Presented at
Seventeenth European American Nuclear Data Committee
Tokyo, Japan
March 25-30, 1974

OPTICAL MODEL CALCULATIONS

AT

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* Research supported by the USAEC under Contract AT(11-1)-3058.

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ABSTRACT

Experimental evidence of deep minima in the p-wave neutron strength function about mass numbers 55 and 160 has been studied via optical model calculation. By employing a spherical optical model with an angular momentum dependent (l) imaginary potential strength ($W^{(l)}$), a global optical model parameter set has been determined which accurately predicts the s and p-wave neutron strength functions and potential scattering radius over mass numbers 40-240. Extension of the angular momentum dependent optical potential to coupled-channel calculations treating 0^+-2^+ collective state coupling, improved the agreement between prediction and experimental data. The values $W^{(0)}=1.2\text{MeV}$ and $W^{(1)}=1.5\text{MeV}$ employed in the calculations indicate that p-wave neutrons effectively interact less weakly than s-wave neutrons with the target nucleus.

INTRODUCTION

High resolution neutron interaction experiments have made available p-wave neutron strength function (S_1) values, in addition to refined s-wave neutron strength function (S_0) and potential scattering radii (R') values, as a function of mass number (A). Experiments conducted at the RPI Linear Accelerator Laboratory⁽¹⁾ and other facilities revealed strong minima in S_1 , where at $A=55$ and 160 values of $\approx 4 \times 10^{-6}$ and $\approx 1 \times 10^{-5}$ were observed, respectively.

This new data on S_1 has regenerated an interest in the ability of optical model calculations to simultaneously accurately predict S_0 , S_1 and R' versus mass number A from 40 to 240. Previous work performed by Perey-Buck,⁽²⁾ Moldauer,⁽³⁾ and by others⁽⁴⁻⁵⁾ on obtaining a global optical model parameter set was biased towards simultaneous fits to S_0 and R' versus A , since scarce data existed on S_1 values. With interesting S_1 data available, we have attempted to obtain a global optical model parameter set with as few additional free parameters that also accurately predicts S_1 versus A , in addition to S_0 and R' .

II. ANGULAR MOMENTUM INDEPENDENT OPTICAL MODEL

Restricting our discussion to low energy neutron interactions, the basis of optical model calculations is that the interaction of the incident neutron and target nucleus can be modeled by a complex central potential, hence, the optical model Schrödinger's equation becomes

$$-\frac{\hbar^2}{2m} \nabla^2 \psi_I(\vec{r}) + V_{Op}(|\vec{r}|) \psi_I(\vec{r}) = E \psi_I(\vec{r}) \quad (1)$$

where

$$V_{Op}(|\vec{r}|) = V_{Real}(|\vec{r}|) + i V_{Imag}(|\vec{r}|). \quad (2)$$

Physically the real potential accounts for shape elastic scattering; whereas, the imaginary potential accounts for excitations of the target nucleus which would generally remove the incident neutron from its entrance channel and lead to resonance behavior. Hence, the magnitude of $V_{Imag}(|\vec{r}|)$ can be interpreted as the entrance channel removal interaction strength exerted on the incident neutron by the target nucleus.

Noting the simplicity of the Hamiltonian operator in Eq. (1), the incident neutron's wave function $\psi_I(\vec{r})$ is easily numerically determined. We have employed the ABACUS II computer-code⁽⁶⁾ for the numerical determination of $\psi_I(\vec{r})$. Once having determined this wave function, the energy averaged neutron total, shape elastic and removal cross sections can be computed. Alternately, the neutron strength function and potential scattering radius values can be evaluated, where as usual, we define the angular momentum dependent (ℓ) strength function by

$$S_l = \frac{1}{2l+1} \sum_J \frac{g_J \langle \Gamma_l^J \rangle}{\sqrt{E} V_l \langle D^J \rangle} \quad (3)$$

