International Atomic Energy Agency

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A Computer Code for Nuclear Optical Model Calculations

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July 1995

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Reproduced by the IAEA in Austria
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ABSTRACT

The report describes the details of the spherical optical model code developed by the author. The details include mathematical formulations and their methods of solutions. The code computes differential elastic scattering cross sections for neutrons and protons, nuclear polarization, Mott-Schwinger polarization and total cross sections for neutrons. The code also gives volume integrals of potentials and average values of potential radii, potential scattering length and strength functions. A comparison of the calculations of the present code with those done using other codes is also provided.

Contents

1. Introduction

The nuclear optical model plays a fundamental role in nuclear reaction calculations for nuclear data. It is widely used for computation of elastic differential scattering cross sections, polarizations, reaction cross sections, neutron total cross sections, S-wave and P-wave strength functions, and scattering lengths. The wave functions derived from optical model potentials are used in DWBA calculations and penetrabilities based on optical model are used in Hauser-Feshbach calculations. Recently due to the availability of a large amount of scattering data in positive energy range, a considerable interest has been shown in determining an optical model potential nuclear mean field that can explain experimental data in both positive and negative energy ranges giving rise to dispersive optical model analysis [1-5]. However the basis of these calculations still remains the phenomenological optical model analysis which also constitutes the theme of the present report. The report provides the details of the optical model code developed by the author. At this stage it does not have the facility for optimization of optical model parameters. It gives elastic differential scattering cross sections, neutron total cross sections, nuclear and Mott-Schwinger polarization for neutrons, reaction cross sections, S-wave, P-wave and D-wave neutron strength functions and scattering lengths. It also gives volume integrals of real and imaginary potentials as well as the root mean square values of potential radii. The code has already been used in the analysis of 14 MeV neutron scattering data [6-7] and forms a part of the Hauser-Feshbach code developed by the author that will be used for nuclear data calculations. Therefore, it is considered very appropriate to publish the details of the mathematical formulations and the methods of their solutions used in the present code.

2. Mathematical Formulation

2.1 The Optical Model Potential

The optical model regards a nucleus as a 'cloudy crystal ball' that partly transmits and partly absorbs the incident nuclear radiations. The partial absorption of the nuclear radiations is achieved by making the two body nuclear potential a complex one. The imaginary component of the potential gives rise to the absorption of the incident radiation which results in the compound elastic and non-elastic processes. The details of the model and its historical development could be found in the literature [8-11]. The nuclear optical model potential is taken as

$$V(r) = V_c(r) - U\, f(r) - i\left[W_v f(r) + W_D g(r)\right] - \left(U_s + iW_s\right) h(r)\, \underline{\ell}.\underline{\sigma} \qquad (1)$$

where r is the separation of the two interacting particles. $V_c(r)$ is the Coulomb potential and it is taken to be that of a charged sphere of radius $R_c = r_c A^{1/3}$

$$\begin{aligned} V_c(r) &= \frac{Z_i Z_t e^2}{2\,R_c}\left(3 - \frac{r^2}{R_c^2}\right) \text{ for } \quad r \le R_c \\ &= \frac{Z_i Z_t e^2}{r} \qquad \text{for} \quad r > R_c \end{aligned} \qquad (2)$$

where U, W_v and W_D are the real, imaginary volume and imaginary surface components of the central potential respectively. U_s and W_s are the real and imaginary spin-dependent potential. Evidence for spin-dependence of nuclear forces comes from the nuclear shell model and observation of the phenomenon of polarization of particles scattered from nuclei. $\underline{\ell}$ and $\underline{\sigma}$ are the orbital and Pauli spin operators for spin−1/2 particles. The scattering of spin−1/2 particles from nuclei with zero ground state spin is considered in the present code. The f(r), g(r) and h(r) are Saxon-Woods, Saxon-Woods derivative and Thomas-type geometrical form factor that give variation of the potential with the radius of the nucleus. These have the following forms

$$f(r) = \frac{1}{1 + \exp\left(\frac{r - R}{a}\right)} \qquad (3)$$

$$g(r) = -4a\,\frac{df(r)}{dr} \qquad (4)$$

$$\begin{aligned} h(r) &= -\left[\frac{\hbar}{m_\pi c}\right]^2 \frac{1}{r}\,\frac{df(r)}{dr} \\ &= -2\,\frac{1}{r}\,\frac{df(r)}{dr} \end{aligned} \qquad (5)$$

where r, a are in fermis.

