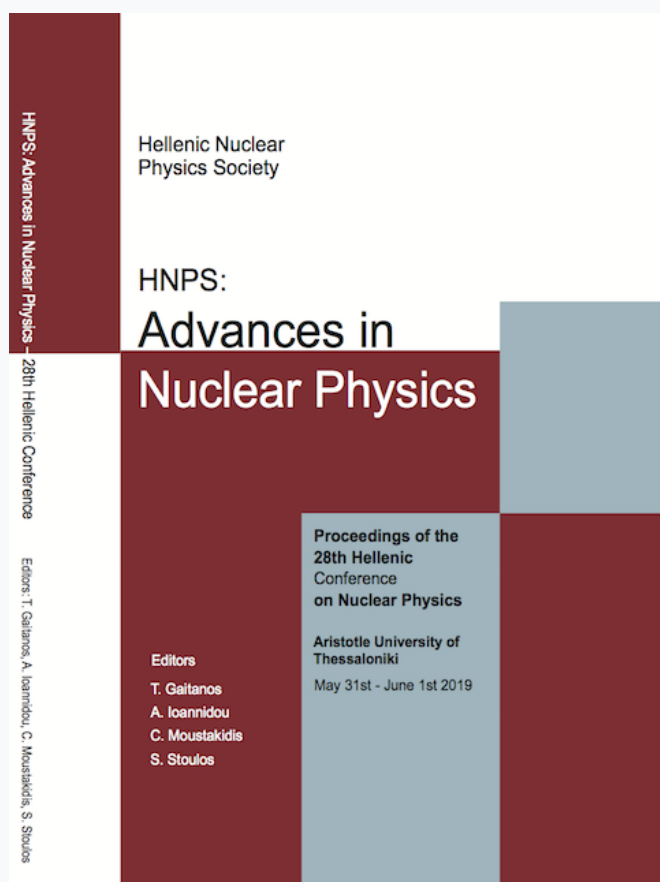


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MottCalc: A new tool for calculating Mott scattering differential cross sections for analytical purposes

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Abstract In the last few years, the popularity of ERDA applications has soared along with the implementation of time of flight (TOF) type measurements. However, ERDA and other forward scattering IBA techniques suffer from the possibility of the occurrence of Mott scattering. This leads to deviations in the elastic differential cross sections which in turn demand special care in the treatment of the obtained experimental spectra. To address this issue, a new code has been developed, called MottCalc (Mott Calculator). Based on the analytical formula, first developed by Mott, which describes the phenomenon, the code is capable of producing theoretical angular and energy distributions of such differential cross sections along with the appropriate R33 files, which in turn can be implemented in all the widely used analytical codes (SIMNRA, DF, POTKU etc.). The electronic screening effect is taken into account in these calculations by implementing the Andersen model. A list of 314 different isotopes is available to choose from as projectile and target nuclei. The list can be expanded with radioactive isotopes. The program is available in two distinct versions, an Excel Spreadsheet and a stand-alone application. Both versions of the program can be freely downloaded from the webpage of the Nuclear Physics group of NTUA (nuclearphysics.ntua.gr/downloads.php). The implementation of the code as well as the features and capabilities of both versions of the program are presented in the current work along with a brief synopsis of the elastic Mott scattering phenomenon.

Keywords Mott scattering, Elastic scattering of identical nuclei, ERDA, MottCalc

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INTRODUCTION

Elastic Recoil Detection Analysis (ERDA) is an experimental method that belongs in the wider family of Ion beam Analysis (IBA) techniques. ERDA offers great accuracy in the identification, quantitative measurement and determination of the depth profiles of light isotopes in near surface layers of a target. In addition, such measurements are least-destructive.

