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Unitary Variational Approximations*

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The problem of generating nonrelativistic three-body scattering amplitudes which satisfy unitarity exactly, at all energies, is studied in the context of an effective-potential theory. It is shown how the nonlinear unitarity relations can be replaced by linear integral equations, simpler in structure than the original Faddeev equations, such that for any set of input amplitudes satisfying standing-wave boundary conditions the output will be unitary. Variational principles for these input amplitudes are derived from the Faddeev equations which define them, so that approximations can be systematically improved. Attention is drawn to a particular class of approximations for which the integral equations to be solved are all of the two-body type. These approximations have the additional virtue that the trial functions which enter into the Schwinger-type variational expression are square-integrable. This property allows for a choice of trial functions based on an "effective-range" type of argument. The Schwinger principle can then be thought of as providing an analytic continuation of the effective potential from an energy domain below the breakup threshold to a limited range above it.

I. INTRODUCTION

An effective-potential approach to the few-body nonrelativistic scattering problem has been studied in some detail during the past few years. For energies below the threshold for target breakup this method benefits significantly from the existence of rigorous maximum and minimum principles for the construction of the effective potential.[1,2] The scattering amplitude can be obtained from a given approximation to the effective potential by numerical solution of a Lippmann-Schwinger equation of the two-body type. Several applications of this approach have been reported recently, in which upper and lower bounds on phase shifts for certain low-energy three-body scattering problems have been obtained.[3-5]

In the present study we are concerned with developing variational methods which preserve the unitarity of the scattering matrix. The effective potential can be thought of as a scattering matrix associated with a modified Hamiltonian with two-particle bound states removed. (The precise definition is given in Sec. II.) It therefore satisfies "unitarity" relations differing from those satisfied by the physical scattering matrix in the absence of sums over intermediate states with a pair bound. Any approximation to the effective potential which satisfies "unitarity" relations of the proper form will lead to a unitary scattering matrix, as shown in Sec. III. It is possible to continue the reduction one step further by introducing an amplitude which is Hermitian (both two- *and* three-body intermediate states removed) from which the effective potential is obtained by solution of a Heitler-type integral equation. (For energies below the breakup threshold the effective potential is itself Hermitian. We are interested here in the general case where all channels are open.) Variational principles for this Hermitian amplitude, of the Kohn and Schwinger types, can then be written down and the correct reality properties imposed without difficulty, as shown in Sec. IV. The Schwinger-type principle can be put in a form which involves only square-integrable trial functions, a property which should prove useful in practice.

In general, three-body (energy-conserving) states appear in the kernel of the above-mentioned Heitler integral equation. Present computational methods may be adequate to deal with equations of this type. It is of interest nevertheless to observe that a simplified model can be defined in which the integral *equation* can be replaced by integrals over known functions without sacrificing the exact unitarity relations for the scattering matrix. In addition the variational nature of the approximation is retained for the elastic and rearrangement components. This model is described in Sec. V and a procedure for choosing trial functions in the spirit of effective-range theory is indicated.

For simplicity we confine our attention throughout to the three-body problem in which the particles interact by means of short-ranged local two-body potentials. The Faddeev equations can then

be used to provide rigorous derivations of the variational principles. The derivations are based on techniques introduced previously for variational treatment of the breakup problem[6] and are suitably modified here to apply to elements of the effective potential rather than to the scattering matrix. The basic approach can be characterized as follows. We take the separable-potential model[7] as a zeroth-order approximation, treating the residual interaction variationally. Unitarity is preserved by formulating this problem in terms of a Heitler equation. The particular virtues of variational principles of the Schwinger type become apparent in this analysis.

II. METHOD OF EFFECTIVE POTENTIALS

For ease of reference and to establish notation the effective-potential formalism previously described[2] will be reviewed here. The starting point is the set of Faddeev equations[8] for the operators ${}^{i}T^{j}(E)$ $(i,j=1,2,3)$, in terms of which the physical scattering amplitudes for energy E can be constructed. These equations can be written in matrix form as

$$\underline{T}(E)=\underline{T}^{D}(E)+\underline{T}^{D}(E)\underline{G}_{0}(E)\underline{T}(E). \tag{2.1}$$

Here

$$[\underline{G}_{0}]_{ij}=G_{0}(1-\delta_{ij}), \tag{2.2}$$

with G_0 expressed in terms of the total kinetic-energy operator as

$$G_{0}=(E-K)^{-1}. \tag{2.3}$$

The disconnected part is given by

$$[\underline{T}^{D}]_{ij}=T_{i}\delta_{ij}. \tag{2.4}$$

The two-body transition operator T_i is defined by

$$T_{i}=V_{i}+V_{i}G_{0}T_{i}, \tag{2.5}$$

where V_i is the potential for pair i. If pair i supports a bound state (for simplicity we assume that no more than one bound state exists for each pair) we write $V_i=V_{iA}+V_{iB}$, where

$$V_{iB}=\frac{V_{i}|\chi_{i}\rangle\langle\chi_{i}|V_{i}}{\langle\chi_{i}|V_{i}|\chi_{i}\rangle}, \tag{2.6}$$

