

Long Range Interactions: A dynamic and thermodynamic study of a discrete mean field model

Miguel Filipe de Sousa Vairinhos Pinhão

Under supervision of Professor Rui Vilela Mendes

Dep. Physics, IST, Lisbon, Portugal

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Abstract

Long Range systems are systems which potential decays at large distances as $V(r) \sim 1/r^\alpha$, with $\alpha \leq d$. The non-additivity of such systems give rise to ensemble inequivalence and strange thermodynamic behaviours. The hamiltonian mean field model (HMF) represents a paradigmatic example of this class of systems. In this study, a review over the basic tools used when studying the thermodynamics of long range interactions. It will also be made a review of the thermodynamic properties of the HMF model as well as a study of its phase transitions in both the canonical and microcanonical ensembles.

Since it is not possible to calculate the exact Lyapunov spectrum of the HMF, a new mean field model will be introduced, so that the dynamics of this model can be thoroughly studied with a relation to the Lyapunov spectrum calculated, and then compared with the dynamic behaviour of the HMF model. The thermodynamic study of the new model will also be made with the purpose of looking for similar phase transitions and thermodynamic behaviour as the ones found in the HMF.

Keywords: long range interaction, hamiltonian mean field, Lyapunov spectrum, ensemble inequivalence, phase transitions

1 Introduction

For systems with long-range interactions, the two-body potential decays at large distance as $V(r) \sim 1/r^\alpha$, with $\alpha \leq d$ where d is the dimension of

the space. Examples of this systems are gravitational systems, two-dimensional elasticity, two-dimensional hydrodynamic, charged and dipolar systems. Although such systems can be made extensive by using a scale-factor, they are intrinsic

sically *non additive*. The sum of the energy of macroscopy subsystems is not equal to the energy of the system. The space accessible macroscopic thermodynamic parameters might be non convex. The violation of this properties is at the origin of the *ensemble inequivalence*.

Long-Range Interactions concern a wide range of interesting problems in physics. As a counterpart, this systems are, to a large extent, only poorly understood, with the main challenge being the thermodynamic treatment of this systems and understanding the differences and analogies between the various and numerous domains of this application. New and promising results have been obtained by combining known tools developed by standard statistical mechanics and methods from dynamical systems. The most exciting results are obtained when studying phase transitions for long range interaction systems (negative specific heat, and temperature jumps).

2 Hamiltonian Mean Field

Mean Field systems are those in which $\alpha = 0$ and thus, the interaction does not depend on the distance. The potential of the model rises from the first mode of the fourier expansion of the potential of the one dimensional gravitational and charged sheet models. In a simpler approach it represents a system of particles all moving on a circle, all coupled by a equal attractive or repulsive interaction.

The most common example is that of N parti-

cles moving on a circle coupled by a cosine. Such hamiltonian is

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

Here the variables p_i are the momenta conjugate to θ_i , which is the angle describing the state of the i th particle.

One can introduce macroscopic variables to help understand the physical meaning of the model. Consider the variance of momentum, $T(t)$, and the modulus of the mean field, $M(t)$, respectively defined as,

$$T(t) = \frac{1}{N} \sum_{j=1}^N p_j(t)^2 \quad \mathbf{M} = M(t) e^{i\phi(t)} = \frac{1}{N} \sum_{j=1}^N e^{i\theta_j(t)} \quad (2)$$

In equilibrium those are nothing more that the temperature and the magnetization of the system, respectively. One can rewrite the Hamiltonian (1),

$$H = \frac{1}{2} \sum_{i=1}^N p_i^2 + \frac{JN}{2} (1 - \mathbf{M}^2) \quad (3)$$

Let's consider the ferromagnetic case, setting $J = 1$ without loss of generality, and let's make a simple review over the canonical and microcanonical thermodynamics of this system.

