Lorentz Integral Transform for Inclusive and Exclusive Cross Sections with the Lanczos Method

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Abstract

The Lorentz Integral Transform (LIT) method is reformulated via the Lanczos algorithm both for inclusive and exclusive reactions. The new technique is tested for the total photoabsorption cross section of $^3$H and $^4$He. Due to the rapid convergence of the algorithm one has a decrease in cpu time by two orders of magnitude, but at the same time an excellent agreement with the results of a conventional LIT calculation. The present work opens up the possibility of ab initio calculations for inclusive and exclusive processes for $A\geq 6$ with inclusion of complete final state interactions.

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I. INTRODUCTION

The study of reaction cross sections is an important tool to reveal the dynamics of particle systems. For systems with a small number of particles one aims at microscopic calculations trying to take into account all relevant degrees of freedom of the considered process. However, calculations via the classical approach, where one employs initial and continuum state wave functions, are very difficult to perform for reactions at energies beyond a possible three-body breakup threshold. On the other hand the calculation can be carried out in an alternative way, namely via the Lorentz Integral Transform (LIT) method [1]. This method allows ab initio calculations which take into account final state interactions correctly, without explicit knowledge of the complicated continuum wave functions. Various applications of this method for reactions of nuclei up to four nucleons can be found in the literature (see e.g. [1–7]).

The LIT is expressed in terms of Lorentz states $\tilde{\Psi}$, which have bound state like asymptotic boundary conditions that are much simpler to treat than the boundary conditions for a continuum state and thus $\tilde{\Psi}$ can be calculated with similar methods as a bound state wave function. Common to many bound state methods is an expansion of the wave function on some basis set. In fact in the above mentioned LIT calculations an expansion on the hyperspherical harmonics basis has been employed for the reactions of nuclei with $A \geq 3$ (with the exception of Ref. [1]). As the Hilbert space increases with the number of particles the calculations face larger and larger hamiltonian matrices, which have to be inverted in order to solve the equations associated with the LIT method. Such an inversion is time consuming and limits the number of possible basis states used in the calculation. The aim of the present paper is to point out that the inversion can be avoided. Inspired by recent condensed matter calculations [8–10] we have adapted the Lanczos method for the calculation of the LIT. In this way we open the possibility to extend the LIT method to problems, where a rather large number of basis functions is needed, e.g., calculations of reactions of the $\alpha$ particle with realistic interactions or calculations of reactions of systems with more than four particles.

The outline of the paper is as follows. In Sections II/III we review the LIT method for inclusive/exclusive reactions briefly and discuss the corresponding implementation of the Lanczos technique. Various checks of the calculation are discussed in Section IV, which also contains a short summary at the end.

II. INCLUSIVE PROCESSES

As pointed out for the case of the Stieltjes transform [11] the integral transform method can be used for the calculation of a variety of reaction cross sections. In this and in the following section we restrict the discussion to inclusive and exclusive cross sections due to an external probe, though the approach can also be applied to other reaction cross sections, e.g., to the elastic scattering of particle systems.

In order to determine inclusive cross sections due to external probes one has to calculate various dynamical functions

$$F_{kk'}(\omega,q) = \int d\psi_f \langle \psi_0 | \hat{O}_k'(q) | \psi_f \rangle \langle \psi_f | \hat{O}_{k'}(q) | \psi_0 \rangle \delta(E_f - E_0 - \omega),$$

(1)
where $\omega$ and $q$ are energy and momentum transfer; $\psi_0$ and $\psi_f$ denote ground and final state wave functions of the considered system with energies $E_0$ and $E_f$, respectively, while the various $\hat{O}_k$ are excitation operators inducing different types of transitions.

For few-body reactions with $A > 2$ one faces very often the problem that $F_{kk'}(\omega, q)$ cannot be calculated exactly, since the microscopic calculation of $\psi_f$ is too complicated. However, via the LIT approach the problem can be reformulated in such a way that the knowledge of $\psi_f$ is not necessary [1]. To this end the LIT of the response function is introduced

$$L_{kk'}(\sigma) = \int d\omega \frac{F_{kk'}(\omega)}{(\omega - \sigma_R)^2 + \sigma_I^2},$$

where

$$\sigma = \sigma_R + i\sigma_I \quad \sigma_R, \sigma_I > 0.$$  

In (2), as well as in the following equations, we suppress the dependence on $q$ of $L_{kk'}(\sigma, q)$ and $F_{kk'}(\omega, q)$.