and potential scattering radii by

$$R'_l = \lim_{E \rightarrow 0} \left(\frac{\langle \sigma_{se} \rangle}{4\pi} \right)^{\frac{1}{2}} \quad (4)$$

with

$$V_l = P_l / kR$$

$$g_J = (2J+1)/2$$

$$P_l$$

$$k$$

$$R$$

$$\langle \Gamma_l^J \rangle$$

$$\langle D^J \rangle$$

$$\langle \sigma_{se} \rangle$$

... statistical spin factor,

... neutron penetration factor
for l -waves,

... neutron wave number,

... channel radius,

... average neutron total width for
angular momentum l and total
momentum J ,

... average resonance spacing for
total momentum J ,

... shape elastic neutron cross section.

It is recognized that the potential scattering radii can be associated with hard sphere elastic scattering interaction; whereas, the strength function indicates the target nucleus strength to enter into resonance reactions with either s or p-wave incident neutrons.

Having defined S_0, S_1 and R' and indicated they can be obtained from the model systems wave function, $\psi_I(\vec{r})$, we now consider the construction of the optical potential, $V_{Op}(|\vec{r}|)$. As usual, we express $V_{Op}(|\vec{r}|)$ as the sum of the potential well and spin-orbit real terms plus an imaginary term, hence

$$V_{Op}(|\vec{r}|) = -V_{Re} f(|\vec{r}|, a_{Re}, R) - V_{so} \frac{\hbar^2}{4m} \frac{\vec{\sigma} \cdot \vec{r}}{r} \frac{1}{r} \left| \frac{df(|\vec{r}|, a_{so}, R)}{dr} \right| \quad (6)$$

$$- 4i W a_{Im} g(|\vec{r}|, a_{Im}, R+b).$$

The real form function, f , has generally been chosen to reflect the target nucleus-nucleon density via the Saxon-Wood's form

$$f(|\vec{r}|, a, R) = \left[1 + \exp\left(\frac{r-R}{a}\right) \right]^{-1} \quad (7)$$

which we have also employed.

By contrast, several imaginary form functions, g , have been employed in the past. In particular Moldauer employed a shifted Gaussian form given by

$$g(\vec{r}, a_{Im}, R+b) = \frac{1}{4a_{Im}} \exp \left[- \left(\frac{r-R-b}{a_{Im}} \right)^2 \right] \quad (8)$$

and Perey-Buck, ourselves and others have used the Saxon-Wood's derivative form

$$g(\vec{r}, a_{Im}, R+b) = \left| \frac{df(r, a_{Im}, R+b)}{dr} \right| \quad (9)$$

where $R=r_0 A^{1/3}$. It will be noted that the only quantum number dependence of the chosen optical potential is contained in the spin-orbit potential via $(\vec{\sigma} \cdot \vec{l})$. Theoretical calculations do indicate considerably more quantum number dependence, but to minimize the number of unknown optical parameters to be determined there is a strong incentive to ignore this fact. We refer to the proposed potential as the angular momentum independent spherical optical potential. (7-8)

Having specified the angular momentum independent optical model form, we have attempted to determine a global optical model parameter set which simultaneously predicts values of S_0 , S_1 , and R' over the mass number range $A=40-240$ consistent with experimental values. We were particularly interested in predicting the recently observed deep minima in S_1 about $A=55$ and 160 . Table I presents the optical parameter set we thus determined and contrasts our set to optical parameter sets proposed by Perey-Buck and Moldauer.

