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Minimal coupling schemes in N-body reaction theory

A. Picklesimer
Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106

P. C. Tandy
Department of Physics, Kent State University, Kent, Ohio 44242

R. M. Thaler
Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106

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A new derivation of the N-body equations of Bencze, Redish, and Sloan is obtained through the use of Watson-type multiple scattering techniques. The derivation establishes an intimate connection between these partition-labeled N-body equations and the particle-labeled Rosenberg equations. This result yields new insight into the implicit role of channel coupling in, and the minimal dimensionality of, the partition-labeled equations.

[NUCLEAR REACTIONS Scattering theory, multiple scattering, connected kernel reaction theory, minimal coupling, coupling schemes.]

We consider the nonrelativistic theory of N interacting (nuclear) particles under the assumption that the (nuclear) force can be represented by two-body potentials, so that the Hamiltonian for the entire system is

$$H=H_0+V=\sum_i K_i+\sum_{i<j} v_{ij}=\sum_i K_i+\sum_p V_p \ . \tag{1}$$

In Eq. (1) K_i is the kinetic energy operator for particle i, with the sum over i taken over the N particles of the system, and V_p is the two-body interaction potential for the particular pair of particles p, with the sum over p taken over the $\frac{1}{2}N(N-1)$ possible pairs. The operator $T^{00}\equiv T$, the N to N transition operator, plays a special role in the N-body reaction theory because T, given by

$$\begin{aligned} T&=VGG_0^{-1}=\sum_p V_pGG_0^{-1}=\sum_p T_p \\ &=\sum_p V_p(E-H+i\eta)^{-1}(E-H_0+i\eta) \ , \end{aligned} \tag{2}$$

with G and G_0 taken to be defined by the final equality in Eq. (2), permits us to express the resolvent identity as

$$G=G_0+G_0TG_0 \ . \tag{3}$$

Thus knowledge of T is equivalent to knowledge of G from which any transition operator $T^{\beta\alpha}$ may be constructed directly.

If the N to N operator T is written as $T=\sum_p T_p$, as in Eq. (2), then Eqs. (2) and (3) may be combined to form the set of $\frac{1}{2}N(N-1)$ coupled integral equations

$$T_p=V_p+V_pG_0\sum_q T_q \ , \tag{4}$$

or equivalently as the matrix integral equation[1]

$$\underline{T}=\underline{V}+\underline{V}G_0\sigma^0\underline{T}=\underline{V}+\underline{K}\underline{T}=[1-\underline{K}]^{-1}\underline{V} \ , \tag{5}$$

in which $\underline{T}$ and $\underline{V}$ are pair-labeled column matrices of dimension $\frac{1}{2}N(N-1)$ and σ^0 is a row matrix, of the same dimensionality, all of whose entries are unity. Thus $T=\sum_p T_p=\sigma^0\underline{T}$ and the kernel $\underline{K}=\underline{V}G_0\sigma^0$. Formally, our ability to solve matrix integral equations of the form of Eq. (5) relates directly to our ability to invert $[1-\underline{K}]$. The N-body reaction theory[2-8] largely concerns itself with recasting Eq. (5) (or its equivalent) into a new integral equation with a kernel $\underline{K}'$ such that either $\underline{K}'$

or $(\underline{K}')^n$ (n finite) is a fully-connected operator.[1-8] Such a kernel is referred to as a connected kernel and this property is a necessary condition for the unambiguous inversion of $[1-\underline{K}']$.

Thus, our first aim is to rewrite Eq. (5) in the form of an integral equation with a connected kernel since such an equation may be amenable to finite matrix methods of numerical solution. In this paper, we employ Watson-type[9] multiple scattering techniques in order to achieve this end. Our first step is to express Eq. (3) as

$$\begin{aligned} T_p &= V_p \left[1+G_0 \sum_{q\neq p} T_q\right] + V_p G_0 T_p \\ &= t_p \left[1+G_0 \sum_{q\neq p} T_q\right], \end{aligned} \tag{6}$$

where

$$t_p = V_p + V_p G_0 t_p \ . \tag{7}$$

In matrix notation Eqs. (6) become components of the matrix equation

$$\begin{aligned} \underline{T} &= \underline{t} + \sum_p \underline{t}(p) G_0 \sigma^p \underline{T} \\ &= \sum_{a_2} \{\underline{T}\}_{a_2} + \left[\sum_{a_2} \{\underline{T}\}_{a_2} G_0 \sigma^{a_2}\right] \underline{T} \\ &= \{\underline{T}\}_2 + \underline{K}_2 \underline{T}, \end{aligned} \tag{8}$$

