General Many-Channel Variational Principles
for Multi-Particle Scattering

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Abstract

A general multi-channel scattering formalism based on Schwinger-type variational principles and capable of treating rearrangements was recently presented by Tobocman. The approach involved combining variational functionals for individual transition operators with new coupled integral equations for these operators derived recently by Baer and Kouri and by Kouri and Levin. In this paper, we present general variational principles whose Euler equations are precisely the new coupled channel $T_{\alpha\beta}$ operator equations obtained by Kouri and Levin. The results are expressions which are stationary with respect to variations in all the $T_{\alpha\beta}$ simultaneously rather than just for a single $T_{\alpha\beta}$ operator. It is shown that such matrix generalizations may be obtained for a variety of functionals. With the specific choice of a channel permuting array (as discussed by Tobocman and by Kouri and Levin), the present formalism provides a valid computational basis for general many-body (e. g. nuclear) reactions, since then the iterated kernels of the resulting coupled channel $T_{\alpha\beta}$ operator equations are completely connected.

I. Introduction

Recently there has been interest in the formulation of variational approaches to many-particle reactions which take proper account of the many-body character of such systems ¹. In their work, Hüfner and Lemmer were unable to include effects of particle rearrangement. Subsequently, Tobocman presented a more general variational formalism which removes this restriction ². In his work, the variational functional was for a single transition, $T_{\alpha\beta}$. In addition, Tobocman made use of new coupled integral equations for the rearrangement transition operators derived by Baer and Kouri ³ and by Kouri and Levin ⁴. These equations contain elements of a matrix W , the channel coupling array, that determine which channels are explicitly coupled. The array W serves several purposes ⁵⁻⁷: (1) it permits one to retain maximum generality in the structure of the coupled T operator equations so that one may avoid prematurely specifying which T operators are to be explicitly coupled to a given $T_{\alpha\beta}$; (2) it enables one quite simply to ensure that all asymptotic boundary conditions are properly incorporated into the coupled equations; (3) one can ensure that the iterated kernel of the resulting coupled integral equations contains only connected diagrams, thereby ensuring compactness of the kernel for sufficiently well behaved potentials; (4) it enables one to finesse problems of non-orthogonality. The combination of these new coupled integral equations (with a W array which Tobocman, and Kouri and Levin showed resulted in a connected iterated kernel) and the variational functional for $T_{\alpha\beta}$ thus leads to a satisfactory basis for calculations of many-particle scattering. ⁵⁻⁷

It would seem desirable, however, to develop a variational formalism in which the coupled equations for all the transition operators enter more directly. That is, in Tobocman's approach ² one is assured of a result in which a single transition operator $T_{\alpha\beta}$ is stationary but which involves the use of the transition operators for all the other

channels. However, a formalism which simultaneously leads to stationary results for all $T_{\alpha\beta}$ seems more suitable and should yield improved numerical results. This involves the development of a functional which possesses, as its Euler equations, the coupled T operator equations developed previously. In this paper we show how such functionals may be constructed. All results regarding connectedness of the kernels of the resulting coupled integral equations will continue to apply.

In Section II we present the various generalized functionals. In Section III we discuss some computational aspects of the equations and compare our results to those of Tobocman.

II. Schwinger-Type Variational Principles for Many-Body Collisions

A. Preliminary Background

We will treat a system comprized of n particles which can be grouped together in N ways. The N groupings are referred to as arrangements or channels. For each channel, there corresponds a splitting of the total Hamiltonian H as

$$H = H_{\alpha} + V_{\alpha} ; \quad \alpha = 1, 2, \dots, N. \quad (1)$$

Here H_{α} describes the non-interacting particle-stable subsystems in the α th channel and V_{α} is the interaction giving rise to scattering. The full state vector for the system satisfies the Schrödinger equation

$$H|\psi_{\beta}(i)\rangle = E|\psi_{\beta}(i)\rangle, \quad (2)$$

where β labels the initial channel arrangement and i denotes the initial internal state. Following Hahn, Kouri and Levin⁸⁻⁹ we split $|\psi_{\beta}(i)\rangle$ into its channel components:

$$|\psi_{\beta}(i)\rangle = \sum_{\lambda=1}^N |\psi(\lambda|\beta|i)\rangle, \quad (3)$$

where $|\psi(\lambda|\beta|i)\rangle$ will have the outgoing scattered waves in the λ th arrangement. Substituting (3) into (2) leads to

$$\sum_{\lambda=1}^N (E-H) |\psi(\lambda|\beta|i)\rangle = 0; \quad (4)$$

use of (1) in (4) yields

$$\sum_{\lambda=1}^N (E - H_{\lambda} - V_{\lambda}) |\psi(\lambda|\beta|i)\rangle = 0. \quad (5)$$

