Survey of (some) statistical and dynamical properties of systems with long-range interactions

STEFANO RUFFO

Dipartimento di Energetica "S. Stecco" and INFN

Center for the Study of Complex Dynamics, Firenze

`Dynamical systems and statistical mechanics,`

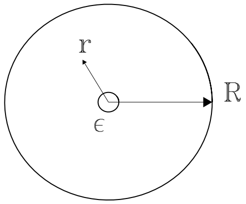
`Durham Symposium, July 3-13 2006`

PLAN

- Introduction
  - Long-range interactions
  - Extensivity vs. additivity
  - Ensemble inequivalence: negative specific heat, temperature jumps
- Models and methods
  - XY models
  - Large deviations
  - Entropy and free energy
  - Free electron laser
- Slow dynamics
  - Quasi-stationary states
  - Metastability
  - Broken ergodicity

Long range interactions

- Energy of a particle at the center of a sphere of radius R where matter is homogeneously distributed



$$U = \int_{\varepsilon}^{R} 4\pi r^2 dr\ \rho\ \frac{1}{r^{\alpha}} = 4\pi\rho \int_{\varepsilon}^{R} r^{2-\alpha} dr \propto \left[r^{3-\alpha} \right]_{\varepsilon}^{R} \sim R^{3-\alpha}$$

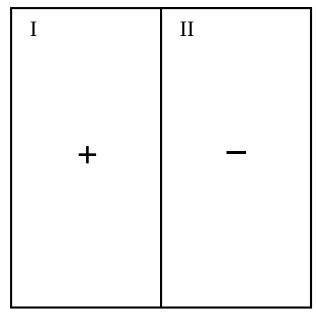
The contribution of the surface of the sphere can be neglected only if $\alpha > 3$.
Long range if $\alpha \leq 3$ ($\alpha \leq d$)

- Physical examples
  - Gravity $\alpha = 1, d = 3$, singularity at the origin
  - Coulomb $\alpha = 1, d = 3$, Debye screening
  - Dipolar $\alpha = 3, d = 3$, shape dependence
  - Onsager vortices $\alpha = 0, d = 2$
  - Mean-Field $\alpha = 0$, any d.

Extensive but not additive

$$H = -\frac{J}{2N} \sum_{i,j} \sigma_i \sigma_j$$

The Curie-Weiss Hamiltonian is EXTENSIVE $H \sim N$ but not ADDITIVE

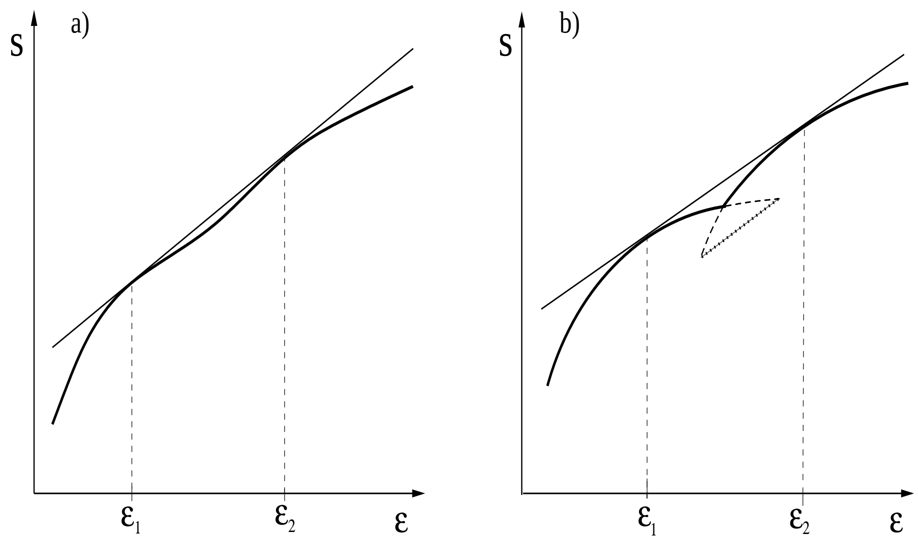


Zero magnetization state $M = \sum_i \sigma_i = 0$
$E_{I+II} = 0$, $E_I = E_{II} = -J/8N$
Hence

$$E_{I+II} \neq E_I + E_{II}$$

Ensemble inequivalence

Convex intruders

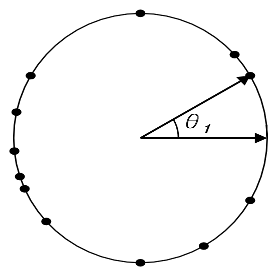


- Negative heat capacity (negative susceptibility, etc.)
- Temperature jumps

XY models

Simple mean-field models with Hamiltonian dynamics

$$H_{XY} = \sum_{i=1}^{N} \frac{p_i^2}{2} - \frac{J}{2N} (\sum_{i=1}^{N} \vec{s}_i)^2 - \frac{K}{4N^3} \left[(\sum_{i=1}^{N} \vec{s}_i)^2 \right]^2 , \quad \vec{s}_i = (\cos\theta_i, \sin\theta_i)$$



Simplifications of

- Gravitational and charged sheet models
- Wave-particle interactions

with D. Mukamel (Weizmann) and P. De Buyl (ULB, Bruxelles)

Large deviations

$\mathbf{X} \in R^d$ a random variable with given PDF
$\mathbf{X}_i$,$i = 1, \ldots, N$, a sample of $\mathbf{X}$.
$\mathbf{M}_N = \frac{1}{N} \sum_i \mathbf{X}_i$ sample mean
What's the PDF of the sample mean? (`Cramèr, Gartner-Ellis`)
Compute the generating function

$$\psi(\lambda) =< \exp(\lambda \cdot \mathbf{X}) >,$$

with $\lambda \in R^d$ and the average $< \cdot >$ performed on the PDF of $\mathbf{X}$
If $\psi(\lambda) < \infty$ and differentiable, then

$$P(\mathbf{M}_N = \mathbf{x}) \sim \exp(-NI(\mathbf{x}))$$

where the rate function $I(\mathbf{x})$ is given by the Legendre-Fenchel transform of $\ln(\psi(\lambda))$

$$I(\mathbf{x}) = \sup_{\lambda \in R^d} (\lambda \cdot \mathbf{x} - \ln(\psi(\lambda)))$$

