Computer Code Abstract

CCRMN – A Program for Calculating Complex Reactions of a Medium-Heavy Nucleus with Six Light Particles

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1. Program of Identification: The CCRMN program is developed for the theoretical calculation of all complex reactions of a medium-heavy nucleus with a neutron or a charged particle in the 1- to 100-MeV-energy region.

2. Description of the Problem Solved: In the CCRMN program, the incoming particles can be neutrons, protons, ^{4}He, deuterons, tritons, and ^{3}He; the outgoing particles are also the foregoing six particles (corresponding to channels 1 through 6, respectively). In CCRMN, we calculate the reactions in the first, second, third, . . . , up to the tenth emitting processes. In the 1- to 100-MeV-energy region, CCRMN can give correct results for optical model quantities and all kinds of reaction cross sections in first, second, third, . . . , up to tenth emitting processes. The emitted particles are all the foregoing six particles (channels 1 through 6) in the first, second, and third processes; neutrons, protons, ^{4}He, and deuterons (channels 1 through 4) in the fourth and fifth processes; neutrons, protons, and ^{4}He (channels 1, 2, and 3) in the sixth and seventh processes; and only neutrons and protons (channels 1 and 2) in the eighth, ninth, and tenth processes.

The output data of CCRMN include the following: the total cross section; the elastic scattering cross section and its angular distribution; the total reaction (or nonelastic) cross section; the radiative capture cross section; the (x,x') reaction and the (x,x_1,x_2) reaction cross sections, where x, x', x_1, and x_2 can be neutrons, protons, ^{4}He, deuterons, tritons, or ^{3}He; and $\sigma_{x,2np}$, $\sigma_{x,3n}, \sigma_{x,4n}, \ldots, \sigma_{x,10n}$.

For convenient comparison with the experimental data, we also give the sum of the cross sections of all the reactions that lead to the same residual nucleus, usually called the isotope yield cross sections; for example, $\sigma_{2n1p} = \sigma_{x,2np} + \sigma_{x,nd} + \sigma_{x,t}$. These cross sections refer to activation or transmutation processes. We also give the total cross section of emitted particle y in reactions $(x,y),(x,yx'),(x,x'y),(x,yx_1x_2),(x,x_1yx_2)$, $(x,x_1x_2y),\ldots,(x,yx_1\ldots x_9),(x,x_1yx_2\ldots x_9),\ldots,$ $(x,x_1x_2\ldots x_9y)$ in the first, second, third, . . . , up to the tenth processes, without regard to what particles $x',x_1,x_2,\ldots,x_9$ are, where y can be a neutron, proton, ^{4}He, deuteron, triton, or ^{3}He. For example,

$$\sigma_{x,p} = \sigma_{x,p} + \sigma_{x,2p} + \sigma_{x,3p} + \ldots + \sigma_{x,10p} + \sigma_{x,px'} + \sigma_{x,x'p} + \ldots + \sigma_{x,px_1x_2\ x_9} + \sigma_{x,x_1px_2\ x_9} + \ldots + \sigma_{x,x_1x_2\ x_9p},$$

$$\sigma_{x,p\ tot} = \sigma_{x,p} + 2\sigma_{x,2p} + 3\sigma_{x,3p} + \ldots + 10\sigma_{x,10p} + \sigma_{x,px'} + \sigma_{x,x'p} + \ldots + \sigma_{x,px_1x_2\ x_9} + \sigma_{x,x_1px_2\ x_9} + \ldots + \sigma_{x,x_1x_2\ x_9p},$$ [a]

$$m_{x,p} = \sigma_{x,p\ tot}/\sigma_{x,p}.$$

These are referred to as inclusive reactions. The value $\sigma_{x,p}$ is called an inclusive cross section, and $m_{x,p}$ is the multiplicity of $\sigma_{x,p}$, corresponding to emitted particle p. All nuclear data are given for the natural element as well as for its isotopes.

