Deuteron Photodisintegration in a Shifted Correlated Gaussian Basis

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June, 2018

Abstract

In this thesis we consider the photodisintegration reaction of the deuteron. The reaction is considered in the dipole approximation and the cross section is calculated numerically using the correlated Gaussian method. It is investigated whether shifted correlated Gaussians are a suitable choice for basis functions for electromagnetic reactions of this kind. Instead of considering the free particle state it was assumed that the photon excites the deuteron to a p-wave state experiencing the harmonic oscillator potential. Initial calculation were done with only including states with projection quantum number $m_l = 0$ using a basis size of 300 Gaussians. Convergence of the cross section was found at an oscillator potential of $\hbar\omega = 0.35$ MeV with slight deviation from experimental data. An attempt at including all states and spin dependent forces in the p-wave triplet was made using a basis size of 700 Gaussians which improved the estimate in the region $E_\gamma < 8$ MeV however an estimate above 8 MeV was not achieved as the degeneracy at the highly excited states is greatly increased by the inclusion of all states and thus preventing us from reaching higher energies. The use of shifted correlated Gaussians was found problematic at highly excited states as it was difficult to reach convergence of the energy levels and cross section. However at lower energies our estimate was in agreement with experimental data and thus found suitable as basis functions for further work on other electromagnetic reactions.

Resume

I denne opgave betragter vi fotodisintegrations reaktionen af deuteron. Reaktionen betragtes i dipole approksimationen og tværsnittet beregnes numerisk ved brug af den korrelerede Gaussiska metode. Det undersøges om skiftede korrelerede Gauss-funktioner er et passende brug af basis funktioner for elektromagnetiske reaktioner af denne type. I stedet for at betragte den fri partikel tilstand antages det at fotonen eksiterer deuteron til en p-bølge tilstand, hvor kernen oplever det harmoniske oscillator potentiale. Tværsnittet estimeres først ved udelukkende at kigge på tilstande med projektions kvantetal $m_l = 0$ i en basis størrelse af 300 Gaussfunktioner. Konvergens af tværsnittet blev fudnet ved et oscillator potentiale med $\hbar\omega = 0.35$ MeV med mindre afvigelse fra eksperimentelle resultater. Et forsøg på at inddrage alle tilstande og et spin-afhængig potentiale i p-bølge tilstanden øgede overensstemmelsen med eksperimentelle værdier i regionen $E_\gamma < 8$ MeV men et estimate for tværsnittet over $E_\gamma < 8$ MeV opnåes ikke da udartningen af energi niveauer øges i en sådan grad at vi ikke når energiniveauer højere. Valget af skiftede Gaussfunktioner som basis funktioner blev da fundet problematisk ved højt exciterede tilstande da det blev fundet svært at nå konvergens af tværsnittet og energiniveauerne. Ved lavere energier opnåes resultater i overensstemmelse med eksperimentelle værdier og da egnede som basisfunktioner til fotoodisintegrations reaktionen.

Contents

Chapter 1

Introduction

As the deuteron is the simplest compound nucleus it has been subject to numerous experimental and theoretical studies. The deuteron allows us to study simple nuclear processes such as the photo disintegration reaction where the nucleus absorbs a gamma photon and decays by emitting a subatomic particle $d + \gamma \rightarrow p + n$. In this thesis we seek to employ the correlated Gaussian method to calculate the cross section of the photo disintegration of the deuteron using a basis of shifted correlated Gaussians. We consider the reaction in the dipole approximation and will use simple potentials to approximate the nucleon interaction in both the initial and final state. Firstly the correlated Gaussian method is introduced then we describe the deuteron system and derive the photo disintegration cross section in the dipole approximation. Finally the cross section is calculated numerically and evaluated with comparison to experimental data and zero-range models.

Chapter 2

The correlated Gaussian method

In this chapter we seek to introduce the correlated Gaussian method. The correlated Gaussian method is a variational method to solve quantum mechanical few-body problems with applications in molecular, atomic and nuclear physics. The following chapter is, if not cited otherwise, based on Suzuki and Varga[1].

2.1 The variational method

The variational method is an approach to estimate both the ground state and excited states of a quantum mechanical system using trial wave functions. We consider a physical system with Hamiltonian $\hat{H}$ and discrete normalized eigenstates Φ_n with corresponding eigenvalues E_n

$$\hat{H}\Phi_n = E_n\Phi_n \quad n = 1, 2, ... \tag{2.1}$$

The eigenvalues are ordered such that $E_1 \leq E_2 \leq ....$ In general it is not easy to solve equation 2.1 even though $\hat{H}$ is known. Instead of trying to solve the eigenvalue problem directly one can get approximate results of Φ_n and E_n using a trial wave function. Formulated in the Ritz theorem.

Ritz Theorem. *For and arbitrary function Ψ the expectation value of Hamiltonian $\hat{H}$ in the state Ψ is such that*

$$E = \frac{\langle\Psi|\,\hat{H}\,|\Psi\rangle}{\langle\Psi|\Psi\rangle} \geq E_1, \tag{2.2}$$

where the equality holds if and only if Ψ is an eigenstate of $\hat{H}$ with eigenvalue E_1.
Thus by using a trial wave function the Ritz theorem yields an upper bound of the ground state energy. The trial wave functions may be chosen arbitrarily, however to reach accurate results with estimates as close to the true eigen state as possible a suitable choice of basis functions is important. The Ritz theorem can be extended to excited states as well. Formulated in the *Mini-max Theorem.*

Mini-Max Theorem. *Let $\hat{H}$ be a Hermitian operator with discrete eigenvalues $E_1 \leq E_2 \leq ...$ Let $\epsilon_1 \leq \epsilon_2 \leq ... \leq e_k$ be the eigenstates of $\hat{H}$ restricted to the subspace $\mathcal{V}_K$ of a linearly independent set of K functions $\Psi(\alpha_1), ..., \Psi(\alpha_k)$. Then*

$$E_1 \leq \epsilon_1, E_2 \leq \epsilon_2, ..., E_K \leq \epsilon_K \tag{2.3}$$

Hence restricting our basis to a subspace $\mathcal{V}_K$ of linearly independent functions allows us to estimate the estimate the ground state and $K-1$ excited states for a K-dimensional basis size. As trial wave functions we shall consider a linear combination

$$|\psi\rangle = \sum_{i=1}^{K} c_i\,|i\rangle \tag{2.4}$$

of a set of basis functions $|i\rangle$ and reformulate the eigenvalue problem. This is considered in the following section.

