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Comparison of the Chandler-Gibson and the Baer, Kouri, Levin, and Tobocman many-body scattering formalisms

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The Chandler-Gibson N-body scattering formalism is shown to be related to the one of Baer, Kouri, Levin, and Tobocman in that both are the result of selecting a set of Lippmann-Schwinger equations to serve as a set of simultaneous coupled integral equations for all the elements in a row or column of the transition operator matrix. The Baer, Kouri, Levin, and Tobocman choice has the advantage that the equations decouple on iteration to give a set of uncoupled connected kernel equations whereas the Chandler-Gibson choice has the advantage of coupling the partitions in a symmetrical manner. This might cause the Chandler-Gibson formalism to be less sensitive than the Baer, Kouri, Levin, and Tobocman formalism to truncations on the spectrum of allowed intermediate virtual states. The Chandler-Gibson formalism is shown to be consistent with unitarity provided the coupling scheme includes all open channels. An alternative method for introducing projectors into the Chandler-Gibson formalism is suggested as a method for generating connected kernel equations. The Chandler-Gibson wave function equations are derived and compared to the coupled reaction channels equations. Finally, we show that like the Baer, Kouri, Levin, and Tobocman equations, the Chandler-Gibson equations decouple and, in fact, reduce to a single wave operator equation of particularly simple form.

[NUCLEAR REACTIONS Chandler-Gibson N-body formalism—unitarity, kernel connectivity, introduction of projection operators, wave function equations, decoupling, comparison with CRC and BKLT formalisms.]

I. INTRODUCTION

The Chandler-Gibson (CG) formalism[1] for N-body scattering has the attractive property that it couples channels belonging to different partitions in a symmetric manner that appears very physical. The Baer, Kouri, Levin, and Tobocman[2] (BKLT) N-body scattering formalism, on the other hand, has a sequential partition coupling scheme which seems most unphysical. This suggests that the CG equations might respond better than the BKLT equations to an approximate treatment employing a truncated set of basis states.

In contrast to the BKLT equations, the CG integral equations are not of the connected kernel type, and this has discouraged interest in the CG equations. However, there have been some recent developments that suggest that kernel connectivity is after all not crucial to the usefulness of a set of coupled integral equations. Therefore, we believe renewed interest in the CG formalism is warranted. This has motivated the present reexamination of the CG formalism.

Connectivity is a necessary condition for compactness, and compactness is sufficient for the validity of the Fredholm alternative. Validity of the Fredholm alternative would guarantee the convergence of a discrete basis expansion that converts the set of linear integral equations into a set of linear algebraic equations.

In a recent publication Kuruoglu and Levin[3] tested the accuracy of an L^2 discretization approximation for solving dynamical integral equation sets for the scattering of a symmetric three-body system. They found that the (nonconnected kernel) coupled reaction channel (CRC) equations worked better than any of the several connected kernel formalisms that were tested. The CRC formalism does not generalize in a *simple* way to a formally exact set of integral equations for the general N-body system.[4] However, the CG formalism is a formally exact set of N-body equations which embody a symmetric coupling scheme similar to that of the CRC treatment.

The method of Kuruoglu and Levin[3] could be applied directly to the CG equations. However, there is another method which may prove to be more powerful. That is the method which Eyre and Osborn[5] tested with good results on a three-body system. Although they used the connected kernel

Karlsson-Zeiger equations, the fact that the method worked very well at a very low level of approximation seems to suggest that the kernel connectivity was not a significant factor. This method uses a Feshbach projection method to introduce a cluster expansion to force the equations into connected form. In addition, there is a set of nonconnected kernel equations for the effective interactions. However, these latter equations prove to be amenable to solution by a few terms of the Neumann series.

We show how the Feshbach projection operator scheme used by Eyre and Osborn[5] can be applied to the CG coupling scheme to get a modified form of the CG equations. This set of equations would then provide a basis for extending the Eyre and Osborn scheme to the general N-body problem.

We also discuss the question of decoupling the CG equations so that one is required to solve only a single integral equation rather than $\mathcal{N}$ coupled equations, where $\mathcal{N}$ is the number of partitions. This can be of great practical importance in numerical calculations. In a discrete basis treatment it reduces the dimension of the matrices to be inverted by a factor of $\mathcal{N}$. Ordinarily, the decoupling is achieved by iterating the coupled equations. Thus, when the BKLT equations are decoupled, the kernel of the resulting equation is the product of the kernels of all the original coupled equations. This is a reflection of the sequential coupling scheme that is characteristic of the BKLT formalism. On the other hand, the CG equations can be decoupled without resorting to iteration. The kernel of the resulting single equation is simply the sum of the kernels of the $\mathcal{N}$ original equations. This reflects the symmetric coupling of the CG formalism.

In Sec. II we show how the CG equations are derived from an appropriate coupling scheme. Verification of consistency with the unitarity constraint is done in Sec. III, and in Sec. IV we discuss the restriction of dynamical development to truncated channel subspaces in the CG formalism. Section V is devoted to the application of the Feshbach projection operator formalism to the special case CG equations. In Sec. VI the CG wave function equations are derived and compared to the coupled reaction channels equations. The CG equations are decoupled and reduced to a single dynamical equation in Sec. VII. A summary and a discussion of the results are given in Sec. VIII.

II. COUPLING SCHEME FOR THE CHANDLER-GIBSON (CG) EQUATIONS

We consider a system of N distinguishable particles interacting with each other via short range potentials. Let the lower case Greek letters label the different ways of partitioning these particles into *two* groups or clusters. Then associated with each such partition α is a division of the Hamiltonian for the system into two terms.

$$H = H_\alpha + V_\alpha \ . \tag{1}$$

Here H_α, the kinetic energy plus the intracluster interaction potentials, is called the partition Hamiltonian for partition α. The term V_α, the partition α residual interaction, is the sum of the intercluster interaction potentials for partition α.