We now introduce the channel coupling array W , whose elements satisfy

$$\sum_{\alpha} W_{\alpha\gamma} = \sum_{\delta} W_{\alpha\delta} = 1, \quad (6)$$

from which it follows that

$$V_{\lambda} = \sum_{\alpha} W_{\alpha\lambda} V_{\alpha} \quad (7)$$

$$= \sum_{\gamma} V_{\gamma} W_{\gamma\lambda}, \quad (8)$$

where the index on W which is not summed is free to be chosen as is convenient. We therefore may write (5) as (setting equal to 0)

$$\sum_{\lambda=1}^N (E - H_{\lambda}) |\psi(\lambda|\beta|i)\rangle - \sum_{\lambda=1}^N \sum_{\alpha=1}^N W_{\alpha\lambda} V_{\alpha} |\psi(\alpha|\beta|i)\rangle = 0, \quad (9)$$

and since the sums over λ and α are finite, we can trivially rewrite (9) as

$$\sum_{\lambda=1}^N (E - H_{\lambda}) |\psi(\lambda|\beta|i)\rangle - \sum_{\lambda=1}^N \sum_{\alpha=1}^N W_{\lambda\alpha} V_{\alpha} |\psi(\alpha|\beta|i)\rangle = 0. \quad (10)$$

Coupled equations for the channel states $|\psi(\alpha|\beta|i)\rangle$ are obtained now by requiring them to obey

$$(E - H_{\alpha}) |\psi(\alpha|\beta|i)\rangle - \sum_{\lambda} W_{\lambda\alpha} V_{\lambda} |\psi(\lambda|\beta|i)\rangle = 0. \quad (11)$$

This is a set of N coupled equations whose properties we briefly discuss.

As shown by Hahn, Kouri and Levin⁸ choosing the $W_{\lambda\alpha}$ to be channel permuting array elements puts (11) into the form of Hahn's reduction method equation (10); these sets of coupled equations possess connected iterated kernels.⁵⁻⁷

The formal solution to these equations is given by

$$|\Psi(\lambda|\beta|i)\rangle = |\varphi(\beta|i)\rangle \delta_{\lambda\beta} + (E + i\epsilon - H_\lambda)^{-1} \sum_{\alpha} W_{\lambda\alpha} V_{\alpha} |\Psi(\alpha|\beta|i)\rangle, \quad (12)$$

where $|\varphi(\beta|i)\rangle$ is an eigenstate of H_β corresponding to initial state i in channel β and consists of products of bound internal states and plane wave relative motion states. In matrix form, Eq. (12) reads

$$|\Psi\rangle = |\varphi\rangle + g^+ W V |\Psi\rangle, \quad (13)$$

where

$$\begin{aligned} (|\Psi\rangle)_{\alpha\beta} &= |\Psi(\alpha|\beta|i)\rangle, \\ (|\varphi\rangle)_{\alpha\beta} &= \delta_{\alpha\beta} |\varphi(\alpha|i)\rangle, \\ (g^+)_{\alpha\beta} &= (E + i\epsilon - H_\alpha)^{-1} \delta_{\alpha\beta} \\ (W)_{\alpha\beta} &= W_{\alpha\beta} \\ \text{and } (V)_{\alpha\beta} &= V_{\alpha} \delta_{\alpha\beta}. \end{aligned} \quad (14)$$

We may now introduce the matrix of arrangement channel transition operators⁵⁻⁶ $\hat{T}$ in an obvious fashion:

$$\hat{T} |\varphi\rangle = W V |\Psi\rangle, \quad (15)$$

where

$$(\hat{T})_{\lambda \beta} = \hat{T}_{\lambda \beta}$$

is the transition operator connecting arrangements β and λ . The channel perturbation causing transitions is now WV rather than V . It is clear from Eq. (11) that the elements of W determine which channels are explicitly coupled in the equations. From Eqs. (13) and (15), we readily deduce that

$$\begin{aligned} \hat{T} &= WV + WV g^+ \hat{T} \\ &= U^T + U^T g^+ \hat{T} \end{aligned} \quad (16)$$

where for simplicity we have defined

$$U = VW^T$$

so that

$$U^T = WV,$$

and where the superscript T means transpose. Equation (16) is the integral equation for the matrix of transition operators T derived in our previous work⁵⁻⁶. The transpose occurs because there is another set of equations involving U itself; these are⁵⁻⁶

$$T = U + U g^+ T. \quad (17)$$

Equations (16) and (17) can be easily shown to have the formal solutions

$$\hat{T} = U^T + U^T \hat{G}^+ U^T \quad (18)$$

and

$$T = U + U G^+ U, \quad (19)$$

where

$$\hat{G}^+ = [(g^+)^{-1} - v^T]^{-1} \quad (20)$$

and

$$G^+ = [(g^+)^{-1} - v]^{-1}. \quad (21)$$

Variational functionals can be determined for both $\hat{T}$ and T ; we shall work with T in this paper, although the functionals derived below can be trivially transformed into ones for $\hat{T}$.

