Models with interactions that decay weakly with distance

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`Theory Seminar, Pisa , march 4, 2014`

Plan

- Long-range interactions
- Non additivity
- α-Ising model
- Non-concave entropies and negative specific heat
- Large deviations and Legendre transforms
- The Kardar-Nagel model
- Broken ergodicity
- Mean-field metastability
- Dipolar needles
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- Vlasov equation and quasistationary states
- Vlasov equation on the lattice
- α-HMF model and zero-mode dominance

Long-range interactions

At large inter particle distance r

$$V(r) \sim r^{-\alpha}$$
$$0 \le \alpha \le d$$

Energy per particle

$$\epsilon = \frac{E}{N} = \int_{\delta}^{R} d^d r \rho \frac{J}{r^{\alpha}} \propto \left[R^{d-\alpha} - \delta^{d-\alpha} \right]$$

- if $\alpha > d$ then $\epsilon \to const$ when $R \to \infty$.
- if $0 \le \alpha \le d$ then $\epsilon \sim V^{1-\alpha/d}$ ($V \sim R^d$)

Off and on lattice

$$U(\overrightarrow{r}_1, \ldots, \overrightarrow{r}_N) = \sum_{1 \le i < j \le N} V(|\overrightarrow{r}_i - \overrightarrow{r}_j|) + h \sum_{i=1,N} V_e(\overrightarrow{r}_i)$$

Gravitational point masses and Coulomb point charges fall into this category.

$$U(\mathbf{q}_1, \ldots, \mathbf{q}_N) = \sum_{1 \le i < j \le N} C_{ij} V(\mathbf{q}_i, \mathbf{q}_j) + h \sum_{i=1}^{N} V_e(\mathbf{q}_i)$$

$\mathbf{q}_i$ represents “internal" degrees of freedom sitting at lattice site $\mathbf{r}_i$ and the coupling

$$C_{ij} = \frac{1}{|\overrightarrow{r}_i - \overrightarrow{r}_j|^\alpha} \qquad , \quad 0 \le \alpha \le d$$

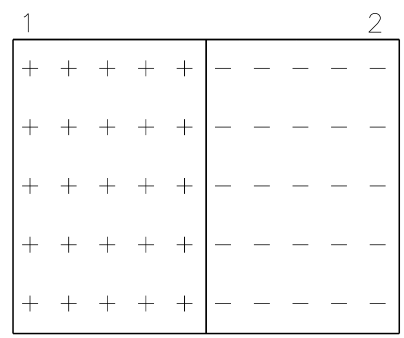
Non additivity

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

Curie-Weiss Hamiltonian

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

with $\sigma_i = \pm 1$.
Zero magnetization state $M = \sum_i \sigma_i = 0$



$$E_{I+II} = 0 \qquad E_I = E_{II} = -J/8N.$$

Energy and free energy

Total energy $E = \epsilon V$

$$\alpha > d \quad E \sim V$$
$$\alpha \leq d \quad E \sim V^{2-\alpha/d}$$

Free energy

$$F = E - TS \quad , \quad S \sim V \quad , \quad s = S/V$$

Kac rescaling in order for the entropy to compete with energy.

$$J \rightarrow JV^{\alpha/d-1} \quad , \quad F \sim V \quad , \quad f = F/V$$

or, alternatively,

$$T \rightarrow TV^{1-\alpha/d} \quad , \quad F \sim V^{2-\alpha/d}$$

α-Ising model

Barré, Bouchet, Dauxois and Ruffo, 2005

$$H_N = -\frac{J}{2\tilde{N}} \sum_{i \neq j} \frac{\sigma_i \sigma_j}{|i-j|^\alpha}$$

with

$$\tilde{N} = \sum_{i=1}^{N} \frac{1}{i^\alpha} \sim N^{1-\alpha} \quad , \quad 0 \leq \alpha \leq 1$$

Continuum limit:Divide the lattice in K boxes, each with $n = N/K$ sites and introduce the box-averaged magnetization m_k, $k = 1, ...K$. Take the limit $N \to \infty$, $K \to \infty$, $1/n = K/N \to 0$. The magnetization becomes a continuous function of $m(x)$ in the interval $[0,1]$ and

$$H_N = NH[m] + o(N)$$

with

$$H[m] = -\frac{J}{2} \int_0^1 dx \int_0^1 dy \frac{m(x)m(y)}{|x-y|^\alpha}$$

Entropy of α-Ising

Large deviation principle for the probability of observing a given magnetization m_k in the k-th box

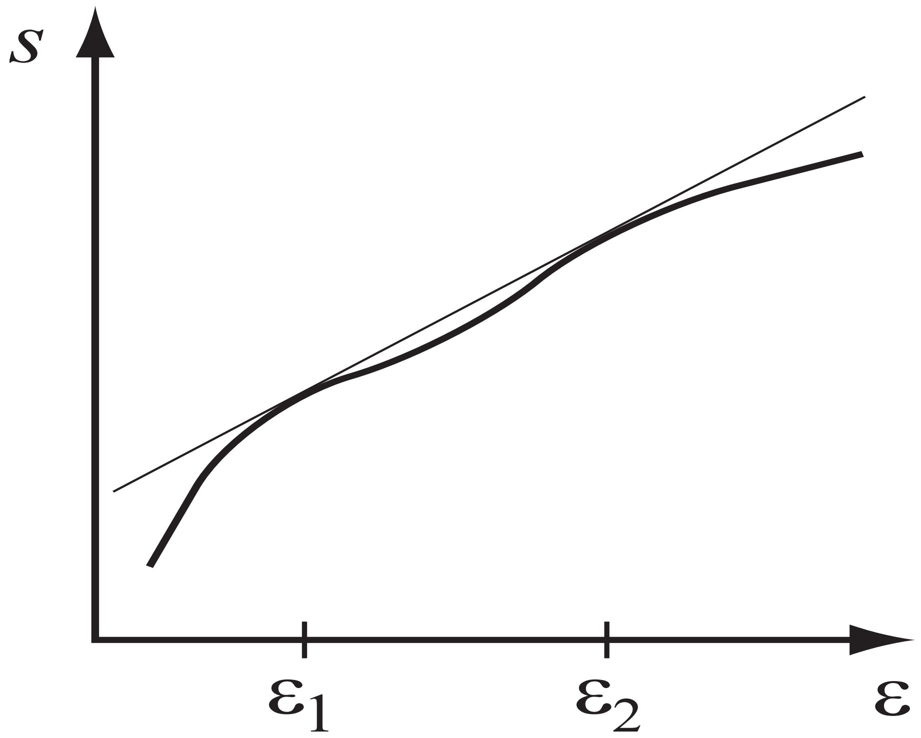
$$P(m_k) \propto \exp(ns(m_k)) = \exp\left[-n(\frac{1+m_k}{2}\ln\frac{1+m_k}{2} + \frac{1-m_k}{2}\ln\frac{1-m_k}{2})\right]$$

Since the microscopic random variables are a-priori independent

$$\begin{aligned} P(m_1, m_2, \ldots, m_K) &= \prod_{k=1}^{K} P(m_k) \simeq \prod_{k=1}^{K} \exp(ns(m_k)) = \\ &= \exp\left[nK\sum_{k=1}^{K}\frac{s(m_k)}{K}\right] \simeq \exp(Ns[m(x)]) \end{aligned}$$

