Wave-function formalisms in the channel coupling array theory of many-body scattering

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Wave-function formalisms corresponding to different channel coupling array transition operators of many-body scattering theory are derived and discussed. The Kouri-Levin transition operators are seen to be in typical Lippmann-Schwinger form and allow for the introduction of wave-function components in a particularly straightforward way. The Baer-Kouri transition operators are not in the Lippmann-Schwinger form and an alternate procedure is used to derive their corresponding wave-function components. In the three-body case, the Kouri-Levin operators $\hat{T}_{jk}$ obtained from the Faddeev-Lovelace choice of channel coupling array are seen to lead to precisely the Faddeev wave-function components. The Baer-Kouri operators are shown to lead to wave-function components obeying inhomogeneous equations. These inhomogeneous equations are used to give an alternate explanation of the nonunitary amplitudes obtained in recent calculations based on approximate forms of the Baer-Kouri operators.

[NUCLEAR REACTIONS Many-body scattering theory, channel coupling array wave-function formalisms, aspects of the bound-state type of approximation method, explanation of some nonunitary numerical results of Baer and Kouri and of Lewanski and Tobocman.]

I. INTRODUCTION

In this paper we investigate wave-function formalisms for some of the channel coupling array[1] (CCA) theories of many-body scattering.[2-8] Our work is in part complementary to that of Vanzani, who has discussed this topic for a number of n-particle scattering theories not based on the CCA method.[9] In contrast to the approaches reviewed by Vanzani, some of the CCA types of scattering equations for transition operators are in matrix Lippmann-Schwinger (LS) form,[10] which allows for the introduction of wave-function equations in a particularly transparent manner, and we discuss examples of this case in some detail.

For those CCA types of equations not in LS form, we introduce an alternate procedure for introducing wave-function equations. This latter procedure is found to lead to *inhomogeneous* differential equations for the wave-function components, rather than to homogeneous ones, as in the LS case. The existence of such inhomogeneous equations provides an alternate explanation to the one given previously[11] for the occurrence of the nonunitary results found in the recent numerical calculations of Baer and Kouri[1] and of Lewanski and Tobocman,[12] as we discuss in detail below.

The organization of this paper is as follows. In Sec. II we introduce our notation. Transition operator equations are stated in Sec. III. Wave-function equations are derived in Sec. IV, and approximations are discussed in Sec. V. Section VI summarizes our work.

II. NOTATION

Our notation mostly follows that of earlier work,[2-6] and we provide only a brief summary here. We consider a scattering system consisting of n, nonrelativistic, distinguishable particles labeled $1 \ldots n$, governed by a Hamiltonian H and obeying the Schrödinger equation

$$(E - H)\,|\Psi\rangle = 0\,. \tag{2.1}$$

The particles can be observed in a variety of m-cluster channels or partitions, $1 \leq m \leq n$. Corresponding to these channels are partitions of H into a channel Hamiltonian H_j, governing the motion of the noninteracting clusters in channel j, and a channel interaction V^j, which goes to zero as the separations between all clusters in channel j become asymptotic:

$$H = H_j + V^j, \quad 0 < j < N\,. \tag{2.2}$$

H_0 is the total kinetic energy operator, and $V^0 = V$ is the sum of all interactions; $j = 0$ thus refers to the n-particle breakup channel.

The asymptotic states $|\Phi_j(E)\rangle$ of the system are eigenstates of H_j with total binding plus kinetic energy equal to E:

$$(E - H_j)\,|\Phi_j(E)\rangle = 0\,. \tag{2.3}$$

The $|\Phi_j(E)\rangle$ are products of a bound state for each cluster in the channel times plane wave states describing the intercluster motion.

Resolvent operators $G(z)$ and $G_j(z)$ are defined

as usual:

$$G(z) \equiv (z - H)^{-1} \tag{2.4}$$

and

$$G_j(z) = (z - H_j)^{-1}\,, \tag{2.5}$$

and are related by the LS equations

$$\begin{aligned} G(z) &= G_j(z) + G_j(z) V^j G(z) \\ &= G_j(z) + G(z) V^j G_j(z)\,. \end{aligned} \tag{2.6}$$

When taken between states $\langle \Phi_j(E) |$ and $|\Phi_k(E)\rangle$, matrix elements of the transition operators $U_{jk}^{(\pm)}(z)$ defined by

$$U_{jk}^{(+)}(z) = V^j + V^j G(z) V^k\,, \tag{2.7}$$

$$U_{jk}^{(-)}(z) = V^k + V^j G(z) V^k \tag{2.8}$$

yield identical transition amplitudes for $z = E + i0$. Equations (2.7) and (2.8) are in the "post" and "prior" forms,[13] respectively. We shall refer to $G(E + i\epsilon)$ and $G_j(E + i\epsilon)$ in the limit $\epsilon \to 0+$ as $G^{(+)}$ and $G_j^{(+)}$, the outgoing wave Green's functions.

The three-body problem ($n = 3$) is of particular interest, and we introduce an additional notation for it. The pair of particles j and k will collectively be referred to as i (the "odd man out" notation) and i, j, and k will be assumed in this case to take on only the values 1, 2, and 3. The channel interactions are

$$V^j \equiv V_{ji} + V_{jk} = V_k + V_i \equiv \sum_{m=1}^{3} \bar{\delta}_{jm} V_m\,, \tag{2.9}$$

where $\bar{\delta}_{jm} = 1 - \delta_{jm}$. From (2.9) it follows that $V = V_j + V^j$ and thus that $H_j = H_0 + V_j$.

The two-particle transition operator $t_j(z)$ acting in the three-particle Hilbert space obeys

$$t_j(z) = V_j + V_j G_0(z) t_j(z) \tag{2.10a}$$

$$= V_j + t_j(z) G_0(z) V_j \tag{2.10b}$$

$$= V_j + V_j G_j(z) V_j\,, \tag{2.10c}$$

and is related to V_j by

$$t_j(z) G_0(z) = V_j G_j(z) \tag{2.11a}$$

and

$$G_0(z) t_j(z) = G_j(z) V_j\,. \tag{2.11b}$$

III. TRANSITION OPERATORS

A. Channel coupling array case

There are two distinct sets of transition operators that can be introduced, depending on how the channel coupling array W is used to partition G over the channels in Eqs. (2.7) and (2.8). Following Tobocman,[7] we shall refer to these as the Kouri-Levin (KL) and the Baer-Kouri (BK) operators.

