Approach to 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 the energy is not low. Within 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 the dynamics calculation is done. Such a calculation is of a bound-state type and continuum spectrum states never enter the game.

Keywords: *Multichannel reactions; microscopic calculations; method of integral transforms*

1 Overview

An approach reviewed in this paper is advantageous, in particular, in problems with many open channels of various nature, i. e., when the 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 within its framework there is no need to specify reaction channels at all. These come into play at merely the kinematics level and only after the dynamics calculation is done. Such a calculation is of a 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 the 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 the form of Eq. (1) are of interest themselves representing observable response functions for inclusive perturbation-induced reactions.

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The "response-like" functions of the form of Eq. (1) are obtained not in terms of 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. This transform is expressed in a closed form and represents a "continuum sum rule" depending on a σ parameter, see 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.

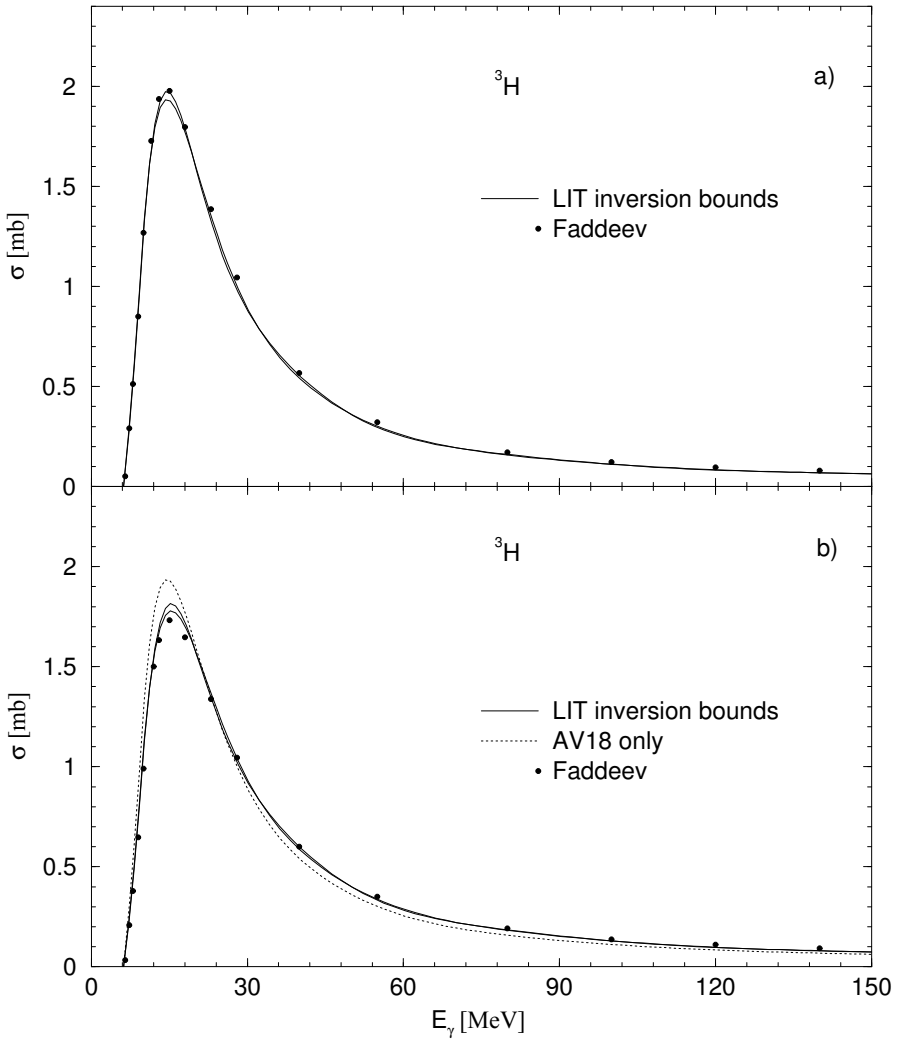

Figure 1: Comparison of Faddeev and LIT results for the total ^{3}H photoabsorption cross section in unretarded dipole approximation a) with NN (AV18) force only and b) with NN(AV18) + NNN(UrbIX) force. Dots are the Faddeev results and two curves represent the bounds for the LIT inversion. Dotted curve in b) is the result with AV18 only.

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

In addition to the stability checks, comparisons with more conventional calculations 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.

