Metastable states, relaxation times and free-energy barriers in finite dimensional glassy systems

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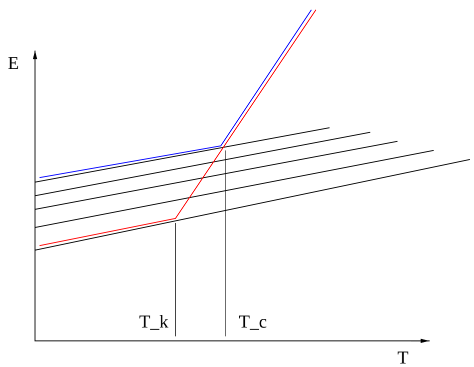
- Introduction
- Metastable states: Lebowitz-Penrose theory
- Disordered Kac model: Dynamics in the Kac limit and metastability
- Relaxation time and Free-energy barrier

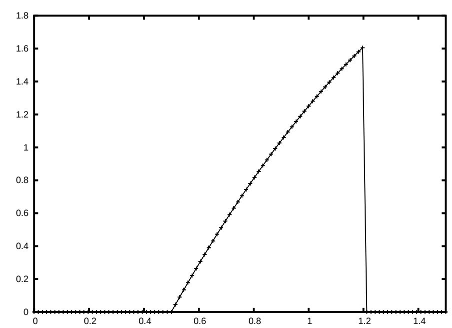
The Problem

Relaxation in Supercooled Liquids

Approximated liquid theories (Mode Coupling Theory) and Mean-field theory (Random 1^{st} order transition 1RSB) [long range p-spin model]:

- Spurious Dynamical Ergodicity Breaking at T_C.
- Power law divergence $\tau \sim |T - T_c|^{-\alpha}$ Infinite life metastable states below T_c.





Two transitions: 1) T_c broken ergodicity transition

- # of ergodic components $\mathcal{N} \sim \exp(N\Sigma(T))$

2) T_k ($< T_c$) entropy crisis transition $\Sigma(T_k) = 0$

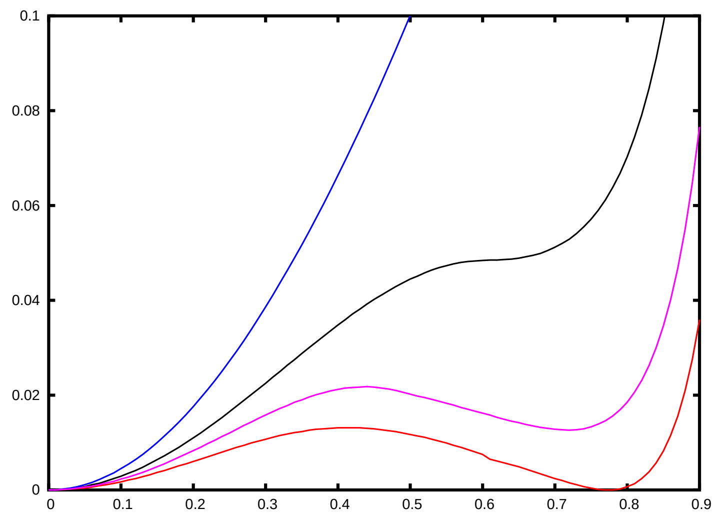
Effective potential

$\mathbf{S^0}$ reference config. chosen with canonical probability $e^{-\beta H(\mathbf{S^0})}$

Order parameter: Overlap

$$q(\mathbf{S},\mathbf{S}') = \frac{1}{N}\sum_i S_i, S_i'$$

$$V(q) = \frac{-T}{N} E_J E_{\mathbf{S_0}} \log \frac{1}{Z}\sum_{\mathbf{S}} e^{-\beta H(\mathbf{S})}\delta(q(\mathbf{S},\mathbf{S^0})-q)$$



$$V(q_{EA}) - V(0) = T\Sigma$$

Non perturbative approach Random 1^{st} order transition

- Kirkpatrick-Thirumalai-Wolynes entropic droplets and mosaic state
- Parisi: effective potential
- Biroli-Bouchaud: mosaic state "explained"
- SF Instanton Calculation of free-energy barrier long-but-finite range (Kac)

Description of supercooled state as Locally mean field-like and glassy; liquid on a large scale **Biroli-Bouchaud argument**

Fix the system at a generic equilibrium configuration outside a ball of radius R.