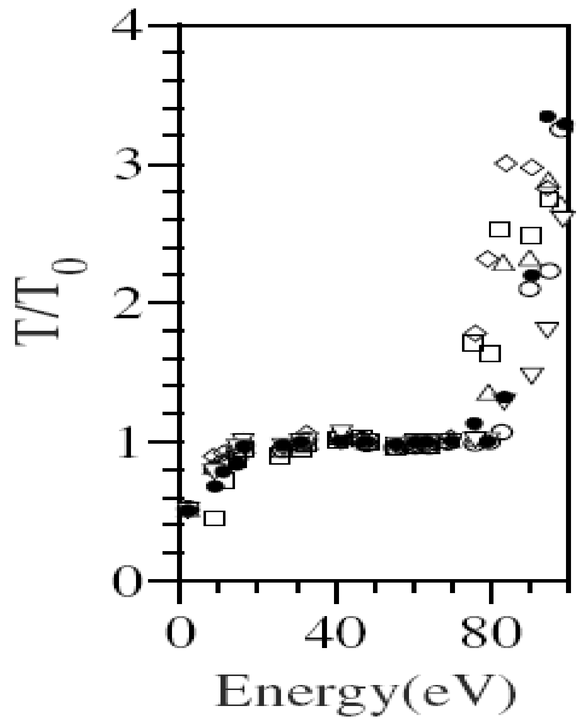
where $s[m(x)] = \int_0^1 dx s(m(x))$ is the entropy functional associated with the global variable $m(x)$. This results implies that entropy is extensive (proportional to N) also for long-range systems.

Non concave entropy



$$\partial^2 s/\partial\epsilon^2 = -(c_V T^2)^{-1}$$

Negative specific heat



F. Gobet et al., 2001

Caloric curve of hydrogen cluster ions $H_3^+(H_2)_{m\leq 14}$ bombarded by Helium projectile (liquid-gas transition), energy and temperature are determined from the size distribution of the fragments.

Large deviations, Legendre transform

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

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

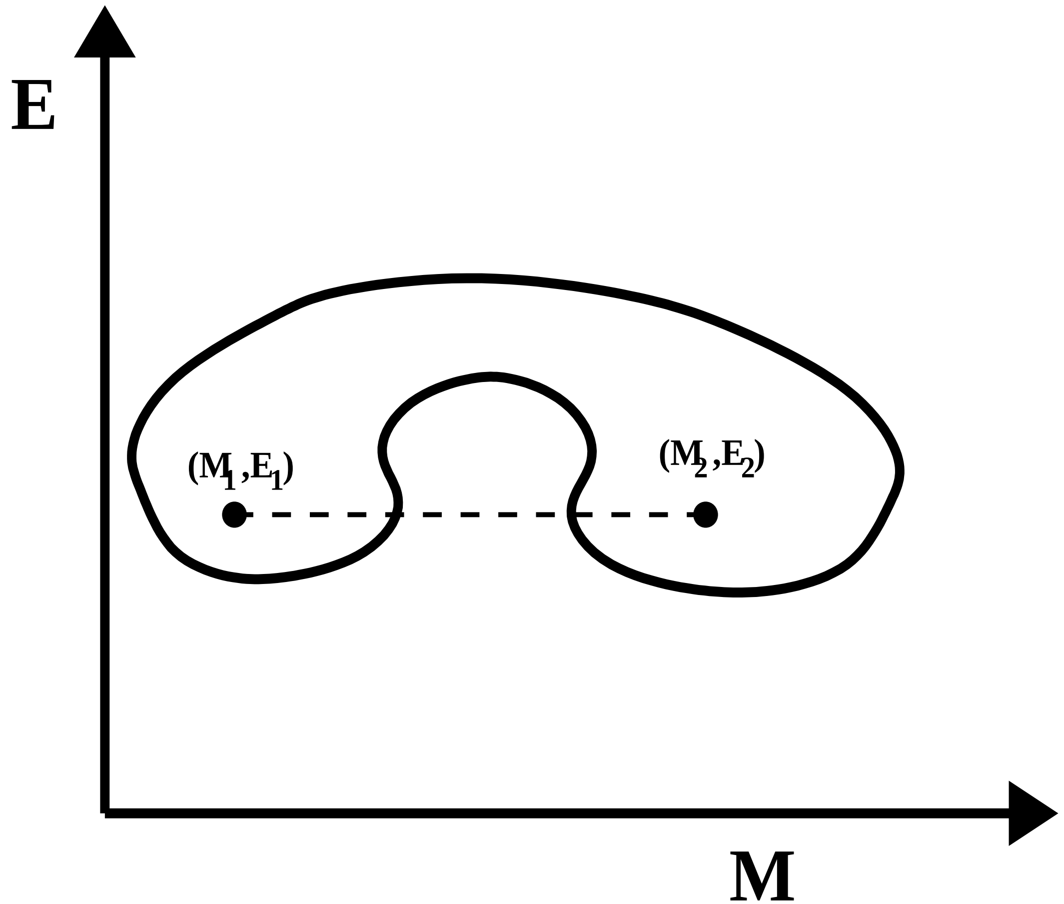
with $\Omega_N(\gamma)$ the number of microscopic configurations with fixed γ.

Step 3 Solve the microcanonical and canonical variational problems

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

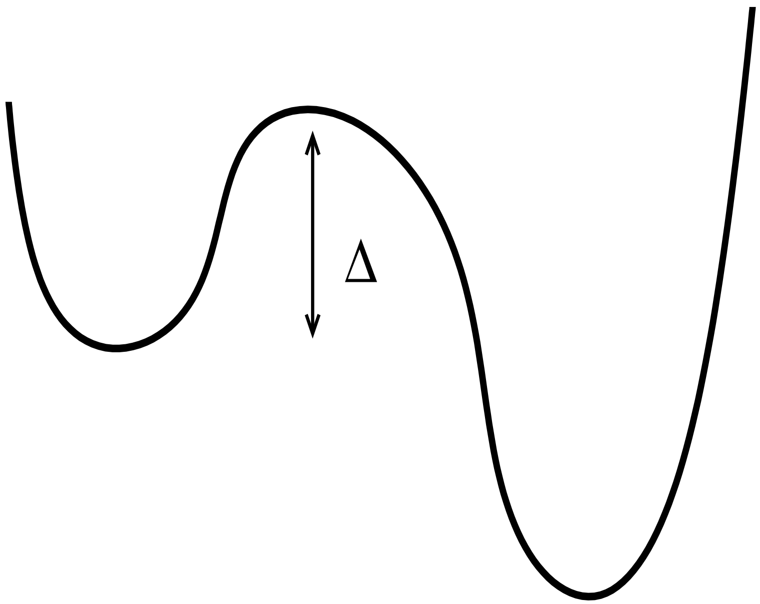
$$\beta f(\beta) = \inf_{\gamma} \left(\beta h(\gamma) - s(\gamma) \right)$$

Concave regions and broken ergodicity



$$E = \lambda E_1 + (1-\lambda) E_2 \quad , \quad M = \lambda M_1 + (1-\lambda) M_2 \quad , \quad 0 \leq \lambda \leq 1$$

Metastability



$$\tau \sim e^{N\frac{\Delta f}{k_B T}} \quad \text{canonical} \quad , \quad \tau \sim e^{N\frac{\Delta s}{k_B}} \quad \text{microcanonical}$$

Griffiths, Weng and Langer, 1966; Antoni, SR and Torcini, 2004; Schreiber, Mukamel and SR, 2005

