Computer Code Abstract

CMUP2

A Program for Calculating Complex Reactions of a Medium-Heavy Nucleus with Charged Particles

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I. INTRODUCTION

Based on MUP2 (Ref. 1), we wrote in 1988 a program called CMUP to meet the needs for calculating the charged-particle induced reactions $^{55}Mn(\alpha,n)^{58}Co$ and $^{55}Mn(\alpha,2n)^{57}Co$. Meanwhile a group at Sichuan University performed experiments on the same type of reactions. The MUP2 code is a program for calculating all kinds of neutron-induced reactions on a medium-heavy nucleus in the energy region below 20 MeV. The CMUP code was only suitable below 20 MeV (or at most up to 25 MeV), although the results of optical model calculations are correct from 3 to 150 MeV, and CMUP could not be used for evaluations of charged-particle–induced reactions at higher energies. To meet the demands for evaluations of charged-particle–induced reactions in the energy region of 3 to ~100 MeV, recently we improved and rewrote CMUP and named it CMUP2. In CMUP and CMUP2, the incoming charged particles can be protons, tritons, ^{3}He, deuterons, or ^{4}He; the outgoing particles are neutrons and the foregoing charged particles, as well as photons. In CMUP2, we calculate the reactions in the first, second, third, and fourth emitting processes.

II. FUNCTION OF CMUP2

• In the 3- to 100-MeV energy region, CMUP2 can give correct results for optical model quantities and all kinds of reaction cross sections in first, second, and third emitting processes. The fourth emitting process includes the contributions in higher order processes. CMUP2 also gives the energy spectra of all the emitted particles in the first and second emitting processes.

The output data of CMUP2 include total cross section; shape-elastic scattering cross section (only for neutron as projectile); total reaction cross section; radiative capture cross section; (x,x') reaction cross sections, (x,x_1x_2) reaction cross sections, and $(x,x_1x_2x_3)$ reaction cross sections, where x', x_1, x_2, and x_3 may be neutrons, protons, tritons, ^{3}He, deuterons, or ^{4}He; $(x,x_1x_2x_3x_4)$ reaction cross sections, where x_1 and x_2 can be neutrons, protons, tritons, ^{3}He, deuterons, or ^{4}He, but x_3 and x_4 can only be neutrons or protons; the elastic scattering angular distribution and the ratio of the elastic scattering differential cross section to the Rutherford differential cross section; and the energy spectra of x' particles in (x,x') reactions, and of x_1 and x_2 particles in (x,x_1x_2) reactions.

To compare with experimental data conveniently, we also give the sum of the cross sections of all reactions that lead to the same residual nucleus, for example, $\sigma_{x,2np} + \sigma_{x,nd} + \sigma_{x,t}$. These cross sections refer to activation or transmutation processes. We also give the total cross section of emitted particle y in reaction (x,yx') in the first and second processes, without regard to what particle x' is, and the corresponding energy spectra of particle y in reaction (x,yx'), where y can be neutrons, protons, tritons, ^{3}He, deuterons, or ^{4}He. For example,

$$\sigma_{x,dx'} = \sigma_{x,d} + \sigma_{x,dn} + \sigma_{x,dp} + \sigma_{x,dt} + \sigma_{x,d\tau} + 2\sigma_{x,dd} + \sigma_{x,d\alpha}$$

with the spectrum distribution function

$$F_{x,dx'} = (\sigma_{x,d}F_{x,d} + \sigma_{x,dn}F_{x,dn} + \dots + 2\sigma_{x,dd}F_{x,dd} + \sigma_{x,d\alpha}F_{x,d\alpha})/\sigma_{x,dx'} .$$

The latter cross sections are referred to as inclusive reactions. All nuclear data are given for the natural element as well as for its isotopes.

The CMUP2 code is written in Fortran-77 and ran on the M-340S computer (made in Japan) at Nankai University originally. There is also a version on a MicroVAX Computer at the Chinese Nuclear Data Centre (CNDC). We have already calculated several reactions ($p + {}^{89}$Y, $p + {}^{56}$Fe, $n + {}^{56}$Fe, $\alpha + {}^{55}$Mn, and $p + {}^{63}$Cu) and obtained quite good results in agreement with the experimental data.

At present, CMUP2 is used at CNDC. The original CMUP2 program and the user's manual for CMUP2 will be submitted to the Nuclear Energy Agency Data Bank by CNDC in 1992.

III. THEORY AND METHODS

The CMUP2 code is constructed within the framework of optical model, pre-equilibrium statistical theory based on the exciton model (with some changes by Zhang et al.[2]) and the evaporation model. In the first, second, and third emitting processes, we consider pre-equilibrium emission and evaporation; in the fourth emitting process, we consider only evaporation. For emission of composite particles, we adopted a pickup reaction mechanism introduced by Zhang et al.[2] 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.[3] The inverse reaction cross sections of the emitted particles used in statistical theory are calculated from the optical model. The partial widths for gamma-ray emission are calculated based on the giant dipole resonance model with two resonances.

In the optical model calculation, we frequently adopt the phenomenological optical potential of Becchetti and Greenlees[4] (the parameters are usually given by a program for automatically searching for the optimum optical model parameters). The CMUP2 code can also do microscopic optical potential calculations based on Skyrme force[5] and the phenomenological optical potential calculation by Varner et al.[6] for the neutron and proton channels. 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.[7]

The CMUP2 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, CMUP2 subtracts the input direct cross sections from the total reaction cross section and then adds them to corresponding statistical cross sections.

In CMUP2, we do not consider Hauser-Feshbach theory. Because pre-equilibrium theory cannot calculate the compound elastic cross section, we assume the compound elastic cross section to be zero at $E > 3$ MeV, which does not affect the use of CMUP2 in real calculations.[a] We consider CMUP2 valid at $E > 3$ MeV because pre-equilibrium theory usually does not apply at $E < 3$ MeV.

[a]The reason is that when $E < 3$ MeV, the total reaction cross section is <10 mb, which is nearly equal to the cross section of the (x, n) reaction, and the sum of the compound elastic and inelastic cross sections is <1 mb; when $E > 3$ MeV, the compound elastic cross section is always <1 mb.

IV. CONCLUSIONS AND REMARKS

The CMUP2 code is suitable for calculating charged-particle-induced reaction cross sections on medium-heavy nuclei with three outgoing particles to ~50 MeV, although its calculated results of the optical model and in first, second, and third processes are correct up to 100 MeV or even higher energy. It cannot completely meet all demands of evaluation of charged-particle-induced reactions, so we intend to further improve and develop it, and name it CMUP3, in the future.

In CMUP3, besides neutrons, protons, tritons, ^{3}He, deuterons, and ^{4}He, we will add ^{6}Li, ^{7}Li, ^{7}Be, and ^{9}Be as emitted particles in the first and second processes. For neutron and proton emission, we will consider up to nine processes. Perhaps we need also to consider fission channels in the first, second, and third processes. To realize this objective, we must solve a lot of problems both in physics and in computation.

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