

FEW-NUCLEON REACTIONS IN THREE DIMENSIONAL FORMALISM*

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In this contribution, we present few-nucleon calculations performed in a three-dimensional framework. References are given to our treatment of two- and three-nucleon bound states as well as for the transition operator in the positive energy range. New results for the transition operator in the negative energy range are shown. Different features of the standard partial wave and three dimensional calculations are presented.

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1. Introduction

The fundamental equations that govern two- and three-particle bound and scattering state calculations were formulated a long time ago [1]. Their application to the two- and three-nucleon systems typically employs the partial wave approach. The advent of powerful computing resources made it possible to construct calculations using three-dimensional (3D) degrees of freedom. Considering 3D momentum vectors together with spin and isospin states is quite natural and incorporates all partial wave states. This gives hope for more precise calculations with a wider spectrum of applications. Our results obtained using this new method are in good agreement with classical partial wave calculations.

In this paper, we give a brief description of the tools that were developed in our group to handle the degrees of freedom of the two- and three-nucleon systems. Section 2 introduces the problems that had to be overcome in order to construct efficient numerical realizations. Section 3 introduces our methods of approaching the calculations. The final section contains a discussion of the results.

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2. Complexity

All our calculations are constructed using non-relativistic quantum mechanics. Our final expressions can be, in a few steps, traced back to the Schrödinger equation, which describes the evolution of the system state $|\psi(t)\rangle$ with the Hamilton operator $\hat{H}$

$$i\hbar\partial_t |\psi(t)\rangle = \hat{H} |\psi(t)\rangle. \quad (1)$$

For scattering, our expressions can always be traced to the Lippmann–Schwinger equation for the transition operator t

$$\check{t}(E) = \check{V} + \check{V}\check{G}_0(E + i\epsilon)\check{t}(E) \quad (2)$$

with $\check{V}$ being the potential operator, $\check{G}_0$ being the free propagator, and E being the energy.

An application of these simple equations to systems with two- and three-nucleons leads to complicated analytical expressions. This is largely an effect of the necessity to introduce additional constraints on the two and three nucleon bound state, the potential and the transition operator [2–4]. These constraints significantly limit the required computational resources and are necessary if a practical numerical realization of the calculations is to be constructed. The complexity arises from the spin and isospin structure of the bound state and from the operator representation of the nuclear forces present in the Hamiltonian. With the suitable choice of basis operators, it is possible to arrive at a finite set of equations for scalar functions of the momentum vectors only and thus to eliminate spin degrees of freedom. The scalar functions play a role of expansion coefficients and contain the full information about the few-nucleon state or about the transition operator [2–4]. The scalar nature of the unknown functions is very important for a construction of numerical solutions.

3. Tools

The complexity and the size of the numerical problems we faced led us to a development of tools that make the process of generating the analytical expressions and their FORTRAN implementation automatic. Numerical realizations require many thousands of lines of a FORTRAN code. Our tools written in the **Mathematica**[®] symbolic programming language are very efficient and reduce the probability of human error.

After introducing conditions from [2–4], equations (1) and (2) take the form of large linear (eigen) equations. The implementation of linear operators involved in the calculations can be constructed from the automatically generated codes. The dimension of the problem is typically very large

($N \approx 10^6$). This is especially true for three-nucleon systems. In order to reduce the dimension of the matrices, Krylov subspace methods are eventually used. However, essential iterations require supercomputer resources. We use the Jülich supercomputer JUQUEEN from the Jülich Supercomputing Centre (JSC) in Germany. The reduced problem (expressed in terms of, for example, 40 by 40 matrices and 40 dimensional vectors) can be solved using standard numerical methods.

4. Results

All calculations utilize a very general form of the two- and three-nucleon potentials. Our framework can be used to test various nuclear force models available in the literature. Our results for the deuteron, transition operator and three-nucleon bound state have been verified and published [2–4]. Like in the partial wave representation, the 3D treatment of the two-nucleon transition operator must account for the pole, which appears at the negative two-nucleon energy corresponding to the deuteron binding energy. The residue is constructed from the deuteron wave function given in the operator form. The essentially analytical expression is easily obtained using our *Mathematica*® routines. The residue result must match the transition operator values, calculated for other negative energies. This is the case, as

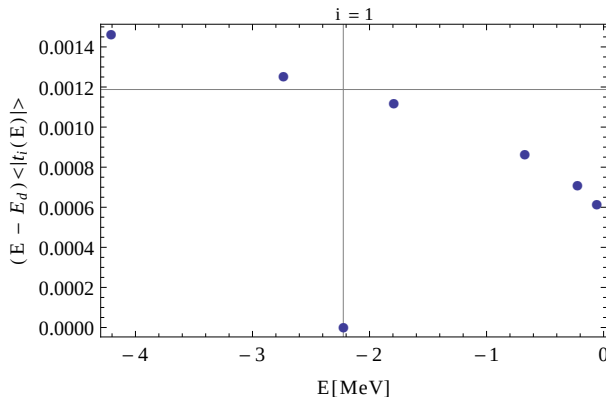


Fig. 1. One ($i = 1$) of the six scalar functions, $t_i(p', p, x'; E)$ in the expansion of the transition operator, for the two-nucleon isospin $t = 0$, as a function of the two-nucleon internal energy E in the vicinity of the deuteron binding energy, $E_d \approx -2.2$ MeV. In this example, $p' = 0.26 \text{ fm}^{-1}$, $p = 0.11 \text{ fm}^{-1}$, $x' = -0.41$. The crossing of the horizontal and vertical lines denotes the residue position (calculated from the deuteron wave function) and matches nicely the dots obtained from the Lippmann-Schwinger equation. A chiral NNLO potential from Epelbaum *et al.* has been used.

shown in Figs. 1 and 2. Our tools can also be applied to processes involving electroweak probes, for example, in the description of deuteron electrodisintegration [5].

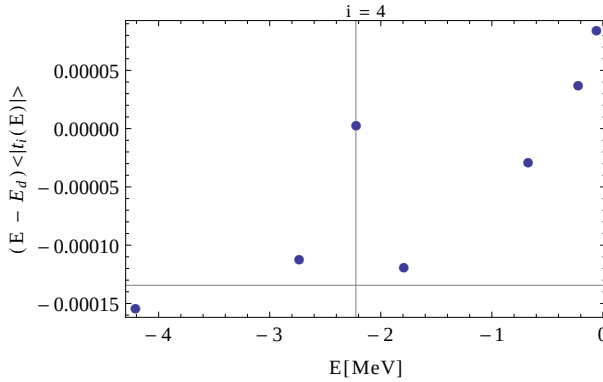


Fig. 2. The same as in Fig. 1, but for the fourth coefficient ($i = 4$).

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