Role of multifragmentation in spallation reactions.

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Abstract
In nuclear reactions induced by hadrons and ions of high energies, nuclei can disintegrate into many fragments during a short time (∼100 fm/c). This phenomenon known as nuclear multifragmentation was under intensive investigation last 20 years. It was established that multifragmentation is an universal process taking place in all reactions when the excitation energy transferred to nuclei is high enough, more than 3 MeV per nucleon, independently on the initial dynamical stage of the reactions. Very known compound nucleus decay processes (sequential evaporation and fission), which are usual for low energies, disappear and multifragmentation dominates at high excitation energy. For this reason, calculation of multifragmentation must be carried on in all cases when production of highly excited nuclei is expected, including spallation reactions. From the other hand, one can consider multifragmentation as manifestation of the liquid-gas phase transition in finite nuclei. This gives way for studying nuclear matter at subnuclear densities and for applications of properties of nuclear matter extracted from multifragmentation reactions in astrophysics. In this contribution, the Statistical Multifragmentation Model (SMM), which combines the compound nucleus processes at low energies and multifragmentation at high energies, is described. The most important ingredients of the model are discussed.

1 Introduction
Statistical approaches have proved to be very successful for description of nuclear reactions. According to the statistical hypothesis, initial dynamical interactions between nucleons lead to re-distribution of the available energy among many degrees of freedom, and the nuclear system evolves towards equilibrium. The most famous example of such an equilibrated nuclear source is the 'compound nucleus' introduced by Niels Bohr in 1936 [1]. It was clearly seen in low-energy nuclear reactions leading to excitation energies of a few tens of MeV. It is remarkable that the statistical concept works also for nuclear reactions induced by particles and ions of intermediate and high energies, when nuclei break-up into many fragments (multifragmentation) [2]. In the most general consideration the process may be subdivided into several stages: (1) a dynamical stage leading to formation of equilibrated nuclear system, (2) disassembly of the system into individual primary fragments, (3) de-excitation of hot primary fragments.
2 Formation of thermalized nuclear system

At present, a number of dynamical models is used for description of nuclear reactions at intermediate energies. The Intranuclear Cascade Model was the first one used for realistic calculations of ensembles of highly excited residual nuclei which undergo multifragmentation, see e.g. [3, 4, 5]. Other more sophisticated models were also used for dynamical simulations of heavy-ion reactions, such as quantum molecular dynamics (QMD), Boltzmann (Vlasov)-Uehling-Uhlenbeck (BUU, VUU) and other similar models (see e.g. refs. [6]). All dynamical models agree that the character of the dynamical evolution changes after a few rescatterings of incident nucleons, when high energy particles (‘participants’) leave the system. This can be seen from distributions of nucleon velocities and density profiles in remaining spectators [7, 8, 9]. However, the time needed for equilibration and transition to the statistical description is still under debate. This time is estimated around or less than 100 fm/c for spectator matter, however, it slightly varies in different models. Parameters of the predicted equilibrated sources, i.e. their excitation energies, mass numbers and charges vary significantly with this time. In this case a reasonable strategy is to use results of the dynamical simulations as a qualitative guideline, but extract parameters of thermalized sources from the analysis of experimental data. In this case, one can avoid uncertainties of dynamical models in description of the thermalization process.

3 Break-up of nuclear system into hot primary fragments

3.1 Evolution from sequential decay to simultaneous break-up

After dynamical formation of a thermalized source, its further evolution depends crucially on the excitation energy and mass number. The standard compound nucleus picture is valid only at low excitation energies when sequential evaporation of light particles and fission are the dominant decay channels [2]. Some modifications of the evaporation/fission approach were proposed in order to include emission of fragments heavier than $\alpha$-particles, see e.g. [10, 11, 12]. However, the concept of the compound nucleus cannot be applied at high excitation energies, $E^* > 3$ MeV/nucleon. The reason is that the time intervals between subsequent fragment emissions, estimated both within the evaporation models [13] and from experimental data [14], become very short, of order of a few tens of fm/c. In this case there will be not enough time for the residual nucleus to reach equilibrium between subsequent emissions. Moreover, the produced fragments will be in the vicinity of each other and, therefore, should interact strongly. The rates of the particle emission calculated as for an isolated compound nucleus will not be reliable in this situation. There are many other theoretical arguments in favour of a simultaneous break-up at high excitation energy. For example, the Hartree-Fock and Thomas-Fermi calculations predict that the compound nucleus will be unstable at high temperatures [15]. Sophisticated
dynamical calculations have also shown that a nearly simultaneous break-up into many
fragments is the only possible way for the evolution of highly-excited systems [16].

