PHYSICAL REVIEW C **93**, 041603(R) (2016)

Bimodality emerges from transport model calculations of heavy ion collisions at intermediate energy

S. Mallik,[1] S. Das Gupta,[2] and G. Chaudhuri[1]

[1]*Theoretical Nuclear Physics Group, Variable Energy Cyclotron Centre, 1/AF Bidhan Nagar, Kolkata 700064, India*

[2]*Physics Department, McGill University, Montréal, Canada H3A 2T8*

(Received 3 February 2016; published 14 April 2016)

This work is a continuation of our effort [S. Mallik, S. Das Gupta, and G. Chaudhuri, Phys. Rev. C **91**, 034616 (2015)] to examine if signatures of a phase transition can be extracted from transport model calculations of heavy ion collisions at intermediate energy. A signature of first-order phase transition is the appearance of a bimodal distribution in $P_m(k)$ in finite systems. Here $P_m(k)$ is the probability that the maximum of the multiplicity distribution occurs at mass number k. Using a well-known model for event generation [Botzmann-Uehling-Uhlenbeck (BUU) plus fluctuation], we study two cases of central collision: mass 40 on mass 40 and mass 120 on mass 120. Bimodality is seen in both the cases. The results are quite similar to those obtained in statistical model calculations. An intriguing feature is seen. We observe that at the energy where bimodality occurs, other phase-transition-like signatures appear. There are breaks in certain first-order derivatives. We then examine if such breaks appear in standard BUU calculations without fluctuations. They do. The implication is interesting. If first-order phase transition occurs, it may be possible to recognize that from ordinary BUU calculations. Probably the reason this has not been seen already is because this aspect was not investigated before.

DOI: 10.1103/PhysRevC.93.041603

Introduction. In a recent paper [1] we used a well-known model of fluctuations [2] in Botzmann-Uehling-Uhlenbeck (BUU) [3] to generate event-by-event simulation of collisions of fairly large (mass 120 on mass 120) ions as well as not so large (mass 40 on mass 40) ions. The multiplicity distribution of the final collision products showed a remarkable similarity with the results given by equilibrium statistical models where we used a canonical thermodynamic model (CTM) [4]. Both canonical [4,5] and grand canonical thermodynamic models [6] predict first-order phase transitions in hot nuclear systems. So the similarity suggested that probably transport model calculations also will give more direct evidence of first-order phase transition. This work is aimed at exploring this further. It is not so obvious how to go about doing this. In canonical and grand canonical models there are two parameters, temperature T (which is the basic parameter) and average energy E. The behavior of E against T can indicate the order of the phase transition. Usually two parameters are needed, but in the transport model calculations that we do here there is only one parameter, the beam energy E. Defining a temperature is quite difficult. Formulas like $\frac{E*}{A}=\frac{3T}{2}$ are obviously inappropriate. One might try $T=(\frac{\partial S}{\partial E})_V$ but that requires obtaining the entropy of an interacting system and an accurate evaluation would be very hard.

We recall that as early as 1998, in compiling existing knowledge from experimental data and comparing these with lattice gas model predictions, it was concluded that in intermediate-energy heavy ion collisions one passes through a first-order phase transition [7]. This was subsequently investigated by many authors with different approaches. One approach uses the idea of "bimodality." A very useful exposition of this can be found in [8] which also has a list of other references using the bimodality approach. The size of the largest cluster k is considered to be an order parameter. Phase transitions occur in very large systems but practical calculations (and experiments with heavy ions) need to be done with finite systems. Gulminelli and Chomaz pointed out that we should expect for $P_m(k)$ (probability that the biggest cluster has mass k) a double humped distribution (hence the name bimodality) if the phase transition is first order. The authors establish this with a lattice gas model. For a relevant study of this in the Ising model, see [9].

