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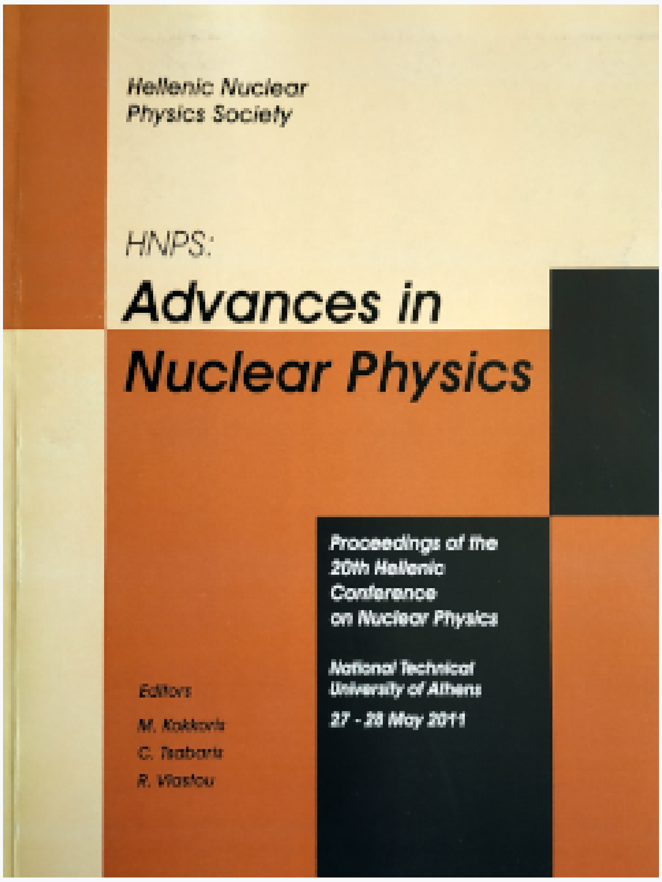

Evaluation of differential cross-sections for light element reactions at low energies using R-matrix calculations: The case of 12C

M. Kokkoris

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Evaluation of differential cross-sections for light element reactions at low energies using R-matrix calculations: The case of ^{12}C

Michael Kokkoris

Department of Physics, National Technical University of Athens, Zografou Campus 157 80, Athens, Greece

Abstract

The theoretical evaluation of differential cross-section values for low-energy reactions of light elements is of great importance in the fields of IBA (Ion Beam Analysis) and nuclear astrophysics. R-matrix theory is generally accepted as the most appropriate one for the analysis of resonance reactions in low-energy nuclear physics. In this approach, the configuration space of the scattering problem is divided into an internal region, corresponding to the compound nucleus, where the total wave function can be expanded into a complete set of eigenstates (in terms of unknown base functions, with the energy eigenvalues and the matrix elements of the base functions being adjustable parameters) and an external region, where the possible combinations of coupled particle pairs exist, corresponding to the reaction channels that emerge from the compound nucleus. This division of space is made by the choice of the boundary of the compound nucleus, i.e. an appropriate nuclear radius is chosen for each reaction channel. The R-matrix takes account of all the interactions which occur inside the nucleus. In the present work, results obtained in the specific case of elastic scattering and charged-particle nuclear reactions, namely for the ^{12}C+p system are presented.

Key words: R-matrix theory, IBA, EBS, NRA.

1 Introduction

When an ion having a kinetic energy of the order of a few hundred keVs up to a few MeVs interacts with matter, it gradually loses energy by interacting mainly with the electrons of the target, but it can also interact (with a much lower probability) at the atomic or nuclear level with the target nuclei as well.

The result of such interactions is the emission of characteristic radiation and/or light charged particles, which can - in principle - provide valuable information about the absolute concentration, as well as, depth distribution of the target nuclei. Interactions of MeV ions with matter permit off-line analysis of light elements in solids (**CPAA** - Charged Particle Activation Analysis - implying the use of high resolution γ-ray spectroscopy) and in-beam microanalysis and imaging of sample constituents using excited X-rays (**PIXE** - Proton Induced X-ray Emission), γ-rays from nuclear reactions (**PIGE** - Proton Induced Gamma-ray Emission), outgoing nuclear reaction particles (**NRA** - Nuclear Reaction Analysis, implying emitted charged particles), elastically scattered ions (**BS** - Backscattering, including **RBS** - Rutherford Backscattering Spectroscopy, implying potential scattering, **EBS** - Elastic Backscattering Spectroscopy, implying non-Rutherford cross-sections, and - in most cases - the implementation of the resonant mechanism in elastic scattering, and **ERDA** - Elastic Recoil Detection Analysis), or visible and infrared emissions from the sample.

