JETIR.ORG ISSN: 2349-5162 | ESTD Year : 2014 | Monthly Issue
JOURNAL OF EMERGING TECHNOLOGIES AND INNOVATIVE RESEARCH (JETIR)
An International Scholarly Open Access, Peer-reviewed, Refereed Journal

Persistence in Kinetic Ising Model of Glass Transition on coupled map lattice.

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Abstract:
We study the persistence in the kinetic Ising model of glass transition by Frederickson and Anderson based on the kinetic Ising model with cooperative spin flip rates. We consider spin models that are standard Ising ferromagnetic ones and not the ones used for modelling spin glasses. We perform a graphical analysis to study the persistence of spins on coupled map lattice. We study Tent map and Logistic map.
Keywords: Persistence; Ising Model; Glass Transition, Coupled Map Lattice.

1. Introduction:

A majority of supercool liquids transit into a metastable glassy state if crystallization is prevented by significant cooling rates. Glass transition is experimentally characterized by relaxation periods of a few minutes or hours. The freezing in of the translational degrees of freedom causes a steady decrease in thermodynamic parameters such as compressibility, specific heat, and thermal expansion, at transition temperature T_g. This is known as the glass transformation range [1]. T_g is sometimes referred to as the "melting point of amorphous materials," and although this term may not sound scientific, it accurately describes the glass transition: polymeric materials are soft and rubbery in the highly viscous region above the T_g, whereas they are hard and brittle below it. However, there is a crucial distinction between glass transition and melting: melting represents a true first-order phase transition, whereas glassification (vitrification) is only a pseudo-second-order transition. In other words, while melting produces a discontinuity in the first derivative of Gibbs free energy (volume, entropy), glassification only causes a (pseudo) discontinuity in the second derivative (e.g., heat capacity, expansion coefficient, etc.).

The actual nature of the glass transition is not widely understood, as it is a complex process controlled by a number of parameters, including heating rate, ageing history, morphology, and molecular weight. Several theories have been proposed to explain the glass transition. It is viewed as a dynamic process in the kinetic theories. The process of "freezing" the motions of chain segments (kinetic units) results in vitrification or glassification. The initial (solid-state) transition starts at extremely low temperatures, at that point, side chain motions and localised bond bending and stretching can happen. This is called the T_γ gamma transition. The material begins to acquire some toughness as the temperature rises and other localised motions involving whole side chain and localised group movements become active. This is called the beta transition (T_β). T_g is reached when the heating continues. Large-scale coordinated motions of the polymer chains take place in this area, and a noticeable shift in characteristics is seen [3].

Leutheusser created a microscopic model of the hard-sphere fluid's glass transition. He developed a straightforward non-linear solution for the time evolution of the density correlation function that forecasts a glass transition by roughly analysing mode coupling equations. A highly cooperative spin-flip rate kinetic Ising model is the foundation of the glass transition microscopic theory. Through graphical analysis, one can derive conclusions for the spin systems that closely resemble Leutheusser's findings for hard spheres. This observation might represent the addition of a universality aspect to the glass transition [4].

2. The Ising Model:

The Ising model is intended to describe how short-range interactions, for example, between molecules in a crystal, result in long-range, correlative behaviour and, in a way, to forecast the possibility of a phase transition. The Ising model has also been used to solve issues in molecular biology, chemistry, and other fields that study the "cooperative" behaviour of complex systems [5] [6]. We assign independent variable $\sigma_i = +1$ or -1 to every lattice site i = 1,2,3, ..., N. Thus, there are only two possible outcomes at each lattice site: *up* or *down* or *occupied* or *vacant*. We create the system's Hamiltonian. The ideal and seemingly extremely severe assumption that only short-range, "nearest-neighbour" interactions and interactions between the lattice sites and an "external field" contribute to the system's energy level is the basis for the definition of the Hamiltonian for the Ising model. For each configuration $\sigma_i = (\sigma_1, \sigma_2, ..., \sigma_N)$ we have,

$$H = H(\sigma) = -\sum_{<i,j>} E\left(\sigma_i \, . \sigma_j\right) - \sum_i J\, \sigma_i$$

where the first sum is over all pairs of the lattice's nearest neighbours and the second sum is over all lattice sites. E and J are the parameters in this equation. For nearest-neighbour interactions and interactions with the external field, respectively, the parameters E and J stand for the "energies" involved. A ferromagnet has an energy level that is lower than a non-magnetized configuration because a "magnetised" configuration (where the majority of nearest-neighbour pairings have parallel moments, $\sigma_i = \sigma_j$) has a positive E. When an "external magnetic field" (represented by the parameter J) is present, the magnetic moments will seek to align with the field's direction, once more "favouring" configurations with shorter energy levels [7].