Entropy and free energy

Step 1 Express the Hamiltonian in terms of global variables γ

$$H_N(\omega_N) = \widetilde{H}_N\left(\gamma(\omega_N)\right) + R_N(\omega_N)$$

(ω_N a phase-space configuration) leading to $h(\gamma) = lim_{N\to\infty} \widetilde{H}_N\left(\gamma(\omega_N)\right)/N$.
Step 2 Compute the entropy functional in terms of the global variables using, e.g., Cramèr's theorem

$$s(\gamma) = \lim_{N\to\infty} \frac{1}{N} \ln \Omega_N(\gamma)$$

with $\Omega_N(\gamma)$ the number of microscopic configurations with fixed γ.
Step 3 Solve the microcanonical and canonical variational problems

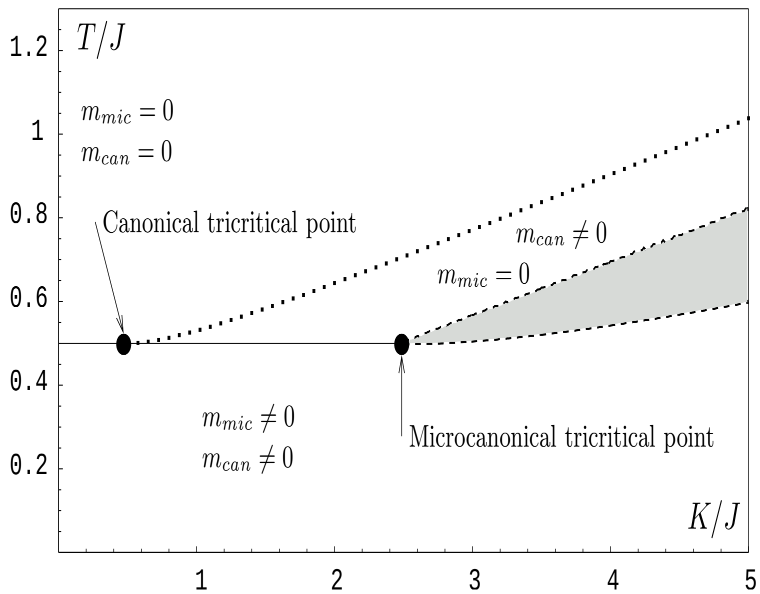
$$S(\epsilon) = \sup_{\gamma} \left(s(\gamma) \mid h(\gamma) = \epsilon\right) ,$$

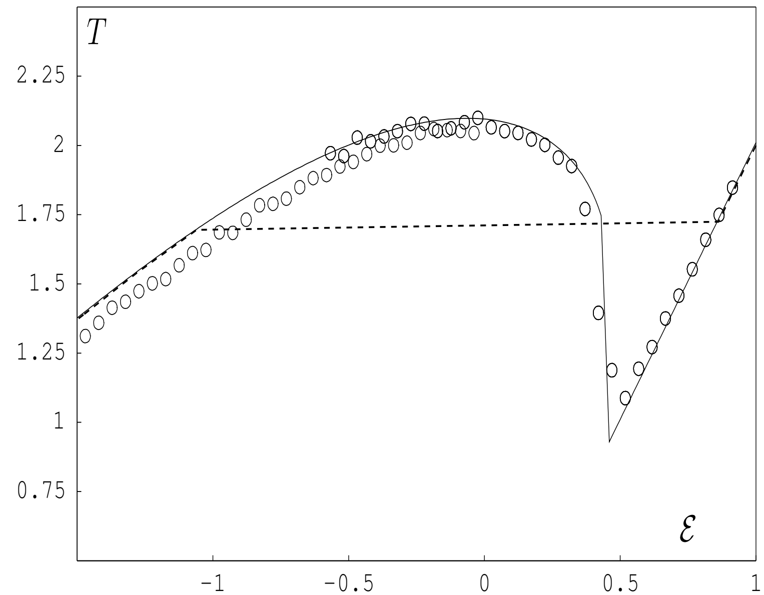
$$\beta F(\beta) = \inf_{\gamma} \left(\beta h(\gamma) - s(\gamma)\right)$$

Solution by large deviations

- Local random variable: $\vec{X} = \big(\cos\theta, \sin\theta, p^2/2\big)$, corresponding to $\sum_i \cos\theta_i/N = m_x$, $\sum_i \sin\theta_i/N = m_y$ (magnetization), $\sum_i p_i^2/2 = \mathcal{E}_K$ (kinetic energy)
- Generating function:$\Psi(\vec{\lambda}) \simeq I_0(\sqrt{\lambda_x^2 + \lambda_y^2})/\sqrt{-\lambda_K}$, where $\vec{\lambda} = (\lambda_x, \lambda_y, \lambda_K)$ and I_0 is the modified Bessel function of zero order.
- Rate function: $I(\vec{x}) = \sup_{\vec{\lambda}}(\lambda_K p^2/2 + \lambda_x m_x + \lambda_y m_y + \ln(-\lambda_K)/2 - \ln(I_0(\sqrt{\lambda_x^2 + \lambda_y^2})))$, where $\vec{x} = (m_x, m_y, \mathcal{E}_K)$
- Entropy: $S(\mathcal{E}) = \sup_{\vec{x}}\{-I(\vec{x})$ with $\mathcal{E}_K = \mathcal{E} + \frac{Jm^2}{2} + \frac{Km^4}{4}\}$