and χ_i is the bound-state wave function. Then $T_i=T_{iA}+T_{iB}$, where T_{iA} satisfies an equation of the form (2.5) with V_i replaced by V_{iA}, and T_{iB} contains the bound-state pole. It will be convenient to express T_{iB} in terms of the operators

$$\mathcal{V}_{0i}^{D}=(1+T_{iA}G_{0})|V_{i}\chi_{i}\rangle \tag{2.7}$$

and

$$\mathcal{V}_{i0}^{D}=\langle\chi_{i}V_{i}|(1+G_{0}T_{iA}), \tag{2.8}$$

which, as will be seen, represent disconnected parts of elements of the effective-potential matrix. We also introduce the propagator

$$\mathcal{G}_{i}=(\langle\chi_{i}|V_{i}|\chi_{i}\rangle-\langle\chi_{i}V_{i}|G_{iA}|V_{i}\chi_{i}\rangle)^{-1}, \tag{2.9}$$

where

$$G_{iA}=(E-K-V_{iA})^{-1}. \tag{2.10}$$

We then can write[2]

$$T_{iB}=\mathcal{V}_{0i}^{D}\mathcal{G}_{i}\mathcal{V}_{i0}^{D}. \tag{2.11}$$

When the above decomposition of T_i is inserted into Eqs. (2.1) the result can be expressed as a set of integral equations for the scattering operators whose momentum-space matrix elements give the physical scattering amplitudes.[9-11] Our notation is such that the elastic and rearrangement amplitudes, with pair j bound in the initial state and pair i bound in the final state, are represented as $\langle\vec{k}_i|\mathcal{T}_{ij}|\vec{k}_j\rangle$, where $\vec{k}_j$ is the momentum of the center of mass of pair j relative to the third particle. We find coupled equations for the operators $\mathcal{T}_{ij}$ in the form of *two*-body Lippmann-Schwinger equations:

$$\mathcal{T}_{ij}=\mathcal{V}_{ij}+\sum_{k=1}^{3}\mathcal{V}_{ik}\mathcal{G}_{k}\mathcal{T}_{kj}, \quad i,j=1,2,3. \tag{2.12}$$

The effective-potential matrix elements $\mathcal{V}_{ij}$ can be constructed in terms of the matrix $\underline{T}_A$, defined by Faddeev equations which have been modified by the replacement of $\underline{T}^D$ with $\underline{T}_A^D$. Explicitly, we have

$$\mathcal{V}_{ij}=\mathcal{V}_{i0}^{D}G_{0}\mathcal{V}_{0j}^{D}(1-\delta_{ij})+\sum_{l\neq i}\sum_{k\neq j}\mathcal{V}_{i0}^{D}G_{0}{}^{l}T_{A}^{k}G_{0}\mathcal{V}_{0j}^{D}. \tag{2.13}$$

With the operators $\mathcal{T}_{ij}$ known the remaining elements of the physical scattering matrix can be obtained by quadratures. The amplitudes for the breakup process and its inverse are represented as $\langle\vec{K}_0|\mathcal{T}_{0i}|\vec{k}_i\rangle$ and $\langle\vec{k}_i|\mathcal{T}_{i0}|\vec{K}_0\rangle$, respectively, where $\vec{K}_0$ is a six-dimensional momentum vector for the state of three free particles in the center-of-mass frame. The $3\to3$ amplitude is represented as $\langle\vec{K}_0'|\mathcal{T}_{00}|\vec{K}_0\rangle$. Let us define the effective-potential matrix elements

$$\mathcal{V}_{0i}=\mathcal{V}_{0i}^{D}+\sum_{k\neq i}T_{A}^{k}G_{0}\mathcal{V}_{0i}^{D}, \tag{2.14}$$

$$\mathcal{V}_{i0}=\mathcal{V}_{i0}^{D}+\sum_{l\neq i}\mathcal{V}_{i0}^{D}G_{0}{}^{l}T_{A}, \tag{2.15}$$

and

$$\mathcal{V}_{00}=T_{A}, \tag{2.16}$$

where we use the notation $\sum_{l=1}^{3}{}^{l}T_{A}^{k}=T_{A}^{k}$, etc. Then the equations which determine the complete scattering matrix take the form

$$\mathcal{T}_{\alpha\beta}=\mathcal{V}_{\alpha\beta}+\sum_{k=1}^{3}\mathcal{V}_{\alpha k}\mathcal{G}_{k}\mathcal{T}_{k\beta}, \quad \alpha,\beta=1,2,3,0. \tag{2.17}$$