Bimodality also emerges in CTM [10] which has a first-order phase transition. The objective of this work is to investigate if bimodality emerges from a transport model calculation. Using what is labeled as QMD (quantum molecular dynamics), Lefevre and Aichelin used ideas from bimodality to show that in some noncentral collisions [11] there is evidence of first-order phase transition [12]. In the calculation the full distribution $P_m(k)$ was not displayed. The complete curves $P_m(k)$ as functions of beam energy are quite interesting and we present them here. In contrast with the QMD work we use central collisions. As we are interested in phase transition under the influence of nuclear force, Coulomb effects will be switched off. The use of central collisions to display bimodality has been questioned before. Also the transport model we use is quite different from QMD.

Model description. The calculations done here follow those of [1] except for small but important details which will be fully presented. For completeness we outline the model. More details are given in [1]. The original model was developed in [2] where the formal structure was discussed and an application was presented. Initially each nucleon in the target and the projectile is given a semiclassical phase-space density. For each nucleon this phase-space density is represented by $\tilde{N}$ test particles where each test particle is generated by Monte Carlo and has a position $\vec{r}$ and a momentum $\vec{p}$. Initially the two nuclei are apart with an impact parameter b (in this work we only consider the central collision i.e., $b=0$) and the projectile starts with a beam velocity toward the target. As they propagate in time, the test particles will move in a mean field and suffer hard scattering. As $\tilde{N}$ test particles will represent a nucleon,

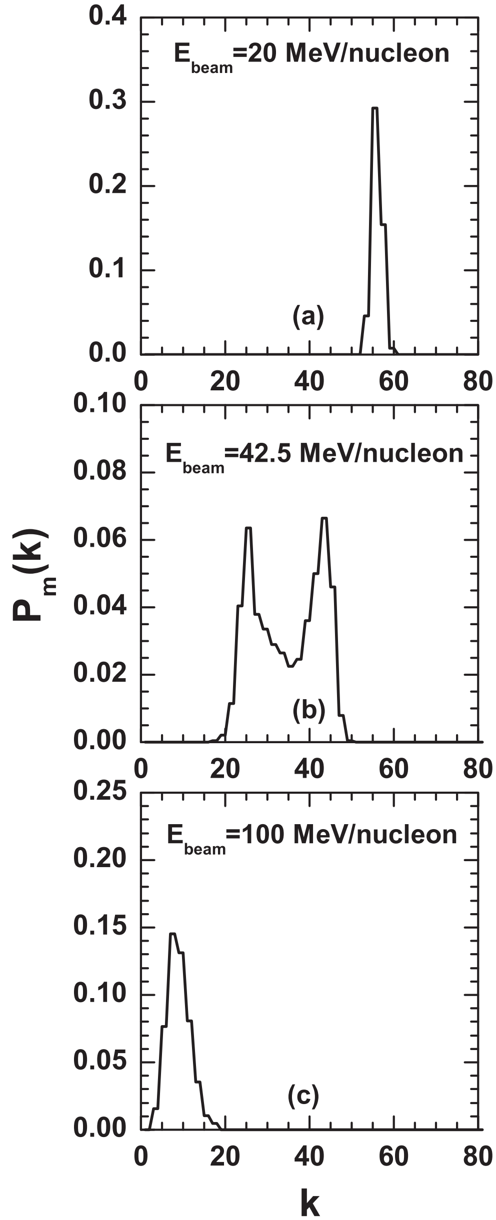

FIG. 1. Largest cluster probability distribution for $A_p = 40$ on $A_t = 40$ reaction at beam energies (a) 20, (b) 42.5, and (c) 100 MeV/nucleon. The average value of 2 mass units are shown. At each energy 1000 events are chosen. The results shown in this figure are calculated at $t = 300$ fm/c.