Since we shall limit ourselves to functionals for T (and its associated matrix of reactance operators K), we only develop the above equations for T and G^+ . From (21), we find

$$G^+ = g^+ + g^+ v G^+ \quad (22)$$

$$= g^+ + G^+ v g^+; \quad (23)$$

use of (23) in (17) then leads to

$$T = v + T g^+ v \quad (24)$$

which is the last equation needed to develop the variational functionals. Equations for $\hat{G}^+$ and $\hat{T}$ analogous to the above are valid as well. We remark here that Eq. (24) also can be derived via the above methods by starting with the Schrödinger equation in the form $0 = \langle \Psi | (E - H)$ and using Eq. (8).

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These integral equations for T and $\hat{T}$ were previously derived using, in the case of Eq. (17), the definition $T_{\alpha\beta} = V_{\alpha} + V_{\alpha} G^+ V_{\beta}$ and in the case Eq. (16), the definition $\hat{T}_{\alpha\beta} = V_{\beta} + V_{\alpha} G^+ V_{\beta}$, where $G^+ = (E + i\epsilon - H)^{-1}$. The earlier derivations involved the use of the relations (first established

by Lippmann

$$\lim_{\epsilon \rightarrow 0^+} G_\gamma^+ (G_\beta^+)^{-1} |\varphi(\beta|i)\rangle = \delta_{\gamma\beta} |\varphi(\beta|i)\rangle \quad (25)$$

and

$$\lim_{\epsilon \rightarrow 0^+} \langle \varphi(\beta|i) | (G_\beta^+)^{-1} G_\gamma^+ = \langle \varphi(\beta|i) | \delta_{\gamma\beta}, \quad (26)$$

with $G_\lambda^+ = (E + i\epsilon - H_\lambda)^{-1}$. The $|\varphi(\beta|i)\rangle$ is an eigenstate of H_β with energy E . There has been some question as to whether (25) or (26) justified writing the integral equations in the form of Eq. (16) - (17). For example; in Tobocean's work the equations for $T_{\alpha\beta}$ or $\hat{T}_{\alpha\beta}$ have been written with the factor $G_\alpha G_\beta^{-1}$ multiplying the matrix elements of U or U^T (see, for example, Ref. 2 or 7). The direct derivation of Eq. (16) and (17) from the Schrödinger equation establishes that our prior use of (25) and (26) was correct, and that one need not retain the factors $G_\alpha G_\beta^{-1}$ in place of the Kroncker delta, $\delta_{\alpha\beta}$, when writing the coupled equations obeyed by $T_{\alpha\beta}$ or $\hat{T}_{\alpha\beta}$.

We also wish to comment on the further and important point of unitarity in connection with Eqs. (16) and (17), and also by implication with Eqs. (11) and (13). Equations (16) and (17) can be thought of as on-shell (physical) values of a more general set of operators, eq. $T(Z)$:

$$T(Z) = U + U g(Z) T(Z) \quad (27)$$

when $Z = E + i\epsilon$ gives the physical value (in the limit $\epsilon \rightarrow 0^+$). Now, the physical value of Z is on the real axis where it is known that the Green's functions possess cuts originating at the various thresholds; i. e., the

$T_{\alpha\beta}$ are singular and need to be carefully defined. Since Eq. (17) is apparently the limiting value of Eq. (27) on these cuts we may ask if an accurate analysis of Eq. (27), taking into account the singularity structure, will actually yield Eq. (17) itself or a modification of it. This question is important, for it is connected with a proper statement of unitarity. We have recently shown that, in fact, Eq. (17) has the wrong structure and by itself does not satisfy the correct unitarity relations.¹⁰ However an analysis of the discontinuity of $T_{\alpha\beta}(z)$ across the real axis (which is the same¹⁰ as $2i \operatorname{Im} T_{\alpha\beta}(z)$), plus the use of Cauchy's theorem, actually leads¹⁰ to a modification of Eq. (16) and (17) in which the matrix $g(z)$ is replaced by $\tilde{g}(z)$, defined by

$$\tilde{g}_{\alpha\beta}(z) = \delta_{\alpha\beta} G_{\alpha}^{+}(z) P(\alpha). \quad (28)$$

Here, $P(\alpha)$ is the projection on to the entire set of bound internal states in channel α ; for the free-particle channel [$\alpha = 0$], we have $P(0) = 1$.