The elements of the prior form of the transition operator matrix are

$$\hat{T}_{\beta\alpha} = V_\alpha + V_\beta \mathcal{G} V_\alpha \ , \tag{2}$$

where

$$\mathcal{G} = \lim_{\epsilon \to 0} (E + i\epsilon - H)^{-1} \ , \tag{3}$$

and E is the energy of the system. $\mathcal{G}$ is the system Green's function operator. Alternatively, this expression may be written

$$\begin{aligned} \hat{T}_{\beta\alpha} &= (1 + V_\beta \mathcal{G}) V_\alpha = (\mathcal{G}^{-1} + V_\beta) \mathcal{G} V_\alpha \\ &= G_\beta{}^{-1} \mathcal{G} V_\alpha \ , \end{aligned} \tag{4}$$

where

$$G_\beta = \lim_{\epsilon \to 0} (E + i\epsilon - H_\beta)^{-1} \tag{5}$$

is the partition β Green's function operator.

The relationship used to get Eq. (4), namely,

$$G_\beta{}^{-1} = \mathcal{G}^{-1} + V_\beta \ , \tag{6}$$

is the equivalent of the resolvent relation

$$\mathcal{G} = G_\beta + G_\beta V_\beta \mathcal{G} = G_\beta + \mathcal{G} V_\beta G_\beta \ . \tag{7}$$

The Lippmann-Schwinger (LS) N-particle equations result from combining Eqs. (2) and (4).

$$\begin{aligned} \hat{T}_{\beta\alpha} &= V_\alpha + V_\beta G_\gamma G_\gamma{}^{-1} \mathcal{G} V_\alpha \\ &= V_\alpha + V_\beta G_\gamma \hat{T}_{\gamma\alpha} \ . \end{aligned} \tag{8}$$

A coupling scheme[6] is defined by the representation of the residual interaction as a partition sum.

$$V_\beta = \sum_\gamma v_{\beta\gamma} \ . \tag{9}$$

The associated set of dynamical equations is the result of combining Eqs. (9), (4), and (2).

$$\begin{aligned} \hat{T}_{\beta\alpha} &= V_\alpha + \sum_\gamma v_{\beta\gamma} G_\gamma G_\gamma{}^{-1} \mathcal{G} V_\alpha \\ &= V_\alpha + \sum_\gamma v_{\beta\gamma} G_\gamma \hat{T}_{\gamma\alpha} \ . \end{aligned} \tag{10}$$

To get the BKLT equations one uses the coupling scheme

$$V_\beta = \sum_\gamma V_\beta \delta_{\gamma,\beta+1} , \tag{11}$$

with the result

$$\hat{T}_{\beta\alpha} = V_\alpha + V_\beta G_{\beta+1} \hat{T}_{\beta+1\alpha} . \tag{12}$$

This is seen to be just the set of LS equations which sequentially couple the elements of a given column of the transition operator matrix.

We use an approach to the CG equations which is due to Polyzou.[7] The coupling scheme that produces one version of the CG equations is just

$$V_\beta = \mathcal{N}^{-1} \sum_\gamma V_\beta , \tag{13}$$

where $\mathcal{N}$ is just the number of two-cluster partitions. Combining Eqs. (13), (4), and (2) gives

$$\begin{aligned} \hat{T}_{\beta\alpha} &= V_\alpha + V_\beta \mathcal{N}^{-1} \sum_\gamma G_\gamma G_\gamma{}^{-1} \mathcal{G} V_\alpha \\ &= V_\alpha + V_\beta \mathcal{N}^{-1} \sum_\gamma G_\gamma \hat{T}_{\gamma\alpha} . \end{aligned} \tag{14}$$

We will call these the special Chandler-Gibson (SCG) equations. This equation can be derived from Eq. (8) by summing both sides on γ and dividing by $\mathcal{N}$. Thus these CG equations are simply a selection of LS equations, as are the BKLT equations, but in each case the selection is different. The BKLT equations have the advantage that they decouple upon iteration to yield connected kernel integral equations for each element of the transition operator matrix. The SCG equations have the advantage that they couple the channels in a symmetric manner.

The above version of the CG equations is a special case of the following set of equations:

$$\hat{T}_{\beta\alpha} = V_\alpha + V_\beta \mathcal{M}^{-1} \sum_\gamma P_\gamma G_\gamma \hat{T}_{\gamma\alpha} . \tag{15}$$

These result from the coupling scheme

$$V_\beta = V_\beta \mathcal{M}^{-1} \sum_\gamma P_\gamma , \tag{16}$$

or equivalently from the following resolution of the identity,

$$1 = \mathcal{M}^{-1} \sum_\gamma P_\gamma . \tag{17}$$

Here P_γ is a projection operator, and evidently,

$$\mathcal{M} = \sum_\gamma P_\gamma . \tag{18}$$

The special case represented by Eq. (14) corresponds to replacing each projector P_γ by the identity. If the sum on the right of Eq. (18) does not span the entire Banach space, then the inverse of $\mathcal{M}$ must be defined on that part of the Banach space which is spanned by $\mathcal{M}$. The resulting set of equations must then be regarded as approximate, since Eq. (17) is not rigorously satisfied.