The above are accomplished via the detection of the elastically scattered recoil nuclei of the target. Usually the beam is composed of an isotope having a mass equal or greater than the one of the target under measurement. This allows the greater part of the system's kinetic energy to be transferred to the light target nucleus which is then scattered in forward angles and subsequently detected. However, the use of heavy isotopes for the beam limits the probing depth. [1]

Moreover, in forward scattering IBA applications the presence of target isotopes identical to the projectiles lead to elastic scattering of identical nuclei, also known as Mott scattering. In such cases, strong deviations appear in the measured differential cross sections compared to the Rutherford ones. These require special care in the treatment of the experimental data. Currently none of the widely used analytical codes (SIMNRA, DF, POTKU) provides theoretical calculations of the differential cross section of Mott scattering. To the best of the authors' knowledge the only software code that partially provides such calculations is LISE++ (developed at MSU); however, without taking into



account the electronic screening effect, or the ability to generate energy distributions and the accompanying necessary R33 files.

Mott Scattering

Mott scattering refers to the elastic scattering of two identical nuclei. Since there are no physical attributes that can be used to distinguish between the projectile and recoil nuclei after the scattering, the resulting differential cross section is the sum of the projectile and recoil scattering cross sections. In addition, due to the indistinguishability principle, this phenomenon must be studied quantum mechanically. As a result an interference term must also be added to the cross section (as shown in [2]).

$$\frac{d\sigma_{total}}{d\Omega} = |f|_{scattered}^2 + |f|_{recoil}^2 \pm 2R|f|_{scattered}|f|_{recoil} \quad (1)$$

The sign of the interference term changes depending on whether the identical colliding nuclei follow a bosonic or a fermionic distribution (integer or half-integer nuclear spins of the ground state accordingly). For isotopes with a ground state spin other than 0, the spin multiplicity must also be taken into account. This leads to a sum of the various possible differential cross sections in the form of equation 1, along with their respective weighting factors.

Taking all the above into account, the total differential cross section in the Center of Mass reference frame for the elastic scattering of two identical nuclei with atomic number Z , ground state spin s and mass m , for detection angle θ , when the initial kinetic energy of the projectile is K , is given in a compact form by the analytical Mott formula [3], which also takes into account the spin multiplicity. All the parameters refer to the Center of Mass frame of reference unless stated otherwise.

$$\frac{d\sigma}{d\Omega} = \left(\frac{1}{4\pi\epsilon_0} \frac{Z^2 e^2}{4K}\right)^2 \left\{ \frac{1}{\sin^4\left(\frac{\theta}{2}\right)} + \frac{1}{\cos^4\left(\frac{\theta}{2}\right)} + \frac{2(-1)^{2s} \cos [n_s \ln (\tan^2\left(\frac{\theta}{2}\right))]}{2s+1 \sin^2\left(\frac{\theta}{2}\right) \cos^2\left(\frac{\theta}{2}\right)} \right\} \quad (2)$$

The first term corresponds to the projectile's differential cross section, the second to the recoil's one and the third is the interference term. The first and second terms follow the Rutherford formula, while the interference term causes the differential cross section to oscillate around the expected Rutherford values in both angular and energy distributions (see Fig. 1). This oscillatory behavior depends on the spin of the ground state of the isotope, the detection angle θ and the Sommerfeld parameter n_s .

$$n_s = \frac{Z^2 e^2}{\hbar} \sqrt{\frac{m_{red}}{2E_{lab}}} \quad (3)$$

The term E_{lab} refers to the initial kinetic energy of the projectile nucleus in the Lab reference frame, while the term m_{red} symbolizes the reduced mass of the system. It should be noted that the elastic scattering of identical nuclei is a forward only scattering process, meaning that the allowed angular range is between 0° and 180° degrees in the centre of mass reference frame and 0° to 90° degrees in the Lab one.

The position of the maxima and the minima of the differential cross section is opposite between fermions (half-integer ground state spin) and bosons (integer ground state spin) as seen in Fig. 2. This is due to the different sign of the interference term (positive for bosons and negative for fermions) that the spins create, which ensures that the corresponding distribution is followed (expression 2). The

numeric value of the spin also influences the amplitude of the oscillations (Fig. 2).