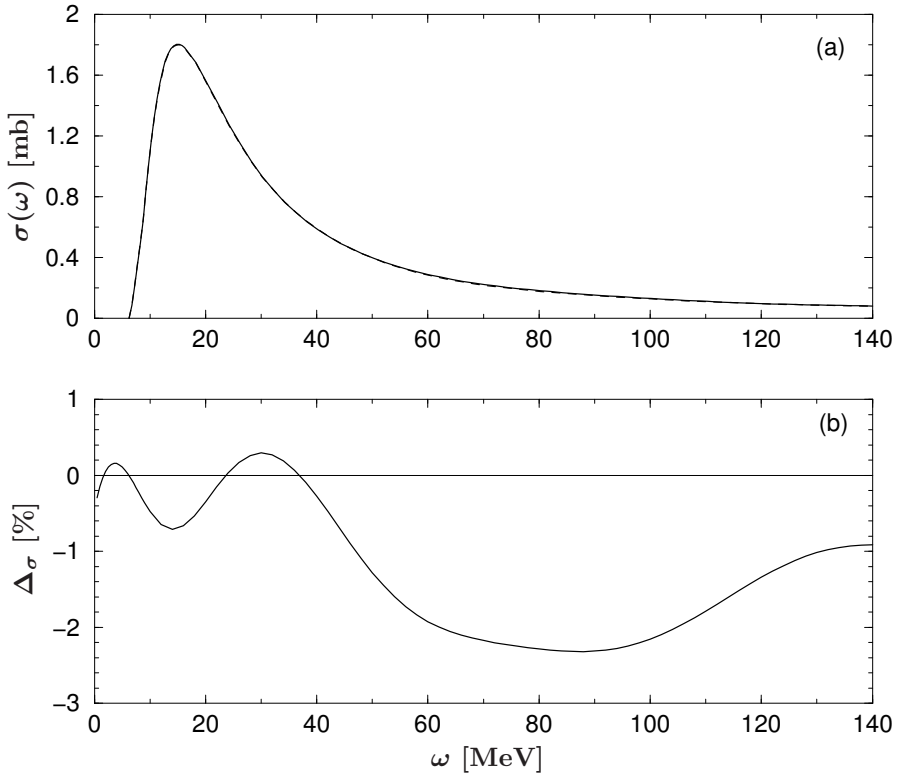

Figure 2: (a) The same cross section calculated with the same $NN + NNN$ force as in Fig. 1(b) ($E_\gamma \to \omega$). It is obtained with the help of LIT at solving the dynamics equation in two ways. Full and dashed curves represent the results gained using the CHH and EIHH expansions, respectively. (b) Relative difference $\Delta_\sigma = [\sigma(\mathrm{CHH}) - \sigma(\mathrm{EIHH})]/\sigma(\mathrm{CHH})$ between these cross sections.

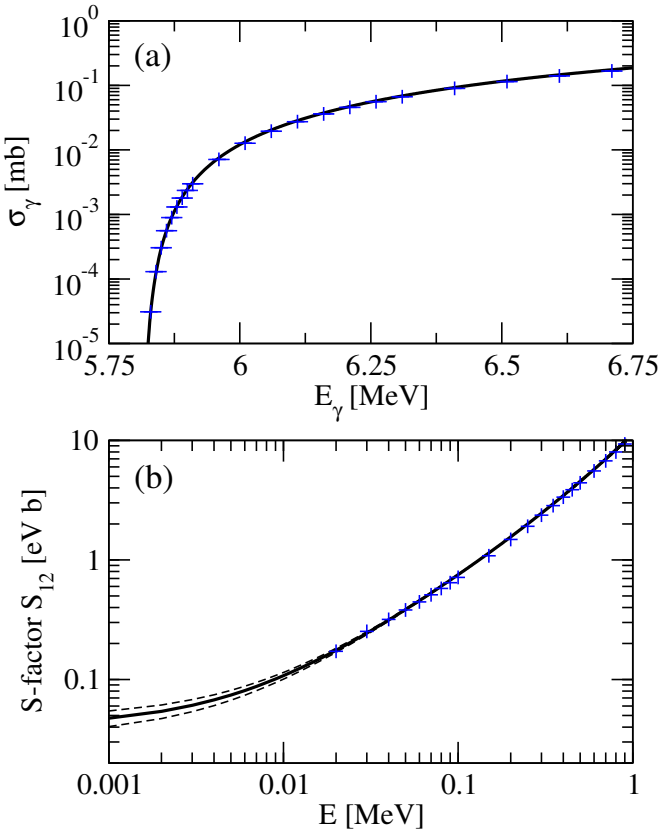

Figure 3: (a) Total ^{3}He photoabsorption cross section in the threshold region calculated with the MT NN potential. Full curve — LIT results; plus signs — direct calculation utilizing explicit continuum wave functions. (b) The same as (a) but rescaled in order to determine the S-factor. The inversion error bounds are shown by dashed lines. E denotes the $p-d$ relative motion energy.