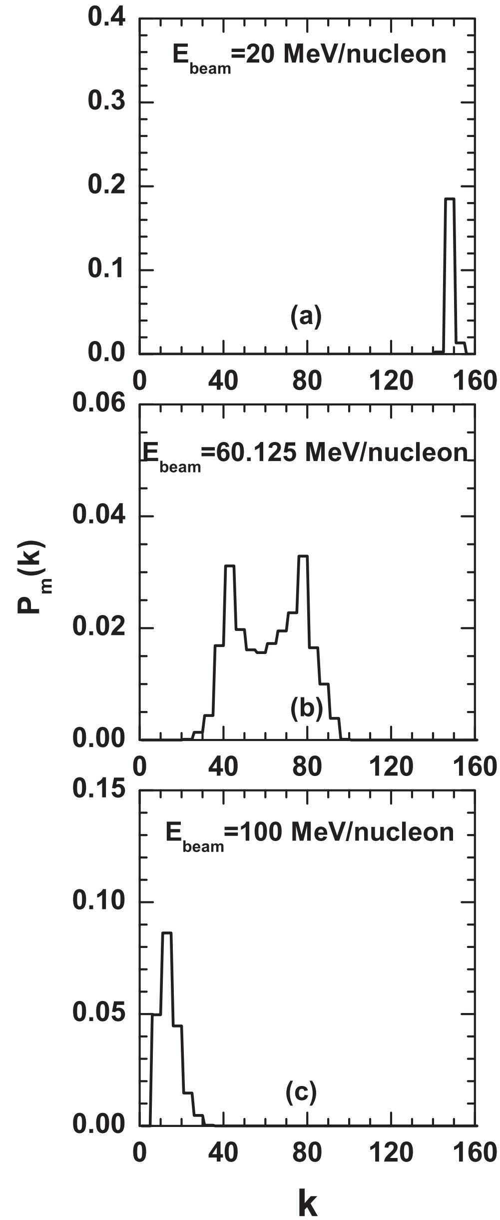

FIG. 2. Largest cluster probability distribution for $A_p = 120$ on $A_t = 120$ reaction at beam energies (a) 20, (b) 60.125, and (c) 100 MeV/nucleon. The average value of 5 mass units are shown. At each energy 1000 events are chosen. The results shown here are calculated at $t = 600$ fm/c.

the collision cross section between test particles is reduced to $\sigma_{nn}/\tilde{N}$ where σ_{nn} is the nucleon-nucleon cross section. In [2], to simulate an event, the cross section is further reduced by a factor $\tilde{N}$ but if a collision happens not only the the two test particles go from $\vec{p}_1$ to $\vec{p}_1 + \Delta\vec{p}$ and from $\vec{p}_2$ to $\vec{p}_2 - \Delta\vec{p}$, but also $\tilde{N} - 1$ test particles contiguous to test particle 1 undergo momentum change $\Delta\vec{p}$ and $\tilde{N} - 1$ test particles contiguous to test particle 2 undergo momentum change $-\Delta\vec{p}$. This is followed in time till the collisions are over and we have one event. To simulate another event we start with initial positions of the ions and generate by Monte Carlo fresh sets of test particles. Many events are needed before any comparison with experiments can be made.

The calculation for each event is quite large as collisions between $(A_p + A_t)\tilde{N}$ test particles need to be checked. Here A_p is the number of nucleons in the projectile and A_t is the number of nucleons in the target and $\tilde{N}$ is rather large (usually about 100). It was shown in [1] that the problem can be reduced, for each event, to checking collisions between just $(A_p + A_t)$ test particles. This feature makes it possible for us to do large systems. We refer to Sec. II of [1] for details. No compromise to theory or numerical accuracy is introduced.