It should be recalled that both of the previous works were primarily concerned with predicting S_0 and R' , since little data on S_1 was then available. In Figures (1-3) values of S_0 , S_1 , and R' versus mass number A are presented respectively, as calculated by Percy-Buck, Moldauer and our work and experimentally determined. Moldauer predicts S_0 very accurately; whereas, our work underpredicts the S_0 minima due to our heavy bias on accurately predicting S_1 . Figure (2) reveals that indeed we have improved upon former works in predicting S_1 versus A , particularly in the deep S_1 minima. It is quite surprising that Moldauer's work predicted the deep S_1 minima about $A=55$ before any strong supporting experimental evidence. Finally, Figure (3) clearly illustrates the trouble we encountered in accurately predicting R' in conjunction with S_0 and S_1 . With considerable effort expended on obtaining a global optical parameter set that simultaneously predicts S_0 , S_1 , and R' versus A and the poor results indicated in Figures (1-3), we concluded that the employed angular momentum independent spherical optical model was inadequate.

III. ANGULAR MOMENTUM DEPENDENT OPTICAL MODEL

Concluding that an angular momentum dependent spherical optical model was required, we have attempted to construct such a model with a minimum of additional unknown optical parameters. With bound state calculations indicating only a weak dependence [other than spin-orbit force] of the real potential, $V_{\text{Real}}(|\vec{r}|)$, on the bound state particle angular momentum, we chose to place the total angular momentum dependence of the optical potential on the imaginary term, $V_{\text{Imag}}(|\vec{r}|)$.

To minimize the additional number of optical parameters introduced, angular momentum dependence was restricted to the potential strength, hence

$$V_{\text{Imag}}(i\vec{r}) = -4W^{(l)}a_{\text{Im}} \left| \frac{df(i\vec{r}, a_{\text{Im}}, R+b)}{dr} \right|. \quad (10)$$

Theoretical derivations⁽⁷⁻⁸⁾ of the optical potential indicate angular momentum dependence, but little information exists to support the form we have assumed.

The proposed angular momentum dependent spherical optical potential was then employed to obtain an associated set of global optical parameters which would simultaneously predict S_0 , S_1 , and R' from $A=40-240$. Table II presents the values we obtained, and contrasts them (Table I) to optical parameter values obtained by Perey-Buck and Moldauer. It is noted that our real potential employs a smaller diffuseness length, a_{Re} , implying a sharper nucleon surface. In contrast to previous work which has chosen to restrict $a_{\text{So}} = a_{\text{Re}}$, we have chosen $a_{\text{So}} = a_{\text{Im}}$. The imaginary potential shape employed by Moldauer and our work were found very similar, even though different imaginary form functions, g , were employed. Most interestingly, we determined $W^{(o)} = 12 \text{ MeV}$ and $W^{(l)} = 1.5 \text{ MeV}$. The optimum value of $W^{(l)}$ to employ was found not very uniquely specified, but all acceptable values of $W^{(l)}$ were considerably smaller than $W^{(o)}$. We conclude from the larger magnitude of $(W^{(o)}/W^{(l)})$ that s-wave neutrons effectively interact the target nucleus much stronger than p-wave neutrons. A theoretical derivation of the optical potential in a (2 particle-1-hole) basis is underway to determine whether a simple mechanism for this behavior can be identified.

Values of S_0 , S_1 , and R' versus mass number A are presented in Figure (4-6) using the angular momentum dependent spherical optical model. The simultaneous fit to these three quantities is very accurate over a majority of the mass number range. As illustrated, calculations using the ABACUS II computer code were performed at three different neutron energies, revealing the care that should be exercised in interpreting the adequacy of the fit in the energy sensitive strength function peaks. For certain mass number ranges where either S_0 or S_1 reach maxima or minima, agreement between prediction and data is less adequate. Following the work of Perey-Buck⁽²⁾, we attributed this disagreement to be due to the presence of low lying collective target nucleus states which could easily be excited by the incident neutron. With our spherical optical model not modeling such collective state excitations, we extended our angular momentum dependent optical model to coupled-channel calculations anticipating improved agreement in predicted and measured S_0 , S_1 , and R' values.