2.2 The Generalized Eigenvalue problem

In the correlated Gaussian method one uses Gaussians as basis functions. Gaussians are not mutually orthogonal allowing us to formulate the eigenvalue problem differently. Again we consider a system with time-independent Hamiltonian $\hat{H}$ and

discrete eigenvalues of $\hat{H}$. We are interested in finding the eigen energies ϵ and the corresponding eigenstates. The Schrödinger equation reads:

$$\hat{H}\left|\psi\right\rangle = \epsilon\left|\psi\right\rangle. \tag{2.5}$$

We now write our wave function ψ as a linear combination of a set of basis functions and insert into the Schrödinger equation

$$\hat{H}\sum_{i=1}^{K} c_i\left|i\right\rangle = \epsilon\sum_{i=1}^{K} c_i\left|i\right\rangle \tag{2.6}$$

Taking inner product on a basis function $|k\rangle$ yields

$$\sum_{i=1}^{K} c_i\left\langle k\right|\hat{H}\left|i\right\rangle = \epsilon\sum_{i=1}^{K} c_i\left\langle k|i\right\rangle, \tag{2.7}$$

or in matrix notation

$$\mathcal{H}\mathbf{c} = \epsilon\mathcal{N}\mathbf{c} \tag{2.8}$$

Where $\mathcal{H}$ and $\mathcal{N}$ are respectively the Hamiltonian and overlap matrices with the matrix elements:

$$\mathcal{H}_{kj} = \left\langle k\right|\hat{H}\left|i\right\rangle, \quad \mathcal{N} = \left\langle k|i\right\rangle \tag{2.9}$$

Equation 2.8 is called the generalized eigenvalue problem. If the basis function were orthogonal it would reduce to the normal eigenvalue problem, however as we use Gaussians this is not the case. The generalized eigenvalue problem can be solved through Cholesky decomposition [4] if the overlap matrix is positive definite. The overlap $\mathcal{N}$ is written as the product of a lower triangular matrix and its transposed

$$\mathcal{N} = LL^T \tag{2.10}$$

Rewriting the generalized eigenvalue problem of equation 2.8 gives

$$L^{-1}\mathcal{H}(L^T)^{-1}L^T\mathbf{c} = \epsilon L^T\mathbf{c}, \tag{2.11}$$

switching notation yields

$$\mathcal{H}'\mathbf{c}' = \epsilon\mathbf{c}' \tag{2.12}$$

and the generalized eigenvalue problem reduces to the normal eigenvalue problem.

2.3 Basis functions

As stated by the Ritz theorem one can use an arbitrary function as trial wave functions. When choosing basis functions one should consider which the properties of the functions and whether they fit the system of interest. Firstly Gaussians are advantageous because they are easily generalized for an N-body system and the matrix elements of equation 2.9 are all analytical. A possible choice are the correlated Gaussians

$$\exp\left(-\mathbf{x}^T A\mathbf{x}\right) = \exp\left(-\sum_{i=1}^{N-1}\sum_{i=j}^{N-1} A_{ij}\mathbf{x}_i\mathbf{x}_j\right), \tag{2.13}$$

where the matrix elements A_{ij} are non-linear parameters and $\mathbf{x}$ the coordinates of the system (see section . However these functions are spherical and wont allow us to describe states with quantum numbers different from $l = 0$. To describe non-spherical states on has to multiply the basis function by a orbital angular function

$$|g : A\rangle = \theta_{l,m}(\mathbf{r}) \exp\left(-\mathbf{x}^T A\mathbf{x}\right), \tag{2.14}$$

where $\theta_{l,m}$ is a spherical harmonic function. Trial wave functions projected on a spherical harmonic function have the advantage that on can pre-define the angular momentum of the desired states. The calculation of matrix elements however becomes easier if one chooses a generating function. A generating function that generates correlated Gaussians of the type in equation 2.14 are the shifted correlated Gaussians

$$|g : A, s\rangle = \exp\left(-\mathbf{x}^T A\mathbf{x} + \mathbf{s}^T\mathbf{x}\right) \tag{2.15}$$

The shifted correlated Gaussians contain additional variational parameters in the form of a shift vector $\mathbf{s}$ allowing one to describe non-spherical states. That is if one does not put restrictions on the shift vectors the function $|g : A, s\rangle$ generates states of all angular momenta. The shifted Gaussians are not eigenfunctions of the square of the total orbital angular momentum operator, however using a large set of basis functions with sufficient variational flexibility results in a wave function that approaches the correct symmetry because the Hamiltonian commutes with symmetry operators[2]. Gaussians with prefactors have previously been used to calculate the

cross section of the deuteron photo disintegration with good results [3]. In this thesis we use shifted correlated Gaussians and investigate whether this is a suitable choice of basis functions or not.

2.4 Coordinates

To describe intrinsic excitations of the system it is important to separate the center of mass motion from the intrinsic motion of the system. This is done by introducing a suitable set of relative coordinates. In the following we refer to the laboratory frame coordinates as $\tilde{\mathbf{r}} = (\mathbf{r}_1, ..., \mathbf{r}_N)$ for a system containing N particles and to the relative coordinate set as $\tilde{\mathbf{x}} = (\mathbf{x}_1, ..., \mathbf{x}_N)$, where $\mathbf{x}_N$ is the center of mass coordinate. The two coordinate sets are related by a linear transformation

$$\tilde{\mathbf{x}} = \mathcal{U}\tilde{\mathbf{r}}. \tag{2.16}$$

The transformation matrix $\mathcal{U}$ depends of the choice of relative coordinate set. We choose the Jacobi coordinate set in which the transformation matrix is given as

$$\mathcal{U} = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 \\ \frac{m_1}{m_1+m_2} & \frac{m_2}{m_1+m_2} & -1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{m_1}{m_1+...+m_N} & \frac{m_2}{m_1+...+m_N} & \cdots & \cdots & \frac{m_N}{m_1+...+m_N} \end{pmatrix}. \tag{2.17}$$

To separate the kinetic energy of the center of mass motion we first express the momentum in the relative coordinate set. The momentum $\mathbf{p}_i$ corresponding to the relative coordinates can be found by applying the inverse transformation of 2.17 to the laboratory momenta $\mathbf{q}_i$.

$$\mathbf{p}_i = \sum_{j=1}^{N} U_{ij}^{-1} \mathbf{q}_j, \tag{2.18}$$

The kinetic energy operator can be written

$$T = \frac{1}{2} \sum_{i,j=1}^{N-1} \mathbf{p}_i \cdot \mathbf{p}_j + T_{c.m.}, \tag{2.19}$$

which without the center of mass kinetic energy $T_{c.m.}$ is

$$= \frac{1}{2} \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} \Lambda_{ij} \boldsymbol{\pi}_i \boldsymbol{\pi}_j, \tag{2.20}$$

where Λ is the $(N-1) \times (N-1)$ matrix with elements

$$\Lambda_{ij} = \sum_{k=1}^{N} U_{ik} U_{jk} \frac{1}{m_k} \quad (i, j = 1, ..., N-1). \tag{2.21}$$

To evaluate potential energy matrix elements the inter particle distance between two particles with coordinates $\mathbf{r_i}$ and $\mathbf{r}_j$ in terms of the relative coordinate set is

$$\mathbf{r}_i - \mathbf{r}_j = \sum_{k=1}^{N-1} \left(\left(U^{-1} \right)_{ik} - \left(U^{-1} \right) \right) \mathbf{x}_k = w^{ij} \mathbf{x} \tag{2.22}$$

2.5 Basis optimization

When one has chosen a suitable set of basis functions one has to optimize the trial wave function with respect to the variational parameters to reach convergence to the true eigen state. Optimization strategies can be divided into two categories: deterministic optimization and stochastic optimization. Deterministic optimization strategies follow a well-defined strategy and given a starting point always reach the same minimum, they have the disadvantage that they however have a tendency to converge towards the first local minimum that they encounter. Stochastic optimization strategies omit this problem by using a random trial and error procedure. The parameters are chosen randomly until the function appears to have converged towards the global minimum. In this thesis stochastic optimization is chosen and in the follow it is explained how it has been implemented in Matlab. Our program starts by generating a K-dimensional set of basis functions that each depend on a set of variational parameters. The program calculates the $K \times K$ Hamiltonian and overlap matrices of the generalized eigenvalue problem equation 2.8 and solves it through Cholesky decomposition. This is done using the Matlab function "eig(H,N,'chol')" which, given

the H and N matrices, solves the generalized eigenvalue problem through Cholesky decomposition and returns eigenvalues and corresponding eigen vectors.