1. KL operators T_{jk} and $\hat{T}_{jk}$

These operators obey[3,5]

$$T_{jk}(z) = V^j W_{lk} + V^j \sum_m W_{lm} G_m(z) T_{mk}(z) \tag{3.1}$$

and

$$\hat{T}_{jk}(z) = W_{jl} V^k + \sum_m \hat{T}_{jm}(z) G_m(z) W_{ml} V^k\,, \tag{3.2}$$

where l is a free channel index to be chosen as is convenient.[2,4] They are related to the transition operators $U_{jk}^{(\pm)}$ via[7]

$$U_{jk}^{(+)}(z) = \sum_m T_{jm}(z) G_m(z) G_k^{-1}(z) \tag{3.3}$$

and

$$U_{jk}^{(-)}(z) = \sum_m G_j^{-1}(z) G_m(z) \hat{T}_{mk}(z)\,. \tag{3.4}$$

If channel $k(j)$ in Eq. (3.3) [Eq. (3.4)] is a two-cluster channel, then in limit $z \to E + i0$,

$$U_{jk}^{(+)}(E + i0) \,|\, \Phi_k(E)\rangle = T_{jk}(E + i0) \,|\, \Phi_k(E)\rangle$$

and

$$\langle \Phi_j(E) \,|\, U_{jk}^{(-)}(E + i0) = \langle \Phi_j(E) \,|\, \hat{T}_{jk}(E + i0)\,,$$

results that follow from Lippmann's identity,[14] e.g.,

$$G_m^{(+)} G_k^{(+)-1} \,|\, \Phi_k(E)\rangle = |\, \Phi_k(E)\rangle \delta_{mk}\,.$$

Suppressing the complex energy parameter z and defining the matrices T, $\mathfrak{g}$, $\mathfrak{V}$, and $\hat{\mathfrak{V}}$ by

$$\begin{aligned} &(T)_{jk} = T_{jk}, \quad (\mathfrak{g})_{jk} = G_j \delta_{jk}\,, \\ &(\mathfrak{V})_{jk} = V^j W_{lk}, \quad (\hat{\mathfrak{V}}) = W_{jl} V^k\,, \end{aligned} \tag{3.5}$$

Eqs. (3.1) and (3.2) can be written in matrix notation as

$$T = \mathfrak{V} + \mathfrak{V} \mathfrak{g} T \tag{3.6a}$$

and

$$\hat{T} = \hat{\mathfrak{V}} + \hat{T} \mathfrak{g} \hat{\mathfrak{V}}\,. \tag{3.7a}$$

These latter two equations are in typical LS form and as such can also be expressed as

$$T = \mathfrak{V} + T \mathfrak{g} \mathfrak{V} \tag{3.6b}$$

and

$$\hat{T} = \hat{\mathfrak{V}} + \hat{\mathfrak{V}} \mathfrak{g} \hat{T}\,. \tag{3.7b}$$

From Eqs. (3.6a) and (3.7b) it is trivial to deduce wave-function equations, as we demonstrate below.

We next consider choices for W. For arbitrary

n, the most studied case is that of the channel permuting array (CPA),[4,7] while for $n=3$, an additional coupling scheme, the Faddeev-Lovelace (FL) choice of W, has also been used.[2] We consider each in turn, using only the right-hand forms for T and $\hat{T}$.

(*a*) *CPA choice of W.* Following Refs. 4 and 7, Eqs. (3.6a) and (3.7b) become

$$T_{jk}=V^j\delta_{jN_2}+V^jG_{j+1}T_{j+1,k} \tag{3.8a}$$

and

$$\hat{T}_{j1}=V^1\delta_{jN_2}+V^{j+1}G_{j+1}\hat{T}_{j+1,1}\,. \tag{3.8b}$$

When j runs over the set of $N_2=2^{n-1}-1$ two-cluster channels,[15] Eqs. (3.8a) and (3.8b) are minimally coupled.[16] They are also asymmetric, which can lead to time-reversal noninvariance when approximations are made, although the calculations carried out so far indicate that such effects are smaller than those due to channel coupling.[17]

(*b*) *FL choice of W.* Here we restrict ourselves to the case $n=3$. The T and $\hat{T}$ equations become[2,4,5]

$$T_{jk}=\bar{\delta}_{jk}V_k+\sum_{m=1}^{3}\bar{\delta}_{jm}V_mG_mT_{mk} \tag{3.9a}$$

and

$$\hat{T}_{jk}=V_j\bar{\delta}_{jk}+V_j\sum_{m=1}^{3}\bar{\delta}_{jm}G_m\hat{T}_{mk}\,, \tag{3.9b}$$

where the pair index notation is used. The operator T_{jk} defined by Eq. (3.9a) has been shown by Kouri, Levin, and Sandhas[5] to be phase equivalent to the Alt-Grassberger-Sandhas (AGS) transition operator[18] [Eq. (3.16a)]. As noted below, this is also true for the $\hat{T}_{jk}$ defined by Eq. (3.9b). In addition, matrix elements of this $\hat{T}_{jk}$ occur directly in the asymptotic form of the solution to the Faddeev wave-function component equations.

2. *BK operators X_{jk} and $\hat{X}_{jk}$*

The operators X_{jk} obey

$$X_{jk}=V^j+\sum_m X_{jm}G_m(z)W_{ml}V^k\,. \tag{3.10a}$$

For the CPA choice of $W(l=k)$, Eq. (3.10a) was first published by Tobocman.[7] The operators $\hat{X}_{jk}$ are given by[2]

$$\hat{X}_{jk}=V^k+\sum_m V^jW_{lm}G_m\hat{X}_{mk}\,. \tag{3.10b}$$

Equation (3.10b) is a generalization of the original two-channel Baer-Kouri equations.[1] Since Eqs. (3.10a) and (3.10b) are developed directly from the $U_{jk}^{(\pm)}$ without the intervention of terms such as $G_mG_k^{-1}$, the matrix elements of X_{jk} and $U_{jk}^{(+)}$, and also of $\hat{X}_{jk}$ and $U_{jk}^{(-)}$, are equal for j and k arbitrary m-cluster channels.

Matrix versions of (3.10a) and (3.10b) are easily written out with the aid of the matrix N, whose elements are all unity[19] ($N_{jk}=1$, all j and k):

$$X=VN+X\,g\,\hat{U} \tag{3.11a}$$

and

$$\hat{X}=NV+U\,g\,\hat{X}\,, \tag{3.11b}$$

where V in these equations is a diagonal matrix with elements $V_{jk}=\delta_{jk}V^j$. Since $VN\neq\hat{U}$, it is clear that neither (3.11a) nor (3.11b) is in LS form. Detailed forms for Eqs. (3.11) may be obtained by using the CPA and FL choices of W, as we now demonstrate.

(*a*) *CPA choice of W.* The standard CPA choice[4,7] for W leads to

$$X_{1k}=V^1+X_{1,k-1}G_{k-1}V^k \tag{3.12a}$$

and

$$\hat{X}_{j1}=V^1+V^jG_{j+1}\hat{X}_{j+1,1}\,. \tag{3.12b}$$

These are also minimally coupled sets of equations. While they do not suffer from time-reversal noninvariance, approximate solutions to them have yielded nonunitary results.[1,12,20] An explanation of this nonunitary feature, applicable to both Refs. 1 and 12, has previously been given.[11] We present an alternate explanation based on the wave-function formalism associated with Eq. (3.12b) in Sec. V.

(*b*) *FL choice of W.* Insertion of the FL choice of W into Eqs. (3.10a) and (3.10b) yields for the case $n=3$

$$X_{jk}=\sum_m\bar{\delta}_{jm}V_m+\sum_m X_{jm}G_mV_m\bar{\delta}_{mk} \tag{3.13a}$$

and

$$\hat{X}_{jk}=\sum_m V_m\bar{\delta}_{mk}+\sum_m\bar{\delta}_{jm}V_mG_m\hat{X}_{mk}\,. \tag{3.13b}$$

These are precisely the equations derived by Lovelace[21] for the post and prior transition operators $U_{jk}^{(\pm)}$; hence X_{jk} of (3.13a) is to be identified with the $U_{jk}^{(+)}$, and $\hat{X}_{jk}$ of (3.13b) is similarly to be identified with the $U_{jk}^{(-)}$, as defined by Lovelace's three-body equations.

