89-238

L 63

M. Lewitowicz, S. Kliczewski

ELPHIC-PC: A NEW VERSION OF THE MONTE-CARLO CODE FOR KINEMATIC SIMULATION OF HEAVY ION-INDUCED REACTIONS

1989

1. INTRODUCTION

The ELPHIC-PC programme has been written for Monte-Carlo simulation of nuclear reactions with heavy ions. In recent years several such simulation programmes appeared, e.g.: LINDA[1], ELPHIC[2], GANES[3]. Using the statistical model assumptions, these simulation programmes give, as a result, the charge and energy spectra and angular distributions in the laboratory system - both for fission fragments, evaporation residues and light particles emitted in different stages of reaction.

The comparison of experimental data (e.g., light charged particle spectra) for calculations of different input parameters and different possible emission sources enables us to conclude about the reaction scheme. Using the programmes mentioned above or the programme ELPHIC-PC one may simulate planned multi-detector experiments both inclusive and correlated. Such simulation gives the possibility of selecting the best geometry of experiment and indicates the influence of different kinematic effects.

As a result of calculations one may obtain for an inclusive experiment:

- the energy spectra and angular distributions of light particles (three kinds of particles with any A and Z) emitted from different sources (direct reaction, evaporation from compound nucleus and evaporation from fission fragments);
- the energy, mass and charge spectra and angular distributions of heavy reaction products (fission fragments and evaporation residues);

and for correlation experiments:

- the energy spectra and angular distributions of light particles in coincidence with two heavy fragments or evaporation residue:
- the energy, mass and charge spectra and angular distributions of heavy fragments in coicidence with the second heavy fragment.

The programme ELPHIC-PC has been written for calculations on personal computers PC - XT/AT. The widespread use of these computers gives (though these computers are slower than the

1

big ones) the possibility of very effective work using the DOS operating system. The ELPHIC-PC programme has been written in the TURBO-PASCAL v.3.0 language. Programmes written in this language are fast, especially for personal computers equipped with arithmetic coprocessors. This language also enables very easy modifications of the source version of the programme.

The scheme of the ELPHIC-PC calculations is similar to the typical scheme of the physical experiment. The programme is divided into two main parts, analogously to two successive parts of an experiment - measurement and data presentation:
ELP - the main programme for simulation of the nuclear reaction with heavy ions, storing results event-by-event in binary form on the disc file,
ELPRI - the programme for sorting and selection of one- and two-dimensional spectra and for printing them.The sorted data can also be recorded on disc file to be used by the DOS-system graphic code.
The full description of these programmes, input data and results as well as the examples of calculations are included in the ELP.HLP file (see chapter 6).

2. THE PROGRAMME ELP - METHOD OF CALCULATION

The combined standard-weighed Monte-Carlo method is used in the ELP programme[4]. The standard method has been used for simulation of the fission process, and the weighed method for light particle emission from all sources. This combination enables one to obtain the energy and angular spectra of light particle with accuracy independent of the emitted particle kinetic energy. The scheme of nuclear reaction with heavy ions may be divided into the following stages:
a) collision, composite system formation and direct emission of the light particles in the case of incomplete fusion;
b) compound nucleus formation and evaporation of light particles;
c) fission of the compound nucleus into two heavy fragments or evaporation residue formation;
d) evaporation of light particles from fission fragments.
Flow-diagram of the programme ELP is presented in Fig.1.

