UCRL-JC-106542
PREPRINT

Received by OSTI
AUG 26 1991

**Advanced Modeling of Reaction
Cross Sections for Light Nuclei**

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**This paper was prepared for submittal to
Strong, Weak, and Electromagnetic
Interactions in Nuclei and Astrophysics**

MASTER

January 3-4, 1991

Lawrence
Livermore
National
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ADVANCED MODELING OF
REACTION CROSS SECTIONS FOR LIGHT NUCLEIDavid A. Resler
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ABSTRACT

The shell model/R-matrix technique of calculating nuclear reaction cross sections for light projectiles incident on light nuclei is discussed, particularly in the application of the technique to thermonuclear reactions. Details are presented on the computational methods for the shell model which display how easily the calculations can be performed. Results of the shell model/R-matrix technique are discussed as are some of the problems encountered in picking an appropriate nucleon-nucleon interaction for the large model spaces which must be used for current problems. The status of our work on developing an effective nucleon-nucleon interaction for use in large-basis shell model calculations is presented. This new interaction is based on a combination of global constraints and microscopic nuclear data.

INTRODUCTION

Many applications require nuclear reaction cross sections of light projectiles (n, p, d, t, ^3He , α) incident on light nuclei ($A \leq 20$). Ideally, these cross sections should be *measured*. But in practice this is not always feasible because of time and/or cost. Further, some cross sections may be impossible to measure. Therefore, the ability to *calculate* such cross sections with reasonable accuracy is necessary.

The accuracy of a calculation can be tested by making comparisons with existing cross section data. For example, Lawrence Livermore National Laboratory has the only comprehensive evaluated cross section library for charged-particle reactions¹ (ECPL). New evaluations for the thermonuclear reactions $^2\text{H}(d,n)^3\text{He}$, $^2\text{H}(d,p)^3\text{H}$, $^3\text{H}(d,n)^4\text{He}$, and $^3\text{He}(d,p)^4\text{He}$ have recently been completed.² These evaluations, based on all available experimental information, have uncertainties on the order of a few percent. We intend to use these cross sections for testing the accuracy of our computational methods. If these cross sections can be calculated accurately, then the method can be employed confidently in regions of interest where little or no experimental data are currently available.

In the next section, the shell model/R-matrix technique for calculating nuclear reaction cross sections will be discussed. The following sections will discuss aspects of the computational methods, results using this technique, problems encountered, and our work on solving those problems by developing a new effective nucleon-nucleon interaction.

SHELL MODEL/R-MATRIX TECHNIQUE

In general, nuclear reaction cross sections for light projectiles (n , p , d , t , ^3He , α) of low-energy ($E \leq 20$ MeV) incident on light nuclei ($A \leq 20$) are dominated by isolated and overlapping resonance behavior. These resonances derive from the formation of nuclear states in the intermediate or compound nucleus. The standard method for analysing experimental cross section data for these reactions is to employ the R-matrix formalism.³ Parameters of the R-matrix can be determined by fitting the available data. (For example refer to some of the work from Ohio University.^{4,5}) These R-matrix parameters (e.g., level energies and reduced-width amplitudes) are related to nuclear structure properties (excitation energies and spectroscopic amplitudes). For example, consider the $d+d$ reaction at a given energy. The probability of producing the compound system, ^4He , depends on how much ^4He at the corresponding energy "looks like" two deuterons coupled together. Whether the ^4He then decays back to $d+d$ or $n+^3\text{He}$ depends on how much ^4He at that energy "looks like" two deuterons coupled together compared with a neutron and ^3He coupled together.

The nuclear shell model can be used to obtain structure information—level energies and wavefunctions. It can also be used to calculate spectroscopic amplitudes—the quantification of "looks like" discussed above. In the nuclear shell model, the nucleons are placed in single-particle basis states obtained from a three-dimensional harmonic oscillator. In performing the nuclear shell model calculation, there are two major decisions to be made. First, a model space must be chosen, i.e., what subset of all possible configurations should be used—a configuration being a single placement of the nucleons of the nucleus in question into the harmonic oscillator basis states. Second, an effective nucleon-nucleon interaction must be chosen for describing how the nucleons interact with one another.

Fig. 1. General scheme of the shell model/R-matrix technique of calculating reaction cross sections.

The general scheme of the shell model/R-matrix technique of calculating reaction cross sections is shown in Figure 1. This technique starts with an effective nucleon-nucleon interaction. By using the nuclear shell model, the appropriate nuclear structure information is calculated and transformed to input for the R-matrix calculation. The R-matrix formalism is used to calculate the reaction cross section. Because of the fundamental nature of the calculations, i.e., starting from a nucleon-nucleon interaction, if the method can be used to accurately calculate reaction cross sections where one has data to compare with, then the method can be used with confidence where little or no data exist. Before describing results using this technique, some of the computational aspects will now be discussed.

