Empirical Estimates of the Neutron-Nucleus Scattering Cross Sections

S.S.V. Surya Narayan†∗, Rajesh S. Gowda† and S. Ganesan†

† Nuclear Physics Division, ‡ Reactor Physics Design Division,
Bhabha Atomic Research Centre, Trombay, Mumbai 400 085, India
(Dated: October 31, 2018)

Theoretical study of systematics of neutron scattering cross sections on various materials for neutron energies up to several hundred MeV are of practical importance. In this paper, we analysed various cross sections of neutron-nucleus (n-N) scattering for several systems in the energy range of 50-250 MeV, predicted by the optical model using Koning-Delaroche potentials. We propose an empirical approach to successfully predict the energy dependence of total, shape elastic, reaction cross sections and zero degree scattering angular distributions. We demonstrate that owing to two conditions, only two out of these four cross sections need to be fitted empirically. Further, we modified the Wick’s approximation for the zero degree angular distributions and use this approach for estimating various cross sections for any nucleus from Aluminum to Lead.

Keywords: Optical Model, total cross section, reaction, shape elastic, forward elastic cross sections, n-N scattering, Wick’s limit, empirical formulae.

PACS numbers: 24.10.Ht, 25.40.-h, 28.20.Cz

In recent times, the concept of an accelerator driven subcritical (ADS) system is drawing worldwide attention [1, 2]. In this ADS system, neutrons are produced by bombarding a heavy element target with a high energy proton beam of typically above 1.0GeV with a current of > 10mA [3]. Such a system serves a dual purpose of energy multiplication and waste incineration. In this context, theoretical study of systematics of neutron scattering cross sections on various materials for neutron energies up to several hundred MeV are of practical importance. In this paper, we propose an empirical approach to successfully predict the energy dependence of total cross sections (σtot), shape elastic cross sections (σsc), reaction cross sections (σreac) and zero degree scattering angular distributions (σ0 or σ(θ = 0)), of the neutron-nucleus (n-N) scattering. The total cross sections are usually fitted by using the Ramsauer model. The nuclear Ramsauer model was first proposed by Lawson in the year 1953 as a simple means to understand the energy dependence of total cross sections of neutron nucleus scattering. In order to appreciate this model, it is necessary to discuss briefly the optical model (OM) description of neutron scattering. In the OM approach, complex optical model potentials (OMP) are used and the Schrodinger’s equation is solved to obtain the scattering amplitude. The real part of the OMP describes the scattering and the imaginary part results in attenuation or absorption of the incident wave. This absorption gives an estimate of the optical model reaction cross section. The calculations are usually performed using partial wave expansion method and the phase shifts (ηℓ = αℓe iβℓ) are determined. These complex phase shifts are strongly angular momentum and energy dependent for a given set of potentials.

\[ \sigma_{tot} = 2\pi \lambda^2 \sum \ell (2\ell + 1) [1 - \Re \eta\ell] \]  
\[ \sigma_{sc} = \pi \lambda^2 \sum \ell (2\ell + 1) |\eta\ell|^2 \]  
\[ \sigma_{reac} = \pi \lambda^2 \sum \ell (2\ell + 1) (1 - |\eta\ell|^2) \]  
\[ \frac{d\sigma}{d\Omega}(\theta) = \frac{\lambda^2}{4} \sum \ell (2\ell + 1)(1 - \eta\ell) P_\ell(\cos \theta)^2 \]