The canonical solution to this problem can be easily derived. Start by calculating the partition function. For this calculation we will use the hamiltonian obtained in (3). The integral over the momenta is a straightforward gaussian integral,

$$Z = \left(\frac{2\pi}{\beta}\right)^{N/2} \int_{-\pi}^{\pi} d^N \theta_i e^{\frac{-\beta J N}{2}(1-M^2)} \quad (4)$$

Using the Hubbard-Stratonovich transformation one obtains

$$Z = \left(\frac{2\pi}{\beta}\right)^{N/2} e^{\frac{-\beta J N}{2}} L \quad (5)$$

with

$$L = \frac{1}{P_i} \int_{-\pi}^{\pi} d^N \theta_i \int_{-\infty}^{+\infty} d\mathbf{y} e^{-\mathbf{y}^2 + \sqrt{2\mu} \mathbf{M} \cdot \mathbf{y}} \quad (6)$$

and $\mu = \beta J N$. We will now use the definition of the magnetization in (2) and exchange the order of the integrals, factorizing the integration over the coordinates of the particles. Also rescaling the variable $\mathbf{y} \rightarrow \mathbf{y} \sqrt{N/2\beta J}$, one gets the following expression for the partition function,

$$Z = \left(\frac{2\pi}{\beta}\right)^{N/2} \frac{N}{2\pi\beta J} e^{\frac{-\beta J N}{2}} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} e^{\frac{y^2}{2\beta J} - \ln(2\pi I_0(y))} \quad (7)$$

The last integral can be evaluated by using the saddle point method. This means that one gets for the rescaled free energy in the thermodynamic limit,

$$\phi = \beta f = - \lim_{N \rightarrow +\infty} \frac{\ln Z}{N} = -\frac{1}{2} \ln \left(\frac{2\pi}{\beta}\right) + \frac{J\beta}{2} + \max_y \left(\frac{y^2}{2\beta J} - \ln(2\pi I_0(y)) \right) \quad (8)$$

The maximum condition leads to the following consistency equation,

$$\frac{y}{\beta J} = \frac{I_1(y)}{I_0(y)} \quad (9)$$

This equation can be solved graphically, and one sees that for $J < 0$ there is a unique solution that is $y = 0$, which means that in the antiferromagnetic case there is no phase transition. On the other side, in the ferromagnetic case, there are two solutions. Those solutions are easily obtained graphically because I_1/I_0 is positive for $y > 0$. Thus one obtain that for $\beta < 2$ there is a unique solution $y = m^* = 0$ and for $\beta > 2$ the solution increases with β , approaching $m^* = 1$ for $\beta \rightarrow \infty$.

One now calculates the energy per particle by deriving the free energy with respect to β ,

$$\epsilon(\beta) = \frac{1}{2\beta} + \frac{1}{2} - \frac{1}{2} (m^*(\beta))^2 \quad (10)$$

the lower bound to the energy is 0. At the critical temperature the energy is $\epsilon_c = 3/4$.

We will now calculate the entropy in the microcanonical ensemble. The simplicity of the hamiltonian makes it possible to obtain directly the thermodynamic limit of the entropy per particle. The method used here was ‘‘borrowed’’ from self-gravitating systems.

The number of microscopic configurations corresponding to the total energy E is given by,

$$\Omega(E, N) = \int \prod_i dp_i d\theta_i \delta(E - H_N) \quad (11)$$

$$= \int dK \underbrace{\int \prod_i dp_i \delta\left(K - \sum_i \frac{p_i^2}{2}\right)}_{\Omega_{\text{Kin}}(K)} \underbrace{\int \prod_i d\theta_i \delta(E - K - U(\{\theta_i\}))}_{\Omega_{\text{conf}}(E-K)} \quad (12)$$

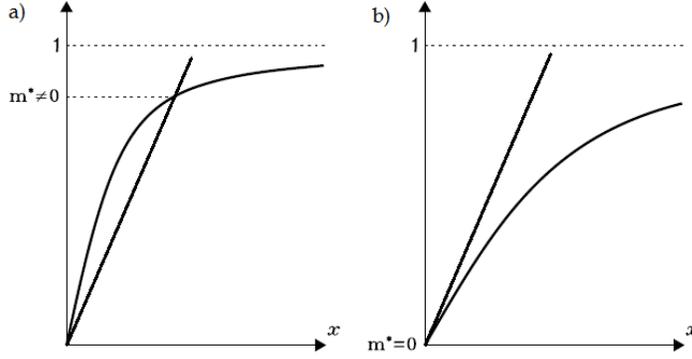


Figure 1: Graphical Resolution for (9). For a) $\beta = 4 > \beta_c = 2$ and the equilibrium solution is $m^* \neq 0$. In b) $\beta = 1.5$, the unique solution is $m^* = 0$.