The LIT method proceeds in two steps. First $L_{kk'}(\sigma)$ is evaluated in a direct way, which does not require the knowledge of $F_{kk'}$, and then in a second step the dynamical function is obtained from an inversion of the LIT. The direct calculation of $L_{kk'}(\sigma)$ is outlined in the following. Starting from the definition of the LIT in (2), substituting for $F_{kk'}(\omega)$ the expression in (1) and using the completeness relation of the Hamiltonian eigenstates,

$$\int df \langle \psi_f | \psi_f \rangle = 1,$$

one finds

$$L_{kk'}(\sigma) = \langle \tilde{\psi}_k | \tilde{\psi}_{k'} \rangle.$$  

It is evident that the solutions of the equations

$$(\hat{H} - E_0 - \sigma_R + i\sigma_I)|\tilde{\psi}_l\rangle = \hat{O}_l|\psi_0\rangle; \quad l = k, k'$$

lead directly to the searched transform:

$$L_{kk'}(\sigma) = \langle \tilde{\psi}_k | \tilde{\psi}_{k'} \rangle.$$  

Physical solutions for the Lorentz states $|\tilde{\psi}_l\rangle$ of (1) have asymptotic boundary conditions like a bound state. Moreover the solutions are unique, since due to the hermiticity of $\hat{H}$ the homogeneous equation

$$(\hat{H} - E_0 - \sigma_R + i\sigma_I)|\tilde{\psi}_l\rangle = 0$$

has only the trivial solution $|\tilde{\psi}_l\rangle = 0$.

The inversion of the calculated $L_{kk'}(\sigma)$ leads to the dynamical functions $F_{kk'}(\omega)$. For details on the inversion procedure see, e.g., Ref. [3]. The LIT method leads to reliable results as shown in test calculations for two- and three-body systems [1,2].
If one solves \((\hat{\psi}_i)\) expanding \(|\tilde{\psi}_i\rangle\) on a set of basis functions \(|\mu\rangle\) one has to invert the corresponding hamiltonian matrix \(H_{\mu,\mu'}\). For a large number of basis functions this is a time consuming calculation, moreover, for dense matrices this task rapidly becomes prohibitive. As we will show, the Lanczos method can help to overcome this problem.

Basically the Lanczos method \([12]\) is used to tridiagonalize matrices. If one is interested in calculating the ground state energy of an hamiltonian matrix \(\hat{H}_{\mu,\mu'}\) one has first to choose a starter, a vector \(|\phi_0\rangle\), which must have a non-zero overlap with the ground state \(|\psi_0\rangle\). One can then build the Lanczos orthonormal basis \(|\phi_i\rangle, i = 0, \ldots, n\rangle\) by applying the Lanczos algorithm recursively

\[
b_{i+1}|\phi_{i+1}\rangle = \hat{H}|\phi_i\rangle - a_i|\phi_i\rangle - b_i|\phi_{i-1}\rangle,
\]

where

\[
|\phi_{-1}\rangle = 0, \quad \langle \phi_i|\phi_j\rangle = \delta_{ij}.
\]

The Lanczos coefficients \(a_i\) and \(b_i\) are defined as

\[
a_i = \langle \phi_i|\hat{H}|\phi_i\rangle, \quad b_i = \| b_i|\phi_i\|, \quad b_0 = 0.
\]

If one applies \(M\) Lanczos steps to an \(M \times M\) matrix, then the original matrix is reduced into a tridiagonal form. However, the power of the Lanczos algorithm lays in the fact that even after \(m << M\) steps the eigenvalues of the \(m \times m\) tridiagonal Lanczos matrix are good approximations of the extreme eigenvalues of \(H\). These eigenvalues converge rapidly with increasing number of Lanczos steps. Working with finite precision, it is necessary to recall that at each step there are round-off errors so that after a certain number of steps the Lanczos vectors loose their orthogonality. In order to obtain accurate results this loss has to remain small, otherwise one has to apply an additional reorthogonalization procedure.

