Master 2ème année
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Exam of the lecture "Physics of Long-Range Interacting Systems"

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13h30-16h : Handwritten lecture notes allowed

Self-gravitating particles

1 Klimontovich and Vlasov equations

Let us consider N self-gravitating particles of mass m interacting through the gravitational interaction.

1(a) Give the equations of motion of the point particle i of mass m located in the position $\mathbf{r}_i$ in the three-dimensional configuration space and denoting its velocity by $\mathbf{v}_i$. It is useful to introduce the gravitational potential $\phi(\mathbf{r}, t)$.

1(b) Define the associate discrete time-dependent density function f_d.

1(c) Give the relation between the microscopic density $n(\mathbf{r}, t)$ and the discrete density function f_d.

1(d) By differentiating with respect to time the density function, derive the Klimontovich equation (Hint: it involves derivatives of the gravitational field).

1(e) What are the advantages and the difficulties of the Klimontovich equation?

1(f) Explain the strategy to go further.

1(g) Derive the Vlasov equation for the gravitational interaction.

2 The infinite mass problem

2.1 The singular isothermal sphere profile

2.1(a) Using the Boltzmann entropy

$$S = -\int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, f(\mathbf{r}, \mathbf{v}, t) \ln f(\mathbf{r}, \mathbf{v}, t) \tag{1}$$

and the constraints on the number of particles N and on the total energy E, derive the expression for the one-particle distribution function $f(\mathbf{r}, \mathbf{v}, t)$.

2.1(b) Recall briefly the method used during the lecture on gravitation to obtain the equation

$$\Delta\phi = 4\pi\mathcal{G}mB\exp(-\beta m\phi), \tag{2}$$

for self-gravitating particles.

2.1(c) Show that $\phi(r) = [1/(m\beta)] \ln(Cr^2)$ is solution. Give the constant C.

2.1(d) Give the expression of the number density $n(r)$. Explain why it is called the singular isothermal sphere profile.

2.1(e) Derive from the density number the total mass M. What is your conclusion?

2.2 The non singular isothermal sphere profile

A first tentative to solve this issue is to consider non singular solutions by considering the mean-field equation as

$$\Delta\phi = 4\pi\mathcal{G}mn_0 \exp[-\beta m(\phi - \phi_0)], \tag{3}$$

in which n_0 and ϕ_0 are the central number density and potential.

2.2(a) Rewrite the equation using the new variables $\psi = m\beta(\phi - \phi_0)$ and $\rho = r\sqrt{4\pi\mathcal{G}m^2n_0\beta}$.

2.2(b) To derive the asymptotic behavior of ψ at long distance (r or $\rho \to \infty$), it is convenient to introduce $\theta = \ln\rho$ and $u = -\psi + 2\theta$. Show that one gets

$$\frac{\mathrm{d}^2u}{\mathrm{d}\theta^2} + \frac{\mathrm{d}u}{\mathrm{d}\theta} + \alpha\exp(u) - \gamma = 0. \tag{4}$$

Give the value of α and γ.

2.2(c) Using a simple mechanical analogy derive the $\lim_{\theta\to\infty} u$.

2.2(d) From the previous result, derive the asymptotic expression for the number density at long distance.

2.2(e) What is your conclusion?

3 The virial theorem and its consequence

3(a) Using the Newton's law, give two different expressions for $\mathbf{F}_i$, the force on the particle i.

3(b) Multiplying above expressions by $\mathbf{r}_i$ and summing on all particles, show that one leads directly to the potential energy E_p, while the other leads to $\dot{S} - 2E_c$ with E_c the kinetic energy and $S = \sum_i \mathbf{r}_i\mathbf{p}_i$.

3(c) What is the relationship between kinetic and potential energy for a stationary system?

3(d) If one introduces the time average, $\langle K\rangle_\tau = \frac{1}{\tau}\int_0^\tau K$, show that $\langle E_p\rangle_\tau + 2\langle E_c\rangle_\tau \simeq 0$.

3(e) Recalling that the total energy E is constant, propose a simple argument which justifies the presence of a negative specific heat for this gravitational system.

3(f) How does one generalize the virial theorem if the force between any two particles of the system results from a potential energy $V(r) = A\,r^\alpha$?

