Method of integral transforms for calculating few–body reactions

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Abstract

A non–conventional approach to calculating reactions in quantum mechanics is presented. Reaction observables are obtained with bound state calculation techniques. The accuracy of the method to calculate few–nucleon response functions is discussed.

\textsuperscript{*}supported by INFN and the Russian Foundation for Basic Research (grant no. 97-02-17003).
I. INTRODUCTION

The purpose of the method discussed is to solve reaction problems with bound state calculation techniques. The approach can be applied to both perturbation and strong interaction induced inclusive and exclusive processes. Below the case of inclusive perturbation induced reactions is considered.

The general procedure was introduced in 1985 [1]. The originally proposed Stieltjes transform led to stability problems [2]. In Ref. [3] it was found that a Lorentzian kernel allowed to cure the instabilities. Accurate results on three- and four-nucleon response functions were obtained with this kernel [4–7].

In Sec. 2 the procedure is outlined. In Sec. 3 the stability issue is explained and the inversion technique is described. In Sec. 4 the choice of the transform kernel is discussed. In Sec. 5 the accuracy of the method in the “exactly solvable” $(e,e'np)$ problem is demonstrated, and its features in the calculations of the three- and four-nucleon response functions are discussed.

II. OUTLINE OF THE METHOD

We need to obtain the response functions of the form

$$R(\epsilon) = \int df |\langle \Psi_f |\hat{O} |\Psi_0 \rangle|^2 \delta(E_f - E_0 - \epsilon)$$  \hspace{1cm} (1)

starting from a few–body Hamiltonian. Here $\epsilon$ is the excitation energy, $\Psi_0$ is the ground state wave function, $\Psi_f$ is a complete set of the final state wave functions, and $\hat{O}$ is a transition operator. In general the continuum wave functions $\Psi_f$ include infinite numbers of various channels with three or more fragments. The number of these functions is infinite as well. Therefore the calculation of $R$ via direct use of Eq. (1) would in general be impractical. Complications may occur even at very low energy due to the Coulomb interaction in channels with more than two fragments. The present method circumvents the above problems due to the fact that the continuum wave functions $\Psi_f$ do not enter the calculation at all.

The method proceeds in two steps. At the first step an integral transform of $R$ with a smooth kernel $K$

$$\Phi(\sigma) = \int K(\sigma, \epsilon) R(\epsilon) d\epsilon,$$  \hspace{1cm} (2)

is calculated instead of $R$ itself. Using sum–rule techniques one can see that

$$\Phi(\sigma) = \langle \Psi_0 |\hat{O}^\dagger \hat{K}(\sigma, \hat{H} - E_0) \hat{O} |\Psi_0 \rangle,$$  \hspace{1cm} (3)

$\hat{H}$ and $E_0$ being the Hamiltonian and the ground state energy, respectively. Expression (3) is evaluated with bound–state techniques as described below. As a second step Eq. (2) is considered as an integral equation to invert and thus one gets $R(\epsilon)$ from $\Phi(\sigma)$. 

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III. INVERSION OF THE TRANSFORM AND ISSUE OF STABILITY

Let us suppose that the transform (3) is evaluated and consider the subsequent inversion of Eq. (2). As it is known solutions to such type of equations are unstable with respect to high frequency oscillations. Indeed, let us add an oscillating increment \( \Delta R \) to the right-hand side of Eq. (2). The transform will get the increment \( \Delta \Phi \), and if the oscillations are rapid enough \( \Delta \Phi \) may be small even if the oscillation amplitudes are not small. The quantity \( \Delta \Phi \) might become less than possible errors in the numerical calculation of the transform and the corresponding rapidly oscillating increment \( \Delta R \) could not then be discriminated. It is known that a regularization procedure can cure the instability. The mathematical justification of such procedures can be found e.g. in Ref. \([8]\). The regularization suppresses rapid oscillations. The higher an accuracy in \( \Phi \) the higher might be the frequency level at which the suppression occurs and the finer are the details of a true response that can be reproduced with an approximate solution. A stability of the solution with respect to changes in the regularization parameter would then indicate that the high frequencies suppressed are insignificant for reproducing a response.

The inversion procedure in the calculations \([1–7]\) was the following. The response was sought for in the form

\[
R(\epsilon) = \sum_{n=1}^{N} c_n \chi_n(\epsilon, \alpha),
\]

where \( \chi_n \) are known functions including nonlinear parameters \( \alpha \). If one substitutes this form into the right hand side of Eq. (2) one has

\[
\Phi(\sigma) = \sum_{n=1}^{N} c_n \tilde{\chi}_n(\sigma, \alpha),
\]

where the \( \tilde{\chi}_n(\sigma, \alpha) \) are the transformed basis functions. The parameters \( c_n \) and \( \alpha \) are obtained fitting the transform of Eq. (5) to the known results obtained by Eq. (3) at many \( \sigma \) points. The number of functions \( N \) plays the role of the regularization parameter and is chosen within the above mentioned stability region.

Features of a response known beforehand such as its low energy behavior and possible information on narrow levels could easily be incorporated into the set \( \{\chi_n\} \). This increases the accuracy of the inversion. The longitudinal \((e, e')\) few-body responses behave in a rather peculiar way at small \( \epsilon \). This is caused by the fact that lower multipole contributions to the continuum part of the responses can have maxima in the threshold region, while higher multipoles exhibit maxima only in the quasielastic peak region. We applied the method separately to those lower multipole responses and to the sum of all others retained \([3,5]\). This substantially increased the accuracy of the results at low energy. The reason is that for simple functions \( \chi_n \) one can better describe the behavior of those pieces of the response function with sufficiently low \( N \) values in Eq. (4) than the total response function.