The CCRMN code is constructed within the framework of optical model, preequilibrium statistical theory based on the exciton model (with some changes by Zhang et al.[1]) and the evaporation model. In the first, second, and third emitting processes, we consider preequilibrium emission and evaporation; in the fourth through tenth emitting processes, we consider only evaporation. For emission of composite particles, we adopt a pickup reaction mechanism introduced by

[a]Note that $x',x_1,x_2,\ldots,$ or x_9 is not equal to p here.

Zhang et al.[1] In the calculation of state densities for the exciton model, we accommodate the Pauli principle. All nuclear level densities required in the evaporation model are calculated by the formula of Gilbert and Cameron.[2] The inverse reaction cross sections of the emitted particles used in statistical theory are calculated from the optical model. In CCRMN, for gamma-ray emission, in addition to the evaporation we also consider preequilibrium emission; furthermore, the partial widths are calculated based on the giant dipole resonance model with one or two resonances.

In the optical model calculation, we frequently adopt the phenomenological optical potential of Becchetti and Greenlees[3] (the parameters are usually given by a program for automatically searching for the optimum optical model parameters). The CCRMN code can also do microscopic optical potential calculations based on Skyrme force[4] and the phenomenological optical potential calculation with CH89 or CH86 parameters[5] for the neutron and proton channels.

The CCRMN code does not calculate direct reactions, but it can accept direct reaction cross sections calculated by other programs as input for six outgoing channels in the first process. First, CCRMN subtracts the input direct cross sections from the total reaction cross section and then adds them to corresponding statistical cross sections.

In CCRMN, we do not directly do the Hauser-Feshbach calculation, but it can accept the compound-nucleus elastic-scattering cross section and its angular distribution calculated by other programs as input. CCRMN adds them to the shape elastic-scattering cross section and its angular distribution, respectively, and subtracts the input compound-nucleus elastic-scattering cross section from the total reaction cross section. At the same time, we change the lower limit of the integration of excited energy in the first emitted process at the emitting channel corresponding to the incoming channel from zero to the first excited level energy.

3. Methods of Solution: In the optical model calculation, we use Neumanove methods to solve the radial equation. The step length is 0.1 fm, and there are 150 step numbers in solving the radial equation. The maximum number of fractional waves in the optical model calculation is 60. The coulomb wave functions used in the optical model are calculated by the continued fraction method.[6]

The most important difference between CCRMN and CMUP2 (Ref. 7) is the integral method in the preequilibrium and evaporation calculation. In CMUP2 and many other programs, arguments in the integrand are always kinetic energies of emitted particles: first, we must do the innermost integration corresponding to the last emitted particle and then do the second innermost integration corresponding to the emitted particle before the last emitted one, . . . ; finally, we do the outermost integration corresponding to the first emitted particle. So, the multifold number of the integration in preequilibrium and evaporation calculation is equal to the number of emitted particles. Limited by the computer running time, usually one can do a fourfold integration at most, so previously, one could consider only up to the fourth emitting process. In CCRMN, through transforming the integral argument from the kinetic energy $E_1, E_2, E_3, \ldots$, of the emitted particle in the first, second, third, . . . , emitting processes to the excited energy $u_1, u_2, u_3, \ldots$, of the residual nucleus after the first, second, third, . . . , emitting processes, respectively, and inversing the integral sequence from

$$\int \ldots du_1\, du_2\, du_3 \ldots \text{ to } \int \ldots \ldots du_3\, du_2\, du_1 \ ,$$

we can find a method to change multifold (higher than twofold) integration to twofold integration, and then in principle, we can do the preequilibrium and evaporation calculation up to a very high emitting process (in CCRMN, we really calculate up to the tenth emitting process). To simplify expressions, here we omit the index of the channel at first and let

E = excited energy of the compound nucleus formed from the target nucleus absorbing the incoming particle

$B_1, B_2, B_3, \ldots$ = combined energy of the residual nucleus and the outgoing particle in the first, second, third, . . . , emitting processes, respectively

$Z_1, Z_2, Z_3, \ldots$ = minimum kinetic energy of the emitting particle at which the inverse cross section is larger than 5×10^{-7} b in the first, second, third, . . . , emitting processes, respectively.