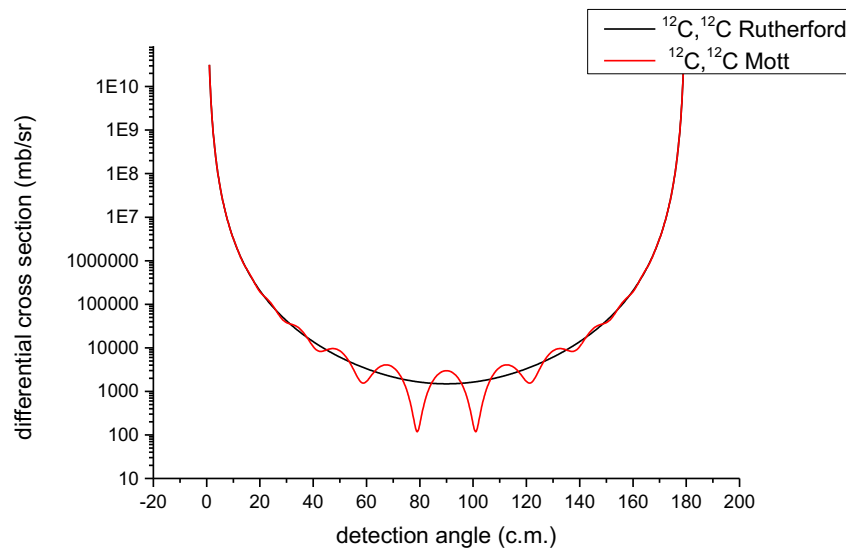


Figure 1. Angular distribution of the differential cross section of the elastic Mott Scattering (red) and the expected Rutherford values (black) of ^{12}C for $K = 3 \text{ MeV}$ in the Center of Mass Reference frame.

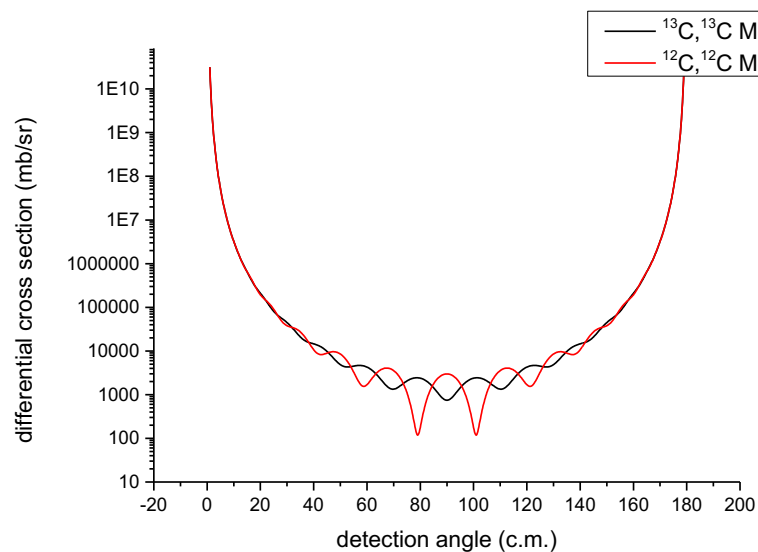


Figure 2. Angular distribution of the Mott scattering differential cross section of ^{13}C (black) with a spin $\frac{1}{2}$ and of ^{12}C (red) with a spin 0 in the Center of Mass reference frame for $K = 3 \text{ MeV}$.

The interference term also depends on the mass of the isotope (expression 2). The mass influences both the amplitude of the oscillations and their frequency in a proportional way, as greater mass leads to greater amplitude and frequency values (figure 3).

