Slow dynamics in systems with long-range interactions

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Systems with long range interactions

two-body interaction

 $v(r) \propto rac{1}{r^{d+\sigma}}$ in d dimensions

for $\sigma < 0$

 $E \propto V R^{-\sigma} \propto V^{1-\sigma/d}$

and the energy is not extensive

| self gravitating system | s (1/r) | σ=-2 |
|-------------------------|-----------|------|
| ferromagnets | $(1/r^3)$ | σ=0 |
| 2d vortices | log(r) | σ=-2 |

driven systems out of thermal equilibrium

Free Energy:
$$F = E - TS$$

since
$$E \propto V^{1-\sigma/d}$$
, $S \propto V$

S << E the entropy may be neglected in the thermodynamic limit.

In finite systems, although E>>S, if T is high enough E may be comparable to TS, and the full free energy need to be considered. (Self gravitating systems, e.g. globular clusters)

Globular clusters are gravitationally bound concentrations of approximately ten thousand to one million stars, spread over a volume of several tens to about 200 light years in diameter.



For a typical cluster (M2) N=150,000 stars R= 175 light years F = E - TS $M = 2 \cdot 10^{30}$ Kg

$$E \sim \frac{GN^2M^2}{R} \quad S \sim k_BN$$
$$\frac{E}{S} \sim \frac{1}{k_B} \frac{GNM^2}{R} \sim 10^{61} \text{ K}$$

 $\frac{1}{2}k_B T = \frac{1}{3}Mv^2 \qquad v \approx 10 \text{ km/sec}$

Thus although $E \propto V^{5/3}$ and $S \propto V$ E may be comparable to TS One may implement the large T limit by rescaling the Hamiltonian

$$H \to V^{\sigma/d} H \implies E \propto V$$

Ferromagnetic dipolar systems

$$v(r) = \frac{s_i s_j}{r^3} - 3 \frac{(s_i r)(s_j r)}{r^5} \qquad \sigma = 0$$
$$H \to H - \frac{D}{V} M^2 \qquad \text{(for ellipsoidal samples)}$$

D is the shape dependent demagnetization factor

$$H \to H - \frac{J}{N} \left(\sum_{i=1}^{N} S_i\right)^2$$

Models of this type, although they look extensive, are non-additive.

 $v(r) \propto \frac{1}{r^{d+\sigma}}$

For σ >0 the energy is additive, however long-range effects show up in the thermodynamic functions for $0<\sigma\leq 2$

- $0 < \sigma \le 2$ weak long-range interactions
- $\sigma < 0$ strong long-range interactions

interactions with σ >0, although additive, affect the thermodynamic properties of the system



Long-range interactions (whether weak or strong) tend to suppress fluctuations and enhance long-range order.

For example while there is no long-range order in d=1 in systems with short range interactions, it can take place when long range interactions are present.

Strong long-range interactions: σ<0 features which result from non-additivity

Thermodynamics

- Negative specific heat in microcanonical ensemble
- Inequivalence of microcanonical (MCE) and canonical (CE) ensembles
- Temperature discontinuity in MCE
- Similarly, inequivalence between CE and GCE, discontinuity in chemical potential in CE.

Dynamics

Slow dynamics, diverging relaxation time

Breaking of ergodicity in microcanonical ensemble

- Systems with short range interactions- S is concave
- On the other hand in systems with long range interactions (non-additive), in the region E₁<E<E₂



$$S_0 = xS_1 + (1-x)S_2$$

 $E_0 \neq xE_1 + (1-x)E_2$

The entropy may thus follow the homogeneous system curve, the entropy is not concave. and the microcanonical specific heat becomes negative $C_V < 0$.

compared with canonical ensemble where

 $T^2 C_V = \langle E^2 \rangle - \langle E \rangle^2 \ge 0$

Ising model with long- and short-range interactions.

$$H = -\frac{J}{2N} \left(\sum_{i=1}^{N} S_{i}\right)^{2} - \frac{K}{2} \sum_{i=1}^{N} \left(S_{i} S_{i+1} - 1\right)$$

d=1 dimensional geometry, ferromagnetic long range interaction J>0

The model has been analyzed within the canonical ensemble Nagel (1970), Kardar (1983)



-1/2

0

K/J

Canonical (T,K) phase diagram



Microcanonical analysis

$$H = -\frac{J}{2N} (\sum_{i=1}^{N} S_i)^2 - \frac{K}{2} \sum_{i=1}^{N} (S_i S_{i+1} - 1)$$
$$E = -\frac{J}{2N} M^2 + KU$$