2.1. Direct Emission of Light Particles

The formation of a composite system can be regarded as complete or incomplete. In the case of incomplete fusion the forward peaked direct emission of light particles is possible.
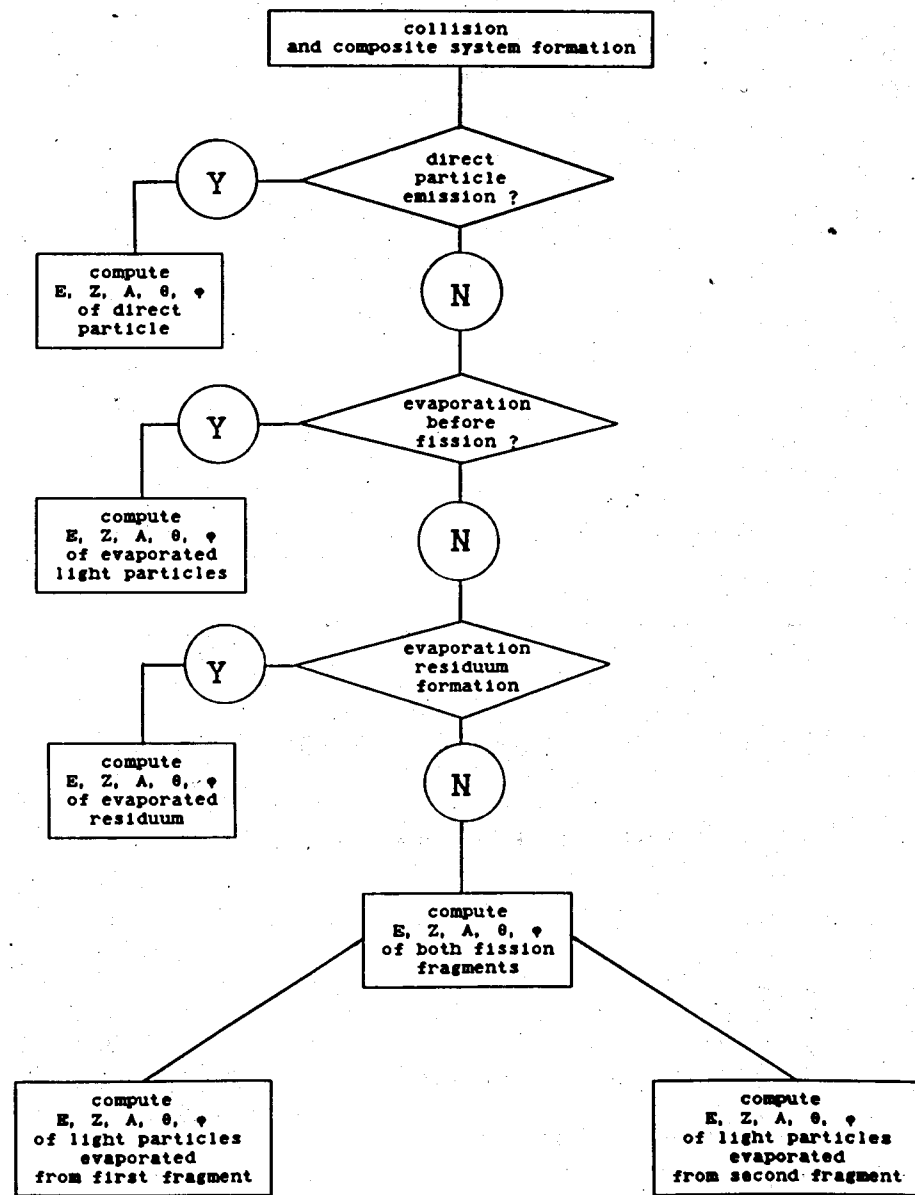

Fig.1. Flow-diagram of the ELP programme.

The mass and charge of projectile and target and the lab. energy of incoming particle are read as input data. For the composite system the mass-excess is calculated using a semiempirical formula without regarding the orbital momentum transfer. This mass-excess value can also be read from input data. Three types of directly emitted light particles are allowed. Energy spectra and angular distributions in the center-of-mass system of directly emitted particles are introduced phenomenologically as input data. The following options are possible here:

- the maximum emission angle and the angle for which the value of $(\frac{d\sigma}{d\Omega})_{c.M.}$ is decreased by a factor of two with respect to its maximum are determined,
- the energy spectrum can be determined in the following modes:

a) the monochromatic spectrum;
b) the energy of particles decreases exponentially with increasing emission angle;
c) the Maxwellian energy distribution with constant temperature,
d) the Maxwellian energy distribution with temperature decreasing exponentially with increasing emission angle;
e) an asymmetric Gaussian energy spectrum;
f) an asymmetric Gaussian energy spectrum with both half-widths decreasing exponentially with increasing emission angle;
g) an asymmetric Gaussian energy spectrum with both half-widths depending linearly on emission angle.

