Ab initio calculation of $^7\text{Li}$ photodisintegration

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Abstract

The $^7\text{Li}$ total photoabsorption cross section is calculated microscopically. As nucleon-nucleon interaction the semi-realistic central AV4′ potential with S- and P-wave forces is taken. The interaction of the final 7-nucleon system is fully taken into account via the Lorentz Integral Transform (LIT) method. For the calculation of the LIT we use expansions in hyperspherical harmonics (HH) in conjunction with the HH effective interaction (EIHH) approach. The convergence of the LIT expansion is discussed in detail. The calculated cross section agrees quite well with the available experimental data, which cover an energy range from threshold up to 100 MeV.

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The electromagnetic response of an \( A \)-body nucleus is a basic property in nuclear physics. It contains important information about the dynamical structure of the system. For this reason microscopic calculations are needed in order to investigate the details of the reaction mechanism and the underlying dynamics. Traditionally such studies could only be made for few-body systems with \( A \leq 3 \). The explicit calculation of final state wave functions constitutes the main limitation of standard approaches. On the other hand these difficulties can be avoided in the Lorentz Integral Transform (LIT) method \[1\], where only a bound-state-like problem has to be solved although the full final state interaction (FSI) is rigorously taken into account. First applications of the method were made for electromagnetic responses of \( ^4\text{He} \) \[2\]. Enormous progress has also been achieved in the calculation of bound-state wave functions of systems with \( A > 4 \) (No Core Shell Model \[3\] and Effective Interaction Hyperspherical Harmonics (EIHH) approach \[4\]). The novel methods of LIT and EIHH combined with the help of modern computational resources enabled us to carry out calculations of electromagnetic cross sections of nuclei with \( A = 6 \) \[5, 6\]. Therefore, systems with \( 4 < A < 12 \) are now considered an interesting playground for establishing a bridge between few- and many-body physics and especially for testing many-body approximations.

In this paper we present the first microscopic calculation of a photoabsorption reaction on a nucleus with \( A=7 \), namely \( ^7\text{Li} \). In this calculation we use as nucleon-nucleon interaction the Argonne potential AV4’ \[7\], which is a semirealistic central interaction that contains S- and P-wave forces. In recent work \[6\] we found that the P-wave interaction has a significant influence on the photodisintegration cross section of P-shell nuclei, like \( ^6\text{He} \) and \( ^6\text{Li} \), and leads to a considerably better agreement with experimental data than a central S-wave interaction only. Thus we have chosen this potential model for the present ab initio calculation of the \( ^7\text{Li} \) total photoabsorption cross section. The calculational procedure is described in detail in \[5, 6\]. In the following we will briefly review the main steps only.

The inclusive unpolarized response function \( R(\omega) \) is defined by the total photoabsorption cross section
\[
\sigma(\omega) = 4\pi^2\alpha\omega R(\omega), \tag{1}
\]
where \( \alpha \) denotes the fine structure constant and \( \omega \) the photon energy. In the LIT method \[1\] one obtains \( R(\omega) \) from the inversion of the integral transform
\[
\mathcal{L}(\sigma_R, \sigma_I) = \int d\omega \frac{R(\omega)}{(\omega - \sigma_R)^2 + \sigma_I^2}. \tag{2}
\]
In the unretarded dipole approximation one has

\[
\mathcal{L}(\sigma_R, \sigma_I) = \frac{1}{2L_0 + 1} \sum_{M_0^L, M_0^S} \frac{1}{\sigma_I} \sum_{M_0^L, M_0^S} \frac{1}{\sigma_I} \Im\{\langle \Psi_0(M_0^L, M_0^S) | \hat{D}_z | H - \sigma_R - i\sigma_I | \hat{D}_z | \Psi_0(M_0^L, M_0^S) \rangle\},
\]

(3)

where \( \hat{D}_z \) denotes the dipole operator, \( H \) the nuclear Hamiltonian, and \( L_0 \) and \( S_0 \) are the angular momentum and spin of the ground state \( |\Psi_0(M_0^L, M_0^S)\rangle \), with projections \( M_0^L \) and \( M_0^S \), respectively (since we work with central forces, \( L_0 \) and \( S_0 \) are good quantum numbers).