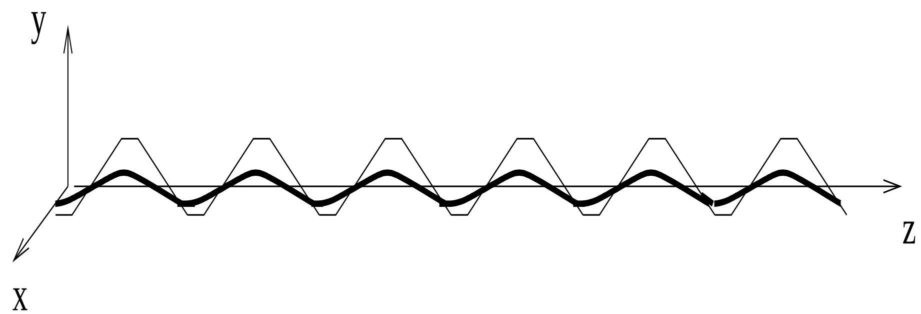
Phase diagram and caloric curves





- At $K/J = 0$ (HMF model), second order phase transition at $T/J = 0.5$. Ensembles are equivalent.
- For $K/J > 1/2$ ensembles are inequivalent. Negative specific heat for $1/2 < K \leq 5/2$; Temperature jumps for $K > 5/2$.
- Right figure shows the caloric curve for $K/J = 10$. The points are results of a molecular dynamics simulation with $N = 100$

Free Electron Laser



Colson-Bonifacio model

$$
\begin{aligned}
\frac{d\theta_j}{dz} &= p_j \\
\frac{dp_j}{dz} &= -\mathbf{A}e^{i\theta_j} - \mathbf{A}^* e^{-i\theta_j} \\
\frac{d\mathbf{A}}{dz} &= i\delta\mathbf{A} + \frac{1}{N}\sum_j e^{-i\theta_j}
\end{aligned}
$$

with A. Antoniazzi (Florence), J. Barré (Nice), T. Dauxois (ENS-Lyon), D. Fanelli (Florence and Stockholm), G. De Ninno (Sincrotrone Trieste)

Microcanonical solution

Hamiltonian

$$H_N = \sum_{j=1}^{N} \frac{p_j^2}{2} - N\delta A^2 + 2A \sum_{j=1}^{N} \sin(\theta_j - \varphi)$$

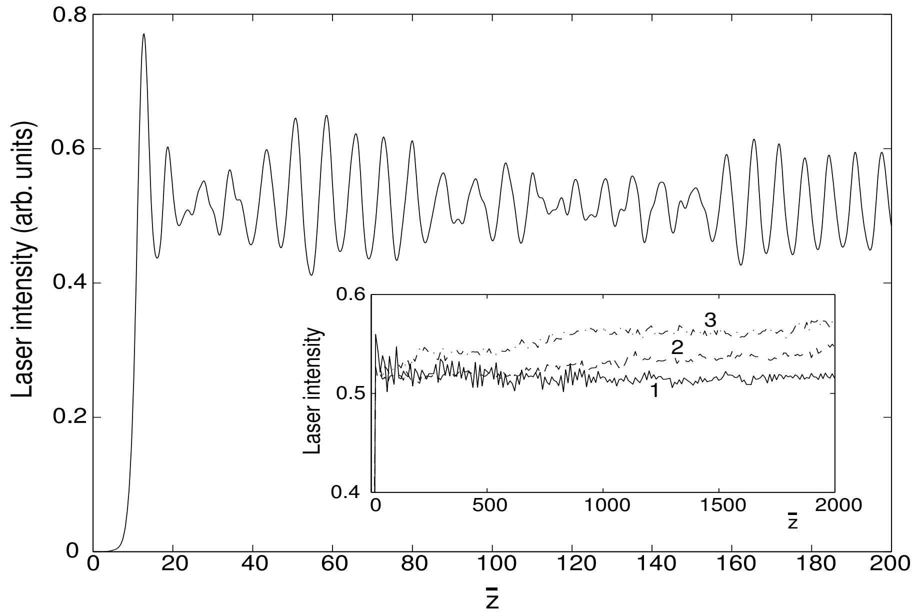
where $A = \sqrt{\mathbf{A}\mathbf{A}^*}$.
Entropy

$$S(\varepsilon, \sigma, \delta) = \sup_{A,M} \left[\frac{1}{2} \ln \left[2 \left(\varepsilon - \frac{\sigma^2}{2} \right) + 4AM + 2(\delta - \sigma)A^2 - A^4 \right] + s_{conf}(M) \right]$$

where $M = \sqrt{m_x^2 + m_y^2}$, $m_x = \sum_i \cos\theta_i / N$, $m_y = \sum_i \sin\theta_i / N$, σ is the total average momentum $\sum_i p_i / N$ and

$$s_{conf}(M) = -\sup_{\lambda} \left[\lambda M - \ln I_0(\lambda) \right]$$

Quasi-stationary states



$N = 5000$ (curve 1), $N = 400$ (curve 2), $N = 100$ (curve 3)

On a first stage the system converges to a quasi-stationary state. On a longer $O(N)$ time scale, it relaxes to Boltzmann-Gibbs equilibrium.

`Conjecture`

The quasi-stationary state is a Vlasov equilibrium.