Extensive study of the optical model fits of scattering cross sections on various nuclei over wide energy range have been made by several groups. This is owing to the excellent data base of neutron cross sections available in the energy range up to 600 MeV [3, 4, 5]. The most recent work by Koning and Delarosche [6] presents a very exhaustive search for OMP parameters that fit the data very well up to 200 MeV. In the remaining part of our work, we use the OM code SCAT2 [7] with Koning and Delarosche potentials. We treat this as the “experimental data” for shape elastic, reaction, total scattering cross sections with spherical targets. We made a phenomenological Ramsauer model analysis of this data to derive systematics of Ramsauer model parameters and utilize it for further predictions. As mentioned before, the nuclear Ramsauer model [8] provides a simple means to parameterise the energy dependence of neutron nucleus total scattering cross sections. This model assumes that the scattering phase shifts are independent of angular momentum (ℓ) as given in Eq.(5) (η = αℓe iβ ) , in contrast to the predictions of the optical model given in Eq.(1). Further, it was proposed that the ℓ-independent phase shift varies slowly with energy. The model thus implies that the nucleus is seen as a right circular cylinder by the neutrons incident along the axis of symmetry. Owing to this unphysical picture, initially this model did

* The author Surya Narayan’s name appeared also as ”S.V.S. Sastry” in Nuclear physics journals.
not receive much attention, despite a successful demonstration of this model for neutron scattering from various nuclei by Peterson [9, 10]. There were some attempts to put this Ramsauer model on a sound theoretical basis [11, 12, 13, 14] (see references therein). The neutron total cross sections have thus been well studied using this model, over a wide range of nuclear masses as well as neutron energies up to 500 MeV [13, 14, 15, 16, 17, 18, 19]. Various cross sections used in the Ramsauer model are given below.

\[ \sigma_{\text{tot}} = 2\pi(R + \lambda)^2(1 - \alpha \cos \beta) \]  
\[ \alpha = \frac{a_0}{A^{1/3}} \]  
\[ \beta/A_p = a_0 \left( \sqrt{b_0 + c_0 E} - \sqrt{E} \right) \]  
\[ r_0 = 1.25519, \quad a_0 = 1.42042, \quad p = 0.29361 \]  
\[ a_0 = 3.0, \quad b_0 = 5.84633, \quad c_0 = 0.97676 \]

I. ANALYSIS OF TOTAL CROSS SECTIONS

We performed the Ramsauer model fits to total cross sections by using Eq.(5,7) for a set of seven nuclei with \( \chi^2/N = 653.762 \). The \( R, \alpha, \beta \) are functions of atomic mass number and the center of mass energy.

\[ \sigma_{\text{tot}} = 2\pi(R + \lambda)^2(1 - \alpha \cos \beta) \]  
\[ \sigma_{\text{se}} = \pi(R + \lambda)^2 \left[ ((1 - \alpha \cos \beta)^2 + (\alpha \sin \beta)^2 \right] \]

The \( \sigma_{\text{tot}} \) cross sections are shown in Fig. 1 with solid lines representing Ramsauer model fits using Eqs.(7-9) and the symbols represent the results from the optical model code SCAT2 [7]. The fits are obtained with total of six free parameters as given in Eq.(9), over wide mass range of \(^{27}\text{Al}\) to \(^{208}\text{Pb}\) and also covering the neutron energy region (\( E_{\text{cm}} \)) of 50-250 MeV. Similar Ramsauer model fits to total cross sections were already shown by various groups [14, 17] (and see the references therein). In these works, the normalised (relative to \(^{208}\text{Pb}\)) cross sections were shown for various nuclei [17]. Our functional dependence on energy and mass given in Eq.(8) with six global parameters was able to reproduce the SCAT2 results very well. The form of \( \beta \) given in Eq.(8) is chosen such that \( \beta/A_p \) is a global phase function for all nuclei, as shown versus energy in Figure 2. We have chosen this form of \( \alpha, \beta \) which directly scale by some power of mass rather than a polynomial function of mass in order to obtain a global function. The energy dependence of global \( \beta \) function has also been well discussed in literature. The parameter \( b_0 \) is called potential depth and \( c_0 \) (\( \approx 0.90 \)) is the non local parameter. The atomic number dependence of \( \beta \) can also be introduced through these parameters, however at the cost of global function.