Various optimization strategies are possible from here. It is wished to lower the eigenvalues of the desired state retrieved from the generalized eigenvalue problem as close to the true eigenstate as possible. One can choose to enlarge the size of the basis or refine the parameters of an existing basis or a combination of the two. When enlarging a basis one increases the basis size from K to K+1. The parameter set for the K+1 basis function is proposed stochastically and the new matrix elements of the Hamiltonian and overlap matrices are calculated. The eigenvalues of the K+1 dimensional basis are calculated. If the enlargement of the basis has reduced energy of the desired state(s) the K+1 basis function is kept, if not it is discarded and a new set of parameters is proposed for the K+1 basis function. This process is repeated until a good estimate for the desired state(s) has been reached. An advantage of enlarging the size of the basis is that one cannot worsen the calculation of the other eigenvalues making it a suitable strategy of reaching convergence of multiple excited states at once.

When refining the parameters the basis size is kept fixed. Instead one proposes a new set of randomly parameters for one of the existing basis functions. If the new set of parameters lowers the eigen energy of the desired state the new set of parameters is kept and the old set discarded. If the new set does not lower the energy, a new set is proposed. This process is repeated for all basis functions until the eigen energy has converged close to the desired state(s). In our program a combination of refining the parameters of the basis and enlargement of the basis size has been implemented.

Chapter 3

Deuteron photo-disintegration

3.1 The deuteron system

The deuteron is the simplest of all nucleon bound states consisting of one proton and one neutron. The deuteron has ground state energy -2.224575 MeV and root-mean-square radius $r_d = 1.971$ fm [9]. The ground state consists mostly of a $l = 0$ spin-triplet state $^3S_1$ with a 4 % chance of finding the deuteron in the $^3D_1$ state. This admixture can be explained by the tensor components of the nucleon-nucleon interaction[5]. In this thesis we neglect tensor components of the N-N interaction and assume the ground state is purely an S-state. The deuteron may undergo photodisintegration by absorbing a gamma photon and enter an excited state and immediately decay by emitting a neutron

$$d + \gamma \rightarrow p + n. \tag{3.1}$$

To estimate the cross section of the photo-disintegration reaction we need to evaluate transition matrix elements of the form

$$\mathcal{M}_{if} = \langle \psi_f | \hat{V_{int}} | \psi_i \rangle , \tag{3.2}$$

where $\hat{V}_{int}$ is the interaction operator, ψ_f and ψ_i are the final- and initial state wave function. To estimate the states using the correlated Gaussian method it is needed

to introduce appropriate potentials for the ground and excited state. In the ground state we neglect spin-dependent forces and use the two-body potential from Jensen, Johansen and Hansen [6]

$$V_{gs} = V_k \exp\left(-\frac{r^2}{b^2}\right), \tag{3.3}$$

where the parameters V_k and b are adjusted until a potential which reproduces the ground state energy and root-mean radius of the deuteron is reached. As it is in general hard to describe the wave function of multiple free particles instead of describing the proton and neutron in the final state as free particles it is assumed that the photon excites the deuteron to a p-wave state

$$^3S_1 \rightarrow {}^3P_J, \quad J = 0, 1, 2. \tag{3.4}$$

In this excited state we assume that the deuteron in addition to the nucleon-nucleon interaction experiences the harmonic oscillator potential

$$V_{exc} = \frac{1}{2}kr^2 + V_k \exp\left(-\frac{r^2}{b^2}\right). \tag{3.5}$$

where the parameters b and V_k adjusted to the ground state are kept fixed. The oscillator potential is then expanded until it shows continuum-like behaviour of the energy spectrum and convergence in the cross section. The nucleon interaction is of short range hence we expect our energy spectrum in the excited state to resemble that of the harmonic oscillator. A single particle in an isotropic harmonic oscillator potential has known analytical solution therefore in the following we review some properties of the oscillator potential to get an idea of the expected energy spectrum of the deuteron in the excited state. If we consider the deuteron in a single relative coordinate r with reduced mass μ. The Hamiltonian in the excited state takes the form

$$H = -\frac{\hbar^2}{2\mu}\nabla^2 + \frac{1}{2}kr^2. \tag{3.6}$$

The system is spherical symmetric and by separation of variables the energy levels can be found as[7]

$$E_n = \hbar\omega(n + \frac{3}{2}), \quad n = 1, 2, 3... \tag{3.7}$$

with $n = 2k + l$. As k is a non negative integer for every even n we have $l = 0, 2, .., n-2, n$ and for odd n we have $l = 1, 3, ..., n-2, n$. For every value of l we have (2l+1) values of m_l and thus the degeneracy of the n'th energy level is:

$$\sum_{l=,...n-2,n} (2l+1) = \frac{(n+1)(n+2)}{2} \tag{3.8}$$

where the sum starts from 0 if n is even and from 1 if n is odd. As we use shifted correlated Gaussians as basis functions we expect to accommodate states of all angular momenta and therefore expect a highly degenerate spectrum in the excited state.

3.2 Photo disintegration cross section in the dipole approximation

In this section the photodisintegration reaction is considered in the dipole approximation and the cross section is derived. The description of the electromagnetic field is based on Cappelaro [10]. We derive the cross section starting from Fermi's golden rule[5]

$$w = \frac{2\pi}{\hbar} |\mathcal{M}_{fi}|^2 \nu, \tag{3.9}$$

where w is the reaction rate and ν the density of states in the final state. The reaction rate relates to the cross section σ as

$$w = \frac{\sigma \cdot c}{V}, \tag{3.10}$$

where c is the speed of light and V is the spatial volume occupied by the photon. The cross section is then, using 3.9 and 3.10

$$\sigma = \frac{2\pi}{\hbar c} |\mathcal{M}_{fi}|^2 \cdot \nu \cdot V. \tag{3.11}$$

If the transition matrix elements are known the cross section can be calculated using equation 3.11. We consider the photo disintegration reaction in the dipole approximation where the interaction operator is

$$\hat{\mathbf{V}}_{int} = -\hat{\mathbf{d}} \cdot \hat{\mathbf{E}}(\mathbf{0}), \tag{3.12}$$

where $\hat{\mathbf{E}}$ the electric field and $\hat{\mathbf{d}}$ the dipole moment operator

$$\hat{\mathbf{d}} = q\hat{\mathbf{r}}. \tag{3.13}$$

with $q = e$, the elementary charge. The electromagnetic field is considered in the coulomb gauge where the vector potential satisfies

$$\nabla \cdot \mathbf{A} = 0, \tag{3.14}$$

and describe the field using quantum mechanical operators with $\hat{a}_{\mathbf{k}\lambda}$ being the annihilation operator and $\hat{a}^\dagger_{\mathbf{k}\lambda}$ the creation operator where. The operators follow the commutation relations:

$$[\hat{a}_{\mathbf{k}\lambda}, \hat{a}^\dagger_{\mathbf{k}\lambda}] = \delta_{\mathbf{k}'\mathbf{k}}\delta_{\lambda',\lambda} \tag{3.15}$$

where $\lambda = 1, 2$ denotes the two polarizations of light and $\mathbf{k}$ is the wave vector. The Hamiltonian is

$$\hat{H} = \sum_{\lambda=1,2}\sum_{k} \hbar\omega_{\mathbf{k}} \left(\hat{a}^\dagger_{\mathbf{k}\lambda}\hat{a}_{\mathbf{k}\lambda} + \frac{1}{2}\right), \tag{3.16}$$

hence we describe the electromagnetic field as a collection of independent harmonic oscillators with each mode described by a polarization λ and a wave vector $\mathbf{k}$. The creation operator excites the field from the vacuum state $|0\rangle$

$$\hat{a}^\dagger_{\mathbf{k}\alpha}|0\rangle = |1_{\mathbf{k}\lambda}\rangle \tag{3.17}$$

to a state corresponding to a single photon. Correspondingly the annihilation operator deexcites the field from a single photon state to the vacuum state

$$\hat{a}_{\mathbf{k}\alpha}|1_{\mathbf{k}\lambda}\rangle = |0\rangle. \tag{3.18}$$