The transform \( \mathcal{L}(\sigma_R, \sigma_I) \) is evaluated by inserting a complete set of projection operators \( \sum_{C,M^L,M^S} |\Psi_C(M^L, M^S)\rangle \langle \Psi_C(M^L, M^S)| \equiv \sum_{C,M^L,M^S} \hat{P}_{C,M^L,M^S} \hat{P}_{C,M^L,M^S}, \) where \( C = \{ L, S, T, T^z, \pi \} \) stands for the quantum numbers characterizing the channels (angular momentum, spin, isospin and its projection, and parity, respectively), \( M^L \) and \( M^S \) are third components of angular momentum and spin. In the sum only the channels allowed by the dipole selection rules need to be considered and since the dipole operator does not depend on spin, we do not need to average over the initial spin projections \( (M_0^S) \), neither to sum over \( M^S \). Therefore one obtains

\[
\mathcal{L}(\sigma_R, \sigma_I) = \frac{1}{2L_0 + 1} \sum_{C} |\langle \Psi_C | \hat{D}_z | \Psi_0 \rangle|^2 \Im\{\langle \Psi_C | \frac{1}{H - \sigma_R - i\sigma_I} | \Psi_C \rangle\},
\]

where

\[
|\Psi_C\rangle = \frac{\hat{P}_C \hat{D}_z | \Psi_0 \rangle}{\sqrt{\langle \Psi_0 | \hat{D}_z \hat{P}_C \hat{D}_z | \Psi_0 \rangle}}.
\]

(4)

To simplify the notation, in the last two equations we have also omitted the dependences on \( M^L \) and \( M_0^L \), as will be done in the following.

In order to use the Lanczos algorithm (see Ref. [10]) it is convenient to write \( \mathcal{L}(\sigma_R, \sigma_I) = \sum_C N_C^2 F_C \), where \( N_C \) is connected to the norm of \( \hat{P}_C \hat{D}_z | \Psi_0 \rangle \),

\[
N_C^2 = \frac{1}{2L_0 + 1} \sum_{M^L,M_0^L} |\langle \Psi_C | \hat{D}_z | \Psi_0 \rangle|^2 = \frac{1}{2L_0 + 1} \sum_{M^L,M_0^L} \langle \Psi_0 | \hat{D}_z \hat{P}_C \hat{D}_z | \Psi_0 \rangle
\]

(5)

and

\[
F_C = \frac{1}{\sigma_I} \Im\{\langle \Psi_C | \frac{1}{H - \sigma_R - i\sigma_I} | \Psi_C \rangle\}
\]

(6)
TABLE I: Good quantum numbers for the channels $|\Psi_C\rangle$ allowed by the dipole selections rules.

| $\Psi$ | $\Psi_1$ | $\Psi_2$ | $\Psi_3$ | $\Psi_4$ | $\Psi_5$ | $\Psi_6$ |
|-------|-------|-------|-------|-------|-------|-------|
| $L$   | 0     | 0     | 2     | 2     | 1     | 1     |
| $S$   | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ |
| $T$   | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ |
| $T^z$ | $-\frac{1}{2}$ | $-\frac{1}{2}$ | $-\frac{1}{2}$ | $-\frac{1}{2}$ | $-\frac{1}{2}$ | $-\frac{1}{2}$ |

is evaluated as continuous fraction via the Lanczos coefficients. This means that the LIT of the total response is the sum of the Lorentz transforms of the individual channels

$$\mathcal{L}(\sigma_R, \sigma_I) = \sum_C \mathcal{L}_C(\sigma_R, \sigma_I),$$

where for every channel one has $\mathcal{L}_C(\sigma_R, \sigma_I) = N_C^2 F_C$.

In the case of $^7\text{Li}$ one has total angular momentum and parity $J^\pi = \frac{3}{2}^-$ and isospin $T_0 = \frac{1}{2}$ with projection $T_0^z = -\frac{1}{2}$. Using central forces, one has ground state orbital angular momentum $L_0 = 1$ and spin $S_0 = \frac{1}{2}$. There are six different channels allowed by the dipole selection rules corresponding to angular momentum $L = L_0 - 1, L_0, L_0 + 1$, spin $S = S_0$ and isospin $T = T_0, T_0 + 1$ with isospin projection conserved $T^z = T_0^z$. In Table I we show the good quantum numbers of these channels.