 $M = N_{+} - N_{-}$ $N = N_{+} + N_{-}$

U = number of broken bonds in a configuration

U/2 (+) segments U/2 (-) segments

DM, Ruffo, Schreiber (2005)

The number of ways to divide N_{+} spins into U/2 groups

$$\binom{N_+ - 1}{U/2 - 1}$$

Number of microstates with N+ , N_{-} and U:

$$\Omega(N_{+}, N_{-}, U) \approx \binom{N_{+} - 1}{U/2 - 1} \binom{N_{-} - 1}{U/2 - 1}$$

 $M = N_{+} - N_{-}$ $N = N_{+} + N_{-}$

s=S/N, $\mathcal{E}=E/N$, m=M/N, u=U/N

$$s(u,m) = \frac{1}{N} \ln \Omega =$$

$$\frac{1}{2} (1+m) \ln(1+m) + \frac{1}{2} (1-m) \ln(1-m) - u \ln u$$

$$-\frac{1}{2} (1+m-u) \ln(1+m-u) - \frac{1}{2} (1-m-u) \ln(1-m-u)$$

but
$$\mathcal{E} = -\frac{J}{2}m^2 + Ku$$

$$s(u,m) \rightarrow s(\varepsilon,m)$$

Maximize $s(\varepsilon, m)$ to get $m(\varepsilon)$

 $s(\varepsilon) = s(\varepsilon, m(\varepsilon))$ $1/T = \partial s / \partial \varepsilon$



 $1/T = \partial s / \partial \varepsilon$

In a 1st order transition there is a discontinuity in T, and thus there is a T region which is not accessible.





Microcanonical phase diagram



canonical

microcanonical



The two phase diagrams differ in the 1st order region of the canonical diagram

Ruffo, Schreiber, Mukamel (2005)



possible phase diagram - I (critical end point)



possible phase diagram - II

microcanonical

canonical

Dynamics

- Systems with long range interactions exhibit slow relaxation processes.
- This may result in quasi-stationary states (long lived non-equilibrium states whose relaxation time to the equilibrium state diverges with the system size).
- Non-additivity may facilitate breaking of ergodicity which could lead to trapping of systems in non-Equilibrium states.

Slow Relaxation

In systems with short range interaction, typically the relaxation time from an unstable (or metastable) state to a stable one is finite (independent of the system size).



free energy gain of a droplet



 $R_c = \sigma / \Delta f$

critical radius above which the droplet grows.

Since the critical radius is finite, the relaxation time scale in systems with short range interactions is finite.

This is not the case in systems with long range interactions. relaxation processes are typically slow, with relaxation time which grows with the system size.

- In the case of the Ising model, the relaxation time is found to grow as logN.
- In other cases it is found to grow with a power of N.

This results in non-equilibrium, quasi-stationary states.

Microcanonical Monte Carlo Ising dynamics:

$$H = -\frac{J}{2N} \left(\sum_{i=1}^{N} S_i\right)^2 - \frac{K}{2} \sum_{i=1}^{N} \left(S_i S_{i+1} - 1\right)$$

Microcanonical Monte Carlo dynamics: Creutz (1983)

In this algorithm one probes the microstates of the system with energy $\leq E$

This is implemented by adding an auxiliary variable, called a demon such that

$$E_{S} + E_{D} = E$$

system's energy E_s demon's energy $E_D \ge 0$

Creutz algorithm:

- 1. Start with $E_s = E$ $E_D = 0$
- 2. Attempt to flip a spin:

accept the move if energy decreases and give the excess energy to the demon.

$$E_s \rightarrow E_s - \Delta E \qquad E_D \rightarrow E_D + \Delta E , \quad \Delta E > 0$$

if energy increases, take the needed energy from the demon. Reject the move if the demon does not have the needed energy.

$$E_S \rightarrow E_S + \Delta E$$
, $E_D \rightarrow E_D - \Delta E > 0$

$$P(E_D) \propto e^{-\beta E_D} \quad \beta = 1/k_B T$$

Yields the caloric curve T(E).



