AN APPROACH TO THE COMPUTATION OF FEW/MANY–BODY MULTICHANNEL REACTIONS

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Abstract

A method to calculate reactions in quantum mechanics is outlined. It is advantageous, in particular, in problems with many open channels of various nature i.e. when energy is not low. In this method there is no need to specify reaction channels in a dynamics calculation. These channels come into play at merely the kinematics level and only after a dynamics calculation is done. This calculation is of the bound–state type while continuum spectrum states never enter the game.
I. OVERVIEW

The approach reviewed in the paper is advantageous, in particular, in problems with many open channels of various nature i.e. when energy is not low. Conventional approaches dealing with continuum wave functions are impractical in such problems at least at $A > 3$. The approach was successfully applied in nuclear reaction problems with $3 \leq A \leq 7$ and also recently for $A=12$ and $16$ proceeding from NN or NN+NNN forces. Many cases of reactions induced by a perturbation, i.e. electromagnetic or weak interaction, were considered. Both inclusive (mostly) and exclusive processes were studied. Reactions induced by strong interaction still were not considered although this can be done in a similar way, see below.

The main features of the approach are the following. In a dynamics calculation in its framework there is no need to specify reaction channels at all. These come into play at merely the kinematics level and only after a dynamics calculation is done. Such a calculation is of the bound–state type.

Correspondingly, continuum spectrum states never enter the game. In place of them, ”response–like” functions, of the type of Eq. (1) below, are basic ingredients of the approach. Reaction observables are expressed in terms of these functions as quadratures, see Eqs. (3) – (6) below. It should also be noted that in some problems of importance the quantities of Eq. (1) form are of interest themselves representing observable response functions for inclusive perturbation–induced reactions.

And the required ”response–like” functions of Eq. (1) form are obtained not in terms of the complicated continuum spectrum states entering their definition but via a bound–state type calculation. As the first step, an integral transform of such a function is performed. The transform is found in a closed form and represents a ”continuum sum rule” depending on a $\sigma$ parameter, Eq. (12). It is evaluated via a bound–state type calculation. As the next step, this sum rule is considered as an equation determining the ”response–like” function, i.e. its inversion is performed. Once this is done, the above mentioned quadratures giving the reaction observables are readily obtained.

Thus, as claimed above, the specification of reaction channels in the dynamics calculation and dealing with continuum wave functions are avoided in this approach. The criterion of accuracy is stability of response–like function obtained.

In addition to checking the stability, comparisons with more conventional calculations
FIG. 1: Comparison of the Faddeev and LIT results for the total $^3$H photoabsorption cross section in unretarded dipole approximation (a) with NN (AV18) force only and (b) with NN(AV18)+NNN(UrbIX) force. The dots are the Faddeev results and the two curves represent the bounds for the inversion of the LIT. The dotted curve in (b) is the result with AV18 only.

that deal with continuum wave functions have been performed. In the benchmark paper [1] the Faddeev results for the $^3$H photoabsorption total cross section are compared with the results [2] obtained via the above described approach. In the framework of this approach, the Lorentz integral transform (LIT), see the next section, was used. The Argonne V18 NN interaction and the Urbana IX NNN potential have been employed. The results are shown in Fig. 1.

A compete agreement is observed in the case when only the NN force is retained while in the case when the NNN force is added such an agreement is observed everywhere except for the peak region where a slight difference is present. In Ref. [3] the LIT results in the same problem have been obtained employing expansions over two different bases at solving the dynamics equation, the correlated hyperspherical basis (CHH) and the effective interaction hyperspherical basis (EIHH). The results are shown in Fig. 2.

These results practically coincide with each other which testifies to that the LIT results in Fig. 1 b) are accurate.
FIG. 2: (a) The same cross section with the same NN+NNN force as in Fig. 1(b) \((E\gamma \rightarrow \omega)\). It is obtained with the help of LIT at solving the dynamics equation in two ways. The full curve and the dashed curve represent its solution using the CHH and EIHH expansions, respectively. (b) The relative difference \([\sigma(\text{CHH}) - \sigma(\text{EIHH})]/\sigma(\text{CHH})\) between the two solutions.