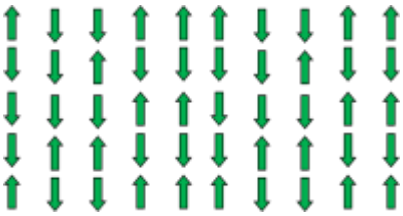

Fig. 1: The Ising model applied to a two-dimensional square lattice. Every arrow is a "spin," a magnetic moment that might point upward or downward.

3. The Model:

We study a variant of the Fredrickson-Andersen model [4] based on an extremely cooperative spin-flip rate kinetic Ising model-based microscopic theory of the glass transition. An n-spin facilitated model is defined as one for which the flip rate of the j^{th} spin is nonzero only if *n* or more near neighbours of spin *j* are in the spin-up state in spin configuration σ [4]. The update rules are as follows:

a) We choose a site randomly on the lattice.
b) If none of the neighbours is 'up' spin, the spin at this site is not changed.
c) If the site has at least one 'up' neighbour, and the site itself has an 'up' spin, it is flipped.
d) If the site has at least one 'up' neighbour and the site itself has a 'down' spin, it is flipped with probability *p*.

An all-spins "down" is the absorbing state for any value of *p*. Spins for *p*=0 will occasionally be "down." This isn't guaranteed for higher values of *p*. We investigate the system's short-time dynamics and memory retention. It is common to observe extended exponential dynamics in glassy systems. For lower values of *p*, the dynamics should be exceedingly sluggish. This will show up as autocorrelation with starting conditions. We have examined the likelihood that the initial conditions will be precisely maintained, or persistence, a stronger quantifier. In this case, it is defined as the fraction of spins that have not altered their original spin state at all until a specific period. Nonzero persistence suggests that the system preserves the initial conditions indefinitely. The decay exponent is referred to as the persistence exponent when the persistence exhibits power-law decay at the critical point. This is a non-Markovian quantity. The exponents are found to be non-trivial even in the simplest of cases [8]. In the previous work, we studied persistence in this model of glass transition and plotted the persistence P(t) vs time t on a semi-logarithmic scale [9]. We obtained a stretched exponential behaviour for all values of probabilities and respective exponents considered.

4. Coupled Map Lattice (CML)

Menon, Sinha, and Ray have extended the Ising model to coupled map Lattice (CML). They suggested that the initial variable value of a site should be represented by (+) spin if it is more than the fixed point and (−) spin if it is less than the fixed point. It is now possible to specify the persistence in a way that is similar to spin systems [10]. We simulate the system of size N= 5 x 10^4 for 10^5 time steps and averaged over 2.5x10^4 configurations. CML was originally introduced to facilitate the study of spatiotemporal chaos, i.e., chaotic dynamics in a spatially extended system [11]. In the spatially extended system, CML is the nonlinear dynamical system. It's a type of iterative system constructed from several similar functions of a single variable that are connected linearly to a network's closest neighbours. The time evolution is given by:

$$x_{t+1}(i) = (1\text{-}\varepsilon)\, f(x_t(i)) + \frac{\varepsilon}{2}\{ f(x_t(i+1)) + f(x_t(i-1))\}$$

where $x_t(i)$ is a continuous variable value x at discrete time t at lattice site i. Here ε is the coupling parameter and f(x) is the underlying map. There are a number of variants to consider, including asymmetric and linear coupling. It is simple to extend the idea to higher-dimensional lattices. Higher-dimensional maps like the Henon map have also used. Nonetheless, logistic and tent maps continue to be the most studied maps.