4 The statistical mechanics of the HMF model using large deviations

The Hamiltonian Mean Field model is defined by the following Hamiltonian

$$H_N = \sum_{i=1}^{N} \frac{p_i^2}{2} + \frac{J}{2N} \sum_{i,j=1}^{N} \left[1 - \cos(\theta_i - \theta_j)\right], \tag{5}$$

where $\theta_i \in [0, 2\pi[$ is the position (angle) of the i-th unit mass particle on a circle and p_i the corresponding conjugated momentum.

4(a) Using trigonometric identities, simplify the potential energy as a function of the magnetization per site m.

4(b) Identify the global variables necessary to apply the large deviation method.

4(c) Give the expression of the energy per particle as a function of these global variables.

4(d) Compute the associated generating function ψ.

4(e) Derive the following expression for the free energy

$$\bar{\phi}(\lambda_u, \lambda_x, \lambda_y) = C + \frac{1}{2} \ln \lambda_u - \ln I_0 \left(\sqrt{\lambda_x^2 + \lambda_y^2} \right), \tag{6}$$

in which one has to determine the constant C.

4(f) Compute the entropy function $\bar{s}(u, m_x, m_y)$. Call B_{inv} the inverse function of I_1/I_0, where $I_0(z)$ and $I_1(z)$ are the modified Bessel function of order 0 and 1, respectively.

4(g) Derive finally the entropy $s(u)$.

4(h) Aiming at comparing the canonical and microcanonical ensembles, we turn to calculate the rescaled canonical free energy. Give the expression relating $\phi(\beta)$ to $\bar{s}(\mu_1, \dots, \mu_n)$.

4(i) Identify an additional global variable, which does not appear in the Hamiltonian, but which is a conserved quantity. By taking into account this additional variable, derive the entropy using a similar procedure.

Let us recall that for integer indices the modified Bessel functions of order n is defined by

$$I_n(z) = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\theta \, e^{z \cos\theta} \cos(n\theta). \tag{7}$$

Correction of the exam

1. Klimontovich and Vlasov equations for self-gravitating particles

1(a) Assume that the point particle i of mass m occupies position $\mathbf{r}_i$ in the three-dimensional configuration space. Its velocity will be denoted by $\mathbf{v}_i$. The position $\mathbf{r}_i$ satisfies

$$\mathbf{v}_i = \dot{\mathbf{r}}_i \tag{8}$$

and likewise the velocity of particles i obeys the following equation

$$m\dot{\mathbf{v}}_i = -m\nabla_{\mathbf{r}_i}\,\phi(\mathbf{r}_i(t), t), \tag{9}$$

where ϕ is defined by the Poisson equation

$$\Delta\,\phi(\mathbf{r}, t) \quad = \quad 4\pi\mathcal{G}m\,n(\mathbf{r}, t), \tag{10}$$

in which $n(\mathbf{r}, t)$ is the microscopic density of particles.

1(b) The kinetic equation of motion can be derived by resorting to the Klimontovich equation. The discrete density $f_d(\mathbf{r}, \mathbf{v}, t)$ of N such particles in the six-dimensional phase space $(\mathbf{r}, \mathbf{v})$ reads

$$f_d(\mathbf{r}, \mathbf{v}, t) = \frac{1}{N}\sum_{i=1}^{N}\delta(\mathbf{r} - \mathbf{r}_i(t))\delta(\mathbf{v} - \mathbf{v}_i(t)). \tag{11}$$

1(c) The microscopic density relation can be written as

$$n(\mathbf{r}, t) = \int \mathrm{d}\mathbf{v}\, f_d(\mathbf{r}, \mathbf{v}, t). \tag{12}$$

1(d) An exact equation for the evolution of the system of charged particles is obtained by taking the time derivative of the density $f_d(\cdot)$. This immediately yields

$$\begin{aligned}\frac{\partial f_d(\mathbf{r}, \mathbf{v}, t)}{\partial t} \quad = \quad & - \quad \frac{1}{N}\sum_{i=1}^{N}\dot{\mathbf{r}}_i \cdot \nabla_{\mathbf{r}}\delta(\mathbf{r} - \mathbf{r}_i(t))\delta(\mathbf{v} - \mathbf{v}_i(t)) \\ & - \quad \frac{1}{N}\sum_{i=1}^{N}\dot{\mathbf{v}}_i \cdot \nabla_{\mathbf{v}}\delta(\mathbf{r} - \mathbf{r}_i(t))\delta(\mathbf{v} - \mathbf{v}_i(t)),\end{aligned} \tag{13}$$

where $\nabla_{\mathbf{r}} = (\partial_x, \partial_y, \partial_z)$ and $\nabla_{\mathbf{v}} = (\partial_{v_x}, \partial_{v_y}, \partial_{v_z})$.