B. The AGS operators

These are the only other operators of interest to us in the present work, and we introduce them because, as noted earlier, they provide interesting connections to the X_{jk}, $\hat{X}_{jk}$ sets and to the T_{jk}, $\hat{T}_{jk}$ sets. The AGS operators U_{jk} obey[18] (recall

that $n=3$ here)

$$U_{jk}(z)=\bar{\delta}_{jk}G_0^{-1}(z)+\sum_m \bar{\delta}_{jm}t_m(z)G_0(z)U_{mk}(z) \tag{3.14a}$$

$$=\bar{\delta}_{jk}G_0^{-1}(z)+\sum_m U_{jm}(z)G_0(z)t_m(z)\bar{\delta}_{mk}\,. \tag{3.14b}$$

Use of (2.12a) and (2.12b) in (3.14a) and (3.14b) allows one to express the latter equations in terms of $V_mG_m(z)$ or $G_m(z)V_m$ rather than $t_m(z)$ and $G_0(z)$. Although it is straightforward to express (3.14a) and (3.14b) as matrix equations, it is unnecessary to do so in order to see that they are not in standard LS form. Nevertheless, they do possess an equivalent wave-function formalism, viz., the Faddeev wave-function component equations, as noted, for example, by Vanzani.[22]

Alt, Grassberger, and Sandhas have shown that their operators U_{jk} are related to those defined by Lovelace, i.e., the X_{jk} and $\hat{X}_{jk}$:

$$U_{jk}(z)=\bar{\delta}_{jk}G_k^{-1}(z)+X_{jk}(z) \tag{3.15a}$$

and

$$U_{jk}(z)=\bar{\delta}_{jk}G_j^{-1}+\hat{X}_{jk}(z)\,. \tag{3.15b}$$

The relation between the U_{jk} and T_{jk} of Eq. (3.9a) is given in Ref. 5:

$$\lim_{\epsilon\to 0+} T_{jk}(E+i\epsilon)=\lim_{\epsilon\to 0+} U_{jk}(E+i\epsilon)G_0(E+i\epsilon)V_k\,. \tag{3.16a}$$

The analogous relation for $\hat{T}_{jk}$ of (3.9b) is

$$\lim_{\epsilon\to 0+} \hat{T}_{jk}(E+i\epsilon)=\lim_{\epsilon\to 0+} V_jG_0(E+i\epsilon)U_{jk}(E+i\epsilon)\,. \tag{3.16b}$$

These last four equations show that on-shell, the exact matrix elements of these various operators are phase equivalent. Nevertheless, the corresponding wave-function formalisms need not be and are not the same. Furthermore, use of an approximation in one of the wave-function formalisms will, in general, not lead to the same form for each of the approximate transition operator equations to which the wave-function equation corresponds. This is, of course, not surprising, since approximations can be viewed as off-shell transformations. What may be surprising, however, are the particular approximate equations themselves, a point discussed in Sec. V.

IV. WAVE-FUNCTION FORMALISMS

A. Methods

The resemblance of Eqs. (3.6a) and (3.7b) to the LS equation (2.10a) suggests that at least for the KL operators it will be simple to obtain wave-function components. This is indeed the case and we first review the relevant procedure for the LS equation $n=2$. The analog of (2.10a) for $n=2$ is

$$t(z)=v+v(z-H_0)^{-1}t(z)\,, \tag{4.1}$$

where $H=H_0+v$, with H_0 the relative-motion kinetic-energy operator and v the interparticle interaction. The LS equation for the state vector $|\Psi\rangle=\lim|\Psi^{(\epsilon)}\rangle$ (i.e., the LS wave-function equation) is obtained from Eq. (4.1) by means of the definition

$$v|\Psi^{(\epsilon)}\rangle\equiv t(E+i\epsilon)|\Phi(E)\rangle\,, \tag{4.2}$$

where $|\Phi(E)\rangle$ is a plane wave state with energy E, the $n=2$ analog of $|\Phi_j(E)\rangle$ of Eq. (2.3).

Applying both sides of (4.1) to $|\Phi(E)\rangle$ for $z=E+i\epsilon$ and using (4.2) yields

$$|\Psi^{(\epsilon)}\rangle=|\Phi(E)\rangle+(E+i\epsilon-H_0)^{-1}v|\Psi^{(\epsilon)}\rangle\,, \tag{4.3}$$

the well-known LS equation.[10] That a similar procedure can be applied to the T and $\hat{T}$ matrix equations[4] is a consequence of the occurrence of $v(\hat{v})$ in both the driving term and the kernel term of these equations. However, since the X and $\hat{X}$ equations (3.11a) and (3.11b) are not of this form, we may anticipate possible problems using the LS type of method for these latter operators.

We shall consider in detail only the right-hand form of the various operator equations, since in left-hand form, e.g., Eq. (3.6b)—one obtains equations for the components $\langle\vec{\psi}|$ rather than $|\vec{\psi}\rangle$. For the case of arbitrary particle number n, the various matrix operator equations take the form

$$O(z)=B(z)+K(z)O(z)\,, \tag{4.4}$$

where O stands for any of the transition operators, B is the Born or driving term, and K is the kernel term.

Of particular interest is the situation wherein $K(z)$ factorizes as

$$K(z)=B(z)\mathcal{G}(z)\,, \tag{4.5}$$

where $\mathcal{G}(z)$ contains outgoing wave Green's functions (in limit $z\to E+i0$). Equations (3.6a), (3.7b), and (3.14a) are all of this form. If K does not factorize or if instead of (4.5), one finds

$$K(z)=C(z)\mathcal{G}(z)\,, \tag{4.6}$$

with $C^{-1}B\neq I\neq B^{-1}C$, I being the unit matrix, then, in general, other methods for obtaining wave-function equations must be sought.

Thus when (4.5) holds, then analogously to (4.2), we define a column vector of state-vector components $|\vec{\psi}\rangle$ via

$$B(E+i0)|\vec{\psi}\rangle \equiv O(E+i0)|\vec{\Phi}\rangle , \tag{4.7}$$

where for future notational simplicity we have omitted the necessary intermediate step of first setting $z=E+i\epsilon$ and writing $|\vec{\psi}^{(\epsilon)}\rangle$, and then taking the limit $\epsilon \to 0^+$. The vector $|\vec{\Phi}\rangle$ is defined by

$$(|\vec{\Phi}\rangle)_j = \delta_{jk}|\Phi_k(E)\rangle , \tag{4.8}$$

where k is arbitrarily taken to be the incident channel (assumed to be a two-cluster channel unless otherwise stated). Correspondingly, we have

$$(|\vec{\psi}\rangle)_j = |\psi_j\rangle \tag{4.9}$$

and the dependence of $|\psi_j\rangle$ on both E and the incident channel index k is suppressed.

From Eqs. (4.4), (4.5), and (4.7) we easily find

$$|\vec{\psi}\rangle = |\vec{\Phi}\rangle + \mathcal{G}(E+i0)B(E+i0)|\vec{\psi}\rangle , \tag{4.10}$$

the desired result in general form. The definition (4.7) immediately allows one to determine the transition amplitudes from the asymptotic form of (4.10) in a coordinate (wave-function) representation.