Configurational entropy as the bulk driving force to ergodicity restoration.

$$\Delta F = -T\Sigma R^d + \Gamma R^\theta$$

Strong correlations for $R > R^*$, $R^* \sim (\Gamma/\Sigma)^{1/(d-\theta)}$ typical "mosaic length"

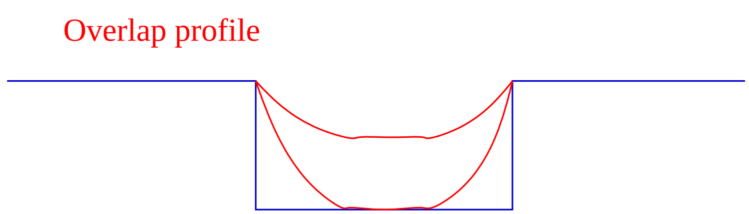
$$\Delta F^* \sim \Gamma^{\frac{d+\theta}{d-\theta}}/\Sigma^{\frac{\theta}{d-\theta}} \sim C/(T-T_K)^{\frac{\theta}{d-\theta}}$$

A first principle approach

Quenched Potential

τ reference, generic equilibrium state.

$$V_Q(\{q_x\}) = -\frac{T}{N} E \frac{1}{Z} \sum_{\tau} e^{-\beta H(\tau)} \log \left[\frac{1}{Z} \sum_{\sigma} e^{-\beta H(\sigma)} \delta\left(q_x(\sigma,\tau) - q_x \right) \right].$$



Study as a function of R if the system remain close to the reference state.

R^* critical radius in a nucleation like theory.

Variant of the replica method to evaluate V_Q.

Computation in long-but-finite range model (Kac).

Finite surface tension $\sigma \rightarrow \theta = d - 1$

No explicit connection between free-energy barrier and relaxation time.

Goal: provide this connection

- Describe metastable states in disordered systems
- Characterize typical liquid configuration as metastable states
- use quasi-equilibrium to relate relaxation time to free-energy barrier
- Kac models: close (but not too much) to Mean Field

Systems with long-but-finite interaction range (Kac 1959)

$$H = -\sum_{i<j} \gamma^d \phi(\gamma|i-j|) S_i S_j - h \sum_i S_i$$

- L System size
- γ^{-1} interaction range; $\approx \gamma^{-d}$ interactions per spin each of strength γ^d

Classical models of Mathematical Statistical Physics

Emphasize the role if the interaction range in the Mean Field pathologies

$$\gamma = 1/L \quad \text{Mean Field}$$

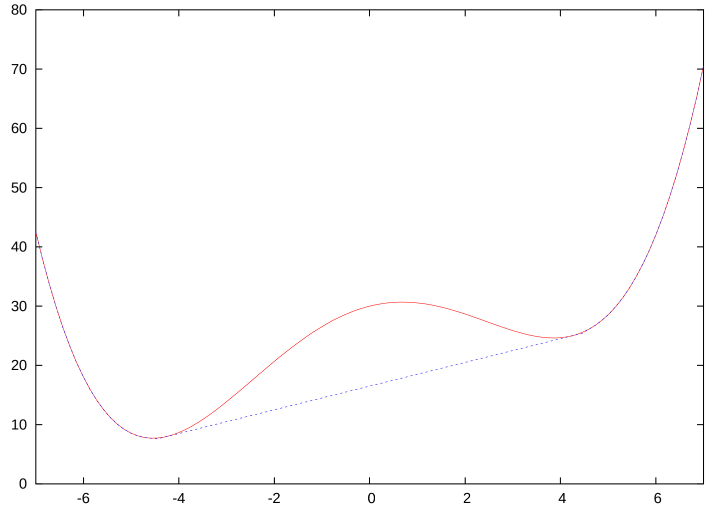
$$\gamma > 0 \quad \text{Finite Range}$$

Kac limit: $\gamma \to 0$ After the thermodynamic limit $L \to \infty$.