COMPUTATIONAL METHODS

The shell model/R-matrix technique is computationally intensive. To carry out a set of calculations, several computer codes, linked together by various data files, must be executed. The most complex code in the set is CRUNCHER⁶—the code which performs the nuclear shell model calculations. This code has been described elsewhere⁶ so only some of its important features are discussed here. CRUNCHER was patterned after the code VLADIMIR,⁷ but only in the external interface with the user. Internally, the codes are different. CRUNCHER was designed for the "small" computer and uses standard FORTRAN 77 whenever possible. This has made the code easy to operate on the present generation of workstations. CRUNCHER uses the m-scheme and the Lanczos process. The Hamiltonians can be used in the one and two-body form of second quantization or can be in the full multiparticle form. The fastest applications of the Hamiltonian come from using the full multiparticle form. In general, however, the multiparticle Hamiltonians are very large and can not always be created because of limited computer resources. In such cases, it is still possible to use the one and two-body form.

A unique feature of CRUNCHER, which is essential to the shell model/R-matrix technique, is its capability to calculate generalized multinucleon spectroscopic amplitudes. In a reaction like $^{13}\text{C}(n,\alpha)^{10}\text{Be}$, for example, overlaps of the compound nuclear ^{14}C wavefunctions with the result of coupling an alpha particle wavefunction onto a ^{10}Be wavefunction must be calculated. These quantities are called multiparticle spectroscopic amplitudes. In the example, the alpha particle is the cluster being transferred. The coding in CRUNCHER allows for any number of nucleons to be in the transferred cluster. In addition, these calculations can be carried out for any size model space.

Because of the complexities in running all the codes which must be executed in sequence to perform a calculation, an interactive controller, SuperCRUNCHER, has been developed. The emphasis on SuperCRUNCHER has been to streamline the structure part of the calculations. By answering a few "simple" questions, it is usually easy to perform the required shell model calculations. An excerpt from a session with SuperCRUNCHER is shown in Figure 2. In this example the first ten eigenstates of ^{13}C were calculated using the (8-16)POT interaction of Cohen and

SuperCRUNCHER

Nuclear Physics Mode

Enter your choice for what to do next...

Dimension ==> generate m-scheme basis dimension
Eigen ==> generate eigenvectors
He4 ==> calculate interaction parameters for He-4
EXIT ==> exit program

eigen

Generate eigenvectors

Enter the name of the nucleus to consider...

Examples: He-4
Li-7.2 <-- special format for A<20; the ".2" signifies to
use a standard 2 hbar omega space
be-8 <-- note that upper or lower case may be used

c-13.0

VECTOR LENGTH = 21

Current eigenvector information:

key	value	description
log	T	save/do not save log files
hgl	F	use/do use Glockner-Lawson Hamiltonian
rvf	sc.tmp	name for the vector files
itr	100	number of Lanczos iterations to do
eig	10	number of eigenstates to obtain

Enter keyword to change a value...

[A blank line indicates all values are OK.]

The following Hamiltonians are available for the "(s)p" model space:

name	description
ak	Amit & Katz, Nucl. Phys. 58, 388 (1964)
ck6-16	(6-16)2BME, Cohen & Kurath, Nucl. Phys. 73, 1 (1965)
ckpot	(8-16)POT, Cohen & Kurath, Nucl. Phys. 73, 1 (1965)
ck8-16	(8-16)2BME, Cohen & Kurath, Nucl. Phys. 73, 1 (1965)
kumar	Kumar, Nucl. Phys. A225, 221 (1974)

Enter the name of the built-in Hamiltonian OR enter "new" to create a different Hamiltonian...

[A blank line returns to the "enter nucleus" request.]

ck8-16

Using built-in Hamiltonian:

"(8-16)2BME, Cohen & Kurath, Nucl. Phys. 73, 1 (1965)"

Start time: 1991/01/01 21:47:35 End time: 1991/01/01 21:48:18

Fig. 2. Excerpt of the console input (circled) and output from running a typical calculation using SuperCRUNCHER. Refer to the text for details.