The result of the replacement $g \rightarrow \tilde{g}$ is that both the equations for $T(E+i0)$ [and $\hat{T}(E+i0)$] and for the matrices of K (reactance) operators discussed below now satisfy the proper kind of unitarity relationship, stated both in terms of $\operatorname{Im} T_{\beta}(E+i0)$ and also in terms of the damping relation between $T(E+i0)$ and the reactance operator $K(E)$. The replacement also means that only bound internal states occur in the expansion of the $G_{\alpha}(z)$ via the states of H_{α} .

Corresponding changes occur in the coupled differential equation for the states $|\Psi\rangle$ as well¹⁰: expansions of the $|\Psi(\lambda|\beta|i)\rangle$ are limited to bound internal states of H_{λ} , except for the case of the free channel ($\lambda=0$), where the full set of n -body plane wave states occur.

Having previously established our notation, we shall not alter it at this point; this means that we suppress the tilde which should now appear over Green's functions in our equations. As long as all G_{α}

are to be interpreted as $G_{\alpha} P(\alpha)$, etc., nothing vital is lost, since we are not so much interested in the detailed structure of our equations here (see Ref. 10) as in the way variational functionals can be formulated. However, we do point out that this change is consistent with the effective orthogonality results found by Hahn¹¹, as discussed elsewhere¹⁰.

Equations (17), (19), (22), (23) and (24) are the basic results we shall employ in developing our matrix Schwinger variational functionals. It is of interest to point out, however, that the structure of the equations for T and N^+ are identical to those for their onebody counterparts. [The only difference (and it is of course a major one) is that T , V , g^+ and N^+ are matrixes of channel operators]. It is this close resemblance to one-body scattering that enables us so easily to generalize the standard variational functionals to the case of many-body collisions. By way of contrast, we note that the T operators used in alternative approaches^{2, 7} involve a post-prior character which is responsible for many of the complications which occur when one attempts to set up variational principles, etc.^{10, 12}. We also note that the present derivation of the coupled T operator equations [see also ref. 9] emphasizes the fact that the present definition of the $T_{\alpha\beta}$ is the one most directly related to that solution of the Schrödinger equation which explicitly incorporates the proper boundary conditions. That is, we note that the more common definitions of $T_{\alpha\beta}$ are based on the Lippmann-Schwinger equation in a form which is well-known to suffer from various difficulties¹³. All these problems can be circumvented by use in eg. (12) of the proper choice of channel coupling array⁵⁻⁷ $W_{\lambda\alpha}$. Thus, we suggest that the equation¹⁹ may be considered (for a proper choice of W) as the optimal definition of the matrix of channel transition operators (or its transpose) in place of the more customary definition¹³. Of course, we do recognize that exact evaluations of eq. (19) of the more customary $T_{\alpha\beta}$ equations will lead to the same on-shell matrix elements, but our point is that in no real physical problem can one obtain exact solutions.^{10, 11}

B. Schwinger-Type Functionals for T and its Matrix Elements.

We are now prepared to derive the Schwinger-type variational functionals whose Euler equations are eqs. (17), (24) or (13). We begin by considering eqs. (17) and (24). We may rearrange eq. (17) to give

$$U = T - U g^+ T \quad (29)$$

and substituting this into eq. (24) results in

$$T = U + T(g^+ - g^+ U g^+) T. \quad (30)$$

We then form the functional

$$[\tilde{T}]_1 = U + U g^+ \tilde{T} + \tilde{T} g^+ U - \tilde{T}(g^+ - g^+ U g^+) \tilde{T}. \quad (31)$$

If we now arbitrarily vary $\tilde{T}$, we find

$$\begin{aligned} \delta[\tilde{T}]_1 = & U g^+ \delta\tilde{T} + \delta\tilde{T} g^+ U - \delta\tilde{T}(g^+ - g^+ U g^+) \tilde{T} \\ & - \tilde{T}(g^+ - g^+ U g^+) \delta\tilde{T}, \end{aligned} \quad (32)$$

and rearranging yields

$$\begin{aligned} \delta[\tilde{T}]_1 = & \{U - \tilde{T} + \tilde{T} g^+ U\} g^+ \delta\tilde{T} \\ & + \delta\tilde{T} g^+ \{U - \tilde{T} + U g^+ \tilde{T}\}. \end{aligned} \quad (33)$$

This is clearly zero when $\tilde{T}$ satisfies eqs. (17) and (19) so we conclude that $[\tilde{T}]_1$ has as its Euler equations precisely the desired coupled T equations. Furthermore, since $[\tilde{T}]_1$ is formed by adding eqs. (22), (28) and subtracting eq. (30), it is obvious that the stationary value of

$[\tilde{T}]_1$ is just T , as desired.