Lebowitz-Penrose theorem (1966): For all D, Mean-Field free-energy + Maxwell construction

Eliminate most evident pathologies

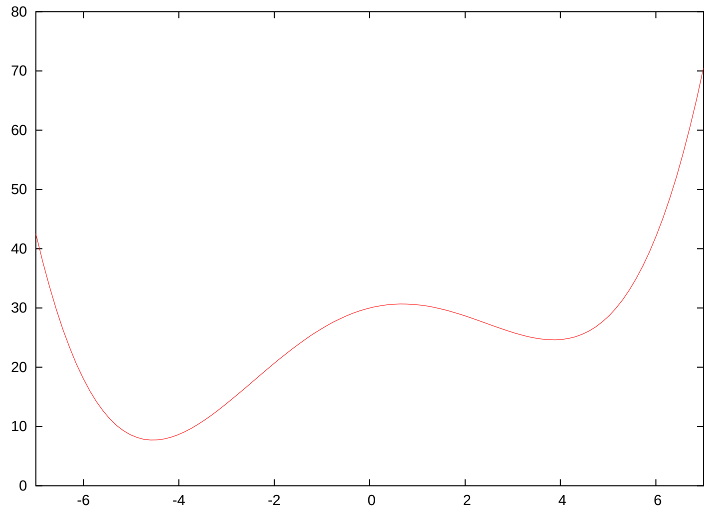
Interfaces restore convexity of free-energy



Ferromagnets: rigorous (asymptotic) expansion around Mean Field

Lebowitz-Penrose Theory of Metastability

Systems with first order transition



Secondary minimum at m^* metastable state

For finite range interaction the life time is finite

Characterization of Metastable States

- Homogeneous states where thermodynamics holds
- "long" life time
- even longer return time(no return)

Kac model again

$$H = -\sum_{i<j} \gamma^d \phi(\gamma|i-j|) S_i S_j - h \sum_i S_i$$

- L System size
- γ^{-1} interaction range
- ℓ homogeneity length

$$\log L << \ell << \gamma^{-1} << L$$

Partition space in boxes B_x of linear size ℓ

Consider $I = [m_-, 1] \ni m^*$, $\quad m_x(\mathbf{S}) = \frac{1}{\ell^d} \sum_{i \in B_x} S_i$

$$R = \{\mathbf{S} | m_x(\mathbf{S}) \in I\}$$

The Metastable state is

$$\mu(\mathbf{S}) = \frac{1}{Z_R} e^{-\beta H(\mathbf{S})} 1_R(\mathbf{S})$$

Relaxation rate

$$\lambda = \sum_{\mathbf{S}' \notin R} \sum_{\mathbf{S} \in R} \mu(\mathbf{S}) W(\mathbf{S} \to \mathbf{S}')$$

Local Dynamics if $\mathbf{S}' \notin R$ and $W \neq 0$ then $\mathbf{S} \in \partial R$

$$\partial R = \{\mathbf{S} \in R | \exists x_0 \quad m_{x_0}(\mathbf{S}) = m_-\}$$

$$\lambda \leq \sum_{\mathbf{S} \in \partial R} \mu(\mathbf{S}) = \frac{Z_{\partial R}}{Z_R} = e^{-\beta \Delta F}$$

Lebowitz-Penrose estimate $\Delta F > C \ell^d$

Self-consistent determination of m_- as the value that maximizes ΔF.

Nucleation theory, instantons... $\Delta F \sim \gamma^{-d}$.

Return rate $Z_R / Z \sim \exp(-A L^d) << \lambda$

The Model

Λ d-Cube of size L

$$H_{\gamma,L,J} = -\frac{1}{p!} \sum_{i_1,\dots i_p \in \Lambda} J_{i_1,\dots i_p} S_{i_1} \dots S_{i_p}$$

$$E(J^2_{i_1,\dots,i_p}) = \gamma^{pd} \sum_{k \in \Lambda} \psi(\gamma|i_1 - k|)\dots\psi(\gamma|i_p - k|)$$

$$\int dx\ \psi(x) = 1$$

γ^{-1} interaction range MF for $\gamma^{-1} = L$.