The Kardar-Nagel model

Nagel, 1970; Kardar, 1983; Schreiber, Mukamel and SR, 2005

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

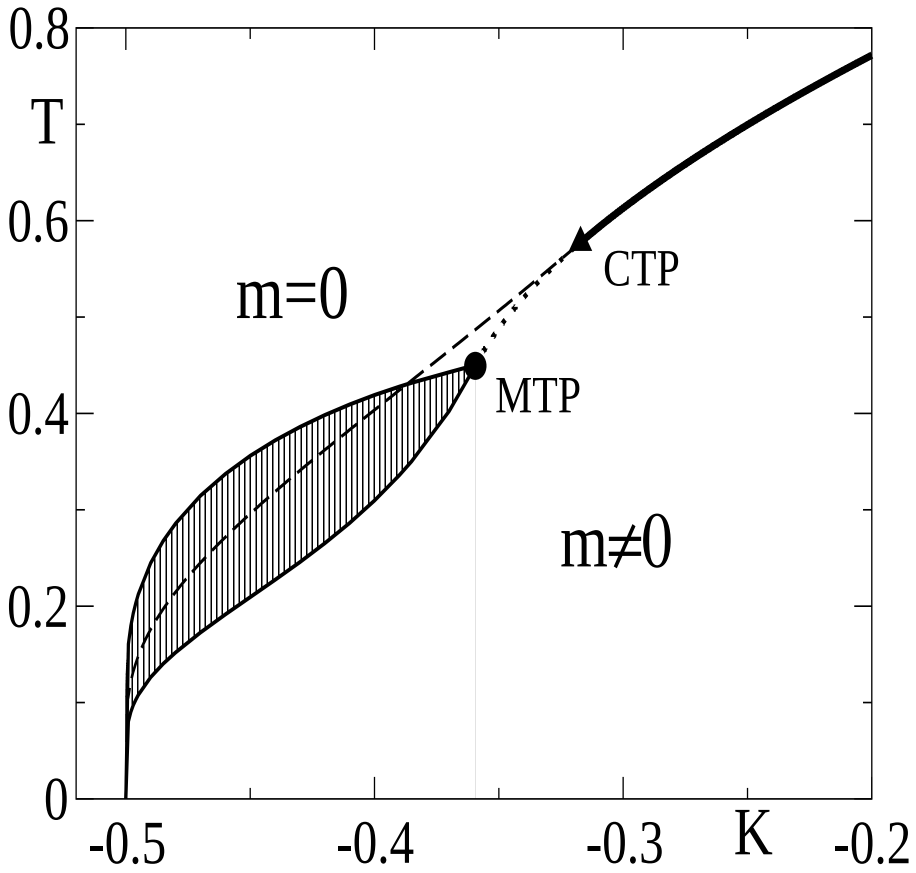
Let $U = -(1/2)\sum_i (S_i S_{i+1} - 1)$ be the number of antiferromagnetic bonds in a given configuration characterized by N_+ up spins and N_- down spins, e.g. $N_+ = 12$, $N_- = 8$, $U/2 = 2$

$$++++++|-----|++++|---|++$$

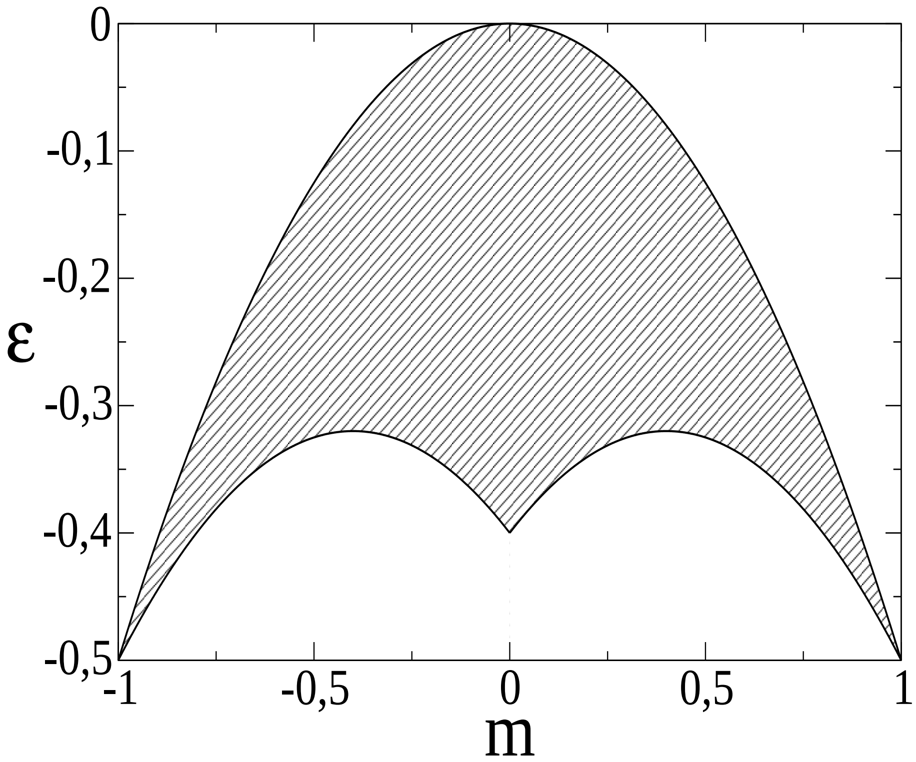
Simple counting arguments yield to leading order

$$\Omega(N_+, N_-, U) \approx \begin{pmatrix} N_+ - 1 \\ U/2 - 1 \end{pmatrix} \begin{pmatrix} N_- - 1 \\ U/2 - 1 \end{pmatrix} .$$