When $K(z)$ does not factorize, or (4.6) holds, one must seek other procedures for introducing wave-function components. The method we follow here is to define components $|\vec{\chi}\rangle$ by

$$|\vec{\chi}\rangle = |\vec{\Phi}\rangle + g(E+i0)O(E+i0)|\vec{\Phi}\rangle , \tag{4.11}$$

where g is given by (3.5). Substituting (4.4) into (4.11) gives

$$|\vec{\chi}\rangle = [I + g(E+i0)B(E+i0)]|\vec{\Phi}\rangle + g(E+i0)K(E+i0)O(E+i0)|\vec{\Phi}\rangle . \tag{4.12}$$

From (4.12) one can try to construct an integral equation for $|\vec{\chi}\rangle$. We apply this procedure below to the operators $\hat{X}$.

Once equations for $|\vec{\psi}\rangle$ or $|\vec{\chi}\rangle$ have been determined, the next step is to relate the components to the Schrödinger state $|\Psi\rangle$. [One is, after all, trying to solve the Schrödinger equation (2.1).] Finally, one may introduce approximations and examine their consequences, a point we consider in Sec. V. We now apply the procedures just outlined to the operators of Sec. III.

B. KL case

We examine these operators first because they are defined by Eqs. (3.6a) and (3.7b), which are precisely in the form of Eq. (4.4). Hence their corresponding wave-function components will obey equations of the form (4.10). Thus for (3.6a) we have

$$|\vec{\psi}\rangle = |\vec{\Phi}\rangle + g\,U|\vec{\psi}\rangle ,$$

and for (3.7b) we find

$$|\hat{\vec{\psi}}\rangle = |\vec{\Phi}\rangle + g\,\hat{U}|\hat{\vec{\psi}}\rangle .$$

The components corresponding to different choices of W will be distinguished by superscripts.

1. FL choice of W

We begin with this $n=3$ choice of W, Eqs. (3.9a) and (3.9b), because of the interesting properties of the corresponding sets of components.

(*a*) *The operators* $\hat{T}$. From Eqs. (3.9b) and (4.7) one easily finds that the components $|\hat{\psi}_j^F\rangle$ corresponding to the $\hat{T}_{jk}$ obey[3,6]

$$|\hat{\psi}_j^F\rangle = |\Phi_k(E)\rangle\delta_{jk} + G_j^{(+)}V_j\sum_{m=1}^{3}\bar{\delta}_{jm}|\hat{\psi}_m^F\rangle , \tag{4.13}$$

which are the Faddeev wave-function component equations;[23] hence the superscript F. In addition, (4.13) also defines the set of components corresponding to the AGS operators.[22] That this is true even though $\mathcal{G}(z)$ for the AGS equations is not equal to $g(z)$ is shown by an easy calculation using Eqs. (3.14a) and (4.7). Such a result might be expected, given the multiplicative relationship (3.16b). Notice, however, that (4.13) follows only from the right-hand equation (3.16) for $\hat{T}_{jk}$. Had the left-hand form been used, the result would have been equations defining the Hermitian conjugate to the components corresponding to T_{jk} of (3.9a). These latter components have quite different properties from the $|\hat{\psi}_j^F\rangle$, despite the fact that both the $\hat{T}_{jk}$ and the T_{jk} are each multiplicatively related to the U_{jk}. We enlarge on this point in subsection (b) below.

Equation (4.13) has two well-known properties[23]:

$$(E-H)\sum_j |\psi_j^F\rangle = 0 \tag{4.14}$$

and

$$|\psi_j^F\rangle = G_0 V_j|\Psi\rangle . \tag{4.15}$$

Taken together these imply

$$\sum_j |\psi_j^F\rangle \equiv |\Psi\rangle , \tag{4.16}$$

illustrating the well-known fact that in integral form the Faddeev wave-function component equations do not admit spurious solutions,[24] i.e., $\sum_j|\hat{\psi}_j^F\rangle \neq 0$.

(*b*) *The operators* T. From Eq. (3.9a) we see that B_{jk} of (4.7) is just $\bar{\delta}_{jk}V_k$, so that the components corresponding to the T_{jk} obey

$$|\psi_j^{FL}\rangle = \delta_{jk}|\Phi_k\rangle + G_j^{(+)}\sum_{m=1}^{3}\bar{\delta}_{jm}V_m|\psi_m^{FL}\rangle . \tag{4.17}$$

Despite the great similarity in structure between Eqs. (3.9a) and (3.9b), their equivalent wave-function components, given by Eqs. (4.13) and

(4.17), are totally dissimilar. As first pointed out by Sandhas,[25] these latter components are each identical to the full Schrödinger state $|\Psi\rangle$. To prove this, one simply operates on both sides of (4.17) by $[G_j^{(+)}]^{-1}$; a little rearranging then yields $(E-H_0)|\psi_j^{\mathrm{FL}}\rangle=\sum_m V_m|\psi_m^{\mathrm{FL}}\rangle$, showing that $|\psi_j^{\mathrm{FL}}\rangle$ is independent of j. The equation that results from utilizing this is the Schrödinger equation. A similar result holds for the components corresponding to the T defined by a CPA (see below).

We thus see that in (4.17), the channel indices on the $|\psi_j^{\mathrm{FL}}\rangle$ act essentially as a bookkeeping device: They remind us that $G_j^{(+)}$ governs the asymptotic behavior of $|\psi_j^{\mathrm{FL}}\rangle$. Unlike the $|\hat{\psi}_j^{F}\rangle$ of Eq. (4.13), which do depend on the channel index and have as bound-state sources only contributions from the "tube" defined by the relative coordinate in channel j becoming large,[26] the $|\psi_j^{\mathrm{FL}}\rangle=|\Psi\rangle$ of (4.17) receive contributions from all asymptotic channels, and hence yield amplitudes for scattering into all channels, not only j.

2. *Channel permuting choice of W*

(*a*) *The $\hat{T}$ operators.* In this case, the operators are defined through Eq. (3.8b) and lead to components obeying

$$|\hat{\psi}_j^{\mathrm{CCA}}\rangle=|\Phi_1(E)\rangle\delta_{j1}+G_j^{(+)}V^{j+1}|\hat{\psi}_{j+1}^{\mathrm{CCA}}\rangle\,, \tag{4.18}$$

where the incident wave is in channel 1. As with the components of Eq. (4.13), those of (4.18) also obey

$$(E-H)\sum_j|\hat{\psi}_j^{\mathrm{CCA}}\rangle=0\,, \tag{4.19}$$

but now in addition to $\sum|\hat{\psi}_j^{\mathrm{CCA}}\rangle=|\Psi\rangle$, one can have a spurious bound-state solution[24] of the form $\sum|\hat{\psi}_j^{\mathrm{CCA}}\rangle=0$. This has not proved to be a serious drawback for the bound-state applications for which (4.18) has been used.[27] In addition, Eq. (4.18) has the advantage over Eq. (4.13), for example, in that it not only applies to an arbitrary number of channels, but this set can also be truncated in a simple fashion, thus permitting a variety of approximations to be studied.[28] Both sets, Eqs. (4.13) and (4.18), have been used for numerical studies of model nuclear reactions.[17] Each of these sets of equations has the "in-principle" advantage that only the jth component yields the amplitude for scattering from an initial two-cluster state in channel k to a final two-cluster (bound) state in channel j: Components $|\hat{\psi}_m\rangle$, $m\neq j$, do not contribute to this amplitude,[6] in contrast to the components, i.e., channel scattering states,[2-4] of Eqs. (4.17) and (4.20) below.

