Dynamical aspects of isoscaling

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(Dated: September 26, 2018)

The origin and dynamical evolution of isoscaling was studied using classical molecular dynamics simulations of \(^{40}\text{Ca} + ^{40}\text{Ca}\), \(^{48}\text{Ca} + ^{48}\text{Ca}\), and \(^{52}\text{Ca} + ^{52}\text{Ca}\), at beam energies ranging from 20 MeV/A to 85 MeV/A. The analysis included a study of the time evolution of this effect. Isoscaling was observed to exist in these reactions from the very early primary isotope distributions (produced by highly non-equilibrated systems) all the way to asymptotic times. This indicates that isoscaling is independent of quantum effects and thermodynamical equilibrium. In summary, collision-produced isoscaling appears to be due more to the mere partitioning of the proton-neutron content of the participant nuclei, than to specific details of the reaction dynamics.

I. INTRODUCTION

Experimental advances, that now permit the study of nuclear reactions involving radioactive isotopes, have propelled the isotopic degree of freedom to the forefront [1, 2, 3, 4, 5]. It is expected, for instance, that this new variable of control could shed light on charge equilibration in heavy ion reactions, and on the role played by the isotope asymmetry terms of the equation of state of nuclear matter [4].

The main tool for inspection of this new observable is based on the isotope yields of central collisions of similar, but isotopically different, reactions [1, 5]. The ratio of isotope yields from reactions 1 and 2, \( R_{21}(N, Z) \), has been found to depend exponentially on the isotope neutron number \( N \) and proton number, \( Z \):

\[
R_{21}(N, Z) = \frac{Y_2(N, Z)}{Y_1(N, Z)} \approx e^{\alpha N + \beta Z},
\]

where \( \alpha \) and \( \beta \) are fitting parameters. Equations of the form of (1) can be linked, under some approximations, to primary isotope yields produced by disassembling infinite equilibrated systems in microcanonical and grand canonical ensembles [4], as well as to breakups in canonical [6] ensembles.

Little reflection is needed to understand that \( R_{21} \) could be affected by many reaction variables. Its direct dependence on the experimentally measured yields, \( Y_1 \) and \( Y_2 \), makes \( R_{21} \) vulnerable to anything that can modify the isotopic content of the initial fragment yield, be this out-of-equilibrium breakup, secondary fission of primordial fragments, light particle emission, \( \beta \)-decay, and the like. As these effects have varying lifetimes, it is very likely that the experimentally-captured yield contains an integral of all of these effects on the primary distribution. This casts a shadow of doubt on the isoscaling-related conclusions obtained by the use of microcanonical, canonical and grand canonical breakup scenarios, and calls for the use of an unconstrained model to ratify the main findings of equilibrium models.

This article aims at elucidating the origin and dynamical evolution of isoscaling using a model not restricted by assumptions such as the existence of freeze-out stages, thermal and chemical equilibration, or unrealistic volume constraints [5]. In the next section, the \( MD \) model used is introduced along with the fragment recognition algorithm selected for this study. The fitting procedure used to extract the isoscaling exponential law (1) from the simulations is presented in section II followed by results consisting of the observation of isoscaling at asymptotic times, its dependence on the reaction energy, the time evolution of such a law during the reaction, and its connection to thermodynamical observables. The manuscript closes with a summary of the main conclusions.

II. MOLECULAR DYNAMICS

To study the origin of isoscaling, a model capable of reproducing both the out-of-equilibrium and the equilibrium parts of a collision is needed. As statistical and other equilibrium models [6,8] lack-by construction-of all relevant collision-induced correlations, a dynamical model is thus needed. Most of such dynamical models, nevertheless, either lack higher-order correlations and have difficulties in producing fragmentation [9,10,11,12,13], or introduce unrealistic volume constraints to the dynamics [14]. In the present work, we use a molecular dynamics (\( MD \)) model that can describe non-equilibrium dynamics, hydrodynamic flow and changes of phase without adjustable parameters. The combination of this \( MD \) code with a fragment-recognition algorithm, has been dubbed “Latino” [15], and in recent
years it has been applied successfully to study, among other things, neck fragmentation \[16\], phase transitions \[17\], critical phenomena \[18\, 19\] and the caloric curve \[20\, 21\] in nuclear reactions.

