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ACTIVITIES AT LOS ALAMOS FOR THE OPTICAL MODEL SEGMENT OF THE RIPL CRP

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1. FORMAT OF THE OPTICAL MODEL PARAMETER LIBRARY

Since the 1995 meeting of the RIPL CRP in Vienna, a number of changes and extensions have been made to the format for optical model parameters. The changes were necessary to accommodate additional forms of optical model potential representations that were encountered in the literature, and to better represent rotational and vibrational models.

As presently formulated, potentials of the form

$$V(r) = V_R f_R(r) + W_V f_V(r) + W_D f_D(r) + V_{SO} f_{SO}(r) + W_{SO} f_{SO}(r) \qquad (1)$$

are allowed. In Eq. (1) V_R and W_V are the real and imaginary volume potential well depths, W_D is the well depth for the surface derivative term, V_{SO} and W_{SO} are the real and imaginary well depths for the spin-orbit potential, and the $f_i(r)$ are radial dependent form factors. Any incident particle is permitted by the format, but we have limited our initial library to incident neutrons, protons, deuterons, tritons, ^{3}He, and ^{4}He particles. Our approach is to supply a general form for optical model potentials that is an extension of the representation implemented in the SCAT2 optical model code [1] and that describes most of the parameterizations that have been commonly used in the past. Additionally, three more specialized formats are formulated that describe particular, less common forms of potentials but which offer promise of being important for applied purposes.

The general form of the optical model potential is the following:

$$\begin{aligned} V_i(E) = {} & \alpha_1 + \alpha_7\eta + \alpha_8\Delta_c + \alpha_9 A + \alpha_{10}A^{1/3} + \alpha_{11}A^{-2/3} + \alpha_{12}\Delta_{c'} + (\alpha_2 + \alpha_{13}\eta + \alpha_{14}A)E \\ & + \alpha_3 E^2 + \alpha_4 E^3 + \alpha_6\sqrt{E} + (\alpha_5 + \alpha_{15}\eta + \alpha_{16}E)\ln(E) + \alpha_{17}\Delta_c E^{-2} \end{aligned} \qquad (2)$$

where $V_i(E)$ designates the i^{th} term of the potential (for example, V_R, W_D, V_{SO}, etc.) at incident laboratory energy E, $\eta = (N\text{-}Z)/A$, N and Z are the neutron and proton numbers of the target nucleus, and A is the atomic mass of the target. Two different forms of correction terms for Coulomb repulsion with incident protons are provided:

$$\Delta_c = \frac{0.4Z}{A^{1/3}} \quad \text{and} \quad \Delta_{c'} = \frac{1.73Z}{R_c} \qquad (3)$$

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where R_c is the Coulomb radius. Δ_c and $\Delta_{c'}$ are zero for incident neutrons. Each of the potential terms in Eq. (1) can be represented over any number of defined energy ranges using as many of the terms given in Eq. (2) as required, with the coefficients of the unused terms set to zero.

The first special form of the potential is used to represent the potential of Smith et al. [2] and to accommodate exponential forms included in the Engelbrecht and Fiedeldey potential [3]:

$$V_i(E) = \alpha_1 + \alpha_2\eta + \alpha_3 \cos\left[2\pi\left(\frac{A-\alpha_4}{\alpha_5}\right)\right] + \alpha_6 \exp(\alpha_7 E + \alpha_8 E^2) + \alpha_9 E \exp(\alpha_{10} E^{\alpha_{11}}) \ . \quad (4)$$

This formulation is activated by setting $\alpha_{18} > 0$.

The second special form is necessary to represent the potential determined in an extensive analysis of proton scattering cross sections and polarizations by Varner et al. [4], as well as an exponential form permitted in the SCAT2 code [1]:

$$V_i(E) = \frac{\alpha_1 + \alpha_2\eta}{1+\exp\left(\frac{\alpha_3 - E + \alpha_4\Delta_{c'}}{\alpha_5}\right)} + \alpha_6 \exp\left(\frac{\alpha_7 E - \alpha_8}{\alpha_6}\right) \ . \quad (5)$$

The formulation in Eq. (5) is activated by setting $\alpha_{19} > 0$.