On the other hand, the picture of a nearly simultaneous break-up in some freeze-out
volume is more justified in this case. Indeed, the time scales of less than 100 fm/c are
extracted for multifragmentation reactions from experimental data [17, 18]. There exist
several analyses of experimental data, which also reject the binary decay mechanism of
fragment production via sequential evaporation from a compound nucleus at high excita-
tion energy. For example, this follows from the fact that a popular sequential GEMINI
code cannot describe the multifragmentation data [19, 20, 21]. We believe that a formal
reason of this failure is that the evaporation approaches always predict larger probabil-
ities for emission of light particles (in particular, neutrons) than for intermediate mass
fragments (IMFs). The GEMINI model, which assumes independent evaporation of frag-
ments, fails also to describe angular correlations of the produced IMFs [22]. The reason
is that at multifragmentation these correlations reflect Coulomb interaction of many frag-
ments, but not a two-body kinematic.

3.2 Statistical multifragmentation model

Several versions of the statistical approach have been proposed for the description of
multifragmentation reactions (see e.g. [2, 23, 24]). As the main de-excitation code we
take the Statistical Multifragmentation Model (SMM), fully described in a review [2].
The reason is that this model was primary constructed for using after initial dynamical
stage, and adjusted for this kind of hybrid calculations.

The model assumes statistical equilibrium of excited nuclear system with mass number
$A_0$, charge $Z_0$, and excitation energy (above the ground state) $E_0$ at a low-density freeze-
out volume. This volume can be parameterized as $V = V_0 + V_f$, so the baryon density is
$\rho = A_0/V$. $V_0$ is the volume of the system at the normal nuclear density $\rho_0 \approx 0.15$ fm$^{-3}$. $V_f$ is the so-called free volume available for translational motion of fragments. In the
excluded volume approximation $V_f$ may be taken as a constant for all break-up channels,
however, under more realistic assumption, it depends on fragment multiplicity $M$ in the
channels [2].

The model considers all break-up channels (ensemble of partitions $\{p\}$) composed of
nucleons and excited fragments taking into account the conservation of baryon number,
electric charge and energy. An important advantage of the SMM is that besides these
break-up channels it includes also the compound nucleus channel, and takes into account
competition between all channels. In this way the SMM includes the conventional evapo-
ration and fission processes at low excitation energy, and provides natural generalization
of the de-excitation process for high excitation energy.

In the model light nuclei with mass number $A \leq 4$ and charge $Z \leq 2$ are treated as
elementary stable particles with masses and spins taken from the nuclear tables (“nuclear
gas”). Only translational degrees of freedom of these particles contribute to the entropy
of the system. Fragments with $A > 4$ are treated as heated nuclear liquid drops. In this
way one may study the nuclear liquid-gas coexistence in the freeze-out volume. Their
individual free energies $F_{AZ}$ are parameterized as a sum of the bulk, surface, Coulomb and symmetry energy contributions

$$F_{AZ} = F_{AZ}^B + F_{AZ}^S + E_{AZ}^C + E_{AZ}^{sym}. \quad (1)$$

The standard expressions for these terms are:

- $F_{AZ}^B = (-W_0 - T^2/\epsilon_0)A$, where $T$ is the temperature, the parameter $\epsilon_0$ is related to the level density, and $W_0 = 16 \text{ MeV}$ is the binding energy of infinite nuclear matter;
- $F_{AZ}^S = B_0 A^{2/3}/(T_c^2 - T^2)^{5/4}$, where $B_0 = 18 \text{ MeV}$ is the surface coefficient, and $T_c = 18 \text{ MeV}$ is the critical temperature of infinite nuclear matter;
- $E_{AZ}^C = cZ^2/A^{1/3}$, where $c = (3/5)(e^2/r_0)(1 - (\rho/\rho_0)^{1/3})$ is the Coulomb parameter (obtained in the Wigner-Seitz approximation), with the charge unit $e$ and $r_0 = 1.17 \text{ fm};$
- $E_{AZ}^{sym} = \gamma (A - 2Z)^2/A$, where $\gamma = 25 \text{ MeV}$ is the symmetry energy parameter. These parameters are those of the Bethe-Weizsäcker formula and correspond to the assumption of isolated fragments with normal density in the freeze-out configuration, an assumption found to be quite successful in many applications. It is to be expected, however, that in a more realistic treatment primary fragments will have to be considered not only excited but also expanded and still subject to a residual nuclear interaction between them. These effects can be accounted for in the fragment free energies by changing the corresponding liquid-drop parameters. The Coulomb interaction of fragments in the freeze-out volume is described within the Wigner-Seitz approximation (see ref. [2] for details).