Using the annihilation and creation operators the vector potential can be written

$$\mathbf{A}(\mathbf{r}) = \sum_{\lambda=1,2}\sum_{k} \sqrt{\frac{2\pi\hbar}{V\omega_{\mathbf{k}}}}\mathbf{e}_{\mathbf{k}\lambda}\left(\hat{a}_{\mathbf{k}\lambda}e^{-i\mathbf{kr}} + \hat{a}^\dagger_{\mathbf{k}\lambda}e^{i\mathbf{kr}}\right), \tag{3.19}$$

with $e_{\mathbf{k}\lambda}$ a unit vector orthogonal on $\mathbf{k}$. The electric field is

$$\mathbf{E}(\mathbf{r}) = \sum_{\lambda=1,2}\sum_{k} \sqrt{\frac{2\pi\hbar\omega_{\mathbf{k}}}{V}}\mathbf{e}_{\mathbf{k}\lambda}\left(\hat{a}_{\mathbf{k}\lambda}e^{-i\mathbf{kr}} - \hat{a}^\dagger_{\mathbf{k}\lambda}e^{i\mathbf{kr}}\right). \tag{3.20}$$

which in the dipole approximating yields $\hat{\mathbf{E}}(\mathbf{0})$ as $e^{i\mathbf{kr}} \approx 1$ for $\mathbf{kr} \ll 1$

$$\hat{\mathbf{E}}(\mathbf{0}) = i \sum_{\lambda=1,2} \sum_{k} \sqrt{\frac{2\pi\hbar\omega_k}{V}} \mathbf{e}_{\mathbf{k}\lambda} \left(\hat{a}_{\mathbf{k}\lambda} - \hat{a}^{\dagger}_{\mathbf{k}\lambda} \right). \tag{3.21}$$

We now calculate the transition matrix elements of equation 3.11. During the photo disintegration reaction a single photon is absorbed, we write the initial state as $|\Psi_i\rangle = |\psi_i\rangle |1_{\mathbf{k}\lambda}\rangle$ and the final state $|\Psi_f\rangle = |\psi_f\rangle |0\rangle$. The matrix element is

$$\mathcal{M}_{fi} = \langle 0| \langle \psi_f| - \hat{\mathbf{d}} \cdot \hat{\mathbf{E}}(\mathbf{0}) |\psi_i\rangle |1_{\mathbf{k}\lambda}\rangle = -ie\sqrt{\frac{2\pi\hbar\omega_k}{V}} \mathbf{e}_{\mathbf{k}\lambda} \mathbf{d}_{fi}, \tag{3.22}$$

as the the modes of the electromagnetic field are orthogonal this is the only lasting term. Here $\mathbf{d}_{fi}$ short for

$$\mathbf{d}_{fi} = \langle \psi_f| \frac{\mathbf{r}}{2} |\psi_i\rangle . \tag{3.23}$$

Inserting into 3.11 yields

$$\sigma = \frac{4\pi^2 e^2 \omega_k \hbar}{\hbar c} |\mathbf{e}_{\mathbf{k}\lambda} \cdot \mathbf{d}_{fi}|^2 \nu, \tag{3.24}$$

where $\alpha = \frac{e^2}{\hbar c}$ is the fine structure constant in our system of units (see section 3.4). If we assume that all directions of $\mathbf{d}_{fi}$ and $\mathbf{e}_{\mathbf{k}\lambda}$ are equally probable the average is [13]

$$\left\langle |\mathbf{e}_{\mathbf{k}\lambda} \cdot \mathbf{d}_{fi}|^2 \right\rangle = \frac{1}{3} |\mathbf{d}_{fi}|^2. \tag{3.25}$$

Inserting into equation 3.24 yields the total cross section

$$\sigma = \frac{4}{3} \pi^2 \hbar \omega_{\mathbf{k}} \alpha |\mathbf{d}_{fi}|^2 \nu. \tag{3.26}$$

where the energy of the absorbed photon is $E_\gamma = \hbar\omega_{\mathbf{k}}$. To calculate the cross section of the photo disintegration of the deuteron we need to find the transition dipole matrix element $|\mathbf{d}_{fi}|$ and the density of states function ν. We find the dipole matrix elements using the initial and final state wave functions from the correlated Gaussian method. The density of states function is calculated by the retrieved spectrum of eigen energies. How this is done is described in the following section.

3.3 The density of states function

In the previous section we derived the total cross section for the photo disintegration of deuteron in the dipole approximation. The total cross section depends on the density of states function which we calculate from the spectrum of eigen energies in the final state. The density of states is defined as the number of available states to be occupied per energy interval. We consider an available state, as a state which gives non-zero transition matrix element from equation 3.23. According to the selection rules for electromagnetic transitions the only allowed transitions are those between states with $\Delta l = \pm 1$ where l is the orbital angular momentum [13]. That is, only p-wave states should give transition matrix elements to the ground state. We consider the spectrum of available states with energy levels

$$\epsilon_n, \quad n = 1, 2, 3... \tag{3.27}$$

Each state of energy ϵ_n corresponds to the absorption of a photon with energy $E_\gamma = \epsilon_n - E_{gs}$ where E_{gs} is the ground state energy. If the energy level of an available state is ϵ_n we calculate the density of states as

$$\nu(\epsilon_n) = \frac{2}{\epsilon_{n+1} - \epsilon_{n-1}}, \tag{3.28}$$

which is the reciprocal of the energy interval around ϵ_n. Every energy level is expected to be a p-state and hence threefold degenerate. If we denote the energy levels ϵ_{nj} with $j = 1, 2, 3$ for the threefold degeneracy and n for the energy level. The three states should be of equal energy however due to numerical imprecision this might not be completely true. The energy level at n is calculated as the mean of the energy of the three degenerate states

$$\epsilon_n = \sum_{j=1}^{3} \frac{\epsilon_{nj}}{3}, \tag{3.29}$$

Finally we calculate the total cross section by summing over the contribution from each of the three states at energy level n.

$$\sigma(\epsilon_n) = \sum_{j=1}^{3} \sigma(\epsilon_{nj}) \tag{3.30}$$

3.4 Unit system and parameter optimization

Unit system

To simplify our numerical calculations it is advantageous to introduce a suitable set of units. In the deuteron system convenient scales of length and energy are MeV and fm which we set to unity along with the reduced Planck constant. Thus in nuclear units (n.u.) we have

$$1 \text{ MeV} = 1 \text{ fm} = \hbar = 1 \text{ n.u.} \tag{3.31}$$

As a consequence of the fore mentioned unit system the mass of the proton and neutron in our unit system is $m_p = 0.02411$ n.u. and the fine structure constant $\alpha = \frac{e^2}{\hbar c}$.