Note that $\mathcal{U}_{ij}$, given by Eq. (2.13), has no disconnected part. This property can be maintained in any approximation generated from Eq. (2.13) by inserting an approximate form for $\underline{T}_A$. Similar approximations based on Eqs. (2.14) and (2.15) will guarantee the correct disconnected parts given by the leading terms. However, in studying the unitarity properties of the effective potential (in Sec. III) we find it convenient to express the effective potential in a different form[12] with the aid of the Faddeev equations satisfied by $\underline{T}_A$. It is easily verified that Eq. (2.13) is equivalent to

$$\mathcal{U}_{ij} = \langle \chi_i V_i | G_A | V_j \chi_j \rangle - \langle \chi_i V_i | G_{iA} | V_j \chi_j \rangle \delta_{ij}, \tag{2.18}$$

where

$$G_A = G_0 + G_0 T_A G_0 . \tag{2.19}$$

Similarly, we have in place of Eqs. (2.14) and (2.15)

$$\mathcal{U}_{0i} = (1 + T_A G_0) | V_i \chi_i \rangle \tag{2.20}$$

and

$$\mathcal{U}_{i0} = \langle \chi_i V_i | (1 + G_0 T_A), \tag{2.21}$$

respectively.

III. UNITARITY PROPERTIES

It is clear that Eqs. (2.17) generate a unitary scattering matrix since they are equivalent to the original Faddeev equations. This unitarity property may be verified directly, as shown below. One identifies in this way the properties of the effective potential and propagator which, if satisfied in any given approximation, will necessarily result in a scattering matrix which satisfies unitarity exactly.

For notational convenience we write Eqs. (2.17) in the matrix form

$$\underline{\mathcal{T}} = \underline{\mathcal{U}} + \underline{\mathcal{U}}\,\underline{\mathcal{G}}\,\underline{\mathcal{T}}, \tag{3.1}$$

or, equivalently,

$$\underline{\mathcal{T}} = \underline{\mathcal{U}} + \underline{\mathcal{T}}\,\underline{\mathcal{G}}\,\underline{\mathcal{U}}. \tag{3.2}$$

The 4×4 matrix $\underline{\mathcal{G}}$ has as its only nonvanishing elements

$$[\underline{\mathcal{G}}]_{ii} = \mathcal{G}_i, \quad i = 1, 2, 3. \tag{3.3}$$

In fact Eqs. (3.1) and (3.2) define two matrices, $\underline{\mathcal{T}}^{(+)}$ and $\underline{\mathcal{T}}^{(-)}$, the superscript indicating the sign of the infinitesimal imaginary part of the energy variable. (When in the following no sign is indicated, the positive sign will be understood.) The identity

$$\begin{aligned}\underline{\mathcal{T}}^{(+)} - \underline{\mathcal{T}}^{(-)} = {} & [\underline{1} + \underline{\mathcal{T}}^{(-)}\underline{\mathcal{G}}^{(-)}][\underline{\mathcal{U}}^{(+)} - \underline{\mathcal{U}}^{(-)}][\underline{1} + \underline{\mathcal{G}}^{(+)}\underline{\mathcal{T}}^{(+)}] \\ & + \underline{\mathcal{T}}^{(-)}[\underline{\mathcal{G}}^{(+)} - \underline{\mathcal{G}}^{(-)}]\underline{\mathcal{T}}^{(+)}\end{aligned} \tag{3.4}$$

is then readily established. From the relation

$$T_A^{(+)} - T_A^{(-)} = -(2\pi i) T_A^{(-)} \delta(E - K) T_A^{(+)}, \tag{3.5}$$

which is also satisfied by the disconnected components T_{iA}, the discontinuity $\mathcal{U}^{(+)} - \mathcal{U}^{(-)}$ can be determined. Thus, from Eq. (2.18) we find

$$\mathcal{U}_{ij}^{(+)} - \mathcal{U}_{ij}^{(-)} = -(2\pi i)[\mathcal{U}_{i0}^{(-)} \delta(E - K) \mathcal{U}_{0j}^{(+)}]_c, \qquad i, j = 1, 2, 3 \tag{3.6}$$

where the subscript c indicates that only the connected part is to be retained. In arriving at this form we used the relation

$$\langle \chi_i V_i | G_{iA}^{(+)} - G_{iA}^{(-)} | V_i \chi_i \rangle = -(2\pi i) \mathcal{U}_{i0}^{(-)D} \delta(E - K) \mathcal{U}_{0i}^{(+)D}. \tag{3.7}$$

The discontinuity relations for the remaining components $\mathcal{U}_{i0}$, $\mathcal{U}_{0i}$, and $\mathcal{U}_{00}$ may be summarized as

$$\mathcal{U}_{\alpha\beta}^{(+)} - \mathcal{U}_{\alpha\beta}^{(-)} = -(2\pi i) \mathcal{U}_{\alpha 0}^{(-)} \delta(E - K) \mathcal{U}_{0\beta}^{(+)}. \tag{3.8}$$

We observe for future reference that matrix elements of the discontinuity shown in Eq. (3.7) vanish on the energy shell. This may be seen by writing $K + V_{iA} = \mathcal{K}_i + H_{iA}$, where $\mathcal{K}_i$ is the kinetic-energy operator of the third particle relative to the center of mass of pair i, and $H_{iA} = K_i + V_{iA}$ is the Hamiltonian for pair i. Then, with E_i representing the bound-state energy, the resolvent equation for G_{iA} becomes

$$\begin{aligned}(E - \mathcal{K}_i - H_{iA})^{-1} = {} & (E_i - H_{iA})^{-1} \\ & - (E_i - H_{iA})^{-1}(E - \mathcal{K}_i - E_i) \\ & \times (E - \mathcal{K}_i - H_{iA})^{-1}.\end{aligned} \tag{3.9}$$

Now the first term on the right is independent of E, and the second term annihilates states on the energy shell due to the factor $(E - \mathcal{K}_i - E_i)$, so the above contention is proved.