As is well known, the number of partitions of medium and heavy systems ($A_0 \sim 100$) is enormous (see e.g. [25]). In order to take them into account the model uses few prescriptions. At small excitation energies the standard SMM code [2] uses a microcanonical treatment, however, taking into account a limited number of disintegration channels: as a rule, only partitions with total fragment multiplicity $M \leq 3$ are considered. This is a very reasonable approximation at low temperature, when the compound nucleus and low-multiplicity channels dominate. Recently, a full microcanonical version of the SMM using the Markov Chain method was introduced [25, 26]. It can be used for exploring all partitions without limitation. However, it is a more time consuming approach, and it is used in special cases only [26].

Within the microcanonical ensemble the statistical weight of a partition $p$ is calculated as

$$W_p \propto \exp S_p, \quad (2)$$

where $S_p$ is the corresponding entropy, which depends on fragments in this partition, as well as on the excitation energy $E_0$, mass number $A_0$, charge $Z_0$, volume $V$ of the system. In the standard treatment we follow a description which corresponds to approximate microcanonical ensemble. Namely, we introduce a temperature $T_p$ characterising all final states in each partition $p$. It is determined from the energy balance equation taking into account the total excitation energy $E_0$ [2]. In the following we determine $S_p$ for the found $T_p$ by using conventional thermodynamical relations. In the standard case, it can be written as

$$S_p = \ln\left(\prod_{A,Z} g_{A,Z}\right) + \ln\left(\prod_{A,Z} A^{3/2}\right) - \ln(A_0^{3/2}) - \ln(\prod_{A,Z} n_{A,Z}!) + \ldots$$
\[(M - 1) \ln \left( \frac{V_f}{\lambda_{T_p}^3} \right) + 1.5(M - 1) + \sum_{A,Z} \left( \frac{2T_p A}{\epsilon_0} - \frac{\partial F_{A,Z}^S(T_p)}{\partial T_p} \right),\]

where \( n_{A,Z} \) is the number of fragments with mass \( A \) and charge \( Z \) in the partition, \( g_{A,Z} = (2s_{A,Z} + 1) \) is the spin degeneracy factor, \( \lambda_{T_p} = (2\pi\hbar^2/m_N T_p)^{1/2} \) is the nucleon thermal wavelength (\( m_N \approx 939 \text{ MeV} \) is the average nucleon mass), and the summation is performed over all fragments of the partition \( p \). We enumerate all considered partitions and select one of them according to its statistical weight by the Monte-Carlo method.

At high excitation energy the standard SMM code makes a transition to the grand-canonical ensemble [2], since the number of partitions with high probability becomes too large. In the grand canonical formulation, after integrating out translational degrees of freedom, one can write the mean multiplicity of nuclear fragments with \( A \) and \( Z \) as

\[
\langle n_{A,Z} \rangle = g_{A,Z} \frac{V_f}{\lambda_T^3} \exp \left[ -\frac{1}{T} \left( F_{A,Z}(T,V) - \mu A - \nu Z \right) \right].
\]

(3)

Here the temperature \( T \) can be found from the total energy balance of the system by taking into account all possible fragments with \( A \) from 1 to \( A_0 \) and with \( Z \) from 0 to \( Z_0 \) [2]. The chemical potentials \( \mu \) and \( \nu \) are found from the mass and charge constraints:

\[
\sum_{A,Z} \langle n_{A,Z} \rangle A = A_0, \quad \sum_{A,Z} \langle n_{A,Z} \rangle Z = Z_0.
\]

(4)

In this case the grand canonical occupations \( \langle n_{A,Z} \rangle \) are used for Monte-Carlo sampling of the fragment partitions [2]. These two methods of partition generation are carefully adjusted to provide a smooth transition from the low energy to the high energy regimes.

4 Propagation and de-excitation of hot fragments

After the Monte-Carlo generation of a partition the temperature of the hot fragments, their excitation energy and momenta can be found from the energy balance. In this approach the temperature may slightly fluctuate from partition to partition, since the total energy of the system \( E_0 \) is always conserved. At the next stage Coulomb acceleration and propagation of fragments must be taken into account. For this purpose the fragments are placed randomly in the freeze-out volume \( V \) (without overlapping), and their positions are adjusted by taking into account that their Coulomb interaction energy must be equal to the value calculated in the Wigner-Seitz approximation. We note that in the case of the Markov Chain SMM version [26] this adjustment is not necessary, since positions of fragments are sampled directly. In the freeze-out volume a possible collective flow of fragments can be also taken into account [2]. Usually it is done by adding additional radial velocities to the fragments (proportional to their distances from the centre of mass) in the beginning of Coulomb acceleration. In the following we resolve the Hamilton equations for motion of fragment from these initial positions in their...
mutual Coulomb field. The energy and momentum balances are strictly respected during this dynamical propagation.