N=400, K=-0.35 E/N=-0.2416 To second order in E_D the demon distribution is

$$P(E_D) \propto e^{-\beta E_D - E_D^2/2C_V T^2}$$

$$\begin{split} S(E_S) &= S(E) - \frac{\partial S}{\partial E} E_D + \frac{1}{2} \frac{\partial^2 S}{\partial E^2} E_D^2 \qquad E_S = E - E_D \\ \frac{\partial S}{\partial E} &= \frac{1}{T} \ , \ \ \frac{\partial^2 S}{\partial E^2} = -\frac{1}{T^2 C_V} \end{split}$$

And it looks as if it is unstable for $C_V < 0$ (particularly near the microcanonical tricritical point where C_V vanishes).

However the distribution is stable as long as the entropy increases with E (namely T>0) since the next to leading term is of order 1/N.



Relaxation of a state with a local minimum of the entropy (thermodynamically unstable)



One would expect the relaxation time of the m=0 state to remain finite for large systems (as is the case of systems with short range interactions..



M=0 is a minimum of the entropy K=-0.25 $\ \mathcal{E}=-0.2$

 $\tau \propto \ln N$

One may understand this result by considering the following Langevin equation for m:

$$\frac{\partial m}{\partial t} = \frac{\partial s}{\partial m} + \xi(t) \qquad <\xi(t)\xi(t') >= D\delta(t-t') \qquad \text{With} \quad D\sim 1/N$$

Why $D\sim 1/N$?

each time unit consists of N flipping attempts

$$\frac{\Delta M}{\Delta t} = \frac{\Delta S}{\Delta M} + \frac{\sqrt{N}}{\Delta t} \zeta \qquad \Delta t \propto N$$

 $\sqrt{N}\zeta$ - sum of N random numbers ±1

$$\frac{1}{\sqrt{N}}\zeta = \xi$$

$$\frac{\partial m}{\partial t} = \frac{\partial s}{\partial m} + \xi(t) \qquad <\xi(t)\xi(t') >= D\delta(t-t') \qquad \text{With} \quad D\sim 1/N$$

$$s(m) = am^2 - bm^4 \qquad a, b > 0$$



Fokker-Planck Equation:

 $P(m,t) \qquad P(m,t=0) = \delta(m)$ $\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial m^2} - \frac{\partial}{\partial m} \left(\frac{\partial s}{\partial m}P\right)$

This is the dynamics of a particle moving in a double well potential V(m)=-s(m), with T~1/N starting at m=0.

$$\frac{\partial P(m,t)}{\partial t} = D \frac{\partial^2 P}{\partial m^2} - \frac{\partial}{\partial m} \left(\frac{-\partial V(m)}{\partial m} P \right)$$



Taking for simplicity $s(m) \sim am^2$, a > 0, the problem becomes that of a particle moving in a potential V(m) $\sim -am^2$ at temperature T $\sim D\sim 1/N$

$$\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial m^2} - a \frac{\partial}{\partial m} (mP)$$

This equation yields at large t $P(m,t) \propto \exp\left(-\frac{am^2 e^{-2at}}{2D}\right)$
Since D~1/N the width of the distribution is $< m^2 >= e^{2at} / aN$

$$e^{2a\tau}/N \approx 1$$
 $\tau \propto \ln N$

The anisotropic XY model

slow relaxation with algebraically increasing time scale

$$H = \frac{1}{2} \sum_{i=1}^{N} p_i^2 + \frac{1}{2N} \sum_{i,j=1}^{N} (1 - \cos(\theta_i - \theta_j)) + W \sum_{i=1}^{N} \cos^2 \theta_i$$

with Hamiltonian, deterministic dynamics

$$\frac{d\theta_i}{dt} = p_i$$

$$\frac{dp_i}{dt} = -m_x \sin \theta_i + m_y \cos \theta_i + W \sin 2\theta_i$$

$$m_x = \frac{1}{N} \sum \cos(\theta_j) \quad , \quad m_y = \frac{1}{N} \sum \sin(\theta_j)$$

Yamaguchi, Barre, Bouchet, Dauxois, Ruffo (2004) Jain, Bouchet, Mukamel, J. Stat. Mech. (2007)

Phase diagram



Distribution function $f(\theta, p, t)$

Vlasov equation

$$\frac{\partial f}{\partial t} + p \frac{\partial f}{\partial \theta} - \frac{\partial V}{\partial \theta} \frac{\partial f}{\partial p} = 0 \qquad (\mathsf{N} \to \infty)$$

$$V(\theta,t) = \int dp' \int_{-\pi}^{\pi} d\theta' (1 - \cos(\theta - \theta')) f(\theta', p', t) + W \cos^2 \theta$$

initial distribution (for the homogeneous case)

$$f_0(p) = \frac{1}{2p_0}$$
 $-p_0 \le p \le p_0$ uniform in θ



$$f_0(\theta, p) = \frac{1}{4\pi p_0} \qquad -p_0 \le p \le p_0 \qquad \text{uniform in } p, \theta$$