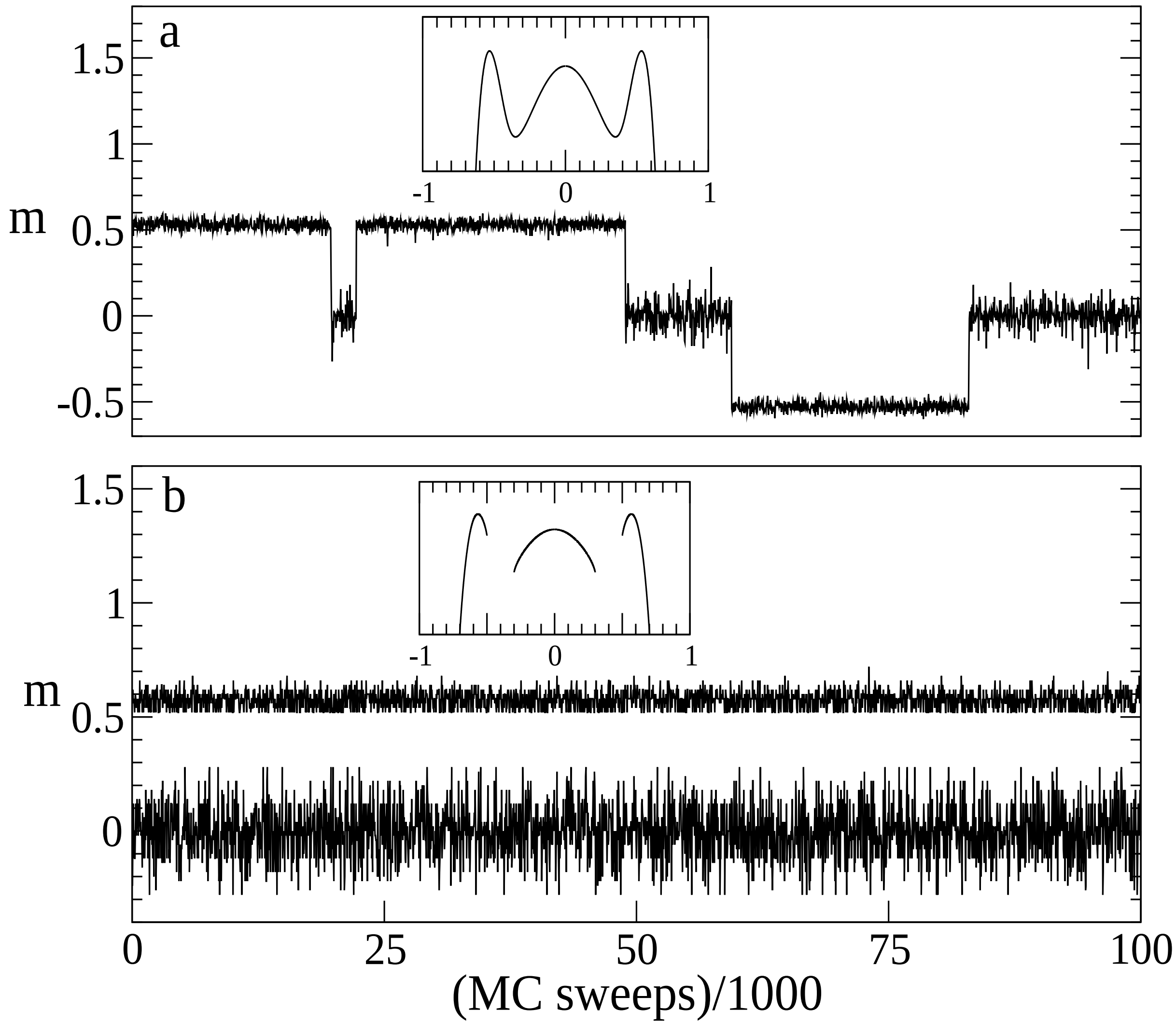
Phase diagram



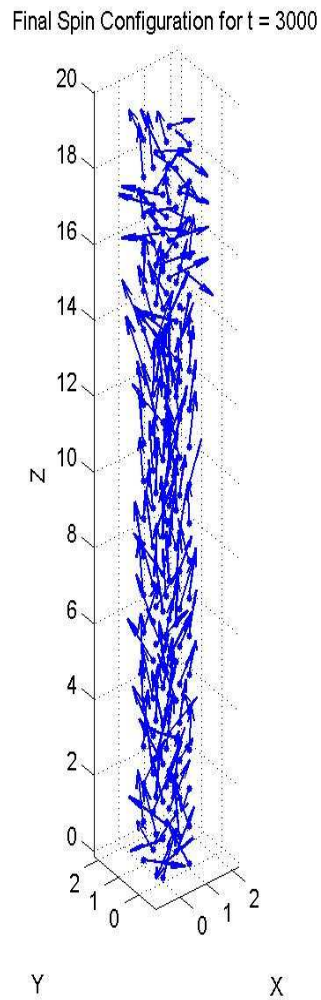
Broken ergodicity

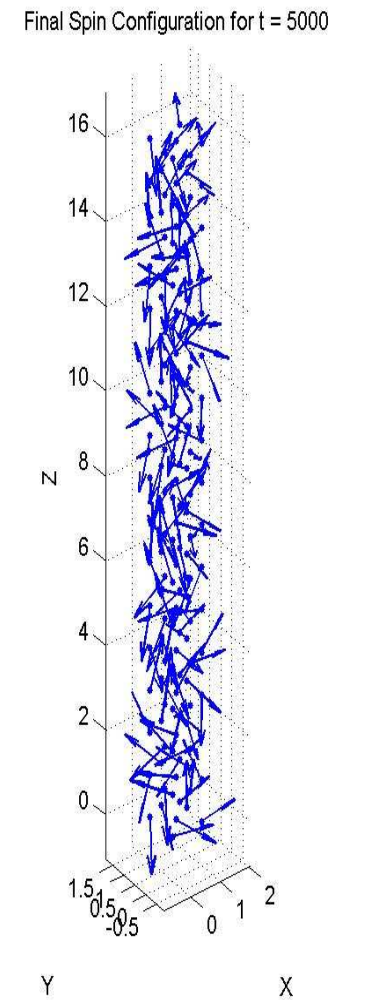


Magnetization flips



Microcanonical dipolar needles





Dipolar interaction and mapping

Miloshevic, Dauxois, Khomeriki and SR, 2013

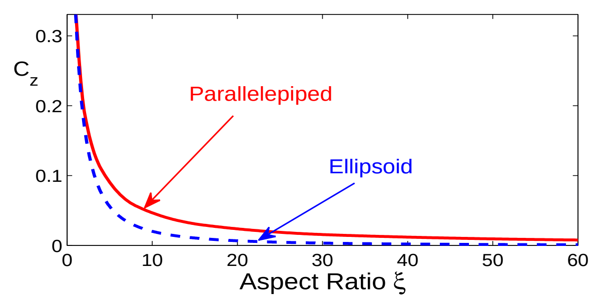
$$\mathcal{H} = \frac{\epsilon}{2} \sum_{i \neq j} \frac{a^3}{r_{ij}^3} \left(\vec{S}_i \cdot \vec{S}_j - 3 \frac{(\vec{S}_i \cdot \vec{r}_{ij})(\vec{S}_j \cdot \vec{r}_{ij})}{r_{ij}^2} \right) \qquad \epsilon = \mu_0 \sigma^2 / (4\pi a^3)$$

Mapping to the Kardar-Nagel model

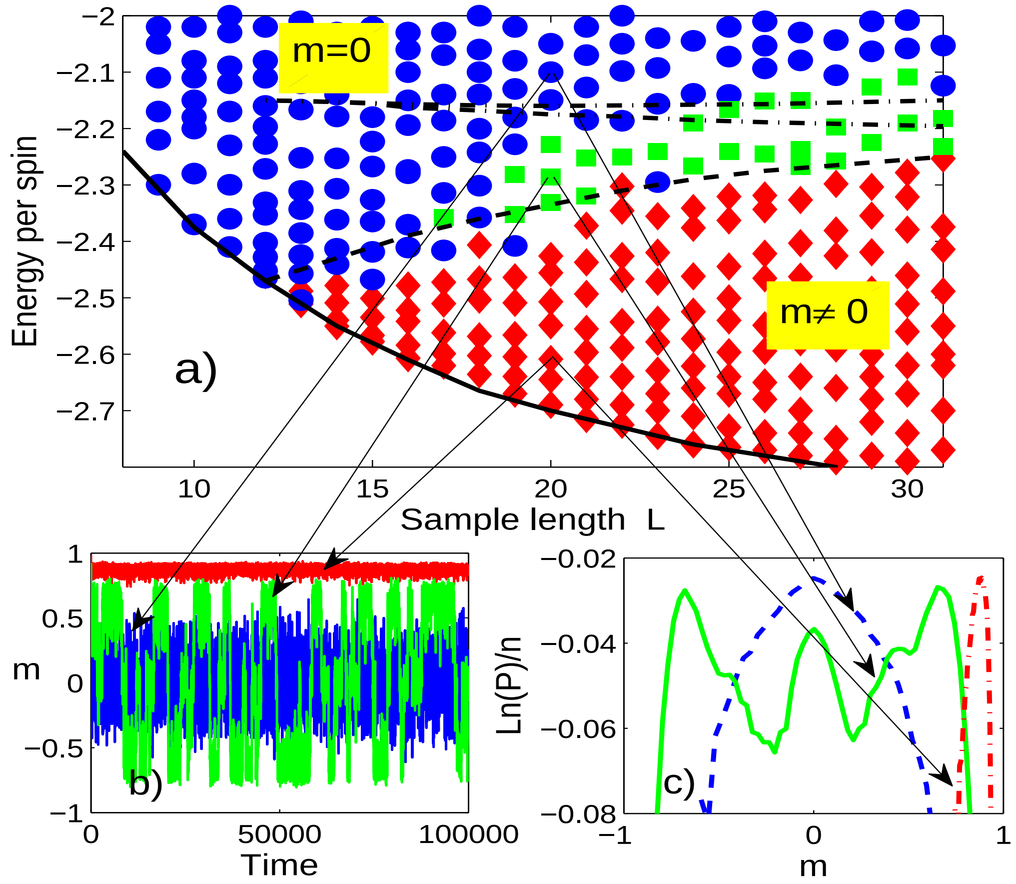
$$\mathcal{H}_{eff} = -\frac{K}{2} \sum_{\langle i,i' \rangle} \left(S_i^z S_{i'}^z - 1 \right) - \frac{J}{2N} \left(\sum_{i=1}^{N} S_i^z \right)^2$$