III. UNITARITY OF THE CHANDLER-GIBSON EQUATIONS

We next address the question of whether the solution of the CG equations is constrained to fulfill the requirement that the collision matrix be unitary. This is not an empty exercise since Benoist-Gueutal[8] has given an example of an LS equation which is not consistent with that constraint. The consistency of the solution of the BKLT equations with unitarity has been established by Kouri and Levin[9] and by Benoist-Gueutal.[10] Our discussion will be similar to theirs except that it will be simplified by making a unique assignment of each channel to a particular partition Green's function operator.

Our first step will be the introduction of an alternative form of the CG equations more suitable to our purpose. We start with the post form of the transition operator matrix

$$\begin{aligned} T_{\beta\alpha} &= V_\beta + V_\beta \mathcal{G} V_\alpha = V_\beta \mathcal{G} \overleftarrow{G}_\alpha{}^{-1} \\ &= V_\beta - V_\alpha + G_\beta{}^{-1} \mathcal{G} V_\alpha . \end{aligned} \tag{19}$$

This is then combined with the partition coupling scheme of Eq. (16)

$$\begin{aligned} T_{\beta\alpha} &= V_\beta \mathcal{M}^{-1} \sum_\gamma P_\gamma G_\gamma \{ \overleftarrow{G}_\gamma{}^{-1} + \overleftarrow{G}_\gamma{}^{-1} \mathcal{G} V_\alpha \} \\ &= V_\beta \mathcal{M}^{-1} \sum_\gamma P_\gamma G_\gamma \{ \overleftarrow{G}_\gamma{}^{-1} + V_\alpha - V_\gamma + T_{\gamma\alpha} \} \\ &= V_\beta \mathcal{M}^{-1} \sum_\gamma P_\gamma G_\gamma \{ \overleftarrow{G}_\alpha{}^{-1} + T_{\gamma\alpha} \} . \end{aligned} \tag{20}$$

Equation (20) is related to Eq. (15) the same way as the post Kouri-Levin BKLT equation is related to the prior Baer-Kouri BKLT equation.

Next we define the auxiliary transition operator matrix t.

$$t_{\beta\alpha} = V_\beta \mathcal{M}^{-1} P_\alpha + V_\beta \mathcal{M}^{-1} \sum_\gamma P_\gamma G_\gamma t_{\gamma\alpha} . \tag{21}$$

This is related to the transition operator matrix T by

$$T_{\beta\alpha} = \sum_\gamma t_{\beta\gamma} G_\gamma \overleftarrow{G}_\alpha{}^{-1} . \tag{22}$$

For convenience we introduce (partition space) matrix notation.

$$t = VU\mathcal{M}^{-1} P + VU\mathcal{M}^{-1} PGt , \tag{21a}$$

$$T = tGU\overleftarrow{G}^{-1} , \tag{22a}$$

where P, G, and V are diagonal matrices, $\mathscr{M}^{-1}$ is a scalar, and U is the units matrix.

$$[U]_{\alpha\beta}=1 \quad (\text{all } \alpha,\beta) . \tag{23}$$

The complex conjugate of the auxiliary T-matrix operator is the solution of

$$\begin{aligned} t^* &= VU\mathscr{M}^{-1}P + VU\mathscr{M}^{-1}PG^*t^* \\ &= (1+t^*G^*)VU\mathscr{M}^{-1}P . \end{aligned} \tag{24}$$

Now combine Eqs. (21a) and (24).

$$\begin{aligned} t &= (1+t^*G^*)VU\mathscr{M}^{-1}P(1+Gt) - t^*G^*t \\ &= t^* + t^*(G-G^*)t . \end{aligned} \tag{25}$$

Matrix elements of the elements of t with respect to asymptotic states are then

$$\begin{aligned} &\langle \phi_{\beta b} \mid t_{\beta a} - t^*_{\beta a} \mid \phi_{aa} \rangle \\ &\qquad = \sum_{\gamma} \langle \phi_{\beta b} \mid t^*_{\beta\gamma}(G_\gamma - G^*_\gamma)t_{\gamma a} \mid \phi_{aa} \rangle , \end{aligned} \tag{26}$$

where the Latin subscripts are channel indices and

$$(E-H_\alpha)\phi_{aa}=0 . \tag{27}$$

The partition Green's function operators have the property

$$\begin{aligned} G_\gamma - G^*_\gamma &= -2\pi i\delta(E-H_\gamma) \\ &= -2\pi i \sum_{c\in\gamma}{}' \mid \phi_{\gamma c} \rangle\langle \phi_{\gamma c} \mid , \end{aligned} \tag{28}$$

where the prime on the sum over channels c indicates that only open channels are to be included. Combining Eqs. (26) and (28) then gives

$$\mathscr{T}_{ba} - \mathscr{T}^*_{ba} = -2\pi i \sum_{\gamma} \sum_{c\in\gamma}{}' \mathscr{T}^*_{bc}\mathscr{T}_{ca} , \tag{29}$$

where

$$\mathscr{T}_{ba} = \langle \phi_{\beta b} \mid t_{\beta a} \mid \phi_{aa} \rangle , \tag{30}$$

and we have used the fact that the channel state wave functions $\phi_{\beta b}$ can be chosen real.

Observe next that by virtue of the Lippmann identity

$$\begin{aligned} \mathscr{T}_{ba} &= \langle \phi_{\beta b} \mid \sum_{\gamma} t_{\beta\gamma}G_\gamma \overleftarrow{G}_\alpha{}^{-1} \mid \phi_{aa} \rangle \\ &= \langle \phi_{\beta b} \mid T_{\beta a} \mid \phi_{aa} \rangle , \end{aligned} \tag{31}$$

so that $\mathscr{T}$ is the transition matrix. Thus Eq. (29) just expresses the unitarity of the collision matrix $\mathscr{S}$,

$$\mathscr{S} = 1 - 2\pi i\mathscr{T} , \tag{32}$$

when the symmetry of $\mathscr{T}$ is taken into account. We conclude that the CG equations do satisfy unitarity.

