Predicting total and total reaction cross sections using a simple functional form

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Abstract

Total reaction cross sections have been predicted for nucleons scattering from nuclei ranging in mass 6 to 238 and for projectile energies from just above noticeable giant resonance excitation to 300 MeV. So also have been the mass variations of those cross sections at selected energies when they have been calculated using coordinate space optical potentials formed by full folding effective two-nucleon ($NN$) interactions with one body density matrix elements (OBDME) of the nuclear ground states. Good comparisons with data result when effective $NN$ interactions defined by medium modification of free $NN t$ matrices are used. However, there is a simple three parameter functional form that reproduces the partial wave total reaction cross section values determined from those optical potential calculations; a functional form also maps the total scattering cross section partial wave elements. Adjusting the theoretical defined parameter values has enabled us to fit the actual measured data values from the scattering involving (15) nuclei spanning the mass range from $^9$Be to $^{238}$U and for proton energies from 10 to 300 MeV. Likewise total cross sections for neutron cross sections for neutron scattering from various nuclei can be equally well reproduced. Of import is that the three parameter values vary smoothly with mass and energy.

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I. INTRODUCTION

Total and total reaction cross sections from the scattering of nucleons by nuclei are required in a number of fields of study which range over problems in basic science as well as many of applied nature. Such as in radioactive waste management, in radiation therapy and radiation protection for patients and in many other fields. In medical radiotherapy absorbed dose distributions in the patient are needed and cannot be measured directly as we should not do nuclear experiment with human body, they must be calculated. For all these purposes an extensive data bank is necessary. Since we do not have the experimental data for all necessary nuclei at all different energies it would be utilitarian if such scattering data were well approximated by a simple convenient function form with which predictions could be made for cases of energies and/or masses as yet to be measured. It has been shown [1, 2, 3, 4] that such forms may exist for proton total reaction cross sections. Herein we consider that concept further to reproduce the measured total reaction cross sections from protons at energies from 10 to 300 MeV and from 15 different nuclei ranging in mass between $^9$Be and $^{238}$U and total cross sections from neutron scattering for energies to 600 MeV and from nine nuclei ranging in mass between $^6$Li and $^{238}$U. These suffice to show that such forms will also be applicable in dealing with other stable nuclei since their neutron total cross sections vary so similarly with energy [5].

Total reaction cross sections for protons and total cross sections for neutrons from nuclei have been well reproduced by using optical potentials. In particular, the data (to 300 MeV) from the same nuclei we consider, compare quite well with predictions made using a $g$-folding method to form nonlocal optical potentials [6], though there are some notable discrepancies. Alternatively, in a recent study Koning and Delaroche [5] gave a detailed specification of phenomenological global optical model potentials determined by fits to quite a vast amount of data, and in particular to the neutron total scattering cross sections we consider herein.

II. FORMALISM

The total and total reaction cross sections for nucleons scattering from nuclei can be expressed in terms of partial wave scattering ($S$) matrices specified at energies $E \propto k^2$, by

$$S_l^\pm \equiv S_l^\pm(k) = e^{2i\delta_l^\pm(k)} = \eta_l^\pm(k)e^{2\Re[\delta_l^\pm(k)]},$$

where $\delta_l^\pm(k)$ are the (complex) scattering phase shifts and $\eta_l^\pm(k)$ are the moduli of the $S$ matrices. The superscript designates $j = l \pm 1/2$. In terms of these quantities, the elastic, reaction (absorption), and total cross sections respectively are given by

$$\sigma_{el}(E) = \frac{\pi}{k^2} \sum_{l=0}^{\infty} \left\{ (l + 1) \left| S_l^+(k) - 1 \right|^2 + l \left| S_l^-(k) - 1 \right|^2 \right\} = \frac{\pi}{k^2} \sum_l \sigma_{l}^{(el)},$$

$$\sigma_{R}(E) = \frac{\pi}{k^2} \sum_{l=0}^{\infty} \left\{ (l + 1) \left[ 1 - \eta_l^+(k)^2 \right] + l \left[ 1 - \eta_l^-(k)^2 \right] \right\} = \frac{\pi}{k^2} \sum_l \sigma_{l}^{(R)},$$

