# Solving the time-dependent few-body Schrödinger equation within a basis expansion method

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**Abstract.** Nuclear responses are a source of information on nuclear structure and re-action dynamics. We develop a method to study the nuclear response by solving time-dependent equation. We expand the wave function by many correlated Gaussian functions. In this paper, the photoabsorption of $^3$He is presented as a simple example. Measured photoabsorption cross sections are reproduced up to 20 MeV.

## 1 Introduction

We can get information on nuclear structure and reaction dynamics from nuclear responses. For example, the photo-absorption reaction, which mainly occurs through the electric dipole ($E1$) transition is one of them. However, one faces difficulty in treating many-body continuum states, since the $E1$ field excites a nucleus not only to discretized states but also to continuum states. Various methods have been developed to avoid this problem, for example, the complex scaling method [1], the Lorentz integral transform method [2], and the time-dependent method [3]. Here we employ the time-dependent method, in which we solve the time-dependent equation directly to obtain the response function. The wave function is expanded by correlated Gaussians [4], which describe many-body correlations explicitly. We extend them into the complex-range to express oscillations of the wave function at a large distance. As a simple example, a calculation for of three-nucleon system, $^3$He, is presented.

In Sec. 2, we explain how to calculate the photoabsorption cross section with the time-dependent method using the complex-range correlated Gaussians basis functions. In Sec. 3 the results are presented. The calculated photoabsorption cross sections are compared with experimental data. The summary is given in Sec. 4.

## 2 Method

We consider the three-nucleon system. The total Hamiltonian of the system is

$$\hat{H} = \sum_{i=1}^{3} \frac{\boldsymbol{p}_i^2}{2m} - T_{CM} + \sum_{j>i} V_{NN}(|\boldsymbol{r}_i - \boldsymbol{r}_j|) + \sum_{j>i} V_{\text{coul}}(|\boldsymbol{r}_i - \boldsymbol{r}_j|), \tag{1}$$

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where $\boldsymbol{r}_i$ is the single particle coordinate of the $i$-th particle, $T_{CM}$ is the kinetic energy of the center of mass, and $V_{NN}$ and $V_{\text{coul}}$ are nucleon-nucleon and Coulomb interactions, respectively. The Minnesota potential [5] is employed as $V_{NN}$. The binding energy of $^3$He is obtained as 7.71 MeV, which agrees with the experimental value.

The photoabsorption cross section is obtained with the formula [6]

$$\sigma_\gamma(E_\gamma) = \frac{4\pi^2}{\hbar c} E_\gamma S(E_\gamma), \tag{2}$$

where $E_\gamma$ is the photon energy, and $S(E_\gamma)$ is the $E1$ response function defined by

$$S(E_\gamma) \equiv \int d^3\boldsymbol{k} \left| \langle \phi_{\boldsymbol{k}} | \hat{D}_{10} | \phi_0 \rangle \right|^2 \delta(E_{\boldsymbol{k}} - E_0 - E_\gamma), \tag{3}$$

where $\phi_{\boldsymbol{k}}$ and $E_{\boldsymbol{k}}$ are the eigenstate and eigenenergy, respectively.

We assume that the ground state nucleus is excited by the electric dipole ($E1$) field at time $t = 0$. The initial state is constructed by multiplying the $E1$ operator $\hat{D}_{10}$ with the ground state wave function $\phi_0$,

$$\psi(0) = \hat{D}_{10}\phi_0. \tag{4}$$

From the time-dependent Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} \psi(\boldsymbol{r}, t) = \hat{H} \psi(\boldsymbol{r}, t), \tag{5}$$

the wave function at $t$ is expressed by multiplying the time evolution operator with the initial state as

$$\psi(\boldsymbol{r}, t) = \mathrm{e}^{-\frac{i\hat{H}}{\hbar}t} \psi(\boldsymbol{r}, 0). \tag{6}$$

We divide the time variation into short time steps $\Delta t$, and approximate the time evolution operator for $\Delta t$. The $E1$ response function $S(E_\gamma)$ can be written as

$$S(E_\gamma) = \frac{1}{\pi} \mathrm{Re} \int_0^\infty d\left(\frac{t}{\hbar}\right) \mathrm{e}^{\frac{i(E_\gamma + E_0 + i\varepsilon)t}{\hbar}} \langle \psi(0) | \psi(t) \rangle, \tag{7}$$

where $\varepsilon$ is a smoothing factor. This allows us to stop the time evolution in a finite time. It is taken to be a small value about 0.05 MeV in our calculation. We only need to calculate the time evolution of the overlap of the wave function with the initial state to obtain the photoabsorption cross section. This allows us to calculate the cross section without the explicit construction of many-body continuum states.

Here we extend this formalism to three-body systems. We expand the time-dependent wave function $\psi(t)$ by time-independent basis functions $\varphi_i(\boldsymbol{x})$, where $\boldsymbol{x} = (\boldsymbol{x}_1, \boldsymbol{x}_2)$, and the Jacobi coordinate is taken as $\boldsymbol{x}_1 = \boldsymbol{r}_1 - \boldsymbol{r}_2, \boldsymbol{x}_2 = (\boldsymbol{r}_1 + \boldsymbol{r}_2)/2 - \boldsymbol{r}_3, \boldsymbol{x}_3 = (\boldsymbol{r}_1 + \boldsymbol{r}_2 + \boldsymbol{r}_3)/3$. The time evolution of the wave function is expressed by the time-dependent coefficients $c_i(t)$,

$$\psi(\boldsymbol{x}, t) = \sum_{i=1}^N c_i(t)\varphi_i(\boldsymbol{x}). \tag{8}$$

Here $N$ is the number of basis functions. The time evolution is described by $\Delta t$ by solving the linear equations,

$$\left(B + \frac{iH}{2\hbar}\Delta t\right) \boldsymbol{c}(t + \Delta t) = \left(B - \frac{iH}{2\hbar}\Delta t\right) \boldsymbol{c}(t), \tag{9}$$

where $B$ and $H$ are $N \times N$ matrix, and their elements are $\langle \varphi_i | \varphi_j \rangle$ and $\langle \varphi_i | \hat{H} | \varphi_j \rangle$, and $\boldsymbol{c}(t)$ is $N$-dimensional vector that consists of $c_i(t)$.

