Study of fragmentation using clusterization algorithm with realistic binding energies

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Abstract

We here study fragmentation using simulated annealing clusterization algorithm (SACA) with binding energy at a microscopic level. In an earlier version, a constant binding energy (4 MeV/nucleon) was used. We improve this binding energy criterion by calculating the binding energy of different clusters using modified Bethe-Weizsäcker mass (BWM) formula. We also compare our calculations with experimental data of ALADiN group. Nearly no effect is visible of this modification.

1 Introduction

In the recent years, several theoretical attempts [1, 2, 3, 4, 5] have been reported on spectator matter fragmentation observed in relativistic heavy-ion (HI) reactions using ALADiN set up [6, 7, 8, 9]. The multifragmentation has been thought to be one of the important phenomena for the understanding of phase transition in nuclei and nuclear equation of state. The multiplicity of intermediate mass fragments (IMFs) in central collisions is reported to first increase

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with the beam energy with a peak at $E \approx 100 \text{ MeV/nucleon} [7, 10]$ and then decline afterwards indicating a complete disassembly of nuclear matter. At relativistic energies, IMF emission becomes preferential only at peripheral collisions [6, 7, 8, 9, 11] where system has relatively low excitation energy. The low energy heavy-ion collisions are dominated by the phenomena such as the deep-inelastic scattering and fusion-fission. The fireball-spectator picture, however, emerges and dominates the physics at relativistic energies where the formation of heavier clusters is a rather unusual phenomenon. The most complete experiments of ALADIN collaboration have shown that fragment emission pattern remains almost unchanged above the incident energy of 400 MeV/nucleon for a given projectile-target combination [9]. This observation is also very often termed as universality of the fragmentation emission and has been discussed in the literature extensively [6, 8, 9, 12]. In these experiments, the correlation between IMF multiplicity and impact parameter 'b' suggests a picture of transition from evaporation to complete disassembly with increasing violence of the collision [6, 8, 11, 13]. At higher incident energies, one also expects complete disassembly or vaporization of the colliding matter [7, 10, 14].

It has been reported earlier that fragment multiplicities predicted by quantum molecular dynamics (QMD) model [15, 16, 17] coupled with conventional clustering technique such as *minimum spanning tree* (MST) algorithm are significantly underestimated for larger values of impact parameters [3, 8, 7]. The choice of different nuclear incompressibilities (*i.e.* equations of state) was found to have only marginal influence on the predicted IMF multiplicities and light charged particles yield [8]. About decade ago, Dorso et al. [18] advanced a new algorithm in which fragments if already formed can be identified earlier. The scope of this approach was limited to light systems like Ca+Ca where only a few fragments are produced. The results indicated a quite early formation. However, for the understanding of multifragmentation, the multifragment events observed in the collision of heavy systems have to be analyzed. Unfortunately, the computing time for the algorithm employed [18] increase by roughly N!, where N is the number of nucleons in the system. Hence a completely new numerical procedure was invented to extend the approach to larger and more relevant systems [19]. Due to small surface, heavier nuclei are close to nuclear matter and hence are ideal to study the physics.

The basic principle behind this algorithm [19] is that fragment structure was

achieved via energy minimization using simulated annealing technique which yields maximum binding energy of the system consisting of fragments of all sizes produced in a reaction. In this algorithm, each cluster is subjected to a binding energy check. As a first attempt, a constant average binding energy check of -4 MeV/nucleon was employed for the all clusters. This algorithm (labeled as simulated annealing clusterization algorithm i.e. SACA) yielded quite encouraging results. For instance, one could explain the fragment distribution for the reactions of O+ Ag/Br at incident energies 25-200 AMeV [20, 21]. For the first time, this microscopic approach [3] could also reproduce the fragment multiplicities in ¹⁹⁷Au +¹⁹⁷Au reaction at E=600 AMeV measured by ALADiN collaboration. It is worth mentioning that the MST approach failed badly to reproduce this experimental trend [3, 8, 7]. A comparison of SACA (without binding energy cut of -4 MeV/nucleon) and one developed by Dorso *et al.* [18] yielded the same results for lighter colliding nuclei.

As discussed above, each fragment in SACA method was subjected to a constant binding energy of -4 MeV/nucleon. We know that the binding energy depends on the mass of the fragment/nucleus. One is always wondering whether this criterion of average binding energy is justified or not. In this paper, we wish to address the above question by subjecting each fragment to its true binding energy that has now been measured to a very precise level with reference to unstable and stable isobars, proton-rich and neutron-rich nuclei. We shall show that this improvement does not yield different results justifying the validity of the algorithm.