The ion beam can also be channeled down crystal axes and planes (channeling related phenomena). Many of these techniques can be combined with channeling to study the lattice location of species. In general, MeV light ions are very penetrating while producing very little sample damage.

These qualities permit the in situ, least destructive analysis and imaging of buried structures such as solid and fluid inclusions in minerals. All the above mentioned techniques are integral parts of Ion Beam Analysis (**IBA**), a strong, interdisciplinary field, combining Nuclear Physics and Material Science, which is continuously enriched and evolving. Among IBA techniques, RBS, EBS, ERDA, PIGE (when narrow resonances exist) and NRA are more commonly implemented for elemental depth profiling.

It is evident that in all cases, the most important factors that need to be known with high accuracy in order to determine the yield and the energy of the detected particles are: a) The stopping power values of incoming beam ions (and possibly outgoing reaction products) which is usually well-known for light ions, with only a few existing exceptions (e.g. [1]) and b) The differential cross-sections (corresponding to the probability of occurrence at a specific angle where the detector is set) of the implemented nuclear reactions. Other important experimental issues involve the determination of the detector efficiency (for PIGE measurements), the effects of energy and lateral straggling, the precise assessment of the total number of impinging beam ions, and the solid angle subtended by the detector, but in sophisticated experimental setups, and for experienced research groups, they can - in general - be under control. Thus, in essence, it is the knowledge of the differential cross-sections of the implemented nuclear reactions that has a fundamental importance in all low-energy nuclear techniques.

2 Motivation

Recently, as a result of the pioneer efforts of the past, a new, comprehensive library, IBANDL (Ion Beam Analysis Nuclear Data Library) has been created, according to the recommendations of the IAEA Technical Meeting held at the IAEA Headquarters in Vienna (29 to 30 October 2003). This data collection is a result of the old merging SigmaBase and NRABASE, along with more recent experimental differential cross-section data suitable for EBS, NRA and PIGE. Nowadays IBANDL contains most of the available experimental nuclear cross-sections relevant to Ion Beam Analysis, but also naturally represents a dynamically developing collection, depending on the activity of all members of the IBA community. Excitation functions are presented both as graphs and data files. All the entries are supplied with a reference to the data source. The data published only in a graphical form are digitized using a precise technique. There is also a direct link with the standard EXFOR nuclear data library (see www-nds.iaea.org/exfor/). The activity of the IBA community in the field of nuclear data has recently been supported by IAEA through the Coordinated Research Project (CRP) 'Development of a Reference Database for Ion Beam Analysis'. As a result of this project, a few key-reactions for NRA have been assessed and validated, e.g. ^{28}Si(d,p_0) and ^{27}Al(d,p_0), and most importantly a new online calculator, SigmaCalc [2–4], based on theoretical R-matrix calculations, has been incorporated in IBANDL. Moreover, through SigmaCalc, NRA users can obtain evaluated, though not yet benchmarked, differential cross-section values for a certain, very limited number of selected reactions, such as the ^{12}C(d,p_0) or the ^{12}O(d,p_0) ones.

These values, in ASCII format, can be directly incorporated in the existing sophisticated simulation codes. Nevertheless, there is a huge amount of work still pending, since there are many important reactions in NRA where the evaluation is impeded by the, often discrepant, experimental data. It should also be noted here that the theoretical evaluation is a dynamical process, based on the availability of precise experimental data over a wide range of beam energies and detector angles and can be tested through carefully designed benchmarking experiments. After the last 5 years of significant efforts, IBANDL is still an unfinished project, since differential cross-section measurements and theoretical evaluations are a vast research field and the questions of accuracy, benchmarking experiments and use of alternate reactions, including PIGE for light element depth profiling, need further investigation and coordinated efforts from the scientific community. Nevertheless, recent advances in the field, concerning R-matrix codes, constitute a real breakthrough for EBS, PIGE, NRA studies, and other low-energy nuclear physics applications, such as nuclear astrophysics [5].