Parameter optimization

As described in section 2.5 we use stochastic optimization with respect to the variational parameters of the trial wave function. The parameters are chosen stochastically however from an exponential distribution to speed up the optimization process. As we are dealing with a two-body problem in reduced coordinates each basis function depends on a three component shift vector $\mathbf{s}$ and a $(N-1) \times (N-1)$ matrix which is just a single parameter. As mentioned in section 2.8 the overlap matrix $\mathcal{N}$ has to be positive definite in order to solve the generalized eigenvalue problem through Cholesky decomposition. As $\mathcal{N}$ is an overlap matrix this is condition is satisfied however only if each component of the trial wave function are not too alike. To assure positive definiteness we put restrictions on each set of proposed parameters so that for all components of the wave function

$$\frac{\langle \psi_i | \psi_j \rangle}{\sqrt{\langle \psi_i | \psi_i \rangle \langle \psi_j | \psi_j \rangle}} < \text{T}, \quad i \neq j, \tag{3.32}$$

where T is some threshold $0 < \text{T} < 1$. The magnitude of T depends on the amount of variational parameters and the size of the basis.

Chapter 4

Results

In this section we present the results produced using the correlated Gaussian method. First the results of the deuteron ground state is presented and then the energy spectrum in the excited state. Finally we expand our oscillator potential to reach convergence of the photo-disintegration cross section. The expectation values of a superposition state with operator $\hat{O}$ have been calculated calculated as

$$\left\langle \hat{O} \right\rangle = \mathbf{c}_k^T \mathcal{O} \mathbf{c}_k, \tag{4.1}$$

where $\mathcal{O}$ is a matrix with elements $\mathcal{O}_{ki} = \langle k | \hat{O} | i \rangle$ and $\mathbf{c}_k$ is the eigenvector belonging to the k'th eigenstate. Here the wave functions are normalized so that $\mathbf{c}_k^T \mathcal{N} \mathbf{c}_k = 1$ for all k with $\mathcal{N}$ being the overlap matrix. All matrix elements used in the calculations can be found in the Appendix.

4.1 The deuteron ground state

In section 3.1 it was assumed that the nucleon-nucleon potential could be approximated as

$$V = V_k \exp\left(-\frac{r^2}{b^2}\right). \tag{4.2}$$

Table 4.1: Estimate the ground state energy and root mean square radius of the deuteron from the correlated Gaussian method.

	Exp. value	Result
E_{gs} [MeV]	-2.224575	-2.224571
r_d [fm]	1.971	1.970
L^2	0	0.000

The parameters b and V_k were adjusted until the experimental data of the deuteron ground state was reproduced. The parameters

$$V_k = 61.4925 \text{ MeV}, \; b = 1.635 \text{ fm}, \tag{4.3}$$

were found to reproduce the ground state of the deuteron. A trial wave function of 50 components was used while allowing the shift vectors to point in all directions. The ground state energy $\mathrm{E_{gs}}$, root-mean-square radius r_d and orbital angular momentum produced using this potential can be seen in table 4.1. For all further calculations we use this wave function of this section as our ground state.

4.2 Excited state and cross section

As we expect a highly degenerate spectrum in the excited state to reduce computations we restrict our calculations to include only states with the projection quantum number $m_l = 0$. To account for the threefold degeneracy of the p-states the retrieved cross section is then multiplied by three. To accommodate only $m_l = 0$ states in our spectrum we restrict our shift vectors to only have non-zero components in the z-direction. The matrix element of the L_z operator is [1]

$$\langle g| \, L_z \, |g'\rangle = -i \sum_{ij} \left(B^{-1}\right)_{ij} \left(\mathbf{s} \times \mathbf{s}'\right)_z M. \tag{4.4}$$

If all shift vectors have only z-components the cross product is zero and all matrix elements of the L_z-operator are equal to zero, hence we expect to accommodate only

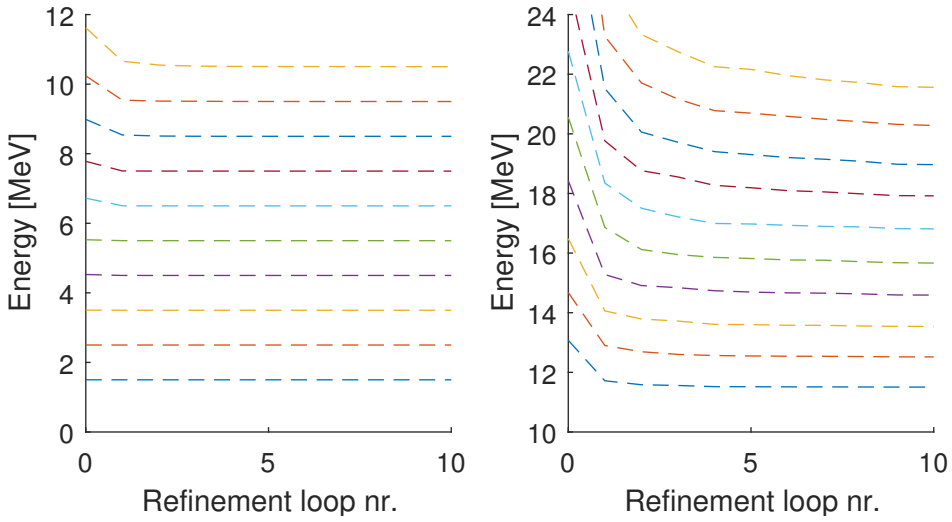

Figure 4.1: Estimate of the first 20 energy levels in the harmonic oscillator potential with $\hbar\omega = 1$ MeV using a basis size of 300 Gaussians. The figure shows the mean value of the degenerate states with quantum number $m_l = 0$ at each energy level.

states with $m_l = 0$. To do initial tests on our method we see if we can produce the expected energy spectrum of the harmonic oscillator potential. For the oscillator potential we set $\hbar\omega = 1$ MeV and use a trial wave function of 300 components. The overlap threshold is set at T = 0.975 and we optimize the basis through refinement. The convergence of the first 20 energy levels can be seen in figure 4.1 and the numerical results in table 4.2. It is seen that we are able to produce the expected spectrum of eigen energies in the oscillator potential. The energies converge close to the true value at the first 15 energy levels, at highly excited states we note that there is some deviation from the expected values. It is also noted that by restricting our shift vectors to have only z-components the degeneracy has been reduced as expected.

Now the potential is altered by including our estimate of nucleon-nucleon potential from the ground state in addition to the oscillator potential. As an initial estimate the basis size is kept at $K = 300$ and the overlap threshold set to $T = 0.975$. We start with $\hbar\omega = 1$ MeV and lower $\hbar\omega$ until convergence in the cross section is achieved. The retrieved cross sections can be seen in figure 4.2. In spite of altering

Table 4.2: Estimates of the first 20 energy levels of the harmonic oscillator potential with $\hbar\omega = 1$ MeV. The table shows the mean value of the degenerate states with quantum number $m_l = 0$ at each energy level.