The basis function is

$$\varphi_i(\boldsymbol{x}) = \mathcal{A}\left\{ e^{-\frac{1}{2}\tilde{\boldsymbol{x}} A_i \boldsymbol{x}} \mathcal{Y}_{LM}(\tilde{u}\boldsymbol{x}) \chi_S \eta_{M_T} \right\}, \tag{10}$$

where $\mathcal{A}$ is the antisymmetrizer. The ~-symbol means the transpose of vectors, $\chi_S$ and $\eta_{M_T}$ are spin and isospin wave function, and $S$ and $M_T$ are total spin and $z$ component of isospin, respectively. The 2-dimensional vector $u$ is determined by the $E1$ operator to make $\tilde{u}\boldsymbol{x}$ correspond with the single particle coordinate of protons. The spacial part is called correlated Gaussian [4], in which $A_i$ is a positive-definite $2 \times 2$ symmetric matrix. $\tilde{\boldsymbol{x}} A \boldsymbol{x}$ is a quadratic form for $\boldsymbol{x}$,

$$\tilde{\boldsymbol{x}} A \boldsymbol{x} = A_{11} \boldsymbol{x}_1^2 + 2 A_{12} \boldsymbol{x}_1 \cdot \boldsymbol{x}_2 + A_{22} \boldsymbol{x}_2^2. \tag{11}$$

The off-diagonal element $A_{12}$ describes the correlation between the relative coordinates. Although the matrix elements of $A$ are usually taken as real numbers, we extend them to complex numbers [7]. This increases the flexibility of the set of basis functions to express oscillations at a large distance.

## 3 Results

In the time evolution of the wave function, artificial reflection waves appear from the model space boundaries. This brings some oscillations to the overlap of the wave function with the initial state. In order to exclude them, we add an imaginary potential to the Hamiltonian in order to absorb the reflected waves [8].
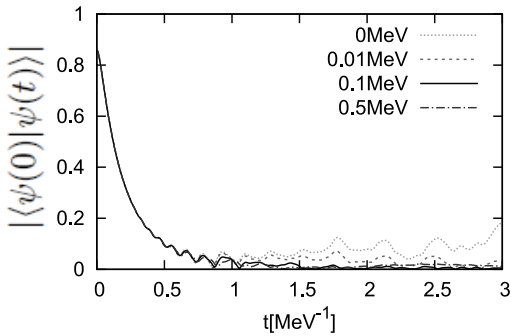
$$\hat{H} \rightarrow \hat{H} + i \sum_{i=1}^{3} W(|\boldsymbol{r}_i - \boldsymbol{x}_3|), \tag{12}$$
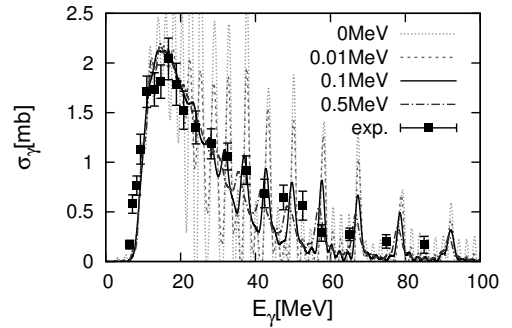
$$W(r) = W_0 \theta(r - R)(r - R)^2, \tag{13}$$

where $\boldsymbol{x}_3$ represents the position of the center of mass of the three nucleons, and $\theta(r - R)$ is a step function. The absorbing potential has two parameters, the one is the strength of the potential $W_0$, and the other is the potential starting position $R$. We calculate photoabsorption cross section with some different values of $W_0$. Fig.1 and Fig.2 display the absolute value of the overlap $\langle \psi(0) | \psi(t) \rangle$ and photoabsorption cross sections calculated with four different $W_0$. $R$ is commonly taken to be 15 fm. Without the absorbing potential, namely $W_0 = 0$, the overlap and the cross section show terrible oscillations. However, when $W_0$ is too large, i.e. 0.5 MeV, there are some reflection after $t = 2.0$, which are considered as the reflection by the absorbing potential. No value of $W_0$ exists, that completely removes the artificial reflection. Some oscillations appear in higher energy region of the cross section. In case of $W_0 = 0.1$, where the reflection effect is smallest, the calculated cross section is found to reproduce the experimental data up to 20MeV.

## 4 Summary

We obtain the photoabsorption cross section of $^3$He within the time-dependent method. We expand the wave function by correlated Gaussian functions extended to the complex-range in order to efficiently describe oscillatory wave function at large distances. Photoabsorption cross section data is reproduced up to 20 MeV. However, the artificial reflection from model space boundaries is not completely removed by imaginary absorbing potential. This problem has to be resolved. Future plans include the application to more-particle systems and use of more realistic interactions.

**Figure 1.** Time evolution of the absolute value of the overlap between the wave function and initial state calculated with different $W_0$. $R$ is commonly taken to be 15 fm. See text for details.



**Figure 2.** Calculated photoabsorption cross sections are shown. The experimental value is taken from Ref. [9].

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