$$J = \frac{4\pi \varepsilon a^3 (1 - 3C_z)}{3 v_0} \quad , \quad C_z = -\frac{1}{4\pi V} \int_V d^3 r \int_V d^3 r_1 \frac{\partial^2}{\partial z^2} \left(\frac{1}{|\vec{r} - \vec{r}_1|} \right).$$

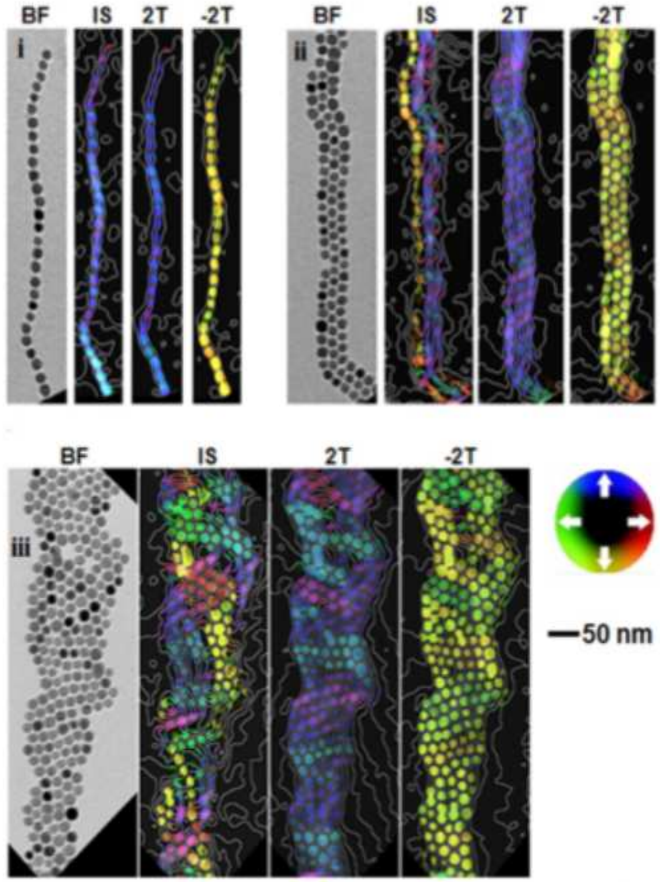
K is negative in units of ϵ and depends on the lattice type: simple cubic, body-centered cubic, face-centered cubic, etc.