In the following we show how the Lanczos algorithm can be applied to the LIT method for inclusive processes. To this end we rewrite the LIT in the following form

\[
\frac{\sigma_I}{\pi} L_{kk'}(\sigma) = -\frac{1}{\pi} \text{Im} \left\{ \langle \psi_0|\hat{O}_{k'}^{\dagger} \frac{1}{\sigma_R + i\sigma_I + E_0 - \hat{H}} \hat{O}_k|\psi_0\rangle \right\}.
\]

A similar relation connects the dynamical functions \(F_{kk'}\) to the Green’s function

\[
F_{kk'}(\omega) = -\frac{1}{\pi} \text{Im} \left\{ \lim_{\eta \to 0} G(\omega + i\eta + E_0) \right\}; \quad G(z) = \langle \psi_0|\hat{O}_{k'}^{\dagger} \frac{1}{z - \hat{H}} \hat{O}_k|\psi_0\rangle,
\]

provided that \(z = \omega + i\eta\) is replaced by \(\sigma_R + i\sigma_I\). This is not surprising since for \(\sigma_I \to 0\) the properly normalized Lorentzian kernel tends to \(\delta(\omega - \sigma_R)\) and thus \(L_{kk'}(\sigma_R)\sigma_I/\pi \to F_{kk'}(\sigma_R)\).

In condensed matter calculations \([8-10]\) the Lanczos algorithm has been applied to the calculation of the Green function with a small value of \(\eta\), and its imaginary part has been interpreted as \(F_{kk'}(\omega)\) directly. This can be done if the spectrum is discrete (or discretized) and \(\eta\) is sufficiently small. In our case we have a genuine continuum problem and we want to avoid any discretization, therefore we calculate \(L_{kk'}(\sigma_R)\) in the same way i.e. with finite \(\sigma_I\) using the Lanczos algorithm, but then we antitransform \(L_{kk'}(\sigma_R)\) in order to obtain \(F_{kk'}(\omega)\).

Choosing
\[|\phi_0\rangle = \frac{\hat{O}|\psi_0\rangle}{\sqrt{\langle \psi_0 | \hat{O}^\dagger \hat{O} | \psi_0 \rangle}} \]  

as starting vector for the Lanczos basis and setting \( z = E_0 + \sigma_R + i\sigma_I \) one finds

\[
L(\sigma) = \frac{1}{\sigma_I} \langle \psi_0 | \hat{O}^\dagger \hat{O} | \psi_0 \rangle \Im \left\{ \frac{1}{z - \hat{H}} \langle \phi_0 | \right\}
\]

showing that the LIT depends on the matrix element

\[
x_{00} = \langle \phi_0 | \frac{1}{z - \hat{H}} | \phi_0 \rangle .
\]

One can calculate \( x_{00} \) applying Cramer’s rule to the solution of the linear system

\[
\sum_n (z - \hat{H})_{mn} x_{n0} = \delta_{m0}
\]

that arises from the expansion of the identity

\[
(z - \hat{H})(z - \hat{H})^{-1} = I
\]

over the Lanczos basis \( \{|\phi_i\rangle, i = 0, \ldots, n\} \). In this way one is able to write \( x_{00} \) as a continued fraction containing the Lanczos coefficients \( a_i \) and \( b_i \),

\[
x_{00} = \frac{1}{(z - a_0) - \frac{b_1^2}{(z - a_1) - \frac{b_2^2}{(z - a_2) - \frac{b_3^2}{\ldots}}}} ,
\]

and thus also the LIT becomes a function of the Lanczos coefficients

\[
L(\sigma) = \frac{1}{\sigma_I} \Im \left\{ -\frac{\langle \psi_0 | \hat{O}^\dagger \hat{O} | \psi_0 \rangle}{(z - a_0) - \frac{b_1^2}{(z - a_1) - \frac{b_2^2}{(z - a_2) - \frac{b_3^2}{\ldots}}}} \right\} .
\]

This illustrates that the Lanczos method allows to determine \( L(\sigma) \) without solving the differential equation (6), i.e. without inverting the hamiltonian matrix.

