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A CLASSICAL STATISTICAL MODEL OF HEAVY ION COLLISIONS.

II. Description of the Computer Code TRAJEC

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1. INTRODUCTION

In the first paper [1] we presented a classical statistical model of heavy ion collisions. In this model the relative motion of two ions is described by Newton-type equations of motion including frictional forces. The mass transfer between the two nuclei is included and treated dynamically. The deformation energy is taken into account by modifying the exit-channel interaction potential. In the model the statistical fluctuations around the classical mean values of the trajectory are taken into account and obtained from a linear Fokker-Planck equation in the phase space of the collective degrees of freedom. The solution of the Fokker-Planck equation is a Gaussian with mean values as they follow from the solution of the Newton-type equation. For the second moments a coupled set of first order differential equations has been derived. It must be solved simultaneously with the Newton-type equations. We assume that relative motion and mass transfer are statistically uncorrelated. The total distribution function can be used to calculate various multi-differential cross sections of deep inelastic reaction products.

The basic formulas as well as the parameters of the model are summarized in ref. [1]. In this paper we describe the computer code TRAJEC which represents the numerical realization of the model in ref. [1].

2. DESCRIPTION OF THE PROGRAM

The FORTRAN code contains tha main program TRAJEC and 34 SUBROUTINEs and FUNCTIONs. A summary of the UP's is given in the Table. We use the predictor-corrector method by Milne and Hamming [2] to solve the system of coupled differential equations. The service program library of the computer has to contain the UP's GRAPH1 (function plot) and GAUSS1 (integration procedure). In the main program the whole input and output is carried out.

The input data contain the reaction characteristics (mass and charge numbers of projectile and target and bombarding energy) and some control integers for the print options, step widths and ranges for the calculation of the multiple diffe-

Table

SUBROUTINEs and FUNCTIONs

FUN RUNKU HAMM FE	solution of the differential equations
DEF DEFF	deformation
VPR	proximity potential
FPR	derivation of the proximity potential
VCOUL	Coulomb potential
FCOUL	derivation of the Coulomb potential
VPOT	total potential
POTENT	potential print
GRAZIN	integration of the Coulomb trajectory
STIF	stiffness tensor
STICK	sticking form factor
PT	θ-distribution
PZ	Z_1-distribution
PZT	Z_1,θ-distribution
PETZ	E, Z_1, θ-distribution
PEZ	E, Z_1-distribution
PET	E, θ-distribution
RINT1...RINT6	integration SUBROUTINEs
MATRA MATRB MATRC MASSET	mass transfer
TRACO	mass transport coefficients
GRAPH1	deflection function plot *
GAUSS1	integration SUBROUTINE*

*The TRAJEC deck does not contain this UP's. They have to be within the service library of the computer.

rential cross sections. In a standard run the model parameters are fixed in the program corresponding to the values given in eq. (15) in ref. [1], although there exists a possibility to change the radial friction strength. In this case the tangential friction strength and the deformation parameter are calculated in the program according to eq. (16) in ref. [1]. The equations of motions are solved for different relative angular momenta L with the step widths of $\Delta L=2$, starting with the grazing angular momentum ℓ_{gr} and terminating with the critical angular momentum for fusion. The maximal value of the grazing angular momentum that can be used in the program is restricted to 600 ($\ell_{gr} \leq 600$).

Two main different types of calculations are possible and controled by the input integer IS (cf. input, card 2). If this control integer is equal to zero (IS = 0) the Newton-type differential equations are solved only. The results of such a calculation (interaction time, deflection angle, turning point, radial and tangential energy loss, deformation energy, total kinetic energy loss, kinetic energy in the exit channel, scission radius, mean values of the mass and charge of the projectile like reaction-product, variance of the element distribution) can be printed as function of the initial relative angular momentum (cf. output). If the control integer IS is equal to one (IS=1) the code solves, in addition to the Newton-equations, the coupled set of 13 first order differential equations for the second moments. This exceeds the running time considerably and is needed only in the cases where differential cross sections should be calculated.

Typical examples of input data sets for both types of calculations are presented in section 5.