The above conclusion requires one qualification. One must remember that the projector P_α is implicit as a final factor in the definition of $t_{\beta\alpha}$. Thus the sum in Eq. (29) includes only those channels which are contained in the projectors $\{P_\gamma\}$. Therefore the unitarity sum will be complete only if the set of projectors $\{P_\gamma\}$ contains all the open channels.

IV. ROLE OF THE PROJECTION OPERATORS

What sets the CG N-particle scattering formalism apart from all others is the manner in which the projectors are introduced. In principle, the projectors P_γ that appear in Eqs. (15)–(18) are arbitrary. The explicit construction of the inverse of $\mathscr{M}$ (called JJ^* by Chandler and Gibson) might be done in the following way: by introducing a convenient discrete basis $\{ \mid m \rangle \}$ for the Banach space. These states might be products of single particle harmonic oscillator states. Then we can form the matrix $\underline{\mathscr{M}}^{(N_0)}$ with elements

$$\begin{aligned} \mathscr{M}^{(N_0)}_{mn} &= \sum_{\gamma} \langle m \mid P_\gamma \mid n \rangle \\ &= [\underline{\mathscr{M}}^{(N_0)}]_{mn} \quad (m,n \le N_0) . \end{aligned} \tag{33}$$

The dimension of this matrix is labeled N_0. Then we have

$$\mathscr{M} = \lim_{N_0\to\infty} \mathscr{M}^{(N_0)} , \tag{34a}$$

$$\mathscr{M}^{(N_0)} = \sum_{m=1}^{N_0}\sum_{n=1}^{N_0} \mid m \rangle \mathscr{M}^{(N_0)}_{mn} \langle n \mid , \tag{34b}$$

and, accordingly,

$$\mathscr{M}^{-1} = \lim_{N_0\to\infty} \mathscr{M}^{(N_0)-1} , \tag{35a}$$

$$\mathscr{M}^{(N_0)-1} = \sum_{m=1}^{N_0}\sum_{n=1}^{N_0} \mid m \rangle [\underline{\mathscr{M}}^{(N_0)-1}]_{mn} \langle n \mid . \tag{35b}$$

In practice, we expect that if $\mathscr{M}$ does not span the entire Banach space, then there will be an upper limit $\bar{N}_0$ for N_0 above which $\underline{\mathscr{M}}^{(N_0)-1}$ does not exist. Then one would have to be content with the approximation

$$\mathscr{M}^{-1} \approx \mathscr{M}^{(\bar{N}_0)-1} . \tag{36}$$

Next let us consider the sort of projectors one would want to use. Consider the resolution of the identity in terms of the partition asymptotic states,

that is to say, in terms of the eigenstates of H_γ.

$$1=\sum_{c\in\gamma} |\phi_{\gamma c}\rangle\langle\phi_{\gamma c}| \ . \tag{37}$$

The sum on c is understood to include an integral on energy. There will be additional integrals for the relative motion kinetic energies in those channels c describing three or more clusters, i.e., the breakup channels.

In any practical calculation for a complex system a reasonable approximation would be to neglect transitions to virtual intermediate states $\phi_{\gamma c}$ which are far from the energy shell or which have a very different structure from that in the incident channel. Thus in the dynamical equations one would replace the partition Green's function operators G_γ by $P_\gamma G_\gamma$, where

$$P_\gamma=\sum_{c\in\gamma}'' |\phi_{\gamma c}\rangle\langle\phi_{\gamma c}| \ , \tag{38}$$

and where the double prime indicates that the sum on channels has been truncated in some suitable way.

This represents an approximation. However, the CG coupling scheme permits the introduction of the normalization operator $\mathscr{M}^{-1}$ which mitigates to a certain extent the harm caused by the introduction of the projection operators. Indeed, if the projection operators span the Banach space, then the presence of $\mathscr{M}^{-1}$ compensates entirely for the intermediate state contributions suppressed by the projection operators.

Thus it appears that the CG formalism is less sensitive to truncations of the spectrum of allowed intermediate virtual states than is the BKLT scattering formalism. The cost paid for this, dynamical integral equations with disconnected kernels, is very high. Some hope in this regard is provided by a connected kernel formalism by Polyzou, Gibson, and Chandler[11] which is a modification of the CG formalism.

An alternative method for compensating for the deletions caused by the introduction of projection operators is provided by the Feshbach projection operator method. This will be discussed in the next section.

V. APPLICATION OF THE FESHBACH PROJECTION OPERATOR METHOD TO THE COUPLED EQUATIONS FORMALISM

The Feshbach projection operator method has been applied to the BKLT formalism by Goldflam and Tobocman.[12] We will now consider the application of this method to the SCG equations to produce a formally exact alternative to the CG equations. We expect that these alternative Chandler-Gibson (ACG) equations will provide a practical basis for calculations.

The SCG equations displayed in Eqs. (14) and (20) (with $\mathscr{M}$ and P_γ set equal to $\mathscr{N}$ and 1, respectively) can be written in the form

$$T_{\beta\alpha}=M_{\beta\alpha}+\sum_\gamma V_\beta W_{\beta\gamma} G_\gamma T_{\gamma\alpha} \ . \tag{39}$$

Let us use matrix notation and write this equation as

$$T=M+VWGT \ , \tag{40}$$

where V and G are diagonal matrices in partition space. In Eq. (40) the elements of the matrix W are

$$W_{\alpha\beta}=\mathscr{N}^{-1} \ \text{(SCG)} \ . \tag{41}$$

By changing to

$$W_{\alpha\beta}=\delta_{\alpha,\beta-1} \ \text{(BKLT)} \ , \tag{42}$$

and making the appropriate change in the definition of M, we can convert Eq. (40) from SCG to BKLT.