The MD code uses a two-body potential composed of the Coulomb interaction plus a nuclear part \[22\] that correctly reproduces nucleon-nucleon cross sections, as well as the correct binding energies and densities of real nuclei. The “nuclear” part of the interaction potential is

\[
V_{np}(r) = V_\rho \left[ \frac{\exp(-\rho r)}{r} - \frac{\exp(-\rho r_c)}{r_c} \right] - V_a \left[ \frac{\exp(-a r)}{r} - \frac{\exp(-a r_a)}{r_a} \right]
\]

\[
V_{nn}(r) = V_{pp}(r) = V_0 \left[ \frac{\exp(-\rho_0 r)}{r} - \frac{\exp(-\rho_0 r_c)}{r_c} \right]
\]

(2)

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 \[22\] correspond to an equation of state of infinite nuclear matter with an equilibrium density of \( \rho_0 = 0.16\ \text{fm}^{-3} \), a binding energy \( E(\rho_0) = -16\ \text{MeV/nucleon} \), and a compressibility of around 250 MeV.

To study collisions, this potential is first used along with dissipative molecular dynamics to construct “nuclei” by grouping “nucleons” at the binding energies and radii of real nuclei, and stable for times longer than the reaction time. These nuclei are then used as targets and projectiles by rotating the relative orientation of the target-nuclei combination, boosting the center-of-mass velocity of the projectile to a desired energy, and leaving the target initially at rest. The trajectories of motion of individual nucleons are then calculated using the standard Verlet algorithm with an energy conservation of \( O(0.01\%) \).

The collision information, initially composed by the values of \( \vec{r}, \vec{p} \) of the nucleons, is then transformed into fragment information by means of a cluster-detection algorithm which, in this case, is the MSE method which was introduced decades ago \[23\], but was recently adapted for this field, fully analyzed and compared with other fragment recognition algorithms \[24\]. According to this prescription, a particle \( i \) belongs to a cluster \( C \) if there is a particle \( j \) in \( C \) to which \( i \) is bound in the sense of \( p_{ij}^2/4\mu < v_{ij} \), where \( p_{ij} \) is the relative momentum, \( \mu \) the reduced mass, and \( v_{ij} \) the interparticle potential. In this cluster definition the effect of the relative momentum between the particles that form the cluster is taken into account in an approximate way; of course, at some time during the reaction, MSE yields the asymptotic cluster distribution. The resulting information contains details about the nucleon content of the emitted fragments and, as this is available at all times during the collision, it allows the study of the time evolution of quantities such as the isoscaling law.

Before we turn to a description of the analysis performed on these collisions, a word of caution is needed to underline the fact that the MD model here described is fully classical. Since all quantal effects (such as the exclusion principle) and isotopic content-modifying phenomena (such as \( \beta \)-decay) are excluded, means that, if any of them is responsible for isoscaling, this study should not reproduce this effect. On the contrary, if isoscaling is well predicted by this classical model, this will exclude any purely quantum phenomenon as the sole cause of isotopic scaling.

III. ISOSCALING

The collisions \(^{40}\text{Ca}+^{40}\text{Ca},\ 48\text{Ca}+^{48}\text{Ca},\ 52\text{Ca}+^{52}\text{Ca}\), were studied at beam energies of 20, 25, 35, 45, 65 and 85 MeV/A with two thousand collisions performed at each energy. Data from these collisions were used to construct the corresponding yield matrices \( Y_i(N, Z) \), where \( i \) stands for the reaction, and \( N \) and \( Z \) for the neutron and proton numbers, respectively. These matrices were then used to calculate the ratio \( R_{21}(N, Z) = Y_2(N, Z)/Y_1(N, Z) \) for the combinations of reactions \(^{40}\text{Ca}+^{48}\text{Ca},\ ^{40}\text{Ca}+^{52}\text{Ca},\ 48\text{Ca}+^{52}\text{Ca}\) at each of the energy values. These ratios were calculated at different reaction times starting at impact \( t = 0 \) and ending at \( 5000\ \text{fm}/c \); this last time corresponds, practically, to an asymptotic value. Fits to the isoscaling exponential law \[11\] were obtained using a standard least squares method for each reaction and energy, procedure which yielded values of the parameters \( \alpha \) and \( \beta \) for each of the calculated times. Next, studies of the energy dependence of isoscaling at long times and its behavior during the dense part of the reaction are presented.