The discontinuity $\underline{\mathcal{G}}^{(+)} - \underline{\mathcal{G}}^{(-)}$ in Eq. (3.4) has two contributions, arising from the branch points at the elastic and breakup thresholds. These two contributions can be computed by using Eq. (3.9), along with the relation

$$(E_i - H_{iA})^{-1} V_i | \chi_i \rangle = | \chi_i \rangle \tag{3.10}$$

(which follows from the homogeneous integral equation satisfied by χ_i and the fact that $V_{iA}|\chi_i\rangle = 0$), to express Eq. (2.9) in the form

$$\mathcal{G}_i = \frac{1}{E - \mathcal{K}_i - E_i} + \frac{1 - \langle \chi_i | G_{iA} V_i | \chi_i \rangle}{\langle \chi_i | V_i | \chi_i \rangle - \langle \chi_i | V_i G_{iA} V_i | \chi_i \rangle}. \tag{3.11}$$

When evaluated in momentum space the first term on the right-hand side will have a branch point at $E = E_i$ which is absent from the second term. The branch point at $E = 0$ arises from the singularity of G_{iA}, and the associated discontinuity can be com-

puted directly from Eq. (2.9). In this way we find that

$$\mathcal{G}_i^{(+)} - \mathcal{G}_i^{(-)} = -(2\pi i)\delta(E - \mathcal{K}_i - E_i) - (2\pi i)\mathcal{G}_i^{(-)}\mathcal{V}_{i0}^{(-)D}\delta(E-K)\mathcal{V}_{0i}^{(+)D}\mathcal{G}_i^{(+)}, \tag{3.12}$$

where we have used Eq. (3.7) in writing the second term.

The above discontinuity relations can now be used in Eq. (3.4), with the result (for $\alpha, \beta = 1, 2, 3, 0$)

$$\mathcal{T}_{\alpha\beta}^{(+)} - \mathcal{T}_{\alpha\beta}^{(-)} = -(2\pi i)\mathcal{T}_{\alpha 0}^{(-)}\delta(E-K)\mathcal{T}_{0\beta}^{(+)} - (2\pi i)\sum_{i=1}^{3}\mathcal{T}_{\alpha i}^{(-)}\delta(E - \mathcal{K}_i - E_i)\mathcal{T}_{i\beta}^{(+)} \tag{3.13}$$

plus terms which vanish when on-shell matrix elements of these operator relations are constructed. Equations (3.13) are equivalent to the usual unitarity relations since $\mathcal{T}_{\alpha\beta}^{(-)} = \mathcal{T}_{\beta\alpha}^{(+)\dagger}$.

The preceding discussion shows that the problem of preserving unitarity, i.e., of satisfying Eqs. (3.13) in a given approximation, can be transferred to the problem of finding solutions to Eqs. (3.6), (3.8), and (3.12). The advantage of this reformulation lies in the simpler structure of Eqs. (3.6) and (3.8); the elastic and rearrangement components do not appear on the right-hand sides.

We can think of Eqs. (2.17) as representing a partial linearization of the unitarity relations. This process can be completed by the introduction of a Heitler-type transformation of the equations which define the effective potential. To do this it is convenient to express Eq. (2.19) in the form

$$G_A = G_0 + G_0 V_A G_A, \tag{3.14}$$

with

$$V_A = \sum_{i=1}^{3} V_{iA}.$$

If we write

$$G_0 = G_0^P - i\pi\,\delta(E-K), \tag{3.15}$$

and introduce G_A^P as the solution of

$$G_A^P = G_0^P + G_A^P V_A G_0^P, \tag{3.16}$$

we have the identity

$$G_A = G_A^P - i\pi(G_A^P V_A + 1)\delta(E-K)(1 + V_A G_A). \tag{3.17}$$

Similarly, we see that

$$G_{iA} = G_{iA}^P - i\pi(G_{iA}^P V_{iA} + 1)\delta(E-K)(1 + V_{iA}G_{iA}). \tag{3.18}$$