For every channel the LIT is calculated by expanding $|\Psi_0\rangle$ and $|\Psi_C\rangle$ in terms of the 7-body anti-symmetrized hyperspherical harmonics (HH) up to a maximum HH hyperangular momentum $K^\text{max}$, i.e. $K^\text{max}_0$ for the ground state $|\Psi_0\rangle$ and $K^\text{max}_C$ for the channels $|\Psi_C\rangle$. The convergence of the HH expansion is improved by using the EIHH approach. Our procedure consists in fixing first $K^\text{max}_0$ such that convergence for the binding energy is reached, and then we study the behavior of the LIT with increasing $K^\text{max}_C$. As already pointed out in [6], the rate of convergence for a potential that includes a central P-wave interaction, like the AV4', can be slower than that of a purely central S-wave force. Nevertheless, in the case of $^7\text{Li}$ we have obtained a satisfactory convergence in terms of hyperangular momentum, both for ground state energy and LIT. For the ground state of $^7\text{Li}$ good convergence is reached with $K^\text{max}_0 = 9$ with a binding energy of 45.28 MeV. Further increase to $K^\text{max}_0 = 11$ leads only to a small change of the binding energy by 0.05 MeV. Because of the dipole selection rule $K = K_0 \pm 1$ between states with hyperangular momenta $K$ and $K_0$, an expansion of
TABLE II: Reduction of basis states for channel $C = 3$ for $K_{\text{max}} = 10$. Each symmetry is represented by a Young tableau. The total number of states for each symmetry is listed as $N^{\text{sym}}$, while $N^{\text{sym}}_{\text{used}}$ lists the actual number of states in the calculation.

| Symmetry | [111111] | [211111] | [221111] | [311111] | [22211] | [32111] | [41111] | [32211] | [33111] | [42111] | [43111] |
|----------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| $N^{\text{sym}}$ | 5       | 69      | 240     | 314     | 315     | 977     | 693     | 698     | 780     | 1515    | 742     |
| $N^{\text{sym}}_{\text{used}}$ | 0       | 0       | 0       | 0       | 0       | 693     | 0       | 780     | 1515    | 742     |         |

the ground state up to a certain $K^0_{\text{max}}$ implies that in $|\Psi_C\rangle$ only states with hyperangular momentum $K \leq K_{\text{max}} = K^0_{\text{max}} + 1$ contribute to the LIT. Thus it is expected that for sufficiently high $K^0_{\text{max}}$ a further increase of $K_{\text{max}}$ beyond $K^0_{\text{max}} + 1$ will not result in a significant change. In this case a check of the convergence with respect to $K^0_{\text{max}}$ only will be sufficient.

In the present work, the best calculation of the LIT corresponds to a final state with $K_{\text{max}} = 10$. In this case the number of HH-basis states to be included becomes quite large, especially for the channels with $L_C = 1$ and 2. For example, already for channel $C = 3$ and $K_{\text{max}} = 10$ one has 6348 hyperspherical states. This number has to be multiplied by the number of hyperradial states, about 30, to obtain the total number of states needed in the expansion. Therefore, it is desirable to discard those HH states which give only negligible contributions to the LIT. To this end we have studied the importance of the HH states according to their spatial symmetry and found that quite a few of them can be safely neglected (see Table II). We have checked this approximation by performing calculations with the complete set of states for lower values of $K_{\text{max}}$ (6 and 8) and compared the results with those using a truncated set. Whenever the differences between results with the reduced and the full basis were negligible (below 0.5%) we concluded that the omitted states were negligible also for higher $K_{\text{max}}$. In this way we accomplished for $K_{\text{max}} = 10$ a sizable reduction from $N = 190\,440$ to $N = 111\,900$ basis functions. In an analogous way we carried out the calculations for all the other channels. The estimated error introduced by these truncations is of the order of 0.5%.