Exact [MeV]	Result [MeV]	Exact [MeV]	Result [MeV]
1.5	1.500	11.5	11.50
2.5	2.500	12.5	12.52
3.5	3.500	13.5	13.54
4.5	4.500	14.5	14.59
5.5	5.500	15.5	15.67
6.5	6.500	16.5	16.8
7.5	7.500	17.5	17.92
8.5	8.500	18.5	18.97
9.5	9.500	19.5	20.28
10.5	10.50	20.5	21.56

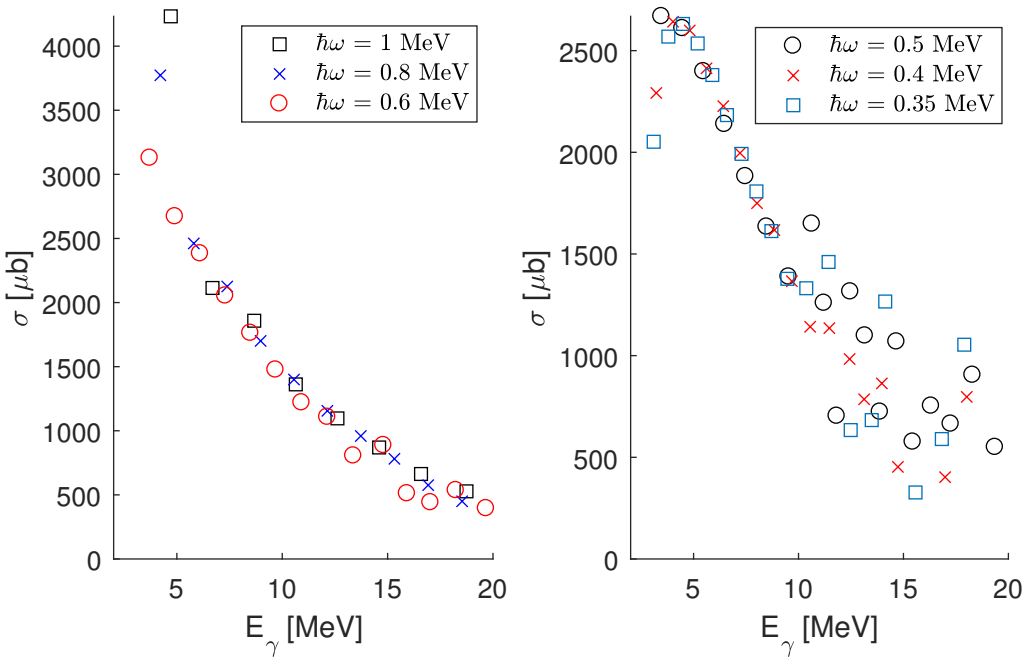

Figure 4.2: Convergence of the deuteron photo disintegration cross section by lowering $\hbar\omega$ of the oscillator potential in a basis of 300 Gaussians.

the potential the retrieved spectrum resembles that of the harmonic oscillator, the energy levels are approximately spaced $\hbar\omega$ and the degeneracy at each energy level is equal to the possible values of l. For the first 16 energy levels non-zero transition matrix elements are spaced $2\hbar\omega$ and all other states give 0 transition matrix elements to the ground state in agreement with the selection rules of electromagnetic transitions. However at highly excited states we see non-zero transition matrix elements at multiple degenerate energy levels. As we wish to use all states that give non-zero transition matrix elements in our calculation, for degenerate states with non-zero transition matrix elements we add the contribution from the states in order to avoid division with zero when calculating the density of states and use the mean of the energy levels. In the region $E_\gamma < 10$ MeV the cross section seems to have converged at $\hbar\omega = 0.35$MeV. At highly excited states it could seem the problem with reaching convergence of the energy levels in the oscillator potential is redundant in our altered potential and thus in our calculation of the cross section.

In order to try to improve convergence in the higher energy region we increase our basis size to from $K = 300$ to $= 650$ Gaussians demanding each basis function to lower the energy of one or more of the highly excited states. The result can be seen in figure 4.3 along with experimental data from Arenhövel, H. and Sanzone, M [12]. It is seen that expanding the size of our trial wave function has improved our estimate noticeably however convergence of the highly excited states is still not fully achieved. One could try to expand the wave function even further however significant improvements were not found above $K = 600$. Lower values of $\hbar\omega$ and close to $\hbar\omega = 0.35$ MeV were also tried but did not improve the results. The current estimate is slightly too high around 5 MeV and too low above 16 MeV. The present model does take into account the d-state admixture of the deuteron ground state or spin dependent forces. In the following section we try to implement the latter.

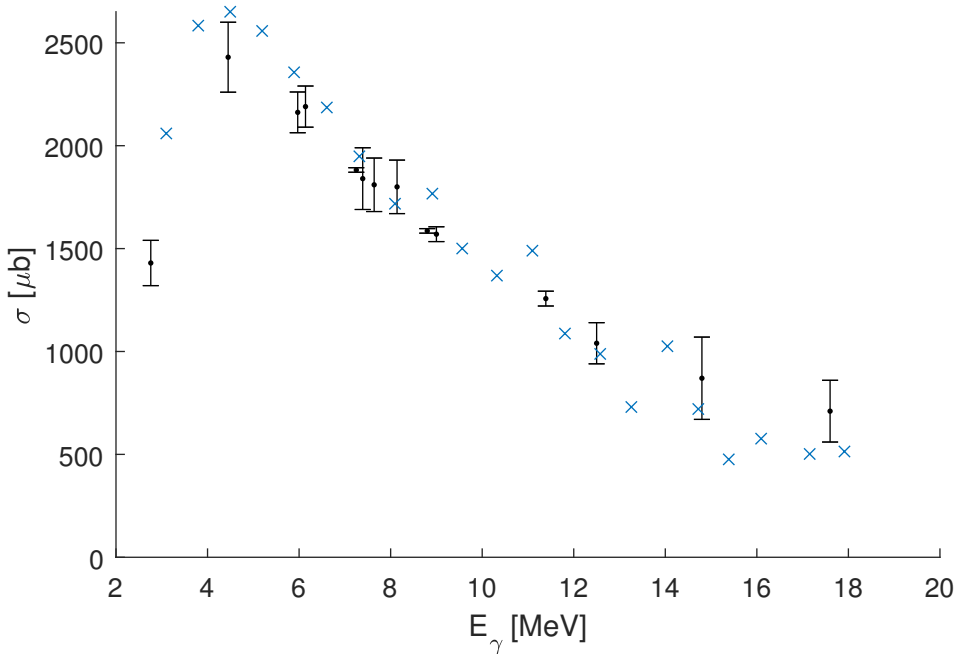

Figure 4.3: Total cross section of the deuteron photo disintegration in a basis size of 650 Gaussians. The estimate is plot along with experimental data from [12].