Vlasov equation

In the $N \to \infty$ limit, the single particle distribution function $f(\theta, p, t)$ obeys a Vlasov equation.

$$
\begin{aligned}
\frac{\partial f}{\partial z} &= -p\frac{\partial f}{\partial \theta} + 2(A_x \cos\theta - A_y \sin\theta)\frac{\partial f}{\partial p} \quad , \\
\frac{\partial A_x}{\partial z} &= -\delta A_y + \frac{1}{2\pi}\int f \cos\theta \, d\theta dp \quad , \\
\frac{\partial A_y}{\partial z} &= \delta A_x - \frac{1}{2\pi}\int f \sin\theta \, d\theta dp \; .
\end{aligned}
$$

with $\mathbf{A} = A_x + iA_y = \sqrt{I}\exp(-i\varphi)$

Vlasov equilibria

Coarse grained entropy maximization (Lynden-Bell 1968, Chavanis, 1996)

$$s(\bar{f}) = -\int dpd\theta \left(\frac{\bar{f}}{f_0} \ln \frac{\bar{f}}{f_0} + \left(1 - \frac{\bar{f}}{f_0}\right) \ln \left(1 - \frac{\bar{f}}{f_0}\right) \right) .$$

$$S(\varepsilon, \sigma) = \max_{\bar{f}, A_x, A_y} [s(\bar{f}) | H(\bar{f}, A_x, A_y) = N\varepsilon; \int d\theta dp \bar{f} = 1; P(\bar{f}, A_x, A_y) = \sigma].$$

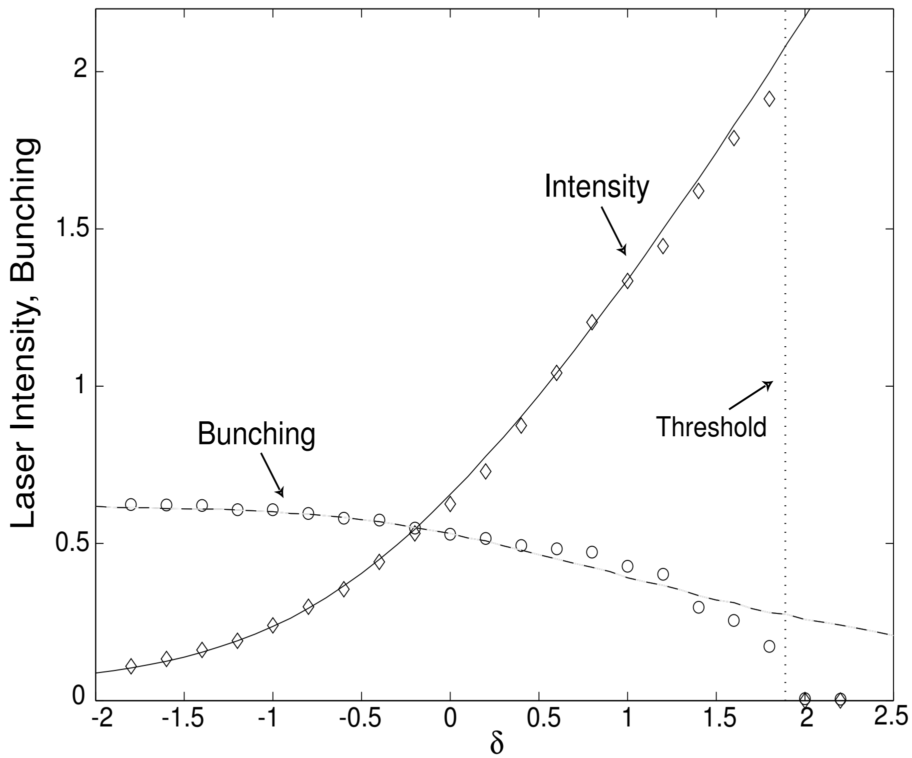
Non Gaussian momentum distribution

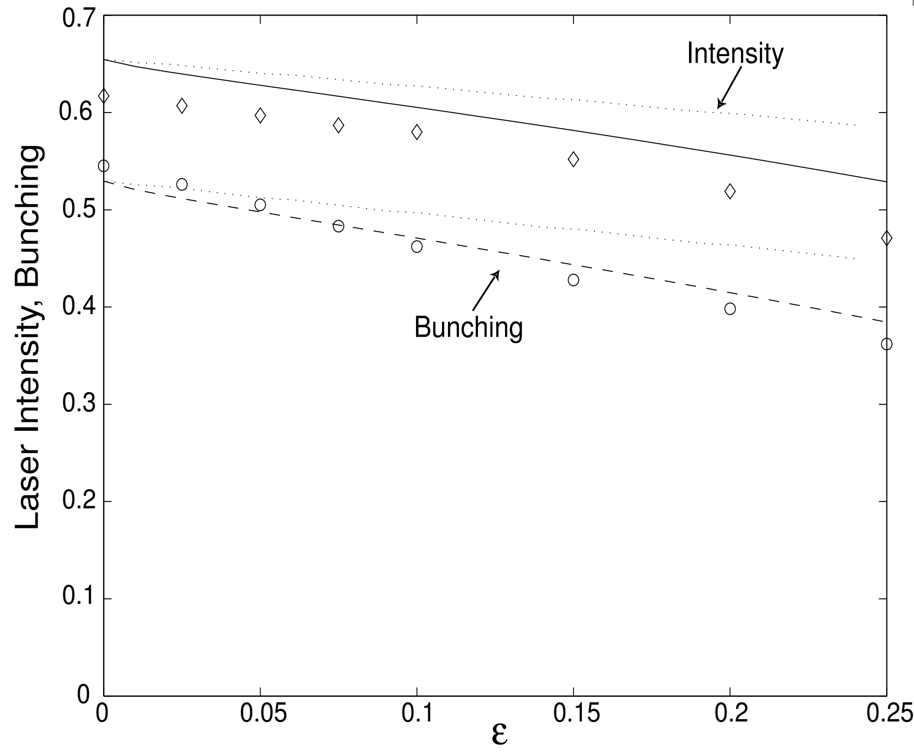
$$\bar{f} = f_0 \frac{e^{-\beta(p^2/2 + 2A\sin\theta) - \lambda p - \mu}}{1 + e^{-\beta(p^2/2 + 2A\sin\theta) - \lambda p - \mu}} .$$