Briefly reviewing the basis of coupled-channel calculations and employing the notation of Tamura⁽⁹⁾, the coupled-channel model Schrödinger equation is given by

$$\left[H_T - \frac{\hbar^2}{2m} \nabla_{\vec{r}}^2 + V_{Op}(\vec{r}) \right] \Psi_I(\vec{r}, \vec{g}) = E \Psi_I(\vec{r}, \vec{g}) \quad (11)$$

where $\vec{r}$ denotes the incident neutron coordinates and $\vec{R}$ the collective target nucleus coordinates. Now the collective target nucleus wave function, $\Phi_{I_n M_n}$, satisfies the Hamiltonian

$$\mathcal{H}_T[\Phi_{I_n M_n}] = \omega_n \Phi_{I_n M_n} \quad (12)$$

for intrinsic momentum I_n and projection M_n for energy state n . The solution of the collective state Hamiltonian equation is well known for vibrator and rotator states and totally specified by the excitation energy, ω_n , and deformation parameter, β , associated with each state. Thus by expanding the total system wave function, Ψ , in the collective state basis, Eq. (11) can be numerically solved, from which energy averaged cross sections, S_0 , S_1 , and R' values can be determined. The JUPITER computer code⁽⁹⁾ was used for these calculations. We recognize that S_0 , S_1 , and R' values are not only sensitive to the optical parameter set employed, but also the parameters specifying the collective states. In our calculations, the collective state parameters are not free to choose but set to values determined in fitting other data (electromagnetic transition strengths, etc.).

Restricting our coupled-channel calculations to $0^+ - 2^+$ target nucleus collective states, S_0 , S_1 , and R' were computed employing the angular momentum dependent optical parameter set previously given in Table II. The excellent results are presented in Figures (4-6). Both the vibrator state splitting of the S_0 peak about $A=150$ and minima filling about $A=100$ and 240 are accurately predicted.

Figure (5) illustrates the excellent prediction of the deep S_1 minima, where the presence of vibrator states is noted to fill the S_1 minima about $A=160$ which does not contradict the existing data. Of particular interest is the S_1 peak about $A=100$. Contradicting experimental evidence as to whether this S_1 peak is split has once again appeared.⁽¹⁰⁾ Both our spherical and collective optical model calculations do predict splitting. To help understand the mechanism of this splitting, in Figure (7) the $p^{1/2}$ and $p^{3/2}$ strength functions are presented as calculated by the spherical and collective angular momentum dependent optical model. The spherical optical model results indicate that the split S_1 peaks about $A=100$ can be uniquely associated with either the $p^{1/2}$ or $p^{3/2}$ states, hence caused by the spin-orbit force. However, when the presence of collective states is modeled via coupled-channel calculations, no such unique identification is possible. Finally, the scarce data on the potential scattering radii is seen in Figure (6) to be accurately fitted via coupled-channel calculations employing the angular momentum dependent optical model.

Having demonstrated that a set of global optical parameters exists for the proposed angular momentum dependent optical model that accurately predicts S_0 , S_1 , and R' from $A=40-240$, we have employed this model to also compute the energy averaged total neutron cross section. Indeed from a practical viewpoint, we are most interested in obtaining a model that accurately predicts cross sections for use in reactor physics calculations. Figure (8) contrasts predictions of the total neutron cross section energy averaged about 100 keV, obtained by Perey-Buck and our work for both the spherical and collective models. Our work predicts considerably more structure than Perey-Buck's work, which the data weakly supports.

Both models fail to correctly predict the total cross section peak about $A=150$, caused by the split S_0 peak. To study the energy sensitivity of our model, the energy averaged total neutron cross section was calculated and contrasted to experimental data in Figure (9) at 30, 100 and 300 keV. As in the previous figure, the data has considerable scatter but does indicate the expected trend of increased total cross section peaks with decreasing neutron energy due to single particle binding. The previously discussed total cross section peak about $A=150$ is noted to be quite energy sensitive in our calculations, hence difficult to accurately predict. Scatter of data does not enable us to make a firm statement as to the adequacy of our angular momentum optical model in computing the energy averaged total neutron cross section, but we can conclude that general trends are adequately predicted.