3. INPUT

Card 1   IP1, IP2,IP3,IP4 (print options)
FORMAT(4I5)

- IP1 =1, print the time dependence of the classical trajectory after each tenth time integration step. In a standard run IP1 = 0. If IP1 = -1 the calculation stops. (cf.card 3,5)
- IP2 =1, print the results of the classical trajectory calculation (interaction time, turning point, energy loss,..., cf.output) for each initial angular momentum.
- IP3 =1, the deflection function is plotted.
- IP4 =1, the program prints the proximity potential and the Coulomb potential.

If the integers IP1,IP2,IP3,IP4 are put equal to zero the corresponding prints are not carried out.

Card 2   IC,NN,IR,IT,ID,IS,IFF,IW,IEL,IEZ (control integers)
FORMAT(10I5)

- IC =0, program calculates Coulomb trajectories.
  =1, standard run.

NN =0, radial friction strength is fixed as a_R = 12 fm/c MeV.
=1, a_R must be read by an additional card (cf. card 4).

IR =0, calculation without radial friction.
=1, standard run.

IT =0, calculation without tangential friction.
=1, standard run.

ID =0, calculation without deformations.
=1, calculation with deformations.

IS =0, calculation without fluctuations, only the classical trajectory is calculated.
=1, calculation of fluctuations, cross sections are calculated.

IFF =2 in any case.

IW =0, calculation of $d\sigma/d\Omega$.
=1, calculation of $d\sigma/d\Omega$ and $d^2\sigma/dEd\theta$.
=2, calculations of $d\sigma/d\Omega$, $d^2\sigma/dEd\theta$ and $d^3\sigma/dEd\theta dZ_1$.

IEL =0, calculation without mass transfer.
=1, with dynamical mass transfer. (The calculation of $d\sigma/dZ_1$ and $d^2\sigma/d\theta dZ_1$ is carried out if also IS=1).

If IW=2 the value of IEL should be chosen to be equal one (IEL=1).

IEZ =0, no calculation of $d^2\sigma/dE_1dZ_1$.
=1, calculation of $d^2\sigma/dE_1dZ_1$.

E_1 represents the total kinetic energy loss. If IEZ=1 the value of IEL should be chosen to be equal one (IEL=1).

Card 3 A1,A2,Z1,Z2 (masses and charges)
FORMAT (4F10.2)

A1 projectile mass number A_1
A2 target mass number A_2
Z1 projectile charge number Z_1
Z2 target charge number Z_2

If A1=-1, a new run is created beginning with the reading of the card 1 (cf. cards 1,5).

Card 4 DELTA (radial friction strength)
FORMAT (F10.2)

DELTA radial friction strength a_R *

This card is needed only if NN=1.

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* The quantities a_θ and α are then calculated according to eq.(16) in ref./1/.

Card 5 ELAB (laboratory energy)
FORMAT (F10.2)
ELAB laboratory energy of the projectile E_{lab} in MeV.
If ELAB=-1., a new run is created beginning with the reading of the card 3 (cf. cards 1,3).

Card 6 LMAXE,IEMIN,IEMAX,IEDEL (LMAXE is the maximal angular momentum and IEMIN, IEMAX, IEDEL control the energies at which $d^2\sigma/d\theta dE$ and $d^3\sigma/d\theta dE dZ_1$ are printed).
FORMAT(4I5)
LMAXE grazing angular momentum ℓ_{gr} in units of $\hbar$.
LMAXE is also used as maximal angular momentum for the calculation of $d\sigma/d\Omega$, $d^2\sigma/d\theta dE$ and $d^3\sigma/d\theta dE dZ_1$.
If LMAXE=-1, ℓ_{gr} is calculated within the program according to

$$\ell_{gr} = \frac{r_0(A_1^{1/3} + A_2^{1/3}) + 0.5\,\mathrm{fm}}{\lambda\!\!\!^-}\sqrt{1 - \frac{V_{CB}}{E_{CM}}}$$

with the center of mass energy E_{CM}, the Coulomb barrier V_{CB} and $\lambda\!\!\!^- = (2\mu E_{CM})^{-1/2}$ and $r_0 = 1.2$ fm.
IEMIN minimal value of the exit kinetic energy E_{min} for the calculation of $d^2\sigma/d\theta dE$ and $d^3\sigma/d\theta dE dZ_1$.
IEMAX maximal value of the exit kinetic energy E_{max} for the calculation of $d^2\sigma/d\theta dE$ and $d^3\sigma/d\theta dE dZ_1$.
IEDEL energy step width ΔE for the calculation of $d^2\sigma/d\theta dE$ and $d^3\sigma/d\theta dE dZ_1$.
The value of (IEMAX - IEMIN)/IEDEL must be integer. and smaller than 15.