Non-equilibrium field amplitude

$$A = \sqrt{A_x^2 + A_y^2} = \frac{\beta}{\beta\delta - \lambda} \int dpd\theta \, \sin\theta \bar{f}(\theta, p).$$

Results


Laser Intensity, Bunching
Intensity
Bunching
Threshold
δ


Laser Intensity, Bunching
Intensity
Bunching
ε

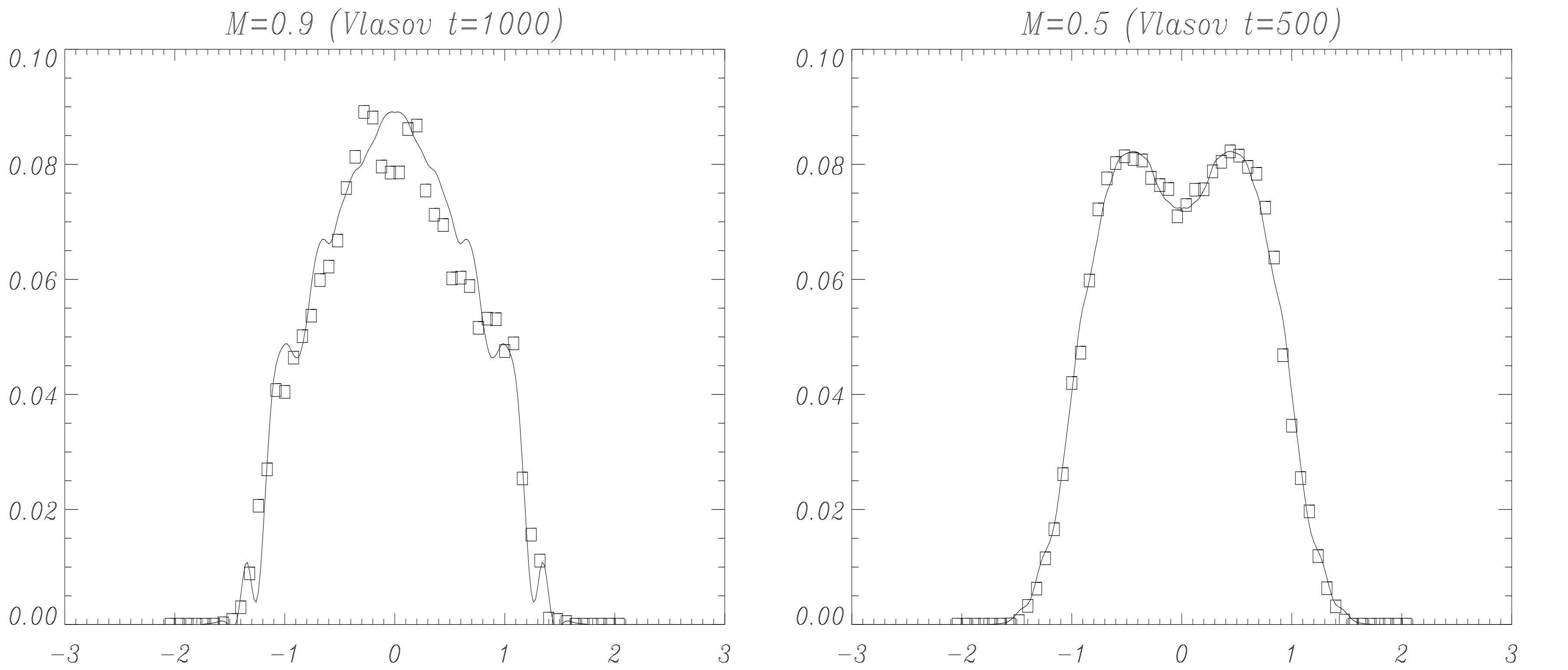
HMF Vlasov equation

$$\frac{\partial f}{\partial t} + p\frac{\partial f}{\partial \theta} - \frac{dV}{d\theta}\frac{\partial f}{\partial p} = 0 \quad ,$$

$$\begin{aligned} V(\theta)[f] &= 1 - M_x[f]\cos(\theta) - M_y[f]\sin(\theta) \ , \\ M_x[f] &= \int f(\theta, p, t)\ \cos\theta \mathrm{d}\theta \mathrm{d}p \quad , \\ M_y[f] &= \int f(\theta, p, t)\ \sin\theta \mathrm{d}\theta \mathrm{d}p \quad . \end{aligned}$$

Specific energy
$e[f] = \int (p^2/2) f(\theta, p, t) \mathrm{d}\theta \mathrm{d}p + 1/2 - (M_x^2 + M_y^2)/2$ and momentum $P[f] = \int p f(\theta, p, t) \mathrm{d}\theta \mathrm{d}p$ are conserved.

Vlasov simulations



Maximal Lynden-Bell entropy state

$$\bar{f}(\theta,p) = f_0 \frac{e^{-\beta(p^2/2 - M_y[\bar{f}]\sin\theta - M_x[\bar{f}]\cos\theta) - \lambda p - \mu}}{1 + e^{-\beta(p^2/2 - M_y[\bar{f}]\sin\theta - M_x[\bar{f}]\cos\theta) - \lambda p - \mu}}.$$

$$f_0 \quad \frac{x}{\sqrt{\beta}} \int \mathrm{d}\theta e^{\beta \mathbf{M}\cdot\mathbf{m}} F_0\left(x e^{\beta \mathbf{M}\cdot\mathbf{m}}\right) = 1$$

$$f_0 \quad \frac{x}{2\beta^{3/2}} \int \mathrm{d}\theta e^{\beta \mathbf{M}\cdot\mathbf{m}} F_2\left(x e^{\beta \mathbf{M}\cdot\mathbf{m}}\right) = e + \frac{M^2 - 1}{2}$$