Kurath.⁸ The results from the main log file are shown in Figure 3.

```

Summary of the vector file sc.tmp

==> INITLAN <==
Operator used for Lanczos process: ..... OPHGL   sc.tmp2
Pseudoenergy limit: ..... 9

==> RUNLAN <==
Number of Lanczos vectors saved: ..... 21
Number of Lanczos iterations completed: ..... 21
Length of longest vector: ..... 21
Form of the vector file: ..... Stable
Condition of basis: ..... Saturated

==> DIAG <==
Number of eigenvectors saved: ..... 10
Iteration at which diagonalization was performed: ..... 21
Operator used for J square: ..... OPJSQR   sc.tmp2
Operator used for T square: ..... OPTSQR   sc.tmp2
Operator used for parity: ..... OPPAR     sc.tmp2
Operator used for HCM: .....

Ground state energy: -7.54057116097507d+01

  I  2IPI 2T   Energy      HCM      J Err      P Err      T Err      E Err      C Err
  1  1 ~ 1   0.000000      1.d-04    1.d-08    1.d-04    0.d+00
  2  3 ~ 1   3.673267      2.d-04    1.d-08    1.d-04    0.d+00
  3  5 ~ 1   7.466057      0.d+00    1.d-04    1.d-04    0.d+00
  4  1 ~ 1   8.639347      1.d-04    0.d+00    0.d+00    0.d+00
  5  3 ~ 1  10.626189      2.d-04    1.d-08    1.d-04    0.d+00
  6  7 ~ 1  11.107986      5.d-04    1.d-08    1.d-04    0.d+00
  7  5 ~ 1  13.762624      4.d-04    0.d+00    1.d-04    0.d+00
  8  1 ~ 1  13.812678      1.d-04    0.d+00    1.d-04    0.d+00
  9  3 ~ 1  14.276023      2.d-04    1.d-08    1.d-04    0.d+00
 10  3 ~ 3  14.669414      0.d+00    2.d-08    2.d-04    0.d+00
>>> ALL STATES HAVE CONVERGED <<<

```

Fig. 3. Results from the calculation shown in Figure 2.

RESULTS USING THE SHELL MODEL/R-MATRIX TECHNIQUE

The shell model/R-matrix technique has worked well where it has been tested.^{4,9,10} So far the most complicated problem involved the calculation of the $^{14}\text{N}(n,xy)$ spectrum for E_n up to 14 MeV. The 32 reaction channels which were included in the R-matrix part of the calculation are listed in Table I. Shell model calculations were performed for ^{11}B , ^{12}C , ^{13}C , ^{14}C , ^{14}N , and ^{15}N using an interaction, parameter set D, derived for a previous study.¹¹ Of the 32 reaction channels listed in Table I, 27 result in gamma-ray production since the excited residual nuclei are below particle emission thresholds. By calculating the cross sections for these reactions and knowing the branching ratios for the subsequent gamma-ray decays (assuming isotropic emission) and, with broadening the lines to match the experimental resolution, the spectrum in Fig. 4 was produced. The calculation compares well with the experimental results by Dickens, *et al.*¹²

Table I. Channels included in the calculation of the $^{14}\text{N}(n,xy)$ spectrum.

^{15}N compound system	(11) $p_0+^{14}\text{C}$	(22) $t_0+^{12}\text{C}$
	(12) $p_1+^{14}\text{C}^*$ (6.09)	(23) $t_1+^{12}\text{C}^*$ (4.44)
(1) $n_0+^{14}\text{N}$	(13) $p_2+^{14}\text{C}^*$ (6.59)	(24) $\alpha_0+^{11}\text{B}$
(2) $n_1+^{14}\text{N}^*$ (2.31)	(14) $p_3+^{14}\text{C}^*$ (6.73)	(25) $\alpha_1+^{11}\text{B}^*$ (2.12)
(3) $n_2+^{14}\text{N}^*$ (3.95)	(15) $p_4+^{14}\text{C}^*$ (6.90)	(26) $\alpha_2+^{11}\text{B}^*$ (4.44)
(4) $n_3+^{14}\text{N}^*$ (4.92)	(16) $p_5+^{14}\text{C}^*$ (7.01)	(27) $\alpha_3+^{11}\text{B}^*$ (5.02)
(5) $n_4+^{14}\text{N}^*$ (5.11)	(17) $p_6+^{14}\text{C}^*$ (7.34)	(28) $\alpha_4+^{11}\text{B}^*$ (6.74)
(6) $n_5+^{14}\text{N}^*$ (5.69)	(18) $d_0+^{13}\text{C}$	(29) $\alpha_5+^{11}\text{B}^*$ (6.79)
(7) $n_6+^{14}\text{N}^*$ (5.83)		(30) $\alpha_6+^{11}\text{B}^*$ (7.29)
(8) $n_7+^{14}\text{N}^*$ (6.20)		(31) $\alpha_7+^{11}\text{B}^*$ (7.98)
(9) $n_8+^{14}\text{N}^*$ (6.45)		(32) $\alpha_8+^{11}\text{B}^*$ (8.56)
(10) $n_9+^{14}\text{N}^*$ (7.03)		
	(19) $d_1+^{13}\text{C}^*$ (3.09)	
	(20) $d_2+^{13}\text{C}^*$ (3.68)	
	(21) $d_3+^{13}\text{C}^*$ (3.85)

Fig. 4. Comparison of the calculated gamma-ray spectrum to experimental data.