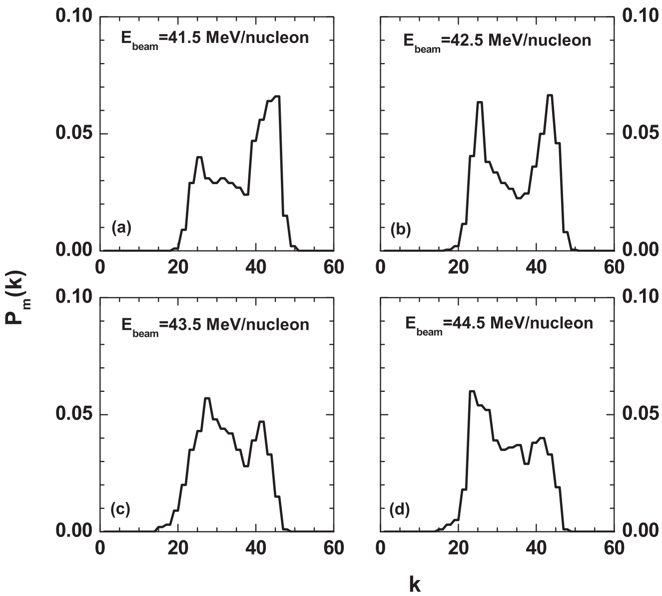

FIG. 3. Largest cluster probability distribution for $A_p = 40$ on $A_t = 40$ reaction at beam energies (a) 41.5, (b) 42.5, (c)43.5, and (d) 44.5 MeV/nucleon. The average value of 2 mass units are shown. At each energy 1000 events are chosen. The results shown in this figure are calculated at $t = 300$ fm/c

Some details of the simulation. For completeness, we provide some details of the calculation that will be needed to explain our cluster recognition algorithm. Collisions are treated as in [3]. For Vlasov propagation we use the lattice Hamiltonian method [13] which accurately conserves energy and momentum. The mean field is also taken from [13]. The configuration space is divided into cubic lattices. The lattice points are l fm apart. Thus the configuration space is discretized into boxes of size l^3 fm^3. Density at the lattice point $\vec{r_\alpha}$ is given by

$$\rho_L(\vec{r_\alpha}) = \sum_i S(\vec{r_\alpha} - \vec{r_i}). \tag{1}$$

Here the sum over i goes over all the test particles and the form factor is

$$S(\vec{r}) = \frac{1}{\tilde{N}(nl)^6} g(x)g(y)g(z), \tag{2}$$

where

$$g(q) = (nl - |q|)\Theta(nl - |q|). \tag{3}$$

In this work we have used $n = 1$ and $l = 1$ fm. Because of this choice, at a given time, if two test particles are more than 2 fm apart, they cannot affect each other's motion directly. This prompts us to prescribe the following algorithm. Two test particles are part of the same cluster if the distance between them is less than or equal to 2 fm. Two clusters are distinct if none of the test particles of cluster 1 is within a distance of 2 fm from any of the test particles of cluster 2. With this prescription, the number of clusters and their sizes will change as a function of time at early times. Because of the momenta that test particles carry, two test particles which are less than 2 fm apart (or more than 2 fm apart) may not remain so at a later time. The physical picture we depend upon is that when two heavy ions collide, clusters are formed which begin to move away from one another. If this is true then at large times, the momentum $\vec{p_i}$ and position $\vec{r_i}$ in each individual cluster are strongly correlated and the transfer of test particles between different clusters will disappear. One can test this by plotting the multiplicity distribution as a function of time. We find that for 40 on 40, near constancy is observed around 300 fm/c, and for 120 on 120 (because this is a much larger system) around 600 fm/c. From the multiplicity distributions of 1000 events, we construct $P_m(k)$, the probability that the largest cluster in an event has k nucleons. Examples are shown in Figs. 1 and 2. Our algorithm for enumerating cluster numbers and their sizes has some similarities and also some differences with the method used in [14] in QMD.