2.2 Solution of the Schrodinger Equation

The determination of the cross section is carried out employing the method of partial wave phase shift analysis [12] using the Schrodinger equation

$$\nabla^2 \psi + \frac{2\mu}{\hbar^2}(E - V(r))\psi = 0 \tag{6}$$

where μ and E are the reduced mass and the centre-of-mass energy of the incident particle. The total wave function ψ is expressed in terms of radial wave function, spherical harmonics and spin wave function as follows.

$$\psi = \sum_{jlm} \frac{u_{jl}(r)}{r} \sum_{\mu\lambda} C^{jls}_{m\lambda\mu}\, y_l^{\lambda}(\theta,\phi)\, X_s^{\mu} \tag{7}$$

where $C^{jls}_{m\lambda\mu}$ is Clebsch-Gordan coefficient. The eigen values of $\underline{\ell} \, . \, \underline{\sigma}$ for the spin of the particle being parallel and antiparallel corresponding to the two j-values of (ℓ +1/2) and (ℓ -1/2) are ℓ and -(ℓ +1) that correspond to the radial wave functions $u_\ell^+(r)$ and $u_\ell^-(r)$ respectively. The two wave functions are solution of the following two equations.

$$\frac{d^2u_\ell^+(\rho)}{d\rho^2} + \left[1 - \frac{V_c(\rho)}{E} + \frac{Uf(\rho) + iW_D g(\rho) + iW_v f(\rho)}{E} + \frac{\ell(U_s + iW_s)h(\rho)}{E} - \frac{\ell(\ell+1)}{\rho^2}\right] u_\ell^+(\rho) = 0 \tag{8(a)}$$

$$\frac{d^2u_\ell^-(\rho)}{d\rho^2} + \left[1 - \frac{V_c(\rho)}{E} + \frac{Uf(\rho) + iW_D g(\rho) + iW_v f(\rho)}{E} - \frac{(\ell+1)(U_s + iW_s)h(\rho)}{E} - \frac{\ell(\ell+1)}{\rho^2}\right] u_\ell^-(\rho) = 0 \tag{8(b)}$$

where $\rho = kr$, k being the wave number given by

$$k = \frac{\sqrt{2\mu E}}{\hbar} = 0.218728(\mu\, E)^{\frac{1}{2}} fm^{-1} \tag{9}$$

E, the centre of mass energy, is the energy in MeV and μ, the reduced mass, is given by $A_i A_t / (A_i + A_t)$; A_i and A_t are the masses of the incident and target nuclei in amu.

The radial wave functions are zero at the origin and beyond the nuclear field they tend asymptotically to the forms

$$u_\ell^\pm(\rho) = F_\ell(\rho)+iG_\ell(\rho)+S_\ell^\pm(F_\ell(\rho)-iG_\ell(\rho)) \tag{10}$$

where

$$S_\ell^\pm = \exp(2i\delta_\ell^\pm) \tag{11}$$

are the complex elements of the scattering matrix. $F_\ell(\rho)$ and $G_\ell(\rho)$ are regular and irregular wave functions which are the solutions of eq. (8) without the nuclear potentials. These functions are taken to have the asymptotic forms

$$F_\ell(\rho) \underset{\rho\to\infty}{\to} \sin\left[\rho-\eta\ \ln(2\rho)-\ell\frac{\pi}{2}+\sigma_\ell\right] \tag{12}$$

$$G_\ell(\rho) \underset{\rho\to\infty}{\to} \cos\left[\rho-\eta\ \ln(2\rho)-\ell\frac{\pi}{2}+\sigma_\ell\right] \tag{13}$$

where

$$\eta = \frac{\mu Z_I Z_T e^2}{k\hbar^2} = 0.157454\, Z_I Z_T\ (A_i/E_o)^{1/2} \tag{14}$$

where E_o is the energy of incident particle in the laboratory system and is expressed in MeV. Z_I and Z_T represent the charge states of the incident and target nuclei. σ_ℓ is the Coulomb phase-shift of the ℓth partial wave. The non spin-flip and the spin flip scattering amplitudes are given by

$$A(\theta) = f_c(\theta)+\left(\frac{1}{2ik}\right)\sum_{\ell=0}^{\infty}\{(\ell+1)S_\ell^+ +\ell S_\ell^- -(2\ell+1)\}P_\ell(\cos\theta)\exp(2i\sigma_\ell) \tag{15}$$

$$B(\theta) = \left(\frac{1}{2ik}\right)\sum_{\ell=0}^{\infty}\{S_\ell^+ - S_\ell^-\}P_\ell^1(\cos\theta)\exp(2i\sigma_\ell) \tag{16}$$

where $P_\ell(\cos\theta)$ and $P_\ell^1(\cos\theta)$ are Legendre polynomials and associated Legendre functions. $f_c(\theta)$ is Coulomb scattering amplitude and it is given by

$$f_c(\theta) = -\left(\frac{\eta}{2k}\right)\operatorname{cosec}^2\left(\theta/2\right)\exp\left[2i\sigma_o - 2i\eta\ \ln\left\{\sin\left(\theta/2\right)\right\}\right] \tag{17}$$

2.3 Nuclear Scattering Cross Sections and Polarization

The differential scattering cross section is given by

$$\sigma(\theta) = |A(\theta)|^2 + |B(\theta)|^2 \tag{18}$$

The polarization of the elastically scattered particles is given by

$$P(\theta) = \frac{2\mathrm{Im}\,(AB^*)}{|A|^2 + |B|^2}\,\underline{n} \tag{19}$$

where

$$\underline{n} = \frac{\underline{k}_i \times \underline{k}_f}{|\underline{k}_i \times \underline{k}_f|} \tag{20}$$