A. Isoscaling in asymptotia

Experimental results always correspond to asymptotic values, taking into account that, at the energies listed below, the crossing time is of the order of a few \( \text{fm}/c \), it is safe to consider times of, say, 1000 \( \text{fm}/c \) as asymptotic; in this study, nevertheless, the calculation was extended to five times this value.

Figure \[11\] shows the obtained values of \( R_{21}(N, Z) \) and the corresponding fit to the isoscaling exponential law \[11\] for the case \(^{40}\text{Ca} -^{48}\text{Ca}\) at 35 MeV/A at 1250 \( \text{fm}/c \). The fact that \( \text{Latino} \) reproduces the reactions sufficiently well as
FIG. 1: Asymptotic behavior of isoscaling. Typical fit to $R_{21}(N, Z)$ for the case $^{40}\text{Ca} - ^{48}\text{Ca}$ at 35 MeV/A at 1250 fm/c.

to produce isoscaling at long times is obvious from this figure. Other reactions (i.e. with other masses and energies) yield similar results.

Upon applying the fitting procedures described in III for each of the three ratios of reactions, values of $\alpha$ and $\beta$ were obtained for each of the energies. Figure 2 shows the values of these fitting parameters at asymptotic times (5000 fm/c) as a function of beam energy per nucleon for the ratios of the reactions $^{40}\text{Ca} - ^{48}\text{Ca}$, $^{40}\text{Ca} - ^{52}\text{Ca}$, and $^{48}\text{Ca} - ^{52}\text{Ca}$. The smooth trends of $\alpha$ and $\beta$ are in the range of values obtained by other investigators [4, 5, 14, 25, 26].

It is instructive to compare these results to those recently obtained using quantal molecular dynamics simulations with the AMD-V model [14]. In that work, collisions between $^{40}\text{Ca}+^{40}\text{Ca}$, $^{48}\text{Ca}+^{48}\text{Ca}$ and $^{60}\text{Ca}+^{60}\text{Ca}$ at 35 MeV/A were performed, and an isoscaling-looking behavior was observed for their $R_{21}$. The power-law fit obtained for the ratio of $^{48}\text{Ca} + ^{48}\text{Ca}$ to of $^{40}\text{Ca} + ^{40}\text{Ca}$ yielded an $\alpha = 1.03$ and $\beta = 1.22$. These values agree with the results here obtained here for a similar case: $\alpha = 1.07$ and $\beta = 1.22$ (cf. figure 2); other AMD-V results are also in line with our classical MD simulations.

As stated before, since this study is based on a classical MD model, the fact that isospin is well reproduced by it, implies that this effect is not due to quantum effects that could modify the isotopic content of the fragments, such as $\beta$-decay. To gain a deeper insight into the origin of isoscaling, we now turn to a study to its time evolution during the reaction.

### B. Evolution of isoscaling

As the nucleon information is available throughout the reaction, the yields and, thus, the ratio $R_{21}$ can be calculated at any time during the collision. Figure 3 shows early (at 125 fm/c) values of $R_{21}(N, Z)$ and the corresponding fit to the isoscaling exponential law $\Pi$, for the case $^{40}\text{Ca} - ^{48}\text{Ca}$ at 35 MeV/A. The observed goodness of the isoscaling exponential law appears to be as good in early times as in asymptotic times. Other reactions yield similar results.