We employ quantum molecular dynamics (QMD) model as primary model to follow the time evolution of nucleons. Section 2 describes the primary QMD model along with details of *simulated annealing clusterization algorithm* (SACA) and its extension. Section 3 deals with the calculations and illustrative results, which are summarized in section 4.

2 The Model

2.1 Quantum Molecular Dynamics (QMD) model

The quantum molecular dynamics is an n-body theory that simulates the heavyion reactions between 30 AMeV and 1AGeV on event by event basis. This is based on a molecular dynamics picture where nucleons interact via two and three-body interactions. The explicit two and three-body interactions preserve the fluctuations and correlations which are important for n-body phenomenon such as multifragmentation [15, 16, 17]. Nucleons follow the classical trajectories obtained by Hamilton's equations of motion:

$$\dot{\mathbf{r}}_{\alpha} = \nabla_{\mathbf{p}_{\alpha}} \langle \mathcal{H} \rangle, \alpha = 1, ..., N;$$

$$\dot{\mathbf{p}}_{\alpha} = -\nabla_{\mathbf{r}_{\alpha}} \langle \mathcal{H} \rangle, \alpha = 1, ..., N.$$

$$(1)$$

Here, nucleons interact via n-n interactions and stochastic elastic and inelastic collisions. For further details of the model, the reader is referred to Ref. [15].

2.2 Extended SACA formalism

As discussed in the previous section, earlier versions of clustering algorithm such as minimum spanning tree (MST) rely on the spatial correlation principle to identify the fragment configuration [15]. In this algorithm, two nucleons are considered to be a part of the same fragment if their inter-nucleon distance is smaller than r_C (in fm). One generally takes $2 \leq r_C \leq 4$. Naturally, it cannot address the time scale of fragmentation. This failure led to the development of more sophisticated algorithm based on the simulated annealing technique. This approach, known as *simulated annealing clusterization algorithm* (SACA), is based on the principle of energy minimization which requires that a group of nucleons can form a bound fragment if their total fragment energy per nucleon ζ_i is below certain binding energy E_{bind} *i.e.*

$$\zeta_{i} = \frac{1}{N_{f}} \sum_{\alpha=1}^{N_{f}} \left[\sqrt{\left(\mathbf{p}_{\alpha} - \mathbf{P}_{N_{f}}\right)^{2} + m_{\alpha}^{2}} - m_{\alpha} + \frac{1}{2} \sum_{\beta \neq \alpha}^{N_{f}} V_{\alpha\beta}\left(\mathbf{r}_{\alpha}, \mathbf{r}_{\beta}\right) \right] < -E_{Bind}.$$
(2)

In the original SACA version [19], we take $E_{bind} = 4.0$ AMeV if $N_f \ge 3$ and $E_{bind} = 0$ otherwise. In this equation, N_f is the number of nucleons in a fragment, P_{N_f} is the average momentum of the nucleons bound in the fragment. To find the most bound configuration, we start with a random configuration and the energy of each cluster is calculated using Eq. (2). Let the total energy of a configuration k be E_k ($=\sum_i N_f \zeta_i$), with ζ_i is the energy per nucleon associated with that fragment.

Now to generate new configuration k', we assume that this can be achieved by (a) transferring a nucleon from some randomly chosen fragment to another fragment, by (b) setting a nucleon free or, by (c) absorbing a free nucleon into a fragment] has total energy E'_k . If the difference between energies of the old and the new configurations, $\Delta E(=E'_k-E_k)$ is negative, the new configuration is always accepted. If not, the new configuration $k^{'}$ may nevertheless be accepted with a probability of $exp(-\Delta E/c)$, where 'c' is called control parameter. This procedure is known as Metropolis algorithm. The control parameter is decreased in small steps. This algorithm will yield eventually the most bound configuration (MBC). Since this combination of Metropolis algorithm with decreasing control parameter is known as simulated annealing, this approach was dubbed as simulated annealing clusterization algorithm (SACA) [19]. The present algorithm with a constant average binding energy check is labeled as SACA (1.1). For further details, we refer the reader to Refs. [19, 20, 21, 22]. In Fig. 1, we show the calculated multiplicities of different fragments as well as the mean size of the largest fragment $\langle A^{max} \rangle$ as a function of different binding energy cuts using original SACA. The multiplicities of light charged particles LCPs $[2 \le A \le 4]$ and size of the largest fragment $\langle A^{max} \rangle$ remains almost unaffected by changing the binding energy cut. However, the multiplicities of medium mass fragments MMFs $[5 \le A \le 20]$ and intermediate mass fragments IMFs $[5 \le A \le 65]$ show strong sensitivity towards the imposed binding energy. From this analysis, it would be interesting to study the effect of binding energy on average fragment production. The choice of proper binding energy can be based on either experimental information or on theoretical information. Since experimental information is range bound, we shall use theoretical formulation.