IV. THE CHOICE OF THE TRANSFORM KERNEL

At a given accuracy in the transform \( \Phi \) the resulting response \( R \) will be most accurate if the kernel is chosen as ”narrow” as possible. Indeed, only changes in \( R \) occurring at the
intervals $\Delta \epsilon$ smaller than the range of the kernel may be hard to resolve since they may tend to cancel at integrating in Eq. (2).

The following choice proved to be efficient [3]. Let the transform variable $\sigma$ be complex and consider the kernel of the Lorentz form

$$K(\sigma = -\sigma_R + i\sigma_I, \epsilon) = \frac{1}{(\sigma^* + \epsilon)(\sigma + \epsilon)} = \frac{1}{[(\sigma_R - \epsilon)^2 + \sigma_I^2]}, \quad (6)$$

$\sigma_I$ being ”sufficiently small”. According to Eq. (3) this leads to the transform

$$\Phi(\sigma) = \langle \Psi_0 | \hat{O}^\dagger \frac{1}{H - E_0 + \sigma^*} \frac{1}{H - E_0 + \sigma} \hat{O} | \Psi_0 \rangle. \quad (7)$$

Eq. (7) can be written as

$$\Phi(\sigma) = \langle \tilde{\Psi}(\sigma) | \tilde{\Psi}(\sigma) \rangle, \quad (8)$$

where $\tilde{\Psi}$ is the unique solution to the Schrödinger–like equation with a source,

$$(H - E_0 - \sigma_R + i\sigma_I)\tilde{\Psi} = Q, \quad Q = \hat{O}\Psi_0. \quad (9)$$

Since $\Phi$ and thus $\langle \tilde{\Psi} | \tilde{\Psi} \rangle$ does exists, $\tilde{\Psi}$ is localized! Hence bound–state type methods can be applied to solve Eq. (9).

V. CALCULATIONS OF FEW–NUCLEON RESPONSES

The accuracy of the method was tested with the two–body longitudinal $d(e, e')$ response. To approach the situation with $A=3$ and 4, several percent errors were artificially introduced into the transform, see [3]. Fig. 1 demonstrates that even in presence of the errors the response obtained practically coincides with the exact one calculated in the conventional way.

Longitudinal $(e, e')$ response functions [4,5] and total photoabsorption cross sections [6,7] were studied for three- and four-nucleon cases. In [4] Reid and Bonn realistic NN forces were employed. Eq. (9) was cast into the form of inhomogeneous Faddeev–type equations. In [5–7] local NN (Malfliet–Tjon type) potentials reproducing $s$–wave NN phase shifts up to the pion threshold were used. Eq. (9) was solved with the help of the Jastrow correlated hyperspherical harmonic basis (CHH). The $\sigma_I$ values were taken from the interval $5 \text{ MeV} \leq \sigma_I \leq 20 \text{ MeV}$. The smaller $\sigma_I$ the more accurate is the inversion but the larger is the number of CHH basis functions required to achieve the same accuracy in the transform. In fact for $\sigma_I$ tending to zero the scattering regime is recovered. In other problems, such as the response of the $^{11}\text{Li}$ nucleus in the 3–cluster model much lower $\sigma_I$ values can easily be used. For an efficient inversion the transform should be obtained in the $\sigma_R$ region covering the interval of $\epsilon$ values of interest. Besides $\sigma_I = \text{const}$, the choice $\sigma_I = \sigma_I(\sigma_R)$ is possible. In Refs. [4,6] the $\sigma_I$ values were taken to increase with $\sigma_R$. This improved the accuracy in $R$ at low energy.

To judge the quality of the responses obtained the following criteria were applied. First, the input transform should be obtained from the dynamic equation (9) with a sufficient accuracy. A typical trend of convergence is demonstrated in Fig. 2. The quantity $K_{\text{max}}$ intervals $\Delta \epsilon$ smaller than the range of the kernel may be hard to resolve since they may tend to cancel at integrating in Eq. (2).
governs the number of the CHH basis functions retained at solving Eq. (9). The $K_{\text{max}}$ values in Fig. 2 are sufficient to provide an accurate response and they are substantially lower than those required in the bound–state calculation with the same NN potential. Second, as said above, the responses obtained should be stable with respect to a change in $N$ in Eq. (4) in some $\Delta N$ interval. This is the most important criterion. In the harder 4-nucleon calculations we had $\Delta N \simeq 3 - 4$. In some easier cases the $\Delta N$ values were much larger. Third, various choices of $\sigma_I$ in Eq. (9) and sets $\{\chi_n\}$ in Eq. (4) should lead to approximately the same responses provided that the above mentioned criterion is fulfilled, and this also tested in our calculations as well. An additional check is provided by sum rules. The quantities $\int R(\epsilon)d\epsilon$ and $\int R(\epsilon)\epsilon d\epsilon$ were compared with the sum rule expressions evaluated independently. The differences were about 1% or less for the non–energy weighted and less than 2% for the energy–weighted sum rules.

To sum up, the method proved to be a practical tool for studying few–nucleon responses. It would be of interest to try the approach also for exclusive and strong interaction induced reactions.
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FIGURES

FIG. 1. Longitudinal deutron form factor at $q^2 = 5 \text{ fm}^{-2}$. Conventional calculation: full curve; from inversion of the Lorentz transform: dashed curve.

FIG. 2. The Lorentz Transform with various $K_{\text{max}}$ values.
$R(E_{np}) \left[10^{-3} \text{ MeV}^{-1}\right]$ vs. $E_{np} \ [\text{MeV}]$