The secondary de-excitation of primary hot fragments includes several mechanisms. For light primary fragments (with \( A \leq 16 \)) produced in multifragmentation even a relatively small excitation energy may be comparable with their total binding energy. In this case we assume that the principal mechanism of de-excitation is the explosive decay of the excited nucleus into several smaller clusters (the Fermi break-up) \([11, 2]\). In this decay the statistical weight of the channel \( p \) containing \( n \) particles with masses \( m_i \) (\( i = 1, \cdots, n \)) in volume \( V_p \) can be calculated in microcanonical approximation:

\[
\Delta \Gamma_p \propto \frac{S}{G} \left( \frac{V_p}{(2\pi \hbar)^3} \right)^{n-1} \left( \frac{\prod_{i=1}^{n} m_i}{m_0} \right)^{3/2} \left( \frac{2\pi \hbar^2}{\Gamma(n)} \right)^{3(n-1)/2} \frac{(E_{\text{kin}} - U_p^C)^n}{G(n)},
\]

where \( m_0 = \sum_{i=1}^{n} m_i \) is the mass of the decaying nucleus, \( S = \prod_{i=1}^{n} (2s_i + 1) \) is the degeneracy factor (\( s_i \) is the \( i \)-th particle spin), \( G = \prod_{j=1}^{n} n_j! \) is the particle identity factor (\( n_j \) is the number of particles of kind \( j \)). \( E_{\text{kin}} \) is the total kinetic energy of particles at infinity which can be found through the energy balance by taking into account the fragment excitation energy, \( U_p^C \) is the Coulomb barrier for this decay. We have slightly modified this model \([11]\) by including fragment excited states stable with respect to the nucleon emission as well as some long-lived unstable nuclei.

The successive particle emission from hot primary fragments with \( A > 16 \) is assumed to be their basic de-excitation mechanism, as in the case of the compound nucleus decay. Due to the high excitation energy of these fragments, the standard Weisskopf evaporation scheme was modified to take into account the heavier ejectiles up to \(^{18}\text{O}\), besides light particles (nucleons, \( d, t, \alpha \)), in ground and particle-stable excited states \([11]\). The width for the emission of a particle \( j \) from the compound nucleus \((A, Z)\) is given by:

\[
\Gamma_j = \sum_{i=1}^{n} \int_{B_j - E_{s_j}^{(i)}}^{E_{s_j}^{(i)} + B_j} \frac{\mu_j g_j^{(i)}}{\pi^2 \hbar^3} \sigma_j(E) \frac{\rho_{A'Z'}(E_{AZ}^* - B_j - E)}{\rho_{AZ}(E_{AZ}^*)} E dE.
\]

Here the sum is taken over the ground and all particle-stable excited states \( s_j^{(i)} \) (\( i = 0, 1, \cdots, n \)) of the fragment \( j \), \( g_j^{(i)} = (2s_j^{(i)} + 1) \) is the spin degeneracy factor of the \( i \)-th excited state, \( \mu_j \) and \( B_j \) are corresponding reduced mass and separation energy, \( E_{AZ}^* \) is the excitation energy of the initial nucleus, \( E \) is the kinetic energy of an emitted particle in the centre-of-mass frame. In eq. \((6)\) \( \rho_{AZ} \) and \( \rho_{A'Z'} \) are the level densities of the initial \((A, Z)\) and final \((A', Z')\) compound nuclei. The cross section \( \sigma_j(E) \) of the inverse reaction \((A', Z') + j = (A, Z)\) was calculated using the optical model with nucleus-nucleus potential \([11]\). The evaporation process was simulated by the Monte Carlo method and the conservation of energy and momentum was strictly controlled in each emission step.

An important channel of de-excitation of heavy nuclei \((A > 100)\) is fission. This process competes with particle emission, and it is also simulated with the Monte-Carlo method. Following the Bohr-Wheeler statistical approach we assume that the partial
width for the compound nucleus fission is proportional to the level density at the saddle point $\rho_{sp}(E)$ [2]:

$$\Gamma_f = \frac{1}{2\pi \rho_{AZ}(E_{AZ})^2} \int_0^{E_{AZ}-B_f} \rho_{sp}(E_{AZ} - B_f - E) dE,$$

(7)

where $B_f$ is the height of the fission barrier which is determined by the Myers-Swiatecki prescription. For approximation of $\rho_{sp}$ we used the results of the extensive analysis of nuclear fissility and $\Gamma_n/\Gamma_f$ branching ratios, see ref. [2] for details.