Local Spherical Constraint: length ℓ. Partition of Λ in boxes B_x of linear size ℓ

$$\sum_{i \in B_x} S_i^2 = \ell^d$$

Thermodynamics in the Kac limit

(SF and F.L. Toninelli)

$\gamma \to 0$ *after* $L \to \infty$

Theorem 1 *For all dimension D, temperatures T magnetic field h, and p even, the infinite volume free-energy of the Kac model tends to the free-energy of the mean-field p-spin model in the Kac limit $\gamma \to 0$.*

Theorem 2 *The local order parameter (local overlap probability distribution on scales γ^{-1}) tends to the MF order parameter for $\gamma \to 0$.*

Equilibrium Dynamics

$$1 << \ell << \gamma^{-1} << L$$

$$\ell >> \log L$$

Suppress events with a prob. $\sim L^d \exp(-a\ell^d)$

e.g. $\ell = \gamma^{-\delta}$, $0 < \delta < 1$

Langevin dynamics for spherical spins

Analysis of Correlation function $C_x(t) = \frac{1}{\ell^d} \sum_{i \in B_x} S_i(t) S_i(0)$

$$S(0) \to \exp(-\beta H(S_0))$$

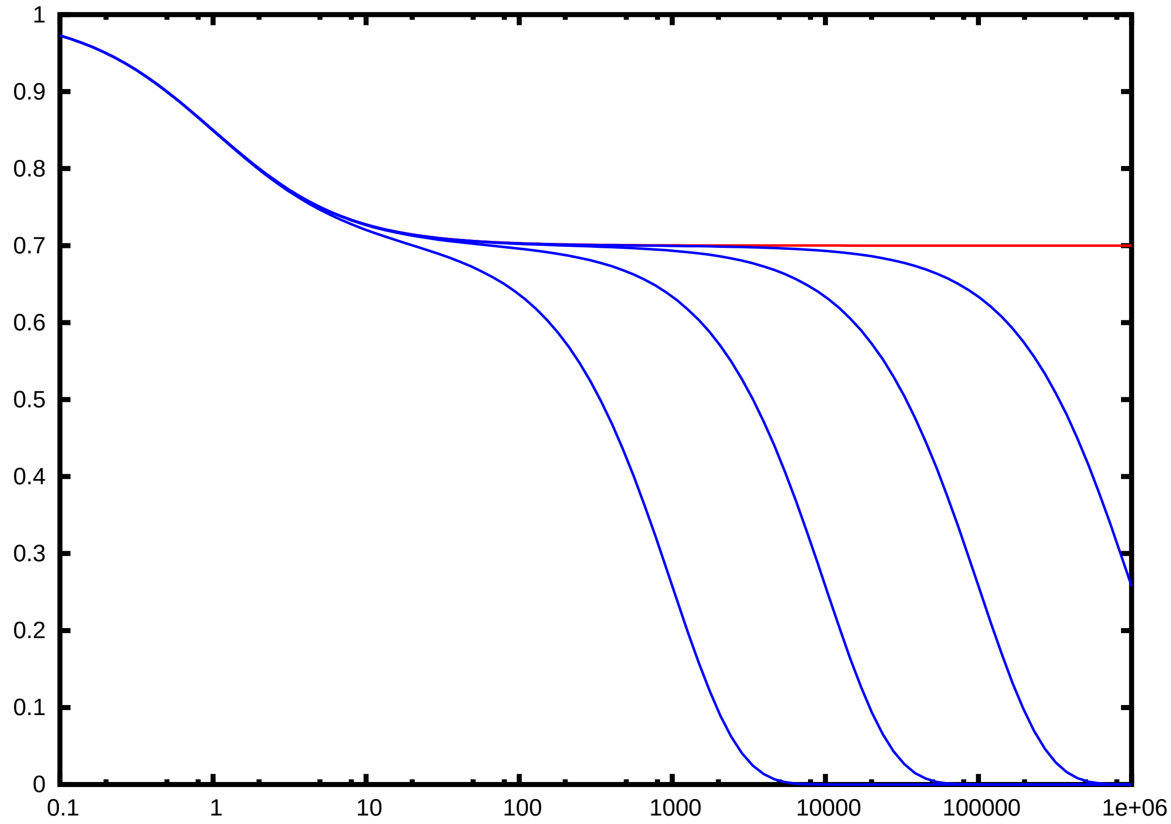
Kac limit: $L \to \infty$, $\gamma \to 0$ for $t < \infty$ $C_x(t) \to C(t)$ homogeneous in space and verifies the MF equation

$$\frac{dC(t)}{dt} = -TC(t) + \frac{p\beta}{2} \int_0^t ds\, C^{p-1}(t-s) \frac{dC(s)}{ds}.$$

MSR or dynamical cavity show that γ^{-d} plays the role of N in the usual MF derivation.