(*b*) *The T operators.* These operators, which are defined by Eq. (3.8a), yield components superficially similar to those of (4.19), viz.,

$$|\psi_j^{\mathrm{CCA}}\rangle=|\Phi_1(E)\rangle\delta_{j1}+G_j^{(+)}V^j|\psi_{j+1}^{\mathrm{CCA}}\rangle\,. \tag{4.20}$$

The similarity ends here, however, since (4.20) defines channel scattering states having the same properties as those of Eq. (4.17), i.e., they are independent of the subscript j and are each equal to the Schrödinger state $|\Phi\rangle$. This feature has been discussed in Ref. 4; we now present a much simpler demonstration of it.[29]

First, we note that in the present case, Eq. (4.7) takes the simple form

$$T_{j1}(E+i0)|\Phi_1(E)\rangle=V^j|\psi_{j+1}^{\mathrm{CCA}}\rangle\,, \tag{4.21}$$

where $|\Phi_1(E)\rangle$ is now specifically assumed to be an incident two-cluster state. From this latter assumption, it follows that if both sides of (3.3) are applied to $|\Phi_1(E)\rangle$ $(k=1)$, we get

$$\begin{aligned}U_{j1}^{(+)}(E+i0)|\Phi_1(E)\rangle&=T_{j1}(E+i0)|\Phi_1(E)\rangle\\&=V^j|\psi_{j+1}^{\mathrm{CCA}}\rangle\,,\end{aligned} \tag{4.22}$$

the second line being a result of (4.21). But Eq. (2.7) may be written as $U_{j1}^{(+)}=V^jGG_1^{-1}$, while $|\Psi\rangle$ is given by

$$|\Psi\rangle=\lim G(E+i\epsilon)G_1^{-1}(E+i\epsilon)|\Phi_1(E)\rangle\,.$$

Putting these results into (4.22) thus yields

$$V^j|\Psi\rangle=V^j|\psi_{j+1}^{\mathrm{CCA}}\rangle\,, \tag{4.23}$$

i.e.,

$$|\psi_{j+1}^{\mathrm{CCA}}\rangle=|\Psi\rangle\,, \tag{4.24}$$

a result that obviously holds for all j and is thus independent of j.

That components based on the T operators are in fact equal to $|\Psi\rangle$ is essentially the reason for the more complicated derivation presented in Ref. 26 of the "true" wave-function components for the BRS transition operators. It is also this same fact that renders the $|\psi_j^{\mathrm{CCA}}\rangle$ of (4.20) less useful than those based on the $\hat{T}$ operators, should one introduce approximations which include breakup, rather than keeping strictly to bound-state approximations. However, we do note that since $|\psi_j^{\mathrm{CCA}}\rangle\equiv|\Psi\rangle$, Eq. (4.20) is just the set uniquely defining $|\Psi\rangle$.[30]

C. BK case

We have presented the results in the previous section in some detail, as they illustrate the ease with which one can derive wave-function equations when the transition operators obey equations of LS type, e.g., (3.7). In contrast to this, (3.11b) is not in standard LS form, and thus one encounters difficulties in deriving associated wave functions.

We shall illustrate this using Eq. (3.12b), the CPA version of (3.11b).

The matrix equation (3.11b) can be written as

$$\hat{X}(z)=B(z)+C(z)g(z)\hat{X}(z)\,, \tag{4.25}$$

where $B=NV$ and $C=\mathcal{U}$. In seeking to apply relation (4.7), we may try to define components $|\hat{\vec{\psi}}\rangle$ via either

$$NV|\hat{\vec{\psi}}\rangle=\hat{X}|\vec{\Phi}\rangle \tag{4.26a}$$

or

$$V|\hat{\vec{\psi}}\rangle=\hat{X}|\vec{\Phi}\rangle\,. \tag{4.26b}$$

Neither of these definitions leads to a satisfactory equation for $|\hat{\psi}\rangle$, in the first instance because N^{-1} does not exist and in the second because a proper plane wave term $|\Phi\rangle$ does not occur. To remedy this, we shall derive components using Eqs. (4.11) and (4.12) for which it suffices to work out the two-channel case. Before doing so, we establish the validity of such a procedure by applying it to Eq. (3.8b) for $\hat{T}$, for which we have already derived components.

In the two-channel case (3.8b) becomes

$$\hat{T}_{11}=V^2G_2\hat{T}_{21} \tag{4.27a}$$

and

$$\hat{T}_{21}=V^1+V^1G_1\hat{T}_{11}\,, \tag{4.27b}$$

where the dependence on $E+i0$ is suppressed.

Now "define" components $|\hat{\psi}_1^{\rm CCA}\rangle$ and $|\hat{\psi}_2^{\rm CCA}\rangle$ via

$$|\hat{\psi}_j^{\rm CCA}\rangle=\delta_{j1}|\Phi_1\rangle+G_j^{(+)}\hat{T}_{j1}|\Phi_1\rangle\,, \tag{4.28}$$

following (4.11). Substituting (4.27) into (4.28) and then using (4.28) on the right-hand sides of the resulting equations yields Eq. (4.18) for the two-channel case, just as predicted. Hence the procedure is a proper one to follow, although in the present instance it does not emphasize the essential LS structure of the equations.

We now turn to the operators of interest, defined by Eq. (3.11b). For the two-channel case they are

$$\hat{X}_{11}=V^1+V^1G_2\hat{X}_{21} \tag{4.29a}$$

and

$$\hat{X}_{21}=V^1+V^2G_1\hat{X}_{11}\,. \tag{4.29b}$$

The equations defining the corresponding "components" $|\hat{\chi}_j^{\rm CCA}\rangle$ are

$$|\hat{\chi}_1^{\rm CCA}\rangle=|\Phi_1(E)\rangle+G_1^{(+)}\hat{X}_{11}|\Phi_1(E)\rangle \tag{4.30a}$$

and

$$|\hat{\chi}_2^{\rm CCA}\rangle=G_2^{(+)}\hat{X}_{21}|\Phi_1(E)\rangle\,. \tag{4.30b}$$

Substituting (4.29) into (4.30) and using (4.30) in the resulting equations leads to

$$|\hat{\chi}_1^{\rm CCA}\rangle=|\Phi_1(E)\rangle+G_1^{(+)}V^1|\Phi_1(E)\rangle+G_1^{(+)}V^1|\hat{\chi}_2^{\rm CCA}\rangle \tag{4.31}$$

and

$$|\hat{\chi}_2^{\rm CCA}\rangle=G_2^{(+)}(V^1-V^2)|\Phi_1(E)\rangle+G_2^{(+)}V^2|\hat{\chi}_1^{\rm CCA}\rangle\,. \tag{4.32a}$$

Equation (4.32a) can be simplified by using in it Lippmann's identity,[14]

$$G_2^{(+)}(V^1-V^2)|\Phi_1(E)\rangle=-|\Phi_1(E)\rangle\,.$$

This gives

$$|\hat{\chi}_2^{\rm CCA}\rangle=-|\Phi_1(E)\rangle+G_2^{(+)}V^2|\hat{\chi}_1^{\rm CCA}\rangle\,. \tag{4.32b}$$