The effective-potential matrix associated with the "standing wave" resolvent G_A^P can be defined as follows:

$$\mathcal{V}_{ij}^P = \langle \chi_i V_i \,|\, G_A^P \,|\, V_j \chi_j\rangle - \langle \chi_i V_i \,|\, G_{iA}^P \,|\, V_i \chi_i\rangle \delta_{ij}, \tag{3.19}$$

$$\mathcal{V}_{0i}^P = (1 + V_A G_A^P)\,|\, V_i \chi_i\rangle, \tag{3.20}$$

$$\mathcal{V}_{i0}^P = \langle \chi_i V_i \,|\, (1 + G_A^P V_A), \tag{3.21}$$

$$\mathcal{V}_{00}^P = V_A + V_A G_A^P V_A. \tag{3.22}$$

When Eqs. (3.17) and (3.18) are used in the expressions for the effective-potential matrix given at the end of Sec. II we obtain the equations

$$\mathcal{V}_{ij} = \mathcal{V}_{ij}^P - i\pi[\mathcal{V}_{i0}^P\delta(E-K)\mathcal{V}_{0j}]_c, \tag{3.23}$$

for $i, j = 1, 2, 3$, while the remaining elements $\mathcal{V}_{0i}$, $\mathcal{V}_{i0}$, and $\mathcal{V}_{00}$ satisfy

$$\mathcal{V}_{\alpha\beta} = \mathcal{V}_{\alpha\beta}^P - i\pi\mathcal{V}_{\alpha 0}^P\delta(E-K)\mathcal{V}_{0\beta}. \tag{3.24}$$

The usual property of Heitler-type equations hold here: Given any set $\mathcal{V}_{\alpha\beta}^P$ with no discontinuity, the correct discontinuity relations are guaranteed for solutions of the above set of linear integral equations.

The operators $\mathcal{V}_{\alpha\beta}^P$ may be determined from equations of the form (2.13)–(2.16), in which all singularities have been evaluated with the principal-value prescription. The leading terms in the expansion of the Faddeev T matrix in these equations may provide a reasonable approximation at high energies.[13] In the next section we set up a more general scheme for generating approximations for $\mathcal{V}_{\alpha\beta}^P$.

Different methods for constructing unitary three-body theories can be found in the work of Kowalski[13] and Cahill.[14]

IV. VARIATIONAL PRINCIPLES

The equations which determine the effective-potential matrix can be put in variational form. Since the derivations closely follow the methods developed in an earlier study of the breakup problem[6] we need only sketch the procedure here. When the trial functions introduced below are chosen to satisfy standing-wave boundary conditions the variational principles apply to the elements $\mathcal{V}_{\alpha\beta}^P$ which appear in Eqs. (3.23) and (3.24). This provides a systematic procedure for generating approximations to the scattering matrix which are variational in nature and which satisfy unitarity exactly.

We first consider the elastic and rearrangement elements of the effective potential, defined by Eq. (2.13) or, equivalently, by Eq. (2.18). While both definitions can be put in stationary form we shall work here with Eq. (2.13); the correct connectedness property is then incorporated at the outset. [Precisely the same result is obtained if, in the variational principle based on Eq. (2.18), the trial functions are constrained to have the correct dis-

connected parts.]

For energies below the breakup threshold a Kohn-type variational principle for $\mathcal{U}_{ij}$ has been derived with the aid of a variational principle for the resolvent G_A.[2] That derivation breaks down, however, for positive energy scattering (since G_A is no longer a two-sided inverse of $E - H_A$). Instead we work with a variational formulation of the Faddeev equations which define the matrix $\underline{T}_A$ in Eq. (2.13). We have the identity[11]

$$\underline{T}_A = \underline{T}_A^D + \underline{T}_A^D \underline{G}_0 \underline{T}_{At} + \underline{T}_A \underline{G}_0 \underline{T}_A^D - \underline{T}_A \underline{G}_0 \underline{T}_{At} + \underline{T}_A \underline{G}_0 \underline{T}_A^D \underline{G}_0 \underline{T}_{At}, \tag{4.1}$$

where $\underline{T}_{At}$ is some estimate of $\underline{T}_A$. The result of combining Eqs. (4.1) and (2.13) can be expressed in convenient form with the definitions

$$|\tilde{\psi}_{jt}^{(+)}\rangle = \sum_{k \neq j} G_0 T_{At}^k |\chi_j^{(+)}; \vec{k}_j\rangle, \tag{4.2}$$

$$\langle \tilde{\psi}_i^{(-)}| = \sum_{k \neq i} \langle \chi_i^{(-)}; \vec{k}_i|^k T_A G_0, \tag{4.3}$$

where

$$|\chi_j^{(\pm)}; \vec{k}_j\rangle = G_{jA}^{(\pm)} V_j |\chi_j\rangle |\vec{k}_j\rangle. \tag{4.4}$$

After some algebra we arrive at the identity

$$\langle \vec{k}_i | \mathcal{U}_{ij} | \vec{k}_j \rangle = \langle \chi_i^{(-)}; \vec{k}_i | (E-K) | \chi_j^{(+)}; \vec{k}_j \rangle (1 - \delta_{ij}) + \sum_{l \neq i,j} \langle \chi_i^{(-)}; \vec{k}_i | V_{lA} | \chi_j^{(+)}; \vec{k}_j \rangle + \sum_{l \neq i} \langle \chi_i^{(-)}; \vec{k}_i | V_{lA} | \tilde{\psi}_{jt}^{(+)} \rangle + \sum_{l \neq j} \langle \tilde{\psi}_i^{(-)} | V_{lA} | \chi_j^{(+)}; \vec{k}_j \rangle + \langle \tilde{\psi}_i^{(-)} | (H_A - E) | \tilde{\psi}_{jt}^{(+)} \rangle. \tag{4.5}$$

When $\tilde{\psi}_i^{(-)}$ is replaced by an estimate, $\tilde{\psi}_{it}^{(-)}$, the resultant expression is stationary with respect to independent variations of the trial functions $\tilde{\psi}_{jt}^{(+)}$ and $\tilde{\psi}_{it}^{(-)}$ about the correct values.