4.3 Inclusion of spin

In this section we seek to include spin dependent forces on the nucleon-nucleon potential in the excited state. The deuteron ground state is a spin triplet the possible spin configurations are

$$|\uparrow\uparrow\rangle\,, \quad |\downarrow\downarrow\rangle\,, \quad \frac{1}{\sqrt{2}}\left(\uparrow\downarrow + \downarrow\uparrow\right), \tag{4.5}$$

which in the dipole approximation does not change in the transition to the excited state. To include the spin dependent forces in the p-wave stat we now consider the two-body potential from Garrido, Fedorov and Jensen[8] which has been used to describe a triplet p-wave nucleon-nucleon potential

$$V_{nn} = \left(V_c + V_{ss}\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 + V_{so}\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}\right) \exp\left\{-\frac{r^2}{b_{nn}^2}\right\}, \tag{4.6}$$

where $\hat{\mathbf{s}}_1$ and $\hat{\mathbf{s}}_2$ are the spins of each nucleon, $\hat{\mathbf{S}}$ is the total spin operator and $\hat{\mathbf{L}}$ is the relative orbital momentum operator. V_c, V_{ss} and V_{so} are strength parameters. The

parameters of the potential are

$$V_c = 2.92 \text{ MeV},\ V_{ss} = 45.22 \text{ MeV},\ V_{so} = -12.08 \text{ MeV},\ b_{nn} = 1.8 \text{ fm}. \tag{4.7}$$

The expectation values of the spin operators $\langle\chi_b| \hat{\mathbf{S}} |\chi_a\rangle$ and $\langle\chi_b| \hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 |\chi_a\rangle$ have been calculated using the Pauli spin matrices[13]. To include the new spin dependent potential we average over the three spin triplet states. In addition we also allow our shift vectors to take all directions. When allowing our shift vectors to take any direction the degeneracy of each energy level is that of equation 3.8 with spacing approximately equal to $\hbar\omega$. The eigenvalues ϵ_n are ordered such that $\epsilon_1 \leq$ and $\epsilon_2, ..., \leq \epsilon_n$ and for a K-dimensional basis we get at most K-eigenvalues. It is apparent that with $\hbar\omega = 0.35$ MeV one would need a very large basis size to receive eigenvalues in the range up to 20 MeV. Using a basis size of $K = 700$ we were able to estimate the cross section in the range 2 MeV $\leq E_\gamma \leq$ 8 MeV. The result can be seen in figure 4.4. One could try to implement spin dependent forces for only $m_l = 0$ states but the spin-orbit term would vanish as the matrix element involves the cross-product between the shift vectors see 5.8 in the Appendix and has therefore not been attempted.

It seems that our inclusion of spin in the final state potential has slightly increased our estimates agreement with the experimental data, however as we were not able to calculate the cross section above 8 MeV this is not conclusive in the full range. The Garrido, Fedorov, Jensen contains a tensor term as well which was neglected in our calculations. Further work improvements to our current estimate in the range up to 8MeV would be to include tensor components in the excited state potential as well taking into account the d-state admixture.

In this project is was chosen to use shifted Gaussians as basis functions, this choice as basis functions have been found to produce good results when the degeneracy of the desired states is not too high. For highly excited states it was found hard to reach convergence of the energy levels and the cross section. For a spectrum with continuum-like behaviour using basis functions with predefined angular momentum might be more suitable as one accommodates only the states of interest and wont

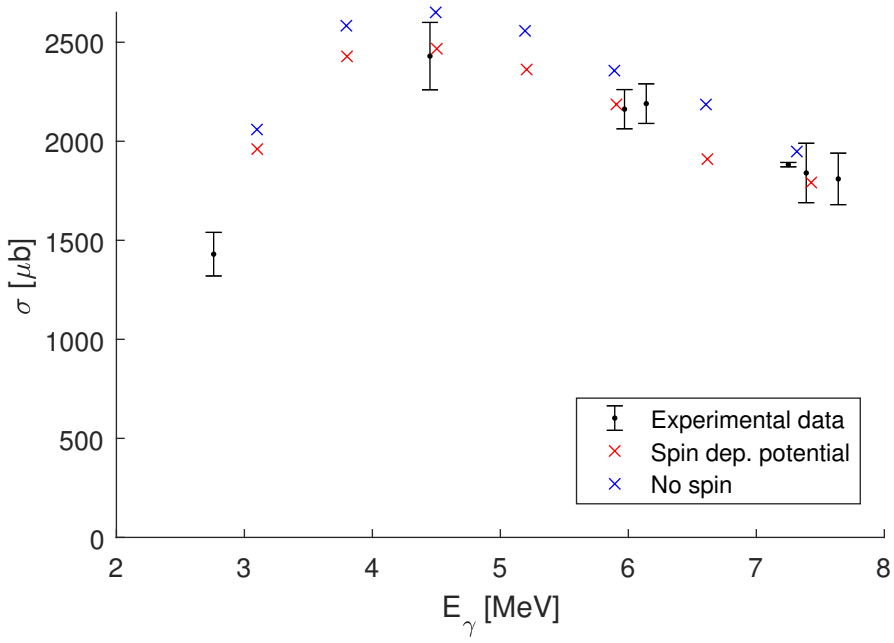

Figure 4.4: Estimate of the deuteron photo disintegration cross section with and without a spin dependent interaction in the excited state. Blue data points are the same as in figure 4.3.

have to worry about convergence of all the other states. In general it is hard to reproduce highly excited states with a Gaussian basis set [2]. The problem has been alleviated in [14] by Hiyama, Kino and Kaminura by using variational parameters with a complex phase $A = a + ib$ where numerical tests have shown to give orders of magnitude better estimate of highly excited states in the harmonic oscillator. Such types of basis functions could be subject to further work.

In [3] the cross section was calculated using prefactored Gaussians as basis functions and convergence was reached at a much lower $\hbar\omega \approx 0.03$ MeV. Using $\hbar\omega$ of this magnitude gives more data points and convergence was achieved better for the highly excited states. Using such low $\hbar\omega$ was not found possible in our use of shifted correlated Gaussians as the degeneracy is highly increasing at each energy level and the difficulty of reaching convergence as well. Compared to our use of shifted Gaussians they do not seem advantageous over prefactored Gaussians for a reaction of this type involving states with continuum like behaviour.

4.4 Deuteron photo-disintegration cross section in the zero range approximation

In this section we compare the results of our Gaussian model with the cross section calculated in the zero-range approximation. The following theory is based on[12]. In the zero-range approximation it is assumed that the nucleon-nucleon interaction can be described using a delta function potential

$$V(r) = -V_0\delta(r). \tag{4.8}$$

This force acts only in the S-state and has the bound state solution

$$\psi_i = \frac{1}{\sqrt{4\pi}}\frac{u_0(r)}{r}. \tag{4.9}$$

For the final state wave function of the transition matrix element we use a plane wave

$$\psi_f = Ae^{-i\mathbf{pr}}, \tag{4.10}$$

where A is a normalization constant and $\mathbf{p}$ is the final state relative momentum between the proton and the neutron. The differential cross section in the dipole approximation is

$$\frac{d\sigma}{d\Omega} = 2\pi^2 e^2 \omega k M \left|\mathbf{d}_{fi} \cdot \epsilon^2\right|, \tag{4.11}$$

where M is the average nucleon mass and ϵ is the photon polarization vector. Averaging over the photon polarizations and using the bound state solution of the delta function potential for the initial state wave function and the plane wave for the final state yields the total cross section

$$\sigma(\gamma) = \frac{8\pi}{3}\frac{e^2}{\alpha^2}\frac{(\gamma-1)^{3/2}}{\gamma^3}, \tag{4.12}$$

where $\gamma = \frac{\hbar\omega}{\epsilon}$ with $\hbar\omega$ being the energy of the photon and ϵ the ground state energy of the deuteron. The constant α is related to the deuteron binding energy by

$$\alpha = \sqrt{M\epsilon}, \tag{4.13}$$

In figure 4.5 we plot the cross section in the photon energy range 2 MeV $< E_\gamma <$ 20 MeV. It is seen that the retrieved cross section agrees well in shape however compared to experimental data it is approximately larger by a factor of 1.7. The underestimation is related to the finite size of the zero-range nucleon-nucleon interaction. Comparing with the cross section of our Gaussian model it is seen that our estimate agrees better in terms of magnitude however our model has difficulties reaching the correct shape at higher energies.