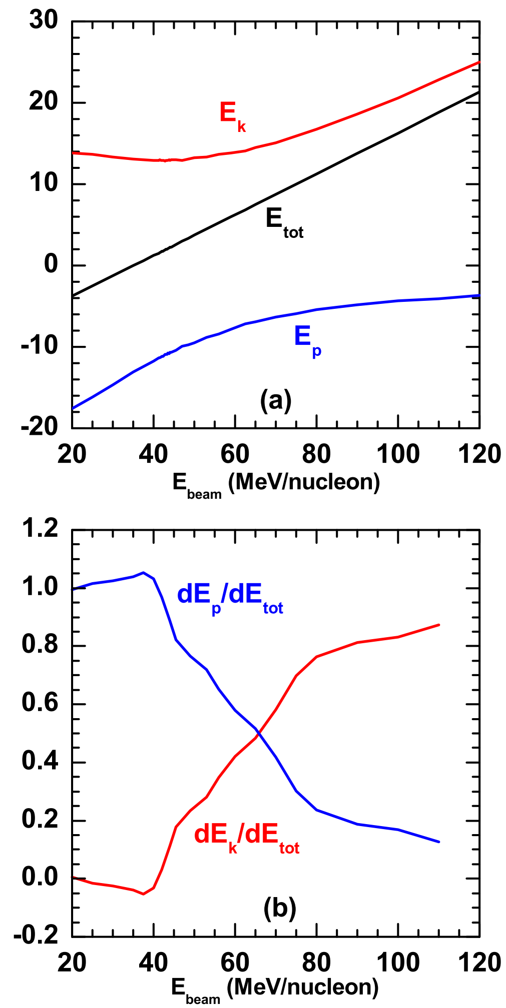

FIG. 4. Upper panel: Dependence of kinetic energy per nucleon (red), potential energy per nucleon (blue), and total energy per nucleon (black) for the $A_p = 40$ on $A_t = 40$ reaction on the projectile beam energy per nucleon. Lower panel: Dependence of first-order derivatives of kinetic energy and potential energy with respect to total energy on total energy per nucleon for the $A_p = 40$ on $A_t = 40$ reaction.

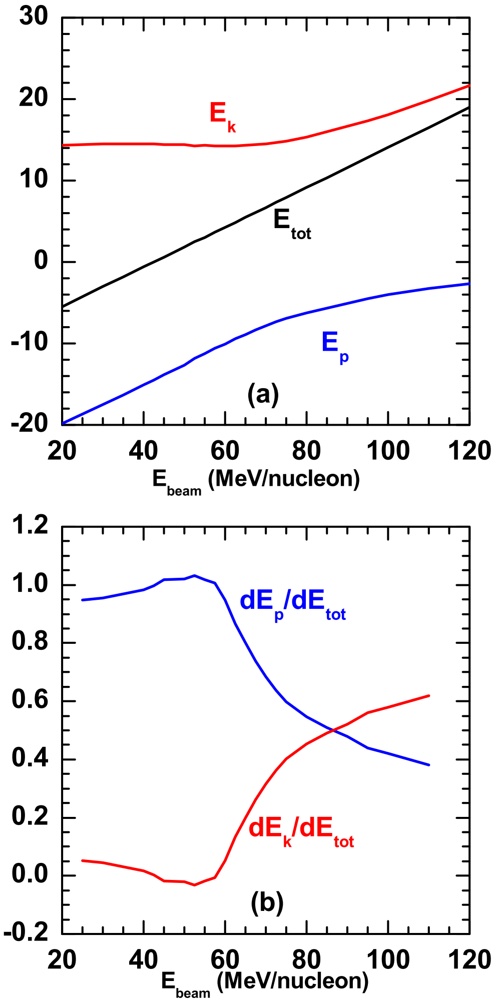

FIG. 5. Same as Fig. 4 but here the nuclear reaction is $A_p = 120$ on $A_t = 120$.