In Fig. 3 one more test is presented [4]. The total cross section of the \(^3\text{He}(\gamma,\text{p})\text{d}\) reaction in the threshold region is calculated in two ways, from the LIT, as above, and via a direct calculation of the pd continuum wave functions. In this case, there is no real need for use of the method of integral transforms since the problem is a one-channel one. Another point is that the problem considered is unfavorable for this method since the cross section at the threshold is tiny and the values of the response function at such energies contribute extremely little to the integral pertaining to the corresponding integral equation of Eq. (12) and therefore to the input to solve the equation. Despite this, a complete agreement of the results of the two methods is observed. This is most clearly seen from Fig. 3 (b) where the quickly varying Gamow factor is factored out from the cross section, and the remaining astrophysical \(S\)–factor is presented. The central Malfliet–Tjon NN potential was employed in this calculation. Let us also mention that the pd continuum wave functions that have led to the results in Fig. 3 provide phase shifts practically coinciding with those of the other group [5].
FIG. 3: (a) The total $^3$He photoabsorption cross section in the threshold region calculated with the MT NN potential. The full curve represents the LIT results and the plus signs represent the results from the direct calculation with explicit continuum wave functions; (b) same results as in (a) but rescaled in order to determine the $S$–factor. The inversion error bounds are shown by dashed lines. $E$ denotes the p–d relative motion energy

In the next section basic points of the approach are presented, and Sec. 3 contains further comments.

II. BASICS OF THE METHOD

Let us consider “response–like” quantities having the structure

$$ R(E) = \sum_n \langle Q' | \Psi_n \rangle \langle \Psi_n | Q \rangle \delta (E - E_n) + \int d\gamma \langle Q' | \Psi_\gamma \rangle \langle \Psi_\gamma | Q \rangle \delta (E - E_\gamma). \quad (1) $$

Here $\Psi_n$ and $\Psi_\gamma$ denote, respectively, bound states and continuum spectrum states with energies $E_n$ and $E_\gamma$ pertaining to the Hamiltonian of a problem. The $\gamma$ subscript labeling the states may include both continuous and discrete variables which is reflected in the sum over integral symbol. The set of states is complete which may be written in the form

$$ \sum_n |\Psi_n\rangle \langle \Psi_n| + \int d\gamma |\Psi_\gamma\rangle \langle \Psi_\gamma| = I \quad (2) $$
where \( I \) is the identity operator. This implies the normalizations \( \langle \Psi_n | \Psi_{n'} \rangle = \delta_{n,n'} \) and \( \langle \Psi_{\gamma} | \Psi_{\gamma'} \rangle = \delta(\gamma - \gamma') \). As said above, in the present approach reaction observables are expressed in terms of quantities (1) as quadratures. First we shall discuss this point. After that, the above mentioned evaluation of quantities (1) via bound–state methods will be outlined.

Consider the case of a reaction induced by strong interaction. Let \( \phi_i(E) \) be the product of bound states of fragments and of a factor representing their free relative motion in the initial state. Let \( \phi_f(E) \) be such products pertaining to final states. Let us denote \( A \) the operator of antisymmetrization with \( A^2 = A \). So that \( A \phi_i(E) \) and \( A \phi_f(E) \) are the anti-symmetrized "free–motion" states [6]. Let us use the notation \( \tilde{\phi}_i(E) = A(\mathcal{H} - E)\phi_i(E) \) and \( \tilde{\phi}_f(E) = A(\mathcal{H} - E)\phi_f(E) \) where \( \mathcal{H} \) is the Hamiltonian. This may be written as \( \tilde{\phi}_i = AV_{res}^i \phi_i \) and \( \tilde{\phi}_f = AV_{res}^f \phi_f \) where \( V_{res}^i,f \) are interactions between fragments pertaining to a channel. These interactions are assumed here to be of a short range. The point on long–range inter–fragment Coulomb interactions is commented below.

The reaction \( T \) matrix is [6]

\[
T_{fi} = T_{fi}^{\text{Born}} + \langle \tilde{\phi}_f(E) | (E - H + i\epsilon)^{-1} | \tilde{\phi}_i(E) \rangle,
\]

where \( \epsilon \to +0 \). Here \( T_{fi}^{\text{Born}} \) denotes the Born contribution,

\[
T_{fi}^{\text{Born}} = \langle \phi_f | \phi_i \rangle = \langle \tilde{\phi}_f | \tilde{\phi}_i \rangle.
\]

