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Searching for the origin of isoscaling: confinement and expansion

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In this article the dynamical origin of isoscaling, the phenomenon first observed in heavy ion reactions, is explored by studying classical molecular dynamics simulations. Systems composed of neutron and proton-like particles and resembling a compound nucleus produced in heavy ion reactions are allowed to undergo a phase transition into clusters both while confined and during free expansion. Varying the isotopic number while maintaining the same atomic number, these simulations are used to obtain isoscaling fits of the ratio of fragment yields, and to elucidate the effect the dynamics of the reaction has on the isoscaling coefficients. It is observed that breakups at high density and before their final expansion are dominant in setting the values of the isoscaling coefficients $\alpha$ and $\beta$.

Keywords: Isoscaling; nuclear matter; equation of state; molecular dynamics; nuclear reactions; fragmentation.

En este artículo se explora el origen dinámico de la isoescala, fenómeno observado originalmente en reacciones de iones pesados, usando simulaciones de dinámica molecular clásica. Sistemas compuestos de partículas similares a neutrones y protones y representando un núcleo compuesto producido en reacciones de iones pesados son permitidos sufrir un cambio de fase hacia cúmulos durante un confinamiento y una expansión libre. Variando el número isotópico manteniendo el número atómico constante, estas simulaciones son usadas para obtener ajustes de isoescala en el proceso de las divisiones de fragmentos, y para elucidar el efecto de la dinámica que la reacción tiene en los coeficientes de isoescala. Se observa que los rompimientos a altas densidades y anteriores a la expansión final dominan al determinar el valor de los coeficientes de isoescala $\alpha$ y $\beta$.

Descriptores: Isoescala; material nuclear; ecuación de estado; dinámica molecular; reacciones nucleares; fragmentación.

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1. Introduction

Nuclear reactions using unstable isotopes have allowed the study of nuclear matter beyond the valley of stability, i.e. of systems with excess neutrons as compared to stable systems [1-5]. The initial interest was to describe the novel reactions by comparing them to the regular collisions. In the case of reactions leading to fragmentation, such comparison was first done by means of the respective yields of fragments produced in the collisions performed with stable and unstable nuclei; those studies led to the discovery of a rule relating such yields now known as isoscaling.

Isoscaling stems out of the study of isotope yields of central collisions of similar, but isotopically different, reactions [1,5]. The ratio of isotope yields from, say, reactions 1 and 2, $R_{21}(N,Z)$, has been found to depend exponentially on the neutron and proton numbers, $N$ and $Z$:

$$R_{21}(N,Z) = C e^{\alpha N + \beta Z}$$  \hspace{1cm} (1)

where $C$, $\alpha$ and $\beta$ are fitting parameters. The interest on such scaling law comes from the fact that the parameters $\alpha$ and $\beta$, under some approximations, can be linked to the symmetry term of the equation of state (EOS) of nuclear matter [4,6,7], $C_{\text{sym}}$:

$$\alpha = \frac{4C_{\text{sym}}}{T} \left[ \left( \frac{Z_1}{A_1} \right)^2 - \left( \frac{Z_2}{A_2} \right)^2 \right]$$  \hspace{1cm} (2)

with a similar expression for the parameter $\beta$.

Previous studies [8-13] based both on dynamic and geometrical models have shown that isoscaling is not inherent to nuclear physics and that such scaling property is also found in non-nuclear phenomena. Indeed isoscaling can be originated both from the dynamics of the nuclear reaction as well as from the pure probabilistic aspects of the disassembly. Although the probabilistic source of isoscaling, symmetry, is by now known from a theoretical point of view [9-12], the first cause of isoscaling, dynamics, has not been fully explored. Thus, this article focuses on studying the role played by a component of the dynamics of the breakup on the establishment of isoscaling: the breakup volume and the post-breakup expansion. Using classical molecular dynamics we will study isoscaling produced in systems that fragment while confined and compare them to the isoscaling obtained from clusterings observed in expanding systems.

In the following section we introduce the molecular dynamics model used. Afterwards we study the isoscaling of confined and expanding systems. The manuscript closes with a summary of the main conclusions.

2. The model

In the present study systems resembling nuclei with a given number of protons and neutrons were created using molecular dynamics. The "nuclei" were equilibrated using interaction potentials that endow them with nuclei-like properties...
such as proper binding energy, radii and nucleon-nucleon cross sections.

