Coupling the Lorentz Integral Transform (LIT) and the Coupled Cluster (CC) Methods: A way towards continuum spectra of “not-so-few-body” systems.

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Abstract

Here we summarize how the LIT and CC methods can be coupled, in order to allow for \textit{ab initio} calculations of reactions in medium mass nuclei. Results on $^{16}$O are reviewed and preliminary calculations on $^{40}$Ca are presented.
I. INTRODUCTION

A striking characteristic of the nuclear photo-absorption cross section is a very pronounced peak around 10–20 MeV called the giant dipole resonance (GDR). Historical semi-classical interpretations are based on a dipole collective motion of protons against neutrons [1]. Later, both collective and in microscopic many-body approaches have tried to account for its centroid and width [2, 3]. For \textit{ab initio} approaches the difficulty is the position of the resonance in the continuum part of the spectrum.

The LIT method [4] reduces the continuum problem into a bound state problem. Its application however, has been restricted to $A < 8$ nuclei [5]. Therefore it is expedient to try to couple it with the CC method [6, 7], which is very powerful in dealing with bound states of many-body systems.

II. FORMALISM

The main point of the LIT method is that the function $S(\omega)$ entering the photonuclear cross section ($\sigma_\gamma(\omega) = 4 \pi^2 \alpha \omega S(\omega)$) can be accessed via inversion of its integral transform with a Lorentzian kernel

$$L(\omega_0, \Gamma) = \frac{\Gamma}{\pi} \int d\omega \frac{S(\omega)}{(\omega - \omega_0)^2 + \Gamma^2},$$  

(1)

In dipole approximation $S(\omega)$ is given by

$$S(\omega) = \sum_n |\langle \Psi_n | D | \Psi_0 \rangle|^2 \delta(\omega - E_n + E_0),$$  

(2)

where $\omega$ is the photon energy and $E_0, E_n$ and $|\Psi_0\rangle, |\Psi_n\rangle$ are ground and excited state eigenvalues and eigenstates, respectively. The completeness property of the hamiltonian eigenstates allows to write

$$L(\omega_0, \Gamma) = \langle \Psi_0 | D \frac{1}{(H - E_0 - \omega_0 - i\Gamma)(H - E_0 - \omega_0 + i\Gamma)} D | \Psi_0 \rangle \equiv \langle \tilde{\Psi} | \tilde{\Psi} \rangle.$$

(3)

Since the integral in (1) is finite $|\tilde{\Psi}\rangle$ is bound, therefore bound state techniques can be used to calculate its norm $L(\omega_0, \Gamma)$, for fixed values of $\Gamma$ and many values of $\omega_0$. For $A < 8$ hyperspherical harmonics (HH) expansions have been used [8]. Accurate enough results for $L$ have allowed its inversion [9, 10] to give the required response function. Here we
reformulate the LIT within the CC approach. To this aim we rewrite Eq. (3) introducing a similarity transformation $e^T$:

$$L(\omega_0, \Gamma) = \langle \Psi_0 | e^T e^{-T} \frac{1}{(H - E_0 - \omega_0 - i\Gamma)} e^T e^{-T} \frac{1}{(H - E_0 - \omega_0 + i\Gamma)} e^T e^{-T} D e^T e^{-T} | \Psi_0 \rangle$$

$$\equiv \langle 0_L | \tilde{D} \frac{1}{(H - E_0 - \omega_0 - i\Gamma)} \frac{1}{(H - E_0 - \omega_0 + i\Gamma)} \tilde{D} | 0_R \rangle \equiv \langle \tilde{\Psi}_L | \tilde{\Psi}_R \rangle \quad (4)$$

Notice that $\langle 0_L |$ is different from $| 0_R \rangle$. In the CC approach the operator $T$ is such that $| 0_R \rangle \equiv e^{-T} | \Psi_0 \rangle$ is a single Slater determinant, and in the single-double (CCSD) approximation it is chosen as a linear combination of one-particle-one-hole (1p-1h) and two-particle-two-hole (2p-2h) operators, only. The amplitudes of $T$ are obtained by solving the CC equations [11].

To calculate the LIT within the CC method one has the additional problem to find $| \tilde{\Psi}_R \rangle$ and $\langle \tilde{\Psi}_L |$, which are solutions of the following equations:

$$\langle \tilde{\Psi}_L | (\tilde{H} - E_0 - \omega_0 - i\Gamma) \tilde{\Psi}_R \rangle = \langle 0_L | \tilde{D} \rangle ;$$

$$\langle \tilde{\Psi}_L | (\tilde{H} - E_0 - \omega_0 + i\Gamma) | \tilde{\Psi}_R \rangle = \tilde{D} | 0_R \rangle . \quad (5)$$

To this aim one may use the equation of motion (EoM) method, namely one can write $| \tilde{\Psi}_R \rangle = R | 0_R \rangle$ and $\langle \tilde{\Psi}_L | = \langle 0_L | L$ , where $R$ and $L$ are linear combinations of 1p-1h and 2p2h excitation operators, similar to $T$. Their amplitudes are obtained by solving the following equations

$$[\tilde{H}, R] | 0_R \rangle = (\omega_0 - i\Gamma) R | 0_R \rangle + \tilde{D} | 0_R \rangle ;$$

$$\langle 0_L | \tilde{H}, L \rangle = \langle 0_L | L (\omega_0 + i\Gamma) + \langle 0_L | \tilde{D} . \quad (6)$$

They differ from the CC EoM only by the presence of the source terms $\tilde{D} | 0_R \rangle$ and $\langle 0_L | \tilde{D}$.  