All these models for secondary de-excitation were tested by numerical comparisons with experimental data on decay of compound nuclei with excitation energies less than 2–3 MeV per nucleons. It is important that after all stages the SMM provides event by event simulation of the whole break-up process and allows for direct comparison with experimental events.

5 Verification and applications of the SMM

As was shown already in first publications [2, 4] the SMM gives very good description of experimental data in the case when fragments are emitted from equilibrated sources. Later on, many experimental groups have successfully applied SMM for interpretation of their data: ALADIN (GSI, Germany) [27], EOS (Purdue University, USA) [28], ISIS (Indiana University, USA) [22], Miniball-Multics (MSU, USA and INFN, Italy) [29], INDRA (GANIL, France) [30], FAZA (Dubna, Russia) [31], and others. In particular, the SMM describes charge (mass) distributions of produced fragments and their evolution with excitation energy, isotope distributions, multiplicities of produced particles and fragments, charge distributions of first, second, third fragments in the system, correlation functions (charge, angle, velocity ones) of the fragments, fragment kinetic energy distributions. Simultaneously, this model reproduces global characteristics of the systems, such as caloric curves, critical indexes for the phase transition, different moments of the fragment charge distribution. Otherwords, the model can describe nearly completely experimental events, and, in some cases, it can be used as event generator. Importance of multifragmentation channels for nuclear reactions is now widely recognized. The SMM is included in many complex codes designed to describe transport of particles and isotope production in matter, for example, in GEANT4 (CERN) [32].

From the other hand, systematic studies of multifragmentation have brought important information about the nuclear liquid-gas phase transition [33, 34]. Multifragmentation reaction opens the unique possibility for investigating the phase diagram of nuclear matter at temperatures $T \approx 3 – 8$ MeV and densities around $\rho \approx 0.1 – 0.3\rho_0$, which are expected in the freeze-out volume. Previously, only theoretical calculations without experimental verification were available for this phase diagram region. This information is crucial, for example, for construction of a reliable equation of state of stellar matter and modelling nuclear composition in supernovae explosions, where the same thermodynamical conditions of nuclear matter exist [35].
One of the promising application of multifragmentation reactions is investigation of properties of excited nuclei embedded in surrounding of other nuclear species. They can be modified in comparison with the properties of isolated nuclei, since in the freeze-out volume fragments can interact with each other with Coulomb and residual nuclear forces. This study can not be performed in conventional nuclear reactions involving only a compound nucleus channel. However, the new properties of fragments can be extracted from analysis of experimental multifragmentation data. As was found there are essential modifications of symmetry and surface energies of hot fragments \[36, 37, 38, 39\]. These modified properties of fragments should be also taken into account during their secondary de-excitation \[40\].

6 Conclusion

Nearly 60 years ago nuclear physicists started to investigate the spallation reaction. Primary it was considered as emission of few nucleons and light charged particles (and, eventually, fission) from a heavy nucleus. Only these processes were clearly observed that time, since the accelerators could provide projectile beams with relatively low energy (few hundred MeV). During last 15 years we have obtained solid evidences that at high projectile energies, and in heavy-ion collisions, a heavy nucleus can be completely disintegrated into light and intermediate mass fragments. This multifragmentation reaction is universal, and it is a natural fast decay taking place at high energies. The multifragmentation channels take as much as 10–15% of the total cross section in high-energy hadron-nucleus reactions, and about twice more in high-energy nucleus-nucleus collisions. Moreover, multifragmentation reactions are responsible for production of most intermediate mass fragments and some specific isotopes.

The traditional evaporation and fission models can not describe correctly this fast multifragmentation, since they are based on the hypothesis of a long-lived compound nucleus. There is a statistical approach, realized in the Statistical Multifragmentation Model (SMM), which allows for natural extension of conventional cascade-evaporation calculations for the multifragmentation reaction. At low excitation energy it includes compound nucleus processes, however, at high excitations it describes the simultaneous break-up. Already at present the SMM demonstrates very good description of experimental data, especially at high excitation energy of nuclear systems (more than 3 MeV/nucleon). The problems, which are necessary to resolve within this approach, concern mainly a better description of transition from the compound nucleus to the multifragmentation decay. This is important for calculation of reactions initiated by low energy projectiles (up to 1 GeV), when very few equilibrated nuclei have a high excitation energy sufficient for multifragmentation.

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