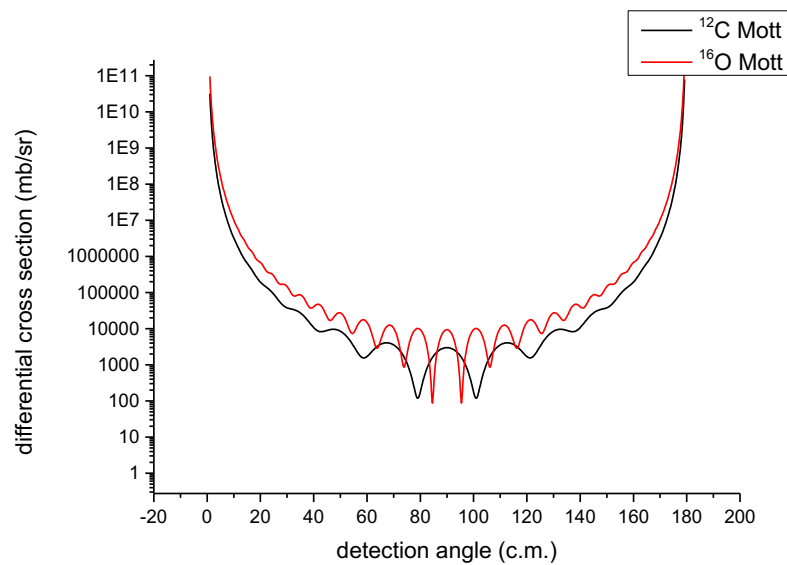


Figure 3. Angular distribution of the Mott Scattering differential cross section for the isotopes ^{12}C (black) and ^{16}O (red) for $K = 3 \text{ MeV}$ in the Center of Mass reference frame. Both isotopes have ground state spin equal to zero but differ slightly in their respective masses.

Finally, the initial kinetic energy K of the projectile plays a crucial role in the determination of the differential cross section of Mott scattering and its oscillatory behavior as it appears in both expressions 2 and 3. A higher energy leads to reductions in both the amplitude and the frequency as seen in figure 4. It should also be noted that for higher energies, reaction channels other than the elastic one are initiated, which in turn lead to a decrease in the differential cross section of Mott Scattering. As a rule of thumb, for energies near or exceeding the Coulomb barrier (as shown in [4]), other reactions occur along with the elastic scattering.

$$U_{Coulomb} = \frac{1.438 Z_1 Z_2}{0.5 + 1.36 \cdot (A_1^{1/3} + A_2^{1/3})} \quad (4)$$

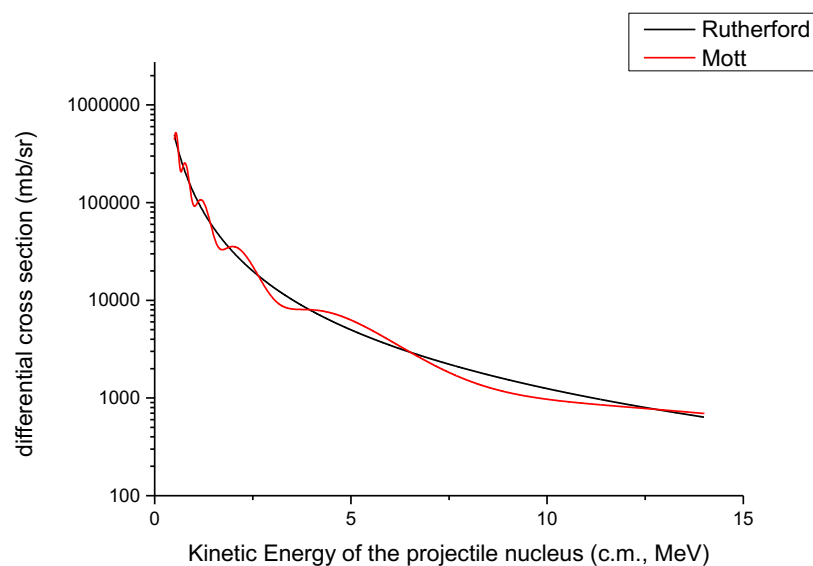


Figure 4. Energy distribution of the Mott scattering differential cross section for the isotope ^{12}C (red) for the detection angle at 40° in the Center of Mass frame. The expected total Rutherford values are shown in black.