and

$$\sigma_{TOT}(E) = \sigma_{el}(E) + \sigma_{R}(E) = \frac{\pi}{k^2} \left[ \sigma_{l}^{(el)} + \sigma_{l}^{(R)} \right] = \frac{2\pi}{k^2} \sum_l \sigma_{l}^{(TOT)},$$

$$\sigma_{l}^{(TOT)} = (l + 1) \left\{ 1 - \eta_l^+(k) \cos(2\Re[\delta_l^+(k)]) \right\} + l \left\{ 1 - \eta_l^-(k) \cos(2\Re[\delta_l^-(k)]) \right\}. \tag{4}$$
Therein the $\sigma_l^{(X)}$ are defined as partial cross sections of the total elastic, total reaction, and total scattering itself. For proton scattering, because Coulomb amplitudes diverge at zero degree scattering, only total reaction cross sections are measured. Nonetheless study of such data established that partial total reaction cross sections $\sigma_l^{(R)}(E)$ may be described by the simple function form

$$\sigma_l^{(R)}(E) = (2l + 1) \left[ 1 + e^{\frac{(l-l_0)}{a}} \right]^{-1} + \epsilon (2l_0 + 1) e^{\frac{(l-l_0)}{a}} \left[ 1 + e^{\frac{(l-l_0)}{a}} \right]^{-2},$$

with the tabulated values of $l_0(E, A)$, $a(E, A)$, and $\epsilon(E, A)$ all varying smoothly with energy and mass. Those studies were initiated with the partial reaction cross sections determined by using complex, non-local, energy-dependent, optical potentials generated from a $g$-folding formalism. While those $g$-folding calculations did not always give excellent reproduction of the measured data (from $\sim$ 20 to 300 MeV for which one may assume that the method of analysis is credible), they did show a pattern for the partial reaction cross sections that suggest the simple function form given in Eq. (5). With that form excellent reproduction of the proton total reaction cross sections for many targets and over a wide range of energies were found with parameter values that varied smoothly with energy and mass.

Herein we establish that the partial reaction cross sections for scattering of protons and total cross sections for scattering of neutrons from nuclei can also be so expressed and we suggest forms, at least first average result forms, for the characteristic energy and mass variations of the three parameters involved. Fifteen nuclei, $^9$Be, $^{12}$C, $^{16}$O, $^{19}$F, $^{27}$Al, $^{40}$Ca, $^{63}$Cu, $^{90}$Zr, $^{118}$Sn, $^{140}$Ce, $^{159}$Tb, $^{181}$Ta, $^{197}$Au, $^{208}$Pb and $^{238}$U, are considered for proton case and nine nuclei, $^6$Li, $^{12}$C, $^{19}$F, $^{40}$Ca, $^{89}$Y, $^{184}$W, $^{197}$Au, $^{208}$Pb and $^{238}$U, for which a large set of experimental data exist, are considered for neutron case. Also those nuclei span essentially the whole range of target mass. However, to set up an appropriate simple function form, initial partial total cross sections must be defined by some method that is physically reasonable. Thereafter the measured total cross-section values themselves can be used to tune details, and of the parameter $l_0$ in particular. We chose to use results from $g$-folding optical potential calculations to give those starting values.

### III. RESULTS AND DISCUSSIONS

The function form results we display in the following set of figures were obtained by starting with $g$-folding model results, for proton case at energies of 10 to 100 MeV in steps of 10 MeV, then to 300 MeV in steps of 50 MeV, and for neutron case, at energies of 10 to 100 MeV in steps of 10 MeV, then to 350 MeV in steps of 25 MeV, and thereafter in steps of 50 MeV to 600 MeV. The $g$-matrices used above pion threshold were those obtained from an optical potential correction to the BonnB force, which, while approximating the effects of resonance terms such as virtual excitation of the $\Delta$, may still be somewhat inadequate for use in nucleon-nucleus scattering above 300 MeV. Also relativistic effects in scattering, other than simply the use of relativistic kinematics in the distorted wave approximation (DWA) approach, are to be expected. Nonetheless the DWA results are used only to find a sensible starting set of the function form parameters $l_0$, $a$, and $\epsilon$ from which to find ones that reproduce the measured total cross-section data. One must also note that the $g$-folding potentials for most of the nuclei considered were formed using extremely simple model prescriptions of their ground states. A previous study revealed that with good spectroscopy the $g$-folding approach gives much better results in comparison with data than
that approach did when simple packed shell prescriptions for the structure of targets were used. That was also the case when scattering from exotic, so-called nucleon halo, nuclei were studied [7, 9].