Card 7 LMAXZ, IZMIN,IZMAX,IZDEL (control the maximal angular momentum and the charge numbers at which the charge distribution is printed).
FORMAT(4I5)
LMAXZ maximal angular momentum ℓ^z_{max} for calculating $d\sigma/dZ_1$ and $d^2\sigma/d\theta dZ_1$.
IZMIN minimal charge number Z_{min} for calculating $d\sigma/dZ_1$, $d^2\sigma/d\theta dZ_1$ and $d^3\sigma/d\theta dE dZ_1$.
IZMAX maximal charge number Z_{max} for calculating $d\sigma/dZ_1$, $d^2\sigma/d\theta dZ_1$ and $d^3\sigma/d\theta dE dZ_1$.
IZDEL charge step width ΔZ for calculating

$d\sigma/dZ_1$, $d^2\sigma/d\theta dZ_1$ and $d^3\sigma/d\theta dE dZ_1$.
This card is needed only if IEL=1. The value of (IZMAX - IZMIN)/IZDEL must be integer and smaller than 10.

Card 8 IELMIN,IELMAX,IELDEL (control the total kinetic energy loss at which $d^2\sigma/dE_\ell dZ_1$ is printed)
FORMAT(3I5)

IELMIN minimal value of total kinetic energy loss $TKEL_{min}$ for calculation $d^2\sigma/dE_\ell\, dZ_1$. (E_ℓ has the meaning of TKEL).

IELMAX maximal value of total kinetic energy loss $TKEL_{max}$ for calculating $d^2\sigma/dE_\ell dZ_1$.

IELDEL total kinetic energy loss step width ΔE for calculating $d^2\sigma/dE_\ell dZ_1$.

This card is needed only if IEZ=1. The value of (IELMAX - IELMIN)/IELDEL must be integer and smaller than 15.

The simplest data set contains five cards (card 1,2,3,5,6). After the run the input of a new data set can be performed. The new input begins with card 5. That is if one wants to repeat the calculation for the same target-projectile combination but at other bombarding energy as in the preceding run. If at card 5 ELAB=-1, the new data set begins with card 3. In this case one wants to calculate another reaction but with the same print options and control integers as in the preceding run. If at card 3 A1=-1, the input of the new run begins with card 1. If at card 1 IP1=-1 the calculation stops.

4. OUTPUT

In any case the following quantities are printed:

A1,A2,Z1,Z2

R1 projectile radius R_1 calculated according to
$R_1 = 1.128\ \mathrm{fm}\, A_1^{1/3}\ (1-0.786\ A_1^{-2/3}\ )$

R2 target radius R_2 calculated according to
$R_2 = 1.128\ \mathrm{fm}\ A_2^{1/3}\ (1-0.786\ A_2^{-2/3})$

R12 radius R_{12} according to $R_{12} = R_1 + R_2$

MUE reduced mass number μ /AMU

RO parameter r_0 in the proximity potential (r_0 = 1.17 fm)

SO parameter s_0 in the proximity potential

K	parameter k in the Coulomb potential V_c (k=0.15) *
N	parameter n in the Coulomb potential V_c (n=2.8)*
VB	Coulomb barrier V_B
RB	barrier radius R_B
DELTA	radial friction parameter a_R
DELTAT	tangential friction parameter a_θ
ALPHA	deformation parameter α.
RREAC	interaction radius R_{int}

If IP4=1 the proximity V_p and the Coulomb potential V_c are printed in the range of 0 to 20 fm.

The following quantities are the results of a classical trajectory calculation. They are printed in a table for each initial angular momentum ℓ_i only if IP2=1.