2.2. Light Particle Evaporation from the Compound Nucleus

The evaporation of light particles following fusion and compound nucleus formation is considered. Three types of light particles (with any A and Z) are allowed. Practically only neutron, proton and light charged particle with low Z are considered. The kinetic energy of light particles is picked randomly using Maxwellian distribution[1]:

$$\rho(E) \sim (E - C) \cdot \exp(-\frac{E-C}{T}),$$

with temperature $T = \sqrt{8U/A}$, where C is the Coulomb barrier height, U and A are the excitation energy and mass number of the emitting nucleus, respectively. The C value is calculated from the formula:

$$C = 1.44 \frac{Z_P(Z_N - Z_P)}{r_o} \text{ [MeV]},$$

where

$$r_o = 1.222(A_P^{1/3} + (A_N - A_P)^{1/3}) + 2 \text{ [fm]}.$$

Here Z_P, Z_N, A_P and A_N are the charges and masses of the light particle and the emitting nucleus, respectively[5]. The direction of emission is picked randomly using the formula[6]:

$$\frac{d\sigma}{d\Omega}(\theta_{LAB}) \sim 1 + B\cos^2(\theta_{LAB}).$$

where B is a phenomenological parameter. It may be emphasized, that this code works only for spherical nuclei and does not take into account the nuclear spin.

The sum of the emission probabilities of all three light particles must be equal to unity. These probabilities may be estimated from any statistical code (e.g. ALICE[7]) calculations or taken from the literature.

The binding energies of light particles in the compound nucleus are read as input data. The anticipated range of the masses of compound nuclei is divided into three parts, and the average binding energy is introduced for each area. The energies may be easily calculated using tables of nuclear masses.

For any emitted light particle E_{LAB}, θ_{LAB} and ϕ_{LAB} are determined. The mass, charge, E_{LAB}, θ_{LAB} and ϕ_{LAB} for the compound nucleus after emission of all light particles are also determined.

2.3. Decay of the Compound Nucleus

After emission of light particles the compound nucleus may deexcite by emitting photons and forming evaporation residues, or may undergo fission. The probability of evaporation residue formation is introduced as input data. Fission into two heavy fragments proceeds when the assumed number of light particles has been emitted or the excitation energy of the compound nucleus has decreased below the preset value. The above-mentioned values are introduced as input data.

The total kinetic energy distribution (TKE) of fragments is assumed to be Gaussian. The average $\overline{TKE}$ is calculated from Viola systematics[8]:

$$\overline{TKE} = 0.1189 \frac{Z^2}{A^{1/3}} + 7.3 \text{ [MeV]}.$$

The half-widths of the TKE distributions: σ_{TKE} (TKE) and $\sigma_{TKE}(A_{FF})$ where A_{FF} is the mass of fission fragment, are introduced as input data. This tabulated data are collected in review papers, e.g.[9].

The angular distribution of fission fragments is assumed to be $\sim \dfrac{1}{\sin(\theta_F)}$, where θ_F is the angle between fragment emission and the direction of the fissioning system movement. The distribution of radial angle ϕ is assumed to be isotropic.

The fission fragment mass distribution is also assumed to be Gaussian. The fragment mass ratio A/A_{F1} is read as input data. Changing the A/A_{F1} ratio we can simulate the decay of the compound nucleus as a result of deep-inelastic interactions. The half-width of the fission fragment mass distribution $\sigma_A(A_{FF})$ is read as input data. The possible values of fission fragment mass may be restricted by introducing the maximum and minimum values of A_{FF} as input data.

2.4. Evaporation of Light Particles from Fission Fragments

The programme can also simulate evaporation of light particles from both fragments of fission. Here, as in the case of compound nucleus, three kinds of light particles can also be emitted. The same simple method of calculating the light particle kinetic energy and its emission direction as for evaporation from compound nucleus is used. The light particle emission probabilities must be determined once again, e.g. by using the statistical code[7]. The maximum and minimum energies of evaporated light particles are also read as input data. The number of light particles evaporated from each fission fragment is determined assuming a minimum energy threshold.