We use the molecular dynamics (MD) model first introduced in the Revista Mexicana de Física back in 1999 [14]. This model has proven to be capable of reproducing both the out-of-equilibrium and the equilibrium parts of a collision, as well as hydrodynamic flow, changes of phase, etc. all without any adjustable parameters, and has been very fruitful in studies of, among other phenomena, neck fragmentation [15], phase transitions [16,17], and—of course—isoscaling [8-13,18]; readers are directed to these references for further details on the model.

The interaction potential is composed of a nuclear part plus Coulomb [19]. The nuclear interaction potentials are

\[ V_{np}(r) = V_r \left( \frac{e^{-\mu r}}{r} - \frac{e^{-\mu r_c}}{r_c} \right) - V_a \left( \frac{e^{-\mu_a r_c}}{r_c} - \frac{e^{-\mu_a r}}{r} \right) \]  
\[ (3) \]

and

\[ V_{nn}(r) = V_{pp}(r) = V_0 \left( \frac{e^{-\mu_0 r}}{r} - \frac{e^{-\mu_0 r_c}}{r_c} \right). \]  
\[ (4) \]

where the cutoff radius is \( r_c = 5.4 \text{ fm} \), \( V_{np} \) is the potential between a neutron and a proton while \( V_{nn} \) is that between identical nucleons. The values of the parameters of the Yukawa potentials correspond to an equation of state of infinite nuclear matter with an equilibrium density of \( \rho_0 = 0.016 \text{ fm}^{-3} \), a binding energy \( E(\rho_0) = 16 \text{ MeV/nucleon} \), and a compressibility of 535 MeV for the stiff model. As an example, Fig. 1 shows the binding energy obtained from this procedure for a number of isotopes for the \( Z = 10 \) and \( Z = 20 \) nuclei.

It is convenient to remark that the model used is purely classical and it excludes all quantal effects, such as the exclusion principle and isotopic content-modifying phenomena. The Fermi motion, although formally absent, is somewhat included by the internal motion of the “nucleons” which is needed for these nuclei to achieve the proper binding energy in their “ground states”. Therefore, any observed variations to isoscaling will be entirely due to the effect of confinement or expansion.

3. Simulating the breakup

The systems constructed are either allowed to undergo a phase transition while confined or during a free expansion. The confined systems are placed in a closed spherical container at a fixed density and allowed to cluster. The expanding systems were also placed at an initial density and allowed to undergo a free expansion during which fragmentation took place. Such types of disassemblies were performed for nuclei with stable N to Z ratios as well as with nuclei with large N to Z ratio; comparisons between yields obtained from systems differing in the number of neutrons were used to obtain the corresponding ratio \( R_{21} (N, Z) \) and the fitting parameters \( \alpha \) and \( \beta \).

As in the past we have studied the collisions of \( ^{40}\text{Ca} + ^{40}\text{Ca}, ^{48}\text{Ca} + ^{48}\text{Ca} \) and \( ^{56}\text{Ca} + ^{56}\text{Ca} \), here we study the evolution of constrained compound “nuclei” of \((N,Z)=(40,40)\) and \((56,40)\) corresponding to the compound nuclei presumably formed during the merging of the colliding partners in our previous works.

As explained before, we have used dissipative molecular dynamics to build nuclei in their ground states. Once these systems are available, they are placed cold inside a spherical container with a radius fixed to obtain values of the number density of 0.003 fm\(^{-3}\) and 0.016 fm\(^{-3}\). The excitation energy is added to such system by scaling the momenta of the particles. The trajectories of individual nucleons are then obtained using an standard Verlet algorithm with an energy conservation of O(0.01\%).

After an initial long run is performed to equilibrate the system, a much longer run is carried out and time snapshots of the evolution are recorded. Such microscopic information

\[ \text{FIGURE 1. Binding energy obtained from the nuclei constructed with the molecular dynamics procedure for isotopes of the } Z = 10 \text{ and } Z = 20 \text{ nuclei.} \]

\[ \text{FIGURE 2. Mass distribution obtained in the clustering of the system } (N,Z) = (40,40) \text{ during confinement at the listed energies per particle.} \]
of the evolution provides the position and momentum of the nucleons, \((\vec{r}, \vec{p})\), and it is used to identify the fragment structure of the system by means of the MSTE cluster-detection algorithm of [20] and refined by [21]. The systems were studied at excitation energies ranging from \(-5\) to \(8\) MeV/A and for the two different values of the number density with two thousand snapshots recorded at each energy. Figures 2 and 3 show examples of the mass distributions of the fragments obtained in confined and expanding experiments.

