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Ambiguities in statistical calculations of nuclear fragmentation

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In standard statistical approaches on nuclear disassembly, the fragmentation pattern is decided at the "freeze-out" volume, generally taken to be 3–8 times the normal nuclear volume. In this communication, we show that the dynamics of the initially produced fragments may allow pairs of fragments to come well within the nuclear force range resulting in possible recombination in the exit channel. The fused complex may undergo further fragmentation if sufficiently excited. This alters the fragmentation pattern and the associated physical observables considerably. The ambiguity so found calls for critical reanalysis of the different statistical approaches to nuclear multifragmentation.

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Multifragmentation of nuclear systems in energetic nuclear collisions serves a novel window for understanding the properties of hot nuclear matter. It has a sensitive bearing on the nuclear equation of state (EoS) [1,2], focuses our attention on the possibility of liquid-gas phase transition in finite and infinite nuclear systems [3,4] and from the production of rare isotopes holds a promise for a better understanding of the nucleosynthesis in astrophysical context [5]. Various statistical models have been suggested to explain the phenomenon of nuclear multifragmentation. Dynamical models [1,2,6] have also been proposed that are discussed no further because they are not relevant in the present context. Broadly the statistical approaches are classified in two groups, namely, sequential binary decay (SBD) [7,8] and one-step prompt multifragmentation (PM) [9–11]. It is generally believed that at low excitation energy, fragmentation proceeds through SBD, whereas at relatively higher energies, it is possibly a one-step breakup process. Different genres of statistical hierarchy have been employed in the PM picture to explain the nuclear disassembly process, from grandcanonical [11] and canonical [12] to microcanonical [9,13], which have been quite successful in explaining various aspects of experimental data. In all these statistical calculations, a freeze-out volume, around $3V_0$ to $8V_0$ (V_0 being the normal nuclear volume of the fragmenting system) is employed when the PM process takes place. The fragments so generated are the primary fragments which are in general in the excited states. Secondary decay from these hot fragments may occur and have been taken into account [14,15]. In the PM models the fragments are distributed in the freeze-out volume and Coulomb trajectories are calculated for an improved description of the momentum distribution of the charged fragments. At high excitation energies a collective motion further needs to be added to the fragments [1,2]. The assumption of *freeze-out* implies that the mass distribution of the primary fragments is decided at the freeze-out boundary; beyond it there is no further interaction among the fragments to alter the primary mass distribution. This is certainly true provided the motion of the fragments at freeze-out is predominantly flowlike. In the standard application of the statistical models, however, this is not assured. In the canonical or the grandcanonical formulation, the momentum distribution is Maxwellian at the relevant temperature and therefore some pairs of fragments leave chances to come close enough to be under the influence of nuclear force beyond the freeze-out volume and may recombine to form an excited heavier fragment that may or may not decay further. In the different variants of the microcanonical models [9,13,16], the momentum distribution, though non-Maxwellian, is not flowlike; chances of recombination then cannot be ruled out. In models like MMMC [9], the positions and momenta of the fragments are not decoupled; the probability of having, say, two heavy fragments nearby is strongly reduced by the Coulomb repulsion. The effects of recombination may then possibly be reduced, but only actual calculations involving large CPU time can substantiate it. Conversely, in grandcanonical or canonical approaches that are mostly used in the literature to compare with experimental data, positions and momenta of the fragments are uncoupled.

The conceptual contradictions so encountered call for an actual calculation on the evolution of the fragments under the combined action of the Coulomb and nuclear fields. This has not been considered so far except the one reported in Ref. [17] where the primary fragment yield was generated in the grandcanonical formulation. It was found that due to recombination, the yield of relatively heavier fragments was enhanced significantly, implying considerable change in the mass, charge, or isotopic yield and momentum distribution. These calculations have, however, been restricted to only a fixed freeze-out volume V_f and excitation energy E^*. Further nuances of the model may be better understood from variations of these parameters. We have addressed these in some detail here. Furthermore, isotopic yields from multifragmentation have been employed to infer about important physical observables such as the temperature of the fragmenting system [18] and the associated liquid-gas phase transition in finite nuclei. Recombination is expected to influence the isotopic yield. Extraction of temperature from the experimental isotopic double ratio then seems to be under a cloud. We have investigated this aspect also in the present communication.