The total absorption cross section is given by

$$\sigma_A = \frac{\pi}{k^2}\sum_{\ell=0}^{\infty}\left\{(\ell+1)\left(1-|S_\ell^+|^2\right)+\ell\left(1-|S_\ell^-|^2\right)\right\} \tag{21}$$

If the incident particles are uncharged, $V_c(\rho)$, $f_c(\theta)$ and σ_ℓ are all zero and the total elastic cross section is finite and given by

$$\sigma_E = \frac{\pi}{k^2}\sum_{\ell=0}^{\infty}\left\{(\ell+1)\,|1-S_\ell^+|^2 + \ell\,|1-S_\ell^-|^2\right\} \tag{22}$$

The total cross section is given by

$$\sigma_t = \frac{2\pi}{k^2}\sum_{\ell=0}^{\infty}\left\{(\ell+1)(1-\mathrm{Re}\;S_\ell^+)+\ell(1-\mathrm{Re}\;S_\ell^-)\right\} \tag{23}$$

In practice only a finite number of partial waves are included in the above summation and higher partial waves whose contributions are negligible are excluded.

2.4 Mott-Schwinger Polarization

Neutrons get also polarized due to their magnetic moment while moving in the Coulomb field of the nucleus. Schwinger [13] using Born approximation gave the following expression for the neutron polarization while assuming no nuclear spin orbit potential.

$$P_m(\theta) = \frac{-2\gamma \cot(\theta/2) \ \mathrm{Im}(A(\theta))}{|A(\theta)|^2 + \gamma^2 \cot^2(\theta/2)} \quad (24)$$

where A(θ) is the nuclear scattering amplitude with no-spin orbit potential and γ is given by

$$\gamma = \frac{\mu_n Ze^2}{2Mc^2} = 1.46Z \times 10^{-3}\,\mathrm{fm} \quad (25)$$

Here μ_n is the numerical value of the magnetic moment (1.91) in the units of Bohr nuclear magnetons. M is the mass of the neutron and c is the velocity of light.

2.5 Volume Integrals and Average Potential Radii

The formulas for volume integrals of potentials, and average potential radii are derived in the appendix using approximations given by Elton [14]. The volume integral of the real potential is given by

$$J_v = \frac{4\pi}{A}\int_0^\infty U(r)r^2dr = \frac{4\pi}{3}r_v^3\left(1+\left(\frac{\pi a}{R}\right)^2\right)U_o \quad (26)$$

where a Saxon-Woods geometrical form factor is used. U_o is the strength of the potential, a is the diffusness parameter and $R = r_v A^{1/3}$.

The volume integral of the surface imaginary potential is given by

$$J_W = \frac{4\pi}{A}\int_0^\infty W(r)r^2dr = \frac{16\pi R^2}{A}aW_o\left[1+\frac{1}{3}\left(\frac{\pi a}{R}\right)^2\right] \quad (27)$$

where W_o is the strength of surface potential. Volume integral of the imaginary potential representing volume absorption is given by eq. (26) with V_o replaced by W_v and $R=r_i A^{1/3}$.

The mean square radius of potential assuming Saxon-Woods geometrical factor is given by

$$< r^2 >_{SW} \;=\; \frac{3}{5}R_v^2\left[\frac{1+\frac{10}{3}\left(\frac{\pi a}{R_v}\right)^2+\frac{7}{3}\left(\frac{\pi a}{R_v}\right)^4}{1+\left(\frac{\pi a}{R_v}\right)^2}\right] \tag{28}$$

The average mean square radius of the potential of the surface absorption nature is given by

$$< r^2 >_{SWD} \;=\; R_d^2\left[\frac{1+2\left(\frac{\pi a}{R_d}\right)^2+\frac{7}{15}\left(\frac{\pi a}{R_d}\right)^4}{1+\frac{1}{3}\left(\frac{\pi a}{R_d}\right)^2}\right] \tag{29}$$

2.6 Strength Functions and Scattering Length

Below 100 KeV the total cross section for S-wave neutron is written as

$$\sigma_T \;=\; \frac{2\pi}{k^2}\, S_o + 4\pi R_{pot}^2 \tag{30}$$

where the first term represents the absorption cross section and the second term represents the potential or shape elastic scattering. S_o is the S-wave strength function and R_{pot} is potential scattering length. In general the normalized strength function for ℓ-wave is defined as

$$S_\ell \;=\; \frac{T_\ell}{2\pi}\;\frac{1}{v_\ell}\;\left(\frac{E_1}{E_o}\right)^{1/2} \tag{31}$$

where

v_ℓ	=	Penetrability of centrifugal barrier for a neutron having orbital angular momentum quantum number ℓ
E_o	=	Energy of the incident particle