Also, we suppose

$$EB_1 = E - B_1 \ , \quad EB_2 = EB_1 - B_2 \ , \quad EB_3 = EB_2 - B_3 \ ,$$

$$BZ_2 = B_2 + Z_2 \ , \quad BZ_3 = B_3 + Z_3, \ldots \ ;$$

for the first emitting process,

$$\int_{Z_1}^{EB_1} \ldots dE_1 \rightarrow \int_0^{EB_1 - Z_1} \ldots du_1 \ ;$$

for the second emitting process,

$$\int_{Z_1}^{EB_2 - Z_2} \ldots dE_1 \int_{Z_2}^{EB_2 - E_1} \ldots dE_2 \rightarrow \int_0^{EB_2 - Z_1 - Z_2} \ldots du_2 \int_{u_2 + BZ_2}^{EB_1 - Z_1} \ldots du_1 \ ;$$

and for the third emitting process,

$$\int_{Z_1}^{EB_3 - Z_2 - Z_3} \ldots dE_1 \int_{Z_2}^{EB_3 - Z_3 - E_1} \ldots dE_2 \times \int_{Z_3}^{EB_3 - E_1 - E_2} \ldots dE_3 \rightarrow \int_0^{EB_3 - Z_1 - Z_2 - Z_3} \ldots du_3 \int_{u_3 + BZ_3}^{EB_2 - Z_1 - Z_2} \ldots du_2 \times \int_{u_2 + BZ_2}^{EB_1 - Z_1} \ldots du_1 \ .$$

From these expressions, we can see that the only difference between the integral for u_1 in the first and in the second processes is the lower limit of the integral. When we do the numerical integration for u_1 in first process, we can keep the values of the integrand at all integral base points, and then we can get values of the integrand for u_1 in the second process by linear interpolation. The integral for u_1 in the second and in the third processes is identical; after completing this integral in the second process, there is no need to do it again in the third process. Furthermore, the only difference between the integral for u_2 in the second and in the third processes is also the lower limit of the integral. Therefore, when we do the numerical integration for u_2 in the second process, we can also keep the values of the integrand at all integral base points, and then we can get values of the integrand for u_2 in the third process by linear interpolation. In this way, we change the threefold integral in the third process to a twofold integral, and in the inner integral, we can obtain the values of the integrand by linear interpolation to reduce the computing quantity. Repeating this argument for the fourth, fifth,..., to the tenth processes, we can change the integral to twofold in any emitting process.

4. Related Material: No additional programs are required.

5. Restrictions: The target is a medium-heavy nucleus ($A = 28$ to 208). The target element consists of only one isotope, or six isotopes at most, in which the difference in mass number of the heaviest and lightest isotopes should be ≤ 10. The incidental energies should be within 1 to 100 MeV, in which the maximum number of the incidental energy points is 40 in one calculation.

6. Special Features of the Program: The main character and advantage of CCRMN is the calculational method in it: Besides the first emitting process, the integral is always changed to twofold in any emitting process. So, in CCRMN, as an increase of the emitting process, only the number of channels increases; the multifold number of the integral in any emitting process is always two and does not increase. In this way, we can easily finish the calculation and get the reaction cross section in any high emitting process.

7. Computers: The original computer was an M340-S; the other computer was an HP station, SUN station.

8. Typical Running Time: The running time depends on the numbers of energy points, how they are distributed, and in what energy region. For example, the calculation of ($p + {}^{28}$Si) (there are 40 energy points distributed in the region below 30 MeV) lasts only ~5 CPU min at the HP Station; however, the same calculation for 4 energy points (30.0, 40.0, 50.0, and 60.0 MeV) lasts ~40.5 CPU min and for 1 energy point (80 MeV) lasts ~1 CPU h at the HP station.

9. Machine Requirements: Disks and a printer are necessary for output; the amount of memory needed is 8192 kbytes.

10. Program Language: FORTRAN 77.

11. Operating System: FACOM OS IV/F4; UNIX.

12. Other Programming or Operating Information or Restrictions: Double-precision arithmetic is necessary for some parts of the calculation. The unit numbers are 4 for input and 7 for output.

13. Material Available: User's Manual for CCRMN and input data file for ($p + {}^{28}$Si).

14. References:

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