II. RELATIONS BETWEEN VARIOUS CROSS SECTIONS

The total scattering cross section is defined as a sum of shape elastic and reaction cross sections given in Eq.(10).

\[ \sigma_{\text{tot}} = \sigma_{\text{se}} + \sigma_{\text{reac}} \]

Further, it has been observed [20, 21] earlier that the ratio (see Eq.(11)) of zero degree elastic cross section and the shape elastic cross sections shows linearity with...
energy. In the present work, we study this linearity in the energy range of 50-250 MeV. We observed that the linear relation is quite good at higher energy region above 150 MeV and this linearity remains valid over a large energy range at high energies. These ratios from SCAT2 for various nuclei are shown in Fig. 3 by symbols. They have been parameterised well (see solid lines in figure) by a function of the form given by Eq.(12). Making use of the Ramsauer assumption for these cross sections in Eqs.(2,4), it can be shown that the ratio has a simple form as in Eq.(12). This is because, the ratio involves \((\ell_{\text{max}} + 1)\) where we use \(\ell_{\text{max}} = \frac{4}{\lambda} + \frac{1}{2}\). For \(\gamma_0\) fits we used \(R = 1.254A^{1/3}\)fm in Eq.(12).

\[
\gamma_0 = \frac{d\sigma(\theta = 0)}{\sigma_{\text{se}}} \tag{11}
\]

\[
\gamma_0 = \left(\frac{R}{\lambda} + 1.5\right)^2 / 4\pi \tag{12}
\]

Therefore, inverting this equation and using the known shape elastic cross sections, we can obtain the zero degree elastic cross sections for a given energy. Therefore, \(\gamma_0\) serves as a relation between \(\sigma_{\text{se}}\) and \(\sigma(\theta = 0)\).

\[
\frac{d\sigma}{d\Omega}(\theta = 0) = \gamma_0 \sigma_{\text{se}} \tag{13}
\]

III. ANALYSIS OF REACTION CROSS SECTIONS

As mentioned in the introduction, we need to fit only two quantities and the other two will be derived. In section I, we parameterised the \(\sigma_{\text{tot}}(A, E)\) for all nuclei. The two important relations between various cross sections have been discussed in the previous section. Therefore, it suffices to parameterise one of the three remaining cross sections \(\sigma_{\text{reac}}, \sigma(\theta = 0), \sigma_{\text{se}}\). In this section we analyse the \(\sigma_{\text{reac}}\), the reaction cross sections and obtain \(\sigma(\theta = 0), \sigma_{\text{se}}\) as derived quantities. As shown in Eq.(3), the reaction cross sections involves only the transmission function \(i.e., (1-|\eta|^2)\). Unlike the \(\sigma_{\text{tot}}, \sigma_{\text{se}}\) and the angular distributions, the reaction cross sections do not involve \(\beta\) phase function. Therefore, we proceed to obtain the empirical fits to the reaction cross sections predicted by SCAT2 code. For this fits, we used the functional form and parameters given below, yielding a \(\chi^2/N=323.641\)

\[
\sigma_{\text{reac}} = \pi (R + 1.5\lambda)^2 e^{-\alpha} ; \quad \alpha = \alpha_0 \sqrt{E}/A_{\text{c}} \tag{14}
\]

\[
\alpha_0 = 0.20873 ; \quad r_0 = 1.38413 ; \quad p = 0.42507 \tag{15}
\]

It should be noted that the fitted parameters of Eq.(15) may not be equal to the corresponding parameters of Eq.(9), as these are effective parameters representing different phenomenological functional forms. One should also note that the multiplying radius dependence of these two equations are respectively, \(2\pi (R + \lambda)^2\) and \(\pi (R + 1.5\lambda)^2\). These \(\sigma_{\text{reac}}\) fits using three parameters given in Eqs.(14,15), are shown in Fig. 4 for all the nuclei studied. Figures (1,4) show that these cross sections of SCAT2 (symbols) are well reproduced by our empirical fitting functional forms and their parameters (lines in figures). Hence, we proceed to utilise these \(\sigma_{\text{reac}}\) fits to obtain other cross sections predicted by SCAT2 code.