where $\underline{t}$ is a column matrix whose components are t_p, $\underline{t}(p)$ is a column matrix whose sole nonzero entry is t_p in the p position [so that $\underline{t} = \sum_p \underline{t}(p)$], and σ^p is a row matrix whose pth entry is zero and all other entries are unity. In Eqs. (8) we have also employed the usual connectivity and partition notation[1-8] in which $\{\underline{T}\}_{a_n}$ is the part of $\underline{T}$ with connectivity a_n; that is, a_n specifies a partition of the N particle system into $(N-n+1)$ disjoint groups of particles, and $\{\underline{T}\}_{a_n}$ consists of that part of $\underline{T}$ in which all particles within each group are connected to the others by interactions but there is no interaction connecting a particle in one group with particles in another group. It follows that $\{\underline{T}\}_{a_n}$ is an operator which is characterized by $(n-1)$ nonconserved momenta. Thus $\{\underline{T}\}_{a_2}$ is the column matrix whose only nonzero entry is the pth entry, which is t_p, in the case that the partition a_2 corresponds to the separation of the system into $(N-2)$ noninteracting particles and one interacting pair, p. In general, the channel selector row matrix[1] σ^{a_n} is defined to have all entries unity except for zeros in positions p for which the pair p is contained within a single group of the partition a_n ($p \subset a_n$).

We note that if $N=3$ then the kernel $\underline{K}_2$ of Eq. (8), unlike that of Eq. (3), is a connected kernel since each element of the matrix $(\underline{K}_2)^2$ is a fully-connected operator. However, if $N>3$ then the kernel $\underline{K}_2$ is not a connected kernel. We therefore extend the procedure which gave us Eq. (6) from Eq. (4) and rewrite Eq. (6) as[1]

$$T_p = t_p + \sum_{q\neq p} T_{pq} \ , \tag{9}$$

so that

$$\begin{aligned} T_{pq} &= t_p G_0 T_q \\ &= t_p G_0 t_q + t_p G_0 t_q G_0 \sum_{s\neq q} T_s \quad (q\neq p) \ . \end{aligned} \tag{10}$$

We now distinguish two cases in our further discussion of the operators T_{pq} which carry two pair labels. In one case, p and q are two disjoint pairs ($p \perp q$) with no particle in common. In the other case ($p||q$), p and q are not disjoint and are thus made up of only three distinct particles. In the first case ($p \perp q$), we obtain from Eq. (10)

$$T_{pq} = t_p G_0 t_q \left[1+G_0 \sum_{s\neq p,q} T_s\right] + t_p G_0 T_{qp} \ , \tag{11}$$

$$T_{qp} = t_q G_0 t_p \left[1+G_0 \sum_{s\neq p,q} T_s\right] + t_q G_0 T_{pq} \ . \tag{12}$$

If we now define the auxiliary quantities $\tilde{T}_{pq}$ and $\tilde{T}_{qp}$ obtained by neglecting the terms in parentheses in Eqs. (11) and (12),

$$\tilde{T}_{pq} = t_p G_0 t_q + t_p G_0 \tilde{T}_{qp} \ , \tag{13}$$

$$\tilde{T}_{qp} = t_q G_0 t_p + t_q G_0 \tilde{T}_{pq} \ , \tag{14}$$

then it follows that[1]

$$T_{pq} = \tilde{T}_{pq} \left[1+G_0 \sum_{s\neq p,q} T_s\right] . \tag{15}$$

From Eqs. (13)-(15) we immediately see that

$$\{T_{pq}\}_{a_3} = \tilde{T}_{pq} \ , \tag{16}$$

where a_3 is the partition which has two interacting pairs (p and q) and $(N-4)$ noninteracting particles. Thus we have

$$T_{pq} = \{T_{pq}\}_{a_3} \left[1+G_0 \sum_{s\not\subset a_3} T_s\right] \quad (p\perp q) \ . \tag{17}$$

We note that Eqs. (13) and (14), which determine $\{T_{pq}\}_{a_3}$, are essentially connected-kernel equations.[10] In the circumstance that the pairs p and q specify only three particles ($p||q$), we note that a third pair r is contained in the partition a_3 defined by p and q: $p,q,r \subset a_3$. It is then necessary to modi-

fy the foregoing treatment in the following manner. In place of Eqs. (11) and (12) we write

$$T_{pq}=t_pG_0t_q\left[1+G_0\sum_{s\neq p,q,r}T_s\right]+t_pG_0(T_{qp}+T_{qr})\,, \tag{18}$$

$$T_{pr}=t_pG_0t_r\left[1+G_0\sum_{s\neq p,q,r}T_s\right]+t_pG_0(T_{rp}+T_{rq})\,. \tag{19}$$