Similarly, by combining Eqs. (4.1) and (2.14) we can derive the identity

$$\langle \vec{K}_0 | \mathcal{U}_{0i} | \vec{k}_i \rangle = \langle \vec{K}_0 | (E-K) | \chi_i^{(+)}; \vec{k}_i \rangle + \sum_{l \neq i} \langle \vec{K}_0 | V_{lA} | \chi_i^{(+)}; \vec{k}_i \rangle + \sum_{l \neq i} \langle \tilde{\psi}_0^{(-)} | V_{lA} | \chi_i^{(+)}; \vec{k}_i \rangle + \langle \vec{K}_0 | V_A | \tilde{\psi}_{it}^{(+)} \rangle + \langle \tilde{\psi}_0^{(-)} | (H_A - E) | \tilde{\psi}_{it}^{(+)} \rangle, \tag{4.6}$$

where

$$\langle \tilde{\psi}_0^{(-)}| = \langle \vec{K}_0 | T_A G_0. \tag{4.7}$$

A Kohn-type variational expression is obtained by replacing $\tilde{\psi}_0^{(-)}$ by a trial function $\tilde{\psi}_{0t}^{(-)}$. Variational expressions for $\mathcal{U}_{i0}$ and $\mathcal{U}_{00}$ can be written down in a similar way.

We remark in passing that the next-to-last term on the right-hand side of Eq. (4.6) is given by a convergent integral in configuration space, while the analogous term which appears in the expression for the breakup scattering amplitude diverges due to the oscillatory behavior of the integrand at infinity. (The origin and ultimate removal of this divergence is discussed in detail in Ref. 6.) The improved convergence in the case of the effective potential, which can be traced to the absence of two-body bound-state contributions to the asymptotic form of the scattered wave $\tilde{\psi}_{it}^{(+)}$, is a simplifying feature of the effective-potential approach. Similar remarks hold for Schwinger-type versions of the variational expressions, to which we now turn our attention.

Given a variational expression of the Kohn type, the Schwinger version can be derived by using a once-iterated trial function in the Kohn form.[6] We follow this prescription in the case at hand by writing the exact version of Eq. (4.2) as

$$|\tilde{\psi}_j^{(+)}\rangle = \sum_{k \neq j} G_0 T_A^k |\chi_j^{(+)}; \vec{k}_j\rangle. \tag{4.8}$$

Now the exact amplitude satisfies

$$T_A^k = V_{kA} + V_A G_0 T_A^k, \tag{4.9}$$

so that

$$|\tilde{\psi}_j^{(+)}\rangle = \sum_{k \neq j} G_0 V_{kA} |\chi_j^{(+)}; \vec{k}_j\rangle + G_0 V_A |\tilde{\psi}_j^{(+)}\rangle. \tag{4.10}$$

Then, given a trial function $\tilde{\psi}_{jS}^{(+)}$ (the subscript S anticipates that it will appear as a trial function in a Schwinger-type variational expression) the once-iterated trial function is

$$|\tilde{\psi}_{jt}^{(+)}\rangle = \sum_{k \neq j} G_0 V_{kA} |\chi_j^{(+)}; \vec{k}_j\rangle + G_0 V_A |\tilde{\psi}_{jS}^{(+)}\rangle. \tag{4.11}$$

If we combine Eqs. (4.11) and (4.5), and define

$$|U_{jS}^{l(+)}\rangle = (1 - \delta_{lj}) V_{lA} |\chi_j^{(+)}; \vec{k}_j\rangle + V_{lA} |\tilde{\psi}_{jS}^{(+)}\rangle, \tag{4.12}$$

$$\langle U_i^{l(-)}| = \langle \chi_i^{(-)}; \vec{k}_i | V_{lA} (1 - \delta_{li}) + \langle \tilde{\psi}_i^{(-)} | V_{lA}, \tag{4.13}$$

we obtain the identity

$$\langle \vec{k}_i | \mathcal{U}_{ij} | \vec{k}_j \rangle = \langle \chi_i^{(-)}; \vec{k}_i | (E-K) | \chi_j^{(+)}; \vec{k}_j \rangle (1 - \delta_{ij}) + \sum_{l \neq i,j} \langle \chi_i^{(-)}; \vec{k}_i | V_{lA} | \chi_j^{(+)}; \vec{k}_j \rangle + \sum_l \sum_k \langle U_i^{l(-)} | G_0 | U_{jS}^{k(+)} \rangle - \langle \tilde{\psi}_i^{(-)} | V_A | \tilde{\psi}_{jS}^{(+)} \rangle. \tag{4.14}$$