$E_l \quad = \quad 1 \text{ eV}$

$T_\ell \quad = \quad 1-|S_\ell|^2$

The strength functions, S_o, S_1 and S_2 for S-, P- and D- wave neutrons respectively are

$$S_o = \left(\frac{T_o}{2\pi}\right)\left(\frac{E_l}{E_o}\right)^{1/2}$$

$$S_1 = \left(\frac{T_l}{2\pi}\right)\left(\frac{1+k^2R^2}{k^2R^2}\right)\left(\frac{E_l}{E_o}\right)^{1/2}$$

$$S_2 = \left(\frac{T_2}{2\pi}\right)\left(\frac{9+3k^2R^2+k^4R^4}{k^4R^4}\right)\left(\frac{E_l}{E_o}\right)^{1/2}$$

R_{pot} is given by

$$R_{pot} = \sqrt{\frac{\sigma_E}{4\pi}} \qquad (32)$$

Here k is the wave number and $R=1.35A^{1/3}$

3. Methods of Computations

The methods of computations described in Refs.[15-16] were adopted in the present code. The determination of all observable quantities involves the knowledge of scattering matrix S_ℓ which is calculated by equating the logarithmic derivative of the internal and external wave functions at the boundary of the nucleus or matching radius. The external wave function contains regular and irregular Coulomb wave functions. The regular Coulomb wave functions have been determined by Miller's method [17]. This method sets $F_{\ell+1}(\rho)=0$ and $F_\ell(\rho)= \in$ where $\in$ is a very small number. Here $\ell=\ell_{max}+10$ is considered adequate where ℓ_{max} is the maximum partial wave contributing to the cross sections. α is a constant which is determined using the Wronskian

$$F_o'(\rho)\, G_o(\rho) - F_o(\rho)\, G_o'(\rho) = 1 \qquad (33)$$

All the lower values of regular Coulomb wave functions were determined from the following recurrence relation

$$\frac{[\eta^2+\ell^2]^{1/2}}{\ell}\,F_{\ell-1}(\rho)=(2\ell+1)\left[\frac{\eta}{\ell(\ell+1)}+\frac{1}{\rho}\right]F_\ell(\rho)-\left[\frac{\{\eta^2+(\ell+1)^2\}^{1/2}}{\ell+1}\right]F_{\ell+1}(\rho) \qquad (34)$$

and $F_o'(\rho)$ was calculated from the recurrence relation

$$\left[\frac{\eta}{\ell+1}+\frac{\ell+1}{\rho}\right]F_\ell(\rho)-F_\ell'(\rho)=\frac{[\eta^2+(\ell+1)^2]^{1/2}}{\ell+1}F_{\ell+1}(\rho) \qquad (35)$$

$G_o(\rho)$ and $G_o'(\rho)$ were calculated as describe below.

The irregular Coulomb wave functions and their derivatives were determined using the following expressions.

$$\begin{aligned} G_o(\rho) &= s\ \cos\ \theta - t\sin\theta \\ G_o'(\rho) &= S\cos\theta - T\ \sin\ \theta \end{aligned} \qquad (36)$$

where

$$\theta=-\eta\ \ln(2\rho)+\rho+\sigma_o$$

s, t, S and T are given by

$$s=\sum_{n=0}^{25}s_n,\quad t=\sum_{n=0}^{25}t_n,\quad S=\sum_{n=0}^{25}S_n,\quad T=\sum_{n=0}^{25}T_n \qquad (37)$$

The required terms in the above series are calculated from the following relations

$$\begin{aligned} s_{n+1} &= \frac{A_1}{A_2}s_n-\frac{A_3}{A_2}t_n \\ t_{n+1} &= \frac{A_1}{A_2}t_n+\frac{A_3}{A_2}s_n \\ S_{n+1} &= \frac{A_1}{A_2}S_n-\frac{A_3}{A_2}T_n-\frac{s_{n+1}}{\rho} \\ T_{n+1} &= \frac{A_1}{A_2}T_n+\frac{A_3}{A_2}S_n-\frac{t_{n+1}}{\rho} \end{aligned} \qquad (38)$$

where

$$A_1 = (2n+1)\eta$$
$$A_2 = 2\rho\ (n+1)\eta$$
$$A_3 = \eta^2 - n(n+1)$$

with the following initial values

$$\begin{aligned}
&s_o = 1\,, \qquad s_1 = \frac{\eta}{2\rho}\,; \qquad S_o = 0\,,\\
&S_1 = \frac{\eta^3 - \eta^2}{2\rho^2} - \frac{\eta^2}{2\rho}\,;\\
&t_o = 0\,, \qquad t_1 = \frac{\eta^2}{2\rho}\,; \qquad T_o = 1 - \frac{\eta}{\rho}\\
&T_1 = \frac{-\eta^2}{\rho^2} + \frac{\eta}{2\rho}\,;
\end{aligned} \tag{39}$$