One of the earlier attempts to reproduce the gross features of nuclear binding energies was made by Weizsäcker *et al.* [23]. The Bethe-Weizsäcker (BW) mass formula for the binding energy of a nucleus reads as [24]:

$$E_{bind} = a_v N_f - a_s N_f^{2/3} - a_c \frac{N_f^z (N_f^z - 1)}{N_f^{1/3}} - a_{sym} \frac{(N_f - 2N_f^z)^2}{N_f} + \delta.$$
(3)

Here, N_f^z stands for the proton number of a fragment. The various terms involved in this mass formula are the volume, surface, Coulomb, asymmetry and pairing terms. The strength of different parameters is: $a_v=15.777$ MeV, $a_s=18.34$ MeV, $a_c=0.71$ MeV and $a_{sym}=23.21$ MeV respectively [24]. The pairing term δ is given by:

$$\delta = +a_p N_f^{-1/2} \text{ for even } N_f^z \text{ and even } N_f^n, \tag{4}$$

$$\delta = -a_p N_f^{-1/2} \text{ for odd } N_f^z \text{ and odd } N_f^n, \tag{5}$$



Figure 1: The average mass of the heaviest fragment $\langle A^{max} \rangle$, mean multiplicities of light charged particles LCPs, medium mass fragments MMFs, and intermediate mass fragments IMFs as a function of binding energy check imposed for the reaction of $^{197}Au + ^{197}Au$ at 600 MeV/nucleon and at an impact parameter of 12 fm.

$$\delta = 0 \ for \ odd \ N_f \ nuclei, \tag{6}$$

with $a_p = 12$ MeV and N_f^n being the neutron number of a fragment. This formula reproduces the binding energy of stable nuclei but faces serious problem for light nuclei along the drip line and with nuclei having rich neutron or proton content. The inadequacy of BW mass formula for lighter nuclei was removed by Samanta *et al.* [24] by modifying its asymmetry and pairing terms. This modified formula was dubbed as modified Bethe-Weizsäcker mass (BWM) formula [24]. The beauty of BWM formula lies in its ability to reproduce the binding energies for light nuclei near the drip line [24]. For a large number of unstable isobars, isotones and halo nuclei, it was shown in Ref. [24] that this modified formula reproduces the experimental binding energies quite precisely. In the BWM formula, the binding energy of a fragment is defined as [24]:

$$E_{bind} = a_v N_f - a_s N_f^{2/3} - a_c \frac{N_f^z (N_f^z - 1)}{N_f^{1/3}} - a_{sym} \frac{(N_f - 2N_f^z)^2}{N_f (1 + e^{-N_f / 17})} + \delta_{new}.$$
 (7)

The strength of various parameters now reads: $a_v=15.777$ MeV, $a_s=18.34$ MeV, $a_c=0.71$ MeV and $a_{sym}=23.21$ MeV, respectively. The pairing term δ_{new} is given by:

$$\delta_{new} = +a_p N_f^{-1/2} \ (1 - e^{-N_f/30}) \ for \ even \ N_f^z \ and \ even \ N_f^n, \tag{8}$$

$$\delta_{new} = -a_p N_f^{-1/2} (1 - e^{-N_f/30}) \text{ for odd } N_f^z \text{ and odd } N_f^n, \tag{9}$$

$$\delta_{new} = 0 \ for \ odd \ N_f \ nuclei, \tag{10}$$

with $a_p = 12$ MeV.

We extend the SACA method by incorporating this binding energy formula during the formation of the clusters. Each fragment at the end of the procedure is subjected to this new binding energy (Eq.(7)) instead of a constant -4 MeV/nucleon binding energy. Any fragment that fails to fulfil the above binding energy criterion is treated as a group of free nucleons. At the end, all fragments are properly bound. This version is labeled as SACA (2.1). We have also tested the spectrum for actual experimental binding energies [25]. Only small difference is seen for lighter fragments only.