The problem lies in calculating the non–Born contribution involving the Green function \( (E - H + i\epsilon)^{-1} \). Let us introduce the quantity

\[
R_E(E') = \sum_n \langle \tilde{\phi}_f(E) | \Psi_n \rangle \langle \Psi_n | \tilde{\phi}_i(E) \rangle \delta(E' - E_n)
+ \int d\gamma \langle \tilde{\phi}_f(E) | \Psi_{\gamma} \rangle \langle \Psi_{\gamma} | \tilde{\phi}_i(E) \rangle \delta(E' - E_{\gamma}).
\]

This quantity has the same structure as that in Eq. (1) (with the replacement \( E \to E' \)). And the contribution to the \( T \) matrix we discuss may readily be calculated in its terms as

\[
\int dE' R_E(E')(E - E' + i\epsilon)^{-1} \equiv -i\pi R_E(E) + P \int dE' R_E(E')(E - E')^{-1}.
\]

Thus, indeed, reaction cross sections may be expressed in terms of the "response–like" quantities of Eq. (1) as quadratures.
The amplitude of a perturbation–induced reaction is \( \langle \Psi_f | \hat{O} | \Psi_0 \rangle \) where \( \hat{O} \) is a perturbation, \( \Psi_0 \) is an unperturbed initial bound state, and \( \Psi_f \) is a continuum spectrum state. To calculate this amplitude let us substitute the expression \[6\] in it. Then

\[
\langle \Psi_f | O | \Psi_0 \rangle = \langle \phi_f | O | \Psi_0 \rangle + \langle \tilde{\phi}_f | (E - H + i\epsilon)^{-1} | O \Psi_0 \rangle
\] (6)

and one may proceed as above with the replacement \( \tilde{\phi}_i \rightarrow \hat{O}\Psi_0 \) there.

A modification of the above relations required to incorporate the long–range inter–fragment Coulomb interactions is outlined in Ref. \[7\]. (And if the response function itself is the objective of a calculation then the Coulomb interaction requires no special consideration as seen from below.) This modification leads to modified \( Q \) and \( Q' \) states which include Coulomb functions in the inner region of the relative motion of fragments. Of course, it is very easy to obtain such Coulomb functions in the case of two–fragment reaction channels.

Now we need to consider the calculation of quantities having the “response–like” structure of Eq. (1). We write them as

\[
R(E) = \sum_n R_n \delta(E - E_n) + f(E), \quad R_n = \langle Q' | \Psi_n \rangle \langle \Psi_n | Q \rangle,
\] (7)

\[
f(E) = \sum \int d\gamma \langle Q' | \Psi_\gamma \rangle \langle \Psi_\gamma | Q \rangle \delta(E - E_\gamma).
\] (8)

The main problem consists in calculating the contribution \( \langle Q' | Q \rangle \). And this should be done avoiding the calculation of multiparticle continuum states entering it.

First let us list the simple sum–rule result. With the help of Eq. (2) one obtains

\[
\int_{E_{thr}}^\infty f(E) dE + \sum_n R_n = \langle Q' | Q \rangle.
\] (9)

Here \( E_{thr} \) is the continuum spectrum threshold value so that \( f(E) \) varies in the range \( E_{thr} \leq E \leq \infty \). While this single sum rule does not determine \( R(E) \), this goal can be achieved with the help of “generalized” sums of the form

\[
\int K(\sigma, E) R(E) dE
\] (10)

depending on a continuous parameter. They are equal to

\[
\sum \int d\gamma \langle Q' | \Psi_\gamma \rangle K(\sigma, E_\gamma) \langle \Psi_\gamma | Q \rangle + \sum_n \langle Q' | \Psi_n \rangle K(\sigma, E_n) \langle \Psi_n | Q \rangle.
\] (11)
Taking into account Eq. (2) this quantity can be represented as $\langle Q'|K(\sigma,H)|Q \rangle$ where, as above, $H$ is the Hamiltonian of a problem. Thus, one comes to the relation

$$\int_{E_{thr}}^{\infty} K(\sigma,E)f(E)dE + \sum_n K(\sigma,E_n)R_n = \Phi(\sigma), \quad \Phi(\sigma) \equiv \langle Q'|K(\sigma,H)|Q \rangle$$

(12)

where $f(E)$ and $R_n$ are the continuous part of the response–like function $R(E)$ and discrete contributions to it, see Eqs. (8) and (7). Since this relation is valid for any $\sigma$ it may be considered as an equation to determine $R(E)$, i.e. $f(E)$ and $R_n$, provided that one is able to calculate the quantity $\langle Q'|K(\sigma,H)|Q \rangle$. At many $K$ kernels this equation determines $f(E)$ and $R_n$ in a unique way.