5. Results:

We study Coupled Tent and Logistic Map. We consider two values of probability p<1 (p=0.8 in this case) and p=1 for both the maps.

a) Tent Map

The canonical form of Tent map is:

$$x_{i+1} = f(x_i) = \mu x_i \quad \text{for} \quad x_i < \frac{1}{2} \quad \text{and}$$
$$= \mu(1 - x_i) \quad \text{for} \quad x_i \geq \frac{1}{2}$$

where μ=1.47. We study phase diagram for p=0.8 for various combination of μ (in range 1.2-2) and ε (in range 0-0.4) (See **Fig:2**). We plot the persistence exponent for various values of ε in the range [0.291:301]. We do not observe a power law in this case as seen in

Fig.3. In the case of p=1, we plot the phase diagram for various combinations of μ (in the range 1-2) and ε (in the range 0-0.45) (See **Fig:4**). We obtain power-law decay of persistence $P(t) \sim t^{-\theta}$, where θ is the decay exponent, at ε=0.314 (θ=0.122 as seen in **Fig:5**).

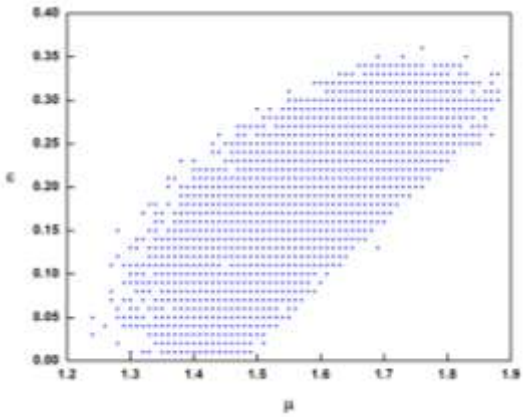

Fig.2: Shows phase diagram for p=0.8 for several combinations of μ and ε in case of coupled tent map.

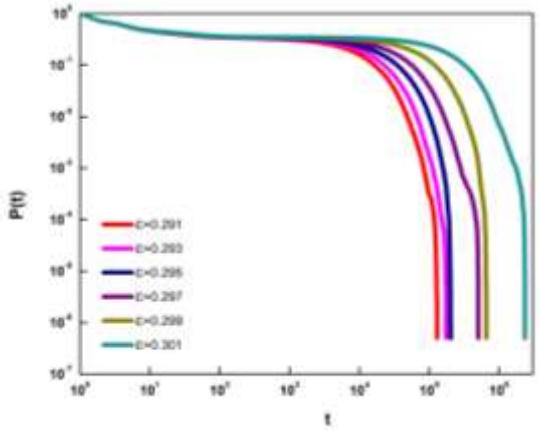

Fig.3: Shows the time evolution of persistence P(t) on log-log scale for several values of ε in the range [0.291:301] for coupled tent map.

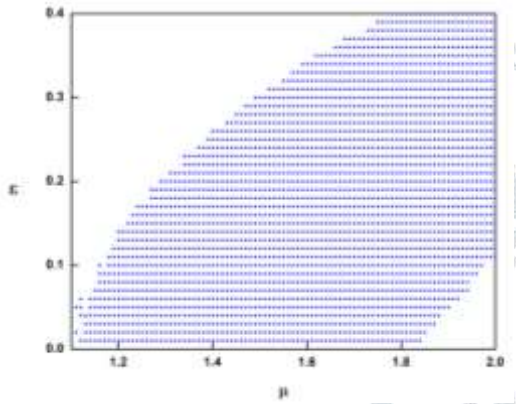

Fig.4: Shows phase diagram for p=1 for several combinations of μ and ε in case of coupled tent map.

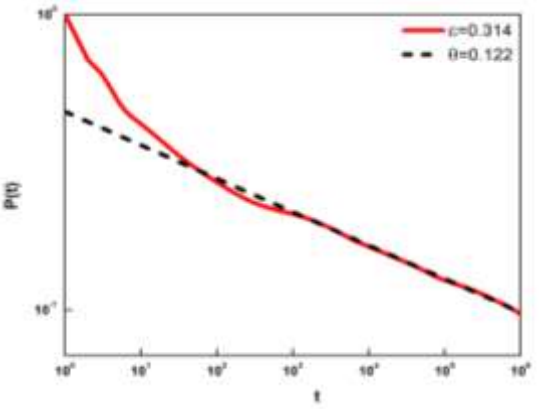

Fig.5: Shows the time evolution of persistence P(t) on log-log scale. We obtain power law at ε=0.314. The decay exponent θ= 0.122 for coupled tent map.

b) Logistic map

The canonical form of Logistic map is:

$$x_{i+1} = f(x_i) = \mu x_i(1 - x_i)$$

where μ=3.474. We study the phase diagram for p=0.8 for various combinations of μ (in the range 3-4) and ε (in the range 0-0.3) (See **Fig:6**). We plot time variation of the persistence on log-log scale. We obtain power law $P(t) \sim t^{-\theta}$ at ε=0.168. θ=0.37 as shown on **Fig.7.** In case of p=1, we plot the phase diagram for various combination of μ (in range 3-4) and ε (in range 0-0.3) (See **Fig:8**). We do not obtain power law in the case as seen in **Fig:9**.