In the form (31), the functional may depend on normalization of the T . It is easy to derive a functional $[\tilde{T}]_2$ which avoids this problem. We simply notice that by eqs. (17), (24) and (30),

$$Tg^+v = v g^+ T \quad (34)$$

$$= T(g^+ - g^+ v g^+) T. \quad (35)$$

Hence, an alternative functional is

$$[\tilde{T}]_2 = v + \tilde{T} g^+ v [\tilde{T} (g^+ - g^+ v g^+) \tilde{T}]^{-1} v g^+ \tilde{T}. \quad (36)$$

It is quite easy to show that this form is also stationary about T given as the exact solution of eqs. (17) and (19), and we simply state it without proof. We remark that we can also obtain variational functionals for the actual T matrix elements (as opposed to the above operator equations). To do this, we note that the T matrix is given by

$$\langle \psi' | T | \psi \rangle = \langle \psi' | v | \psi \rangle. \quad (36)$$

We next note that, by use of eq. (19), $\langle \psi' | T | \psi \rangle$ is also given by

$$\langle \psi' | T | \psi \rangle = \langle \psi' | (v + v M^+ v) | \psi \rangle, \quad (37)$$

and rearranging this gives

$$\langle \psi' | T | \psi \rangle = \{ \langle \psi' | + \langle \psi' | v M^+ \} v | \psi \rangle. \quad (38)$$

We therefore introduce the state $\langle \psi' |$ by

$$\langle \psi' | = \langle \varphi' | + \langle \varphi' | V H^+ \quad (39)$$

and obtain

$$\langle \varphi' | T | \varphi \rangle = \langle \psi' | V | \varphi \rangle. \quad (40)$$

If we now rewrite eq. (13) as

$$| \varphi \rangle = | \psi \rangle - g^+ V | \psi \rangle, \quad (41)$$

then eq. (40) becomes

$$\langle \varphi' | T | \varphi \rangle = \langle \psi' | \{ V - V g^+ V \} | \psi \rangle. \quad (42)$$

We finally combine these forms of $\langle \varphi' | T | \varphi \rangle$, eqs. (36), (40) and (41) to obtain

$$[\widetilde{\langle \varphi' | T | \varphi \rangle}] = \langle \tilde{\psi}' | V | \varphi \rangle [\langle \tilde{\psi}' | \{ V - V g^+ V \} | \tilde{\psi} \rangle]^{-1} \langle \varphi' | V | \tilde{\psi} \rangle \quad (43)$$

as our variational functional for the actual T matrix of numbers. We remark that our derivation of these functionals has been tremendously simplified by the very strong similarity of our coupled equations (in abstract or matrix form) to the more familiar non-reactive equations.

C. Variational Functionals for Channel Reactance (K) Operators.

It is also quite easy to derive coupled channel reactance (K) operator equations for which one may obtain functionals having these as their Euler equations. For example, in place of the outgoing wave solution to the coupled Schrödinger equations, eq. (13), we can write a solution with standing wave unperturbed Green functions:

$$|\psi^p(\lambda|\beta i)\rangle = |\varphi(\beta i)\rangle \delta_{\lambda\beta} + [P/(E-H_\lambda)] \sum_{\alpha} W_{\lambda\alpha} V_{\alpha} |\psi^p(\lambda|\beta i)\rangle. \quad (44)$$

In our matrix notation, we have

$$|\psi^p\rangle = |\varphi\rangle + g^p w v |\psi^p\rangle. \quad (45)$$

By exact analogy to the definition of $\hat{T}$ in eq. (15), the matrix of channel K operators is defined by

$$K|\varphi\rangle = v |\psi^p\rangle, \quad (46)$$

so that from eq. (45), one finds

$$K = v + v g^p K, \quad (47)$$

with

$$(K)_{\lambda\beta} = K_{\lambda\beta} \quad (48)$$

and

$$(g^p)_{\lambda\beta} = \delta_{\lambda\beta} \frac{P}{E-H_\lambda}. \quad (49)$$

