (14), (16), and the results of Sec. IV, this means that this integral is given essentially by the Jost function $F_l(k)$:

$$\int_0^\infty dq\, q^2 q^l \psi_{l,k}^{(+)}(q)=\frac{k^l}{F_l(k)}\ . \tag{A7}$$

This finding makes the similarity between Eqs. (8) and (13) even greater, because in both cases the inhomogeneities are multiplied by integrals over the corresponding wave functions: by the integral (10) for the bound state equation (8) and by (A7) for the scattering equation (13). And again, the existence of the integral (A7) is precisely equivalent to the regularity of the coordinate space transform of $\psi_{l,k}^{(+)}(q)$,

$$\tilde{\psi}_{l,k}^{(+)}(r)=\int_0^\infty dq\, q^2 q^l j_l(qr)\psi_{l,k}^{(+)}(q)\ , \tag{A8}$$

because from Eq. (22) it follows that

$$\lim_{r\to 0} r^{-l}\tilde{\psi}_{l,k}^{(+)}(r)=\frac{1}{(2l+1)!!}\frac{k^l}{F_l(k)}\ . \tag{A9}$$

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