These results practically coincide with each other which testifies to that the LIT results in Fig. 1(b) are accurate.

One more test [4] is presented in Fig. 3. The total cross section of the $^3\mathrm{He}(\gamma, p)d$ reaction in the threshold region is calculated in two ways, by means of the LIT as discussed above, and via a direct calculation of the pd continuum wave functions. In this case, there is no real need to use the method of integral transforms since the problem is single-channel. 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 (12) and therefore to the input to solving this equation. Despite this, a complete agreement of the results of 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 the phase shifts practically indistinguishable from those of another group [5].

The basic points of the approach are presented in the next Section, and Section 3 contains further comments.

2 Basics of the method

As said above, "response-like" quantities of the type

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

are the basic ingredients of the approach. Here Ψ_n are bound states and Ψ_γ are continuum spectrum states. They represent a complete set of eigenstates of the Hamiltonian of a problem. The subscript γ denotes collectively a set of continuous and discrete variables labeling the states which is symbolized in the summation over integration notation. The normalizations $\langle\Psi_n|\Psi_{n'}\rangle = \delta_{n,n'}$ and $\langle\Psi_\gamma|\Psi_{\gamma'}\rangle = \delta(\gamma-\gamma')$ are adopted, so that

$$\sum_n |\Psi_n\rangle\langle\Psi_n| + \sum\!\!\!\!\!\!\int d\gamma\,|\Psi_\gamma\rangle\langle\Psi_\gamma| = I, \quad (2)$$

I being the identity operator.

In the method discussed, the quantities $R(E)$ of Eq. (1) are obtained not in terms of complicated states Ψ_γ entering their definition but via a bound-state type calculation. Reaction observables are expressed in terms of $R(E)$ as quadratures.

Let us first explain the latter of these points. Consider a strong interaction induced reaction. Denote $\mathcal{A}\,\phi_i(E)$ and $\mathcal{A}\,\phi_f(E)$ the antisymmetrized "channel free-motion states". Here the subscript i (f) refers to the initial (final) state of the reaction, $\phi_{i,f}(E)$ are products of fragment bound states and of factors describing their free relative motion [6], and $\mathcal{A}$ denotes the operator realizing antisymmetrization with respect to identical particles ($\mathcal{A}^2 = \mathcal{A}$) [6]. Denote $\bar\phi_i(E) = \mathcal{A}(H-E)\phi_i(E)$ and $\bar\phi_f(E) = \mathcal{A}(H-E)\phi_f(E)$ where H is the Hamiltonian. One has $\bar\phi_i = \mathcal{A}V_i^{res}\phi_i$ and $\bar\phi_f = \mathcal{A}V_f^{res}\phi_f$, where $V_{i,f}^{res}$ are interactions between fragments in the initial and final states. Here it is assumed that these interactions are of a short range so that the outer parts of the long-range inter-fragment Coulomb interaction are disregarded. This point is reconsidered below.

The T matrix determining the reaction rates is [6]

$$T_{fi} = T_{fi}^{Born} + \langle\bar\phi_f(E)|(E-H+i\epsilon)^{-1}|\bar\phi_i(E)\rangle, \qquad \epsilon\to+0. \quad (3)$$

Here T_{fi}^{Born} is the simple Born contribution,

$$T_{fi}^{Born} = \langle\phi_f|\bar\phi_i\rangle = \langle\bar\phi_f|\phi_i\rangle,$$

and the main problem is a calculation of the second term in Eq. (3) that includes the Green function $(E-H+i\epsilon)^{-1}$. This contribution may be presented as

$$\int dE'\,R_E(E')\,(E-E'+i\epsilon)^{-1} \equiv -i\pi R_E(E) + P\int dE'\,R_E(E')\,(E-E')^{-1}, \quad (4)$$

where

$$R_E(E') = \sum_n \langle\bar\phi_f(E)|\Psi_n\rangle\langle\Psi_n|\bar\phi_i(E)\rangle\,\delta(E'-E_n) + \sum\!\!\!\!\!\!\int d\gamma\,\langle\bar\phi_f(E)|\Psi_\gamma\rangle\langle\Psi_\gamma|\bar\phi_i(E)\rangle\,\delta(E'-E_\gamma). \quad (5)$$

The quantity (5) is just of the structure of Eq. (1) (with the $E \to E'$ replacement). Thus, indeed, to calculate matrix elements of the T matrix it is sufficient to have the quantities of this structure. Once they are available, the integrations in Eq. (4) are readily done.