We now wish to show that a "left hand" form of (47) is also valid. To do so, we note that subtraction of eqs. (47) and (17) leads us to

$$T = K - i\pi K \Delta T, \quad (50)$$

where

$$(\Delta)_{\lambda\beta} = \delta_{\lambda\beta} \delta(E - H_\lambda) \rho(\lambda). \quad (51)$$

We next substitute eq. (24) into (50) above to obtain

$$U + T g^+ v = K - i\pi K \Delta U - i\pi K \Delta T g^+ v, \quad (52)$$

and use of eq. (50) on the r. h. s. of eq. (52) yields

$$U + T g^+ v = K - i\pi K \Delta U + \{T - K\} g^+ v. \quad (53)$$

Finally, we note that

$$g^+ = g^p - i\pi \Delta \quad (54)$$

so that we find

$$K = U + K g^p v. \quad (55)$$

Green eqs. (47) and (55), we are now able to repeat all the analysis of the preceding discussion of variational functionals for T , so that

$$[\tilde{K}]_1 = v + v g^p \tilde{K} + \tilde{K} g^p v - \tilde{K} \{g^p - g^p v g^p\} \tilde{K} \quad (56)$$

and

$$[\tilde{K}]_2 = v + \tilde{K} g^P v [\tilde{K} (g^P - g^P v g^P) \tilde{K}]^{-1} v g^P \tilde{K}. \quad (57)$$

It is easy to show that these are stationary about the solutions of eqs. (47) and (55). Furthermore, because T and K are related ab initio via eq. (50), it is easy to assure unitary approximations to T which render (56) and (57) stationary and also eqs. (31) and (36). Finally we note that a variational functional analogous to eq. (43), for the matrix element of K may be easily obtained as

$$[\langle \psi' | K | \psi \rangle] = \langle \tilde{\psi}' | v | \psi \rangle [\langle \tilde{\psi}' | \{v - v g^P v\} | \tilde{\psi} \rangle]^{-1} \langle \psi' | v | \tilde{\psi} \rangle, \quad (58)$$

where now $\langle \tilde{\psi}' |$ and $|\tilde{\psi}\rangle$ are the trial standing wave solutions the Schrödinger equations, eq. (45), and the exact $\langle \psi' |$ satisfies

$$\langle \psi' | = \langle \psi' | + \langle \psi' | K g^P. \quad (59)$$

D. Variational Functionals for Wave Operators and Quasi-Green Functions.

An alternative operator which can be used in carrying out calculations is defined by

$$\Gamma = v^{-1} T v^{-1}, \quad (60)$$

so that by eq. (24), we have

$$\Gamma = v^{-1} + M^+. \quad (61)$$

From the above form of Γ , we interpret it as a Green's function - like quantity. Furthermore, one may introduce wave operators Ω and Ω' by

$$T = U \Omega \quad (62)$$

$$= \Omega' U. \quad (63)$$

Again by eq. (24),

$$\Omega = 1 + H^+ U \quad (64)$$

and

$$\Omega' = 1 + U H^+. \quad (65)$$

The operators Γ , Ω and Ω' also satisfy Lippmann-Schwinger-type equations, obtained using eq. (22) - (23). Thus,

$$\Gamma = U^{-1} + g^+ U \Gamma \quad (66)$$

$$= U^{-1} + \Gamma U g^+, \quad (67)$$

and

$$\Omega = 1 + g^+ U \Omega, \quad (68)$$

$$\Omega' = 1 + \Omega' U g^+. \quad (69)$$

One may obtain variational functionals for the Γ , Ω and Ω' by using them to re-express the functionals for T and $\langle \varphi' | T | \varphi \rangle$ in new forms. For example, eq. (43) may be expressed in terms of the

Γ by

$$[\widetilde{\langle \varphi' | T | \varphi \rangle}] = \langle \varphi' | v \tilde{\Gamma} v | \varphi \rangle [\langle \varphi' | v \tilde{\Gamma} \{v - v g^+ v\} \tilde{\Gamma} v | \varphi \rangle]^{-1} \langle \varphi' | v \tilde{\Gamma} v | \varphi \rangle. \quad (68)$$

By noting that

$$\Omega = \Gamma v \quad (69)$$

and

$$\Omega' = v \Gamma, \quad (70)$$

it is easy to rewrite eq. (68) in the form

$$[\widetilde{\langle \varphi' | T | \varphi \rangle}] = \langle \varphi' | \tilde{\Omega}' v | \varphi \rangle [\langle \varphi' | \tilde{\Omega}' \{v - v g^+ v\} \tilde{\Omega} | \varphi \rangle]^{-1} \langle \varphi' | v \tilde{\Omega} | \varphi \rangle. \quad (71)$$