Upon combining Eqs. (18) and (19) with the aid of the definition

$$T_{p,qr}\equiv T_{pq}+T_{pr}\,, \tag{20}$$

we have

$$T_{p,qr}=t_pG_0(t_q+t_r)\left[1+G_0\sum_{s\neq p,q,r}T_s\right]+t_pG_0(T_{q,pr}+T_{r,pq})\,, \tag{21}$$

while analogous equations for $T_{q,pr}$ and $T_{r,pq}$ follow from Eq. (21) upon cyclic permutation of p, q, and r. If we now define auxiliary quantities as the solutions of Eq. (21) when the right-most factor of the inhomogeneous term is ignored, viz.,

$$\tilde{T}_{p,qr}=t_pG_0(t_q+t_r)+t_pG_0(\tilde{T}_{q,pr}+\tilde{T}_{r,pq})\,, \tag{22}$$

then we find that

$$T_{p,qr}=\tilde{T}_{p,qr}\left[1+G_0\sum_{s\neq p,q,r}T_s\right]. \tag{23}$$

Thus

$$\{T_{p,qr}\}_{a_3}=\tilde{T}_{p,qr}\,, \tag{24}$$

and so

$$T_{p,qr}=\{T_{p,qr}\}_{a_3}\left[1+G_0\sum_{s\not\subset a_3}T_s\right]\quad(p||q)\,. \tag{25}$$

Evidently, both Eq. (17) and Eq. (25) can be written in the more concise form

$$T_{p,a_3}=\{T_p\}_{a_3}\left[1+G_0\sum_{s\not\subset a_3}T_s\right], \tag{26}$$

where we have used T_{p,a_3} to denote that part of T in which the pair p interacts last and a different pair in the partition a_3 [q for $(p\perp q)$ or q and r for $(q||p)$], interacts next to last. Combining Eq. (9) with Eq. (26) yields

$$T_p=t_p+\sum_{a_3}\{T_p\}_{a_3}\left[1+G_0\sum_{s\not\subset a_3}T_s\right], \tag{27}$$

or in matrix notation

$$\underline{T}=\underline{t}+\sum_{a_3}\{\underline{T}\}_{a_3}\left[1+G_0\sum_{s\not\subset a_3}T_s\right] \tag{28}$$

$$=\{\underline{T}\}_2+\{\underline{T}\}_3+\sum_{a_3}\{\underline{T}\}_{a_3}G_0\sigma^{a_3}\underline{T} \tag{29}$$

$$=\sum_{n=2}^{3}\{\underline{T}\}_n+\underline{K}_3\underline{T}\,. \tag{30}$$

The matrix integral equation, Eq. (30), has a connected kernel for $N=4$ just as Eq. (8) has a connected kernel for $N=3$. Continuation of the process outlined above yields after the appropriate number of steps[1]

$$\underline{T}=\sum_{n=2}^{N-1}\{\underline{T}\}_n+\left[\sum_{a_{N-1}}\{\underline{T}\}_{a_{N-1}}G_0\sigma^{a_{N-1}}\right]\underline{T}$$

$$=\{\underline{T}\}_{\text{disconnected}}+\underline{K}_{N-1}\underline{T}\,. \tag{31}$$

We note that the partitions a_{N-1} are necessarily two-cluster partitions. The connected kernel of Eq. (31) is the rank $\frac{1}{2}N(N-1)$ square matrix in the square brackets in Eq. (31), and each element of $(\underline{K}_{N-1})^2$ is a fully-connected operator. Equations (31) are essentially the particle-labeled Rosenberg equations[2] and they are also intimately related to the Bencze, Redish, and Sloan (BRS)[3–6] partition-labeled formulation in a way which is described next.

Since the a_{N-1} in the first of Eqs. (31) are two-cluster channels, we may rewrite this equation as

$$\underline{T}=\sum_{n=2}^{N-1}\{\underline{T}\}_n+\sum_{\gamma}\{\underline{T}\}_\gamma G_0\sigma^\gamma\underline{T}\,, \tag{32}$$

where the sum runs over all two-cluster channels γ. Furthermore, we note that

$$\sigma^\gamma\underline{T}=\underline{\sigma}^\gamma\underline{V}GG_0{}^{-1}=T^{\gamma 0}\,, \tag{33}$$

so that upon multiplication of Eq. (32) by an arbitrary two-cluster channel selector row matrix[1] σ^β we find

$$T^{\beta 0}=\sum_{n=2}^{N-1}\{T^{\beta 0}\}_n+\sum_{\gamma}\{T^{\beta 0}\}_\gamma G_0T^{\gamma 0}\,. \tag{34}$$

If we take α to be an arbitrary, but fixed, two-cluster channel and note that

$$T^{\beta\alpha}=T^{\beta 0}G_0G_\alpha{}^{-1}$$

then Eq. (34) becomes

$$T^{\beta\alpha}=\sum_{n=2}^{N-1}\{T^{\beta 0}\}_nG_0G_\alpha{}^{-1}+\sum_{\gamma}\{T^{\beta 0}\}_\gamma G_0T^{\gamma\alpha}\,. \tag{35}$$

The set of equations represented by Eq. (35) has a connected (matrix) kernel and Eq. (35) is one form in which the BRS equations are often written. The canonical BRS form follows from Eq. (35) upon the application of an off-shell transformation[1,5]; we have no need for it here.