Finally, the third special form, which was developed by Delaroche, is activated by setting $\alpha_{20} > 0$ and is used by Koning, van Wijk, and Delaroche [5] in a recent analysis of neutron reactions with isotopes of Zr:

$$V_i(E) = \alpha_1 + \alpha_2 E + \alpha_3 \exp\left[-\alpha_4(E - \alpha_5 E_f)\right] + \frac{\alpha_6[(E-E_f)^{\alpha_8}]}{(E-E_f)^{\alpha_8} + (\alpha_7)^{\alpha_8}} \quad (6)$$

where E_f is the Fermi energy in MeV and is given by:

$$\begin{aligned} E_f = \ & -0.5\,[S_n(Z,A) + S_n(Z,A+1)] \quad \text{(for incident neutrons)} \\ & -0.5\,[S_p(Z,A) + S_p(Z+1,A+1)] \quad \text{(for incident protons),} \end{aligned} \quad (7)$$

where $S_n(Z,A)$ and $S_p(Z,A)$ are the neutron and proton separation energies for nucleus (Z,A).

Either Woods-Saxon or Gaussian form factors are permitted for the $f_i(r)$ terms in Eq. (1), that is,

$$f_i(r) = \frac{1}{1+\exp\left(\frac{r-R_i}{a_i}\right)} \quad \text{(Woods-Saxon form)} \tag{8}$$

or

$$f_i(r) = \exp\left(\frac{-(r-R_i)^2}{a_i^2}\right) \quad \text{(Gaussian form)} \tag{9}$$

The nuclear radius is given by $R_i = r_i A^{1/3}$ where r_i is given by

$$r_i(E) = \beta_1 + \beta_2 E + \beta_3 \eta + \beta_4 A^{-1} + \beta_5 A^{-1/2} + \beta_6 A^{2/3} + \beta_7 A + \beta_8 A^{2/3} + \beta_9 A^3 + \beta_{10} A^{1/3} + \beta_{11} A^{-1/3} \tag{10}$$

and a similar form is used for the diffuseness, a_i,

$$a_i(E) = \delta_1 + \delta_2 E + \delta_3 \eta + \delta_4 A^{-1} + \delta_5 A^{-1/2} + \delta_6 A^{2/3} + \delta_7 A + \delta_8 A^2 + \delta_9 A^3 + \delta_{10} A^{1/3} + \delta_{11} A^{-1/3} \tag{11}$$

Note that the $\beta_{11} A^{-1/3}$ term in Eq. 7 permits the inclusion of a constant (A-independent) quantity to the radius, that is, $R_i = r_o + r_i' A^{1/3} = \beta_{11} + r_i' A^{1/3}$.

The format also permits inputting of the relevant parameters for coupled-channel rotational, vibrational, and non-axial deformed models, including energies, spins and parities of vibrational and rotational states, deformation parameters, softness parameters, etc., that are required for the various model. At present the format is considered reasonably complete for spherical and rotational models but extensions are needed for the vibrational and non-axial deformed models.

Details of the format for the optical model parameterizations is given in Appendix A. The description in App. A is included in the RIPL data base at the IAEA.

2. CONTENTS OF THE LIBRARY

A computer code was developed that permitted the various potentials compiled at Bombay to be included in the library. Subroutines were developed for reading and writing the library, and a simple code was written to produce a summary of the potentials in the library. Additionally, a number of new potentials were added to the library.

To date, some 107 optical model parameterizations are included in the library. The library contains 75 parameterizations for incident neutrons, 21 parameterizations for incident protons, 2 for incident deuterons, 1 each for incident tritons and ^{3}He particles, and 7 parameterizations for incident alpha particles. These potentials have been selected mainly from analyses made at Los Alamos for various applied calculations [6,7], from a set of parameters supplied by JAERI and others specifically for the RIPL library, and from several well known global optical model parameterizations. Each potential included is given a unique reference number, according to a numbering system that is described in App. 2. This system was adopted in order to separate the potentials for different incident particles into different reference number regions, and to provide approximate information on the sources of the various potentials by geographical region. The latter information might be used, for example, if one wished to use only potentials from a particular source for a given set of calculations (for example, JAERI). To be very useful, of course, many more potentials must be added to the library, for example, from China, Russia, Bologna, and the JEFF and ENDF communities in general. In addition to the numbering rules given in App. B, we are following an informal numbering convention for neutron and proton potentials that are related through isospin by means of the Lane model [8]; that is, we assign a 3-digit reference number to the potential and then add 3000 for incident neutrons and 5000 for incident protons.

