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A NOTE ON NON-ORTHOGONALITY EFFECTS IN COUPLED CHANNEL METHODS FOR REARRANGEMENT REACTIONS

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A NOTE ON NON-ORTHOGONALITY EFFECTS IN COUPLED CHANNEL METHODS FOR REARRANGEMENT REACTIONS

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ABSTRACT

Arguments are given that the presence of non-orthogonality terms in coupled channel formulations of rearrangement scattering is the consequence of inconsistent treatment of multichannel dynamics.

АННОТАЦИЯ

Указывается, что наличие неортогональных членов в формулировках типа связанных каналов процессов рассеяния с перераспределением частиц является следствием некорректной трактовки многоканальной динамики.

KIVONAT

Megmutatjuk, hogy az átrendezõdéses reakciók csatolt egyenleteken alapuló leirásánál a nem-ortogonalitási tagok fellépte a sokcsatornás dinamika következetlen tárgyalásának az eredménye.

The method of coupled reaction channels /CRC/ has been extensively used in nuclear physics to describe elastic and inelastic scattering of composite nuclear particles [1]. This method introduces into the Schrödinger equation a truncated wave function composed of pieces selected from reaction channels to be treated explicitly. However, it has also been known for a long time that the CRC method when applied to rearrangement scattering presents both theoretical and practical difficulties because the wave function components corresponding to different arrangement channels are not orthogonal. Consequently, in the resulting set of coupled equations there appear coupling terms which involve direct overlap as well as matrix elements of the kinetic energy operator between different channel components. It is the presence of such terms which prevents the use of Feshbach's projection operator technique for rearrangement reactions [2]. A solution to this problem was proposed several years ago by Hahn [3] and applied to direct reactions by the author [4]. However, the implications of Hahn's method can be fully appreciated only in the frame of an exact multiparticle scattering theory.

On the other hand coupled equation methods /CEM/ can also be developed on the basis of exact multiparticle scattering theories, e.g. Faddeev's three-body integral equations or their generalisations to N-particle systems. These methods typically seek to obtain coupled differential or integrodifferential equations which are easier to handle than the exact multivariable integral equations [5, 6]. In such formulations "non-orthogonality terms" are usually absent and the method is flexible enough to meet even certain requirements regarding calculational advantages [7, 8]. In the practical applications of the various coupled channel

approaches, however, the Hilbert space of the multiparticle system is drastically truncated. In such circumstances it is not clear whether the conventional CRC method or a truncated form of a formally exact CEM is to be preferred. Also the question of "non-orthogonality terms" is not settled as yet. In a recent preprint [9] actually preference is given to the CRC method by arguing that it is based directly on the Schrödinger equation.

The aim of the present note is to investigate the problem of non-orthogonality effects in the various coupled channel formalisms. It will be shown that non-orthogonality effects are the manifestations of the inconsistent truncation of the Hilbert space, i.e. inconsistent treatment of multichannel dynamics.

For the sake of simplicity let us consider a three-particle system with the Hamiltonian

$$H = H_o + V \equiv H_o + \sum_{i=1}^{3} V_i \quad , \tag{1}$$

where H_o denotes the kinetic energy operator of the system and $V_i \equiv V_{jk}$, i=1,2,3 are the two-body interactions in the usual three-body notation [7]. Let P_i, i=1,2,3 denote the projectors onto the subspace of bound states of the two-body subsystems, i.e.

$$P_i = \sum_{s=1}^{N_i} |\Phi_i^s><\Phi_i^s| \quad , \quad P_i^2 = P_i \quad , \quad i=1,2,3 \quad , \tag{2}$$

where Φ_i^s are the normalised two-body bound state wave functions. In the CRC method the three-body Hilbert space is truncated according to the Ansatz

$$\Psi \approx P_1\Psi + P_2\Psi + P_3\Psi \quad . \tag{3}$$

By substituting (3) into the Schrödinger equation the following set of coupled equations can be immediately derived

$$(E-H_o-P_iVP_i)P_i\Psi = \sum_{k\neq i} P_iVP_k\Psi + \sum_{k\neq i} P_i(H_o-E)P_k\Psi \quad . \tag{4}$$

The "non-orthogonality terms" appear in the second sum on the r.h.s. of eq.(4) and vanish only if $P_iP_k=0$, since P_i commute with H_o. It is important to note that in ref.[7] this terminology is used in a different context, i.e. there "non-orthogonality terms" mean actually nonlocal coupling but always contain interactions as well. Since in multichannel systems $P_iP_k \neq \delta_{ik}P_i$ in general, hence in the CRC method non-orthogonality terms are always present.