By inserting Eq. (8) and Eq. (9) into Eq. (13), one eventually obtains

$$\begin{aligned}\frac{\partial f_d(\mathbf{r}, \mathbf{v}, t)}{\partial t} \quad = \quad & - \quad \frac{1}{N}\sum_{i=1}^{N}\mathbf{v}_i \cdot \nabla_{\mathbf{r}}\delta(\mathbf{r} - \mathbf{r}_i(t))\delta(\mathbf{v} - \mathbf{v}_i(t)) \qquad (14) \\ & - \quad \frac{1}{N}\sum_{i=1}^{N}(-\nabla_{\mathbf{r}_i}\,\phi(\mathbf{r}_i(t), t)) \cdot \nabla_{\mathbf{v}}\delta(\mathbf{r} - \mathbf{r}_i(t))\delta(\mathbf{v} - \mathbf{v}_i(t)).\end{aligned}$$

Using the properties of the Dirac function $a\,\delta(a-b) = b\,\delta(a-b)$ yields

$$\frac{\partial f_d(\mathbf{r},\mathbf{v},t)}{\partial t} = - \frac{1}{N}(\mathbf{v}\cdot\nabla_{\mathbf{r}}\sum_{i=1}^{N}\delta(\mathbf{r}-\mathbf{r}_i(t))\delta(\mathbf{v}-\mathbf{v}_i(t)) - (-\nabla_{\mathbf{r}}\,\phi(\mathbf{r},t))\cdot\nabla_{\mathbf{v}}\sum_{i=1}^{N}\delta(\mathbf{r}-\mathbf{r}_i(t))\delta(\mathbf{v}-\mathbf{v}_i(t))), \tag{15}$$

and recalling the definition $f_d(\cdot)$, the previous equation can be cast in the form

$$\frac{\partial f_d(\mathbf{r},\mathbf{v},t)}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{r}} f_d(\mathbf{r},\mathbf{v},t) - \nabla_{\mathbf{r}}\,\phi(\mathbf{r},t)\cdot\nabla_{\mathbf{v}} f_d(\mathbf{r},\mathbf{v},t) = 0, \tag{16}$$

the *Klimontovich equation* which, together with the Poisson-Newton equation

$$\Delta\,\phi(\mathbf{r},t) = 4\pi\mathcal{G}m\int \mathrm{d}\mathbf{v}\, f_d(\mathbf{r},\mathbf{v},t), \tag{17}$$

provides an exact and general description of any self-gravitating system.

1(e) By assigning initial particles position and velocity, one can clearly reconstruct the associated densities $f_d(\mathbf{r},\mathbf{v},t=0)$. The system is hence completely deterministic and both density and gravitational field can be in principle traced as a function of time and in any position of the generalized phase space. This is an exact equation.

However the amount of information embedded in the Klimontovich description is enormous. Equation (16) explicitly contains in fact the orbits of each individual microscopic entity belonging to the system.

1(f) When looking at average quantities, one is primarily interested in knowing how many particles found in a small volume $(\Delta\mathbf{r},\Delta\mathbf{v})$ of phase space, positioned in $(\mathbf{r},\mathbf{v})$. In other terms, it is tempting to invoke an appropriate ensemble average $\langle\cdot\rangle$. This is an average over realizations of the system prepared according to assigned prescriptions. Therefore, we focus on the smooth function

$$f_0(\mathbf{r},\mathbf{v},t) = \langle f_d(\mathbf{r},\mathbf{v},t))\rangle. \tag{18}$$

An equation for the time evolution of the distribution function $f_0(\mathbf{r},\mathbf{v},t)$ can be recovered from the Klimontovich Eq. (16) by this ensemble averaging. To this end we define the quantities $\delta f$and δB as obeying the following relations

$$f_d(\mathbf{r},\mathbf{v},t) = f_0(\mathbf{r},\mathbf{v},t)) + \frac{1}{\sqrt{N}}\delta f(\mathbf{r},\mathbf{v},t), \tag{19}$$

$$\phi(\mathbf{r},\mathbf{v},t) = \phi_0(\mathbf{r},\mathbf{v},t)) + \frac{1}{\sqrt{N}}\delta\phi(\mathbf{r},\mathbf{v},t). \tag{20}$$

The index 0 labels the averaged quantities, namely $\phi_0 = \langle\phi\rangle$, and the factor $1/\sqrt{N}$ takes into account the typical size of relative fluctuations.