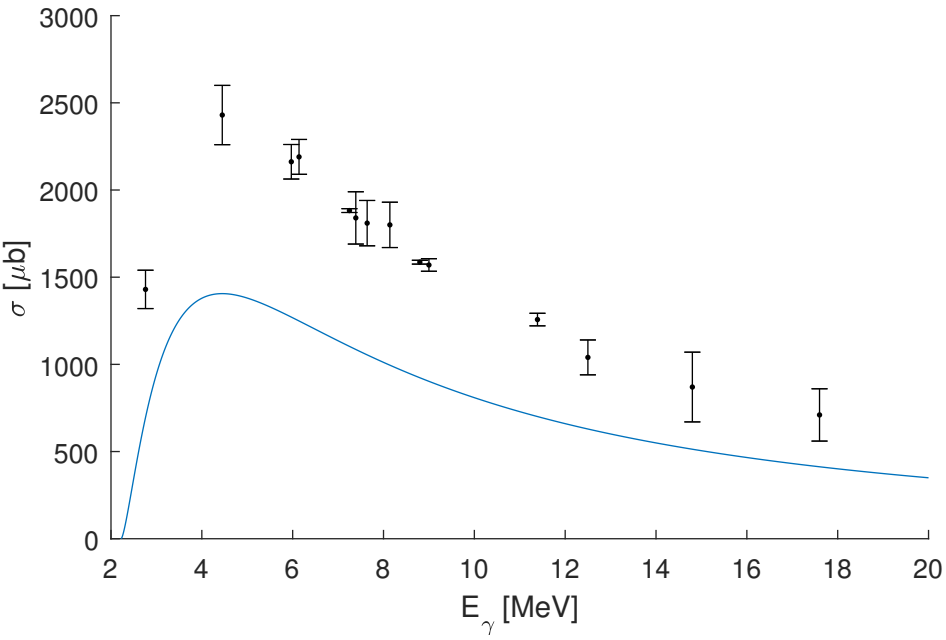

Figure 4.5: The estimated cross section in the zero range approximation blue curve plot along with experimental data from [9].

Chapter 5

Conclusion

In this thesis we employed the correlated Gaussian method to estimate the photo disintegration cross section of the deuteron. Using shifted correlated Gaussians as basis functions we were able to estimate the cross section in the dipole approximation with small deviation from experimental data when using ony $m_l = 0$ states. An implementation of spin did seem to improve our estimate of the total cross section however as we were only able to estimate states in up to 8 MeV this is not conclusive in the full range. Our choice of basis functions produced good results in the low energy range but had the drawback of accommodating states of all angular momenta which increases the computational load and the difficulty of reaching convergence in the highly excited states. Basis functions with a predefined angular momentum may be more suitable for reactions with continuum states as it leaves less states to worry about. Throughout our calculations the d-state admixture of the ground state as well as tensor components of the p-wave nucleon interaction were neglected which could both form the basis for further work. Finally our estimate was compared to the cross section calculated in the zero-range approximation, it was found that our estimate agrees better with experiment in terms of magnitude.

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Appendix

In this appendix we list the matrix elements used in the numerical computations. The matrix elements have all been taken from Fedorov [11] except from the total angular momentum operator $\mathbf{L}^2$ which is from Suzuki and Varga [1]. The matrix elements are presented in general form for a system of N-particles with coordinates $\mathbf{r} = (\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_n)$. All matrix elements have been implemented in the relative coordinates as described in section 2.4 which for a two-body system reduces to that of a single relative coordinate. In the following the basis function is denoted as

$$|g\rangle = e^{-\mathbf{r}^T A \mathbf{r} + s^T \mathbf{r}} \tag{5.1}$$

where A is a size-N square matrix. The overlap matrix element for two basis functions $|g\rangle$ and $|g'\rangle$ is given as

$$\langle g'|g\rangle = e^{\frac{1}{4}\mathbf{v}^T B^{-1}\mathbf{v}} \left(\frac{\pi^N}{\det(B)}\right)^{3/2} \equiv M. \tag{5.2}$$

where $B = A + A'$, $\mathbf{v} = \mathbf{s} + \mathbf{s}'$ and $\mathbf{u} = \frac{1}{2}B^{-1}\mathbf{v}$. The kinetic energy matrix element is

$$\langle g'| -\frac{1}{2}\frac{\partial}{\partial \mathbf{r}}\Lambda\frac{\partial}{\partial \mathbf{r}^T}|g\rangle = \frac{1}{2}\left(6\,\mathrm{tr}\left(A'\Lambda A B^{-1}\right) + (\mathbf{s}' - 2A'\mathbf{u})^T \Lambda(\mathbf{s} - 2A\mathbf{u}\right) M \tag{5.3}$$

where Λ is the matrix of 2.21. For the deuteron ground state a potential with a Gaussian form factor was chosen $V\left(\mathbf{w}^T\mathbf{r}\right) \propto e^{\gamma \mathbf{r}^T \mathbf{w}\mathbf{w}^T \mathbf{r}}$. The matrix element is

$$\langle g'|\, e^{\gamma \mathbf{r}^T \mathbf{w}\mathbf{w}^T \mathbf{r}}\, |g\rangle = e^{\frac{1}{4}\mathbf{v}^T B'^{-1}\mathbf{v}} \left(\frac{\pi^N}{\det(B')}\right)^{3/2} \tag{5.4}$$

where $\mathbf{w}$ is a size-N coloumn with all entrances equal to zero except $w_i = -w_j = 1$ for a two-body potential. B' is the matrix $B' = B + \gamma \mathbf{w}\mathbf{w}^T$. The oscillator potential

was used for the deuteron in the excited state, it has the matrix element

$$\langle g'|\,\mathbf{r}^T w w^T \mathbf{r}\,|g\rangle = \left(\frac{3}{2} w^T B^{-1} w + \mathbf{u}^T w w^T \mathbf{u}\right) M \tag{5.5}$$

which was also used to calculate the root-mean-square radius of the deuteron. The total angular momentum $\mathbf{L}^2$ matrix element is

$$\langle g'|\,\mathbf{L}^2\,|g\rangle = \left(2\mathbf{s}'^T (2B)^{-1}\,\mathbf{s} - \left((2B)^{-1}\,\mathbf{s}' \times \mathbf{s}\right)\right)^2 M \tag{5.6}$$

To calculate the transition dipole moment we need the matrix element

$$\langle g'|\,\mathbf{r}\,|g\rangle = \mathbf{u}M. \tag{5.7}$$

In the excited state the Garrido, Fedorov and Jensen potential included a spin-orbit term. The orbital angular momentum operator can be written $\mathbf{L} = \frac{-i}{2}\left(w^T\mathbf{r} \times w^T \frac{\partial}{\partial \mathbf{r}^T}\right)$. The spin-orbit matrix element with a Gaussian form factor is

$$\frac{-i}{2}\,\langle\chi'|\,\langle g'|\,e^{-\gamma \mathbf{r}^T w w^T \mathbf{r}} \left(w^T\mathbf{r} \times w^T \frac{\partial}{\partial \mathbf{r}^T}\right) \cdot \hat{\mathbf{S}}\,|g\rangle\,|\chi\rangle =$$

$$\frac{-i}{4} w^T B'^{-1}\mathbf{v} \times \left(w^T\mathbf{s} - w^T A B'^{-1}\mathbf{v}\right) M\,\langle\chi'|\,\hat{\mathbf{S}}\,|\chi\rangle \tag{5.8}$$

where $\hat{\mathbf{S}}$ is the total spin operator and $|\chi\rangle$ is the spin wave function.