Ergodicity breaking for $\gamma \to 0$, ergodicity for any $\gamma > 0$

- $\lim_{\gamma \to 0} C_x^\gamma(t) = C(t) \to q_{EA}$ ($t \to \infty$ equilibrium in one state)
- $\lim_{t \to \infty} C_x^\gamma(t) = 0 = \ Equilibrium \ \ value$ ($\gamma > 0$ ergodicity)



Time scale separation: $\tau_\gamma^{erg} >> \tau_{MF}$

Metastable States

$I = [q_-, 1] \ni q_{EA}$

$\tau = S(0)$ initial state of the dynamics Typical equil. configuration

$q_n(\sigma, \tau) = \frac{1}{\ell^d} \sum_{i \in B_n} \sigma_i \tau_i$

$$R = \{\sigma | q_n(\sigma, \tau) \in I\}$$

Previous discussion: Equilibrium in R before relaxing further

Lebowitz-Penrose characterization

- Homogeneities and thermodynamics
- large time to escape
- huge time to come back

Dynamics dominated by Metastable states.

Relaxation rate

Initially

$$\mu(\sigma) = \frac{1}{Z_R} e^{-\beta H(\sigma)} 1_R(\sigma)$$

Escape rate

$$\lambda = \sum_{\sigma' \in R; \sigma \notin R} W(\sigma \leftarrow \sigma') \mu(\sigma') \leq \sum_{\sigma' \in \partial R} \mu(\sigma') = Z_{\partial R} / Z_R$$

$$\partial R = \{\sigma \in R \mid \exists\, n,\ q_n(\sigma, \tau) = q_-\}$$

Typical value of $\lambda = \lambda(\tau, J)$:

$$\log \lambda_{typ} = E_J E_\tau (\log Z_{\partial R} - \log Z_R)$$

Starting point for a purely statical computation of the relaxation rate.

Replica method evaluation of $E_J E_\tau Z_R$ and $E_J E_\tau Z_{\partial R}$

Results

- Precise definition of metastable configurations
- Identification typical liquid configuration as metastable states
- Shown that Lebowitz-Penrose criteria are respected
- Identified a free-energy barrier related to the relaxation time.

Q: is this free-energy barrier the one that appear to describe the mosaic state ?

Free-energy barrier

By the previous discussion one has that Z_R is dominated by the constant profile $q_x = q_{EA} \quad \forall\, x$.

$$Z_R \approx e^{L^d V_{MF}(q_{EA})}$$

Consider for finite L, the constrained free-energy $W_\tau[q_x]$ defined by

$$e^{-\frac{\beta}{\gamma^d} W_\tau[q_x]} = \sum_S e^{-\beta H(S)} \prod_x \delta(q_x(S,\tau) - q_x)$$

$$V[q_x] = E_J E_\tau \left(W_\tau[q_x]\right)$$

then

$$Z_{\partial R} = \sum_{x_0} \int_{q_x \in I;\ \ q_{x_0} = q_-} \mathcal{D}q\; e^{-\frac{\beta}{\gamma^d} W_\tau[q_x]}$$

One can expect that a single $J-\tau$ dependent profile dominates each term of the sum.

Is the knowledge of $V[q_x]$ enough ?

Previous calculations aimed to compute:

$$Z_{\partial R} \approx \left(\frac{L}{\ell}\right)^d \int_{q_x \in I;\ \ q_0 = q_-} \mathcal{D}q\ e^{-\frac{\beta}{\gamma^d} V[q_x]}$$

Nucleation theory

$$\Delta F = R^d T \Sigma - \nu R^{d-1}$$

Istanton calculation based on V give: $\nu(T_K) > 0$

$$\Delta F \approx \frac{\nu^d}{\gamma^d \Sigma^{d-1}} \approx \frac{1}{\gamma^d (T - T_K)^{d-1}}$$

Strong hypothesis

Almost all sites x_0 give similar contributions and these dominate the relaxation rate. In that case, denote q_x^* the profile maximizing $V[q_x]$

$$\lambda = \left(\frac{L}{\ell}\right)^d e^{-\frac{\beta}{\gamma^d}(V[q_x^*]-V[q_x=q_{EA}])}.$$

The incipient spatial heterogeneities on a scale γ^{-1} responsible for relaxation, have for almost all J, τ equal probability of appearing in any point of space.

Is this hypothesis true ?

Compute directly $Z_{\partial R}$ (e.g. with replicas) and see.

Possible way of changing the annoying $d-1$ exponent in the Vogel-Fulcher like relation.