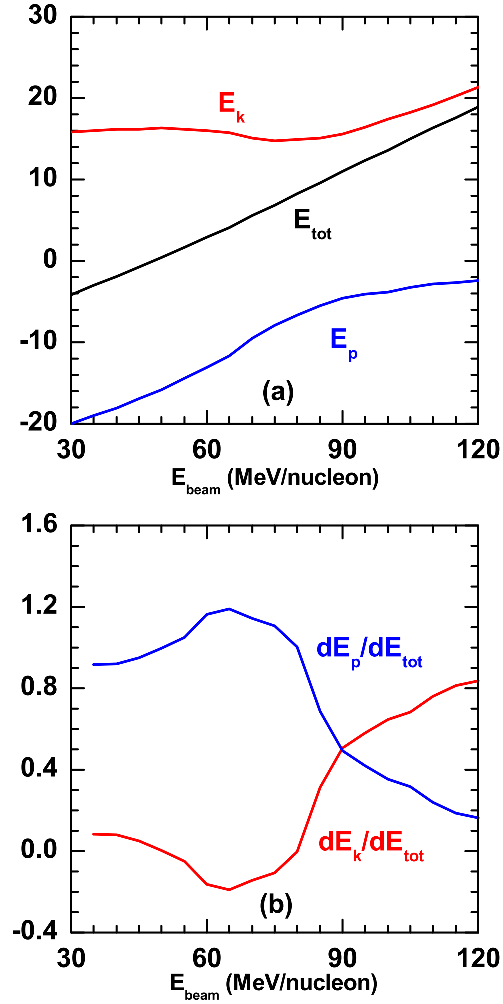

FIG. 6. Same as Fig. 5 but here the calculation is done by the standard BUU method (i.e., without fluctuation).

Results. To study bimodality from our event generation model (BUU plus fluctuation) we simulate central collisions of mass 40 on mass 40 and mass 120 on mass 120 at different projectile beam energies. For 40 on 40 reaction the largest cluster probability distribution is plotted in Fig. 1 for $E_{\rm beam} = 20, 42.5$, and 100 MeV/nucleon. At each energy 1000 events are taken, and for each event, calculation is done up to $t = 300$ fm/c. The results shown are averages for graphs of 2 consecutive mass number at $t = 300$ fm/c. At projectile beam energy $E_{\rm beam} = 20$ MeV/nucleon, the $P_m(k)$ is peaked at around mass 60 which represents the liquid phase whereas at $E_{\rm beam} = 100$ MeV/nucleon, the probability distribution peaks at very low mass, i.e., it suggests the system is in the gas phase. In between these two extremes, at $E_{\rm beam} = 42.5$ MeV/nucleon the largest cluster probability distribution shows the bimodal behavior where the heights of the two peaks are almost the same. Figure 2 shows similar features for a much heavier system: 120 on 120. Here we take the results at 600 fm/c. Several points are worth mentioning. Whether in the case of 40 on 40 or 120 on 120, bimodality occurs in a very narrow range of energy. For 40 on 40 we demonstrate that in Fig. 3. Thus to locate bimodality in experiments, the beam energy variation has to be done in small energy steps. The narrow width of energy over which bimodality appears is common in CTM also.

A phase-transition-like behavior emerges more directly from our calculations. This is quite revealing. For 40 on 40 (and 120 on 120) we do our calculation as a function of beam energy. For example for 40 on 40 we did our calculation from beam energy 20 to 100 MeV/nucleon. For each beam energy 1000 events were generated. From these events we compute the average total energy $E_{\rm tot}$, the average kinetic energy E_k, and the average potential energy E_p per particle. Let us plot the total energy $E_{\rm tot}$ in the center of mass (c.m.) frame. This will of course increase in value as the $E_{\rm beam}$ (MeV/nucleon) increases. This energy $E_{\rm tot}$ is the sum of kinetic energy E_k and potential energy E_p. The origin of E_k is more complicated. It arises from Fermi motion of the test particles and also the c.m. kinetic energy of each cluster. The quantity E_p is more straightforward. It arises from the potential energy of the clusters. Insight is obtained by examining the derivative $dE_p/dE_{\rm tot}$. A sudden change in the derivative $dE_p/dE_{\rm tot}$ occurs at the point where bimodality is observed. This type of break in the first derivative is typical of first-order phase transitions. We might consider this break to be an additional signature of a first-order phase transition.