1(g) Inserting these definitions in Eq. (16) and performing the ensemble averaging, we get

$$\frac{\partial f_0(\mathbf{r},\mathbf{v},t)}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{r}} f_0(\mathbf{r},\mathbf{v},t) - \nabla_{\mathbf{r}}\,\phi_0(\mathbf{r},t)\cdot\nabla_{\mathbf{v}} f_0(\mathbf{r},\mathbf{v},t) = -\frac{1}{N}\langle\nabla_{\mathbf{r}}\,\delta\phi(\mathbf{r},t)\cdot\nabla_{\mathbf{v}}\delta f(\mathbf{r},\mathbf{v},t)\rangle. \tag{21}$$

The right-hand side of Eq. (21) is sensitive to the discrete nature of the fluid, while the left-hand side deals with collective variables. In the limit of large systems ($N \to \infty$), one can neglect the right-hand side and consequently obtain the Vlasov equation

$$\frac{\partial f_0^s(\mathbf{r},\mathbf{v},t)}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{r}} f_0^s(\mathbf{r},\mathbf{v},t) - \nabla_{\mathbf{r}}\,\phi_0(\mathbf{r},t)\cdot\nabla_{\mathbf{v}} f_0^s(\mathbf{r},\mathbf{v},t) = 0, \tag{22}$$

in which the ensemble averaged field ϕ_0 satisfies the ensemble averaged Poisson equation

$$\Delta\phi_0(\mathbf{r},t) = 4\pi\mathcal{G}m\, n_0(\mathbf{r},t), \qquad \text{with} \qquad n_0(\mathbf{r},t) = \int \mathrm{d}\mathbf{v}\, f_0(\mathbf{r},\mathbf{v},t). \tag{23}$$

2. The infinite mass problem

2.1 The singular isothermal sphere profile

2.1(a) The problem is to maximize the entropy S keeping the energy E and the number N constant. Consequently, introducing the associated Lagrange multipliers that we denote respectively by β and α, one obtains the most probable density by canceling the first variation, which leads to

$$\delta S - \beta\delta E - \alpha\delta N = 0. \tag{24}$$

After some algebra, one can write the energy variation δE as

$$\delta E = \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\,\delta f\left(\frac{p^2}{2m} + m\phi(\mathbf{r},t)\right) \tag{25}$$

where the mean gravitational field $\phi(\mathbf{r},t)$ follows from the Poisson equation

$$\Delta\phi(\mathbf{r},t) = 4\pi\mathcal{G}m\, n(\mathbf{r}), \tag{26}$$

and reads

$$\phi(\mathbf{r},t) = -\mathcal{G}\int \mathrm{d}\mathbf{r}'\,\frac{m\, n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}. \tag{27}$$

Taking advantage from the above expression for δE and substituting into (24), one eventually gets

$$-\int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\,\delta f\left[\log f + 1 + \beta\left(mv^2/2 + m\phi\right) + \alpha\right] = 0, \tag{28}$$

which returns

$$\log f + 1 + \beta\left(mv^2/2 + m\phi\right) + \alpha = 0, \tag{29}$$

and finally

$$f = A\exp(-\beta(mv^2/2 + m\phi)), \tag{30}$$

where $A = \exp(-\alpha - 1)$. The two constants A and β are determined by the constraints.

2.1(b) Using the definition $n(\mathbf{r},t) = \int \mathrm{d}^3\mathbf{v}\ f(\mathbf{r},\mathbf{v},t)$ and expression (30), the use of the Poisson equation leads directly to the equation (2) with $B = A(2\pi/(m\beta))^{3/2}$.

