Critical Nucleation in Colossal Magnetoresistance

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Abstract

Critical exponents have been obtained for a 3D spin particle system. Clusters are formed and system reaches a critical behavior when fragment size distribution follows a power law, as predicted by Fisher Liquid Droplet Model. Also, spontaneous magnetization critical temperature is in agreement with other theoretical studies. System evolution is reproduced via a genetic algorithm that performs minimal genetic fluctuations until a stationary state is attained. Critical exponents are in the range of those belonging to Heavy Ion collisions previously reported, and therefore belong to the same universality class.

1 Introduction

Theoretical and experimental studies have shown that homogeneous nucleation is fundamental for nuclear systems meanwhile inhomogeneous nucleation is relevant for macroscopic systems. According to Grassberger universality hypothesis, models exhibiting a continuous phase transition to an absorbing state belong to the same universality class as directed percolation [1]. Rossi *et.al.* have introduced a conservative gas lattice with a short range stochastic interaction that exhibits a continuous phase transition to an absorbing state for a critical value of the density of particles [2].

In this study we obtain critical exponents of the Colossal Magnetoresistance (Fig. 1), namely $\tau = 2.38$ and $\beta = 0.38$ (Fig. 2), which are equal to those recently reported by Kudzia et. al for Heavy Ions collisions [3]. Critical temperature is in the range of 4.5K (Fig. 3) and nuclear collisions critical temperature is in the range of 4.5 MeV. Power law critical exponent is the same as the one found by Mader *et.al.* in his study about reducibility and thermal scaling in the Ising model, where a critical exponent $\tau = 2.39$ was obtained [4]. Therefore both phenomena belong to the same universality class.

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The manuscript introduces the basic ingredients required to study critical phenomena thermodynamics in section 2. Critical exponents for colossal magnetoresistance are computed in section 3. Critical exponents for collision Molecular Dynamics simulations are obtained in section 4. Finally, conclusions are established in section 5.

2 Nucleation Critical Exponents

The general shape of a Nuclear Model phase diagram is shown in fig. 4, where nucleus is considered a collection of protons and neutrons into a potential well, interacting via a phenomenological interaction [5, 6].

Stability conditions for asymmetric nuclear matter are given by:

$$\left(\frac{\partial E}{\partial T}\right)_{\rho,\delta} > 0, \tag{1}$$

$$\left(\frac{\partial P}{\partial \rho}\right)_{T,\delta} \geq 0, \tag{2}$$

$$\left(\frac{\partial \mu_n}{\partial \delta}\right)_{P,T} \geq 0, \tag{3}$$

where E,P and μ_n are the energy per nucleon, pressure and neutron chemical potential. These three equations are related to thermodynamic, mechanic and diffusive equilibriums.

According to fluctuations theory [7], the probability of having a liquid droplet of radius r and A vapor nucleons at temperature T, is given by $P_r(A) \propto e^{-\Delta G/T}$, with ΔG equal to the difference between the Gibbs Free energy for both phases.

Using the ΔG given by the surface, curvature and bulk terms, we obtain [5]:

$$P_r(A) = Y_0 A^{-\tau} e^{-\left[\left(\mu_l - \mu_g\right)A + 4\pi r_0^2 \sigma(T) A^{2/3}\right]/T} ,$$

with Y_0 a normalization constant. The graph of this functional form in the supersaturated region has a U shape. Nevertheless, in the coexistence region, $(\mu_l - \mu_g) = 0$, and $P_r(A) = Y_0 A^{-\tau} \exp[-4\pi r_0^2 \sigma(T) A^{2/3}/T]$, describing a power law times an exponential decay relevant for big masses. Finally, in the critical point $(\mu_l - \mu_g) = 0$, since liquid and gas are indistinguishable at this point, surface tension is null, $\sigma(T_c) = 0$, and hence the following distribution is expected:

$$P_r(A) = Y_0 A^{-\tau} , \tag{4}$$

which is a power law, and as such, scale free.

The exponent τ of the droplet size distribution (4), is known as the critical exponent since it is a dimensionless constant with a common value for different systems. In this case τ can be obtained from a power law fit on the mass distribution, as will be shown hereby.