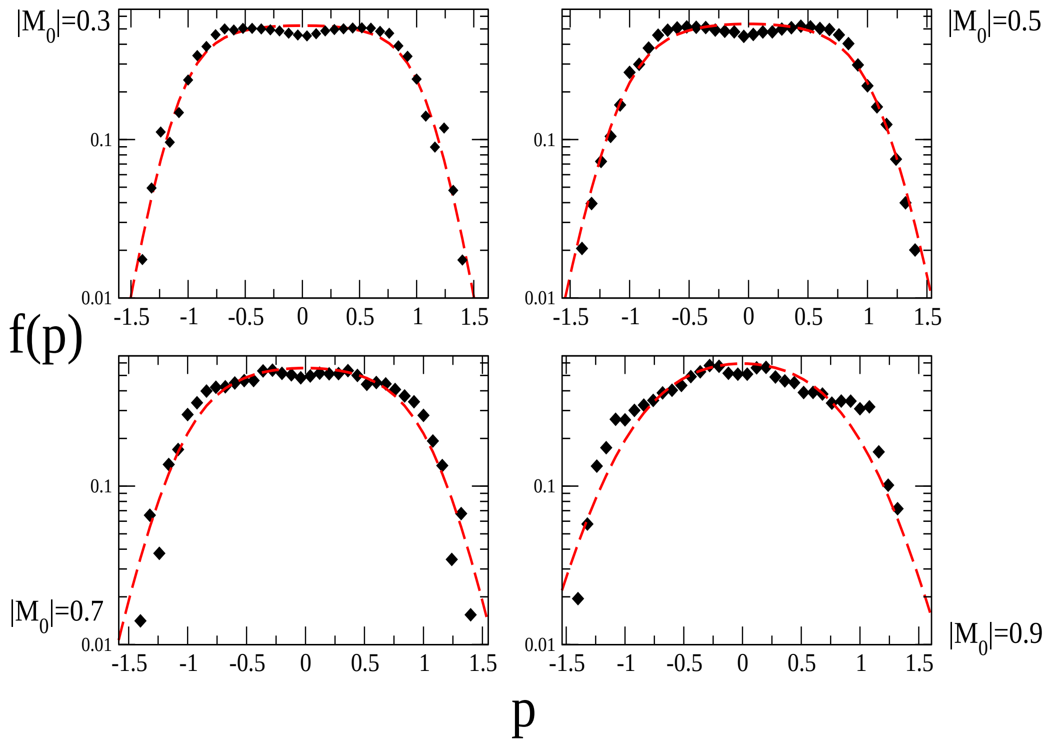
$$f_0 \quad \frac{x}{\sqrt{\beta}} \int \mathrm{d}\theta \cos\theta e^{\beta \mathbf{M}\cdot\mathbf{m}} F_0\left(x e^{\beta \mathbf{M}\cdot\mathbf{m}}\right) = M_x$$

$$f_0 \quad \frac{x}{\sqrt{\beta}} \int \mathrm{d}\theta \sin\theta e^{\beta \mathbf{M}\cdot\mathbf{m}} F_0\left(x e^{\beta \mathbf{M}\cdot\mathbf{m}}\right) = M_y$$

$\mathbf{M} = (M_x, M_y)$, $\mathbf{m} = (\cos\theta, \sin\theta)$.
$F_0(y) = \int \exp(-v^2/2)/(1 + y\exp(-v^2/2))\mathrm{d}v$,
$F_2(y) = \int v^2 \exp(-v^2/2)/(1 + y\exp(-v^2/2))\mathrm{d}v$.
$f_0 = 1/(4\Delta\theta_0\Delta p_0)$