3. VALIDATION OF THE OPTICAL MODEL LIBRARY

Validation of the potentials in the library must be carried out at two levels: (1) ensuring that the potentials in the library are both complete and accurate, and (2) testing how well the potentials agree with the available experimental data base. Some effort has been directed at checking the accuracy of entries into the file by careful proofreading, resulting in the removal of a number of errors. Additional efforts are needed in this area and, in particular, a processing code should be developed that will retrieve information from the file and print it out in standard, easily readable form.

A visit was hosted by Los Alamos of Dr. A. Kumar in order to begin efforts to compare a few of the potentials with experimental data [9]. In this study neutron total, reaction, and elastic scattering cross sections are compared with experimental data for 6 global potentials and 5 regional or nuclide-specific potentials.

4. CONCLUSIONS AND RECOMMENDATIONS

Because of the limited number of potentials included in the library thus far and, especially, because of the very limited testing done, it is difficult to make general recommendations for global optical model potentials at present. However, some general comments can be made. In every case where local potentials were compared by Kumar et al. [9] to global potentials, the local parameterizations produced better agreement with the experimental data than did the global potentials. So one firm conclusion is that additional, carefully chosen nuclide-specific potentials should be included in the RIPL library. Also it was observed that, if a global optical potential must be used for incident neutrons, then the Wilmore and Hodgson [10] potential often gave reasonable results below 30 MeV in the limited tests performed, and the Madland Semmering

potential [11] usually gave reasonable results for both neutrons and protons from ~30 to 200 MeV. Again, it should be emphasized that the parameterizations included and the comparisons with experiment that were made were very limited in scope and should be expanded.

The largest differences in the reaction cross sections calculated with the various potentials by Kumar et al. occurred at fairly low energies, which were not tested in the comparisons. To test the low energy reaction and elastic cross section predictions requires performing Hauser-Feshbach calculations. Such tests should clearly be carried out.

In conclusion, it can be said that we have succeeded in developing an initial or starter file of optical model parameterizations in a format that is easily expanded, together with initial codes and subroutines for handling the data. While the existing library already promises to be useful, it is essential that follow on activities occur to enhance its usefulness. A summary of improvements or areas where additional work is needed includes:

1. Additional potentials must be incorporated into the library. For example, potentials from programs in China, Russia, Bologna, and the JEFF and ENDF communities must be added.
2. Additional processing codes should be developed for checking, displaying, linking of the library to optical model codes, and comparing predictions from the parameter file with experimental data.
3. Extensive checking and validation of the library, especially when more processing codes become available.

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APPENDIX A

OPTICAL MODEL PARAMETER FORMAT FOR RIPL LIBRARY

```
iref
author
reference
summary
emin,emax
izmin,izmax
iamin,iamax
imodel,izproj,iaproj

       *****LOOP: i=1,5
jrange(i)
       *****LOOP j=1,jrange
epot(i,j)
(rco(i,j,k), k=1,11)
(aco(i,j,k), k=1,11)
(pot(i,j,k), k=1,20)
       *****END i AND j LOOPS

jcoul
       *****LOOP j=1,jcoul
ecoul(j),rcoul(j),rcoul0(j),beta(j)
       *****END j LOOP

    (1)*****SKIP TO (2)***** IF IMODEL NOT EQUAL TO 1

nisotopes
       *****LOOP n=1,nisotopes
iz(n),ia(n),ncoll(n),lmax(n),idef(n),bandk(n),[def(j,n),
                                              j=2,idef(n),2]
       *****LOOP k=1,ncoll(n)
ex(k,n),spin(k,n),ipar(k,n)
       *****END k AND n LOOPS

    (2)*****SKIP TO (3)***** IF IMODEL NOT EQUAL TO 2

nisotopes
       *****LOOP n=1,nisotopes
iz(n),ia(n),nvib(n)
       *****LOOP k=1,nvib(n)
exv(k,n),spinv(k,n),iparv(k,n),nph(k,n),defv(k,n),thetm(k,n)
       *****END k LOOP
       *****END n LOOP

    (3)*****SKIP REMAINING LINES IF IMODEL NOT EQUAL TO 3

nisotopes
       *****LOOP n=1,nisotopes
iz(n),ia(n),beta0(n),gamma0(n),xmubeta(n)
       *****END n LOOP
```