The amplitude of a perturbation-induced reaction is $\langle \Psi_f^- | \hat{O} | \Psi_0 \rangle$ where $\hat{O}$ is a perturbation, Ψ_0 is an unperturbed initial bound state, and Ψ_f^- is a continuum spectrum state. To calculate this amplitude, let us substitute $\langle \Psi_f^- |$ in it by the expression [6]

$$\langle \Psi_f^- | = \langle \phi_f | + \langle \bar{\phi}_f | (E - H + i\epsilon)^{-1}.$$

Then

$$\langle \Psi_f^- | \hat{O} | \Psi_0 \rangle = \langle \phi_f | \hat{O} | \Psi_0 \rangle + \langle \bar{\phi}_f | (E - H + i\epsilon)^{-1} | \hat{O} \Psi_0 \rangle, \tag{6}$$

and one may proceed as above with the replacement $\bar{\phi}_i \to \hat{O}\Psi_0$.

Modifications of the above relations required to incorporate the long-range interfragment Coulomb interaction are outlined in Ref. [7]. (If the response function itself is the objective of the calculation, the Coulomb interaction does not require a special consideration as will be seen below.) These modifications consist in changes of the Q and Q' states which include the 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 let us explain the above mentioned point by calculating the quantities expressed by Eq. (1). Let us rewrite Eq. (1) as

$$R(E) = \sum_n R_n \, \delta(E - E_n) + f(E), \qquad R_n = \langle Q' | \Psi_n \rangle \langle \Psi_n | Q \rangle, \tag{7}$$

$$f(E) = \sum\!\!\!\!\!\!\int d\gamma \, \langle Q' | \Psi_\gamma \rangle \langle \Psi_\gamma | Q \rangle \, \delta(E - E_\gamma). \tag{8}$$

The contribution (8) includes an integration over few- or many-body continuum states Ψ_γ that are very complicated except for low energies, and the main problem is just the calculation of this contribution. If E_{thr} denotes the threshold value for the continuum state energies then $f(E)$ is different from zero at $E_{thr} \le E \le \infty$.

An easy task is the sum rule calculation. Using Eq. (2) one gets

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

Obviously, knowing the quantity (9) is not enough to reconstruct the $R(E)$ itself. To achieve this goal, let us consider "generalized sums" of the form

$$\int K(\sigma, E) \, R(E) \, dE. \tag{10}$$

These sums are equal to

$$\sum\!\!\!\!\!\!\int d\gamma \, \langle Q' | \Psi_\gamma \rangle K(\sigma, E_\gamma) \langle \Psi_\gamma | Q \rangle + \sum_n \langle Q' | \Psi_n \rangle K(\sigma, E_n) \langle \Psi_n | Q \rangle. \tag{11}$$

Since Eq. (2) is valid, this quantity is equal to $\langle Q' | K(\sigma, H) | Q \rangle$ where, as above, H is the Hamiltonian of a problem. Thus one comes to the relation

$$\int_{E_{thr}}^{\infty} K(\sigma, E) \, f(E) \, dE + \sum_n K(\sigma, E_n) \, R_n = \Phi(\sigma), \qquad \Phi(\sigma) \equiv \langle Q' | K(\sigma, H) | Q \rangle, \tag{12}$$

where $f(E)$ and R_n are the continuous part and discrete contributions to the response-like function $R(E)$, see Eqs. (8) and (7). Since this relation is valid for any σ, 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 $\langle Q'|K(\sigma,H)|Q\rangle$.

3 Further comments

Thus an equation of the form given by Eq. (12) is to be solved. First, one needs to calculate the 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 an approximation of the type

$$\langle Q'|K(\sigma,H)|Q\rangle \simeq \sum_{n=1}^{N}\langle Q'|\varphi_n^N\rangle K(\sigma,E_n^N)\langle\varphi_n^N|Q\rangle. \tag{13}$$