The Fisher liquid droplet model (FDM) for nucleation [8] refines the probability (4) to obtain a critical liquid droplet mass distribution, normalized to the size of the system:

$$n_A = q_o A^{-\tau} \tag{5}$$

with a proportionality constant q_o that can be obtained from the first moment, $M_1 = \sum_A n_A A$, of the normalized mass distribution, (*i.e.* $M_1 = 1$). Since at the critical point $q_0 = n_A A^\tau$, the moment comes out to be $M_1 = q_o \sum_A A^{(1-\tau)} = 1$, and q_o could be obtained through the following relation: $q_o = 1/\sum_A A^{(1-\tau)}$. Notice that, since in the critical point any liquid droplet can be excluded, the sum is carried out on the clusters belonging to the gas phase.

Critical multiplicity provides a best χ^2 fit [9]. This technique is used in section 3 with data generated by the genetic algorithm describing colossal magnetoresistance and in section 4 on Molecular Dynamics.

Critical exponents are given by the following expressions [10]:

$$M_2 \sim |\epsilon|^{-\gamma} \tag{6}$$

$$A_{max} \sim |\epsilon|^{\beta} \tag{7}$$

$$n_A \sim A^{-\tau} \tag{8}$$

where $m = m_c$. And satisfy the following equation:

$$\tau = 2 + \frac{\beta}{\beta + \gamma} \tag{9}$$

Asymptotic mass distribution moments are given by:

$$m_k^{(j)} = \frac{\sum_A A^k n^{(j)}(A)}{A_{tot}} \tag{10}$$

when $k = 2$ this moment is proportional to the isothermal compressibility.

Assuming scaling in fragment size distribution, close to the critical point:

$$M_k \sim |T - T_c|^{(-1-k+\tau)/\sigma}\,, \tag{11}$$

where: $2 < \tau < 3$.

3 Colossal magnetoresistance critical exponent τ

Flory introduced percolation in the context of polymer gelation, and it has been used ever since in a great variety of techniques [11]. For a wide spectra of spin models there is a mapping of a equivalent graphical representation with a percolating transition related to the spin model phase transition [12].

In a percolation cluster the activated bonds extend from one side of the lattice to the opposite side. For infinite systems, there is a well defined "critical occupation probability" p_c, above which the probability of

finding a percolation cluster is 1, meanwhile below p_c this probability is 0. For finite lattices, this transition is soft, *i.e.* the probability of finding a percolation cluster is different of 0 for any occupation probability.

Mader *et.al.* have found thermal scaling and reducibility properties in the Ising model, obtaining a value of $\tau = 2.39$ [4]. Chayes et.al. have shown that infinite clusters scale with a critical exponent $\tau - 2 = 1/2$ and finite clusters scale with a critical exponent $\tau - 2 = 1/3$ [13]. In the percolation model the weight of a given configuration C with n bonds is given by:

$$W(C) = p^n(1-p)^{N-n} \tag{12}$$

where N is the number of vertices in the lattice. Close to the percolation threshold, the critical behavior is characterized by the following critical exponents:

$$P_\infty = 1 - \sum sn(s,p) \sim |p - p_C|^\beta \tag{13}$$

and:

$$S(P) = \sum s^2 n(s,p) \sim |p - p_C|^\gamma \tag{14}$$

The cluster distribution satisfies the following scaling relation:

$$n(s,p) = s^{-\tau} f((p - p_C)s^\sigma) \tag{15}$$

therefore in the critical point a power law is expected:

$$n(s,p) = s^{-\tau} f(0) \tag{16}$$

Starting from these three last relations, the following relations can be obtained among σ, τ and the exponents β and γ :

$$\tau = 2 + \frac{\beta}{\beta + \gamma} \tag{17}$$

$$\sigma = \frac{1}{\beta + \gamma} \tag{18}$$

In 3D, the best estimation gives $\tau = 2.18$ and $\sigma = 0.45$ [14]

Harreis and Bauer introduced a method to deal with N components percolation, finding new first order phase transitions and new empirical relations for the percolation threshold as a function of component concentration[15]. Bauer introduced percolation in the study of fragmentation [16, 17], for greater details of this computation, readers are referred to the article of Stauffer [18]. We can say that a power law arises in Fisher liquid droplet model as well as in percolation. Therefore we can pose the question whether both belong to the same universality class. In both cases, we expect to find finite size and geometry effects. Though we are dealing with systems whose physical nature is different, the fact that correlations are increased close to the critical point, allows us to consider the possibility of both systems belonging to the same universality class.

Lübeck has computed the critical exponents of the order parameter and the fluctuations of this parameter, in the case of a conservative lattice, finding that the maximum critical dimension for this gas is 4 [19].