We are also able to check the error introduced by the symmetry truncation in a second way. In fact a good check of the quality of the calculation is obtained by considering the
sum over the norms $N_C^2$ defined in (5). Using completeness one finds

$$\sum_C N_C^2 = \frac{1}{2L_0 + 1} \sum_{C,M,L,M_0} |\langle \Psi_C | \hat{D}_z | \Psi_0 \rangle|^2 = \frac{1}{2L_0 + 1} \sum_{M_0} \langle \Psi_0 | \hat{D}_0^\dagger \hat{D}_z | \Psi_0 \rangle,$$

(8)

where the last expression is nothing else than the mean expectation value of the operator $\hat{D}_z^\dagger \hat{D}_z$ in the ground state, that can be easily calculated (see Ref. [5]). With respect to Eq. (8) we obtained 1.877 [fm²] for the ground state expectation value with $K_{max}^0 = 9$, while using a symmetry truncated expansion for $|\Psi_C\rangle$ up to $K_{max} = 10$ we get 1.871 [fm²]. The small difference of 0.3% reflects the small error introduced by the symmetry truncation.

FIG. 1: Upper panel (a): Relative change $R_{K_{max}^0}^{C}$ for the LIT of channel $C=6$ ($\sigma_I = 10$ MeV). Lower panel (b): $R_{K_{max}^0}^{C}$ for the same channel (see text for details).

As next point we address the quality of convergence of the LIT with respect to the HH expansion. For this reason, we first introduce the notation $L_C^{K_{max}^0(\pm)}$ for the LIT calculated with an expansion up to $K_{max}^0$ for the ground state and up to $K_{max}^\pm = K_{max}^0 \pm 1$ for $|\Psi_C\rangle$. 

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respectively. That means $L_{C_{\text{max}}}^{K_{\text{max}}(\pm)}$ represents the LIT of channel C calculated with a maximal hyperangular momentum for those states which can be reached by a dipole transition from the ground state, whereas for $L_{C_{\text{max}}}^{K_{\text{max}}(\pm)}$ the expansion of channel C is taken up to one step below this value. Then we define

$$R_{C_{\text{max}}(\pm)}^{K_{\text{max}}(\pm)} = \frac{L_{C_{\text{max}}}^{K_{\text{max}}(\pm)} - L_{C_{\text{max}}}^{K_{\text{max}}(\pm)-2}(\pm)}{L_{C_{\text{max}}}^{K_{\text{max}}(\pm)}} \times 100,$$

where $R_{C_{\text{max}}(\pm)}^{K_{\text{max}}(\pm)}$ represents the relative percentage change for increasing $K_{\text{max}}$ by 2 together with a corresponding increase of $K_{\text{max}}$ while $R_{C_{\text{max}}(\pm)}^{K_{\text{max}}(\pm)}$ represents the relative change for increasing $K_{\text{max}}$ by 2 but keeping $K_{\text{max}}$ fixed.

In Fig. 1 (a) we show the convergence pattern of $R_{C_{\text{max}}(\pm)}^{K_{\text{max}}(\pm)}$ for one of the more important of the six C channels, namely $C = 6$. One readily sees that increasing $K_{\text{max}}$ results in a considerable reduction of $R_{C_{\text{max}}(\pm)}^{K_{\text{max}}(\pm)}$. For example, changing $K_{\text{max}}$ from 7 to 9 yields a $R_{6}^{9(+)}$ between 5 and 15 %, where the lower value refers to the region of the maximum of the LIT (compare Fig. 2), which however is still not negligible. It is very likely, that a further increase to $K_{\text{max}} = 11$ would lead to a significant improvement of the convergence. Although the calculation of the ground state for $K_{\text{max}} = 11$ can be performed, the corresponding calculation of the final state with $K_{\text{max}} = 12$ is beyond our present technical capabilities whereas it can be done for $K_{\text{max}} = 10$, i.e. $L_{C}^{10(-)}$ can be calculated. Thus the question now is, how much is the convergence improved in going from $L_{C}^{9(+)}$ to $L_{C}^{11(-)}$. To this end we show $R_{C_{\text{max}}(\pm)}^{K_{\text{max}}(\pm)}$ in Fig. 1 (b) for $K_{\text{max}} = 7, 9, 11$. Again one notes a considerable decrease of $R_{C_{\text{max}}(\pm)}^{K_{\text{max}}(\pm)}$ with increasing $K_{\text{max}}$ and for the highest value $K_{\text{max}} = 11$ of the order of 5 % in the region $\sigma_{R} \leq 60$ MeV where the LIT is more sizable. Furthermore, comparing panels (a) and (b) of Fig. 1 one can see that for a given $K_{\text{max}}$ the relative change $R_{6}^{K_{\text{max}}(\pm)}$ is smaller than that of $R_{6}^{K_{\text{max}}(\pm)}$. Therefore, we expect that a further increase to $L_{6}^{11(+)}$ would lead to a relative change with respect to $L_{6}^{9(+)}$ smaller than 5%. Since the other channels behave similarly, we estimate a total uncertainty of about 5%.