The summations s, S, t and T are required to satisfy the following relation

$$sT - St = 1 \tag{40}$$

Since the convergence of the above series improves as ρ increases, a value of ρ substantially greater than ρ_m must be used. To ensure accuracy, ρ is first set to a suitable starting value and the series are summed. If the eq. (40) is satisfied to 1 part in 10^4, the values are accepted if not ρ is increased in steps until the relation is satisfied in the required accuracy limit. since the values of $G_o(\rho)$ and $G'_o(\rho)$ are calculated at a distance greater than the matching radius $\rho_{m,}$ the values of $G_o(\rho)$ and $G'_o(\rho)$ at the matching radius are obtained by integrating numerically in the inward direction the following equation

$$\begin{aligned}
&\frac{d^2u_\ell(\rho)}{d\rho^2} + \left[1 - \frac{2\eta}{\ell} - \frac{\ell(\ell+1)}{\rho^2}\right]u_\ell(\rho) = 0\\
&\frac{d^2u_\ell(\rho)}{d\rho^2} = -\left[1 - \frac{2\eta}{\ell} - \frac{\ell(\ell+1)}{\rho^2}\right]u_\ell(\rho)\\
&u''(\rho) = F(\rho, u_\ell)\\
&u''(\rho) = A(\rho)\ u_\ell(\rho)
\end{aligned} \tag{41}$$

In the present case $\ell = 0$ and $u_o(\ell) = G_o(\rho)$ and $u'_o(\rho) = G'_o(\rho)$. We drop ℓ from u's. The inward integration is done using Runge-Kutta method [18]. Given the function and its derivative at the ith step, the function and its derivative at the (i+1)th step are calculated as follows.

$$
\begin{aligned}
&u''_{i,1} = F(\rho_i,\ u_{i,1}) && u_{i,2} = u_{i,1} + \frac{h}{2}u''_i \\
&u''_{i,2} = F\left(\rho_i + \frac{h}{2},\ u_{i,2}\right) && u_{i,3} = u_{i,2} + \frac{h^2}{4}u_{i,1} \\
&u''_{i,3} = F\left(\rho_i + \frac{h}{2},\ u_{i,3}\right) && u_{i,4} = u_{i,2} + \frac{h}{2}u'_{i,1} + \frac{h^2}{2}u''_{i,2} \\
&u''_{i,4} = F(\rho_i + h,\ u_{i,4}) && \\
&u_{i+1,1} = u_{i,1} + \frac{h^2}{6}\left(u''_{i,1} + u''_{i,2} + u''_{i,3}\right) + hu'_{i,1} && \\
&u'_{i+1,1} = u'_{i,1} + \frac{h}{6}\left(u''_{i,1} + 2u''_{i,2} + 2u''_{i,3} + u''_{i,4}\right) &&
\end{aligned}
\tag{42}
$$

Where h is the basic integrating step.

$G_\ell(\rho)$ and $G_\ell(\rho_m)$ were calculated using the relationship expressed by the eq. (34).

The values of the internal wave functions at the matching radius are obtained by integrating eq. 8 numerically up to ρ_m=kR+7ka where R is the maximum value of the radius of the potential ($R=r_oA^{1/3}$). The Fox-Goodwin method [19] was used for the numerical integration of eq. 8 for internal region.

$$
u_{i+1}(\rho) = \frac{\left[2 + \frac{5}{6}h^2 A_i(\rho)\right]u_i(\rho) - \left[1 - \frac{h^2}{12}A_{i-1}(\rho)\right]u_{i-1}(\rho)}{1 - \left(\frac{h^2}{12}\right)A_{i+1}(\rho)}
\tag{43}
$$

As the technique does not involve the evaluation of the first order differential during the integration it is to be evaluated by using the following expression

$$u_i'(\rho) = \left(\frac{1}{60h}\right)\left[45\left(u_{i+1}(\rho) - u_{i-1}(\rho)\right) - 9\left(u_{i+2}(\rho) - u_{i-2}(\rho)\right) + \left(u_{i+3}(\rho) - u_{i-3}(\rho)\right)\right] \quad (44)$$

The initial values are taken as $u_0(\rho)=0$, $u_1(\rho)=C$ where C is a small number with the stipulation that $A_o(\rho)u_o(\rho) = 0$ for $\ell \neq 1$ and $A_o(\rho)u_o(\rho) = 2$ for $\ell = 1$.

4. Comparison with other Codes

In order to check on any serious mistakes in the present code it is necessary to compare the calculations done using the present code with published calculations based on other codes. Such a comparison is provided for 17 MeV protons scattered from Gold in table 1. The calculations of the present code are in good agreement with calculations reported by Buck et al [15]. The present code was run on VAX/780. In table 2 a comparison of the present calculations of 3.5 MeV neutrons scattered from ^{58}Ni is provided with those done using 'ABAREX CODE' [21] and SCAT2 Code [22]. Similarly table 3 lists a comparison of these codes for 10 keV neutrons scattered from ^{56}Fe. The 'ABAREX' results of cross sections given in the laboratory system have been converted for comparison to centre of mass system by using appropriate solid angle-ratio values. The results of the present calculations are in a good agreement with the calculations of the codes included for the comparison.