Finally, one can write functionals directly for the quasi-Green's function $\tilde{\Gamma}$, e. g.,

$$[\tilde{\Gamma}]_1 = v^{-1} + g^+ v \tilde{\Gamma} + \tilde{\Gamma} v g^+ - \tilde{\Gamma} v \{g^+ - g^+ v g^+\} v \tilde{\Gamma} \quad (72)$$

and

$$[\tilde{\Gamma}]_2 = v^{-1} + \tilde{\Gamma} v g^+ [\tilde{\Gamma} v \{g^+ - g^+ v g^+\} v \tilde{\Gamma}]^{-1} g^+ v \tilde{\Gamma}. \quad (73)$$

These are obvious analogues of the functionals $[\tilde{T}]_1$ and $[\tilde{T}]_2$.

III. Computational Aspects of the Formalism and Comparisons with the Tobocman Single $T_{\lambda 0}$ Approach

The present approach to the many-body collision problem is well suited for actual computation. For example, the equations specialized to the case of two arrangements have been applied to low-energy $e^- + H$ scattering with good results¹². In those studies, no attempt was made to utilize the variational aspect of the formalism. Rather, the equations (22) were solved by a truncated expansion, using the channel permuting array choice of W ^{3, 5-7}.

In this section, we remark on certain features of the coupled equations which enable one to simplify their solution. We shall begin by considering the basic equations for the transition operators, which have the formal solution

$$T = (1 - v g^+)^{-1} v \quad (74)$$

$$= v (1 - g^+ v)^{-1}. \quad (75)$$

Following Tobocman², we write

$$(1 - g^+ v)^{-1} = \left[\sum_{n=0}^{N-1} (g^+ v)^n \right] (1 - [g^+ v]^N)^{-1} \quad (76)$$

where N is the number of arrangements. However, we note that $[g^+ v]^N$ contains only diagonal elements when the channel permuting array choice

of W is employed in $U = WV$, so that the inversion of $1 - [g^+v]^N$ is greatly simplified compared to $1 - g^+v$. This fact was first noted by Kouri and Levin who employed it in obtaining simple expressions for the optical potential governing scattering in any particular arrangement^{6, 14}. It was independently found by Tobocman in his single transition approach² but we here see that it also affords important simplifications in our general variational approach. We remark that the off-diagonal character of $(1 - g^+v)^{-1}$ is generated solely by the terms $(g^+v)^n$ in the summation.

A similar simplification may be obtained in any of the equations satisfied by $|\psi\rangle$, Γ or Ω . For example, Γ may be expressed as

$$\Gamma = v^{-1} + g^+v\Gamma \quad (77)$$

$$= (1 - g^+v)^{-1} v^{-1}, \quad (78)$$

and obviously the same analysis may be employed to simplify $(1 - g^+v)^{-1}$. However, the presence of v^{-1} makes the above expression somewhat less convenient than eqs. (74) - (76) for the T matrix of operators itself. The reason is that the construction of the inverse U^{-1} will require inversion of the full potential matrix whose dimensions will be $(\sum_{\lambda=1}^N M_{\lambda}) \times (\sum_{\lambda=1}^N M_{\lambda})$. Here, M_{λ} is the number of expansion functions for a given arrangement. By contrast, use of eq. (76) combined with eq. (75) requires inversion separately of N sub-matrixes, whose individual dimensions are $M_{\lambda} \times M_{\lambda}$. This is, of course, much simpler. In this instance, there appears to be somewhat less work required in Tobocman's approach since it requires that one invert only one of the N separate sub-matrixes comprising $1 - [g^+v]^N$. It is clear that we must invert all N simply because our functionals render all transition operators stationary while Tobocman's causes only one $T_{\alpha\beta}$ at a time to be stationary. The main attraction of the present approach compared to Tobocman's is that since all the $T_{\alpha\beta}$, $\lambda = 1, 2, \dots, N$ enter in the calculation of a single $T_{\alpha\beta}$, one may

gain in accuracy by using expressions which treat all the transition operators on an equal basis.