Now we turn to the results for photodisintegration. In order to obtain the total photoabsorption cross section $\sigma(\omega)$, we first invert the LITs of the response functions for the various channels (for details see [11]). Then one obtains the contribution to the cross section of each channel using the relation [11]. Summing up all contributions finally yields the total cross section $\sigma(\omega)$. In Fig. 2 we show both the calculated total cross section and the contributions of the separate channels. The energetically lowest open channel is the $T = \frac{1}{2}$
FIG. 2: Contribution of various channels to the total cross section. Panels (a) and (b) show the separate contributions of the different channels and their sum for $T = 1/2$ and $T = 3/2$, respectively. Panel (c) shows again the $T = 1/2$ and $T = 3/2$ contributions and the total cross section.

Associated with the reaction $^7\text{Li} + \gamma \rightarrow ^4\text{He} + t$ with a threshold of 2.47 MeV (the theoretical threshold obtained with the AV4’ potential is 4.70 MeV), whereas the lowest open $T = \frac{3}{2}$ channel corresponds to $^7\text{Li} + \gamma \rightarrow ^6\text{He} + p$, whose threshold is 9.975 MeV (the theoretical value is 12.41 MeV). In Fig. 2 the theoretical thresholds have been used.

For the $T = 1/2$-channels in Fig. 2 (a) one readily sees that by far the largest contribution comes from channel 3 rising steeply above threshold, reaching a maximum around 17 MeV.
and falling off only slowly. Channel 5 is the next in importance rising only slowly above 10 MeV with a maximum near 33 MeV and becoming then comparable in size to channel 3. Only in the very near threshold region channel 1 is dominant but then becomes much smaller than the other two channels. In Fig. 2 (b) the $T = 3/2$ channels have two dominant contributions, almost similar in size. Channel 4 is slightly larger showing also a steep rise at threshold and slow fall-off with a maximum near 23 MeV whereas the second in importance, channel 6, shows a slow rise and a peak around 40 MeV. Compared to these two channels, the remaining channel 2 appears quite marginal. In view of the two maxima of almost equal height with a separation by about 17 MeV the total $T = 3/2$-contribution exhibits a broader distribution than the $T = 1/2$-contribution with a shoulder on the low-energy side. The maxima of both contributions have about the same size but are separated by about 20 MeV. Thus, the resulting total cross section in Fig. 2 (c) shows also a broad distribution with a steep rise right above threshold, a slight shoulder above the maximum and a slow fall-off at higher energies.

This characteristic behavior is indeed exhibited by the experimental data on $^7$Li in Fig. 3 where we show a comparison of the theoretical result to experimental data from \[12\]. Note that the theoretical cross section is shifted here from the theoretical threshold to the experimental one. One readily notes that the gross properties of the data, steep rise, broad maximum and slow fall off, are very well reproduced quantitatively over the whole energy range.
region by the theory. It is worthwhile to emphasize that this result is based on an ab initio calculation in which the complicated final state interaction of the 7N-system is rigorously taken into account by application of the LIT method. No adjustable parameters were used, the sole ingredient being the AV4’ NN potential model. It remains to be seen whether the slight variation of the data near and above the maximum will also be found in an experiment with improved accuracy. Therefore, a new measurement of the total cross section with a higher precision would be very desirable. In particular, this could clarify the question whether a simple semi-realistic potential like the AV4’ model is sufficient for an accurate theoretical description of this reaction or whether a more realistic nuclear force including a 3N-force is needed.

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