Repeating the fitting procedure described in $\Pi$ it is possible to obtain values of $\alpha$ and $\beta$ at different times. Figure 4 shows the time evolution of $\alpha$ and $\beta$ obtained from the ratio of yields of $^{40}\text{Ca} - ^{48}\text{Ca}$ at 35 MeV/A as a function of reaction time.
As attested by figure 3 and with varying values of $\alpha$ and $\beta$ (cf. figure 4), isoscaling appears to be present in the reaction from very early times. This, in agreement with the findings of [4], rules out long-time effects, such as secondary decays, as the cause of isoscaling. Thus, our search for the origin of this effect should now be directed to earlier times of the reaction, those in which the system is still very dense and highly interacting.

### C. Isoscaling and dynamics

As outlined in reference [1], the parameters $\alpha$ and $\beta$ of the power law (1), can be linked to the differences between the neutron and proton separation energies for the two reactions. Assuming that the reactions populate a grand canonical ensemble, and that the secondary decays have little impact on the resulting $R_{21}$, it can be shown that $\alpha = (\mu_n - \mu_{n1})/T$ and $\beta = (\mu_p - \mu_{p1})/T$, where $\mu_n$, and $\mu_p$ are the neutron and proton chemical potentials of reaction $i$, and $T$ is the equilibrium temperature of the reaction, assumed to be the same for both reactions of the isoscaling comparison.

The main assumption of the preceding arguments, namely, the existence of thermodynamic equilibrium, is questionable in systems which are finite, expanding and disassembling. Added to this concern, of course, is the assumption of a common temperature in both reactions, as well as unique separation energies throughout the disassembling systems. Although these assumptions are difficult to verify, next we extract related information to better understand these premises.

As the temperature of a fragmenting system is not well defined, we focus only on the dynamical properties of the largest fragment. Figure 5 shows the time evolution of the average temperature, mass, collective radial velocity, and total kinetic energy of the biggest fragments obtained in one thousand collisions of $^{40}$Ca on $^{40}$Ca (circles) and of $^{48}$Ca on $^{48}$Ca (triangles) both at 35 $MeV/A$. The temperature was calculated as two thirds of the internal kinetic energy, i.e. of the amount of kinetic energy left after removing the energy stored in the collective expansion. The maximum temperatures observed (between 2.5 and 3.5 $MeV$) are consistent with those derived from alternative analyses [27]. Analyses of other reactions at different energies also yielded similar results.

Figure 5 indicates that the time evolution of the dynamical observables of both reactions is, on average, very similar...
FIG. 3: Early behavior of isoscaling. Typical fit to $R_{21}(N,Z)$ for the case $^{40}\text{Ca} - ^{48}\text{Ca}$ at 35 MeV/A at 125 fm/c.

except at very early times. In the beginning of the reaction, while isoscaling sets in, the largest fragments of both reactions suffer similar compressions and expansions, but with very different average temperatures. As indicated by the rapid increase and decrease of the mass and radial velocity, the largest fragments of both types of reactions appear to undergo a fast period of compression and expansion in the beginning of the reaction. But, although both systems appear to be in synchrony in this compression-expansion, their average temperatures differ by a factor of the order of 30%.

Even though this difference in temperature vanishes for later times, its importance cannot be underestimated as it occurs precisely when the $n$ to $p$ ratios and, thus, $R_{21}$ are being established. This discrepancy in temperatures casts serious doubts about the proposed relationship between $\alpha$ and $\beta$ and the neutron and proton chemical potentials. This would, indeed, lead to relationships of the type $\alpha = (\mu_n/T - \mu_p/T) \propto T^2$ and $\beta = (\mu_n/T - \mu_p/T)$. Although the existence of different source temperatures could possibly be handled [25], the dependence of $\mu$ on $T (\mu(T) - \mu(0) \propto T^2)$ combined with the rapid cooling in early times, makes it difficult to argue for the existence of well defined separation energies that could apply throughout the reaction. At best, what exists at, say, 125 fm/c is the sum of fragments emitted at earlier times which might have undergone subsequent decay. The final yield ratio $R_{21}$ can only be said to be a product of the time integral of decays that occurred under different values of the chemical potentials.

Besides ruling out the chemical potential as the decisive factor in establishing isoscaling, the previous results introduce the need to consider the addition of decays and other nucleon-rearranging processes that take place at different times during the reaction. The importance of this factor can be quantified by inspecting the time evolution of the particle production for different types of particles.