3. THE GEOMETRY OF THE SIMULATED EXPERIMENT

The experimental set-up consists of the following detectors:
a) fission fragment detectors, the so - called trigger (TR) and sweeper (SW), with positions determined by θ and ϕ and the chosen angular aperture. For saving computer time the angular range around fission fragment detectors should be determined, as in[1,2];
b) evaporation residue detector (ERD) with position determined by θ and ϕ and chosen angular aperture;

c) up to 20 light particle detectors (LPD) with positions also determined by θ and ϕ angles and angular aperture. The geometry of the experiment presented in Fig.2 has been chosen similarly as in[2]. The angles are the same as in the description included in the ELP.HLP file. There is possible simulation of three kinds of experiments:
a) inclusive experiment: registration of light particles of all three kinds;
b) coincidence experiment: registration of coincidence of two heavy fragments;
c) coincidence experiment: registration of light particles of all three kinds in coincidence with two heavy fission fragments or evaporation residue.
The following light particle emission sources are possible: direct reactions, evaporation from the compound nucleus, evaporation from the first (trigger) and from the second (sweeper) fission fragments.

The events which have hit the detectors, according to the above mentioned requirements, are recorded in binary form on
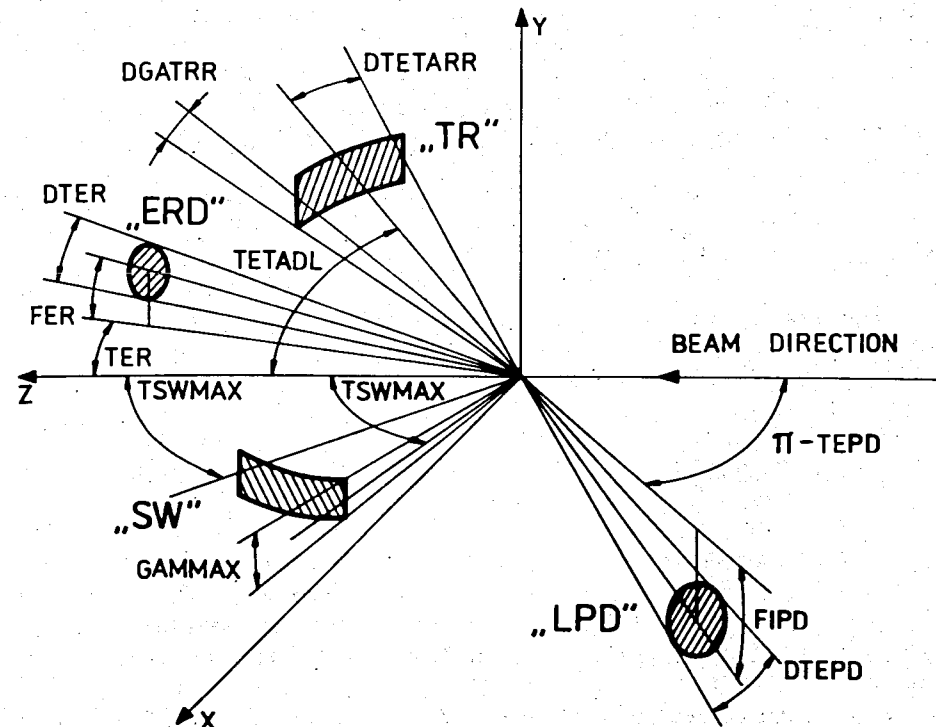

Fig.2. The geometry of the simulated experiment.

the disc file. The detailed description of the chosen number of initial simulations is displayed on request for checking.

4. THE PROGRAMME ELPRI - SORTING OF SPECTRA

The programme ELPRI can create up to 5 one-dimensional 40-channel and two-dimensional 20x25-channel spectra with constant logarithmic or linear scale using the data obtained from the simulation programme. In the ELPRI programme description of the list of parameters for light particles, both heavy fragments and evaporation residues are enclosed. The parameters are charge Z, mass A, kinetic energy, θ and ϕ angles and the sum of linear momenta of both heavy fragments.

5. THE PROGRAMME ELPCUT - PREPARATION OF INPUT FILE FOR THE PROGRAM ELPRI

The output file of program ELP is the input file for ELPRI. This file is written event-by-event in the binary record form and has a header in character form for easy identification by the user. In the case of interrupted work of the ELP programme the last record of this file may be incomplete. The ELPCUT programme truncates the header and the last record of the ELP output file.