The first integral gives,

$$\Omega_{\text{Kin}} = \frac{2\pi^{N/2} R^{N-2}}{\Gamma(N/2)} \quad (13)$$

and with a definition of configurational entropy per particle,

$$s_{\text{conf}}(\tilde{u}) = \frac{\ln \Omega_{\text{conf}}(N\tilde{u})}{N} \quad (14)$$

where $\tilde{u} = U/N = (E - K)/N = \epsilon - u/2$, the formula (12) can be rewritten as

$$\Omega(N\epsilon, N) \sim \frac{N}{2} \int du \exp \left[N \left(\frac{1}{2} + \frac{\ln(2\pi)}{2} + \frac{1}{2} \ln u + s_{\text{conf}}(\tilde{u}) \right) \right] \quad (15)$$

if $N \rightarrow \infty$. Hence, solving the integral in the saddle point approximation, one obtains the following entropy

$$s(\epsilon) = \lim_{N \rightarrow \infty} \frac{1}{N} \ln \Omega_N(\epsilon N) \quad (16)$$

$$= \frac{1}{2} + \frac{1}{2} \ln(2\pi) + \sup_u \left[\frac{1}{2} \ln u + s_{\text{conf}}(\tilde{u}) \right] \quad (17)$$

One can use the fact that the potential energy of the HMF model, as seen in (3), is a very simple function of the magnetization. If we define,

$$\Omega_m(M) = \int \prod_i d\theta_i \delta \left(\sum_i \cos \theta_i - NM \right) \delta \left(\sum_i \sin \theta_i \right) \quad (18)$$

we have that this function will be proportional to Ω_{conf} for $\tilde{u} = U/N = (1/2 - M^2/2)$. The above integral can be computed using the Fourier representation of the δ -function,

$$\Omega_m(M) = \left(\frac{1}{2\pi} \right)^2 \int_{-\infty}^{\infty} dq_1 \int_{-\infty}^{\infty} dq_2 \exp \left[N \left(-iq_1 M + \ln J_0 \left((q_1^2 + q_2^2)^{1/2} \right) \right) \right] \quad (19)$$

To solve the integral (19) using the saddle point method, we have to consider q_1 and q_2 as complex variables. The saddle point has to satisfy the following equations,

$$-iM - \frac{J_1}{J_0} \left((q_1^2 + q_2^2)^{1/2} \right) \frac{q_1}{(q_1^2 + q_2^2)^{1/2}} = 0 \quad (20)$$

$$-\frac{J_1}{J_0} \left((q_1^2 + q_2^2)^{1/2} \right) \frac{q_2}{(q_1^2 + q_2^2)^{1/2}} = 0 \quad (21)$$

The solution to these equations is $q_2 = 0$ and $q_1 = i\gamma$ where γ is the solution to the already seen in the canonical ensemble equation,

$$\frac{I_1(\gamma)}{I_0(\gamma)} = M \quad (22)$$

Also, if one uses the properties of the Bessel functions $J_0(iz) = I_0(z)$ and $J_1(iz) = iI_1(z)$ and denote by B_{inv} the inverse function of I_1/I_0 , one gets for the entropy of the configurations the following expression,

$$s_{\text{conf}} \left(\frac{1}{2} - \frac{1}{2}M^2 \right) = \lim_{N \rightarrow \infty} \frac{1}{N} \ln \Omega_m(M) = -MB_{\text{inv}}(M) + \ln I_0(B_{\text{inv}}(M)) \quad (23)$$

Substituting (23) in (17), knowing that $u = 2(\epsilon - 1/2 + M^2/2)$, and performing equivalently a maximization over M instead of u , one gets,

$$s(\epsilon) = \frac{1}{2} + \frac{1}{2} \ln(2\pi) + \frac{1}{2} \ln 2 + \sup_{M > M_0} \left[\frac{1}{2} \ln \left(\epsilon - \frac{1}{2} + \frac{1}{2}M^2 \right) - MB_{\text{inv}}(M) + \ln I_0(B_{\text{inv}}(M)) \right] \quad (24)$$

with $M_0^2 = \sup[0, 1 - 2\epsilon]$. The maximization problem can be solved graphically just by looking for the solutions of the equation,

$$\frac{M}{2\epsilon - 1 + M^2} - B_{\text{inv}}(M) = 0 \quad (25)$$

The graphical solution is shown in Fig. , and it gives the following results. For $0 \leq \epsilon \leq 3/4$,

the magnetization $M(\epsilon)$ decreases monotonically from 1 to 0, while for $\epsilon > 3/4$ the solution is always $M = 0$. At $\epsilon = 3/4$, there is a second order phase transition, which is the first sign that the two ensembles give equivalent predictions.