Vlasov equation
$$\frac{\partial f}{\partial t} + p \frac{\partial f}{\partial \theta} - \frac{\partial V}{\partial \theta} \frac{\partial f}{\partial p} = 0$$

Linear stability analysis:

$$f(\theta, p, t) = \frac{1}{2\pi} f_0(p) + \lambda f_1(\theta, p, t) \qquad \lambda \propto \frac{1}{\sqrt{N}}$$

 $\varepsilon^*(W) < \varepsilon < \varepsilon_c(W)$ linearly stable, power law relaxation time

 $\mathcal{E} < \mathcal{E}^{*}(W)$ linearly unstable, logarithmic relaxation time

$$\varepsilon_{c}(W=0) = 3/4$$
 $\varepsilon^{*}(W=0) = 7/12$



Dynamical phase diagram of the anisotropic XY model Relaxation of the thermodynamically unstable m=0 state

One would expect the relaxation time of the m=0 state to remain finite for large systems (as is the case of systems with short range interactions.



Yamaguchi, Barre, Bouchet, Dauxois, Ruffo (2004) Jain, Bouchet, Mukamel, J. Stat. Mech. (2007)

Relaxation of the quasi-stationary m=0 state:



Relaxation in the presence of stochastic dynamical processes. Baldovin, Orlandini, Chavanis; Gupta, Mukamel

HMF model with mixed dynamics:

- 1. the model evolves by the usual deterministic dynamics for some time interval.
- This evolution is interrupted with probability r (typically small) and microcanonical Monte Carlo sweep is carried out.

stochastic dynamics



deterministic HMF dynamics



mixed dynamics

$$m \propto \frac{1}{\sqrt{N}} e^{rt + (1-r)t/N^{\gamma}}$$

$$m \propto \frac{1}{\sqrt{N}} e^{rt + (1-r)t/N^{\gamma}}$$

for m~1 $t \propto \ln N \left(\frac{1}{r} + N^{\gamma}\right)$
 $t \propto \frac{1}{r} \ln N f(rN^{\gamma})$ scaling form



Breaking of Ergodicity in Microcanonical dynamics.

Borgonovi, Celardo, Maianti, Pedersoli (2004); Mukamel, Ruffo, Schreiber (2005).

Systems with short range interactions are defined on a convex region of their extensive parameter space.



If there are two microstates with magnetizations M_1 and M_2 Then there are microstates corresponding to any magnetization $M_1 < M < M_2$ This is not correct for systems with long range interactions where the domain over which the model is defined need not be convex.



Ising model with long and short range interactions

$$H = -\frac{J}{2N} (\sum_{i=1}^{N} S_i)^2 - \frac{K}{2} \sum_{i=1}^{N} (S_i S_{i+1} - 1)$$
$$E = -\frac{J}{2N} M^2 + KU$$

 $M = N_{+} - N_{-}$ U = number of broken bonds in a configuration $N = N_{+} + N_{-}$

U/2 (+) segments U/2 (-) segments

Ising model with long and short range interactions

$$\varepsilon = -\frac{J}{2}m^2 + Ku$$

 $m=M/N=(N_{+} - N_{-})/N$ u =U/N = number of broken bonds per site in a configuration

for
$$N_+ > N_-$$
 one has $U \le 2N_- = N - M$

corresponding to isolated down spins

Hence:

$$0 \le u \le 1 - m$$

The available (ε, m) is not convex.







- Local dynamics cannot make the system cross from one segment to another.
- Ergodicity is thus broken even for a finite system.









Summary

- ★ Long range interactions are not additive, resulting in uncommon properties
- Negative specific heat in microcanonical ensembles; ensembles are not equivalent particularly near first order transitions.
- ★ Breaking of ergodicity in microcanonical dynamics due to non-convexity of the domain over which the model exists.
- \star Long time scales, diverging with the system size.

Quasi-staionary states in the case of deterministic dynamics.
★
The results were derived for mean field long range interactions
★ but they are expected to be valid for algebraically decaying potentials.

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- J. Barre, (Nice)
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