Mari *et.al.* have performed corrections on the finite system size, for the Binder parameter computation of the 3D binomial spins Ising glass

[20]. Janssen *et.al.* have shown that for a vector magnetic system of order N, when temperature is considerably greater than the critical temperature, dynamical scaling arises in the early evolution as system is suddenly compressed up to the critical state [21].

Ying *et.al.* have found a nexus between the binding randomness and the critical universality in the Potts random binding ferromagnet with a compressed disorders trinary distribution in triangular lattices [22].

Simões *et.al.* have studied the early dynamical evolution of the bidimensional Ising model with three spin interactions in a direction, considering both Hamiltonian symmetry and boundary conditions when computing magnetization, obtaining critical exponents equal to those of four states Potts model [23].

Ying *et.al.* have studied the early dynamics and critical universality of Potts model with q=2 and q=3 in bidimensional triangular lattices, obtaining the same critical exponents as those of a square bidimensional lattice, therefore belonging to the same universality class [24].

In this study 3D configurations are randomly generated assigning spin values $S = -1, 0, 1$, with the Hamiltonian:

$$H = -J \sum_{i,j} S_i S_j - H \sum_i S_i. \tag{19}$$

Spin values are randomly changed in a site and the subsequent change of the Hamiltonian is evaluated, maintaining this change with a probability equal to:

$$p = \frac{e^{-\Delta H}/T}{1 + e^{-\Delta H/T}} \tag{20}$$

The value of τ for the colossal magnetoresistance obtained this way is equal to 2.39, cf. fig. 2. Also, we computed an exponent value $\beta = 0.38$, therefore colossal magnetoresistance belongs to the same universality class as Heavy Ions collisions, as shown in Table 1. The β value is close to those previously reported by Kudzia *et.al.* in Au emulsion fragmentation experiments [3]. Critical temperature for Heavy Ion collisions is in the range of 4.5 MeV.

4 Simulated collisions critical exponent τ

Among the signatures used to study nucleation in nuclear systems, the presence of a maximum in specific heat has been used as a signature of a phase transition for periodical systems [25]. Another signature explored is the controversial power law of the fragment size distribution, expected to appear close to the critical point of a liquid-gas phase transition [26]. In the relativistic energy range of Heavy Ion collisions, a phase transition has been identified with the onset of shock front instabilities [27] .

In Heavy Ion collisions, phase diagram is expected to show a first-order phase transition turning into a second order phase transition close to the critical point. Experimental measurements of Au+Au collision performed by GSI Collaboration, lead to a caloric curve giving evidence of phase coexistence, in agreement with predictions of statistical multifragmentation models excluding volume [28].

Other experiments performed in Bevalac extracted critical exponents and studied the dependence between the charge distribution second moment and the biggest fragment size as a function of the charged particle multiplicity. Showing that these data are consistent with a second order phase transition predicted by the percolation model [29].

L. Shi et. al. have proved that due to the dependence between asymmetry energy and density, some exceeding neutrons belonging to a high density phase must be released to the low density phase. The fragment build up in this gas phase, tends to overcome this tendency making the gas phase more similar to the liquid phase and reducing the asymmetry in the gas phase. An interesting aspect related to phase transition is the mid-rapidity region in heavy ion collisions at intermediate energy. In simulated semi-peripherical collision simulations, a neck forming region is observed that contributes to mean velocity. The low density region in contact with the high density region (projectile and target) opens the possibility for a coexistence between liquid and gas as well as phase conversion [30].

Since gases do not show first neighbor correlations, and liquids exhibit a strong two body first neighbor correlation, close to the critical point the correlations grow up to include all system particles. The behavior close to the critical point is characterized by a loss of the time and space scales, what makes that all of the critical phenomena have the same characteristics independently of system specifics.

Nevertheless, considering finite and transient systems, the most important scales are given by system size and reaction duration though critical phenomena not always exist. Hence it is important to prove the possibility of such phenomena in transient dynamical systems as those of nuclear reactions.

Concretely, models shall be used to produce similar data resembling a phase transition. These data will be dissected to extract, in the best possible way, those data produced close to the critical point. The resulting subsets will be used to extract the critical exponents. A computation of τ close to the expected values should be an indication of the plausibility of criticality in small and transient processes, such as those of heavy ion reactions

4.1 Molecular Dynamics

Heavy Ion collisions have been studied with Molecular Dynamics, a method based on Newtonian Mechanics, which is the only one able to describe without adjustable parameters phase transitions, hydrodynamic flow and far from equilibrium dynamics. The virtues of Molecular Dynamics to study nuclear collisions have been listed in the existing literature [31].