We now wish to look at the explicit form of the coupled $T_{\lambda\alpha}$ operator equations to demonstrate a second simplification which is related to the above but which can be used in a different fashion. That is, instead of formally solving the equations in the form of eqs. (74) - (75), we may first rearrange them somewhat. Here we follow the analysis given by Kouri and Levin. We take again a channel permuting array for W so that ^{3, 5-7}

$$W_{\lambda, \lambda+1} = 1 \quad , \quad \lambda = 1, 2, \dots, N-1; \quad (79)$$

$$W_{N1} = 1 \quad (80)$$

and all other $W_{\lambda\lambda'}$, are precisely zero. If this is substituted into eqs. (17) - (18) and (21), we obtain

$$T_{\lambda\alpha} = W_{\lambda\alpha} V_{\alpha} + \sum_{\gamma} W_{\lambda\gamma} V_{\gamma} G_{\gamma}^+ T_{\gamma\alpha} \quad (81)$$

which becomes

$$\begin{aligned} T_{1\alpha} &= \delta_{2,\alpha} V_{\alpha} + V_2 G_2^+ T_{2\alpha}, \\ T_{2\alpha} &= \delta_{3,\alpha} V_{\alpha} + V_3 G_3^+ T_{3\alpha}, \\ &\vdots \\ T_{N\alpha} &= \delta_{1,\alpha} V_{\alpha} + V_1 G_1^+ T_{1\alpha}. \end{aligned} \quad (82)$$

For simplicity of illustration, we may take α to be 1 resulting in

$$\begin{aligned}
T_{11} &= V_2 G_2^+ T_{21}, \\
T_{21} &= V_3 G_3^+ T_{31}, \\
&\vdots \\
T_{N1} &= V_1 + V_1 G_1^+ T_{11}.
\end{aligned}$$

(83)

We now note that by successive backsubstitution, we may completely uncouple these equations to obtain

$$T_{11} = V_2 G_2^+ V_3 G_3^+ \dots V_N G_N^+ V_1 (1 + G_1^+ T_{11}), \quad (84)$$

$$T_{21} = V_3 G_3^+ V_4 G_4^+ \dots V_N G_N^+ V_1 (1 + G_1^+ V_2 G_2^+ T_{21}), \quad (85)$$

$$T_{31} = V_4 G_4^+ \dots V_N G_N^+ V_1 (1 + G_1^+ V_2 G_2^+ V_3 G_3^+ T_{31}), \quad (86)$$

$$\begin{aligned}
&\vdots \\
T_{N1} &= V_1 (1 + G_1^+ V_2 G_2^+ V_3 G_3^+ \dots V_N G_N^+ T_{N1}).
\end{aligned} \quad (87)$$

These equations are extremely interesting and they have been discussed extensively in earlier work by Kouri and Levin⁶. Similar, but not identical, results were also formed in Tobocman's approach. In his method, it appears necessary to make use of the fact that, in the limit $\epsilon \rightarrow 0_+$, $G_Y^+ (G_\beta^+)^{-1}$ will vanish, for $\gamma \neq \beta$, when applied to the initial state in arrangement β . Here we see that the result follows without these arguments when one employs the particular definition of the $T_{\lambda\beta}$ which we have introduced⁸. We also note that the kernel in each equation above will be completely connected by the same arguments used in earlier discussions⁵⁻⁷.

We notice that the eqs. (84) - (87) may be expressed in terms of Tobocman's² $V_\alpha^{(-)}$ operators and new operators $U_\alpha^{(-)}$ so that²

$$V_{\alpha}^{(-)} = V_{\alpha+1} G_{\alpha+1}^{+} V_{\alpha+2} G_{\alpha+2}^{+} \dots V_N G_N^{+} \dots V_{\alpha-1} G_{\alpha-1}^{+} V_{\alpha} \quad (88)$$

and

$$U_{\alpha 1}^{(-)} = V_{\alpha+1} G_{\alpha+1}^{+} V_{\alpha+2} G_{\alpha+2}^{+} \dots V_N G_N^{+} V_1. \quad (89)$$

With these definitions, eqs. (84) - (87) become

$$T_{\lambda 1} = U_{\lambda 1}^{(-)} + V_{\lambda}^{(-)} G_{\lambda}^{+} T_{\lambda 1}. \quad (90)$$

Similar expressions hold for other choices of the arrangement channel index. We finally note that equations of the above sort may be used as the starting point for approximate evaluations of the $T_{\lambda \beta}$, which may then be employed in the variational functionals presented earlier in this paper. The simplifying feature of these equations is they enable one to deal with uncoupled equations which nevertheless retain kernels which are completely connected. This assures one that standard expansion methods will yield convergent results. The present approach is also seen to be not greatly more complicated than the approach suggested by Tobocman². This additional complexity results from our ensuring that all $T_{\lambda \beta}$ that enter the calculation are stationary about the exact solutions of the coupled channel equations.