The model employed in the present calculation is the same as that in Ref. [17]. For the sake of completeness, only the salient features of the methodology are discussed here. In the first step, the fragment multiplicities n_i for the various fragments are evaluated in the grandcanonical model (GCM). They are given by the following:

$$n_i = V_f \left(\frac{mA_i}{2\pi\hbar^2\beta}\right)^{3/2} \phi_i(\beta) \exp[-\beta(B - B_i + V_i - \mu_n N_i - \mu_p Z_i)], \quad (1)$$

where β is the inverse of the temperature T; m is the nucleon mass; A_i, N_i, and Z_i are the mass, neutron, and charge numbers of the fragment species i; Bs are the ground state binding energies of the fragmenting system and the generated species, μs are the nucleonic chemical potentials; and $\phi_i(\beta)$s are the internal partition function. The internal partition function is calculated with the assumption that the excitation of the fragment is below the particle emission threshold. The single-particle potential V_i is the sum of the Coulomb and nuclear interaction of the ith fragment with the rest of the fragments and is evaluated in the complementary fragment approximation [19,20]. Employing the GCM fragment formation probability $p_i = n_i / \sum n_i$, microcanonical events are generated following the method similar to that given by Fai and Randrup [21]. After generation of fragments in a microcanonical event, the fragments are placed in a nonoverlapping manner within the freeze-out volume with no correlation among the fragment positions. The true "microcanonical temperature" T_m can be evaluated from the derivative of entropy with respect to energy. However, this is quite difficult a task from the numerical point of view. For fairly large number of fragments, it is approximated from [22] as follows:

$$\frac{3}{2}(M-1)T_m = E_{\rm kin} \quad (2)$$

where M is the total fragment multiplicity in an event and $E_{\rm kin}$ is the kinetic energy of the fragments evaluated from energy conservation [17]. The applicability of Eq. (2) at low excitation energy is restricted because the multiplicity M may be small. The fragment velocities are generated from a Maxwell-Boltzmann distribution commensurate with the microcanonical temperature, which varies from event to event. At this stage the role of thermal statistics is over, the mass partition is supposedly frozen, but a further dynamical evolution with Coulomb force is generally considered for a better description of the momentum distribution. If the introduction of dynamics in the model is accepted, one should be consistent and include the nuclear forces as well because some of the nuclear fragments with imparted random velocities may come close to each other. Two fragments in the exit channel are assumed to coalesce when they touch each other. If the excitation energy of the coalesced fragment is above the particle emission threshold (taken as 8 MeV), the fragment is assumed to undergo binary decay; the decay probability is calculated in the transition state model of Swiatecki [23].

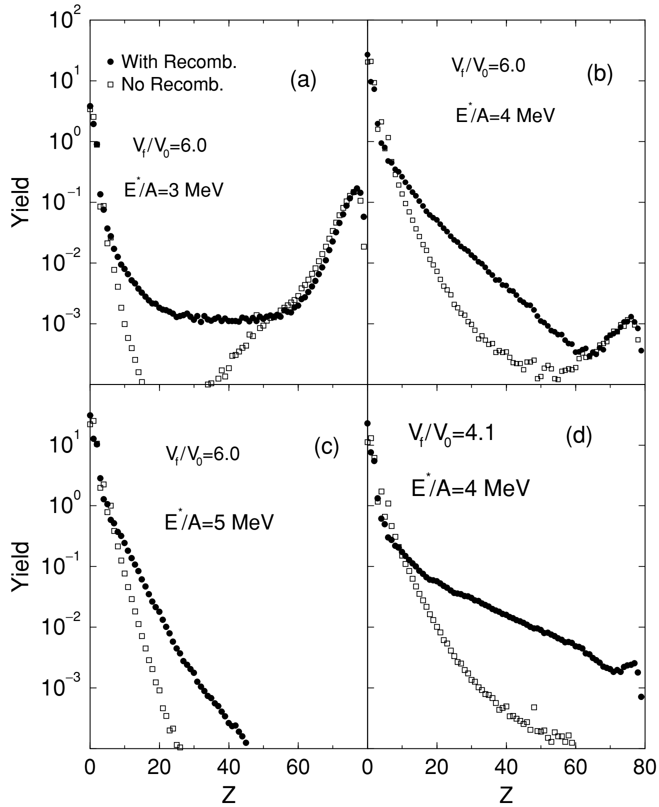

FIG. 1. Charge distributions from the fragmenting system ^{197}Au with and without recombination at different excitation energies and freeze-out volumes as indicated in the figure.