**III. EXCLUSIVE PROCESSES**

Different from an inclusive reaction where the final state of the studied particle system is unobserved, for an exclusive process one has to determine the cross section of a specific breakup channel for specific angles of the outgoing fragments. For instance, the unpolarized cross section for a two-body breakup induced by an external probe is given by

\[
\frac{d\sigma}{d\Omega_f} = \sum_{kk'} c_{kk'}(\omega, q, \phi_f) f_{kk'}(\omega, q, \theta_f) ,
\]
where $\Omega_f = (\theta_f, \phi_f)$ is the spherical angle of one of the outgoing fragments. In (21) the $c_{kk'}$ are known kinematical functions, while the dynamics of the particle system is contained in the structure functions

$$f_{kk'}(\omega, q, \theta_f) = \sum_{cm} T_{akm}^*(E_f) T_{ak'm}(E_f).$$

The above transition matrix elements are defined as follows

$$T_{akm}(E_f) = \langle \psi_{f,\alpha} | \hat{O}_k(q) | \psi_{0,m} \rangle,$$

where $\alpha$ stands for a set of quantum numbers of the final state function $\psi_f$ with energy $E_f$ in the specific breakup channel and $m$ is the projection of the total angular momentum of the initial state wave function $\psi_0$.

Different from the inclusive cross section, where an integral method leads to the direct determination of the dynamical function $F_{kk'}$, one has to determine any single transition matrix element $T_{akm}(E_f)$ in order to calculate the exclusive cross section [11].

We illustrate the derivation of the integral transform method for the exclusive case restricting ourselves to a breakup of the A-body system in two fragments. In this case the final state of the system can be written using the Lippmann-Schwinger equation

$$\langle \psi_f, \alpha | = \langle \phi_{PW}^{\alpha} | + \langle \phi_{PW}^{\alpha} | \hat{V}_{12} \frac{1}{E_f + i\epsilon - \hat{H}},$$

where $|\phi_{PW}^{\alpha}\rangle$ describes the plane wave relative motion of the two fragments with the same set of quantum numbers $\alpha$ as $\psi_{f,\alpha}$, while $\hat{V}_{12}$ denotes the interaction of the constituents of one fragment with the constituents of the other fragment. In coordinate space the plane wave has the following form

$$\phi_{PW}^{\alpha}(\vec{r}) = A \psi_1 \psi_2 e^{-i\vec{p} \cdot \vec{r}} (2\pi)^{3/2},$$

where $A$ is an antisymmetrization operator acting on the constituents of both fragments, $\psi_1$ and $\psi_2$ are the internal wave functions of the two fragments, while $\vec{p}$ is the relative momentum and $\vec{r}$ the relative coordinate of the two fragments. Note that internal coordinates and quantum numbers of $\psi_1$ and $\psi_2$ are suppressed in (25).

Substituting (24) into (23) one finds that the transition matrix element is described by the sum of two pieces, a Born term

$$T_{akm}^{Born}(E_f) = \langle \phi_{PW}^{\alpha} | \hat{O}_k | \psi_{0,m} \rangle,$$

and a final state interaction (FSI) term

$$T_{akm}^{FSI}(E_f) = \langle \phi_{PW}^{\alpha} | \hat{V}_{12} \frac{1}{E_f + i\epsilon - \hat{H}} \hat{O}_k | \psi_{0,m} \rangle.$$

While the Born term can be calculated without major problems the FSI term is more difficult. Using the completeness of the eigenstates $|\psi_p(E_p)\rangle$ of $\hat{H}$ one gets for the FSI term
\[ T^{FSI}_{akm}(E_f) = \int df' \langle \phi^PW_{\alpha}(V_{12} | \psi'_{f}(E_{f}')) \langle \psi'_{f}(E_{f}'') | \hat{O}_{k} | \psi_{0,m} \rangle \frac{1}{E_f + i\epsilon - \hat{H}} \hat{O}_k | \psi_{0,m} \rangle \]  

(28)

\[ = \int df' \langle \phi^PW_{\alpha}(V_{12} | \psi'_{f}(E_{f}')) \langle \psi'_{f}(E_{f}'') | \hat{O}_{k} | \psi_{0,m} \rangle \frac{1}{E_f + i\epsilon - E_{f}'} \]  

(29)

\[ = -i\pi F_{akm}(E_f) + P \int_{E_0 - \delta}^{\infty} dE' \frac{F_{akm}(E_{f}')}{E_f - E_{f}'} \]  

(30)

with

\[ F_{akm}(E_{f}') = \sum_{f'} \langle \phi^PW_{\alpha}(V_{12} | \psi'_{f}(E_{f}')) \langle \psi'_{f}(E_{f}'') | \hat{O}_{k} | \psi_{0,m} \rangle, \]  

(31)

where the sum over \( f' \) stands for a possible degeneracy of the states \( |\psi'_{f} \rangle \) with energy \( E_{f}' \).