3.1. Isoscaling

The fragment mass multiplicity obtained from the evolutions were used to construct the corresponding yield matrices \(Y_1(N,Z)\) and \(Y_2(N,Z)\) which were then used to calculate the ratio \(R_{21}(N,Z) = Y_2(N,Z)/Y_1(N,Z)\) for the systems \(^{40}\text{Ca}^+^{40}\text{Ca}\) and compared to \(^{48}\text{Ca}^+^{48}\text{Ca}\). Fits to the isoscaling exponential law, Eq. (1), were obtained using a least squares method for all points corresponding to each reaction and energy; this yielded values of the parameters \(\alpha\) and \(\beta\) for each of the calculated times.

Figures 4 and 5 show the behavior of the parameter \(\alpha\) for different energies per particle for both the confined and expanding clusterings and for densities \(\rho = 0.016\) fm\(^{-3}\) and \(\rho = 0.003\) fm\(^{-3}\), respectively.

The solid horizontal line represents the symmetropy value of \(\alpha\) expected for this reaction. Symmetropy, recently introduced in Refs. 9 and 10, predicts isoscaling even in the absence of reactions, with values of the parameters \(\alpha\) and \(\beta\) given by

\[
\alpha = \ln \left( \frac{N_2/A_2}{N_1/A_1} \right)
\]

and a similar expression for \(\beta\) in terms of the proton numbers. It is convenient to recall that the symmetropy values are independent of the dynamics of the reaction, energy or density achieved in the collision; indeed these values only depend on the relative probabilities of a nucleon being a proton or a neutron.

Figures 4 and 5 underline the role played by the expanding dynamics of the reaction. Disassemblies both at high \((\rho = 0.016\) fm\(^{-3}\)\) and at low densities \((\rho = 0.016\) fm\(^{-3}\)\) appear to achieve isoscaling parameters about 30% larger than those obtained while the system expands freely; this effect also appears to disappear at high negative energies per particle \((E \approx -2\) MeV/A\) when, presumably, the system is over-bound as to disassembly in all possible partitions.

A similar effect is observed as a function of the density. Systems decaying at around normal density values (cf. Fig. 4) show a more pronounced effect of the confinement than those breaking up at lower densities (cf. Fig. 4). The overall values of the \(\alpha\) obtained at high densities are also substantially larger than those at low densities, for instance at \(E \approx -2\) MeV/A,

\[
\alpha(\rho = 0.016\text{fm}^{-3}) \approx 1.1 > \alpha(\rho = 0.016\text{fm}^{-3}) \approx 0.8
\]

for both confined and expanding cases.

It is important to notice that, as observed in regular simulations of isoscaling reactions [8], \(\alpha\) is a decreasing function of the energy of the system. Likewise, as observed in
such simulations as well as in comparisons to experimental
data [13], α converges to a constant value very close the sym-
mentropy limit given by Eq. (4). These results confirm the
findings of Refs. 12 and 13, namely that in the limit of high
energies isoscaling tends to be purely symmentropic.

4. Conclusions
We have studied the effect that confinement and expansion
have on the isoscaling parameters at different energies and
densities. Using molecular dynamics, breakups of nuclear-
like systems were simulated in confined spaces as well as
during expansions. The fragment production in cases similar
in atomic number but with varying isotopes was computed
with a fragment-recognition algorithm, and used to obtain the
yield ratio \( R_{21}(N,Z) \) which was then fitted with the isoscal-
ing law Eq. (1) to extract the parameter \( \alpha \). The systems
compared were equivalent to those formed by collisions of
\(^{40}\text{Ca}^{+}{^{40}\text{Ca}}\) and \(^{48}\text{Ca}^{+}{^{48}\text{Ca}}\), with energies per particle rang-
ing from -4 to 8 MeV/A.

The comparison of the \( \alpha \)'s obtained for the confined and
expanding cases show that \( \alpha_{\text{confined}} > \alpha_{\text{expanding}} \) except at
low energies and dilute systems. Given that the breakup of
the compound nucleus starts at relatively high densities (pre-
sumably at higher-than-normal densities), and sufficiently
early in the reaction before the expansion reaches its hydro-
dynamic stage, it is to be expected that most of the isoscaling
behavior is crafted during the transition state, and much less
during the post-breakup expansion which kicks off at lower
densities.

This appears to indicate that the values of \( \alpha \) are securely
anchored to the high-density and early-stage of the reaction
where the breakup takes place; contributions to isoscaling
coming form the expansion dynamics are smaller than those
produced during the breakup. As found before [12,13], the
perennial symmentropic contribution to isoscaling appears to
be sizable only at higher energies.

A simultaneous study to be reported elsewhere, [18] will
enlarge this study to incorporate the role of the equation of
state on isoscaling to try to link values of isoscaling to spe-
cific equations of state.

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