III. FURTHER COMMENTS

Thus the equation of Eq. (12) form is to be solved. First, one needs to calculate its right–hand side input. If one is able to diagonalize the Hamiltonian on a sufficiently big subspace of basis functions this can be readily done. In this case, one can use the approximation of the type

$$\langle Q'|K(\sigma,H)|Q \rangle \simeq \sum_{n=1}^{N} \langle Q'|\varphi_n^N \rangle K(\sigma,E_n^N)\langle \varphi_n^N |Q \rangle.$$  

(13)

Here $N$ is the dimension of the subspace and other notation is obvious. Suppose, for example, that the $K(\sigma,E) = \exp[-(\sigma - E)^2/\sigma_0^2]$ kernel is employed. At a given accuracy in the input $\Phi(\sigma)$, smaller $\sigma_0$ values would lead to a better reproduction of details of $f(E)$ at solving Eq. (12). Indeed, at large $\sigma_0$ values, contributions to $\Phi(\sigma)$ from peculiarities of $f(E)$ are spread over large $\sigma$ intervals, and sizes of these contributions may be comparable with sizes of inaccuracies in calculated $\Phi(\sigma)$. At the same time, smaller $\sigma_0$ values require use of subspaces of basis functions of higher dimension. Indeed, accurate $\Phi(\sigma)$ values emerge only at such sizes of these subspaces that (at $\sigma$ values of significance) energy ranges $\sigma - \sigma_0 \leq E \leq \sigma + \sigma_0$ contain sufficiently many $E_n^N$ eigenvalues.

The right–hand side of Eq. (13) represents the result of smoothing the pseudo–response

$$\sum_{n=1}^{N} \langle Q'|\varphi_n^N \rangle \langle \varphi_n^N |Q \rangle \delta(E - E_n^N)$$

with the help of the smoothing function $K(\sigma,E)$. Such type smoothings were performed in the literature and their results were considered as approximations to true responses for
perturbation–induced inclusive reactions. In the difference to this, in the present approach such results are not adopted to be approximations to true responses. Here they play the role of the input to the integral equation and final true responses emerge as its solution. This refinement makes possible to obtain consistent and more accurate results.

At some choices of the kernel $K$ it is possible to calculate the input $\Phi(\sigma)$ to Eq. (12) also without the diagonalization of the Hamiltonian. The simplest case is the Stieltjes kernel $K(\sigma, E) = (\sigma + E)^{-1}$ where $\sigma$ is real and lies apart from the spectrum of a Hamiltonian. In this case one has

$$\Phi(\sigma) = \langle Q'|\tilde{\psi}\rangle, \quad \tilde{\psi} = (H + \sigma)^{-1}Q.$$  

(14)

I.e. $\tilde{\psi}$ is the solution to the inhomogeneous Schrödinger–like equation

$$(H + \sigma)\tilde{\psi} = Q.$$  

(15)

From the fact that $\langle Q|Q\rangle$ is finite it follows that the solution is localized, and such a solution is unique. Another case is the so called Lorentz kernel

$$K(\sigma = \sigma_R + i\sigma_I, E) = 1/[(\sigma_R - E)^2 + \sigma_I^2].$$  

(16)

Writing

$$\frac{1}{(\sigma_R - E)^2 + \sigma_I^2} = \frac{1}{2i\sigma_I}\left(\frac{1}{\sigma_R - E - i\sigma_I} - \frac{1}{\sigma_R - E + i\sigma_I}\right)$$  

(17)

one reduces the calculation in this case to that in the Stiltjes one but with complex kernels. The solutions to the corresponding Eq. (15) type equations are localized and unique also in this case.

Since the Lorentz kernel has a limited range, inversion of the transform is more accurate in the Lorentz case than that in the Stiltjes case at the same accuracy in the input, c.f. the reasoning above. Still, when an expansion over a basis is applied to solve Eq. (15) type equations, convergence of $\Phi(\sigma)$ in the Stiltjes case is faster than that in the Lorentz case with a small $\sigma_I$. Indeed, at $\sigma_I \to 0$ the continuum spectrum regime is recovered at $\sigma_R$ values of interest belonging to the scattering line.