Equations (35) are a closed set of coupled integral equations for the two-cluster transition operators $T^{\gamma\alpha}$. These have been represented as "minimal" in the sense that the equations are closed over the subset of the two-cluster partitions[7,8] without the need for any three or more cluster partitions. There are $(2^{N-1}-1)$ such two-cluster partitions[5] which are all required in this "minimal" form, and Eq. (35) is thus a set of $(2^{N-1}-1)$ coupled equations. On the other hand, the *equivalent equations* [from which Eqs. (35) were derived] in the pair-labeled format represent a closed set of $\frac{1}{2}N(N-1)$ coupled equations for the components T_p. For $N=3$, $2^{N-1}-1=\frac{1}{2}N(N-1)=3$, otherwise as N increases there are increasingly more two-cluster partitions than there are pairs of particles.

Evidently, there are in fact only $\frac{1}{2}N(N-1)$ linearly independent dynamical equations to be solved and the full set of BRS equations, Eqs. (35), is unnecessarily large. This occurs because there are only $\frac{1}{2}N(N-1)$ linearly independent two-cluster transition operators $T^{\gamma\alpha}$, and the additional members of the full set of Eq. (35) merely express the nondynamical relationships among the $T^{\gamma\alpha}$, despite the fact that they are written in a dynamical form.

In order to see this more clearly, let us define[1] a $\frac{1}{2}N(N-1)$ dimensional square matrix, S, such that

$$S=\begin{bmatrix}\sigma^{\alpha}\\ \sigma^{\beta}\\ \sigma^{\gamma}\\ \vdots\end{bmatrix}, \tag{36}$$

where the (otherwise arbitrary) two-cluster channels α, β, γ, ... are linearly independent in the sense that ($V^{\lambda}\equiv\sigma^{\lambda}\underline{V}$).

$$\hat{\underline{V}}\equiv\begin{bmatrix}V^{\alpha}\\ V^{\beta}\\ V^{\gamma}\\ \vdots\end{bmatrix}=S\underline{V} \tag{37}$$

implies that

$$\underline{V}=S^{-1}\hat{\underline{V}}\,. \tag{38}$$

As N increases beyond 4,

$$[2^{N-1}-1]\gg\tfrac{1}{2}N(N-1)$$

so that there are generally many possible choices for S. If we multiply Eq. (32) on the left by S we find

$$\hat{\underline{T}}\equiv\begin{bmatrix}T^{\alpha 0}\\ T^{\beta 0}\\ T^{\gamma 0}\\ \vdots\end{bmatrix}=\sum_{n=2}^{N-1}\{\hat{\underline{T}}\}_n + \left[S\sum_{\gamma}\{\underline{T}\}_{\gamma}G_0\sigma^{\gamma}S^{-1}\right]\hat{\underline{T}}\,, \tag{39}$$

and since every element of $(\underline{K}_{N-1})^2$ is fully connected so is every element of

$$(S\underline{K}_{N-1}S^{-1})^2=S(\underline{K}_{N-1})^2S^{-1}\,.$$

Thus the kernel of Eq. (39) is connected. Furthermore, *any* transition operator $T^{\lambda 0}$ may be obtained from the solution of Eq. (39) by noting that

$$T^{\lambda 0}=\sigma^{\lambda}\underline{T}=(\sigma^{\lambda}S^{-1})\hat{\underline{T}}\,. \tag{40}$$

From these considerations, it is evident that there is generally a large variety of choices among possible coupling schemes within the BRS set of equations. This nonuniqueness allows one the freedom to choose the coupling scheme most suited to the particular physical problem under study. For example, in the $N=4$ case of two neutrons and two protons there are seven two-cluster partitions and only six pairs. Hence one might wish to eliminate from consideration the two-cluster partition consisting of unbound proton and neutron pairs.

It should also be evident that we can directly reduce the dimensionality of the BRS equation given in Eq. (35) (or for that matter the canonical form obtained from it). All that is required is a choice of S. The reduced equation obtained in this manner is simply a partition-labeled restatement of the corresponding particle-labeled equation, involving at most an off-shell transformation.

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[10]The kernel of Eqs. (13) and (14) is not connected in the full *N*-body space. However, the square of the (matrix) kernel is fully connected within the subspace of the *interacting* particles. The disconnected parts of this kernel are contained within the momentum conserving delta functions which factor out of the integral equation.