To study the effect of recombination in nuclear multifragmentation we have considered ^{197}Au as a representative system. To see the effect of recombination on excitation energy, the calculations have been performed at $E^*/A = 3$, 4, and 5 MeV with a fixed freeze-out volume $V_f = 6V_0$. Volume effects have also been considered with E^*/A fixed at 4 MeV. For generation of a microcanonical ensemble, typically 10^5 events have been used. Because we have assumed that the fragments are produced in the particle stable states, the charge or mass distribution is decided at the very onset of fragmentation if there is no recombination. The recombined complex may have excitation above the particle emission threshold and they may undergo sequential binary decay in flight till a particle-stable state is reached. In panels (a), (b), and (c) of Fig. 1, the charge distributions at different excitation energies at $V_f = 6V_0$ are displayed. Except for the very light charge particles, the fragment yield is substantially enhanced. At the lowest excitation energy considered (3 MeV/A), the yield of very heavy fragments is found to be somewhat reduced. The neutron yield is enhanced at all the excitation energies considered. Recombination enhances production of heavier fragments at the cost of lighter fragments, whereas sequential binary decay acts in the opposite direction. The relative importance of the two processes depends on the details of the mass distribution at freeze-out and the evaluated microcanonical temperature.

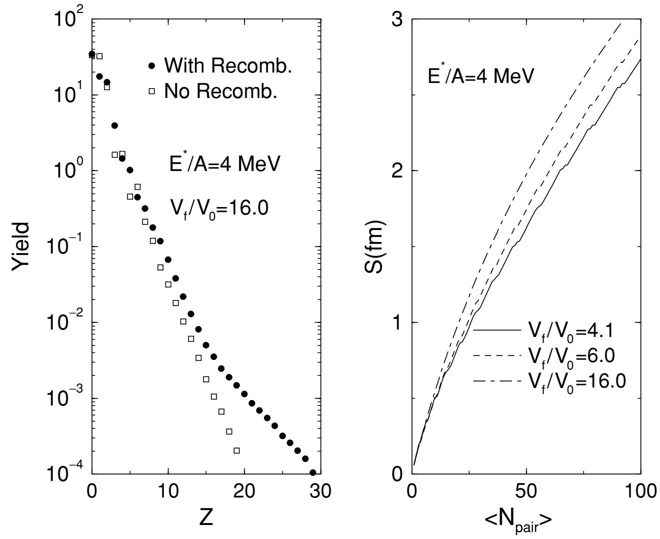

FIG. 2. In the left panel the charge distribution from ^{197}Au at an excitation energy of 4 MeV per nucleon and $V_f = 16V_0$ is displayed. The right panel shows the average number of fragment pairs within a separation distance S at different freeze-out volumes at the same excitation energy.

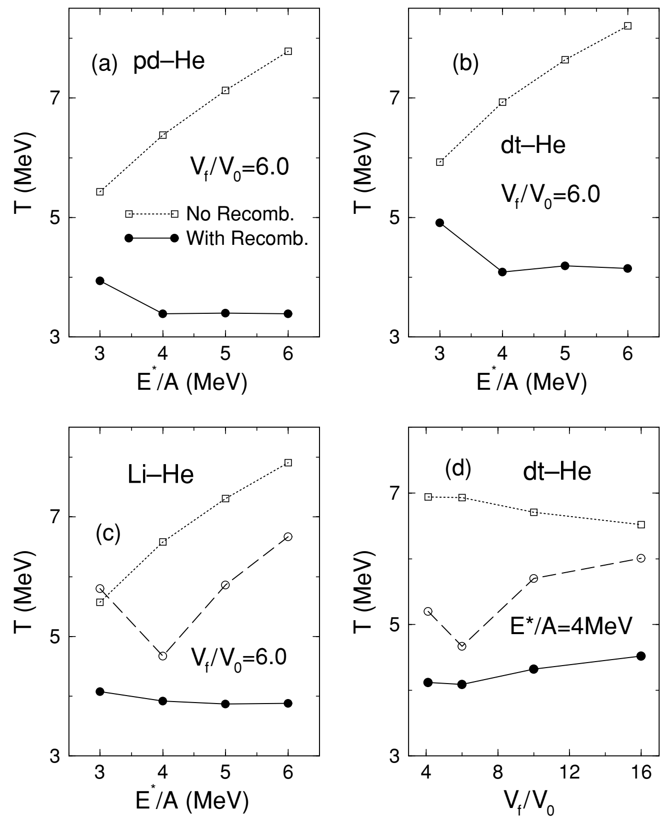

FIG. 3. In (a), (b), and (c), different isotopic double-ratio temperatures for the fragmenting system ^{197}Au are shown at various excitation energies at $V_f = 6V_0$ with and without recombination. In (d), the volume dependence of the double-ratio temperature $(d/t)/(^3\text{He}/^4\text{He})$ at $E^*/A = 4$ MeV is displayed. The ensemble averaged microcanonical temperature $\langle T_m \rangle$ at the relevant excitation energies and freeze-out volume are also displayed in (c) and (d) as open circles joined by dashed lines.