### III. Results

The results presented in the following have been obtained using a realistic chiral effective field theory potential (N3LO [12]). The method has been first validated on the $S(\omega)$ of $^4$He. This has been obtained from the inversion of the LIT calculated by expanding $| \tilde{\Psi} \rangle$ in HH, up to full convergence. Therefore the HH calculation can be considered virtually “exact” and the excellent agreement with the LIT-CC result can be seen in Ref. [13]. From the same reference we report in Fig. [1] the results for $^{16}$O. In Fig. [1], the theoretical LIT is compared
to the LIT of the data \[14\]. The value of $\Gamma$ has been chosen to be 10 MeV, since it is the smallest value for which we are able to obtain a convergent result (the smaller the value of $\Gamma$, the slower the rate of convergence). Nevertheless one can notice that the transform of the data maintains the resonant structure and preserves the peak position. This is due to the fact that the Lorentzian kernel is a representation of the delta-function (for $\Gamma = 0$ the transform coincides with the response). While the comparison shows that the experimental centroid of the GDR is well reproduced by a calculation that neglects three-body forces, the inversion of the transform leads to a less pronounced peak with respect to experiment (see Fig. 2b).

![Comparison of the LIT at $\Gamma = 10$ MeV for $N_{\text{max}} = 18$ and the Lorentz integral transform of Ahrens et al. data \[14\]. (b): Comparison of $S(\omega)$ of $^{16}$O dipole response against experimental data.](image)

FIG. 1: (Color online) (a): Comparison of the LIT at $\Gamma = 10$ MeV for $N_{\text{max}} = 18$ and the Lorentz integral transform of Ahrens et al. data \[14\]. (b): Comparison of $S(\omega)$ of $^{16}$O dipole response against experimental data.

Aiming at addressing \textit{ab initio} the interesting case of $^{48}$Ca, for which recent photoabsorption measurements have been performed \[15\], we have calculated the LIT of its $N=Z$ partner $^{40}$Ca. In Fig. 2b we present preliminary results about the rate of convergence of the
FIG. 2: (Color online) (a): Convergence of $L(\omega_0, \Gamma)$ at $\Gamma = 10$ MeV as a function of $N_{\text{max}}$. (b) Comparison of the LIT at $\Gamma = 10$ MeV for $N_{\text{max}} = 16, 18$ and the LIT of Ahrens et al. data [14].

As for $^{16}$O, in Fig. 2b we show the comparison with the LIT of the data [14]. Three remarks are in order here:

- as can be seen in Fig. 2a full convergence is not yet reached, therefore an inversion is not worth;

- different from the case of $^{16}$O a purely experimental comparison between the peak positions of the data in [14] and of their LIT in Fig 2b shows a slight difference. This is due to the fact that $S(\omega)$ has a tail at higher energies. This tail contributes to the LIT, which differs enough from a delta-function to shift its peak to the right. Therefore the LIT peak position cannot be considered a prediction of the centroid of the GDR, but one needs an inversion;

- the use of larger model spaces seem to move the theoretical result towards the data. However, the agreement in the transforms would not clearly imply an agreement in $S(\omega)$ (as the results on $^{16}$O have also shown), being only a minimal condition. On the other hand, a disagreement in the integral transforms already might give a important
information, pointing to possible shortcomings in the potential (or in the neglect of higher clusters).

IV. CONCLUSIONS

Here we have summarized the CC-LIT method, which allows to calculate response functions in the continuum of not-so-few-body systems. We have presented \textit{ab initio} results obtained with this method and using only the chiral N3LO two-body potential. The application to the GDR of $^{16}\text{O}$ has shown the ability of this potential to reproduce the centroid of the resonance, while a somewhat less pronounced structure has been found inverting the transform. Preliminary results on the application of the method to the GDR of $^{40}\text{Ca}$ show that larger model spaces are still needed to reach a convergent LIT. There are indications that larger and larger model spaces might lead to an agreement between theoretical and experimental LIT’s. Convergent results are needed to attempt an inversion of the transform.

V. ACKNOWLEDGEMENTS

This work was supported by the MIUR grant PRIN-2009TWL3MX, the Natural Sciences and Engineering Research Council, the National Research Council of Canada, the Israel Science Foundation (Grant number 954/09), the US-Israel Binational Science Foundation (Grant No 2012212), the Office of Nuclear Physics, U.S. Department of Energy (Oak Ridge National Laboratory) and \texttt{de-sc0008499} (NUCLEI SciDAC collaboration). Computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This research used resources of the Oak Ridge Leadership Computing Facility located in the Oak Ridge National Laboratory, which is supported by the Office of Science of the Department of Energy under Contract No. DE-AC05-00OR22725, and used computational resources of the National Center for Computational Sciences, the National Institute for Computational Sciences.

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