Here N is the dimensionality of the subspace and other notations are obvious. Suppose, for example, that the kernel $K(\sigma,E)=\exp[-(\sigma-E)^2/\sigma_0^2]$ is employed. At a given accuracy of the input $\Phi(\sigma)$, smaller σ_0 values would lead to a better reproduction of details of $f(E)$ at solving Eq. (12). Indeed, at large σ_0 values, contributions to $\Phi(\sigma)$ from peculiarities of $f(E)$ are spread over large σ intervals, and sizes of these contributions may be comparable with sizes of inaccuracies in calculated $\Phi(\sigma)$. At the same time, smaller σ_0 values require use of subspaces of basis functions of higher dimensionality. Indeed, accurate $\Phi(\sigma)$ values emerge only at such sizes of these subspaces that (at σ values of significance) the energy ranges $\sigma-\sigma_0\le E\le\sigma+\sigma_0$ contain sufficiently large numbers of 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. Contrary to this, within the present approach such results are not adopted as approximations to the true responses. Here they play the role of an input to the integral equation which solution provides the final true responses. This refinement makes it possible to obtain more accurate and consistent results.

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

$$\Phi(\sigma)=\langle Q'|\tilde{\psi}\rangle,\qquad \tilde{\psi}=(H+\sigma)^{-1}Q, \tag{14}$$

i. e., $\tilde{\psi}$ is a solution of the inhomogeneous Schrödinger-like equation

$$(H+\sigma)\tilde{\psi}=Q. \tag{15}$$

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

$$K(\sigma = \sigma_R + i\sigma_I, E) = 1/[(\sigma_R - E)^2 + \sigma_I^2]. \tag{16}$$

By writing

$$\frac{1}{(\sigma_R - E)^2 + \sigma_I^2} = \frac{1}{2i\sigma_I}\left(\frac{1}{\sigma_R - E - i\sigma_I} - \frac{1}{\sigma_R - E + i\sigma_I}\right), \tag{17}$$

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

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

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

We shall not discuss here methods 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 a small number of particles. A new method to solve Eq. (12) has been proposed recently [8]. In this method, the number of maxima and minima of the desired solution 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 much more accurate results than the standard regularization procedure in simple examples considered. However its further study is still required.

The discrete contributions R_n in Eq. (12) may be calculated separately. A convenient way to do this in the cases of the Lorentz or Stieltjes transforms can be found in Ref. [7]. Another option is the following. A general algorithm for solving Eq. (12) suggests to express $f(E)$ through some parameters and to fit these parameters to $\Phi(\sigma)$. The R_n amplitudes may be included in the set of such parameters.

A limitation of the present approach is that in order to reproduce very fine details of spectra of reactions, such as widths of narrow resonances, an increased accuracy in the input $\Phi(\sigma)$ is required. The reason is the same as the discussed above in connection with Eq. (13). This feature is similar to the situation with extracting, say, widths of narrow resonances from experiments measuring scattering or reaction cross sections. However narrow resonances are usually located at low energies whereas the present method is designed for calculations of reactions with many open channels, i. e., not at low energies. Furthermore, the information on the widths of narrow resonances taken from experiment or from alternative calculations may be readily incorporated

in the algorithm of solving Eq. (12). Anyway, the inaccuracies in widths of resonances at low energies in the present method would not lead to inaccuracies at reproducing reaction spectra at higher energy. In addition, the widths of resonances in light nuclei are normally not so narrow. The width about 200 KeV of such a resonance in ^{4}He was reproduced in Ref. [9] with a reasonable accuracy in the framework of the present approach; see also Fig. 3 in this respect.

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., the sum rule calculation of the integral transforms of observable responses $R(E)$, i. e., pertaining to the inclusive perturbation-induced reactions, has been suggested in Ref. [11] in the case of the Stieltjes transform and in Ref. [12] in the case of the Laplace transform. Inversions of the transforms were not considered in those works. An alternative approach [13] in which an observable $R(E)$ is reconstructed from its moments of the type $\langle E^{-n}\rangle$, $n = 0, ..., N$, has been also developed. The quantity of Eq. (9) represents in this case the zero moment. The subsequent moments are calculated recursively. Contrary to the above described method [10] of treatment of general type reactions, i. e., exclusive perturbation- and strong interaction-induced ones, the approach of Ref. [13] is applicable only to the inclusive perturbation-induced reactions. 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'). The Lorentz transform has been introduced in the present context in Ref. [14]. Its evaluation in the form listed above was given in Ref. [7]. In Ref. [15] an efficient algorithm to calculate $\Phi(\sigma)$ by solving Eq. (15) with the help of an expansion in a series of basis functions, has been developed. In the review papers [7] and [16] the transform inversion in the framework of a conventional approach is considered. In Ref. [16] earlier applications performed with the help of the Lorentz transform are reviewed as well. Among later applications, advances in studies of heavier nuclei [17, 18] are to be mentioned.

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