It is one of the virtues of a Schwinger-type variational principle, such as the one shown above, that trial functions appear multiplied by potentials and therefore need only be estimated in the region where these potentials are nonvanishing. If the potentials are local and short-ranged one can define a new trial function as the product of the potential and the original trial function. If this new function is square-integrable it can be expanded in a conveniently chosen set of basis functions.[15,16] The transformation used in Ref. 16 is not immediately applicable to Eq. (4.14) since the potentials V_{iA} are nonlocal and cannot be easily inverted. This difficulty can be surmounted, however, in the following way. Let us define functions $W_{jS}^{I(+)}$ and $W_i^{I(-)}$ by replacing V_{IA} with V_I in Eqs. (4.12) and (4.13), respectively. Now by definition

$$V_{IA} = \omega_I V_I = V_I \omega_I^\dagger ,$$

where

$$\omega_I = 1 - \frac{V_I |\chi_I\rangle\langle\chi_I|}{\langle\chi_I|V_I|\chi_I\rangle} . \tag{4.15}$$

Equation (4.14) then takes the form

$$\langle\vec{k}_i|\mathcal{U}_{ij}|\vec{k}_j\rangle = \langle\chi_i^{(-)};\vec{k}_i|(E-K)|\chi_j^{(+)};\vec{k}_j\rangle(1-\delta_{ij}) + \sum_{I\neq i}\langle\chi_i^{(-)};\vec{k}_i|\omega_I|W_{jS}^{I(+)}\rangle + \sum_{I\neq j}\langle W_i^{I(-)}|\omega_I^\dagger|\chi_j^{(+)};\vec{k}_j\rangle + \sum_I\sum_k\langle W_i^{I(-)}|\omega_I^\dagger G_0\omega_k|W_{jS}^{k(+)}\rangle - \sum_I\langle W_i^{I(-)}|V_I^{-1}\omega_I|W_{jS}^{I(+)}\rangle . \tag{4.16}$$

With the $W_i^{I(-)}$ replaced by trial functions $W_{iS}^{I(-)}$, one can demonstrate the stationary property of the resultant expression. The independent trial functions $W_{jS}^{I(\pm)}$ are all square-integrable. As mentioned above, oscillatory contributions to the asymptotic form corresponding to configurations in which a pair is bound appear in the analogous study of the scattering matrix (or K matrix) but are absent here, thus simplifying the variational calculation.

Variational principles of the Schwinger type for the remaining elements of the effective-potential matrix can be written down in a similar way.

V. A SIMPLIFIED MODEL

With the use of standing-wave boundary conditions the variational methods of the previous section can be applied to construct a matrix $\bar{\mathcal{U}}_{\alpha\beta}^P$ (the bar indicates that it differs from the exact $\mathcal{U}_{\alpha\beta}^P$) to be inserted in Eqs. (3.23) and (3.24). These are linear integral equations in momentum space involving energy-conserving three-body intermediate states. While numerical solutions of such equations may now be feasible,[14] we observe that a simplifying assumption exists which reduces these equations to quadratures. Thus, with $\bar{\mathcal{U}}_{00}^P = 0$, Eq. (3.24) gives $\bar{\mathcal{U}}_{00} = 0$, $\bar{\mathcal{U}}_{0i} = \bar{\mathcal{U}}_{0i}^P$, and $\bar{\mathcal{U}}_{i0} = \bar{\mathcal{U}}_{i0}^P$. Then Eq. (3.23) becomes

$$\bar{\mathcal{U}}_{ij} = \bar{\mathcal{U}}_{ij}^P - i\pi[\bar{\mathcal{U}}_{i0}^P\delta(E-K)\bar{\mathcal{U}}_{0j}^P]_c . \tag{5.1}$$

The correct form of discontinuity relation for the $\bar{\mathcal{U}}_{\alpha\beta}$ is preserved in this approximation. The approximation $\bar{\mathcal{U}}_{00} = 0$ also appears in the separable-potential model,[7] defined by setting $V_{iA} = 0$ for each pair. The remaining elements of the effective-potential matrix are treated more realistically in the present model.

There is another simplifying assumption concerning the choice of input amplitudes $\bar{\mathcal{U}}_{\alpha\beta}^P$ that can be made at this stage. This involves identifying $\bar{\mathcal{U}}_{0i}^P$ and $\bar{\mathcal{U}}_{i0}^P$ with trial functions in a variational calculation of $\bar{\mathcal{U}}_{ij}^P$; unitarity is of course still satisfied exactly. To be able to state this assumption clearly we must return to Eq. (4.14) and rewrite that identity for the elastic and rearrangement components $\mathcal{U}_{ij}$ in a different form.