The difference of the two parameterised cross sections gives shape elastic scattering as given by, \(\sigma_{\text{se}} = \sigma_{\text{tot}} - \sigma_{\text{reac}}\) as shown in Fig. 5(a). Making use of the \(\gamma_0\) and the \(\sigma_{\text{se}}\) of Fig. 5(a), the angular distribution at zero degree versus energy are obtained as shown in Fig. 5(b). In summary, we have fitted total scattering cross sections and reaction excitation functions and hence we derived \(\sigma_{\text{se}}, \sigma_{\text{elas}}(\theta = 0)\). These two derived cross sections also agree very well with the SCAT2 code predictions.

IV. WICKS LIMIT MODIFICATION FOR FORWARD ELASTIC SCATTERING

In this section, we describe the parameterization of energy dependence of zero degree elastic angular distributions and hence the \(\sigma_{\text{reac}}, \sigma_{\text{se}}\) will be derived quantities. It is well known that the optical theorem relates the total scattering cross section to the imaginary part of forward scattering amplitude is given by Eq. (16). However, the forward elastic angular distributions are defined in Eq. (17). In the Wick’s limit \[^{22}\] the real part of the forward scattering amplitude is neglected as in Eq. (18). Therefore,
FIG. 4: Phenomenological fits (lines) to reaction cross sections of optical model code SCAT2. The SCAT2 data (symbols) is fitted by exponential energy dependence multiplied by \((R + 1.5A)^2\) (see text). The fits need three parameters that are given in text. The curves from bottom to top are respectively for Al,Ca,Cu,Y,Sn,W,Pb.

The fractional deviation \(\delta\) of true angular distribution at zero degree for a given energy from the Wick’s limit is defined in Eq. (19).

\[
\begin{align*}
\sigma_{\text{tot}} &= \frac{4\pi}{k} |f(\theta = 0)|^2 = (\Im f(0))^2 + (\Re f(0))^2 \quad (16) \\
\sigma_0 &= |f(\theta = 0)|^2 = (\Im f(0))^2 + (\Re f(0))^2 \quad (17) \\
\sigma_0 &\approx \sigma_0^W = (\Im f(0))^2 - \left(\frac{k}{4\pi} \sigma_{\text{tot}}\right)^2 \quad (18) \\
\delta &= \frac{(\sigma_0 - \sigma_0^W)}{\sigma_0^W} \quad (19)
\end{align*}
\]

Whenever, \(\delta\) is small, Wick’s limit gives a good approximation to zero degree angular distributions. In depth study of this deviation function has been performed for several nuclei by Dietrich et. al.,[19]. They have presented the deviation function derived from optical model predictions and Wick’s limit values. In the present work, following [19], we have constructed the deviation function over 50-250 MeV center of mass energy range for seven target nuclei. We observed that these can be parameterised in terms of a Woods-Saxon function of energy, whose parameters are nuclear mass number dependent. Given below are the functional form for the deviation function and its parameters optimised for all nuclei.

\[
\begin{align*}
\delta &= \frac{(V_1 + V_2 E)}{1 + e^{(E_0 - E)/a_0}} \quad (20) \\
E_0 &= 61.557 + 0.47825A - 9.90931 \times 10^{-4}A^2 \quad (21) \\
V_2 &= 0.00217 - 2.26414 \times 10^{-5}A + 5.164 \times 10^{-8}A^2 \\
V_1 &= 0.15 + 143.04/A^2 \\
a_0 &= 13.48384
\end{align*}
\]

The deviation function derived from SCAT2 and its empirical fits are shown in Fig. 6. As shown in figure, the function with nine free parameters listed above, gives very good fits to data of SCAT2. We have also tried a logarithmic function, which gives similar quality of fits to deviation function with fewer number of parameters. It should be noted here that the \(\delta\) function can be given by some empirical prescription for all nuclei, very much similar to the fits of total cross sections. Once, \(\delta\) of Eq.(19) is known, using \(\sigma_0^W\) of Eq.(18), the zero degree elastic angular distribution versus energy can be obtained, as given by \(\sigma_0 = (1 + \delta)\sigma_0^W\). Consequent to knowing \(\sigma_0\),