Thus the final fragment distributions result from a delicate interplay between fragment recombination and subsequent binary decay. It is expected that with reduction in freeze-out volume, the recombination effect would be more prominent. This is apparent from Fig. 1(b) and 1(d). This is further evident from the left panel of Fig. 2 where the charge distribution has been displayed for a very large freeze-out volume ($16V_0$) at the same excitation energy of 4 MeV per particle. One would expect the recombination effect to be minimal at this large freeze-out volume; however, we find that though it is significantly reduced, it is not negligible, particularly for fragments with $Z > 10$. To understand the persistence of the recombination effect at this large freeze-out volume, we have calculated the surface to surface separation (S) of the different fragment pairs (N_{pair}) produced in a disassembly event at freeze-out. In the right panel of Fig. 2, the ensemble-averaged number of fragment pairs ($\langle N_{\text{pair}} \rangle$) present within the separation distance S is displayed for different freeze-out volumes at $E^*/A = 4$ MeV. The number of fragment pairs within the nuclear force range are the potential candidates to undergo recombination; however, actual recombination would depend on further dynamical evolution. The interfragment nuclear interaction has been broadly classified in three groups depending on the masses of the fragments [17]. The typical range of these interactions is ∼1 fm. It is seen that even at $V_f = 16V_0$, there are significant number of fragment pairs within this distance and that they are not too different from those calculated at the smaller freeze-out volumes.

The knowledge of the temperature of the disassembling system is crucial in drawing many important physical inferences such as liquid-gas phase transition. There is no direct way to measure the temperature in such processes; a number of thermometers have been proposed to that end. Experimentally, it has been the usual practice to resort to the isotopic double ratio [18] to extract the temperature that is based on the statistical multifragmentation model with certain approximations. If the isotopic yield changes due to recombination, the extracted temperature based on this model is questionable. To investigate this aspect, we have calculated temperatures from different isotopic double ratios at a number of excitation energies with and without the effects of recombination. This is displayed in panels (a), (b), and (c) of Fig. 3. It is found that the temperatures extracted without recombination increase with the excitation energies as in the Fermi gas model; however, with inclusion of recombination effects, the extracted temperatures from the isotopic double ratios are reduced dramatically. Recombination introduces a multitude of low-temperature sources in the system that may be responsible for the reduction in the temperature observed. An anomalous fall in temperature at $E^*/A = 4$ MeV is also seen for all the double-ratio thermometers. The temperature extracted after recombination are, however, found to be not too sensitive to the excitation energy (3–6 MeV per nucleon) that we have considered. The dependence of the double-ratio temperature on the freeze-out volume is displayed in Fig. 3(d). We have chosen a representative thermometer $(d/t)/(^3\text{He}/^4\text{He})$ at an excitation energy $E^*/A = 4$ MeV. Even at the very large freeze-out volume of $16V_0$, the temperatures extracted without and with recombination effects are appreciably different, but a very slow approach to a common temperature with increasing V_f is apparent from the figure. For comparison, $\langle T_m \rangle$, the ensemble average of the microcanonical temperature T_m defined in Eq. (2) is displayed in panels (c) and (d). This temperature is independent of the double-isotope ratio and is found to be appreciably different from those calculated from double-isotope ratios with or without recombination. The anomalous rise in $\langle T_m \rangle$ at low excitation energy or at smaller freeze-out volume possibly shows the limitation of Eq. (2) for the evaluation of T_m because of the low multiplicity M.

The concept of freeze-out brings home a close analogy to fission; there one utilizes statistical models to determine the mass distribution frozen out at the saddle point of the potential energy surface. The frozen system then evolves under the combined action of Coulomb, nuclear, and even friction forces without changing the mass distribution. Freeze-out in the fragmentation process, intuitively, refers to such a mass partition on a multidimensional potential energy surface where further dynamical evolution plays no role in mass distribution. In this communication, although discussing the role of nuclear forces in the PM model beyond the chosen freeze-out volume at different excitation energies, we have shown that such an intuitive picture (assumed inherent in the PM model) loses ground. One then has to concur that the description of fragmentation at the freeze-out in the statistical model is either incomplete or, if complete, the import of the parameters entering into the model need be reinterpreted. In a microcanonical statistical model like the MMMC [9] where the positions and momenta of the fragments are not decoupled, the effects of recombination may then possibly be reduced [24] compared to those in the grandcanonical or canonical formulation, but because actual calculations can only quantify it, the role of recombination in a fully microcanonical formulation is worth investigating.

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