The Electronic Screening Effect

The target electrons interact with both the projectile and target nuclei. This interaction leads to a reduction of the effective nuclear charge of both the scattered and recoil nuclei leading to a reduction in the differential cross section of elastic scattering. The influence of this effect can be calculated through phenomenological models. According to the Andersen model the corrected differential cross section is given by the following expressions [5]

$$\sigma(\theta)_{Mott,corrected} = f_{screening}(E, \theta)_{Andersen} \sigma(\theta)_{Mott} \quad (5)$$

$$f_{Andersen} = \frac{(1 + \frac{1}{2} \frac{V_1}{E})^2}{\{1 + \frac{V_1}{E} + [\frac{V_1}{2E \sin(\frac{\theta}{2})}]^2\}^2} \quad (6)$$

$$V_1 (keV) = 0.04873 Z_{projectile} Z_{recoil} \sqrt{Z_{projectile}^{2/3} + Z_{recoil}^{2/3}} \quad (7)$$

THE ANALYTICAL CODE MOTTCALC

Using expression 2, an analytical code, named MottCalc, able to calculate theoretical differential cross section distributions, while taking into account the influence of the electronic screening effect, was developed. The characteristics of these distributions are determined by the user. First the isotope and the type of distribution (angular or energy) are chosen, then the user defines the initial and final values, as well as the step between the values of the distribution. In addition, for angular distributions, the initial beam energy must be determined, while for energy distributions the corresponding detection angle. All the parameters given by the user refer to the Lab reference frame. There is a library of 314 different isotopes available as beam and target nuclei. This library can be expanded to include unstable isotopes, however it should be noted that the code cannot determine the validity of the added isotopes. Subsequently, the code converts the specified parameters to the Center of Mass reference frame and calculates the number of points in the distribution. Using expressions 2, 5, 6 and 7 the specified screened differential cross section distribution is calculated in the Center of Mass reference frame. Afterwards the values of the distribution are converted in the Lab one.

The code is available in two different but user-friendly versions, an Excel Spreadsheet and a stand-alone application. Both versions use the same methodology described above, however each one fulfills a different function. Both versions are freely distributed under the BSD licence, along with their source codes and the list of the available isotopes and their characteristics.

The Excel Spreadsheet

The Excel Spreadsheet is based on the Visual Basic programming language, which is compatible with the Excel program. Its primary function is to provide various information about the specified distribution. It contains 4 different worksheets within, named “Quick Calculation”, “Angular Distribution”, “Energy Distribution” and “Table of Isotopes”.

In the “Quick Calculation” spreadsheet the user chooses the isotope by stating its mass and atomic number as well as the type of the required distribution and its characteristics. By pressing the appropriate button, the specified distribution is calculated and is shown in the spreadsheet as both a graph and in numeric form in the Lab reference frame. Depending on the type of requested distribution, in the spreadsheets “Angular Distribution” and “Energy Distribution” additional info is

shown, including the values of the distribution in both reference frames, the values of the screening effect and the values of the differential cross section according to the Rutherford formula. Also available are graphs comparing the Mott and Rutherford values in both systems. Lastly, the spreadsheet “Table of Isotopes” contains the relevant information about the isotopes that can be used. More isotopes can be added by the user.

The Application

The application was written in the widely used C++ programming language and follows the same methodology as the Excel Spreadsheet. It is an open source application with the graphical interface based on the Qt Company libraries. Its main function is the creation of the appropriate ASCII R33 files of the specified distribution. These files can then be implemented in the various analytical codes used by the experimental Nuclear Physics community (SIMNRA, DF, POTKU, e.t.c.).