3 Simplified Hamiltonian Mean Field

In the previous chapter we have made a thermodynamical solution for a Mean-Field system. In this section we will construct a simplified version of the Hamiltonian Mean-Field. The motivation for this comes when one tries to make a dynamical study of the model. For a dynamical study to be accurate one needs to be able to compute the Lyapunov spectra of the system, in the HMF model it is not possible to calculate the exact Lyapunov Spectra due to the trigonometric function of the potential energy. The idea is to make a plausible substitution of the trigonometric part of the potential, the most common thought is to use a quadratic function,

$$H = \frac{1}{2} \sum_{i=1}^N p_i^2 - \frac{J}{2N} \sum_{i,j=1}^N \alpha (\theta_i - \theta_j)^2 \quad (26)$$

where $\alpha > 0$ is a constant that helps on the approximation of the cosine, a simple value would be $1/\pi$, and p_i is the momenta conjugate to $\theta \in]-\pi, \pi[$. The objective is to make a dynamic and thermodynamic study of this model and make a comparison to those already observed and studied of (1) starting by computing the Lyapunov Spectra.

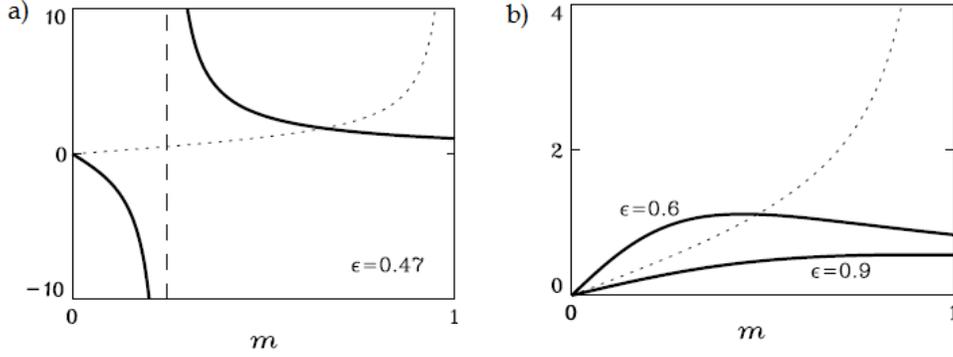


Figure 2: Graphical solution for (25). In a) $\epsilon = 0.47 < 3/4$ there is a unique solution $M \neq 0$. In b) two situations are presented, for $\epsilon = 0.6$ there is one solution $M \neq 0$, for $\epsilon = 0.9$ the unique solution is $M = 0$. In both cases the dotted line represents $B_{\text{inv}}(M)$

Notice that this model is only a valid approximation of the HMF model in the range $\theta \in [-\pi, \pi]$. The qualitative difference between models is the discontinuity on the derivative of the potential on the boundaries $-\pi$ and π .

So that one can compute the Lyapunov Spectra will have to make the map of the model,

$$\dot{\theta}_i = p_i \quad (27)$$

$$\dot{p}_i = -\frac{K}{N} \sum_{j=1}^N (\theta_i - \theta_j) \quad (28)$$

where we introduce the constant $K = J\alpha/N$.