The presence of $-|\Phi_1(E)\rangle$ in (4.32b) and the resulting implication that $|\hat{\chi}_1^{\rm CCA}\rangle+|\hat{\chi}_2^{\rm CCA}\rangle$ cannot be equal to $|\Psi\rangle$ because of the apparent lack in this sum of a plane wave term suggests that the $|\hat{\chi}_j^{\rm CCA}\rangle$ cannot be components in the same sense as the $|\hat{\psi}_j^{\rm CCA}\rangle$ of (4.18). They are, however, very closely related to the $|\psi_j^{\rm CCA}\rangle$ of Eq. (4.20) in that $|\hat{\chi}_j^{\rm CCA}\rangle$ is related to $|\Psi\rangle$ additively [recall Eq. (4.24)]. To see this, we first display the equations uniquely defining $|\Psi\rangle$ (Ref. 30); in the two-channel case, those are, from (4.20) with $N_2=2$ and $|\psi_j^{\rm CCA}\rangle=|\Psi\rangle$,

$$|\Psi\rangle=|\Phi_1(E)\rangle+G_1^{(+)}V^1|\Psi\rangle \tag{4.33a}$$

and

$$|\Psi\rangle=G_2^{(+)}V^2|\Psi\rangle\,. \tag{4.33b}$$

Next consider Eq. (4.32b). As an equation for the sum $|\hat{\chi}_2^{\rm CCA}\rangle+|\Phi_1(E)\rangle$, it becomes similar to (4.20), i.e., similar to (4.33b). We therefore form this combination in each of Eqs. (4.32a) and (4.32b), yielding

$$|\hat{\chi}_1^{\rm CCA}\rangle=|\Phi_1(E)\rangle+G_1^{(+)}V^1[|\hat{\chi}_2^{\rm CCA}\rangle+|\Phi_1(E)\rangle] \tag{4.34a}$$

and

$$[|\hat{\chi}_2^{\rm CCA}\rangle+|\Phi_1(E)\rangle]=G_2^{(+)}V^2|\hat{\chi}_1^{\rm CCA}\rangle\,. \tag{4.34b}$$

The identifications

$$|\hat{\chi}_1^{\rm CCA}\rangle=|\Psi\rangle \tag{4.35a}$$

and

$$|\hat{\chi}_2^{\rm CCA}\rangle=|\Psi\rangle-|\Phi_1(E)\rangle \tag{4.35b}$$

immediately follow on comparison of Eqs. (4.33) and (4.34); (4.35) and (4.35b) are the desired relations.

These identifications notwithstanding, (4.33) and (4.34) differ not only directly in their approaches to solving the Schrödinger equation, but more importantly in their response to approximations. We examine this point in detail in the next section.

We end this section by remarking that the results just obtained [Eqs. (4.35a) and (4.35b)] are

easily generalized beyond the case $N_2=2$. For an arbitrary number of channels N and incident channel $k=1$, one finds

$$|\hat{\chi}_1^{\mathrm{CCA}}\rangle = |\Psi\rangle \tag{4.36a}$$

and

$$|\hat{\chi}_j^{\mathrm{CCA}}\rangle = |\Psi\rangle - |\Phi_1(E)\rangle, \quad j\neq 1\,. \tag{4.36b}$$

This result arises from the cyclic nature of the coupling in Eq. (3.11b), the $N_2=2$ example of which is (4.30).

V. APPROXIMATIONS

Analyses of collision data usually rely on some form of empirical procedure such as the distorted wave Born approximation, the impulse approximation, or a coupled channel approximation. The successful application of such methods has made their justification one of the several goals of many-body scattering theory. Since some of these empirical methods are based on wave-function approaches, the need for approximate wave-function versions of many-body scattering theory is obvious. We consider the Faddeev wave-function components as an example.

In addition to their use in possible attempts to justify empirical approximations, many-body wave-function formalisms may also play the important role of elucidating the results of approximate transition operator calculations. To the extent that they can provide insights into such calculations, they provide a description of multiparticle scattering complementary to that of transition operator formalisms. We show in Sec. V B how the BK wave function components $|\hat{\chi}_j^{\mathrm{CCA}}\rangle$ can be used to understand certain nonunitary numerical results based on approximations to the BK transition operators $\hat{X}_{jk}$.

A. Faddeev wave-function components

The AGS operators U_{jk} defined, e.g., by Eq. (3.14a) are probably the most widely used transition operators for analyses of three-body problems. They have the advantage over the Lovelace and CCA operators of being symmetric and reducing to relatively simple form when separable two-body potentials or t-operator approximations are used. Corresponding to the U_{jk} are the Faddeev wave-function components $|\hat{\psi}_j^F\rangle$. Nevertheless, while the path transition operator $\rightarrow$ wave function leads to $U_{jk}\rightarrow|\hat{\psi}_j^F\rangle$, the reverse process is $|\hat{\psi}_j^F\rangle\rightarrow\hat{T}_{jk}$ and not $|\hat{\psi}_j^F\rangle\rightarrow U_{jk}$.

At first glance, this may seem to be a trivial distinction to emphasize, since on-shell matrix elements of $\hat{T}_{jk}$ and U_{jk} are equal. The aspect of this which we stress is that under identical approximations, $\hat{T}_{jk}$ and U_{jk} will most likely differ on-shell, and under any such approximation, the $|\hat{\psi}_j^F\rangle$ equations will yield the approximate $\hat{T}_{jk}$ amplitudes and not approximate U_{jk} amplitudes. This point is pertinent for the traditional analyses of atomic, molecular, or nuclear collisions when three-body models are used, since such analyses are, as noted above, based on wave-function methods.

We illustrate this by using a particular bound-state approximation which is often referred to as the coupled reaction channel (CRC) method in nuclear physics,[17,31] and as the coupled states (CS) method in molecular physics[32] and in atomic physics[33] (without the additional use of pseudostates).

The approximation procedure is as follows. Consider only two-cluster partitions. Then the channel Hamiltonian H_j can be expressed as

$$H_j = T_j + h_j\,, \tag{5.1}$$

where T_j is the relative-motion kinetic-energy operator and h_j is the Hamiltonian for the internal states of the clusters.

The eigenstates $|\phi_j(\gamma)\rangle$ of h_j obey

$$[\epsilon_j(\gamma) - h_j]\,|\phi_j(\gamma)\rangle = 0\,, \tag{5.2}$$

where $\epsilon_j(\gamma)$ is the energy of the state and γ denotes the set of relevant quantum numbers. Let $\{|\phi_j(\gamma_b)\rangle\}$ denote the subset of the $\{|\phi_j(\gamma)\rangle\}$ which consist of bound internal states only [the former are the states which occur in the $|\Phi_j(E)\rangle$ of Eq. (2.3)]. Now form the projection operators $P_j(\gamma_b)$ and P_j:

$$P_j(\gamma_b) = |\phi_j(\gamma_b)\rangle\langle\phi_j(\gamma_b)| \tag{5.3}$$

and

$$P_j = \sum_{\gamma_b}{}' P_j(\gamma_b)\,, \tag{5.4}$$

where the prime on the γ_b sum in (5.4) means that not all the bound states in channel j need be included in the sum.

The CRC or CS approximation to the solution $|\Psi\rangle$ of the Schrödinger equation (2.1) consists in replacing $|\Psi\rangle$ in Eq. (2.1) by

$$|\tilde{\Psi}\rangle = \sum_j P_j|\Psi\rangle \cong |\Psi\rangle\,, \tag{5.5}$$

projecting the result onto each $\langle\phi(\gamma_b)|$ in turn, and then solving the resulting set of coupled equations for the unknown scattering coefficients $\langle\phi_j(\gamma_b)|\Psi\rangle$, according to the usual outgoing wave boundary conditions.