2.1(c) Using the expression of the Laplacian in spherical coordinates, on has

$$\Delta\phi = \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}(1/(m\beta))\ln(Cr^2)}{\mathrm{d}r}\right) = \frac{1}{m\beta}\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{2}{r}\right) = \frac{2}{m\beta r^2} \tag{31}$$

while

$$4\pi\mathcal{G}mB\exp(-\beta m\phi) = \frac{4\pi\mathcal{G}mB}{Cr^2} \tag{32}$$

and therefore the constant is $C = 2\pi\mathcal{G}m^2B\beta$.

2.1(d) The number density is therefore

$$\begin{aligned} n(r) &= \int \mathrm{d}\mathbf{v}\, f(\mathbf{r},\mathbf{v}) && (33)\\ &= \int \mathrm{d}\mathbf{v}\, A\exp[-\beta(mv^2/2 + m\phi)] && (34)\\ &= \frac{A}{Cr^2}\int \mathrm{d}\mathbf{v}\, \exp[-\beta m v^2/2] && (35)\\ &= \frac{A(2\pi/(m\beta))^{3/2}}{Cr^2} = \frac{B}{2\pi\mathcal{G}m^2B\beta r^2} && (36)\\ &= \frac{1}{2\pi\mathcal{G}m^2\beta r^2}. && (37) \end{aligned}$$

The density therefore decreases at long distance but diverges in the center of the distribution: this is the reason for the name of the singular isothermal sphere profile.

2.1(e) As the system is a priori infinite, one has

$$M = \int_0^{+\infty} n(r)4\pi r^2\mathrm{d}r = \frac{2}{\mathcal{G}m^2\beta}\int_0^{+\infty}\mathrm{d}r \to +\infty \tag{38}$$

The density does not decrease sufficiently fast at long distance, and therefore the total mass diverges.

2.2 The non singular isothermal sphere profile

2.2(a) One gets

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}\rho^2} + \frac{2}{\rho}\frac{\mathrm{d}\psi}{\mathrm{d}\rho} = \exp(-\psi), \tag{39}$$

2.2(b) It is straightforward to get $\alpha = 1$ and $\gamma = 2$.

2.2(c) Above equation is similar to the equation of motion of a damped particle, of mass unity, localized at the pseudo-position u and with the pseudo-time θ moving in the pseudo-potential $V(u) = \exp(u) - 2u$. The particule will oscillate in the potential until reaching, because of the pseudo dissipation, its ground state. Using $V'(u) = 0 = \exp(u) - 2$, one finally gets $u = \ln 2$. One obtains therefore that $\lim_{\theta\to\infty} u = \ln 2$.

2.2(d) Previous result leads to

$$\psi \underset{\rho\to\infty}{\sim} -\ln 2 + 2\ln\rho = \ln(\rho^2/2). \tag{40}$$

and as $\psi = m\beta(\phi - \phi_0)$, one obtains

$$m\beta(\phi - \phi_0) \underset{\rho\to\infty}{\sim} \ln(\rho^2/2), \tag{41}$$

which leads for the density number defined as $n(r) = n_0 \exp[-\beta m(\phi - \phi_0)]$ to the expression

$$n(r) \underset{\rho\to\infty}{\sim} \frac{2n_0}{\rho^2} = \frac{1}{2\pi\mathcal{G}m^2\beta r^2}, \tag{42}$$

We thus get for the asymptotic expression, the function derived within the singular framework.

2.2(e) Consequently the total mass still diverges within this nonsingular isothermal sphere framework. This means that there is no entropy extremum if the system is not bounded. It is always possible to increase the entropy of a self-gravitating system with mass and energy given, spreading the density.

Above result, does not mean however that one should abandon any statistical description. The infinite mass problem and the absence of the equilibrium distribution in the whole space are believed to be wrong problems since, in practice, the relaxation is achieved in subdomains of the whole space and therefore the statistical mechanics applies only in these subdomains.

Several models have been proposed to deal with this incomplete relaxation, and the most well-known is the Michie-King model.

Another possibility is to consider the system bounded in a spherical box of radius R against which stars bounce elastically. Although less realistic, this model is appropriate to pursue the theoretical study as it has been performed during the lecture. Moreover, it leads to valid (and non trivial!) results on the central structure of galaxies, which is only marginally influenced by what happens in the periphery.