To apply the Feshbach projection operator formalism we introduce the complementary projection operator matrices P and Q.

$$P+Q=1 \ , \tag{43a}$$

$$P^2=P \ , \ Q^2=Q \ , \tag{43b}$$

$$Q_{\alpha\beta}=\delta_{\alpha\beta}Q_\beta \ , \ P_{\alpha\beta}=\delta_{\alpha\beta}P_\beta \ . \tag{43c}$$

These are then inserted into Eq. (40).

$$\begin{aligned} T&=M+VWG(P+Q)T \\ &=L+FWGPT \ , \end{aligned} \tag{44}$$

where

$$\begin{aligned} L&=(1-VWGQ)^{-1}M \\ &=M+VWGQL \end{aligned} \tag{45}$$

and

$$\begin{aligned} F&=(1-VWGQ)^{-1}V \\ &=V+VWGQF \ . \end{aligned} \tag{46}$$

Equations (44)—(46) constitute what we will call the alternative Chandler-Gibson formalism. They are formally exact. By making the projectors P_γ sufficiently restrictive we can force the kernel of Eq. (44) to be connected. Then Eq. (44) can be solved for T by conventional methods.

Of course, Eqs. (45) and (46) must be solved to provide the input for Eq. (44), and these equations do not have connected kernels. However, it should be possible to endow P_γ with sufficient strength so that $Q_\gamma V_\gamma$ is a relatively weak interaction. Then instead of solving Eqs. (45) and (46) we can get ade-

quate representations of the solutions from the first few terms of the iteration series.

$$L = M + VWGQM + VWGQVWGQM + \cdots , \tag{47}$$

$$F = V + VWGQV + VWGQVWGQV + \cdots . \tag{48}$$

Thus the ACG formalism appears to be a basis for practical few-body scattering calculations which has the advantage of coupling the partitions in a symmetrical manner.

A comparison of the CG formalism and the Feshbach formalism has been given by Chandler and Gibson.[13] The Feshbach formalism discussed there is the standard one that results from applying the Feshbach projection operator method to the Lippmann-Schwinger equations. The ACG formalism introduced here is produced by applying the Feshbach projection operator method to the SCG equations. Thus these two formalisms are based on different coupling schemes.

VI. WAVE FUNCTION EQUATIONS FOR THE CHANDLER-GIBSON FORMALISM

Hahn, Kouri, and Levin[14] have shown how the BKLT equations may be transformed into a set of coupled equations for the components of the scattering wave function. We will do the same for the CG equations. Our purpose is to compare these equations with those of the coupled reaction channels (CRC) formalism. The two should be closely related because both have a symmetric partition coupling scheme.

We start with Eq. (20) written in matrix notation

$$T = VWGU\overleftarrow{G}^{-1} + VWGT , \tag{49a}$$

$$W = \mathscr{M}^{-1}UP . \tag{49b}$$

Next the wave functions are defined by

$$T\Phi_b = VW\Psi_b , \tag{50a}$$

$$[\Phi_b]_\alpha = \delta_{\alpha\beta}\phi_{\beta b} , \tag{50b}$$

where Ψ_b is the scattering wave function vector and Φ_b is the asymptotic state corresponding to incident flux in channel b belonging to partition β. Then substitution of Eq. (50) into Eq. (49) gives

$$\Psi_b = GUG^{-1}\Phi_b + GVW\Psi_b . \tag{51a}$$

In component notation this is just

$$\psi_{\alpha b} = G_\alpha \overleftarrow{G}_\beta{}^{-1}\phi_{\beta b} + G_\alpha V_\alpha \mathscr{M}^{-1}\sum_{\gamma=1}^{\mathscr{N}} P_\gamma \psi_{\gamma b} . \tag{51b}$$

In contrast to the BKLT case where the coupling is sequential, the coupling here is symmetric. For the special case CG equations where $\mathscr{M} = \mathscr{N}$ and $P_\gamma = 1$, Eq. (51) is recognized as the Lippmann-Schwinger N-body equations for the scattering wave function

$$[\Psi_b]_\alpha = \psi_{\alpha b} , \tag{52a}$$

$$\psi_b = \psi_{\alpha b} = \psi_{\beta b} = \psi_{\gamma b} = \cdots . \tag{52b}$$

Thus we have not found anything very novel, but we have confirmed the identity of the scattering wave function vector Ψ_b.

To proceed further we introduce an alternative version of the CG equations.

$$\begin{aligned} T_{\alpha\beta} &= V_\alpha + V_\alpha \mathscr{G} V_\beta = V_\alpha \mathscr{G} \overleftarrow{G}_\beta{}^{-1} \\ &= V_\alpha + \sum_{\gamma=1}^{\mathscr{N}} V_\alpha \mathscr{G} G_\gamma{}^{-1} G_\gamma P_\gamma \mathscr{M}^{-1} V_\beta \\ &= V_\alpha + \sum_{\gamma} T_{\alpha\gamma} G_\gamma P_\gamma \mathscr{M}^{-1} V_\beta . \end{aligned} \tag{53}$$

In matrix notation this is

$$T = VU + TGWV , \tag{54a}$$

$$W = PU\mathscr{M}^{-1} . \tag{54b}$$

We now substitute the formal solution of Eq. (54a) into Eq. (50a).