This way the equations of motion of the system were obtained. Now a discrete version of the map will be constructed, the momentum at a given instant will be computed using the value of the momentum and position in the previous instant. For the computation of the position one shall use the newly calculated momentum instead of the mo-

mentum in the previous instant much like the semi-implicit Euler method for differential equations,

$$p_i(t+1) = p_i(t) - \frac{K}{N} \sum_{j=1}^N (\theta_i(t) - \theta_j(t)) \quad (29)$$

$$\begin{aligned} \theta_i(t+1) &= p_i(t+1) + \theta_i(t) = \\ \theta_i(t) + p_i(t) &- \frac{K}{N} \sum_{j=1}^N (\theta_i(t) - \theta_j(t)) \quad (30) \end{aligned}$$

Now one has to calculate the Jacobian matrix and its eigenvalues, The Jacobian can be seen on the top of this page. The eigenvectors of this matrix are easy to obtain,

$$v_1 = [1 \ 1 \ \dots \ 1 \ 0 \ 0 \ \dots \ 0]^T \quad (31)$$

and the others eigenvectors are similar, where the first entrance of the vector is always the same α , but the other entrances differ between 0 and $-\alpha$,

$$J = \begin{bmatrix} 1 - \frac{K}{N}(N-1) & \frac{K}{N} & \dots & \frac{K}{N} & 1 & 0 & \dots & 0 \\ \frac{K}{N} & 1 - \frac{K}{N}(N-1) & \dots & \frac{K}{N} & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{K}{N} & \frac{K}{N} & \dots & 1 - \frac{K}{N}(N-1) & 0 & 0 & \dots & 1 \\ -\frac{K}{N}(N-1) & \frac{K}{N} & \dots & \frac{K}{N} & 1 & 0 & \dots & 0 \\ \frac{K}{N} & -\frac{K}{N}(N-1) & \dots & \frac{K}{N} & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{K}{N} & \frac{K}{N} & \dots & -\frac{K}{N}(N-1) & 0 & 0 & \dots & 1 \end{bmatrix}$$

$$v_2 = \left[\alpha \quad -\alpha \quad 0 \quad \dots \quad 0 \quad -1 \quad 1 \quad 0 \quad \dots \quad 0 \right]^T \quad (32)$$

One of the eigenvalues is 1 and the other eigenvalues will obey the relation

$$\begin{cases} \lambda = \frac{\alpha - K\alpha - 1}{N} \\ \lambda = \frac{K\alpha + 1}{1} \end{cases} \quad (33)$$

solving the system one obtains,

$$\lambda_{\pm} = K \left(\frac{1}{K} - \frac{1}{2} \pm \frac{1}{2} \sqrt{1 - \frac{4}{K}} \right) \quad (34)$$

which means that the system has one eigenvalue equal to 1, $(N-1)/2$ with λ_+ , and $(N-1)/2$ with λ_- . One can see that in the interval $K \in]0, 4[$ the value λ_{\pm} is imaginary.

A simple study of these values brings some simple conclusions: the modulus of the eigenvalues obtained here are e^{λ_i} where λ_i are the Lyapunov exponents, there is always one exponent that's equal

to 0 meaning that the system evolves in time never converging to a single point and conserving the total momentum much like a flow; second, for $K < 0$ half of the characteristic exponents obey $|e^{\lambda_i}| > 1$, and the other half $|e^{\lambda_i}| < 1$, making the system chaotic and not stable; third, for $K > 0$ one has to divide the system in two intervals, first when $K \in]0, 4[$, the real part of all the exponents obey $|\text{Re } e^{\lambda_i}| < 1$ meaning that the system will show some stability, in this interval the Lyapunov spectra also has an imaginary part, also notice that the norm of the eigenvalues of the jacobian in this range is 1; in the interval $[4, +\infty[$ the system is again chaotic having half of the exponents $|e^{\lambda_i}| > 1$, and the other half $|e^{\lambda_i}| < 1$.

The dynamic study in all the simulations has a number of particles $N = 10$. First, one has shown that only in the case where $K > 0$ one has an interval where the real part of all the Lyapunov exponents are < 0 , more accurately for $K \in]0, 4[$.

In this regime ($K > 0$) the N bodies are attracting each other. The initial θ_i was obtained randomly in the range $[-\pi, \pi]$ and the initial momenta is 0. The first remark is that this system is extremely sensible to the initial conditions, if the momentum is set to 0 in the initial moment $t = 0$, then the system will mostly show a strange attractor. Although it does not converge, the particles will gather around a fixed point and rotate around it in the phase space, mostly at the same speed, forming a cluster and following the behaviour of that cluster.