3. The virial theorem and its consequence

3(a) Using the Newton law, the force on the particle i is given by

$$\mathbf{F}_i = -\sum_{j\neq i} \mathcal{G}m_i m_j \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3} = m_i \frac{\mathrm{d}^2\mathbf{r}_i}{\mathrm{d}t^2}. \tag{43}$$

3(b) Multiplying above expression by $\mathbf{r}_i$ and summing on all particles, one obtains

$$\sum_i \mathbf{r}_i\mathbf{F}_i = -\sum_{i,j\neq i} \mathcal{G}m_i m_j \frac{\mathbf{r}_i(\mathbf{r}_i - \mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^3} = \sum_i \mathbf{r}_i m_i \frac{\mathrm{d}^2\mathbf{r}_i}{\mathrm{d}t^2} \tag{44}$$

As the indices i and j appearing in the second term are mute, it is possible to write

$$-2\sum_{i,j\neq i} \mathcal{G}m_i m_j \frac{\mathbf{r}_i(\mathbf{r}_i - \mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^3} = -\sum_{i,j\neq i} \mathcal{G}m_i m_j \frac{\mathbf{r}_i(\mathbf{r}_i - \mathbf{r}_j) + \mathbf{r}_j(\mathbf{r}_j - \mathbf{r}_i)}{|\mathbf{r}_i - \mathbf{r}_j|^3} \tag{45}$$

$$= -\sum_{i,j\neq i} \mathcal{G}m_i m_j \frac{(\mathbf{r}_i - \mathbf{r}_j)^2}{|\mathbf{r}_i - \mathbf{r}_j|^3} \tag{46}$$

$$= -\sum_{i,j\neq i} \frac{\mathcal{G}m_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|} = 2E_p \tag{47}$$

as suggested.

For the second expression, one has to use the following identity

$$\frac{\mathrm{d}^2\mathbf{r}_i^2}{\mathrm{d}t^2} = \frac{\mathrm{d}}{\mathrm{d}t}\left(2\mathbf{r}_i\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t}\right) = 2\left(\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t}\right)^2 + 2\mathbf{r}_i\frac{\mathrm{d}^2\mathbf{r}_i}{\mathrm{d}t^2} \tag{48}$$

which leads to

$$\mathbf{r}_i\frac{\mathrm{d}^2\mathbf{r}_i}{\mathrm{d}t^2} = \frac{1}{2}\frac{\mathrm{d}^2\mathbf{r}_i^2}{\mathrm{d}t^2} - \left(\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t}\right)^2. \tag{49}$$

Introducing (47) and(49), Eq. (44) can be simplified as

$$E_p = \sum_i m_i\left(\frac{1}{2}\frac{\mathrm{d}^2\mathbf{r}_i^2}{\mathrm{d}t^2} - \left(\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t}\right)^2\right) \tag{50}$$

$$= \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\left(\sum_i m_i\mathbf{r}_i^2\right) - 2E_c. \tag{51}$$

Introducing the momenta $\mathbf{p}_i$ and the quantity $S = \sum_i m_i\mathbf{r}_i\mathbf{p}_i$, one gets therefore

$$E_p + 2E_c = \frac{\mathrm{d}S}{\mathrm{d}t}. \tag{52}$$

3(c) For a stationary system, on gets $\dot{S} = 0$, and thus $2E_c + E_p = 0$.

3(d) If one introduces the time average, one gets

$$\left\langle\frac{\mathrm{d}S}{\mathrm{d}t}\right\rangle_\tau = \frac{1}{\tau}\int_0^\tau\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{S(\tau) - S(0)}{\tau}. \tag{53}$$

The system being isolated, no mass can escape. Moreover only gravitational interactions being taken into account, there are no collisions. So, the quantity S, which is nothing but the half of the derivative of the moment of inertia $I = \sum_i m_i\mathbf{r}_i^2$, has to be bounded. We have therefore

$$\lim_{\tau\to\infty}\left|\left\langle\frac{\mathrm{d}S}{\mathrm{d}t}\right\rangle_\tau\right| = \lim_{\tau\to\infty}\left|\frac{S(\tau) - S(0)}{\tau}\right| \leq \lim_{\tau\to\infty}\left|\frac{S_{max} - S_{min}}{\tau}\right| = 0. \tag{54}$$

In conclusion, for time averages over sufficiently long times, one has

$$\left|\left\langle\frac{\mathrm{d}S}{\mathrm{d}t}\right\rangle_\tau\right| \simeq 0. \tag{55}$$

Taking the time average of Eq. (52), one ends up with

$$\langle E_p\rangle_\tau + 2\langle E_c\rangle_\tau = \left\langle\frac{\mathrm{d}S}{\mathrm{d}t}\right\rangle_\tau \simeq 0. \tag{56}$$

The word virial derives from vis, the Latin word for “force” or “energy”, and was given its technical definition by Rudolf Clausius in 1870.