The basic inconsistency in the CRC method is that Ansatz (3) is not a projection, because

$$(P_1+P_2+P_3)^2 \neq P_1+P_2+P_3 \quad . \tag{5}$$

This property has the unpleasant consequence that vectors of form (3) do not span a subspace of the Hilbert space, in other words the truncated Hilbert space is actually not itself a Hilbert space. Thus Ansätz (3) cannot in general be systematically improved by a convergent approximation scheme. It is interesting to see that inconsistent truncation rather than the non-orthogonality $P_iP_k \neq \delta_{ik}P_i$ is responsible for the presence of non-orthogonality terms. Let us, namely, assume that the different projectors commute,

$$[P_i, P_k] = 0, \qquad i,k = 1,2,3 \quad . \tag{6}$$

In this case the following operator, constructed in terms of P_i

$$P = P_1+P_2+P_3-P_1P_2-P_1P_3-P_2P_3+P_1P_2P_3 \tag{7}$$

is a projector, i.e. $P^2 = P$[10]. Now, if instead of (3) one starts with the Ansatz

$$\Psi \approx P\Psi \tag{8}$$

which is now a projection, elementary manipulations lead to a set of seven coupled equations with <u>no non-orthogonality terms present.</u> The extra four coupled equations have to be introduced in order to remove the overcompleteness of the states in Ansatz (3).

Unfortunately, in multichannel systems condition (6) is not fulfilled so that the above simple construction does not work. Thus the basic inconsistency in the CRC method cannot be resolved by conventional methods [9].

The solution to this problem proposed by Hahn [3] is based on a simple trick. Let us construct the following matrix of operators

$$\underline{\underline{P}} = \begin{pmatrix} P_1 & 0 & 0 \\ 0 & P_2 & 0 \\ 0 & 0 & P_3 \end{pmatrix} \quad . \tag{9}$$

According to the rules of matrix multiplication it follows immediately that $\underline{\underline{P}}^2 = \underline{\underline{P}}$, irrespectively, whether the channel projectors P_i commute or not. Since construction (10) implies a set of dynamical equations, Hahn also proposed a multichannel generalization of the Schrödinger formalism [3]. Since the exact treatments of multichannel scattering are also based on coupled sets of dynamical equations, Hahn's method can be immediately applied.

Let us write the set of Faddeev equations in differential form

$$(E-H_i)\Psi_i = V_i \sum_{k\neq i} \Psi_k \quad , \qquad i,k=1,2,3 \quad , \tag{10}$$

where $H_i = H_o+V_i$ and in terms of Ψ_i the solution of the Schrödinger equation can be expressed as follows

$$\Psi = \sum_{i=1}^{3} \Psi_i \tag{11}$$

As is well known the Faddeev components Ψ_i contain both two- and three-cluster pieces in the asymptotical region. It is convenient to introduce the following matrix notation.

$$(\underline{\underline{H_o}})_{ik} = H_i \delta_{ik}, \qquad (\underline{\underline{V}})_{ik} = V_i(1-\delta_{ik}) \quad , \tag{12}$$

so that eq.(10) can be rewritten in the form

$$(E\underline{\underline{1}} - \underline{\underline{H_o}})\underline{\Psi} = \underline{\underline{V}}\underline{\Psi} \quad , \tag{13}$$

where $\underline{\Psi} \equiv \{\Psi_1, \Psi_2, \Psi_3\}$ is a three-component vector. The projector (10) projects onto the two-cluster part of the Faddeev components, and the Feshbach projection operator technique leads to the set of equations

$$(E\underline{\underline{1}} - \underline{\underline{PHP}})\underline{\underline{P}}\underline{\Psi} = \underline{\underline{PHQ}}\underline{\Psi} \tag{14}$$

$$(E\underline{\underline{1}} - \underline{\underline{QHQ}})\underline{\underline{Q}}\underline{\Psi} = \underline{\underline{QHP}}\underline{\Psi} \tag{15}$$

where $\underline{\underline{Q}} = \underline{\underline{1}} - \underline{\underline{P}}$. The zeroth order approximation neglects the coupling between subspaces P and Q and corresponds to the Ansatz

$$\underline{\Psi} \approx \underline{\underline{P}}\underline{\Psi} \tag{16}$$

By substituting (16) into (10) the following set of coupled equations is obtained at once

$$(E - H_o - P_i V_i P_i) P_i \Psi_i = \sum_{k \neq i} P_i V_i P_k \Psi_k \quad , \tag{17}$$

again, as expected with no non-orthogonality terms present. In terms of the solution of eq. (17) the approximate solution to the Schrödinger equation is given by

$$\Psi' = \sum_{i=1}^{3} P_i \Psi_i \tag{18}$$

The exact solution to the Schrödinger equation is clearly

$$\Psi = \Psi' + \sum_{i=1}^{3} Q_i \Psi_i \tag{19}$$

Thus by treating $\underline{\underline{Q}}\underline{\Psi}$ in eqs. (14) and (15) a convergent approximation scheme can be obtained. Note that the above considerations are equally valid for any form of distorted Faddeev equations [7] and can be easily generalised to the channel coupling class of N-particle equations as well [11]. The treatment of identical particles, however, is not trivial and more elaborate formalism is needed [12] before any form of a CEM can be derived.