$$\begin{aligned} VW\Psi_b &= VU(1 - GWV)^{-1}\Phi_b \\ &= VPU\mathscr{M}^{-1}\Psi_b . \end{aligned} \tag{55}$$

Finally, let us define

$$U\Xi_b = PU\mathscr{M}^{-1}\Psi_b . \tag{56}$$

Then from Eq. (55) we will have

$$\begin{aligned} \Xi_b &= (1 - GWV)^{-1}\Phi_b \\ &= \Phi_b + GWV\Xi_b . \end{aligned} \tag{57a}$$

In component form this reads

$$\xi_{\alpha b} = \delta_{\alpha\beta}\phi_{\beta b} + G_\alpha P_\alpha \mathscr{M}^{-1}\sum_{\gamma=1}^{\mathscr{N}} V_\gamma \xi_{\gamma b} . \tag{57b}$$

By virtue of Eqs. (50a), (55), and (56) one finds

$$T\Phi_b = VU\Xi_b \tag{58a}$$

or

$$T_{\alpha\beta}\phi_{\beta b} = V_\alpha \sum_{\gamma=1}^{\mathscr{N}} \xi_{\gamma b} . \tag{58b}$$

Equations (57) and (58) constitute the CG wave function formalism. Let us examine the special case where $\mathscr{M} = \mathscr{N}$ and $P_\gamma = 1$.

$$\xi_{\alpha b}=\delta_{\alpha\beta}\phi_{\beta b}+G_\alpha \mathscr{N}^{-1}\sum_{\gamma=1}^{\mathscr{N}} V_\gamma \xi_{\gamma b} \ . \tag{59}$$

The associated integrodifferential equation is

$$(E-H_\alpha)\xi_{\alpha b}=\mathscr{N}^{-1}\sum_{\gamma=1}^{\mathscr{N}} V_\gamma \xi_{\gamma b} \ . \tag{60}$$

Summing both sides of Eq. (60) on α produces

$$\begin{aligned} 0&=\sum_{\alpha=1}^{\mathscr{N}}(E-H_\alpha-V_\alpha)\xi_{\alpha b} \\ &=(E-H)\sum_{\alpha=1}^{\mathscr{N}}\xi_{\alpha b} \ , \end{aligned} \tag{61}$$

which demonstrates that $\sum \xi_{\alpha b}$ is equal to the scattering wave function. This could have been found directly from Eq. (56) in the special case of $\mathscr{M}=\mathscr{N}$ and $P_\gamma=1$.

Now let us compare our result with the coupled reaction channels (CRC) equations. These are derived directly from the Schrödinger equation

$$(E-H_\alpha)\sum_\gamma \xi_{\gamma b}=V_\alpha \sum_\gamma \xi_{\gamma b} \tag{62}$$

by just recombining terms.

$$(E-H_\alpha)\xi_{\alpha b}=\sum_\gamma \{V_\alpha-(1-\delta_{\alpha\gamma})(E-H_\alpha)\}\xi_{\gamma b} \ . \tag{63}$$

Comparing Eqs. (60) and (63) shows that

$$\mathscr{N}^{-1}\sum_\gamma V_\gamma \xi_{\gamma b}=\sum_\gamma \{V_\alpha-(1-\delta_{\alpha\gamma})(E-H_\alpha)\}\xi_{\gamma b} \ . \tag{64}$$

We see that the CRC nonorthogonality terms $(1-\delta_{\alpha\gamma})(E-H_\alpha)$ are absent from the SCG equations. We also see that the coupling is different with V_γ in place of V_α. Evidently, the reduction in coupling strength caused by the factor $\mathscr{N}^{-1}$ is in some way equivalent to the subtraction of strength due to the nonorthogonality terms.

VII. DECOUPLING OF CG COUPLED EQUATIONS

The BKLT N-body equations for the transition operators have the remarkable property that they become decoupled upon iteration. The result is an integral equation for each element of the transition operator matrix. We will show that the CG equations can be also decoupled. This property can be of great practical importance as it reduces the difficulty of numerical solution. This is because one needs only solve a single integral equation instead of a set of coupled integral equations.

Let us first review the decoupling of the BKLT equations. Start with the BKLT equation (12) and iterate it once. The result is

$$\begin{aligned} \hat{T}_{\beta\alpha}&=V_\alpha+V_\beta G_{\beta+1}V_\alpha \\ &\quad +V_\beta G_{\beta+1}V_{\beta+1}G_{\beta+2}\hat{T}_{\beta+2,\alpha} \ . \end{aligned} \tag{65}$$

Suppose there are $\mathscr{N}$ two-cluster partitions possible for the system. Then partition $\beta+\mathscr{N}$ will again be partition β. Thus by iterating Eq. (12) $\mathscr{N}-1$ times we will succeed in finding a decoupled equation for $\hat{T}_{\beta\alpha}$.

$$\hat{T}_{\beta\alpha}=M_{\beta\alpha}+N_\beta G_\beta \hat{T}_{\beta\alpha} \ , \tag{66a}$$

$$\begin{aligned} M_{\beta\alpha}&=(1+V_\beta G_{\beta+1}+V_\beta G_{\beta+1}V_{\beta+1}G_{\beta+2}+\cdots \\ &\quad +V_\beta G_{\beta+1}V_{\beta+1}\cdots G_{\beta-2}V_{\beta-2}G_{\beta-1})V_\alpha \ , \end{aligned} \tag{66b}$$

$$N_\beta=V_\beta G_{\beta+1}V_{\beta+1}\cdots G_{\beta-2}V_{\beta-2}G_{\beta-1}V_{\beta-1} \ . \tag{66c}$$

