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Comparison of the Coupled Reaction Channels and D.W.B.A. Series Approaches to Sequential Transfer Processes

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ABSTRACT

The coupled reaction-channels and D.W.B.A. - series approaches to sequential transfer reactions are formally compared. It is found that coupled-reaction-channels calculations effectively over-predict higher order terms relative to the D.W.B.A. series.

Recently there has been a great deal of interest in reactions which are calculationally allowed to proceed through particle transfer channels. Examples are \(^{(3\text{He}, t)}\) as \(^{(3\text{He}, \alpha)}(\alpha, t)\),\(^{1,2}\) \(^{(p, n)}\) as \(^{(p, d)}(d, n)\)\(^{3}\) and \(^{(p, t)}\) as \(^{(p, d)}(d, t)\).\(^{4,5}\) The most common ways of viewing these first plus second order calculations are either as iterated coupled reaction channels (C.R.C.) calculations or as the first two terms in the D.W.B.A. series. As has been noted\(^{6}\) the two approaches don't obviously give the same answer when extended to third or higher orders or when more than one channel is allowed in second order. It is the purpose of this letter to report a term by term formal comparison which shows that the C.R.C. formalism effectively overpredicts the higher order terms relative to the D.W.B.A. series. In all that follows, spinless particle will be assumed for simplicity of notation.

The C.R.C. equations can be written as\(^{2}\)
where $K_{Y\delta}$ is defined by
\[
F_{Y\delta}(\xi_Y) = K_{Y\delta} \chi_{Y\delta}(r_{\delta}) = \int dr_{\delta} (\psi_{Y\delta} | \hat{V}_Y | \delta) \chi_{\delta}(r_{\delta}),
\]
and
\[
(\psi_{Y\delta} | \hat{V}_Y | \delta) = 0.
\]

Also, the round brackets denote integration over internal coordinates only, $V_Y$ is the exact potential between the two fragments in channel $Y$, $U_Y$ is the optical potential, and $T_Y$ is the relative motion kinetic energy operator. Nonorthogonality effects are neglected throughout.

A series may be generated from Eq. (1) by first defining the incident channel to be $\alpha$ and imposing the proper boundary conditions. This gives
\[
\chi_{\alpha}(r_{\alpha}) = \chi_{\alpha}(r_{\alpha}) + G_{\alpha}(+) \sum_{\delta=1}^{C} K_{\alpha\delta} \chi_{\delta}(r_{\delta})
\]
and
\[
\chi_{Y}(r_{Y}) = G_{Y}(+) \sum_{\delta=1}^{C} K_{Y\delta} \chi(r_{\delta}), \quad (\gamma \neq \alpha)
\]
where
\[
(E_{\alpha} - T_{\alpha} - U_{\alpha}) \chi_{\alpha}(r_{\alpha}) = 0 \quad \text{and}
\]
\[
G_{Y}(+) = (E_{Y}^{+} - T_{Y} - U_{Y})^{-1}
\]

Defining $\beta$ to be the final channel and iterating gives
\[
\chi_{\beta}(r_{\beta}) = G_{\beta}^{(+)} \left[ K_{\beta\alpha} \chi_{\alpha}(r_{\alpha}) + \sum_{\gamma=1}^{C} K_{\beta\gamma} G_{\gamma}(+) K_{\gamma\alpha} \chi_{\alpha}(r_{\alpha})
\right.
\]
\[
+ \sum_{\gamma, \delta=1}^{C} K_{\beta\gamma} G_{\gamma}(+) K_{\gamma\delta} G_{\delta}(+) K_{\delta\alpha} \chi_{\alpha}(r_{\alpha}) + \cdots \]

Identifying the amplitude of the outgoing wave in channel $\beta$ gives an equivalent $T$-matrix element of
\[ T_{\beta\alpha} = \langle \chi_\beta (-) \mid \left( (\beta \mid \hat{V}_\beta \mid \alpha) + \sum_{\gamma=1}^{C} (\beta \mid \hat{V}_\beta \mid \gamma) G_{\gamma}^{(+)} (\gamma \mid \hat{V}_{\gamma} \mid \alpha) \\
+ \sum_{\gamma, \delta=1}^{C} (\beta \mid \hat{V}_\beta \mid \gamma) G_{\gamma}^{(+)} (\gamma \mid \hat{V}_{\gamma} \mid \delta) G_{\delta}^{(+)} (\delta \mid \hat{V}_{\delta} \mid \alpha) + \ldots \right) \rangle_{\chi_\alpha}^{(+)} \]  

(10)

The square bracket denotes integration over the relative coordinate between the two nuclei and a post prior interchange (allowed if nonorthogonality effects are neglected) has been performed in each term. The result expressed in Eq. (10) will be compared below to the D.W.B.A. series.