Although on using Eqs. (3) and (5) to match values of (theoretically) calculated total reaction cross sections led [2] to the three parameters \( l_0(E, A), a(E, A), \) and \( \epsilon(E, A) \) having smooth variations with energy, there are discrepancies between those predictions and the actual measured data. Herein we improve the method of selection of those parameter values to produce more accurate reaction cross section values, while keeping as smooth a variation with energy of those parameters as possible. Specifically, in Eq. (5), we have set the \( \epsilon \) as a constant \((-1.5)\) and so independent of energy and of mass. Further we assume that \( a(E, A) \) varies linearly with the wave vector,

\[
k = \frac{1}{\hbar c} \sqrt{E^2 - m^2 c^4}, \tag{6}
\]

and with the form

\[
a(E, A) \sim 1.02k - 0.25. \tag{7}
\]

Then \( l_0(E, A) \) were adjusted to ensure that all measured total reaction cross section values are matched by using the function form, Eq. (5). The resultant optimized values for the parameter \( l_0 \) are presented in Fig. 1. The different patterns and colors of the lines show the \( l_0 \) values for different nuclei. The legend of the graph indicates the nuclei.

While we have used the partial total cross sections from DWA results for neutron scattering from all the nine nuclei chosen and at all of the energies indicated, from the sets of values that result from the fitting process, the two parameters \( a \) and \( \epsilon \) can themselves be expressed by the parabolic functions

\[
a = 1.29 + 0.00250 E - 1.76 \times 10^{-6} E^2, \tag{8}
\]

\[
\epsilon = -1.47 - 0.00234 E + 4.16 \times 10^{-6} E^2, \tag{8}
\]

where the target energy \( E \) is in MeV. There was no conclusive evidence for a mass variation of them. With \( a \) and \( \epsilon \) so fixed, we then adjusted the values of \( l_0 \) in each case so that actual measured neutron total cross-section data were fit using Eq. (5). Numerical values for \( l_0 \) from that process are presented in a table in Ref. [10]. The values of \( l_0 \) increase monotonically with both mass and energy and that is most evident in Fig. 2 where the optimal values \( l_0(E) \) are presented as different patterned and colored lines. The set for each of the masses (from 6 to 238) are given by those that increase in value respectively at 600 MeV. While that is obvious for most cases, note that there is some degree of overlap in the values for \(^{197}\text{Au}\) and for \(^{208}\text{Pb}\).

In Figs. 3 and 4, we compare the total reaction cross sections generated using the simple functional form and tabled values of \( l_0 \), and displayed by the red curves, with those obtained from calculations made using \( g \)-folding optical potentials [6]. Blue lines represent the predictions obtained from those microscopic optical model calculations. The experimental data [11] are depicted by circles.

The results for scattering from \(^9\text{Be}, ^{12}\text{C}, ^{16}\text{O}, ^{19}\text{F}, ^{27}\text{Al}, ^{40}\text{Ca}, ^{63}\text{Cu}, ^{90}\text{Zr} \) and \(^{118}\text{Sn}\) are displayed in segments (a) through (i) of Fig. 3 respectively. In segment (a), the data are well reproduced by both the \( g \)-folding predictions resulting from the folding with the \(^9\text{Be}\) ground state OBDME found with \((0+2)\hbar\omega\) spectroscopy and by those obtained with the simple functional form method.
Calculated p-$^{12}$C reaction cross sections are compared with the experimental data in segment (b) of Fig. 3. The reaction cross sections obtained from $g$-folding calculations are in good agreement with the experimental data but only in the energy range above 20 MeV. On the other hand, the results obtained from the simple functional method are excellent for all energies, replicating the data very well even in the lower energy range from 10 MeV. There are two data points, at 61 MeV and at 77 MeV, in disagreement with the calculated results however. But, as noted previously [12], these data points should be discounted.