It has been pointed out by Bencze[15] that any coupled equations scattering formalism can be decoupled with the help of the LS N-body equations. Let us use his method to decouple the CG equations shown in Eq. (15). In that equation we substitute for each transition operator $\hat{T}_{\gamma\alpha}$ that appears in the sum the expression for $\hat{T}_{\gamma\alpha}$ in terms of $\hat{T}_{\beta\alpha}$ provided by the LS N-body equations.

$$\hat{T}_{\gamma\alpha}=V_\alpha+V_\gamma G_\beta \hat{T}_{\beta\alpha} \ . \tag{67}$$

The result is a decoupled CG equation for $\hat{T}_{\beta\alpha}$.

$$\hat{T}_{\beta\alpha}=\bar{M}_{\beta\alpha}+\bar{N}_\beta G_\beta \hat{T}_{\beta\alpha} \ , \tag{68a}$$

$$\bar{M}_{\beta\alpha}=\left[1+V_\beta \mathscr{M}^{-1}\sum_\gamma P_\gamma G_\gamma\right]V_\alpha \ , \tag{68b}$$

$$\bar{N}_\beta=V_\beta \mathscr{M}^{-1}\sum_\gamma P_\gamma G_\gamma V_\gamma \ . \tag{68c}$$

This result can be put in simpler form by setting

$$\hat{T}_{\beta\alpha}=Z_\beta V_\alpha \ . \tag{69a}$$

Then Z_β is the solution of

$$Z_\beta=\bar{R}_\beta+\bar{N}_\beta G_\beta Z_\beta \ , \tag{69b}$$

where

$$\bar{R}_\beta=1+V_\beta \mathscr{M}^{-1}\sum_\gamma P_\gamma G_\gamma \ . \tag{69c}$$

Thus one integral equation needs to be solved for each row of the transition operator matrix.

We will now present an alternative method for decoupling the CG equations. The resulting integral equation will have a simpler kernel than the one just derived. In addition, the solution can be used direct-

ly to calculate every element of the transition operator matrix.

We start again with the CG equations shown in Eq. (15). Define the auxiliary quantity $\hat{\tau}_{\beta\alpha}$ as the solution of

$$\hat{\tau}_{\beta\alpha}=V_\beta\mathscr{M}^{-1}+V_\beta\mathscr{M}^{-1}\sum_\gamma P_\gamma G_\gamma\hat{\tau}_{\gamma\alpha}\ . \tag{70}$$

In matrix notation, Eqs. (15) and (70) read

$$\hat{T}=UV+V\mathscr{M}^{-1}UPG\hat{T}\ , \tag{71}$$

$$\begin{aligned}\hat{\tau}&=V\mathscr{M}^{-1}U+V\mathscr{M}^{-1}UPG\hat{\tau}\\&=V\mathscr{M}^{-1}U+\hat{\tau}PGV\mathscr{M}^{-1}U\ .\end{aligned} \tag{72}$$

Now combine Eqs. (71) and (72) as follows:

$$\begin{aligned}\hat{T}&=(1+\hat{\tau}PG)(UV+V\mathscr{M}^{-1}UPG\hat{T})-\hat{\tau}PG\hat{T}\\&=UV+\hat{\tau}PGUV\ .\end{aligned} \tag{73}$$

Thus $\hat{T}$ can be expressed in terms of $\hat{\tau}$.

From Eq. (70) we can see that $\hat{\tau}$ has the form

$$\hat{\tau}_{\beta\alpha}=V_\beta\mathscr{M}^{-1}\hat{\Omega}\ , \tag{74a}$$

where

$$\begin{aligned}\hat{\Omega}&=1+\sum_\gamma P_\gamma G_\gamma V_\gamma\mathscr{M}^{-1}\hat{\Omega}\\&=\left[1-\sum_\gamma P_\gamma G_\gamma V_\gamma\mathscr{M}^{-1}\right]^{-1}\ .\end{aligned} \tag{74b}$$

Combining Eqs. (73) and (74) gives

$$\hat{T}_{\beta\alpha}=V_\alpha+V_\beta\mathscr{M}^{-1}\hat{\Omega}\sum_\gamma P_\gamma G_\gamma V_\alpha\ . \tag{75}$$

This gives all the transition operators in terms of the single wave operator $\hat{\Omega}$. Alternatively, we can write

$$\hat{T}_{\beta\alpha}=V_\alpha+V_\beta\Omega\mathscr{M}^{-1}\sum_\gamma P_\gamma G_\gamma V_\alpha\ , \tag{76a}$$

where

$$\Omega=1+K\Omega=(1-K)^{-1} \tag{76b}$$

and

$$K=\mathscr{M}^{-1}\sum_\gamma P_\gamma G_\gamma V_\gamma\ . \tag{76c}$$

Equation (76) is the alternative decoupled dynamical equation for the CG N-body formalism. Thus we have done more than decouple the CG equations; we have reduced them to just a single equation. This equation can be easily transformed into the version corresponding to the ACG formalism introduced in Sec. V. For the case where all the P_γ's are equal to the identity, Eq. (76c) becomes

$$K=\mathscr{N}^{-1}\sum_\gamma G_\gamma V_\gamma\ . \tag{77}$$

Now introduce the Feshbach projectors

$$\begin{aligned}\Omega&=1+K(P+Q)\Omega\\&=\Omega_Q+\Omega_QKP\Omega\ ,\end{aligned} \tag{78a}$$

where

$$\begin{aligned}\Omega_Q&=(1-KQ)^{-1}\\&=1+KQ\Omega_Q\ .\end{aligned} \tag{78b}$$

The idea is to choose the projector P so that it is restrictive enough so that the kernel KP is a connected operator and yet inclusive enough so that KQ is sufficiently weak so that the power series for Ω_Q,

$$\Omega_Q=1+KQ+(KQ)^2+\cdots\ , \tag{79}$$

is rapidly convergent.