Figure 6 shows the average population of different mass bins obtained at different times for the reaction $^{40}\text{Ca}$ on $^{40}\text{Ca}$ at 35 MeV/A. This time chart clearly illustrates that at times smaller than 100 fm/c, the fragment mass distribution is far from reaching its final value. Furthermore, since, as seen in figure 3, isoscaling is already alive and well at 125 fm/c, i.e. well before the stabilization of most mass bins, the isoscaling power law observed at early times is only a work in progress produced by fragments emitted in previous times.

By induction, all values of $\alpha$ and $\beta$ at a given time include contributions of all earlier fragments, and will pass their own contribution to later values of these exponents. It is, thus, quite obvious that the isoscaling behavior is already present in the initial -and strongly out of equilibrium- stages of the evolution. It does appear as if the origin of isospin...
FIG. 4: Time evolution of $\alpha$ and $\beta$ for the case $^{40}\text{Ca} - ^{48}\text{Ca}$ at 35 MeV/A.

is connected more to the statistical sampling induced by the collision, as observed by Ono et al.\cite{14}, than to specific details of the dynamics of the reaction; this will be explored further in a follow-up investigation\cite{29}.

IV. CONCLUSIONS

The origin and evolution of isoscaling was studied using classical molecular dynamics simulations combined with a fragment-recognition algorithm. Collisions of $^{40}\text{Ca} + ^{40}\text{Ca}$, $^{48}\text{Ca} + ^{48}\text{Ca}$, and $^{52}\text{Ca} + ^{52}\text{Ca}$, at energies from 20 to 85 MeV/A were used to construct the ratios $R_{21}(N,Z)$ and to obtain the fitting parameters $\alpha$ and $\beta$ for the three possible combinations of reactions at all energies and for times from impact to 5000 fm/c.

Isoscaling was found at asymptotic times from 1250 fm/c to 5000 fm/c, the last calculated time. The fitting parameters of the asymptotic $R_{21}$ showed a smooth variation with respect to the beam energy. Although excellent agreement was found with quantal molecular dynamics results, these classical results indicate that the origin of isoscaling is not a quantum effect.

Isoscaling was detected at very early times during the collision (50 fm/c) and it was maintained, with smoothly varying values of $\alpha$ and $\beta$, throughout the reaction. Examining the time evolution of the fragment mass distribution, it is clear that isoscaling exists well before this distribution reaches its final value; whatever produces isoscaling is present in the very early stage of the reaction.

Examining this period of time it was found that the largest fragments of both reactions undergo a compression/heating phase followed by an expansion/cooling period with average temperatures which differ by up to 30%. As this density-$T$ evolution implies a strong variation of the separation energies, the relationship between $\alpha$ and $\beta$ and a unique $\mu$, postulated in other investigations, is obscured.

In summary, we found that isoscaling exists in classical systems, it can be produced in dense systems out of equilibrium, it is accumulative in time and it is maintained in systems expanding and fragmenting. Thus, the existence of isoscaling appears to be independent of the specific characteristics of the dynamics of the reaction. Isoscaling must owe its existence to factors left unexplored in this study, namely, purely geometrical and sampling factors. This will be considered in our following study\cite{29}. 
FIG. 5: Average properties of the biggest fragment. (a) temperature, (b) mass, (c) collective radial velocity, and (d) total kinetic energy. The circles correspond to collisions of $^{40}$Ca on $^{40}$Ca, and the triangles to $^{48}$Ca on $^{48}$Ca, both at 35 MeV/A.

Acknowledgments

C.O.D. acknowledges the support of a grant from the Universidad de Buenos Aires, CONICET through grant 2041, and the hospitality of the University of Texas at El Paso where this project was initiated. The authors are indebted to A. Barrañón for facilitating the initial configurations of the “nuclei” used in these simulations.

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FIG. 6: Population of different mass bins as a function of time for the reaction $^{40}\text{Ca}$ on $^{40}\text{Ca}$ at 35 MeV/A. Circles (3-4), squares (5-6), etc.

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