We first observe that $\sum_I\langle U_i^{I(-)}|$ can be identified as the connected part $\langle\vec{k}_i|\mathcal{U}_{i0} - \langle\vec{k}_i|\mathcal{U}_{i0}^D$. Similarly, $\sum_I|U_{jS}^{I(+)}\rangle$ can be replaced in Eq. (4.14) by $\mathcal{U}_{0jS}|\vec{k}_j\rangle - \mathcal{U}_{0j}^D|\vec{k}_j\rangle$. If we define

$$|\psi_{jS}^{(+)}\rangle = |\chi_j^{(+)};\vec{k}_j\rangle + |\bar{\psi}_{jS}^{(+)}\rangle \tag{5.2}$$

and

$$\langle\psi_i^{(-)}| = \langle\chi_i^{(-)};\vec{k}_i| + \langle\bar{\psi}_i^{(-)}| , \tag{5.3}$$

then Eq. (4.14) can be written, after some algebra, as

$$\langle\vec{k}_i|\mathcal{U}_{ij}|\vec{k}_j\rangle = \langle\vec{k}_i|\mathcal{U}_{i0}G_0\mathcal{U}_{0jS}|\vec{k}_j\rangle_c - \langle\psi_i^{(-)}|V_A|\psi_{jS}^{(+)}\rangle_c . \tag{5.4}$$

Returning now to Eq. (5.1) we make the variational choice

$$\langle\vec{k}_i|\bar{\mathcal{U}}_{ij}^P|\vec{k}_j\rangle = \langle\vec{k}_i|\mathcal{U}_{i0S}^P G_0^P\mathcal{U}_{0jS}^P|\vec{k}_j\rangle_c - \langle\psi_{iS}^P|V_A|\psi_{jS}^P\rangle_c . \tag{5.5}$$

Furthermore, we take $\bar{\mathcal{U}}_{i0}^P = \mathcal{U}_{i0S}^P$ and $\bar{\mathcal{U}}_{0i}^P = \mathcal{U}_{0iS}^P$ so that Eq. (5.1) becomes

$$\langle\vec{k}_i|\bar{\mathcal{U}}_{ij}|\vec{k}_j\rangle = \langle\vec{k}_i|\mathcal{U}_{i0S}^P G_0\mathcal{U}_{0jS}^P|\vec{k}_j\rangle_c - \langle\psi_{iS}^P|V_A|\psi_{jS}^P\rangle_c . \tag{5.6}$$

This is a variational expression of the Schwinger type, but restricted to real trial functions. The discontinuity can then be read directly from Eq. (5.6) since only G_0 is complex. The choice of approximate propagator $\bar{\mathcal{G}}_i$ is governed by the unitarity considerations of Sec. III. Equation (3.12) must be replaced by

$$\bar{\mathcal{G}}_i^{(+)} - \bar{\mathcal{G}}_i^{(-)} = -(2\pi i)\delta(E - \mathcal{K}_i - E_i) - (2\pi i)\bar{\mathcal{G}}_i^{(-)} \mathcal{U}_{i0}^{PD} \delta(E - K) \mathcal{U}_{0i}^{PD} \bar{\mathcal{G}}_i^{(+)}. \quad (5.7)$$

A solution of this discontinuity relation is easily obtained if we use Eq. (3.18) to express the exact propagator, defined by Eq. (2.9), in the form

$$\mathcal{G}_i = [\langle \chi_i | V_i | \chi_i \rangle - \langle \chi_i | V_i G_{iA}^P V_i | \chi_i \rangle + i\pi \mathcal{U}_{i0}^{PD} \delta(E - K) \mathcal{U}_{0i}^{D}]^{-1}. \quad (5.8)$$

If we define $\mathcal{G}_i$ by an expression differing from this by the appearance of $\mathcal{U}_{0i}^{PD}$ in place of $\mathcal{U}_{0i}^{D}$ then Eq. (5.7) may be verified in a manner similar to the derivation of Eq. (3.12). Unitarity is then assured. As in the derivation of Eq. (4.16), Eq. (5.6) can be written in terms of square-integrable trial functions.

For energies not too far above the breakup threshold Eq. (5.6) can be used as the basis for an approximation similar in spirit to that made in the familiar effective-range theory. We recall[17] that the effective-range expansion for low-energy nucleon-nucleon scattering can be derived from the Schwinger variational principle by choosing as trial function the exact zero-energy wave function. This is a reasonable choice since the interior region is of greatest importance in the variational expression and there the wave function will be fairly insensitive to changes in the energy when the potential term dominates the total energy term in the Schrödinger equation. In the present problem the assumption of weak energy dependence of the real, square-integrable trial functions suggests the following procedure for choosing these functions.

Consider a variational calculation based on the negative-energy version of Eq. (4.5); the form is the same except that the trial functions are real and decay asymptotically.[2] Since the variational principle is in fact a minimum principle for negative energies the trial functions can be systematically improved. These trial functions may now be used in the Schwinger form with G_0 evaluated at the correct positive energy. In this way one has effectively performed an analytic continuation of the amplitude from a negative energy to a limited range of positive energies. The correct singularity structure is guaranteed, as it must be for a unitary approximation, by the presence of the free Green's function. Calculations are now being planned to test this procedure.

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