L	initial angular momentum ℓ_i
TAU	mean interaction time τ_{int}
SIGMA	deflection angle θ
RETURN	classical turning point R_{ret}
LFIN	final angular momentum ℓ_f
ELOST-R	radial energy loss ΔE_R
ELOST-T	tangential energy loss ΔE_t
ELOST-D	deformation energy loss ΔE_d
ELOST-SUM	sum of energy losses ΔE
EFIN	final kinetic energy E_f
RSCIS	scission radius R_{sc}
A1	mean mass number in the exit channel $\langle A_1 \rangle$
Z1	mean charge number in the exit channel $\langle Z_1 \rangle$
CHIZZQ	variance of the charge distribution σ^2_{ZZ}
LCR	critical angular momentum for fusion (LCR is printed in any case).

If IP3=1 the plot of the deflection function follows the preceding table.

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$$V_c(r) = \begin{cases} \frac{1}{4\pi\epsilon_0} \frac{Z_1 Z_2 e^2}{r}, & r > R_{12} \\ V_0 - k r^n, & r < R_{12} \end{cases}$$

with

$$V_0 = \frac{3\epsilon^2}{5r_0}\left(\frac{(Z_1+Z_2)^2}{(A_1+A_2)^{1/3}} - \frac{Z_1^2}{A_1^{1/3}} - \frac{Z_2^2}{A_2^{1/3}}\right)$$

and the parameters k and n.

After this plot the differential cross sections are plotted, starting with $d\sigma/d\Omega$ that is given separately for positive and negative deflection angles. Then differential cross sections are plotted with an angle step width of $\Delta\theta = 10°$ and cross sections of positive and negative angle scattering are summed. The step width $\Delta\theta$ for the calculation of the cross sections $d^2\sigma/dEd\theta$ and $d^3\sigma/dEd\theta dZ_1$ can be changed only within the program.

5. TWO EXAMPLES OF DATA SHEETS

1) Calculation of a classical trajectory (IS=0). The calculation should be performed for the $^{86}Kr + ^{166}Er$ reaction with bombarding energies $E_{lab} = 515$ MeV and 650 MeV. The standard model parameters are used. Mass transfer and deformation energy are included. The value of the grazing angular momentum should be calculated within the program. The output contains besides the standard quantities the interaction potential and the plot of the deflection function.

```
Card 1          FORMAT(4I5)
0  1  1  1
Card 2          FORMAT(10I5)
1  0  1  1  1  0  2  0  1  0
Card 3          FORMAT(4F10.2)
86.  166.  36.  68.
Card 5          FORMAT(F10.2)
515.
Card 6          FORMAT(I5)
-1
Card 5          FORMAT(F10.2)
650.
Card 6          FORMAT(I5)
-1
Card 5          FORMAT(F10.2)
-1.
Card 3          FORMAT(F10.2)
-1.
Card 1          FORMAT(I5)
-1
```

2) Calculation of cross sections (IS=1). The calculation should be performed for the reaction $^{86}Kr + ^{166}Er$ ($E_{lab} = 515$ MeV) with the standard model parameters including mass transfer and deformation energy. The grazing angular momentum is 213. The output does not contain the interaction potential

and the plot of the deflection function. Besides the results of the classical trajectory the cross sections $d\sigma/d\Omega$, $d\sigma/dZ$, $d^2\sigma/d\theta dE$, $d^2\sigma/dEdZ_1$ and $d^3\sigma/d\theta dEdZ_1$ are calculated.

```
Card 1        FORMAT(4I5)
0  1  0  0
Card 2        FORMAT(10I5)
1  0  1  1  1  1  2  2  1  1
Card 3        FORMAT(4F10.2)
86.  166.  36.  68.
Card 5        FORMAT(F10.2)
515.
Card 6        FORMAT(4I5)
213  200  340  20
Card 7        FORMAT(4I5)
213  30  48  2
Card 8        FORMAT(3I5)
0  120  20
Card 5        FORMAT(F10.2)
-1.
Card 3        FORMAT(F10.2)
-1.
Card 1        FORMAT(I5)
-1
```

REFERENCES

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