This is not to imply there are no problems with effective nucleon-nucleon interactions. So far, however, the calculations of reaction cross sections have involved model spaces small enough so that the problems either do not appear or have been correctable.

PROBLEMS WITH EFFECTIVE NUCLEON-NUCLEON INTERACTIONS

Earlier, the two major decisions in performing a nuclear shell model calculation were presented. After deciding on a model space, the effective nucleon-nucleon interaction must be chosen. In general, however, all current effective interactions fail in large model spaces. Some terminology on describing the sizes of model spaces must be discussed, so consider, for example, the nucleus ^{12}C . In the simplest configurations, the twelve nucleons are placed in the harmonic oscillator such that four nucleons are located in the $1s$ shell and the remaining eight nucleons are located somewhere in the $1p$ shell. The set of these configurations is referred to as the $0\hbar\omega$ model space. A short hand way of denoting these configurations is $(1s)^4(1p)^8$. If one nucleon is promoted by one major shell, then the new set of configurations make up the $1\hbar\omega$ model space, i.e., $(1s)^3(1p)^9$ and $(1s)^4(1p)^7(2s1d)^1$. For a $2\hbar\omega$ model space, two nucleons are promoted by one major shell or one nucleon is promoted by two major shells. The $0, 2, 4, \dots \hbar\omega$ model spaces describe the states of normal parity and the $1, 3, 5, \dots \hbar\omega$ model spaces describe the states of non-normal parity.

An interaction based on a potential model can work very well for a small model space ($0\hbar\omega$). In general, on increasing the size of the model space ($2\hbar\omega$ and beyond), we find that the original set of eigenstates are separated by many MeV from the additional eigenstates of the larger model space. Large 1-particle, 1-hole configurations are mixed into the original ($0\hbar\omega$) states. Part of the reason for this is that the potential being used does not saturate at the correct oscillator size. Improper mixing of 0 and $2\hbar\omega$ excitations has been discussed by several workers.^{10,13,14,15}

Empirical matrix elements have been obtained for the "small" ($0\hbar\omega$) model spaces; e.g., Cohen and Kurath's 2BME(6-16) interaction⁸ for the p-shell nuclei and Wildenthal's USD interaction^{16,17} for the sd-shell nuclei. Other interactions based on potential models are common. While these interactions can be very successful for their particular applications of nuclei and model space, two questions arise: How can we relate these interactions with one another and how do we expand these interactions to larger model spaces? A final area of concern involves the relationship between the effective nucleon-nucleon interactions used in shell-model calculations and the Skyrme-type interactions used in Hartree-Fock calculations. Each of these points was described by Brown and Wildenthal¹⁸ in their 1988 status report on the nuclear shell model. In discussing "prospects for the future", the following statements were made: "Cross-shell excitations in light nuclei, and in particular the mixing of $2\hbar\omega$ and higher excitations into the low-lying spectra, present another challenge for the future." "A major advance would consist of developing techniques to link information about the effective interaction

from one mass range (model space) to another." "It would also be an important advance to unify the interactions used for Hartree-Fock calculations of closed-shell nuclei with those used for the valence spectra." "Much work remains to be done concerning improvement and unification of effective interactions in nuclei."

QUEST FOR AN IMPROVED NUCLEON-NUCLEON INTERACTION

In collaboration with S. D. Bloom (LLNL) and S. A. Moszkowski (UCLA), a new interaction^{19,20,21} is being developed. This interaction is designed for: (1) use in large model spaces, (2) correctly determining basic properties of nuclei and nuclear matter (i.e., binding energies/nucleon and saturation), and (3) reducing to a Skyrme-like (Hartree-Fock) interaction in the short range limit. In so doing, this work directly addresses all the problems discussed above. The basic phenomenology is outlined below.

Shell model harmonic oscillator basis states are used for the single particle states. Then by using gaussian form factors, closed form expressions for many of the basic properties of ^4He , ^{16}O , and nuclear matter can be obtained. Gaussian form factors in momentum space (equivalent to non-locality) are allowed and result in only slight complications to the closed form expressions. Three components are currently being used; two density-independent and one density-dependent. At first only $N=Z$ nuclei are being considered with the interaction parameters determined from the basic (macroscopic) properties of ^4He , ^{16}O , and nuclear matter.