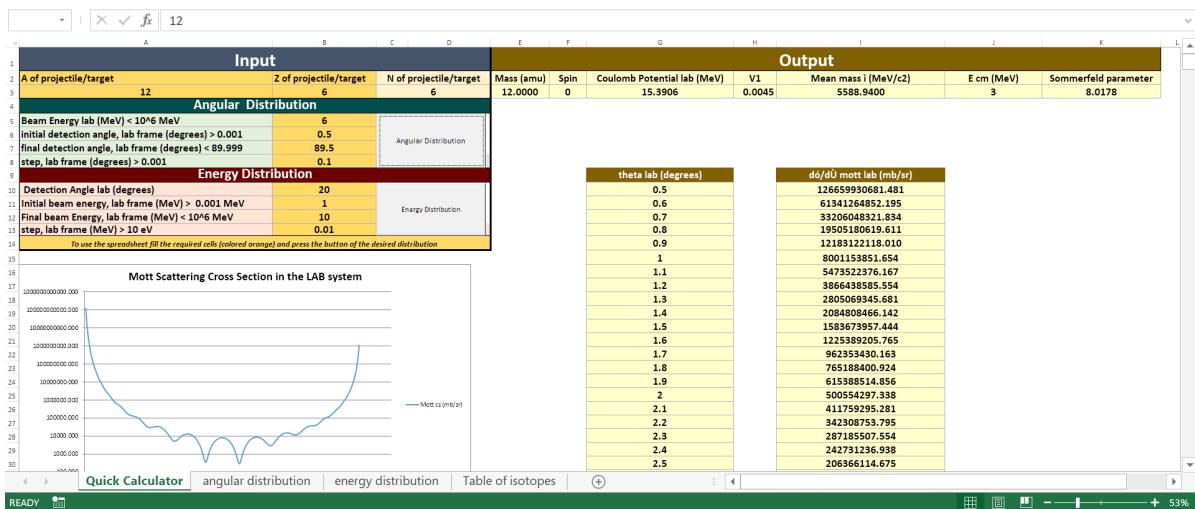


Figure 5. The spreadsheet “Quick Calculator” which serves as the interaction point between the user and the Excel Spreadsheet.

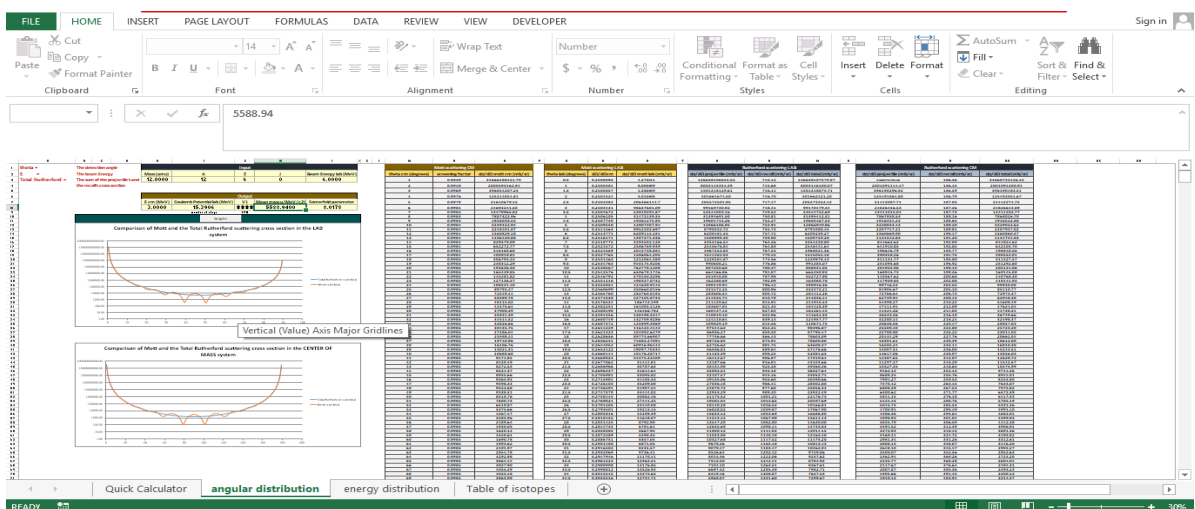


Figure 6. The spreadsheet “Angular Distribution”. Under the yellow banners are the values of the screened Mott Formula in both reference frames while under the blue the corresponding screened Rutherford ones.

	A	B	C	D	E	F	G	H	I	J
1	Symbol	Z	A	Mass (amu)	J					
2	n	0	1	1.008664916	-0.5					
3	p	1	1	1.007825032	0.5					
4	H	1	2	2.014101778	1					
5	H	1	3	3.016049278	0.5					
6	He	2	3	3.01602932	0.5					
7	He	2	4	4.002603254	0					
8	Li	3	6	6.015122887	1					
9	Li	3	7	7.016003437	1.5					
10	Be	4	9	9.012183065	1.5					
11	B	5	10	10.01293695	3					
12	B	5	11	11.00930536	1.5					
13	C	6	12	12	0					
14	C	6	13	13.00335484	0.5					
15	C	6	14	14.00324199	0					
16	N	7	14	14.003074	1					
17	N	7	15	15.0001089	0.5					
18	O	8	16	15.99491462	0					
19	O	8	17	16.99913176	2.5					
20	O	8	18	17.99915961	0					
21	F	9	19	18.99840316	0.5					
22	Ne	10	20	19.99244018	0					
23	Ne	10	21	20.99384669	1.5					
24	Ne	10	22	21.99138511	0					