Since here we plotted values for the average of many events, it is natural to ask, could it be seen in standard BUU which does give average values? This is not obviously so because the average might depend also on the details of fluctuations that were used in our event generation model. However, straightforward BUU as has been used before [3] does produce similar result (Fig. 6). Thus the possibility exists that one might get a signature for first-order phase transition from BUU itself. This is an important step forward. Fluctuation models are numerous and often impossible to implement for realistic situations. The one we have used here is unable to ensure that Pauli principle is satisfied in every step, although estimates in Ref. [1] suggest that such corrections are small. Standard BUU [3] has no such problem, and is highly respected in the nuclear community; if standard BUU also provides signatures of first-order phase transition (although not recognized in any earlier work) it is a very significant step forward.

Discussion. We have studied central collisions of 40 on 40 and 120 on 120 to test the appearance of bimodality which is considered to be a signature of first-order phase transition in finite systems. Bimodality was observed. Since calculations were done with a fixed beam energy, one might be tempted to call it a microcanonical calculation. But even in central collisions at least two different reaction mechanisms operate. One is collision between peripheral parts. Here some nucleons may simply pass by or at most make one collision. We would include preequilibrium emission in this category. The number of nucleons in preequilibrium emission and the energy they carry off will vary from event to event. Thus the number of nucleons which suffer multiple collisions and the energy that is available for such multiple collision events will vary. Presumably such multiple collision events can show signatures of statistical equilibrium, phase transitions, etc., but in experiments and in transport model calculations such as those discussed here, all different reaction mechanisms will play a role. Nonetheless, this calculation shows that a dynamical model describing the collision with just nuclear forces can lead to the observation of first-order phase transitions in intermediate-energy heavy ion collisions.

The similarity between CTM results and transport model results might be exploited to estimate the freeze-out density in statistical models. In CTM a freeze-out density is assumed but there is no such parameter in the transport model. In CTM the temperature at which bimodality appears depends on the assumed freeze-out density. There will be a freeze-out density at which CTM gives the same bimodality temperature as the transport model. This could be an estimate for freeze-out density. Detailed calculations have not been carried out.

Acknowledgement. S. Das Gupta thanks Dr. D. K. Srivastava and Dr. A. K. Chaudhuri for hospitality during visit at Variable Energy Cyclotron Centre.

[1] S. Mallik, S. Das Gupta, and G. Chaudhuri, Phys. Rev. C **91**, 034616 (2015).
[2] W. Bauer, G. F. Bertsch, and S. Das Gupta, Phys. Rev. Lett. **58**, 863 (1987).
[3] G. F. Bertsch and S. Das Gupta, Phys. Rep. **160**, 189 (1988).
[4] C. B. Das, S. Das Gupta, W. G. Lynch, A. Z. Mekjian, and M. B. Tsang, Phys. Rep. **406**, 1 (2005).
[5] S. Das Gupta and A. Z. Mekjian, Phys. Rev. C **57**, 1361 (1998).
[6] K. A. Bugaev, M. I. Gorenstein, I. N. Mishustin, and W. Greiner, Phys. Rev. C **62**, 044320 (2000).
[7] J. Pan, S. Das Gupta, and M. Grant, Phys. Rev. Lett. **80**, 1182 (1998).
[8] F. Gulminelli and Ph. Chomaz, Phys. Rev. C **71**, 054607 (2005).
[9] K. Binder and D. P. Landau, Phys. Rev. B **30**, 1477 (1984).
[10] G. Chaudhuri, S. Das Gupta, and F. Gulminelli, Nucl. Phys. A **815**, 89 (2009).
[11] M. Pichon *et al.*, Nucl. Phys. A **779**, 267 (2006).
[12] A. Le Fevre and J. Aichelin, Phys. Rev. Lett. **100**, 042701 (2008).
[13] R. J. Lenk and V. R. Pandharipande, Phys. Rev. C **39**, 2242 (1989).
[14] Suneel Kumar and Rajeev K. Puri, Phys. Rev. C **58**, 320 (1998).