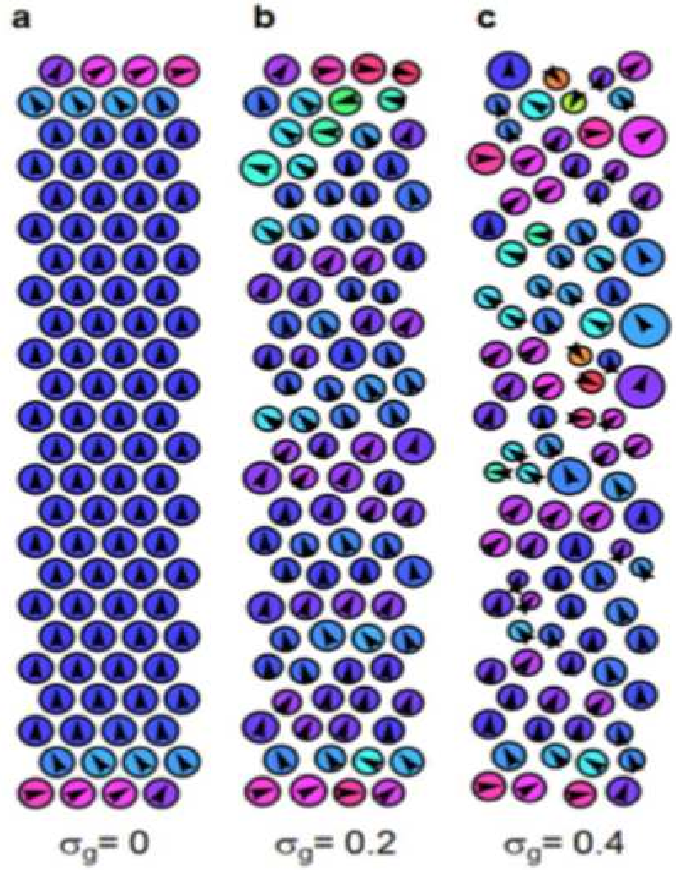


Phase diagram



Co nanoparticles





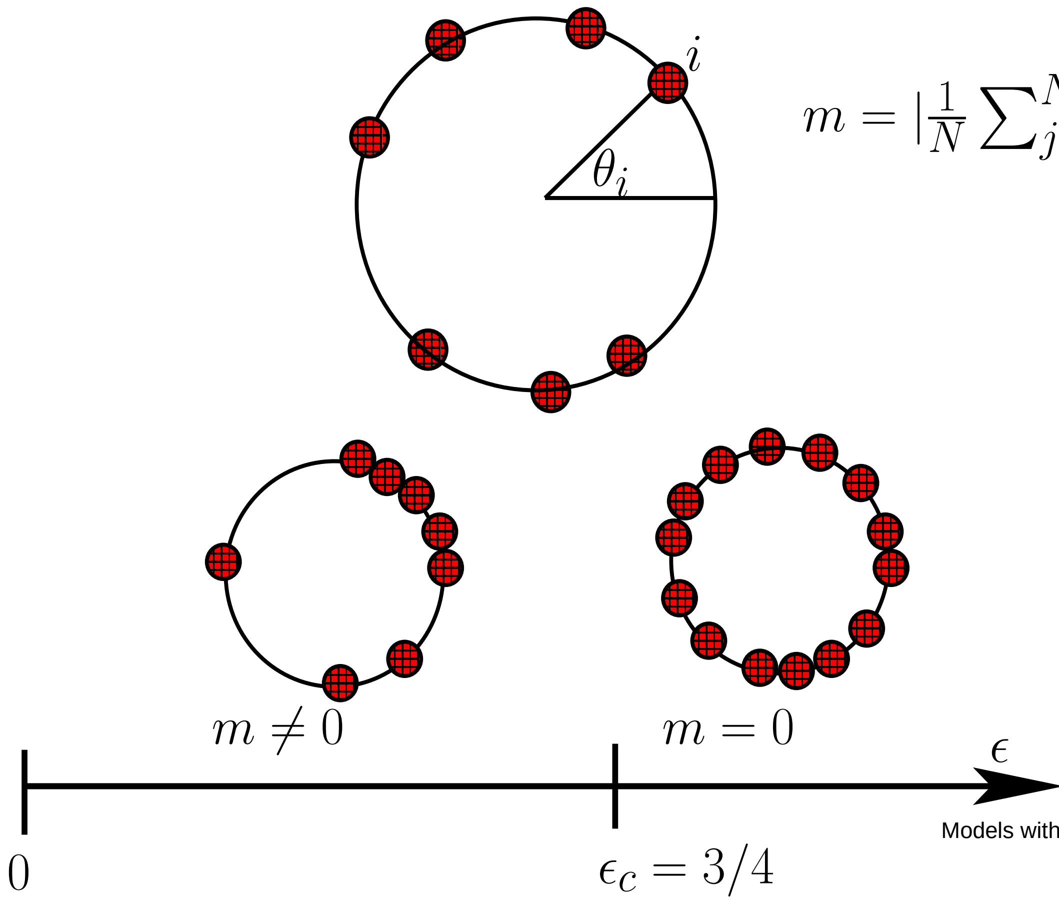
Varon, 2013

The HMF model

Antoni and SR, 1995

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

$$m = \left|\frac{1}{N} \sum_{j=1}^{N} e^{i\theta_j}\right|$$



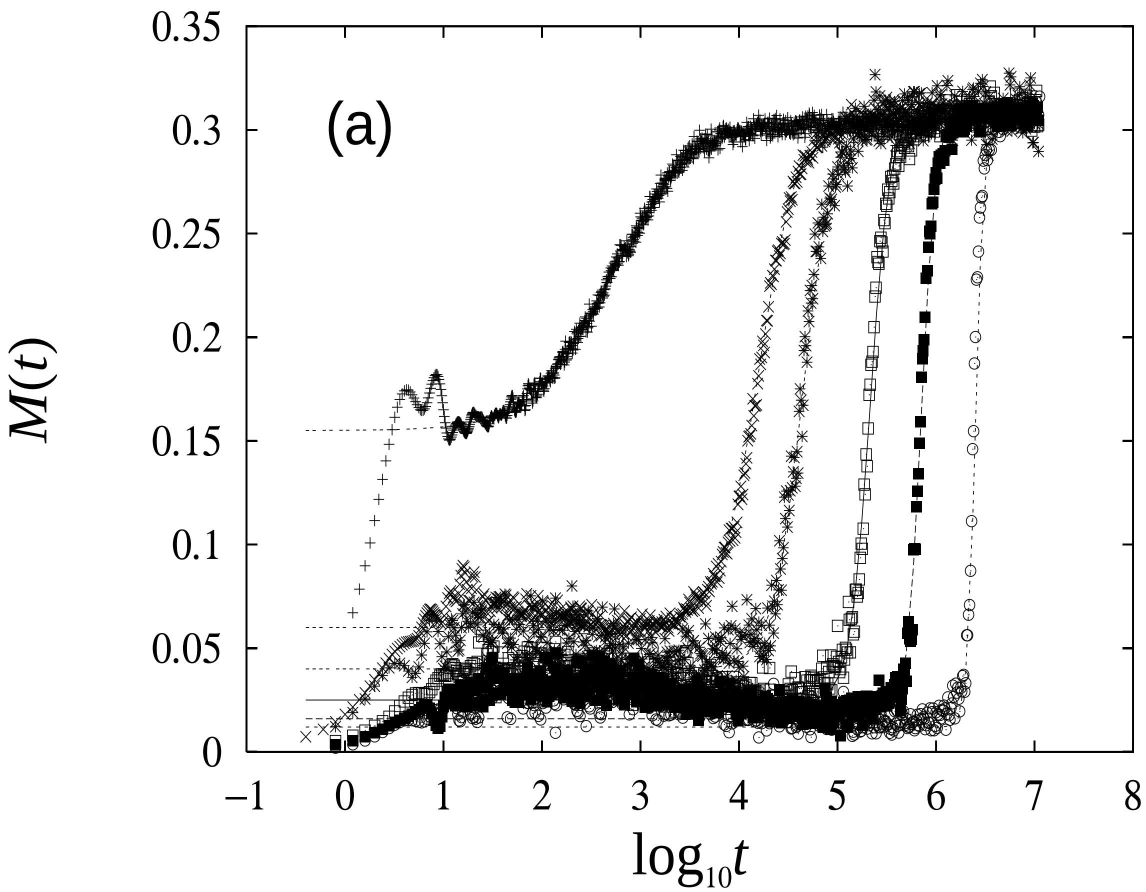
Vlasov equation

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + U(\theta_i) \quad , \quad U(\theta_1, .., \theta_N) = \frac{1}{N} \sum_{i<j}^{N} V(\theta_i - \theta_j)$$

$$\frac{\partial f}{\partial t} + p \frac{\partial f}{\partial \theta} - \frac{\partial \langle v \rangle}{\partial \theta} \frac{\partial f}{\partial p} = \frac{1}{N} \langle \frac{\partial \delta v}{\partial \theta} \frac{\partial \delta f}{\partial p} \rangle$$

$$\langle v \rangle (\theta, t) = \int d\theta' dp' V(\theta - \theta') f(\theta', p', t) \qquad \iint d\theta dp f = 1$$

Slow relaxation



Yamaguchi, Barré, Bouchet, Dauxois and SR, 2004

Quasistationary states

Initial Condition

↓ *Violent* relaxation $\tau_v = O(1)$

Quasistationary state

↓ *Collisional* relaxation $\tau_c = N^q$

Boltzmann's Equilibrium

Scaling law

Bachelard and Kastner, 2013

$$\tau = N^q$$

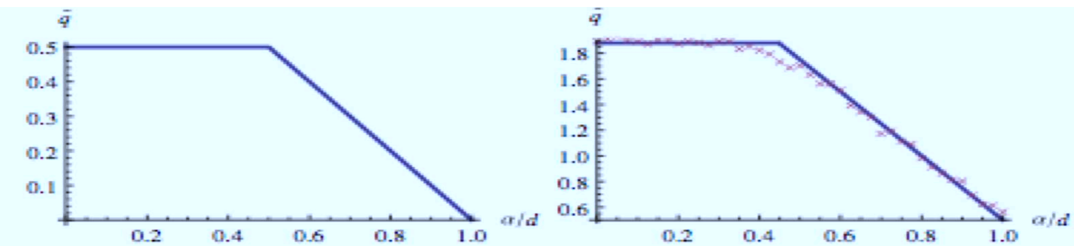
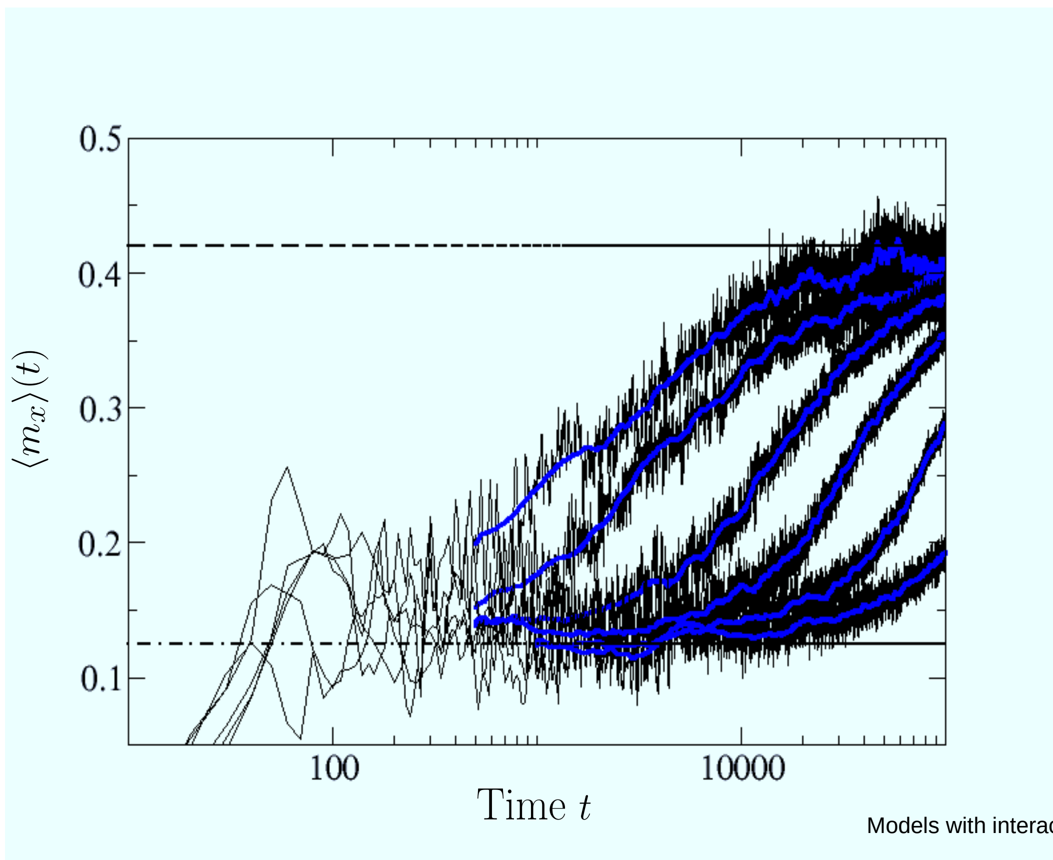