The reason why the simple construction (10) solves the problem of treating rearrangement processes by projection operator technique is intimately connected with the multichannel property of the system and can be best understood in a two-Hilbert space formulation [13]. Let $\mathcal{H}$ denote the Hilbert space of the physical states of the three-body system characterised by the Hamiltonian (1). While the projections $P_i\mathcal{H} \subset \mathcal{H}$, i=1,2,3 are subspaces, their sum is not expected to be, unless $P_iP_k=0$, $i\neq k$. Thus a consistent truncation of $\mathcal{H}$ seems to be very difficult. On the other hand, the three-component vectors $\{\Psi_i\}$ determined by eq. (10) can be regarded as elements of another Hilbert space $\mathcal{H}'$ constructed as a direct sum

$$\mathcal{H}' = \overset{3}{\underset{i=1}{\oplus}} \mathcal{H}_i \tag{20}$$

The communication between spaces $\mathcal{H}'$ and $\mathcal{H}$ is provided by the injection operator $J: \mathcal{H}' \to \mathcal{H}$ defined as

$$J \overset{3}{\underset{i=1}{\oplus}} \Psi_i = \sum_{i=1}^{3} \Psi_i \tag{21}$$

according to (11). In the direct sum Hilbert space $\mathcal{H}'$ construction (10) is clearly a projector, which in turn by means of the injection (21) leads to the required Ansatz (18) of the approximate wave function of the system. The Faddeev formalism presented here differs from the usual two-Hilbert space setting. A consistent two-Hilbert space treatment can be found in the works of Ginibre and Moulin [14] and Yafaev [15].

From the above arguments the following conclusions can be drawn. Presence of non-orthogonality terms in coupled equations formalisms for rearrangement scattering reflects the inconsistent treatment of multichannel dynamics. This inconsistency can be removed only in a CEM based on an exact formulation of multiparticle scattering. The practical problem still to be solved is, which form of a CEM should be truncated to yield the best approximation to the exact solution.

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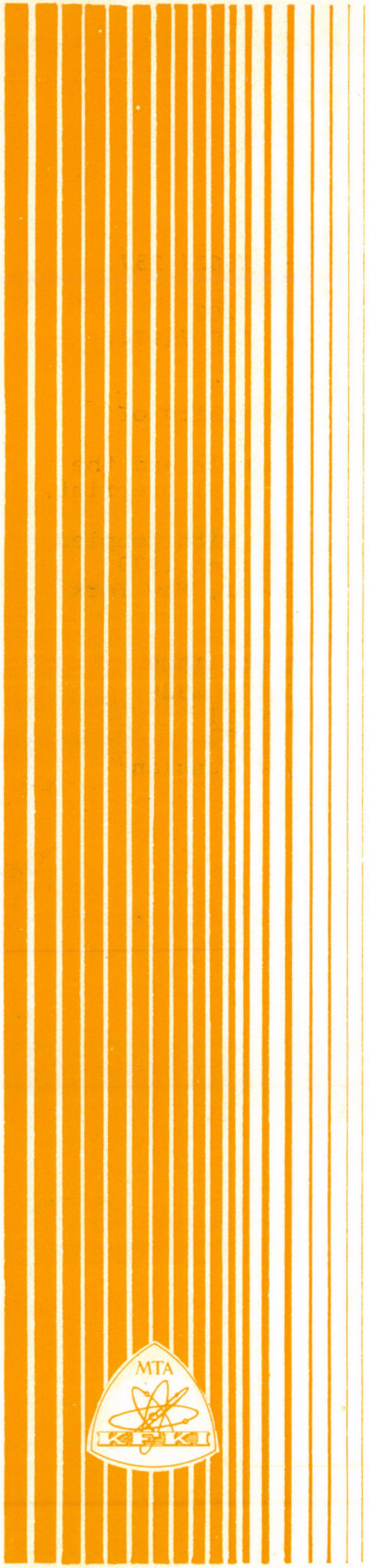

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