Equation (30) is only a formal solution for \( F_{akm}(E) \), since one should know all the eigenstates of \( \hat{H} \). A direct calculation of \( F_{akm}(E) \) is even more difficult than the original problem of Eq. (23), where one needs to know just the eigenstate of energy \( E_{f} \). However, one obtains \( F_{akm} \) indirectly applying the LIT approach:

\[ L_{akm}(\sigma) = \int_{E_0 - \delta}^{\infty} dE \frac{F_{akm}(E)}{(E - \sigma)(E - \sigma^*)} \]  

(32)

\[ = \int_{E_0 - \delta}^{\infty} df' \langle \phi^PW_{\alpha}(V_{12} | \psi'_{f}(E_{f}')) \langle \psi'_{f}(E_{f}'') | \hat{O}_{k} | \psi_{0,m} \rangle \frac{1}{H - \sigma} \frac{1}{H - \sigma^*} \]  

(33)

\[ = \langle \phi^PW_{\alpha}(V_{12} | \psi'_{f}(E_{f}')) \langle \psi'_{f}(E_{f}'') | \hat{O}_{k} | \psi_{0,m} \rangle \]  

(34)

\[ = \langle \tilde{\psi}_{\alpha}(\sigma) | \tilde{\psi}_{km}(\sigma) \rangle . \]  

(35)

The Lorentz state \( \tilde{\psi}_{km}(\sigma) \) is obtained solving essentially the same differential equation as for the inclusive case discussed in the previous chapter:

\[ (\hat{H} - \sigma_{R} + i\sigma_I) | \tilde{\psi}_{km} \rangle = \hat{O}_{k} | \psi_{0,m} \rangle, \]  

(36)

whereas \( \tilde{\psi}_{\alpha}(\sigma) \) is the solution of new differential equation

\[ (\hat{H} - \sigma_{R} + i\sigma_I) | \tilde{\psi}_{\alpha} \rangle = \hat{V}_{12} | \phi^PW_{\alpha} \rangle. \]  

(37)

If \( \hat{V}_{12} \) represents a finite range potential, the term on the right hand side of (37) vanishes for large distances, and one has also for \( \tilde{\psi}_{\alpha} \) an asymptotic bound state boundary condition similar to a bound state. If \( \hat{V}_{12} \) is not of finite range one can reformulate the LIT method accordingly [12][13].

Inverting the various \( L_{akm} \) one gets the functions \( F_{akm} \) and thus the transition matrix elements \( T^{FSI}_{akm} \). An additional calculation of the Born terms \( T^{FSI}_{akm} \) leads to the searched structure functions. Also for exclusive cross sections one obtains reliable results with the LIT method as shown in a test calculation for the \( d(e,e'N) \) reaction [13].

Now we turn to the application of the Lanczos method to the LIT of the exclusive reaction. To this end we first rewrite the LIT in the following form

\[ L_{akm}(\sigma) = \frac{1}{2i\sigma_I} \langle \phi^PW_{\alpha}(V_{12} | \psi'_{f}(E_{f}')) \langle \psi'_{f}(E_{f}'') | \hat{O}_{k} | \psi_{0,m} \rangle \frac{1}{H - \sigma_{R} - i\sigma_I} \frac{1}{H - \sigma_{R} + i\sigma_I} \]  

(38)
Using the completeness relation over the Lanczos vectors \{\phi_i|i = 0, \ldots, n\}, where the starting vector \|\phi_0\rangle is the same as in (14), and setting \(z = \sigma_R + i\sigma_I\) one finds

\[
L_{\alpha km}(\sigma) = \frac{i}{2\sigma_I} \left\{ \sum_{i=0}^{n} \langle \phi_{\alpha}^{PW} | \hat{V}_{12} | \phi_i \rangle \left[ \langle \phi_i | \frac{1}{z - H} \hat{O}_k | \psi_{0,m} \rangle - \langle \phi_i | \frac{1}{z^* - H} \hat{O}_k | \psi_{0,m} \rangle \right] \right\}
\]

\[
= \frac{i\sqrt{\langle \psi_{0,m} | \hat{O}_k^\dagger \hat{O}_k | \psi_{0,m} \rangle}}{2\sigma_I} \left\{ \sum_{i=0}^{n} \langle \phi_{\alpha}^{PW} | \hat{V}_{12} | \phi_i \rangle \left[ \langle \phi_i | \frac{1}{z - H} | \phi_0 \rangle - \langle \phi_i | \frac{1}{z^* - H} | \phi_0 \rangle \right] \right\}
\]

\[
= \frac{i\sqrt{\langle \psi_{0,m} | \hat{O}_k^\dagger \hat{O}_k | \psi_{0,m} \rangle}}{2\sigma_I} \left\{ \sum_{i=0}^{n} \langle \phi_{\alpha}^{PW} | \hat{V}_{12} | \phi_i \rangle \left[ x_{0i} - \bar{x}_{0i} \right] \right\},
\]