DEFINITIONS

```
      iref  = unique fixed point reference number for this
              potential
    author  = authors for this potential (up to 80 characters,
              1 line))
 reference  = reference for this potential (up to 80 characters,
              1 line)
   summary  = short description of the potential (320 characters,
              4 lines)
 emin,emax  = minimum and maximum energies for validity of this
              potential
izmin,izmax = minimum and maximum Z values for this potential
iamin,iamax = minimum and maximum A values for this potential
   imodel   = 0 for spherical potential
            = 1 for coupled-channel, rotational model
            = 2 for vibrational model
            = 3 for non-axial deformed model
   izproj   = Z for incident projectile
   iaproj   = A for incident projectile
   index i  = 1 real potential (Woods-Saxon)
            = 2 surface imaginary potential
            = 3 volume imaginary potential (Woods-Saxon)
            = 4 real spin-orbit potential
            = 5 imaginary spin-orbit potential
   jrange   = number of energy ranges over which the potential is
              specified
            = positive for potential strengths
            = negative for volume integrals
            = 0 if potential of type i not used
  epot(i,j) = upper energy limit for jth energy range for
              potential i
  rco(i,j,k)= coefficients for multiplying A**(1/3) for
              specification of radius R in fm where:

     R(i,j) = {abs[rco(i,j,1)] + rco(i,j,2)*E + rco(i,j,3)*eta
            + rco(i,j,4)/A + rco(i,j,5)/sqrt(A)
            + rco(i,j,6)*A**(2/3) + rco(i,j,7)*A
            + rco(i,j,8)*A**2  + rco(i,j,9)*A**3
            + rco(i,j,10)*A**(1/3)
            + rco(i,j,11)*A**(-1/3)} * [A**(1/3)]
```

and

if rco(2,j,1) >0.0: Woods-Saxon derivative surface potential
if rco(2,j,1) <0.0: Gaussian surface potential.