FIG. 3 (color online). As in Fig. 1, but for scaling exponents $\tilde{q}$ as modified by the presence of an N-dependent prefactor $\mathcal{N}$ in the Hamiltonian. The left plot is for the long-range quantum Ising model, the right for the classical αXY chain.

Response

Patelli, Dauxois, Gupta, Nardini and SR, 2012

$$H(t) = H_0 + H_{\rm ext} = H_0 - h(t) \sum_{i=1}^{N} \cos(q_i)$$



Linearized Vlasov equation

$$f(\theta, p, t) = f_0(p) + \delta f(\theta, p, t)$$

$$\frac{\partial \delta f}{\partial t} + p \frac{\partial \delta f}{\partial \theta} - \frac{\partial \delta v}{\partial \theta} \frac{\partial f_0}{\partial p} = 0.$$

$$\delta f(\theta, p, t) = \hat{f}(p)\, e^{i(k\theta - \omega t)}\, , \; \delta v(\theta, t) = \hat{v}\, e^{i(k\theta - \omega t)}.$$

$$-i\omega\, \hat{f}(p) + p\, ik\, \hat{f}(p) - ik\, \hat{v} f_0'(p) = 0$$

Plasma response dielectric function (HMF) `Inagaki-Konishi (1993)`

$$D(\omega, k) = 1 + \pi k \left(\delta_{k,1} + \delta_{k,-1}\right) \int_{-\infty}^{+\infty} dp \frac{f_0'(p)}{pk - \omega},$$

Dispersion relation

$$D(\omega, k) = 0$$

Stability of the homogeneous state

Stability condition for the homogeneous state of the HMF model

$$I = 1 + \pi \int_{-\infty}^{+\infty} \frac{f_0'(p)}{p}\, dp \geq 0.$$

Gaussian distribution

$$f_g(p) = \frac{1}{2\pi}\sqrt{\frac{\beta}{2\pi}}\exp(-\beta p^2/2)$$

$$I = 1 - \beta/2 \geq 0\,,\; T = 1/\beta > 1/2\,,\; \epsilon \geq 3/4$$

“Waterbag” distribution

$$f_{wb}(p) = \frac{1}{2\pi}\frac{1}{2\Delta p}\left[\Theta(p+\Delta p) - \Theta(p-\Delta p)\right]$$

$$I = 1 - 1/2\Delta p^2 \geq 0\,,\; \Delta p^2 \geq 1/2\,,\; \epsilon \geq 7/12$$

Vlasov equation on a lattice

Bachelard, Dauxois, De Ninno, SR and Staniscia, 2011

$$H = \sum_j \frac{p_j^2}{2} + \frac{1}{2\tilde{N}} \sum_{j,k=1}^{N} \frac{v(q_j, q_k)}{|x_j - x_k|^\alpha}\,,\; x_j = ja\,,\; \tilde{N} = \sum_{i=1}^{N} i^{-\alpha} \propto N^{1-\alpha}\,,\; 0 \le \alpha < 1$$

Continuum limit

$$\dot{q} = p \quad , \quad \dot{p} = -\frac{\partial V_x[f](q,t)}{\partial q}$$

where

$$V_x[f](q,t) = \kappa_\alpha \iiint dq'\,dp'\,dx'\, f(q', p'; x', t)\, \frac{v(q,q')}{|x - x'|^\alpha}\ ,$$

$$\kappa_\alpha^{-1} = \int_{-1/2}^{+1/2} dx/|x|^\alpha$$

Vlasov equation

$$\frac{\partial f}{\partial t} + p\frac{\partial f}{\partial q} - \frac{\partial V_x'[f](q,t)}{\partial q}\frac{\partial f}{\partial p} = 0.$$

Linearized Vlasov equation

Expansion around a homogeneous state

$$f(q,p;x,t) = f_0(p) + \delta f(q,p;x,t)$$

$$\partial_t(\delta f) + p\partial_q(\delta f) - \partial_p f_0(p)\partial_q V_x[\delta f](q,t) = 0.$$

Fourier expansion

$$\delta f_t(q,p;x) = \sum_k e^{\lambda_k t}\hat{f}_k(q,p)\exp(2i\pi kx)$$

Dispersion relation

$$\hat{f}_k(q,p) - c_k(\alpha)\partial_p f_0(p)\frac{e^{-\lambda_k \frac{q}{p}}}{p}\int_{q_0}^{q} e^{\lambda_k \frac{q'}{p}} V[\hat{f}_k](q')dq' = 0$$

where

$$c_k(\alpha) = \kappa_\alpha \int_{-1/2}^{+1/2} \frac{e^{2i\pi ky}}{|y|^\alpha}dy \quad , \quad V[\hat{f}_k](q) = \iint dq'dp'\hat{f}_k(q',p')v(q,q')$$

α-HMF model

Tamarit, Anteneodo (2000), Campa, Giansanti Moroni (2000), Mori (2011,2012)

$$v(q,q') = -\cos(q-q') \quad , \quad V[\hat{f}_k](q) = -\kappa_\alpha \left(m_x[\hat{f}_k]\cos q + m_y[\hat{f}_k]\sin q \right),$$

$$m_x[\hat{f}_k] = \iint dq'\,dp'\,\hat{f}_k(q',p')\cos q' \quad , \quad m_y[\hat{f}_k] = \iint dq'\,dp'\,\hat{f}_k(q',p')\sin q'$$

Dispersion relation

$$\left(1 + \pi c_k(\alpha)\int dp \frac{f_0'(p)}{p\left(1+\frac{{\lambda_k}^2}{p^2}\right)}\right)^2 + \left(\pi c_k(\alpha)\int dp \frac{f_0'(p)}{p^2\left(1+\frac{{\lambda_k}^2}{p^2}\right)}\right)^2 = 0.$$