(39)

with the matrix elements

\[
x_{0i} = \langle \phi_0 | \frac{1}{z - H} | \phi_i \rangle,
\]

(40)

\[
\bar{x}_{0i} = \langle \phi_0 | \frac{1}{z^* - H} | \phi_i \rangle,
\]

(41)

which can be written as continued fractions of the Lanczos coefficients, like in (19).

In the following we describe a simple algorithm for a recursive calculation of all the \(x_{0i}\) starting from \(x_{00}\). Defining

\[
g(\nu) = -\frac{b_\nu^2}{z - a_\nu - \frac{b_{\nu+1}^2}{z - a_{\nu+1} - \bar{x}_{\nu+2}}}
\]

(42)

one has

\[
x_{00} = \frac{1}{z - a_0 + g(1)}.
\]

(43)

The next matrix element \(x_{01}\) can be written as

\[
x_{01} = \frac{1}{(z - a_1)\lambda_0 - b_1 + \lambda_0 g(2)},
\]

(44)

where

\[
\lambda_0 = \frac{z - a_0}{b_1}
\]

(45)

is obtained from \(x_{00}\). Now a new parameter

\[
\lambda_1 = \frac{(z - a_1)\lambda_0 - b_1}{b_2}
\]

(46)

can be obtained from \(x_{01}\) leading to the evaluation of

\[
x_{02} = \frac{1}{(z - a_2)\lambda_1 - b_2\lambda_0 + \lambda_1 g(3)}.
\]

(47)
Proceeding in this way it is easy to show that the $n$-th matrix element $x_{0n}$ can be written as

$$x_{0n} = \frac{1}{(z - a_n)\lambda_{n-1} - b_n\lambda_{n-2} + \lambda_{n-1}g(n + 1)}$$

(48)

with

$$\lambda_n = \frac{(z - a_n)\lambda_{n-1} - b_n\lambda_{n-2}}{b_{n+1}}.$$  

(49)

**IV. RESULTS**

In order to check the accuracy and to quantify the advantages of the Lanczos method for the LIT approach we apply it to the calculation of total photoabsorption cross sections of $^3$H and $^4$He and compare to results which we obtain solving Eq. (6) via an inversion of the hamiltonian matrix.

For the total photoabsorption cross section we use the dipole approximation, where one has a single transition operator, namely

$$\hat{O}_k = \hat{O}_{k'} = \sum_i^A z_i \frac{1 + \tau_z(i)}{2};$$

(50)

here $z_i$ and $\tau_z(i)$ are the third components of the spatial coordinate and of the isospin of particle $i$, respectively. We expand ground and Lorentz states on the hyperspherical harmonics basis making use of the recently developed EIHH approach [16]. As NN interaction model we employ the semirealistic MTI-III potential [17]. We note in passing that calculations of the total photoabsorption cross section of $^3$H and $^4$He via the LIT already exist [4,5,7].

In Fig. 1 we show the LIT for the triton photodisintegration choosing the isospin channel $T = 1/2$ of the disintegrated three-body system. One sees that there is an excellent agreement between both calculations. The relative difference of both results is far below 0.1 %. For the second isospin channel ($T = 3/2$), not shown here, the comparison is of the same excellent quality. In Fig. 2 we show the LIT for the case of the $^4$He photodisintegration, where one has only a single isospin channel of the disintegrated four-body system ($T = 1$) for the considered dipole transition. Again one sees a very good agreement comparing the results with and without application of the Lanczos method. One finds only tiny differences between both results. It is evident from Figs. 1 and 2 that the Lanczos method leads to highly reliable results.