The general form of a component is

$$V e^{-r^2/a^2} e^{-p^2 c^2} \chi \quad (1)$$

The first part of each component is the potential strength. There is a strength for the even states and a strength for the odd states. Since only $N=Z$ is being considered at present, the single/triplet ratios must be determined at a later stage. The second part is the gaussian form factor. While a Yukawa form factor may be more realistic for large r , the gaussian form factor allows for the generation of closed form expressions mentioned earlier and both types are commonly used in the generation of two-body matrix elements.

The third part of (1) when combined with the radial form factor is a schematic representation for non-locality of the following type,

$$V(\vec{r}, \vec{r}') = e^{-(\vec{r} + \vec{r}')^2/4a^2} e^{-(\vec{r} - \vec{r}')^2/4c^2} \quad (2)$$

By a Fourier transformation, (2) is equivalent to

$$V(\vec{r}, \vec{p}) = e^{-r^2/a^2} e^{-p^2 c^2} \quad (3)$$

except for a constant factor. Non-locality of this type is expected at short distances because of the underlying quark structure of the nucleons.²¹ It has also

been shown to be required to accurately describe the deuteron charge radius.²²

The fourth part of (1) is a density-dependent factor. For nuclear matter the density dependence is assumed to scale by the $2/3$'s power, i.e.,

$$\chi = (\rho/\rho_{NM})^{2/3} \quad (4)$$

For nuclei, the density dependence can be written²³ in terms of the harmonic oscillator center-of-mass coordinate R ,

$$\chi = \alpha(1 - \beta R^2/b^2) \quad (5)$$

where α and β are constants for a given nucleus which can be determined through Fermi-Gas arguments and b is the oscillator size parameter.

For the present study, three components of the type shown in (1) are being employed (see Figure 5). The longest range (r) component is assumed to be attractive, density independent, and local ($c=0$). This component is constructed to look like the one pion exchange potential (OPEP). It is this component which leads to the extra clustering that ones finds in ^4He . The second component is of shorter range and is assumed to be attractive, density independent, and non-local. The third component is of still shorter range, repulsive, density dependent, and non-local. The last two components look much like a surface delta interaction and are required for saturation.

Fig. 5. Diagram of the three components used in the present study.

Analytic closed-form expressions have been obtained which allow for macroscopic properties (binding energy/nucleon, saturation, compressibility) of ^4He , ^{16}O , and nuclear matter to be calculated easily from the interaction parameters. The definitions of saturation and compressibility are shown in Table II. The known values for the binding energy/nucleon and the saturation condition are being used to determine the interaction parameters. Several parameter searches have been completed. However, the results are sensitive to how the individual known values are weighted in forming the function to be minimized. The

energy/nucleon curves from one of the parameters searches is shown in Figure 6. Presently, additional constraints are being added to the parameter search.

Table II. Definitions of saturation and compressibility. Compressibility is calculated at saturation.

Definitions	Energy/Nucleon	Saturation	Compressibility
Nuclei	E/A	$b \frac{d(E/A)}{db} = 0$	$b^2 \frac{d(E/A)}{db^2}$
Nuclear Matter	E/A	$k_F \frac{d(E/A)}{dk_F} = 0$	$k_F^2 \frac{d(E/A)}{dk_F^2}$

Fig. 6. Energy/nucleon curves using the results from one of the parameter searches. The asterisks indicate the experimental values.

Preliminary results for $2\hbar\omega$ and $4\hbar\omega$ ${}^4\text{He}$ calculations are very encouraging in that the energies of the original $0\hbar\omega$ states are depressed in energy by less than 1 MeV as compared with many MeV for a non-saturating interaction. By construction, the interaction is global with the parameters currently based on properties of ${}^4\text{He}$, ${}^{16}\text{O}$, and nuclear matter. Finally, this finite-range (shell model) interaction, when taken in the short range limit, reduces to a Skyrme-like (Hartree-Fock) interaction, as is felt to be required for a realistic effective interaction.

SUMMARY

The shell model/R-matrix technique for calculating low-energy ($E \leq 20$ MeV) nuclear reaction cross sections for light projectiles ($n, p, d, t, {}^3\text{He}, \alpha$) incident on light nuclei ($A \leq 20$) has been discussed. The computational methods employed were presented. Results using the shell model/R-matrix technique were discussed as were some of the problems with current effective nucleon-nucleon interactions. The present emphasis on improving the physics in our quest for an improved nucleon-nucleon interaction was presented. In this ongoing work, we are attempting to address the outstanding problems facing the nuclear shell model.

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* Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.