A convenient expression for evaluating the wave operator Ω is provided by

$$\begin{aligned}\Omega=L_Q+N_P+L_QQKPN_P+N_PPKQL_Q\\+L_QQKPN_PPKQL_Q\ ,\end{aligned} \tag{80a}$$

where

$$N_P=(1-PKP-PKQL_QQKP)^{-1}P \tag{80b}$$

and

$$L_Q=(1-QKQ)^{-1}Q\ . \tag{80c}$$

Here we would have a presumably connected kernel integral equation for N_P to solve in P space and a power series for L_Q to sum in Q space.

The fact that only a single dynamical equation needs to be solved in the CG formalism does not really distinguish it very much from the BKLT scattering formalism. Once any element of a given row of the transition operator matrix has been calculated, any other element of that row can be calculated by quadrature by means of the Lippmann-Schwinger N-body equations. Then using the elements of that row the elements in all other rows can be calculated from the Lippmann-Schwinger equations by quadrature.

VIII. SUMMARY AND DISCUSSION

Using the conventional single Hilbert space formulation of scattering theory we have shown how the Chandler-Gibson (CG) many-body scattering theory and the Baer, Kouri, Levin, and Tobocman (BKLT) scattering theory are related to each other. The dynamical equations of the two formalisms have the same structure, differing only in the partition coupling scheme used. Thus the consistency of the CG equations with the unitarity constraint could be demonstrated by the same analysis that had been used for the BKLT equations.

We believe that the symmetric partition coupling scheme of the CG formalism may prove to be of great calculational importance. Recent numerical tests of the BKLT equations on a three body system by Tobocman[16] and by Kuruoglu and Levin[3] have found that the discrete basis method is poorly converging for scattering states. On the other hand, Kuruoglu and Levin[3] have found that this method converges much more rapidly when applied to the coupled reaction channels (CRC) equations.

Like the CG equations, the CRC equations have symmetric partition coupling. This may be the key to the success of Kuruoglu and Levin's CRC calculation and would therefore augur well for discrete basis calculations using the CG equations. It seems likely that in the dynamical development of the symmetric three-body system considered by Kuruoglu and Levin, intermediate state transitions should follow a symmetric pattern that would be more easily reproduced by equations that make this explicit.

We have discussed the introduction of projection operators into the SCG equations to get the CG equations and the role of the normalization operator $\mathscr{M}^{-1}$ in compensating for the resultant deletions. We have indicated how the operator $\mathscr{M}^{-1}$ would be constructed in a discrete basis calculation.

The use of a discrete basis transforms the Banach space into a Hilbert space. One might well question the efficacy of such a basis for representing the noncompact operators appearing in the CG equations. However, the sort of projection operators $P_\alpha, P_\beta, \ldots$, one would want to use would most likely be ones that restrict the wave function to particular two-cluster configurations of the partition in question. Now consider the consequences of this fact for CG equations of the type shown in Eq. (20). By virtue of the fact that

$$T_{\alpha\beta}=V_\alpha \mathscr{G}\overleftarrow{G}_\beta{}^{-1}=V_\alpha \mathscr{J}_\beta \,, \tag{81}$$

Eq. (20) can be written to read

$$\mathscr{J}_\beta=\mathscr{M}^{-1}\sum_\gamma P_\gamma G_\gamma\{\overleftarrow{G}_\beta{}^{-1}+V_\gamma \mathscr{J}_\beta\} \,. \tag{82}$$

Thus the kernel is $\mathscr{M}^{-1}\sum_\gamma P_\gamma G_\gamma V_\gamma$. For the case where all the P_γ's are two-cluster projectors this will be a connected operator.

It is not unreasonable to expect that connected operators of this type would be representable by a discrete basis. As a matter of fact, discrete basis BKLT calculations using projection operators of this sort have had some success.[17]

In discussing their many-body scattering formalism, Chandler and Gibson have attached special significance to the role played by the projection operators in restricting the region of Banach space in which the transition operators must be determined. We agree that the restriction thus imposed on intermediate state propagation can be very helpful in practical calculations, but we observe that the normalization operator $\mathscr{M}^{-1}$ may not be able to compensate for these deletions if they are too severe.

The Feshbach projection operator method has been suggested here as an alternative to the normalization operator as a way to compensate for the introduction of projection operators into the formally exact SCG equations. The advantage of the Feshbach method is that the corrections to the driving term, $L-M$ in Eq. (44), and the corrections to the kernel interaction factor, $F-V$ in Eq. (44), carry contributions from the regions of Banach space excluded by the projectors $P_\alpha, P_\beta, \ldots$. Such contributions cannot be picked up by the CG normalization operator $\mathscr{M}^{-1}$ if they are excluded by all the projectors.

The CG wave function equations are derived and compared to the CRC wave function equations. Like the BKLT equations, the CG equations have no nonorthogonality terms. Like the CRC equations, they have a symmetric partition coupling scheme.

Finally, we have compared the decoupling of the CG equations with that of the BKLT equations. That is, we have shown how the set of coupled integral equations can be replaced by a single integral equation. The resultant BKLT integral equation has a connected kernel while the CG one does not. We have pointed out how projection operators can be used to overcome this difficulty for the CG equations.

The decoupled BKLT equation results from iteration of the BKLT equations. On the other hand, no iterations are required to get the decoupled CG equation. This fact suggests that it may be possible to show that the solution of this equation is unique and free of the possibility of spurious solutions that exists for the decoupled BKLT equation.[18]

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