On the other hand, if the initial momentum is set randomly in the range $] -0.1, 0.1[$, the system starts to show a behaviour similar to the case where $p = 0$ but as the time evolves the system enters in a chaotic kinematics. Until $t = 40$ the system forms a cluster, being periodic in the momentum, but quickly evolving to a chaotic behaviour. This is observed for K in the range $]0, 1[$, the phase space plot shows that in the initial moments the system tends to form limit cycles but then adopt a chaotic form.

For $K = 1$ and initial momentum 0 the system evolves periodically around a point, both θ and the momentum. If on the other hand the momentum is chosen randomly between $] -0.1, 0.1[$ the phase space shows that the system follows lines where the momentum is constant.

In the range $[4, +\infty[$ the Lyapunov spectra becomes pure real, with half of the spectre obeying $\text{Re } \lambda_l < 0$ and the other half approaching

∞ . The behaviour shown by the system is a behaviour mostly chaotic, for both initial momentum 0 and $\neq 0$. No clustering formation or periodicity is found in this case and all the phase space is available for (θ_i, p_i) .

Simple remarks can be made for the attractive case, first, both the periodicity and cluster formation was observed in the interval where the real part of all Lyapunov exponents is lesser than 0, the system in this case shows some stability. Second, although it was only observed in the range $K \in]0, 1[$ with initial momentum not equal to 0, the existence of a small interval of time where the momentum is periodic and θ shows clustering evolving to chaotic behaviour should be expected in all the range $K \in]0, 4[$, it might not have been observed because the time necessary for the system to evolve into a chaotic state is too small to observe. Cases where the formation of clusters was seen only for initial momentum equal to 0 has already been seen by T. Konishi and K. Kaneko [6].

Another interesting out-of-equilibrium starting conditions is the so called "bag of water". All of the particles are clustered with $\theta_0 = 0$ and the momentum following a normal distribution around the point $p = 0$ with a standard deviation of 0.5.

In the range $K \in]0, 4[$, the results obtained do not vary from the ones obtained in the previous case, the system presents clustering in the beginning and soon evolves to a chaotic behaviour. The only difference is in the cases $K = 1$, $K = 2$ e $K = 3$ where one can see that the momentum

evolves between clusters oscillating around 0 and around other values different to 0. In the position this translates into a behaviour where one has clustering evolving in t a chaotic behaviour and then to clustering again. In this case the time for the integration was $t = 200$. The phase space plots also show that the particles tend to evolve around a point while moving as a cluster. For the specific cases of $K = 1$, $K = 2$ and $K = 3$ the phase space shows that particles tend to follow lines in the phase space.

4 Conclusion

Reviewing the overall work done in this thesis one can see that the study of long-range interactions can be split in two: first the thermodynamic study in both the canonical and microcanonical ensemble; second, the dynamic study made by varying different parameters.

The study over the Hamiltonian Mean Field does not show ensemble inequivalence, but has shown the existence of a second order phase transition between a synchronized state (where the magnetization is not null) and a state with no synchronization.

A model has been constructed that could show similar dynamic behaviour to the HMF and its exact Lyapunov spectre has been computed. As expected, a Lyapunov exponent with value 0 has been found, since these models behave like a flow. Also has been shown that when the real part of all

the spectre it's lower than 0 dynamic stable states are found, in this case the Jacobian has imaginary eigenvalues, the modulus of the eigenvalues is 1 in the interval which corresponds to an effective characteristic exponent of 0. The existence of clustering in the HMF might as well be related to the existence of imaginary eigenvalues of the jacobian just like the simplified model studied here. This fact cannot be proved by calculating the local Lyapunov exponent numerically. It has also been showed that different initial conditions have great influence on the behaviour. With initial momentum equal to 0, clustering has been found. With small momentum, a clustering state with finite life-time is found.

For the “bag of water” intital conditions the clustering on the range $K \in]0, 4[$ was clearly seen and for integer K a new behaviour was seen, the clusters have a tendency to reappear even after the system has entered a chaotic behaviour.

This shows that this apparently simple models show a great variety of behaviours. It is also important to try to make a link between the thermodynamics and the dynamics of long range systems, since such investigations are important to make us understand self gravitating systems and plasmas. Also, the phase transitions and clustered states have high importance in understanding the atomic clusters and nuclei. The mean-field models can help us make that important bridge. It is also important to learn more about the out-of-equilibrium states as well as characterize them.

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