[Note that the A dependence of rco(i,j,11) cancels out so that rco(i,j,11) is equivalent to adding a constant of that magnitude to the radius R(i,j)].

```
 aco(i,j,k) = coefficients for specification of diffuseness a in
              fm where:

     a(i,j) = abs(aco(i,j,1)) + aco(i,j,2)*E + aco(i,j,3)*eta
                + aco(i,j,4)/A + aco(i,j,5)/sqrt(A)
                + aco(i,j,6)*A**(2/3) + aco(i,j,7)*A
                + aco(i,j,8)*A**2 + aco(i,j,9)*A**3
                + aco(i,j,10)*A**(1/3) + aco(i,j,11)*A**(-1/3)

 pot(i,j,k) = strength parameters, as follows:

if pot(i,j,k>17) .eq. 0, then

V(i,j) = pot(i,j,1) + pot(i,j,7)*eta + pot(i,j,8)*Ecoul
       + pot(i,j,9)*A + pot(i,j,10)*A**(1/3)
       + pot(i,j,11)*A**(-2/3) + pot(i,j,12)*Ecoul2
       + [pot(i,j,2) + pot(i,j,13)*eta + pot(i,j,14)*A]*E
       + pot(i,j,3)*E*E + pot(i,j,4)*E*E*E + pot(i,j,6)*sqrt(E)
       + [pot(i,j,5) + pot(i,j,15)*eta + pot(i,j,16)*E]*ln(E)
       + pot(i,j,17)*Ecoul/E**2

if pot(i,j,18) .ne. 0, then

V(i,j) = pot(i,j,1) + pot(i,j,2)*eta
       + pot(i,j,3)*cos[2*pi*(A - pot(i,j,4))/pot(i,j,5)]
       + pot(i,j,6)*exp[pot(i,j,7)*E + pot(i,j,8)*E*E]
       + pot(i,j,9)*E*exp[pot(i,j,10)*E**pot(i,j,11)]

if pot(i,j,19) .ne. 0, then

V(i,j) = [pot(i,j,1) + pot(i,j,2)*eta]/
       {1 + exp[(pot(i,j,3) - E + pot(i,j,4)*Ecoul2)/pot(i,j,5)]}
       + pot(i,j,6)*exp[(pot(i,j,7)*E - pot(i,j,8))/pot(i,j,6)]

if pot(i,j,20) .ne. 0, then

V(i,j) = pot(i,j,1) + pot(i,j,2)*E
       + pot(i,j,3)*exp[-pot(i,j,4)*(E - pot(i,j,5)*EF)]
       + pot(i,j,6)*[(E-EF)**pot(i,j,8)]/[(E-EF)**pot(i,j,8)
       + pot(i,j,7)**pot(i,j,8)]
       + pot(i,j,9)*exp[-pot(i,j,10)*(E-EF)]*[(E-EF)**pot(i,j,12)]
       /[(E-EF)**pot(i,j,12) + pot(i,j,11)**pot(i,j,12)]

where
     E      = projectile laboratory energy in MeV
     eta    = (N-Z)/A
     Ecoul  = 0.4Z/A**(1/3)
     Ecoul2 = 1.73*Z/RC
     EF     = Fermi energy in MeV
            = -0.5*[SN(Z,A) + SN(Z,A+1)]   (for incident neutrons)
            = -0.5*[SP(Z,A) + SP(Z+1,A+1)] (for incident protons)
    SN(Z,A) = the neutron separation energy for nucleus (Z,A)
    SP(Z,A) = the proton separation energy for nucleus (Z,A).
```

And, continuing the definitions:

jcoul	= number of energy ranges for specifying coulomb radius and nonlocality range
ecoul(j)	= maximum energy of coulomb energy range j
rcoul(j), rcoul0(j)	= coefficients to determine the coulomb radius, RC, from the expression RC = rcoul*A**(1/3) + rcoul0
beta(j)	= nonlocality range. Note that when beta(j).ne.0., then the imaginary potential is pure derivative Woods-Saxon for energy range j.
nisotopes	= number of isotopes for which deformation parameters and discrete levels are given
iz,ia	= Z and A for the deformation parameters and discrete levels that follow
ncoll	= number of collective states in the coupled-channel rotational model for this iz, ia
lmax	= maximum l value for multipole expansion
idef	= largest order of deformation
bandk	= k for the rotational band
def	= deformation parameters, l=2,4,6,...through lmax
ex	= rotational level excitation energy (MeV)
spin	= rotational level spin
ipar	= rotational level parity
nvib	= number of vibrational states in the model for this iz, ia
exv	= vibrational level excitation energy (MeV)
spinv	= vibrational level spin
iparv	= vibrational level parity
nph	= 1 for pure 1-photon state = 2 for pure 2-photon state = 3 for mixture of 1- and 2-photon states
defv	= vibrational model deformation parameter
thetm	= mixing parameter (degrees) for nph=3
beta0	= beta deformability parameter
gamma0	= gamma deformability parameter
xmubeta	= non-axiality parameter

APPENDIX

REFERENCE NUMBERING SYSTEM FOR RIPL OPTICAL MODEL POTENTIALS

IREF = 1000*I + JREF

Incident Particles (leading digit, I)

IREF	I	Particle
1 - 3999	0 - 3	Neutrons
4000 - 5999	4 - 5	Protons
6000 - 6999	6	Deuterons
7000 - 7999	7	Tritons
8000 - 8999	8	He-3
9000 - 9999	9	He-4

Geographic Indicators (trailing 3 digits, J)

JREF	Region
1- 99	Los Alamos National Laboratory (LANL)
100 - 199	Other U.S. laboratories, universities
200 - 299	Japan, JAERI
300 - 399	Russia
400 - 499	Western Europe, JEF community
500 - 599	China
600 - 649	Former Soviet Union
650 - 699	India, Pakistan
700 - 799	Others
800 - 999	Reserved