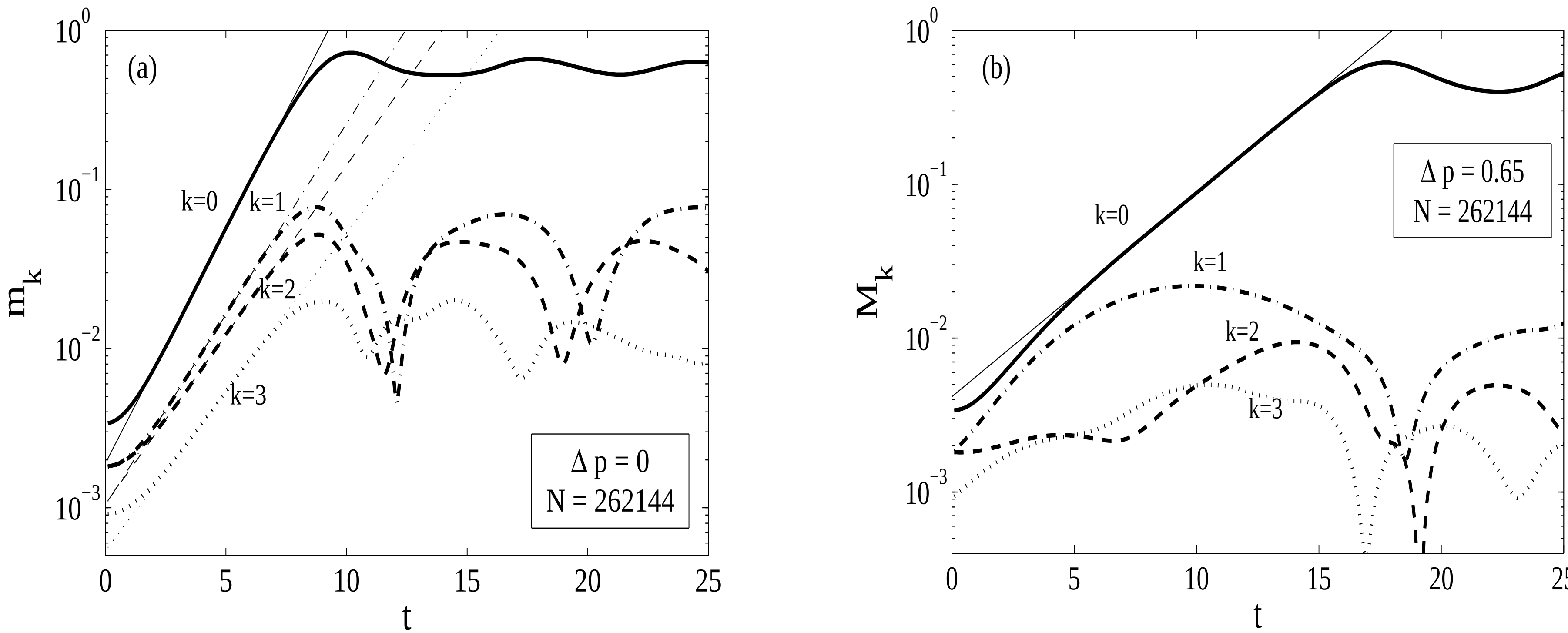
Waterbag distribution

$$f_0(p) = \frac{1}{2\pi}\frac{1}{2\Delta p}\left(\Theta(p+\Delta p) - \Theta(p-\Delta p)\right),$$

The eigenvalue of the k-th Fourier mode is given by

$$\lambda_k = \sqrt{\frac{c_k(\alpha)}{2} - \Delta p^2}.$$

Zero-mode dominance-I



$$m_k = \left| \int e^{-ikx} e^{iq} f(q,p;x,t) dq\, dp \right| \approx \frac{1}{N} \left| \sum_j e^{-ikx_j} e^{iq_j} \right|, \; \alpha = 0.8$$

Overdamped Langevin dynamics

Langevin dynamics (canonical ensemble) Gupta, Campa and SR, 2012

$$\frac{d\theta_i}{dt} = \frac{1}{\widetilde{N}} \sum_{j=1, j\neq i}^{N} \frac{\sin(\theta_j - \theta_i)}{(|j-i|_c)^\alpha} + \eta_i(t)\,,\ \langle \eta_i(t) \rangle = 0\,,\ \langle \eta_i(t)\eta_j(t') \rangle = 2T\delta_{ij}\delta(t-t')$$

$s = i/N \in [0,1]$, local density $\rho(\theta; s, t)$

Smoluchowski equation

$$\frac{\partial \rho}{\partial t} = -\kappa(\alpha)\frac{\partial}{\partial \theta}\Big[\Big(\int d\theta' ds' \frac{\sin(\theta'-\theta)}{(|s'-s|_c)^\alpha}\rho(\theta'; s', t)\Big)\rho\Big] + T\frac{\partial^2 \rho}{\partial \theta^2}.$$

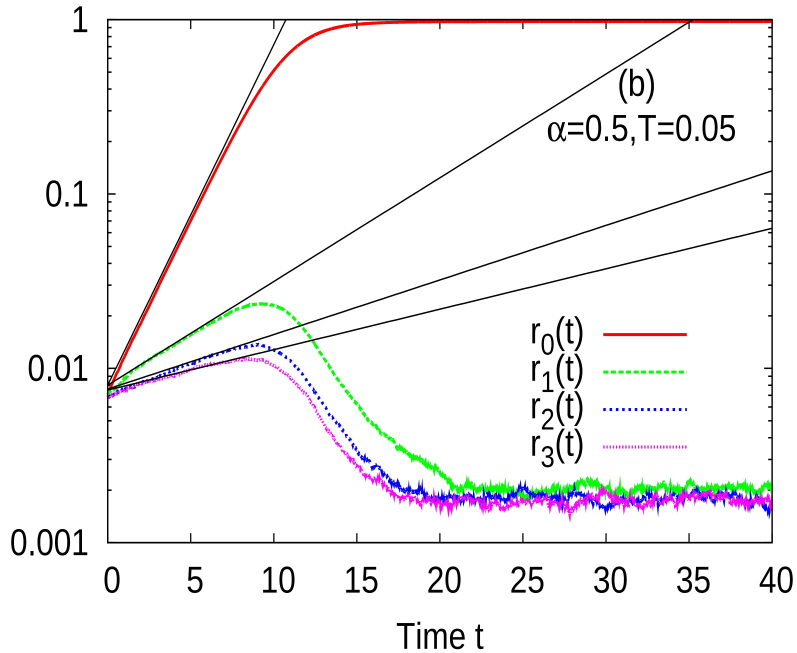
Linearized Smoluchowski equation around the homogeneous state $\rho_0 = 1/(2\pi)$.

$$\frac{\partial \delta\rho}{\partial t} = \frac{\kappa_\alpha}{2\pi}\int d\theta' ds' \, \frac{\cos(\theta'-\theta)}{(|s'-s|_c)^\alpha}\delta\rho(\theta'; s', t) + T\frac{\partial^2 \delta\rho}{\partial \theta^2}.$$

Mode k grows if

$$T < T_{c,k} = \frac{c_k(\alpha)}{2}$$

Zero mode dominance-II



$$r_m(t) = \frac{1}{N}\left|\sum_{j=1}^{N} e^{i(\theta_j + 2\pi jm/N)}\right|; m = 0, 1, 2, \ldots$$

Conclusions

- Long-range interacting systems show unusual properties both in equilibrium and out of equilibrium: ensemble inequivalence, negative specific heat, temperature jumps, quasistationary states, etc.
- These effects could be observable in experimental conditions: dipolar systems, cold atoms, etc.

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