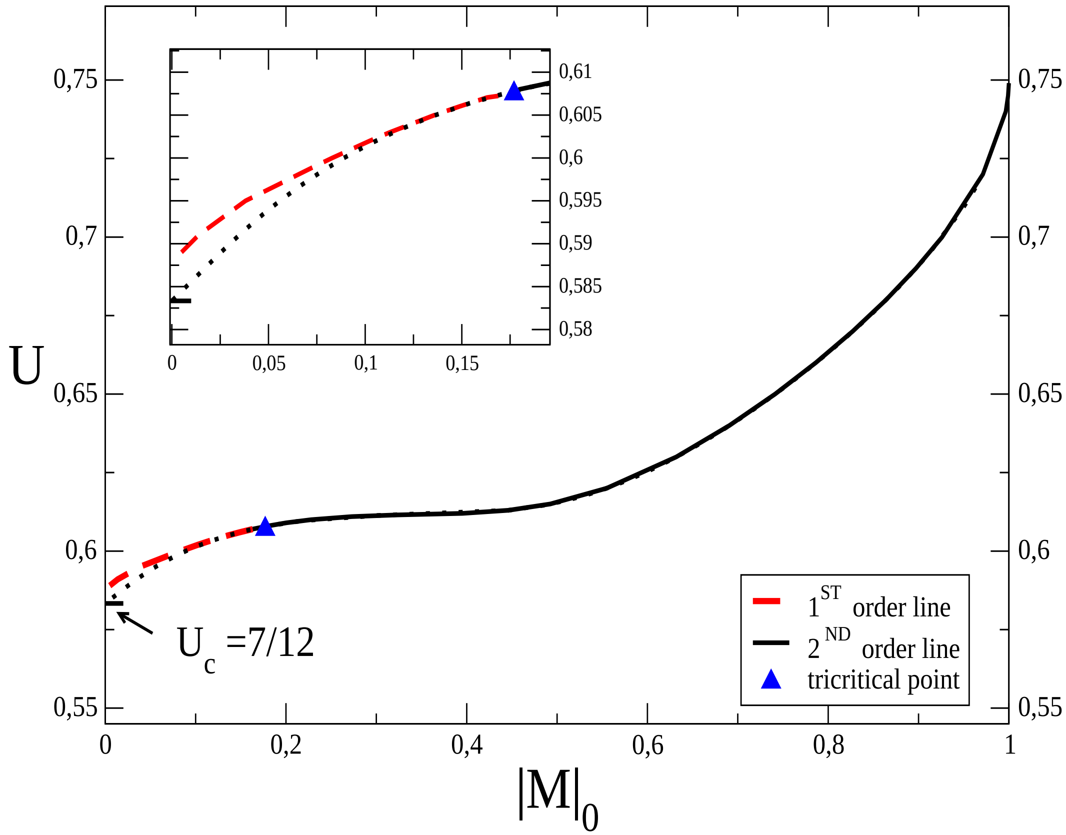
Results

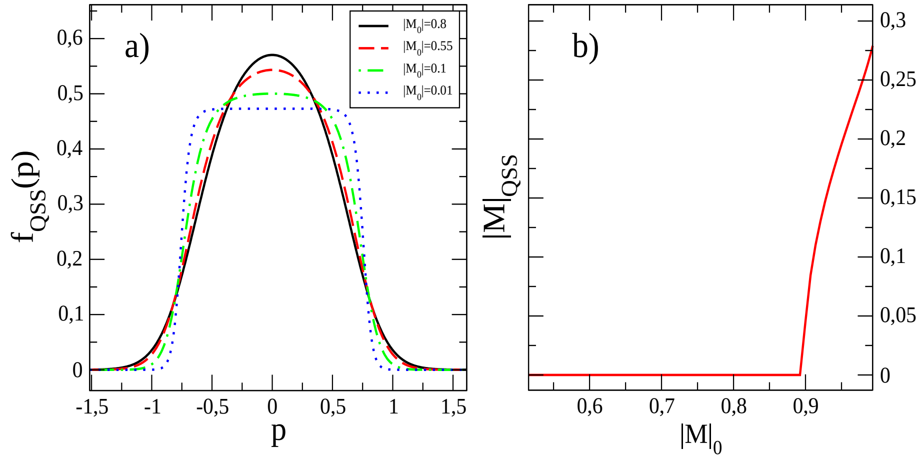
single particle distribution

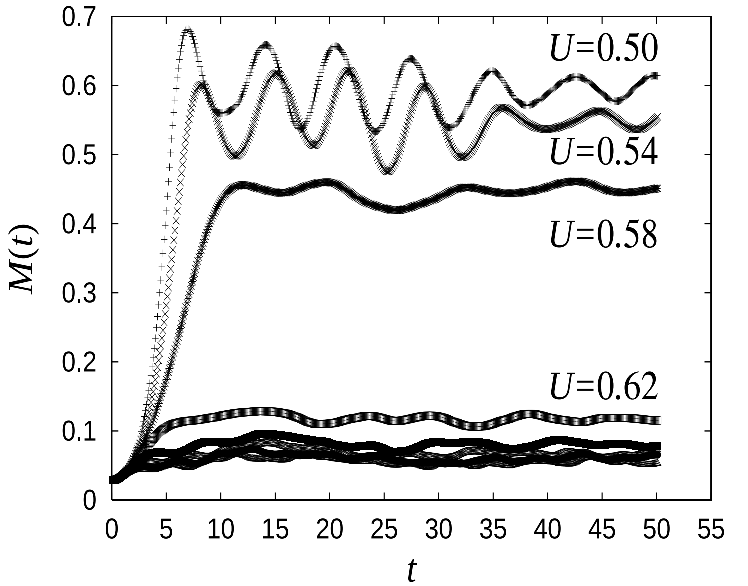


$$|M_0| = \sin(\Delta\theta_0)/\Delta\theta_0$$

Non-concave Lynden-Bell entropy

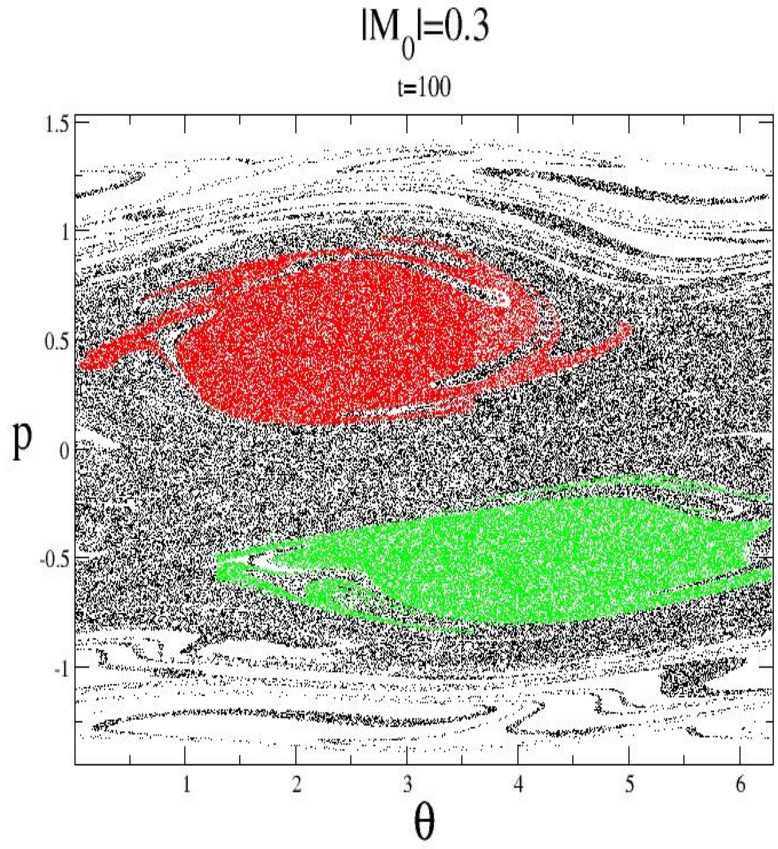



a)
b)
$|M_0|$=0.8
$|M_0|$=0.55
$|M_0|$=0.1
$|M_0|$=0.01
$f_{QSS}(p)$
p
$|M|_{QSS}$
$|M|_0$