3(e) For self-gravitating systems at constant energy (i.e. in the microcanonical ensemble) a simple physical argument which justifies the presence of a negative specific heat has been given by Lynden Bell. It is based on the virial theorem, which, for the gravitational potential, states that $2\langle E_c\rangle + \langle E_p\rangle = 0$. Recalling that the total energy E is constant, we get that

$$E = \langle E_c\rangle + \langle E_p\rangle = -\langle E_c\rangle, \tag{57}$$

Since the kinetic energy defines the temperature, one gets

$$C_V = \frac{\partial E}{\partial T} \propto \frac{\partial E}{\partial E_c} < 0. \tag{58}$$

Loosing its energy, the system becomes hotter.

3(f) If the force between any two particles of the system results from a potential energy $V(r) = A\,r^{\alpha}$ that is proportional to some power α of the inter-particle distance r, one has

$$\begin{aligned}
\sum_i \mathbf{r}_i \mathbf{F}_i &= -\sum_i \sum_{j<i} V'\left(|\mathbf{r}_i - \mathbf{r}_j|\right) |\mathbf{r}_i - \mathbf{r}_j| && (59)\\
&= -\sum_i \sum_{j<i} A\alpha |\mathbf{r}_i - \mathbf{r}_j|^{\alpha-1} |\mathbf{r}_i - \mathbf{r}_j| && (60)\\
&= -\alpha \sum_i \sum_{j<i} A |\mathbf{r}_i - \mathbf{r}_j|^{\alpha} = -\alpha E_p. && (61)
\end{aligned}$$

Consequently, the virial theorem takes the simple form $2\langle E_c\rangle = \alpha\langle E_p\rangle$.

4. The statistical mechanics of the HMF model using large deviations

4(a) Using usual trigonometric identities, one can simplify the potential energy as

$$\begin{aligned}
\sum_{i,j} \cos(\theta_i - \theta_j) &= \sum_{i,j} \left[\cos\theta_i \cos\theta_j + \sin\theta_i \sin\theta_j\right] && (62)\\
&= \sum_i \cos\theta_i \sum_j \cos\theta_j + \sum_i \sin\theta_i \sum_j \sin\theta_j && (63)\\
&= N^2(m_x^2 + m_y^2) = N^2 m^2, && (64)
\end{aligned}$$

with $m = (m_x^2 + m_y^2)^{1/2}$, $m_x = (\sum_{i=1}^N \cos\theta_i)/N$ and $m_y = (\sum_{i=1}^N \sin\theta_i/N)$.

The Hamiltonian of the HMF can thus be rewritten as

$$H_N = \sum_i^N \frac{p_i^2}{2} + N\frac{J}{2}(1 - m^2), \tag{65}$$

4(b) Besides m_x and m_y, the third global variable is

$$u = \frac{1}{N} \sum_i p_i^2. \tag{66}$$

4(c) Hamiltonian (65) can be expressed in terms of the three global variables u, m_x and m_y, and the energy per particle reads

$$\bar{\varepsilon}(u, m_x, m_y) = \frac{1}{2}\left[u + J(1 - m_x^2 - m_y^2)\right] . \tag{67}$$

The above relation is exact for any N.

4(d) To this end we start by computing the generating function ψ

$$\psi(\lambda_u, \lambda_x, \lambda_y) \quad = \quad \int \left(\prod_i \mathrm{d}\theta_i \mathrm{d}p_i\right) \exp\left(-\lambda_u \sum_{i=1}^N p_i^2 - \lambda_x \sum_{i=1}^N \cos\theta_i - \lambda_y \sum_{i=1}^N \sin\theta_i\right), \tag{68}$$

which results in

$$\psi(\lambda_u, \lambda_x, \lambda_y) = \left[\sqrt{\frac{\pi}{\lambda_u}} 2\pi \; I_0\left(\sqrt{\lambda_x^2 + \lambda_y^2}\right)\right]^N . \tag{69}$$

Note that the existence of the integral in Eq. (68) necessarily implies $\lambda_u > 0$.