The main advantage of the Lanczos technique lies in the enormous reduction of the cpu time. In particular one should note that it is not necessary to perform all the Lanczos steps. In fact, checking the convergence of $L(\sigma)$ with respect to the number of Lanczos coefficients used in the continued fraction one finds the following: for $\sigma_R \to \infty$ only the first Lanczos step is necessary, because the entire continued fraction is dominated just by $\sigma_R$. Also in the low $\sigma_R$ region one can expect that the continued fraction converges rapidly, since for $\sigma_R \to 0$ the dominating contribution to the term $1/(z - \hat{H})$ is given by the lowest eigenvalue of $\hat{H}$, which is well approximated using only the first few Lanczos coefficients. Thus one may
hope that in the intermediate $\sigma_R$ region a rather small number of Lanczos coefficients will be sufficient. In Fig. 3 we illustrate the convergence behavior with respect to the number of Lanczos steps for the LIT of the $^4$He photodisintegration for a test case with 1372 basis states. As one can see the transforms are somewhat different from the converged one only if one takes less than 100 Lanczos coefficients. The relative error is already smaller than 0.5% for 150 coefficients and becomes rapidly smaller with a further increasing number of Lanczos steps. One can conclude that 200÷300 steps are completely sufficient in the studied case. Also due to the rapid convergence we obtain a reduction in cpu time of two orders of magnitude comparing with the conventional LIT calculation.

Applying the Lanczos method one has to pay attention to the loss of orthogonality of the Lanczos vectors with an increasing number of steps, since it could reduce the precision of the Lanczos coefficients. We check the orthogonality calculating the scalar products of the 0-th and the $i$-th Lanczos vectors. The results for the LIT case, illustrated in Fig. 3, are shown in Table I. It is evident that after 300 Lanczos steps, where one has a sufficiently converged LIT, one has still a rather good orthogonality. In fact the overlap between the 0-th and the 300-th Lanczos vector is quite small (about $10^{-4}$). However, in other cases one could encounter problems with the orthogonality and thus one would need to reorthogonalize the Lanczos vectors.

In the following we summarize our results briefly. The LIT approach for the calculation of both inclusive and exclusive cross sections including complete final state interactions is reformulated in order to use the Lanczos algorithm. The Lanczos method allows one to calculate the LIT without complete inversion of the hamiltonian matrix. It leads to a huge simplification of the calculation reducing the needed cpu time enormously (about two orders of magnitude) and, even more important, paving the way for calculations with large number of basis functions. We have tested the reliability of the method with great success for the LIT of the total photoabsorption cross sections of $^3$H and $^4$He. The high precision of the method together with the strong reduction of the cpu time opens the way to precise microscopic calculations of reaction cross sections also for more complex few-body systems. Indeed, very recently the new method has been applied to the first microscopic calculation of the total photoabsorption cross section of the A=6 nuclei with complete final state interactions of the six-nucleon system [18].
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TABLES

| $i$  | $\langle \phi_0 | \phi_i \rangle$    |
|------|-----------------------------------|
| 1    | $1.3 \times 10^{-16}$             |
| 150  | $-2.4 \times 10^{-6}$             |
| 200  | $-1.2 \times 10^{-4}$             |
| 250  | $-9.5 \times 10^{-5}$             |
| 300  | $1.1 \times 10^{-4}$              |

TABLE I. Scalar product between the 0-th and $i$-th lanczos vector.
FIGURES

FIG. 1. LIT of the $^3$H photoabsorption cross section for $T = 1/2$ with conventional and Lanczos methods: absolute (a) and relative values (b) setting the conventional LIT result equal to 1 ($\sigma_I = 20$ MeV).

FIG. 2. LIT of the $^4$He photoabsorption cross section with conventional and Lanczos methods: absolute (a) and relative values (b) setting the conventional LIT result equal to 1 ($\sigma_I = 20$ MeV).

FIG. 3. Convergence of the LIT of Fig.2 with respect to the number $n$ of Lanczos coefficients: absolute (a) and relative values (b) setting the LIT result with 1372 Lanczos coefficients equal to 1.
(a) Conventional

(b) $^4$He

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$L [\text{fm}^2 \text{KeV}^{-2}]$

$E_0 + \sigma_R [\text{MeV}]$
(a) \n\n\[ L \left[ \text{fm}^2 \text{Kev}^{-2} \right] \]

(b) \n\[ E_0 + \sigma_R \left[ \text{MeV} \right] \]

\[ 0.996 \quad 1.004 \]

\[ \text{He} \]