U=0.50
U=0.54
U=0.58
U=0.62
M(t)
t

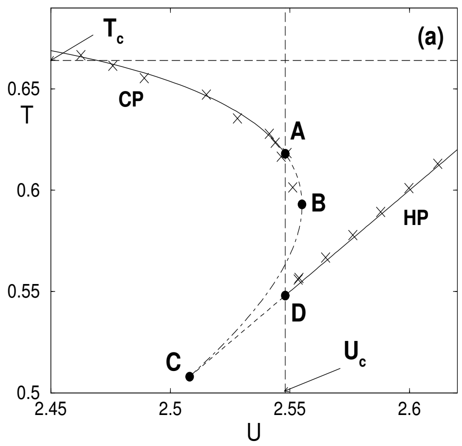
HMF core-halo structure

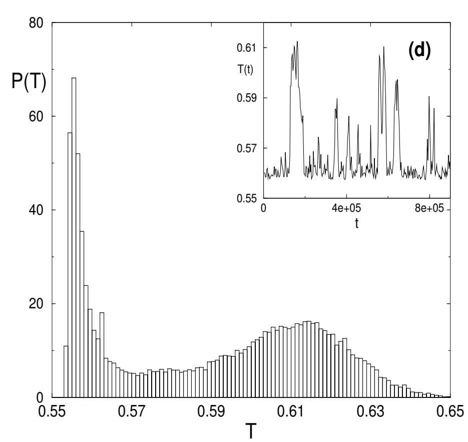
Refinements of maximum entropy methods should take into account the "true" dynamics.

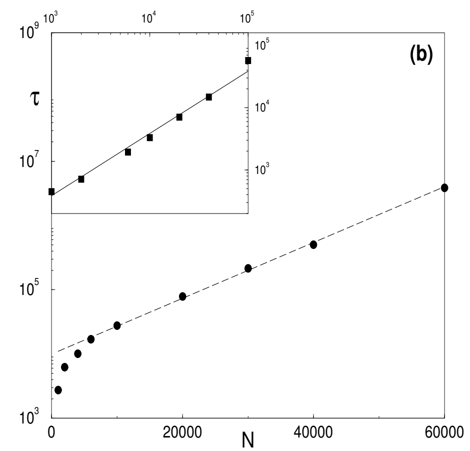


Metastability

At a microcanonical first order transition, temperature has a bimodal distribution.
Once prepared in a local entropy maximum the system relaxes to the global entropy maximum on a time that increases with $\exp(N\Delta s)$, where Δs is the entropy density barrier size.



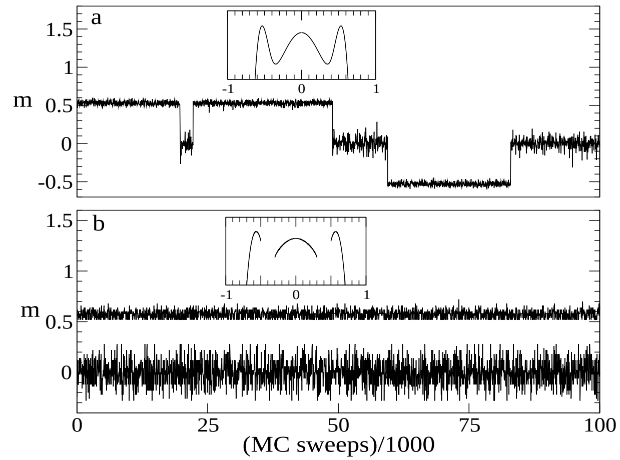




Broken ergodicity

Ising model with short and long-range interactions on a ring

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



with D. Mukamel and N. Schreiber (Weizmann)

Conclusions

- Microcanonical and canonical ensemble disagree for long range interactions at canonical first order transitions.
- Negative specific heat and temperature jumps are typical signatures of *ensemble inequivalence*.
- Collective phenomena for wave-particle interactions (FEL) are the result of constrained maximum entropy principles (Vlasov equilibria).
- Quasi-stationary states appear whose life-time increases with system size.
- Metastable states have a life-time which increases exponentially with system size.
- Due to non-additivity, broken ergodicity is a generic feature of systems with long-range interactions.

References

- T. Dauxois, S. Ruffo, E. Arimondo and M. Wilkens (Eds.) *Dynamics and statistics of systems with long-range interactions*, Springer Lecture Notes in Physics **602** (2002).
- J. Barré, D. Mukamel and S. Ruffo:*Inequivalence of ensembles in a system with long range interactions*, Phys. Rev. Lett., **87**(3), 030601 June (2001).
- J. Barré, F. Bouchet, T. Dauxois and S. Ruffo *Large deviation techniques applied to systems with long-range interactions*, J. Stat. Phys., **119**, 677 (2005).
- P. de Buyl, D. Mukamel and S. Ruffo: *Ensemble inequivalence in a XY model with long-range interactions*, in “Unsolved Problems of Noise and Fluctuations", AIP Conference Proceedings **800**, 533 (2005).
- J. Barré, T. Dauxois, G. De Ninno, D. Fanelli, S. Ruffo:*Statistical theory of high-gain free-electron laser saturation*, Phys. Rev. E, Rapid Comm., **69**, 045501 (R) (2004).
- D. Mukamel, S. Ruffo and N. Schreiber: *Breaking of ergodicity and long relaxation times in systems with long-range interactions*, Phys. Rev. Lett., **95**, 240604 (2005).
- A. Antoniazzi, D. Fanelli, J. Barré, P.H. Chavanis, T. Dauxois and S. Ruffo: *A maximum entropy principle explains quasi-stationary states in systems with long-range interactions: the example of the HMF model*, cond-mat/0603813.