3 The case of p+^{12}C

The proton elastic scattering cross-section demonstrates a complicated structure in the energy range up to 7 MeV. The structure is conditioned by interference of the resonance and potential scattering, the parameters of the resonances being well-known. The R-matrix theory is generally accepted as the most appropriate one for the analysis of resonance reactions in low–energy nuclear physics. In this approach, the configuration space of the scattering problem is divided into an internal region, corresponding to the compound nucleus, where the total wave function can be expanded into a complete set of eigenstates (in terms of unknown base functions, with the energy eigenvalues and the matrix elements of the base functions being adjustable parameters) and an external region, where the possible combinations of coupled particle pairs exist, corresponding to the reaction channels that emerge from the compound nucleus. This division of space is made by the choice of the boundary of the compound nucleus, i.e. an appropriate nuclear radius is chosen for each reaction channel. The wave functions of the internal and external regions, and their derivatives, must match at the boundary surface. The R-matrix takes account of all the interactions which occur inside the nucleus. The external region is generally assumed to contain only long range interactions between the particles, and thus has a complete analytical solution. The hard-sphere scattering phase shifts are conventionally used for the external wave functions. A unified approach [6] combining R-matrix and optical model was shown to be the most appropriate one for cross-section calculations in the case of low energy charged particle scattering. In this approach a Saxon–Woods real potential well along with a surface absorption part are used – together with the standard Coulomb and spin-orbit terms – for the calculation of phase shifts instead of the hard-sphere ones and, as a result, broad, single particle resonances naturally occur, without being artificially, *ab initio,* introduced as in standard R-matrix codes. This seems to constitute a more physical description of the scattering problem, since these resonances are not actually related to the compound nucleus eigenstates, as the other R-matrix components.

The evaluation starts with an assessment of the available data. The potential parameters are found by fitting the non-resonant part of the excitation function, using χ^2 minimization routines. This, above mentioned, data assessment is critical, since, in many cases, there is a lack of adequate and/or reliable data over a wide range of beam energies and detector angles for the reaction under study. In the particular case of proton elastic scattering from carbon, several differential cross-section datasets and angular distributions were considered for the evaluation. The calculations for ^{12}C are relatively simplified by the fact that it is an even–even nucleus ($J^{\pi}=0^{+}$), thus no spin–mixing phenomena are present. In most cases of low-energy scattering of charged particles on light nuclei, the contribution of the reaction channels is negligible, so the imaginary potential is close to zero. In the region of single-particle resonances, the calculated cross-section is extremely sensitive to the potential parameters. The last feature is observed for the $3/2^+$ resonance in the ^{12}C+p system at $E_p \sim$6.5 MeV, which is reproduced in the calculations by fine tuning of the d-wave potential well. To that end a separate real potential depth was used for each one of the l quantum numbers. The imaginary potential could not be retained equal to zero over such a broad energy range interval due to the onset of the competitive ^{12}C(p,p$_1$)^{12}C reaction channel (the energy of the first excited state of ^{12}C being equal to 4.438 MeV). In order to reproduce the right wing of the resonance at $E_p \sim$6.5 MeV, the use of the imaginary potential appeared to be necessary. Its dependence on energy was assumed to be of the form of a sigmoidal curve, with W_0=2.268 MeV, E_0=6.877 MeV,

$$W(E) = W_o \left[1 - \frac{1}{1 + \exp\left(\frac{E - E_o}{\Delta E}\right)} \right]$$

and ΔE=0.193 MeV, meaning that above $\sim$6 MeV the inelastic channel is expected to have a strong influence on the scattering process. In order to take into account the influence of resonance tails, the resonances located up to 11 MeV were included in the calculations. The evaluated cross-sections were matched with the cross-sections of a previous work [7] at 2.7 MeV. A typical result of the evaluation is shown in Fig.1.

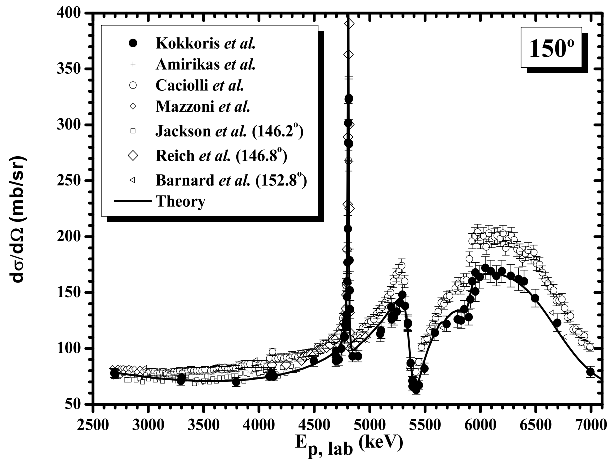

Fig. 1. Evaluated differential cross-sections along with data from literature at 150^o for comparison. For reasons of clarity, in most cases, the errors of older datasets along the y-axis have been omitted.

4 Conclusions

As a result of the present work, reliable differential cross-section values for the elastic scattering of protons on carbon are now available to the scientific community up to $E_{p,lab}$=7 MeV through the online calculator SigmaCalc and the nuclear data library IBANDL, that can be directly incorporated in widely used analytical codes, thus enhancing IBA capabilities. Therefore, as a consequence, the $^{12}C(p,p_0)$ reaction can now be considered as the most important candidate for carbon profiling studies from deep target layers (having a thickness of several μm).

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