Figure 7. The spreadsheet “Table of Isotopes” which contains the symbol, mass number, atomic mass, mass and spin of the available 314 isotopes. The list can be expanded to include unstable isotopes as well.

As before, first an isotope must be selected. The same 314 isotopes as in the Excel Spreadsheet are available in the application by just selecting the appropriate mass and atomic number and clicking the button “Set Isotope”. The user is also able to create a “custom” isotope by filling the mass and atomic numbers along with the mass and the spin of the ground state of the isotope and clicking “Set Custom Isotope”. Secondly, the type of the distribution and its characteristics (initial and final values, step and beam energy or detection angle accordingly) must be specified. By clicking the button “Get Distribution” the values of the differential cross sections are calculated and a graph of the distribution in the Lab reference frame is generated. At this point, the R33 file with the distribution in the Lab system can be created by clicking the button “Save as R33 file”. The user can select the directory where the file is saved.

The Application

The application was written in the widely used C++ programming language and follows the same methodology as the Excel Spreadsheet. It is an open source application with the graphical interface based on the Qt Company libraries. Its main function is the creation of the appropriate ASCII R33 files of the specified distribution. These files can then be implemented in the various analytical codes used by the experimental Nuclear Physics community (SIMNRA, DF, POTKU, e.t.c.). As before, first an isotope must be selected. The same 314 isotopes as in the Excel Spreadsheet are available in the application by just selecting the appropriate mass and atomic number and clicking the button “Set Isotope”. The user is also able to create a “custom” isotope by filling the mass and atomic numbers along with the mass and the spin of the ground state of the isotope and clicking “Set Custom Isotope”. Secondly, the type of the distribution and its characteristics (initial and final values, step and beam energy or detection angle accordingly) must be specified. By clicking the button “Get Distribution” the values of the differential cross sections are calculated and a graph of the distribution in the Lab reference frame is generated. At this point, the R33 file with the distribution in the Lab system can be created by clicking the button “Save as R33 file”. The user can select the directory where the file is saved.