FIG. 5: The derived cross sections for shape elastic (a) and the zero degree elastic angular distributions (b). The shape elastic is obtained as difference of total and reaction cross sections. The zero degree cross sections are obtained by using \(\gamma_0\) factor form shape elastic data.
we can use $\gamma_0$ of Eq.(11) to get the shape elastic cross sections $\sigma_{se}$. By subtracting the $\sigma_{se}$ from total cross section, we can fix the reaction cross section versus energy. We followed this scheme and the results are shown in Fig. 7. The agreement between the derived quantities from fits and the SCAT2 predictions is very good. It should be noted that the deviation function method accomplishes fitting of the zero degree angular distribution without need for a phase $\beta$ function. Otherwise, the angular distributions fits would need a phase function.

V. ANALYSIS OF SHAPE ELASTIC CROSS SECTIONS

In this section, we show the parameterization of the shape elastic cross sections, which need a phase $\beta$ function. The parameterization is performed very much similar to the fits of total cross sections. We followed Eq. (6) for the functional form and searched for the parameters. The $R, \alpha, \beta$ are functions of atomic mass number and the center of mass energy. The best fit functional form and the parameters are given below which yielded $\chi^2/N = 1222.97$ However, in these parameterizations, the $\beta$ function is more complicated, while maintaining the functional forms for other parameters.

$$\sigma_{se} = F \left[ (1 - \alpha \cos \beta)^2 + (\alpha \sin (\beta \alpha))^2 \right]$$

$$F = \pi (R + 1.5A)^2, \quad \gamma_0 = 1.20815$$

$$\alpha = \alpha_0/A^{1/3}; \quad \alpha_2 = \alpha_20/A^{2/3}$$

$$\beta = A^p a_0 \left( \sqrt{b_0 + c_0 E} - \sqrt{E} \right)$$

$$\alpha_0 = 1.08627, \quad \alpha_20 = 12.70632, \quad p = 0.3146$$

$$a_0 = 0.5534, \quad b_0 = 33.0085, \quad c_0 = 0.8626$$

The shape elastic cross sections fits are shown in Fig. 8 for all the systems, and the quality of fits is good. Following the shape elastic parameterization, the forward angular distribution can be obtained using $\gamma_0$ factor. The reaction is given as difference of total and shape elastic cross sections. The two derived quantities, $\sigma_{reaction}, \sigma_0$ agree well with SCAT2 data (not shown here). In summary, we considered three methods in sections III, IV, V where two of the four cross sections were parameterised and the remaining two were derived, as shown in the table.

Conclusion
We have analysed the predictions of optical model code SCAT2 for neutron nucleus scattering using Koning De- laroche potentials. We perform the Ramsauer model parameterization of total scattering cross sections and derive the systematics of the Ramsauer parameters. We have proposed an empirical fits to the reaction cross sections of SCAT2 and using this, the shape elastic cross sections have been obtained as the difference of these two empirical results. Using the $\gamma_0$ factor which is the ratio of forward elastic scattering to the shape elastic scattering, we determine the forward elastic angular distributions. Thus our empirical method is able to predict the SCAT2 results with a good accuracy for all these four quantities, namely $\sigma_{tot}, \sigma_{reac}, \sigma_{se}, \sigma(\theta = 0)$. We have studied the Wick’s limit of the forward elastic cross sections from SCAT2. We parameterised the deviation function of these angular distributions from Wick’s limit and using these as a alternative method, all the remaining cross sections have been obtained which compare well with SCAT2 results. The present method is about empirical estimates of the various cross sections, therefore it will be of practical importance wherever high energy neutron scattering cross sections are required for example for the accelerator driven sub critical assemblies.