The D.W.B.A. series will be generated from

\[ T_{\beta\alpha} = \langle \chi_\beta (-) \mid \left( (\beta \mid \hat{V}_\beta \mid \alpha) + (\beta \mid \hat{V}_\beta \quad G_{\gamma}^{(+)} \quad V_{\gamma} \quad G_{\gamma}^{(+)} \mid \alpha) \right) \mid \chi_\alpha^{(+)} \rangle \]  

(11)

where

\[ G^{(+)} = (E^+ - H)^{-1}, \quad H = H_{Y}^{B} + T_{Y} + V_{Y}, \]  

(12)

and \( H_Y^B \) contains the internal Hamiltonian's for the two nuclei involved.

The form usually used for the exact Green's function is

\[ G^{(+)} = \overline{G}_{\gamma}^{(+)} + \overline{G}_{\gamma}^{(+)} \hat{V}_{\gamma} G^{(+)} , \quad \text{where} \]  

(13)

\[ \overline{G}_{\gamma}^{(+)} = (E^+ - H_{Y}^{B} - T_{Y} - U_{Y})^{-1} . \]  

(14)

An equivalent expression, to be used here, is

\[ G^{(+)} = \frac{1}{C} \sum_{\gamma=1}^{C} \overline{G}_{\gamma}^{(+)} + \frac{1}{C} \sum_{\gamma=1}^{C} G_{\gamma}^{(+)} \hat{V}_{\gamma} G^{(+)} . \]  

(15)

This may be proven by direct formal manipulation. That it is equivalent to Eq. (13) may be seen by iterating Eq. (13) and using it \( C \) times in Eq. (11), redefining \( \gamma \) each time. Adding these \( C \) equations then gives the same second order term as using the iterated version of Eq. (15). The expression, found from Eq. (13), which gave the same second order term may then be used \( C \) times, redefining the new channel that appears in third order
each time, and the same third order term will result when these \( C \) equations are added. By the same procedure, it can be shown to any order that the iterated version of Eq. (15) gives the same answer as following the above procedure with Eq. (13). The channel symmetrized version of the exact Green’s function (Eq. (15)) would seem more desirable since it allows all channels to enter on an equal basis. By contrast, Eq. (13) allows one to pick only one second order intermediate state. The point here, however, is that the channel symmetrized version appears to be formally correct and it allows the desired term by term comparison with the C.R.C. series.

Placing the iterated version of Eq. (15) in Eq. (11) and assuming that only one bound state pair enters in the evaluation of the \( C_{\gamma}^{(+)} \)'s gives the desired form. Namely,

\[
T_{\beta\alpha} = \langle \chi_{\beta}^{(-)} | \left[ (\beta | \hat{V}_{\beta} | \alpha) + \frac{1}{C} \sum_{\gamma=1}^{C} (\beta | \hat{V}_{\beta} | \gamma) G_{\gamma}^{(+)} (\gamma | \hat{V}_{\gamma} | \alpha) \right. \\
+ \frac{1}{C^2} \sum_{\gamma, \delta=1}^{C} (\beta | \hat{V}_{\beta} | \gamma) G_{\gamma}^{(+)} (\gamma | \hat{V}_{\gamma} | \delta) G_{\delta}^{(+)} (\delta | \hat{V}_{\delta} | \alpha) + \ldots \ldots \left. \right] | \chi_{\alpha}^{(+)} \rangle.
\]

(16)

The above result can be compared to the C.R.C. series (Eq. (10)). As is seem, the C.R.C. series overpredicts the higher order terms by factor of \( C^{n-1} \) with \( n \) the order.

The series generated by iterating Eq. (15) may be formally summed to yield

\[
G^{(+)} = \left[ 1 - \frac{1}{C} \sum_{\gamma=1}^{C} G_{\gamma}^{(+)} \right]^{-1} \frac{1}{C} \sum_{\gamma=1}^{C} G_{\gamma}^{(+)}.
\]

(17)

The inverse operator in the above equation can, in principle, be
evaluated by techniques similar to those in Ref. (5). However, it is not clear that this yields a calculationally useful result.

The above comparison says that the C.R.C. formalism over-predicts higher order terms. This implies that such calculations are consistent with the D.W.B.A. series only when the third and higher order terms are effectively zero. When this is true, a C.R.C. calculation, with three included channels, should yield the same answer as first plus second order D.W.B.A. with only one intermediate channel included. The author would like to acknowledge useful conversations with P. D. Kunz, N. K. Glendenning and M. H. Macfarlane.

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