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Table 1

Comparison of the results of the present computer programme with those reported earlier [15] for 17 MeV protons on gold, with U=48 MeV, W=8 MeV, r_o=1.3 fm, r_c=1.3 fm, a=0.5 fm, A_I=1 amu, A_T=197 amu. No spin-orbit potentials were used. Both form factors are Saxon-Woods. All cross sections are in barn/sr.

θ (c.m.)	$\frac{d\sigma}{d\Omega}$ [Buck et al]	$\frac{d\sigma}{d\Omega}$ [Melkanoff]	$\frac{d\sigma}{d\Omega}$ [Present]
20	32.03	32.02	32.10
40	1.549	1.549	1.554
60	0.295	0.295	0.295
80	0.07624	0.06728	0.0684
120	0.01458	0.01460	0.01476
160	0.00781	0.00782	0.00792
σ_R	0.9847 barn	0.9852 barn	0.985 barn

Table 2

Comparison of scattering cross sections of 3.5 MeV neutrons on ^{58}Ni with the following parameters. U=45.1 MeV, r_o=1.298 fm, a_v=0.638 fm, W_v=0, W_d=11.3 MeV, r_w=1.30 fm, a_v=0.334 fm, U_s=5.5 MeV, r_s=1.005 fm, a_s=0.650 fm. All cross sections are in barn and angles in degrees. ABAREX calculations are taken from Ref. [21] and apply to angles given in brackets.

$\theta_{c.m.}$	$\frac{d\sigma}{d\Omega}$ [ABAREX]	($\theta_{c.m.}$)	$\frac{d\sigma}{d\Omega}$ [SCAT2]	$\frac{d\sigma}{d\Omega}$[Present]
0	1.520	(0.0)	1.513	1.529
20	1.129	(20.3)	1.135	1.147
40	0.427	(40.6)	0.443	0.447
60	0.0457	(60.9)	0.0523	0.0525
80	0.0198	(81.1)	0.0175	0.0173
100	0.0813	(101.0)	0.0802	0.0801
120	0.0681	(120.9)	0.0703	0.0702
140	0.0179	(140.6)	0.0190	0.0187
160	0.0179	(160.3)	0.0179	0.0179
180	0.0364	(180.0)	0.0370	0.0373
σ_E	2.070 barn		2.061 barn	2.077 barn
σ_R	1.512 barn		1.513 barn	1.1512 barn

Table 3

Comparison of the calculations of the observables of 0.01 MeV neutrons scattered from ^{56}Fe. The following parameters were used. A_I=1.01 amu, A_T=55.94 amu, V=46 MeV, r_v=1.317fm, a_v=0.62 fm, W_v=0, W_d=14 MeV, r_w=1.447 fm a_w=0.25 fm, U_s=7.0 MeV, W_s=0, r_s=1.317 fm a_s=0.62 fm. All cross sections are in barn. The differential cross sections are in barn/sr and angles are in degrees. Comments in Table 2 for ABAREX apply here too.

$\theta_{c.m.}$	$\frac{d\sigma}{d\Omega}$[SCAT2]	$\frac{d\sigma}{d\Omega}$ [ABAREX]($\theta_{c.m.}$)		$\frac{d\sigma}{d\Omega}$ [Present]
0	0.4227	0.4491	(0.0)	0.4490
15	0.4223	0.4487	(15.3)	0.4489
30	0.4213	0.4481	(30.5)	0.4480
45	0.4201	0.4466	(45.7)	0.4468
60	0.4185	0.4454	(60.5)	0.4451
75	0.4166	0.4433	(76.0)	0.4433
90	0.4146	0.4412	(91.0)	0.4413
105	0.4127	0.4391	(106)	0.4393
120	0.4108	0.4374	(120.9)	0.4375
135	0.4093	0.4360	(135.7)	0.4360
150	0.4081	0.4349	(150.5)	0.4348
165	0.4073	0.4339	(165.3)	0.4340
180	0.4071	0.4340	(180.0)	0.4338

Quantity	SCAT2	ABAREX	Present
σ_R	15.205 barn	14.387 barn	14.381 barn
σ_E	5.219 barn	5.547 barn	5.5460 barn
S_o	3.609×10^{-4}	3.835×10^{-4}	3.325×10^{-4}
S_I	0.3535×10^{-4}	0.3465×10^{-4}	0.3255×10^{-4}
R	6.439 fm	6.508 fm	6.643 fm
J_u	499.39 MeV -fm^3	505.980 MeV -fm^3	505.979 MeV -fm^3
J_w	97.52 MeV -fm^3	96.936 MeV -fm^3	96.966 MeV -fm^3

Appendix

In the appendix we give calculations of the mean square radii of the potentials with Saxon-Woods and Saxon-Wood derivative geometrical form factors. We also give the details of the calculations of the volume integrals of potentials per nuclear for the two types of geometrical form factors.