Predictions for p-$^{16}$O and for p-$^{19}$F scattering are compared with the data in segments (c) and (d) of Fig. 3. For p-$^{16}$O case, there are many data points at the energies between 20 to 40 MeV. Predictions from $g$-folding calculations while replicating the data very well at and above 25 MeV, overestimate at lower energies. That $g$-folding result also underestimates the datum at 250 MeV; the sole datum above 50 MeV. In contrast, the results obtained from the simple functional method are in excellent agreement with the experimental data at all energies. For p-$^{19}$F, although $g$-folding calculations reproduce the data very well, the simple functional form method gives slightly more accurate predictions.

Total reaction cross section predictions for p-$^{27}$Al and for p-$^{40}$Ca are compared with the experimental data in segments (e) and (f) of Fig. 3. Again while $g$-folding calculations reproduce the data quite well to 200 MeV, three data points at 180 to 300 MeV are not
FIG. 2: The values of $l_0$ that fit neutron total scattering cross-section data from the nine nuclei considered and for energies between 10 and 600 MeV. The curves portray the best fits found by taking a function form for $l_0(E)$. The $g$-folding results underestimate them noticeably. But predictions from simple functional form replicate the data very well at all energies. One data point at 61 MeV is exceptional in the set. With $^{40}$Ca, the folding model approach is not expected to be reliable at the energies in the range 10 to 20 MeV, as is the case with $^{12}$C, since for excitation energies of that range, both nuclei have clearly discrete spectra. That is true for most light mass nuclei but little or no total reaction cross sections have been reported for them. Indeed the reaction data from both $^{12}$C and from $^{40}$Ca show rather sharp resonance-like features below 20 MeV. Both the $g$-folding calculations and functional form calculations reproduce the rest of the $^{40}$Ca data very well.

For $^{63}$Cu, our predictions at low energies may be slightly too small and the parameter sets driven too severely by the sole datum at 30 MeV in the range 20 to 70 MeV. Also the data in the range 100 to 300 MeV are quite scattered but the simple functional form gives a good average result.

In segment (h) of Fig. 3 the predicted total reaction cross sections from $p^{90}$Zr scattering are compared with the experimental data. Results from $g$-folding calculations are in very good agreement with the data although the data value at 30 MeV is overestimated. The results obtained from the simple functional form are in excellent agreement with the exper-
Experimental data at the few energies measured, but the shape is not optimally smooth. Lack of data meant that we had to use the $g$-folding values to specify the functional form. That is also the case with masses 140, 159, and 181.

The p-$^{118}$Sn total reaction cross section results are given in segment (i) of Fig. 3 where the two predictions again are compared with the data. Although not as good as the results found for scattering from light mass nuclei, the $g$-folding potential still gives reasonable shape prediction. However, the model underestimates the data by 5 to 10%. But predictions from the simple functional form model form an excellent reproduction of the data at all energies except 61 MeV. This 61 MeV data point is again exceptional being much smaller than other data and the predictions as in the cases of $^{12}$C and $^{27}$Al.

Predictions for p-$^{140}$Ce, p-$^{159}$Tb, p-$^{181}$Ta, p-$^{197}$, p-$^{208}$ and for p-$^{238}$U scattering are compared with the (limited amount of) data in segments (a), (b), (c), (d), (e) and (f) of Fig. 4 respectively. The $g$-folding calculations give very good agreement with that data for p-$^{140}$Ce, slightly underestimate the data for p-$^{159}$Tb, and for p-$^{181}$Ta, underestimate data at the energies to 20 MeV and overestimate data in the energy range 40 to 60 MeV. In all cases results predicted by the simple functional form are excellent reproductions of the experimental data.
For $^{197}$Au, the $g$-folding optical potential calculations are in good agreement with most data; the 29 MeV datum grossly underestimated by the calculations. But that data point is also at odds with the energy trend of the other data. Save for that 29 MeV value, the simple functional form gives even better predictions of the data. The energy variation of the p-$^{208}$Pb reaction cross sections is shown in segment (e) of Fig. 4 where the predictions from $g$-folding optical potential calculations and from the simple functional form calculations are compared with a fairly extensive set of experimental data. In making the $g$-folding potentials, we have used Skyrme-Hartree-Fock wave functions [13] which have been shown to be more realistic than simple oscillator model ones. Still such $g$-folding calculations underestimate the data up to 50 MeV. But simple functional form calculations are in excellent agreement with the experimental data, save that data values at 30, 61 and 77 MeV again are exceptional. The predictions of total reaction cross sections for p-$^{238}$U scattering from the $g$-folding optical potential calculations and from using the simple functional form are compared with the few data in segment (f) of Fig. 4. Given the lack of data the two results are virtually identical.