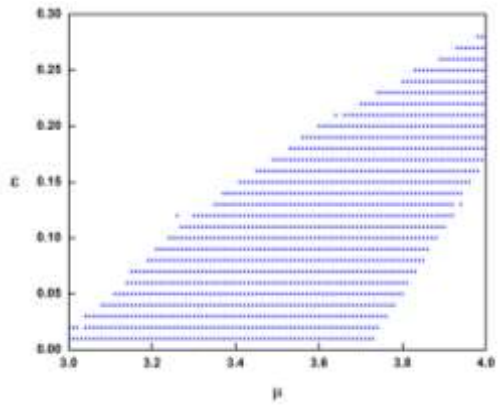

Fig.6: Shows phase diagram for p=0.8 for several combinations of μ and ε in case of coupled Logistic map.

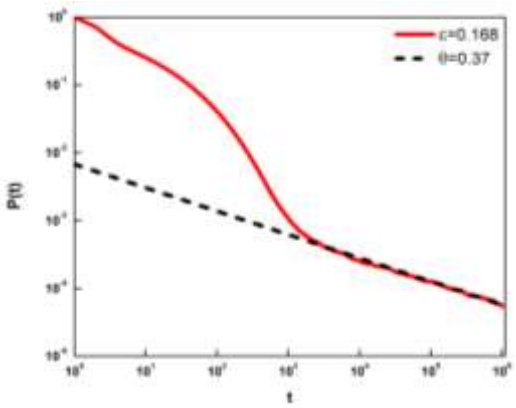

Fig.7: Shows the time evolution of persistence P(t) on log-log scale. We obtain power law at ε=0.168. The decay exponent is θ= 0.37 in the case of coupled Logistic maps.

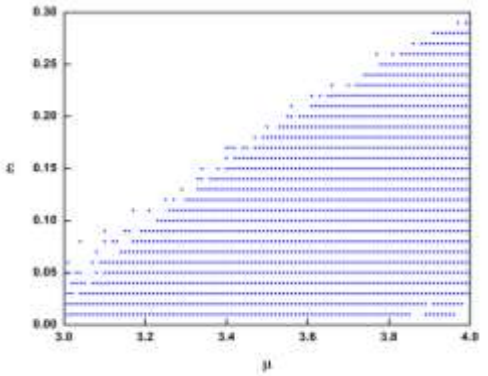

Fig.8: Shows phase diagram for p=1 for several combinations of μ and ε in case of coupled Logistic map.

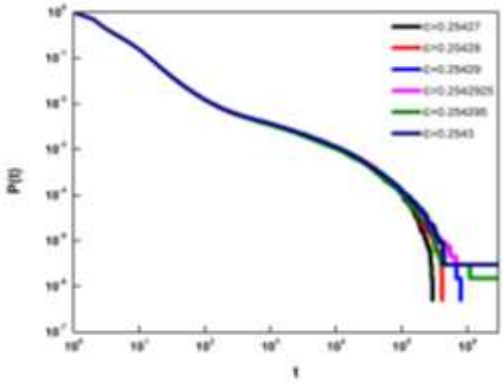

Fig.9: Shows the time evolution of persistence P(t) on log-log scale with ε in the range [0.25427:2543].

6. Summary:

Fredrickson and Andersen introduced the kinetic Ising model of glass transition [4]. In our work, we make a study of the existence of persistence in this model on coupled map lattice where the underlying maps are Tent map and Logistic map. Our function consists of a Hamiltonian that comprises the sum over all pairs of the lattice's nearest neighbours along with the sum over all lattice sites. We consider two cases, p=0.8 and p=1 for the coupled tent map and coupled logistic map. We plot phase diagrams for all of these. For the tent map (p=1) and logistic map (p=0.8) we get a clean power law with exponents θ=0.122 and θ=0.37 respectively.

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