The corresponding approximations for the Faddeev components $|\hat{\psi}_j^F\rangle$, the CCA operators $\hat{T}_{jk}$, and the AGS operators U_{jk} are obtained as follows. In the Faddeev equations (4.13), one first replaces $|\hat{\psi}_j^F\rangle$ by $P_j|\hat{\psi}_j^F\rangle$ and $G_j^{(+)}$ by $\tilde{G}_j^{(+)}\equiv P_jG_j^{(+)}$;

then one solves for the unknown scattering coefficients $\langle\phi_j(\gamma_b)|\hat{\psi}_j^F\rangle$ from

$$\langle\phi_j(\gamma_b)|\hat{\psi}_j^F\rangle=\langle\phi_j(\gamma_b)|\Phi_k(E)\rangle\delta_{jk}+\langle\phi_j(\gamma_b)|\tilde{G}_j^{(+)}V_j\sum_{m=1}^{3}\bar{\delta}_{jm}P_m|\hat{\psi}_m^F\rangle\,. \tag{5.6}$$

The analogous approximations used in (3.9b) for $\hat{T}_{jk}$ lead to

$$\langle\phi_j(\gamma_b)|\hat{T}_{jk}(z)|\phi_k(\alpha_b)\rangle=\langle\phi_j(\gamma_b)|V_j|\phi_k(\alpha_b)\rangle\bar{\delta}_{jk}+\langle\phi_j(\gamma_b)|V_j\sum_m\bar{\delta}_{jm}P_m\tilde{G}_m(z)\hat{T}_{mk}(z)|\phi_k(\alpha_b)\rangle\,, \tag{5.7}$$

while the same approximations inserted into (3.14a) for U_{jk} yield

$$\langle\phi_j(\gamma_b)|U_{jk}(z)|\phi_k(\alpha_b)\rangle=\langle\phi_j(\gamma_b)|G_0^{-1}(z)|\phi_k(\alpha_b)\rangle\bar{\delta}_{jk}+\langle\phi_j(\gamma_b)|\sum_m\bar{\delta}_{jm}V_m\tilde{G}_m(z)P_mU_{mk}(z)|\phi_k(\alpha_b)\rangle\,. \tag{5.8}$$

It is straightforward to verify our earlier remark that Eqs. (5.6) and (5.7) produce the same on-shell amplitude approximations, which are *not* equal to the approximate on-shell amplitudes arising from the AGS operators U_{jk}. This should not be unexpected, since it is only in left-hand form that the approximate $\hat{T}$ operators would be phase equivalent to the approximate operators U_{jk}.

B. The CCA wave-function components

One of the interesting aspects of the CRC or CS approximation (discussed in Sec. V A) is that it is unitary. This follows essentially from the fact that the coupled equations of the method are flux conserving, i.e., there are no sources of or sinks for the incident flux outside of the channels and states coupled to the initial one. In general, however, one does not expect approximations to transition operators to yield transition amplitudes (and thus S matrix elements) which are unitary, the simple Born approximation being a well-known example.

Let us now consider the CCA transition operators defined by Eqs. (3.8) and (3.12) in light of the these comments. Although they and their corresponding wave-function components, defined, e.g., by (4.18) and (4.32), do obey coupled equations, these coupled equations contain asymmetric coupling terms rather than symmetric ones such as occur in the CRC approximation. This suggests that approximations to these CCA equations may not yield unitary amplitudes. The fact that approximations to the KL equations *have* led to unitary results while approximations to the BK equation have not, thus requires explanation.

Before using the BK wave-function components to analyze this, we first review the relevant calculations and the original Kouri, Levin, Craigie, and Secrest analysis.[11] Baer and Kouri[1] found nonunitary elastic scattering amplitudes for e^-+H scattering at energies below the $n=2$ threshold using a symmetrized form of the two-channel BK transition operator equations in the approximation of Sec. V A, in which the P_j are formed from the $1s$ hydrogenic ground state only. Subsequent calculations based on a symmetrized form of the KL transition operator equations using the same approximation yielded a unitary amplitude, i.e., one of the form $\exp(i\delta)\sin\delta$. The phase of the BK amplitude was found to be the same as for the KL amplitude, viz., δ.

Earlier work of Kouri and Levin had established the existence of K or reaction operators related to the KL transition operators by a Heitler damping equation[2]; by contrast, no such relation exists for the BK transition and reaction operators. This fact was used to prove that in the one-state approximation for the P_j, the ratio of the BK and KL amplitudes would be a real number, i.e., that the amplitudes would have the same phase.[11] Lack of unitarity of the BK amplitude was shown to be a consequence of the bound-state approximation for the P_j. In effect, this means that use of P_2 in channel 2 is not the same as (equivalent to) use of P_1 in channel 1: To achieve the effect in channel 2 of P_1 in channel 1, continuum states must be used in P_2. The cause of this behavior of the BK operators is the fact that in Eq. (3.11b), for example, the inhomogeneity NV is not repeated in the kernel term $\mathcal{U}\mathcal{G}$, in contrast to the KL equations; the latter, of course, did yield unitary amplitudes. An analogous incompatibility in apparently equivalent approximations will be seen to be the basis of our alternate explanation, using the inhomogeneous equations obeyed by the components $|\hat{\chi}_j^{\mathrm{CCA}}\rangle$ discussed below.

The Lewanski-Tobocman calculations[12] involve approximations using projection-operator expansions applied to collisions in a system consisting of two light and one infinitely massive particle, the Hulburt-Hirschfelder model.[34] Three sets of calculations were done: those based on a boundary matching procedure employing the Schrödinger equation, those based on BK equations, and those based on KL equations. The first of the three

provided the benchmark against which the other two could be measured. In addition, parameters were changed to allow the two light particles to be identical fermions, thus introducing Pauli principle effects. A maximum of seven expansion states were used in the calculations.

We consider the nonidentical-particle case first. Within this case there are two subcases: all three interactions either not equal or equal. When they are not equal, the KL-based results are found to converge more or less to the same results as those based on the boundary matching procedure, and also to be unitary. For this same case of the three interactions not being equal, the BK-based results are not only nonunitary, they also do not converge to the same numbers to which the other two sets of calculations tend to converge. The other distinguishable particle subcase, that of all three interactions being equal, leads to the opposite results for the BK based calculations: They are not only unitary, but converge to the same numbers as the other two sets of calculations do. This apparently paradoxical situation is easily understood as soon as one realizes that when all three interactions are equal, the matrix elements of each of the channel interactions V^j appearing in the BK equations, when taken betweeen the same initial and the same final states, are *equal*. Hence in this particular situation, the BK equations become a set for which one may expect unitary results, as in the KL case.

The second interesting case examined by Lewanski and Tobocman is that where the two light particles are identical. In this case all three interactions are equal, the three sets of calculations are all unitary (when the seven expansion states are used), and all three converge to the same limits. These results are easily understood in terms of the preceding remarks.

More generally, one can apply the same arguments as used in Ref. 11 to explain the nonunitarity of the Lewanski-Tobocman BK results. Since theirs was a two-channel calculation using equations without a repeated driving term, the inequivalence between the P_1 and P_2 approximations remarked on in connection with the Baer-Kouri results similarly affects the BK results of Ref. 12. Although the latter statement is correct, it is perhaps not as straightforward to apply to the Lewanski-Tobocman computations as to those of Ref. 1. The alternate explanation based on the $|\hat{\chi}_j^{CCA}\rangle$ is, however, much simpler to apply, and we examine it in the following.