IV CONCLUSION

Our work has indicated that an angular momentum (l) dependent optical model employing a global optical parameter set is required to simultaneously and accurately predict S_0 , S_1 , and R' versus mass numbers $A=40-240$. We have chosen the angular momentum dependence of the optical model to be totally contained in the strength of the imaginary potential, $W^{(l)}$ [other than spin orbit force]. Extending this model to coupled-channel calculations, the fine structure of S_0 , S_1 , and R' have been accurately predicted. The large magnitude of $(W^{(c)}/W^{(l)})$ obtained in this work indicates that s-wave neutrons effectively interact much stronger than p-wave neutrons with the target nucleus. Theoretical calculations employing a (2 particle-1 hole) basis are in progress to possibly determine the mechanism of this interaction strength phenomena. ⁽⁸⁾

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FIGURE CAPTIONS:

- Figure (1) The s-wave neutron strength function as calculated by the angular momentum independent spherical optical model.
- Figure (2) The p-wave neutron strength function as calculated by the angular momentum independent spherical optical model.
- Figure (3) The potential scattering radius as calculated by the angular momentum independent spherical optical model.
- Figure (4) The s-wave neutron strength function as calculated by both the angular momentum dependent spherical and collective state optical model.
- Figure (5) The p-wave neutron strength function as calculated by both the angular momentum dependent spherical and collective state optical model.
- Figure (6) The potential scattering radius as calculated by both the angular momentum dependent spherical and collective state optical model.
- Figure (7) The $p_{1/2}$ and $p_{3/2}$ neutron strength functions as calculated by both the angular momentum dependent spherical and collective state optical model.
- Figure (8) The energy averaged total neutron cross section at 100 keV as calculated by both an angular momentum independent (Perey-Buck) and dependent (RPI) spherical and collective state optical model.
- Figure (9) The energy averaged total neutron cross section at 30, 100, and 300 keV as calculated by both the angular momentum dependent spherical and collective state optical model.

TABLE CAPTIONS

- Table (I) The angular momentum independent optical parameter sets employed by Perey-Buck, Moldauer, and ourselves used to obtain results shown in Figures (1-3).
- Table (II) The angular momentum dependent optical parameter set we employed to obtain results shown in Figures (4-9).

FIG. 3.

Figure (4)

s-wave strength function (S_0)

Figure (5)

Figure (6)

Figure (7)

 $E_n = 100 \text{ KeV.}$

p-wave and p-wave strength functions

Figure (8)

Figure C9

TABLE I

UNITS: POTENTIAL-MeV, LENGTH-fm

PEREY-BUCK PARAMETERS

$V_{Re} = 48$

$a_{Re} = 0.65$

$R = 1.27A^{1/3}$

$V_{so} = 6$

$a_{so} = 0.65$

$b = 0.00$

$W = 11$

$a_{Im} = 0.47$

MOLDAUER PARAMETERS

$V_{Re} = 46$

$a_{Re} = 0.62$

$R = 1.16A^{1/3} + 0.6$

$V_{so} = 7$

$a_{so} = 0.62$

$b = 0.50$

$W = 14$

$a_{Im} = 0.50$

RPI PARAMETERS

$V_{Re} = 52$

$a_{Re} = 0.40$

$R = 1.27A^{1/3}$

$V_{so} = 6$

$a_{so} = 0.65$

$b = 0.00$

$W = 4$

$a_{Im} = 0.25$

TABLE II

UNITS: POTENTIAL-MeV, LENGTH-fm

$$V_{\text{Re}}=47$$

$$a_{\text{Re}}=0.52$$

$$R=1.30A^{1/3}$$

$$V_{\text{So}}=6$$

$$a_{\text{So}}=0.23$$

$$W^{(c)}=12$$

$$a_{\text{Im}}=0.23$$

$$b=0.30$$

$$W^{(u)}=1.5$$