6. USER´S GUIDE

The ELPHIC-PC pack includes the following files:
ELP.PAS, ELP.COM, ELPCUT.PAS, ELPCUT.COM, ELPRI.PAS, ELPRI.COM
- the source and compiled versions of programs described in this paper;
DATA.INP - the example input data for ELP programme;
DATA.PRI - the example input data for ELPRI programme;
ELP.HLP - description of input data preparation and output results.
The ELPHIC-PC pack covers 160 kB space on disc.
Input data for the ELP programme should be written on the DATA.INP file. The programme ELP displays on monitor screen the detailed description of the desired number of initial events. This description may be stored on a disc file using DOS redirect command: ELP > OUT.ELP. Simulated events are stored on DATA.OUT file. If a few such output files, obtained for

the same input data exist, then all of them (except one) should be truncated by the ELPCUT programme. Then these files should be concatenated by the DOS command:
COPY DATA1.OUT + ... + DATAn.OUT, where DATA1.OUT is the untruncated file.
The DATA.PRI, written by user, is the input file for ELPRI programme. The output results (histograms) are displayed on the monitor screen. These results may be stored on a disc file using the DOS redirect command: ELPRI > OUT.PRI. The ELPRI programme also creates on request the numeric files including histograms for using them by any graphic code.

Of course, the calculation time strongly depends on the reaction scheme considered. Under the following experimental conditions: the energy of incoming particles of 36 MeV, two neutron detectors, neutron emission from direct reaction, compound nucleus and both fission fragments and for 1000 events, the typical calculation time for the $^{4}He + ^{238}U$ reaction simulation is:

Computer	ELP	ELPRI
Pravetz PC/XT	4500 s	220 s
Pravetz PC/XT/8087	1200 s	150 s
PC AT/8087	700 s	90 s

The largest compiled code ELP.COM requests 51 kB of operation memory.

REFERENCES

1. Duek E. et al. - Comp.Phys.Comm., 1985, v.34, p.395.
2. Lewitowicz M. - JINR Preprint P11-84-284, Dubna, 1984.
3. Ajitanad M.M. et al. - Nucl. Instr. Meth., 1986, v.A243, p.111.
4. Cashwell E.D., Everett C.J. - A Practical Manual of the Monte-Carlo Method for Random Walk Problems, Pergamon, New York, 1959.
5. Volkov V.V. - Yadernye reaktsii glubokoneuprugikh peredach, Moskva, Energoizdat, 1982.
6. Ericson T. - Adv. in Phys., 1960, v.9, p.425.
7. Blann M., Plasil F. - Report COO-3494-10, 1973.
8. Viola V.E. - Phys.Rev., 1985, v.C31, p.1550.
9. Gangrski Yu.P. et al. - Oskolki deleniya yader, Moskva, Energoatomizdat, 1986.

Левитович М., Кличевски С.   E7-89-238

ELPHIC-PC: новая версия программы
кинематического моделирования методом
Монте-Карло ядерных реакций с тяжелыми
ионами

Представляется новая версия программы кинематического
моделирования ядерных реакций с тяжелыми ионами. В про-
грамме использован комбинированный взвешенно-стандартный
метод Монте-Карло, она позволяет моделировать инклюзивные
спектры и корреляции между осколками деления, ядрами отда-
чи и легкими частицами, получая угловые, энергетические
и массовые распределения продуктов реакции в лабораторной
системе. Результаты расчетов программы дают возможность
проверять предсказания теоретических моделей и планировать
новые эксперименты. Эта версия программы написана для пер-
сональных компьютеров класса РС ХТ/АТ.

Работа выполнена в Лаборатории ядерных реакций ОИЯИ.

Lewitowicz M., Kliczewski S.   E7-89-238

ELPHIC-PC: a New Version of Monte-Carlo
Code for Kinematic Simulation of Heavy
Ion-Induced Reactions

A new version of the kinematic simulation programme of
heavy ion-induced reactions has been written. This prog-
ramme uses a combined standard-weigted Monte-Carlo method,
and allows one to simulate both inclusive spectra and cor-
relation between fission fragments, evaporation residues
and light particles. As a result, the angular, energy and
mass distributions of reaction products in the lab.system
are obtained. This programme enables one to check the
theoretical model assumptions and to plan new experiments.
This version of the programme is written for personal com-
puters PC XT/AT.

The investigation has been performed at the Laboratory
of Nuclear Reactions, JINR.