In the two-channel case the $|\hat{\chi}_j^{CCA}\rangle$ obey Eqs. (4.32). These are easily converted into the differential equations

$$(E-H_1)\,|\hat{\chi}_1^{CCA}\rangle - V^1\,|\hat{\chi}_2^{CCA}\rangle = V^1\,|\Phi_1(E)\rangle \tag{5.9a}$$

and

$$(E-H_2)\,|\hat{\chi}_2^{CCA}\rangle - V^2\,|\hat{\chi}_1^{CCA}\rangle = (V^2-V^1)\,|\Phi_1(E)\rangle\,. \tag{5.9b}$$

Equations (5.9) are inhomogeneous differential equations. Subject to the boundary conditions of (4.32), they will yield on-shell matrix elements of the operators $\hat{X}_{jk}$, while if standing wave boundary conditions are imposed, they will yield K matrix elements.

Exact solutions of (5.9) will lead to unitary amplitudes. Suppose, however, that one introduces bound-state approximations via the projection operators P_j of Sec. V A. One then wants to determine the $P_j\,|\hat{\chi}_j^{CCA}\rangle$ rather than the entire component $|\hat{\chi}_j^{CCA}\rangle$. Since (5.9a) and (5.9b) are equations for the channel 1 and 2 components, respectively, the equations one apparently should solve are the projections of (5.9a) and (5.9b) onto P_1 and P_2:

$$(E-H_1)P_1\,|\hat{\chi}_1^{CCA}\rangle - P_1V^1P_2\,|\hat{\chi}_2^{CCA}\rangle = P_1V^1\,|\Phi_1(E)\rangle \tag{5.10a}$$

and

$$(E-H_2)P_2\,|\hat{\chi}_2^{CCA}\rangle - P_2V^2P_1\,|\hat{\chi}_1^{CCA}\rangle = P_2(V^2-V^1)\,|\Phi_1(E)\rangle\,, \tag{5.10b}$$

where we have used $[P_j,H_j]=0$.

The solutions to (5.9) and (5.10) are each a sum of two terms: the complementary function, which satisfies the homogeneous equations and the "particular integral," which involves the inhomogeneities. Although the sum of these two terms will yield a unitary amplitude for (5.9), i.e., when each $P_j=1$, there is no way to guarantee that under the actual projection approximation the sum of the two terms forming the solution of (5.10) will also give a unitary amplitude. That is, one can always postulate an approximation of the form

$$(E-H_1)P_1\,|\hat{\chi}_1^{CCA}\rangle - P_1V^1P_2\,|\hat{\chi}_2^{CCA}\rangle = P_1\eta_1 \tag{5.11a}$$

and

$$(E-H_2)P_2\,|\hat{\chi}_2^{CCA}\rangle - P_2V^2P_1\,|\hat{\chi}_1^{CCA}\rangle = P_2\eta_2\,, \tag{5.11b}$$

such that the sum of the complementary function and the particular integral of (5.11) produces a unitary amplitude, but then we cannot expect that the right-hand sides of (5.10a), (5.10b), and (5.11a), (5.11b) will be equal. In general, they will be unequal, leading to nonunitary amplitudes resulting from (5.10).

The reason for this behavior is the inequivalence in approximating the left- and right-hand sides of an inhomogeneous equation. In other words, while the set (5.9) denotes an equality, the set (5.10) does not form a consistent approxi-

mation to it. The consistent approximation comes from first projecting (5.9) to yield

$$(E-H_1)P_1|\hat{\chi}_1^{CCA}\rangle - P_1V^1|\hat{\chi}_2^{CCA}\rangle = P_1V^1|\Phi_1(E)\rangle \quad (5.12a)$$

and

$$(E-H_2)P_2|\hat{\chi}_2^{CCA}\rangle - P_2V^2|\hat{\chi}_1^{CCA}\rangle = P_2(V^2-V^1)|\Phi_1(E)\rangle\,. \quad (5.12b)$$

Equations (5.12) are not yet in the desired form since the entire term $|\hat{\chi}_j^{CCA}\rangle$ still appears in the second term on the left-hand sides. The next step of the approximation is obtained by defining $Q_j = 1 - P_j$ and putting the Q_j terms in the right-hand sides:

$$(E-H_1)P_1|\hat{\chi}_1^{CCA}\rangle - P_1V^1P_2|\hat{\chi}_2^{CCA}\rangle = P_2V^1|\Phi_1(E)\rangle + P_1V^1Q_2|\hat{\chi}_2^{CCA}\rangle \quad (5.13a)$$

and

$$(E-H_2)P_2|\hat{\chi}_2^{CCA}\rangle - P_2V^2P_1|\hat{\chi}_1^{CCA}\rangle = P_2(V^2-V^1)|\Phi_1(E)\rangle + P_2V^2Q_1|\hat{\chi}_1^{CCA}\rangle\,. \quad (5.13b)$$

Equations (5.10) are obtained from (5.13) by neglecting the terms containing the operators Q_j. But since the inhomogeneous terms also occur on the right-hand side of (5.13), retaining them in full while neglecting the Q_j terms cannot be expected to lead to unitary results. This is the heart of the inconsistency. Thus the final step leading to a consistent, i.e., a unitary, approximation will involve modifying the inhomogeneous terms as well. Doing so will lead in principle to equations of the form of (5.11), not (5.10). Unfortunately, there is in practice no specific procedure available for determining any such modification which is guaranteed to lead to unitary amplitudes. Because the approximate BK transition operator equations used by Baer and Kouri and by Lewanski and Tobocman have corresponding wave-function components obeying equations of the form (5.10) and not (5.11), we immediately see that the amplitudes obtained from such approximate equations cannot be expected to be unitary.

The lack of unitarity of the approximate BK amplitudes of Refs. 1 and 12 illustrate these remarks quite concretely. Similar nonunitarities and an acausal resonance behavior were found in an entirely different $e^- + H$ calculation also based on an approximate inhomogeneous equation.[35] As noted in Ref. 35, caution is obviously called for when using inhomogeneous equations as the basis for approximations.

We have noted above that the approximate KL operators did yield unitary results for $e^- + H$ scattering below the $n=2$ threshold. It is thus interesting to compare the approximate KL wave-function component equations, viz.,

$$(E-H_j)P_j|\hat{\psi}_j^{CCA}\rangle = P_jV^{j+1}P_{j+1}|\hat{\psi}_{j+1}^{CCA}\rangle\,, \quad (5.14)$$

with the inconsistent ones for the $P_j|\hat{\chi}_j^{CCA}\rangle$, Eq. (5.10). Since (5.14) contains no inhomogeneities, it contains no sources of or sinks for flux, immediately leading to the conclusion that these are flux-conserving equations, i.e., the resulting amplitudes will indeed be unitary. However, since the channels are coupled asymmetrically, one also expects time-reversal noninvariant amplitudes, as found numerically.[17]

VI. SUMMARY

We have derived wave-function component equations for the CCA transition operators and discussed their properties in detail. In particular, we have shown that the amplitudes arising from an approximate solution of the Faddeev wave-function component equations are the matrix elements of the KL operators $\hat{T}_{jk}$ and not the AGS operators U_{jk}. We have also shown that in differential form, the BK wave-function component equations are inhomogeneous, and we have used this to give an alternate explanation of the nonunitary character of amplitudes determined from approximate solution of the BK operator equations.

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