One more case is the Laplace kernel $K(\sigma, E) = \exp(-\sigma E)$. The corresponding $\langle Q'|e^{-\sigma H}|Q\rangle$ input can be calculated with the Green Function Monte Carlo method.

We shall not discuss here the point of solving Eq. (12), i.e. the inversion of the transform, referring for this to the literature. Let us mention only that such an equation represents
a classical "ill–posed problem". (This does not mean at all that the problem is a very
difficult one!) A standard regularization procedure was applied in practical calculations and
convergent results have been obtained. Still, with such a procedure a sufficient accuracy of
the input $\Phi(\sigma)$ may be harder to achieve in problems with not small number of particles.
A new method to solve Eq. (12) was proposed recently [8]. In this method, the number of
maxima and minima of the solution sought for is imposed as an additional constraint. The
method does not require a regularization. It has been proved that the method is convergent
at least everywhere except for the points of maxima and minima of $f(E)$. Thus, apart
from this restriction, the problem becomes a well–posed one with the constraint imposed.
With the same approximate inputs the method provides far more accurate results than the
standard regularization procedure in simple examples considered. But its further study is
still required.

The discrete contributions $R_n$ in Eq. (12) may be calculated separately. For a convenient
way to do this in the case of the Lorentz or Stiltjes transform see [7]. Another option is
the following. The general algorithm applied at solving Eq. (12) consisted in writing an
ansatz for $f(E)$ that included parameters and in fitting the parameters to $\Phi(\sigma)$. The $R_n$
amplitudes and, if expedient, $E_n$ energies may be included in the set of such parameters.

A limitation of the present approach is that in order to reproduce fine details of spectra of
reactions, such as the widths of narrow resonances, an increased accuracy in the input $\Phi(\sigma)$
is required. The reason is the same as that discussed above in connection with Eq. (13). This
feature is similar to the situation with extracting widths of narrow resonances from experi-
ments in which scattering or reaction cross sections are measured. Still, narrow resonances
are normally located at low energy whereas the present method is designed for calculations
of reactions when many channels are open, i.e. not at low energy. Then information on
the widths of narrow resonances taken from experiment or from alternative calculations may
be readily incorporated in an algorithm of solving Eq. (12). And, anyway, inaccuracies in
widths of resonances at low energy in the present method would not lead to inaccuracies at
reproducing reaction spectra at higher energy. In addition, in the light nuclei case widths
of resonances are normally not so narrow. In Ref. [9] the width about 200 KeV of such a
resonance in $^4\text{He}$ was reproduced with a reasonable accuracy in the framework of the present
approach. See also Fig. 3 above in this regard.

In conclusion, the relevant literature is listed in addition to the references above. The
approach to calculate reactions described in Sec. 2 has been introduced in Ref. [10]. Its presentation here is close to Ref. [7]. The bound–state type, i.e. sum–rule, calculation of integral transforms of observable responses $R(E)$, i.e. pertaining to inclusive perturbation–induced reactions, has been suggested in [11] considering the Stieltjes transform and in [12] in the Laplace transform case. No inversions of the transforms were considered there. An alternative approach [13] was also developed in which an observable $R(E)$ is reconstructed from its moments of the type $\langle E^{-n} \rangle$, $n = 0, \ldots, N$. The quantity of Eq. (9) represents then the zero moment. Subsequent moments are calculated recursively. That approach referred only to the case of inclusive perturbation–induced reactions, in the difference to the above described method [10] of treatment of general–type reactions, i.e. exclusive perturbation– and strong interaction–induced ones. The described way to calculate $\Phi(\sigma)$ involving Eq. (13) was suggested in Ref. [7] (although at too restrictive conditions imposed on $Q$ and $Q'$).

Prior to this such a calculation of the Lorentz transform in a particular problem has been performed by I.J. Thompson. The Lorentz transform has been introduced in the present context in Ref. [15]. Its evaluation in the form listed above was given in Ref. [7]. In Ref. [14] an efficient algorithm to calculate $\Phi(\sigma)$ at solving Eq. (15) with the help of an expansion over basis functions was developed. In the review papers [7] and [16] the subject of the transform inversion in the framework of the customary approach is considered, in particular. In Ref. [16] earlier applications done with the help of the Lorentz transform are reviewed as well. Among later applications, advances in study of heavier nuclei [17, 18] are to be mentioned. Existing bound–state techniques to solve the multiparticle scattering problem are reviewed in Ref. [19].

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