![Empirical fits of shape elastic cross sections. The fitting functions and parameters are given in Eqs.(22-26)](image)

**Table I:** List of parameterised cross sections and the derived quantities in sections of the text. In above $\sigma_0$ represents zero degree angular distributions.

| Method | Fitted quantities | Derived quantities |
|--------|-------------------|--------------------|
| 1.     | $\sigma_{tot}, \sigma_{reac}$ | $\sigma_{se}, \sigma_0$ |
| 2.     | $\sigma_{tot}, \sigma_0$ | $\sigma_{se}, \sigma_{reac}$ |
| 3.     | $\sigma_{tot}, \sigma_{se}$ | $\sigma_{reac}, \sigma_0$ |

We acknowledge fruitful discussions with Dr. S. Kailas and Dr. A.K. Mohanty. We acknowledge Mr. Mukadam Mayuresh for technical support.

---

[1] C. Rubbia *et al.*, "Conceptual design of a fast Neutron Operated High power Energy Amplifier", CERN Rep, CERN/AT/95-44 (ET), Geneva, 29 Sep. 1995.
[2] IAEA-TEC-DOC-985, Accelerator Driven Systems ; Energy generation and Transmutation of Waste Status Report, Nov 1997, International Atomic Energy Agency, Vienna.
[3] R. W. Finlay, W. P. Abfalterer, G. Fink *et al.*, Phys. Rev. C47, 237 (1993).
[4] F. S. Dietrich, W. P. Abfalterer, *et al.*, LANSE – WNR, Proc. Int. Conf. Nucl. data for Sci. and Tech., Trieste, Italy, May 19-24, 1997, Vol.59, p.402, Italian Phys. Soc. (1997).
[5] W. P. Abfalterer, F. B. Bateman, *et al.*, Phys. Rev C63, 044608, (2001).
[6] A. J. Koning and J. -P. Delaroche, Nucl. Phys. A713, 231 (2003).
[7] O. Bersillon, "SCAT2" Program, Note CEA-N-2227, Centre d’Etudes Nucleaires de Bruyeres-Chatel, Service de Physique et techniques Nucleaires, France (Oct. 1981).
[8] J. D. Lawson, Phil. Mag., 44, 102 (1953).
[9] J. M. Peterson, Phys. Rev. 125, 955 (1962).
[10] A. Bohr and B. Mottelson, Nuclear Structure, Vol. 1 P.166, Benjamin, N.Y. (1969).
[11] V. Franco, Phys. Rev. B140, 1501 (1965).
[12] C. R. Gould *et al.*, Phys. Rev. Lett. 53, 2371 (1986).
[13] J. D. Anderson and S. M. Grimes, Phys. Rev. C41, 2904 (1990).
[14] S. M. Grimes, J. D. Anderson, R. W. Bauer and V. A. Madsen, Nucl. Sci. and Engg. 130, 340 (1998).
[15] V. A. Madsen, J. D. Anderson, S. M. Grimes, V. R. Brown and P. M. Antony, Phys. Rev. C56, 365 (1997).
[16] R. W. Bauer *et al.*, Nucl. Sci. and Engg. 130, 348 (1998).
[17] S. M. Grimes, J. D. Anderson, R. W. Bauer and V. A. Madsen, Nucl. Sci. and Engg. 134, 77 (2000).
[18] S. M. Grimes, J. D. Anderson and R. W. Bauer, Nucl. Sci. and Engg. 135, 296 (2000).
[19] F. S. Dietrich, J. D. Anderson and R. W. Bauer, Phys. Rev. 68, 064608 9(2003).
[20] M. Azam and R. S. Gowda, Nucl. Sci. and Engg. 144, 1 (2003).
[21] R. S. Gowda and S. Ganesan, Submitted to Nucl. Sci. and Engg.
[22] G. C. Wick, Phys. Rev. 75, 1459 (1949).