As a final note regarding many of the exceptional data values so defined in the foregoing, Menet et al. [14] argue that there may be a systematic error in the studies reported in those experiments.

The total neutron scattering cross sections generated using the function form for partial
FIG. 5: Total cross sections for neutrons scattered from (a) $^6$Li, (b) $^{12}$C, (c) $^{19}$F, (d) $^{40}$Ca, (e) $^{89}$Y, (f) $^{184}$W, (g) $^{197}$Au, (h) $^{208}$Pb and (i) $^{238}$U.

total cross sections with the tabled values of $l_0$ and the energy function forms of Eq. (8) for $a$ and $\epsilon$, are shown in Fig. 5. They are displayed by the red lines that closely match the data which are portrayed by circles. The data that was taken from a survey by Abfalterer et al. [15] which includes data measured at LANSCE that are supplementary and additional to those published earlier by Finlay et al. [16]. For comparison we show results obtained from calculations made using $g$-folding optical potentials [6]. Blue lines represent the predictions obtained from those microscopic optical potential calculations. Clearly for energies 300 MeV and higher, those predictions fail.

The total cross sections for neutrons scattered from the nuclei considered are compared with data in Fig. 5. Again the $g$-folding potential results are displayed by the blue curves while those of the function form are shown by the red curves. We show in segment (h) of Fig. 5 the results for neutron scattering from $^{208}$Pb. In this case we used Skyrme-Hartree-Fock model (SKM*) densities [13] to form the $g$-folding optical potentials. That structure when used to analyze proton and neutron scattering differential cross sections at 65 and 200 MeV gave quite excellent results [17]. Indeed those analyzes were able to show selectivity for that SKM* model of structure and for the neutron skin thickness of 0.17 fm that it proposed. Using the SKM* model structure, the $g$-folding optical potentials gave the total cross sections shown by the blue curve in segment (h) of Fig. 5. Of all the results, we believe these for $^{208}$Pb...
point most strongly to a need to improve on the \( g \)-folding prescription as is used currently when energies are at and above pion threshold. Nonetheless, it does do quite well for lower energies, most notably giving a reasonable account of the Ramsauer resonances \( \text{below 100 MeV} \). However, as with the other results, these \( g \)-folding values serve only to define a set of partial cross sections from which an initial guess at the parameter values of the function form is specified. With adjustment that form produces the red curve shown in segment (h) of Fig. 5 which is an excellent reproduction of the data, as it was designed to do. But the key feature is that the optimal fit parameter values still vary smoothly with mass and energy.

Without seeking further functional properties of the parameters, one could proceed as we have done this far but by using many more cases of target mass and scattering energies so that a parameter tabulation as a data base may be formed with which any required value of total scattering cross section might be reasonably predicted (i.e. to within a few percent) by suitable interpolation on the data base, and the result used in Eq. (5).

IV. CONCLUSIONS

Measured reaction cross sections for 10 to 300 MeV proton scattering from nuclei ranging in mass from \( ^9\text{Be} \) to \( ^{238}\text{U} \) are well reproduced by calculations made using the \( g \)-folding model of the optical potential. Measured total cross sections for 10 to 600 MeV neutron scattering from nuclei ranging in mass from \( ^6\text{Li} \) to \( ^{238}\text{U} \) are well reproduced. Those calculated results gave a set of partial reaction cross sections in each case that vary smoothly with target mass and energy. Those variations are well reproduced by a simple three parameter function. Using the simple function form total and total reaction cross sections are well reproduced. This simple functional method can be used to estimate cross sections for many useful applications, such as, medical radiotherapy.

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