1. Mean Square Radius for Saxon-Woods geometrical Form Factor

$$< r^2 >_{SW} = \frac{4\pi\int_0^\infty \frac{r^4 dr}{1+\exp\left(\frac{r-R_v}{a}\right)}}{4\pi\int_0^\infty \frac{r^2 dr}{1+\exp\left(\frac{r-R_v}{a}\right)}} \tag{A1}$$

we put x=r/a which gives dr=adx

$$k = \frac{R_v}{a}$$

$$\text{Numerator} = 4\pi\int_0^\infty \frac{r^4 dr}{1+\exp\left(\frac{r-R_v}{a}\right)} = 4\pi a^5 \int_0^\infty \frac{x^4 dx}{1+e^{x-k}} = 4\pi a^5 F_4(k) \tag{A2}$$

where

$$F_n(k) = \frac{k^{n+1}}{n+1} - \sum_{m=1}^{\infty} \frac{(-1)^m}{m} \left\{ \sum_{r=0}^{n} [1-(-1)^r] \frac{n!}{m^r (n-r)!} k^{n-r} \right\} \tag{A3}$$

for n=4, r=1 and 3 contribute and we get

$$F_4(k) = \frac{k^5}{5} + 8k^3\left[\frac{1}{1^2} - \frac{1}{2^2} + \frac{1}{3^2} + \ldots\right] + 48k\left[\frac{1}{1^4} - \frac{1}{2^4} + \frac{1}{3^4} - \ldots\right]$$

$$F_4(k) = \frac{k^5}{5} + 8k^3\frac{\pi^2}{12} + 48k\frac{7\pi^4}{720} \tag{A4}$$

$$F_4(k) = \frac{R_v^5}{5a^5} + \frac{2\pi^2}{3}\frac{R_v^2}{a^3} + \frac{7}{15}\pi^4\frac{R_v}{a}$$

Therefore the

$$\text{Numerator} = \frac{4\pi}{5}R_v^5\left[1+\frac{10}{3}\left(\frac{\pi a}{R_v}\right)^2+\frac{7}{3}\left(\frac{\pi a}{R_v}\right)^4\right]$$

$$\text{Denominator} = 4\pi\int_0^\infty \frac{r^2 ar}{1+\exp\left(\frac{r-R_v}{a}\right)} = 4\pi a^3\int_0^\infty \frac{.x^2dx}{1+\exp(x-k)} \qquad \text{(A5)}$$

$$= 4\pi a^3 F_2(k)$$

where $$F_2(k) = \int_0^\infty \frac{x^2dx}{1+\exp(x-k)}$$

Now using eq. A3, we get

$$F_2(k) \quad = \quad \frac{k^3}{3}+4k\left[\frac{1}{1^2}-\frac{1}{2^2}+\frac{1}{3^2}+\ \ldots\right]$$

$$= \quad \frac{k^3}{3}+4k\frac{\pi^2}{12}=\frac{k^3}{3}+\frac{\pi^2 k}{3} \qquad \text{(A6)}$$

Therefore the denominator becomes

$$\text{Denominator} \quad = \quad \frac{4\pi a^3}{3}\left[k^3+\pi^2 k\right]$$

$$= \quad 4\pi R_v^3\left[1+\left(\frac{\pi a}{R_v}\right)^2\right] \qquad \text{(A7)}$$

Thus $$\langle r^2\rangle_{sw} \quad = \quad \frac{3}{5}R_v^2\left[\frac{1+\frac{10}{3}\left(\frac{\pi a}{R_v}\right)^2+\frac{7}{3}\left(\frac{\pi a}{R_v}\right)^4}{1+\left(\frac{\pi a}{R_v}\right)^2}\right] \qquad \text{(A8)}$$

2. Mean Square Radius for Derivative Form Factor

The mean square radius for the distribution of derivative form factor is given by

$$\langle r^2 \rangle_{SWD} = \frac{4\pi \int_0^\infty \frac{r^4 \exp\left(\frac{r-R_d}{a}\right) dr}{\left(1+\exp\left(\frac{r-R_d}{a}\right)\right)^2}}{4\pi \int_0^\infty \frac{r^2 \exp\left(\frac{r-R_d}{a}\right) dr}{\left(1+\exp\left(\frac{r-R_d}{a}\right)\right)^2}} \tag{A9}$$

After putting r = ax and $K=R_d/a$ we get for the numerator of eq. (A9)

$$\text{Numerator} = 4\pi a^5 \int_0^\infty \frac{x^4 \exp\ (x-k)\ dx}{1+\exp\ (x-k)}$$