3 Results and Discussions

We simulated the collisions of ${}^{197}Au + {}^{197}Au$ at incident energy of 600 AMeV using a *soft* equation of state along with standard energy dependent *n*-*n* cross section. We display in Fig. 2, the average mass of the largest fragment $\langle A^{max} \rangle$, mean multiplicities of free nucleons, light charged particles LCPs $[2 \le A \le 4]$, medium mass fragments MMFs $[5 \le A \le 20]$, heavy mass fragments HMFs $[21 \le A \le 65]$ and intermediate mass fragments IMFs $[5 \le A \le 65]$ as a function of time for the reaction of ${}^{197}Au + {}^{197}Au$ at 600 AMeV and impact parameter 12 fm. As expected, $\langle A^{max} \rangle$ is nearly independent of the binding energy criterion, whereas insignificant influence can be seen on the multiplicities of free nucleons, LCPs, MMFs and IMFs. Similar trends were also observed for the central reaction of ¹⁹⁷Au +¹⁹⁷Au at 600 AMeV.

To further explore the characteristics of fragment structure obtained with modified SACA (2.1), we show in Fig. 3, the impact parameter dependence of mean multiplicities of various fragments. This will also help to understand the proper energy deposition in the spectator matter. The result obtained with SACA (1.1) and SACA (2.1) are displayed for the reaction of $^{197}Au + ^{197}Au$ at 600 AMeV as a function of impact parameter. The time for realization of different fragments was chosen to be 60 fm/c. This is the time when $\langle A^{max} \rangle$ has minimum size and configuration realized at this stage is most bound [19]. In central collisions, SACA (2.1) predicts smaller $\langle A^{max} \rangle$, whereas trend reverses in the peripheral collisions. As a result, free nucleons also behave accordingly. The yields of IMFs and MMFs do not reduce appreciably for central as well as peripheral geometries using extended version of SACA. This is due to the fact that fragments recognized by SACA method are properly bound, therefore, simple cut also yields same results.

We also attempted to confront our present calculations using extended clusterization approach SACA (2.1) (at t=60 fm/c) with experimental data of AL-ADiN group [9] for the reaction of Au (600 AMeV) + Au. In Fig. 4, we show the mean IMF multiplicity $\langle N_{IMF} \rangle$ (in upper panel) and average charge of the largest fragment $\langle Z^{max} \rangle$ (in lower panel) as a function of impact parameter at 600 AMeV. The calculations with the original SACA (1.1) version are also shown for comparison. All calculations were subjected to experimental cuts of forward hemisphere. The $\langle N_{IMF} \rangle$ and $\langle Z^{max} \rangle$ obtained with different versions of SACA are quite close to each other and to the experimental data. It justifies the use of average binding energy within above algorithm. We have also calculated the yields at incident energies of 400 and 1000 MeV/nucleon. Similar results are also obtained at these incident energies.

4 Summary

Summarizing the work, we have proposed an extension to SACA method by incorporating the binding energy of individual fragments calculated from the



Figure 2: The average mass of heaviest fragment $\langle A^{max} \rangle$ and the mean multiplicities of various kinds of fragments as a function of time for the reaction of $^{197}Au + ^{197}Au$ at 600 MeV/nucleon and at an impact parameter of 12 fm. The solid and dashed lines depict the results due to original SACA and its extension.



Figure 3: The impact parameter dependence of average size of the heaviest fragment $\langle A^{max} \rangle$ and mean multiplicities of various kinds of fragments for the reaction of ${}^{197}Au + {}^{197}Au$ at incident energy 600 MeV/nucelon. The solid and dashed curves depict results of SACA (1.1) and SACA (2.1), respectively.



Figure 4: The mean IMF multiplicity (top panel) and average charge of the heaviest fragment (bottom panel) as a function of impact parameter. Open circles depict the experimental data points [9].

modified Bethe-Weizsäcker mass (BWM) formula. Based on our calculations, we noticed that this extension has little effect on the fragment multiplicities and mean size of the largest fragment at 60 fm/c as well as at asymptotic times. In peripheral collisions, new extension reduces the IMF yield, thereby increasing the size of $\langle A^{max} \rangle$ marginally. Both versions of SACA are clearly close to each other and to ALADiN data.

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