In this section, the evolution of two nuclei collision shall be modeled with MD (Fig. 5). Nucleons will be treated as point particles subject to potential forces (Pandharipande Potential). Colliding nuclei are build out as self-assembling particle clusters with an spherical geometry. Collision is simulated boosting one of these nuclei against the other, and integrating the coupled equations of motion using a Verlet algorithm.

Integration precision is ensured demanding energy conservation to a high level. Following the dynamics of thousands of collisions for different

energies, enough information is obtained in order to understand "nuclei" fragmentation and to obtain a critical exponent τ for the mass distribution of produced fragments. Nevertheless, to reach this stage, Molecular Dynamics is given in terms of point particles and must be transformed in information about fragments.

4.2 Fragment Recognition

In order to convert the particle information provided by Molecular Dynamics in terms of fragment information, an Early Cluster Recognition Algorithm is needed, such as the one that finds the "Most bound partition" of the system [32], *i.e.* the set of clusters $\{C_i\}$ whose fragment internal energies sum reaches a minimum:

$$\begin{aligned} \{C_i\} &= \underset{\{C_i\}}{\text{argmin}} \left[E_{\{C_i\}} = \textstyle\sum_i E_{int}^{C_i}\right] \\ E_{int}^{C_i} &= \sum_i [\sum_{j \in C_i} K_j^{cm} + \sum_{j,k \in C_i j \leq k} V_{j,k}] \end{aligned} \tag{21}$$

where the first sum is over the partition clusters, K_j^{cm} is the kinetic energy of particle j measured in the cluster center of mass containing particle j, and V_{ij} is the internucleonic potential. The algorithm used "simulated annealing" to find the most bound partition and is known as "Early Cluster Recognition Algorithm" ($ECRA$). It has been extensively used in several fragmentation studies [31, 32, 33], helping to discover that excited droplets breakup in a very early stage of collision evolution.

4.3 Critical exponent τ for "realistic" nuclei

A much more realistic model with MD, called "Latino Model" to reflect its Latinamerican origin, was also used. This tri-dimensional model uses binary potentials to reproduce the empirical energy and density of nuclear matter, as well as realistic effective scattering cross sections.

Nuclei used are spherical droplets with the desired number of protons and neutrons, and evolveded to their "ground state" using Molecular Dynamics. Once the spherical nuclear system is produced at a relatively high temperature, it is cooled until it reaches a self-containing state. At this moment, the confining potential is removed and the system is cooled until it reaches a reasonable binding energy.

Considering $Ni + Ni$ collisions, projectile is boosted with the desired energy, once both projectile and target have been randomly rotated. System evolution is reproduced with a Verlet algorithm, ensuring an energy conservation better than a 0.01%. The required fragment size distribution to compute τ is obtained from information provided by MD using $ECRA$, as described in equation (21). Fig. 6 shows mass spectra obtained from collisions with several energies. As can be seen, not all the shapes of these distributions correspond to a power law, *i.e.* not al the break ups happened in the critical point. In order to extract the best critical exponent, only those masses in the range of $A = 2$ to 20 nucleons were

used, *i.e.* most of the evaporation products and the projectile and target residuals were discarded.

Starting from these data, an optimal fit was obtained for each projectile energy, with τ values in the range $2 \sim 3$, and for a projectile energy of 1300 MeV, the value obtained is $\tau = 2.18$. This value coincide with the optimal critical exponent for the percolation model, as mentioned in section 3. The observed values of τ provide enough evidence to consider critical nucleation and confirm other studies of Ni+Ni central collision, where the critical behavior was detected in this projectile energy range [35].

5 Conclusions

Table 1 shows all values of τ obtained for these computations and compared with others reported elsewhere and obtained via percolation as well as with others simulated via bidimensional Molecular Dynamics with a Lennard-Jones potential [36]. Results from both MD collisions and genetic algorithm replicating colossal magnetoresistance, show that critical nucleation occurs in transient and static small fragmenting systems, and that these systems belong to the same universality class.

TABLE 1

Nucleation Model	τ **Value**
Colossal Magnetoresistance	2.38
3-D MD Collision Simulations	2.18
Cubic Lattice Percolation[36]	2.32 ± 0.02
Spherical Lattice Percolation [36]	2.20 ± 0.1
2-D MD Collision Simulations [36]	2.32 ± 0.02

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