Integrating by parts the numerator becomes

$$16\pi a^5 \int_0^\infty \frac{x^3}{1+\exp\ (x-k)} = 16\pi a^5\ F_3(k)$$

From eq. (A3) we get

$$\begin{aligned} F_3(k) &= \frac{k^4}{4} + 6k^2\left[\frac{1}{1^2} - \frac{1}{2^2} + \frac{1}{3^2} + \ldots\right] + 12\left[\frac{1}{1^4} - \frac{1}{2^4} + \frac{1}{3^4}\ldots\right] \\ &= \frac{k^4}{4} + 6k^2\frac{\pi^2}{12} + 12\frac{7\pi^4}{720} \\ &= \frac{k^4}{4} + \frac{\pi^2 k^2}{2} + \frac{7}{60}\pi^4 \end{aligned} \tag{A10}$$

Therefore the numerator becomes

$$\begin{aligned} \text{Numerator} &= 16\pi a^5\left[\frac{R_d^4}{4a^4} + \frac{\pi^2}{2}\frac{R_d^2}{a^2} + \frac{7}{60}\pi^4\right] \\ &= 4\pi a R_d^4\left[1 + 2\left(\frac{\pi a}{R_d}\right)^2 + \frac{7}{15}\left(\frac{\pi a}{R_d}\right)^4\right] \end{aligned} \tag{A11}$$

$$\text{Denominator} = 4\pi a^3 \int_0^\infty \frac{x^2 \exp\ (x-k)\ dx}{(1+\exp\ (x-k))^2}$$

Integration by parts gives

$$= \quad 8\pi a^3 \int_0^\infty \frac{x}{1+e^{x-k}} dx = 8\pi a^3 \; F_1(k)$$

Now $\quad F_1(k) = \frac{k^2}{2} + 2\left[\frac{1}{1^2} - \frac{1}{2^2} + \frac{1}{3^2} - \frac{1}{4^2} + \dots\right]$

$$= \frac{k^2}{2} + 2\frac{\pi^2}{12} = \frac{k^2}{2} + \frac{\pi^2}{6} \qquad \text{(A12)}$$

Therefore the denominator becomes

$$\text{Denomenator} = 4\pi a^3\left[k^2 + \frac{\pi^2}{3}\right]$$

$$= 4\pi a R_d^2\left[1 + \frac{1}{3}\left(\frac{\pi a}{R_d}\right)^2\right] \qquad \text{(A13)}$$

Hence

$$< r^2 >_{SWD} = R_d^2\left[\frac{1 + 2\left(\frac{\pi a}{R_d}\right)^2 + \frac{7}{15}\left(\frac{\pi a}{R_d}\right)^4}{1 + \frac{1}{3}\left(\frac{\pi a}{R_d}\right)^2}\right] \qquad \text{(A14)}$$

3. Volume Integral of Potential with Saxon-Woods Geometrical Factors

The volume integral per nucleon J_v is defined as

$$J_V = \frac{1}{A}\int_0^\infty 4\pi\, V(r)\, r^2 dr = \frac{4\pi}{A} V_o \int_0^\infty \frac{r^2 dr}{1 + \exp\left(\frac{r - R_V}{a}\right)}$$

Putting as before x=r/a and $k=\frac{R_v}{a}$ we get

$$J_v = \frac{4\pi V_o a^3}{A}\int_0^\infty \frac{x^2 dx}{1+\exp(x-k)} = \frac{4\pi V_o a^3}{A} F_2(k)$$

Now from eq. (A6)

$$F_2(k) = \frac{k^3}{3} + \frac{\pi^2 k}{3}$$

and

$$J_v = \frac{4\pi V_o a^3}{A}\left[\frac{R_v^3}{3a^3}+\frac{\pi^2}{3}\frac{R_v}{a}\right]$$

$$= \frac{4\pi V_o}{3}\frac{R_v^3}{A}\left[1+\left(\frac{\pi a}{R_v}\right)^2\right]$$

$$= \frac{4\pi V_o}{3} r_v^3\left[1+\left(\frac{\pi a}{R_v}\right)^2\right] \qquad \text{(A15)}$$

4. Volume Integral of Potential with Saxon-Woods Derivative Form Factor

$$J_W = \frac{16\pi W_o}{A}\int_0^\infty \frac{r^2 \exp\left(\frac{r-R_v}{a}\right)}{\left[1+\exp\left(\frac{r-R_v}{a}\right)\right]^2}$$

Which after putting $x = \frac{r}{a}$ and $k = \frac{R_d}{a}$ becomes

$$J_W = \frac{16\pi W_o}{A} a^3 \int_0^\infty \frac{x^2 \exp(x-k)dx}{[1+\exp(x-k)]^2}$$

Integrating by parts

$$= \frac{32\pi W_o}{A} a^3 \int_0^\infty \frac{xdx}{1+\exp(x-k)} = \frac{32\pi W_o}{A} a^3 F_1(k)$$

Now from eq. (A12), we get

$$J_W = \frac{32\pi W_o a^3}{A}\left[\frac{k^2}{2}+\frac{\pi^2}{6}\right]$$

$$= \frac{16\pi W_o a R_v^2}{A}\left[1+\frac{1}{3}\left(\frac{\pi a}{R_v}\right)^2\right] \qquad \text{(A16)}$$

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