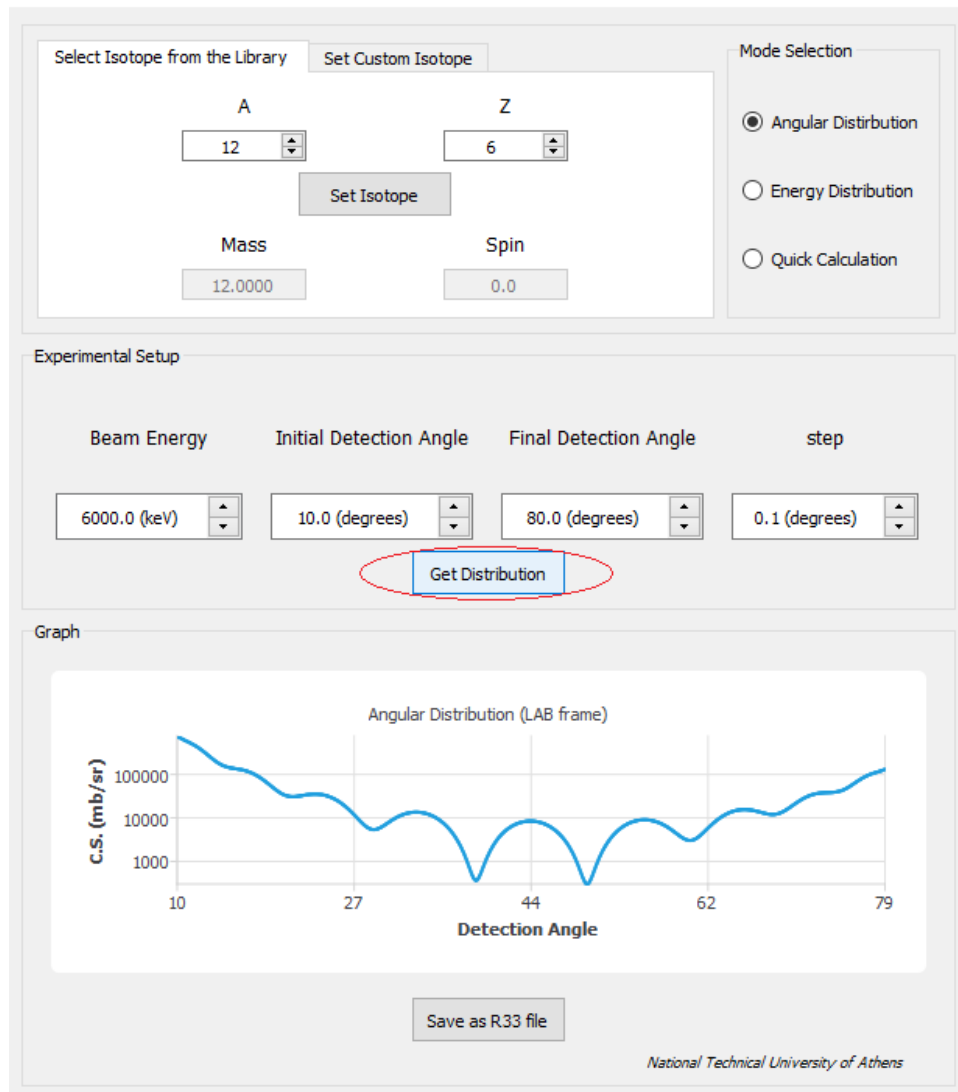


Figure 8. The graphical interface of the application.

RESULTS AND DISCUSSION

As seen in expression 2 and figure 2, the influence of Mott Scattering is greater in isotopes with a ground state spin equal to zero and it wanes as the numeric value of the spin rises. Since even-even isotopes, which are spinless bosons according to the shell model, are widely implemented as projectiles in various IBA applications the effect of Mott scattering can be quite noticeable. The resulting deviations from the expected Rutherford values, where the interference term is omitted, can be up to a factor of 2 as seen in figure 1. The oscillatory behavior is also determined by the detection angle, the mass of the isotopes, as well as the initial beam energy. As is evident from figures 1, 2, 3 and 4 for the angular range that is usually used in forward scattering experimental techniques and in an energy range where elastic scattering would be the primary reaction channel, the presence of Mott Scattering is significant. When the above are combined, the need for a program that can generate theoretical differential cross section distributions becomes apparent.

By taking into account the influence of the electronic screening effect, the theoretical calculations of MottCalc can be used in the analysis of experimental data resulting from Mott scattering. The results of the code have been compared against the more simplistic corresponding

LISE++ calculator and are generally in very good agreement. Figures 1, 2, 3 and 4 were created with the use of MottCalc.

CONCLUSIONS

In summary, an analytical code has been developed, capable of performing theoretical calculations for the determination of differential cross sections relevant to the elastic Mott Scattering. This code was based on the analytical formula for the differential cross section of the elastic scattering of identical nuclei, first developed by Mott, and takes into account the influence of the electronic screening effect on the obtained values. This allows for the use of the code in ERDA measurements and other forward scattering IBA techniques, where the appearance of such a type of scattering is common and leads to significant deviations from the expected Rutherford values.

The program is freely available under the BSD license, along with the source code, in two distinct formats, an Excel spreadsheet which provides a plethora of information and an application for the creation of ASCII R33 files with angular or energy distributions of Mott differential cross sections. Both versions can be downloaded at the webpage of the Nuclear Physics group of NTUA at nuclearphysics.ntua.gr/downloads.php. The current version of MottCalc has been tuned and tested for 32bit and 64bit systems with MS Windows 10. However, since the source code is also available for download, the program can be easily adapted to other operating systems (e.g. Linux, or MacOS) by the user.

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