4(e) The free energy associated with ψ reads

$$\bar{\phi}(\lambda_u, \lambda_x, \lambda_y) = -\frac{1}{2}\ln\pi + \frac{1}{2}\ln\lambda_u - \ln(2\pi) - \ln I_0\left(\sqrt{\lambda_x^2 + \lambda_y^2}\right) . \tag{70}$$

The expression of the constant is therefore $C = -\frac{1}{2}\ln\pi - \ln(2\pi)$.

4(f) We can then calculate the function $\bar{s}$ as

$$\bar{s}(u, m_x, m_y) = \inf_{\lambda_u,\lambda_x,\lambda_y}\left[\lambda_u u + \lambda_x m_x + \lambda_y m_y + \frac{1}{2}\ln\pi - \frac{1}{2}\ln\lambda_u + \ln(2\pi) + \ln I_0\left(\sqrt{\lambda_x^2 + \lambda_y^2}\right)\right] . \tag{71}$$

The above variational problem can be solved explicitly by formally separating the "kinetic" (λ_u) and "configurational" (λ_x, λ_y) subspaces as

$$\bar{s}(u, m_x, m_y) = \bar{s}_{kin}(u) + \bar{s}_{conf}(m_x, m_y). \tag{72}$$

Call B_{inv} the inverse function of I_1/I_0, where $I_0(z)$ and $I_1(z)$ are the modified Bessel function of order 0 and 1, respectively. Then, one obtains

$$\bar{s}_{kin}(u) \quad = \quad \frac{1}{2} + \frac{1}{2}\ln\pi + \ln(2\pi) + \frac{1}{2}\ln 2u \tag{73}$$

$$\bar{s}_{conf}(m) \quad = \quad -mB_{inv}(m) + \ln I_0(B_{inv}(m)). \tag{74}$$

4(g) The next step in the procedure concerns the calculation of the entropy function. Maximizing only with respect to u and m, we obtain

$$s(\varepsilon) \quad = \quad \sup_{u,m}\left[\bar{s}(u, m)\middle|\frac{u}{2} - J\frac{m^2}{2} = \varepsilon\right] \tag{75}$$

$$= \quad \sup_{u,m}\left[\bar{s}_{kin}(u) + \bar{s}_{conf}(m)\middle|\frac{u}{2} - J\frac{m^2}{2} = \varepsilon\right] \tag{76}$$

$$= \quad \frac{1}{2} + \frac{1}{2}\ln 2 + \frac{3}{2}\ln(2\pi) + \frac{1}{2}\ln\left(\varepsilon + J\frac{m^2}{2}\right) - mB_{inv}(m) + \ln I_0(B_{inv}(m)), \tag{77}$$

where m satisfies the self-consistency equation

$$B_{inv}(m) = \frac{Jm}{2\varepsilon + Jm^2}. \tag{78}$$

4(h) The rescaled canonical free energy $\phi(\beta)$ is given by the following extremal problem

$$\phi(\beta) = \beta f(\beta) = \inf_{\mu_1,\ldots,\mu_n} \left[\beta\bar{\varepsilon}(\mu_1,\ldots,\mu_n) - \bar{s}(\mu_1,\ldots,\mu_n)\right]. \tag{79}$$

In the present problem, one gets

$$\phi(\beta) = \frac{\beta J m^2}{2} - \ln(I_0[\beta J m]) + \frac{1}{2}\ln\beta - \frac{3}{2}\ln(2\pi), \tag{80}$$

with m satisfying $B_{inv}(m) = \beta J m$.

4(i) An additional global variable could be identified: the average momentum $v = (\sum_i p_i)/N$, which does not appear in the Hamiltonian, and which is a conserved quantity. Using a similar procedure, one gets the generating function

$$\psi(\lambda_u,\lambda_v,\lambda_x,\lambda_y) = \left[e^{\lambda_v^2/4\lambda_u}\sqrt{\frac{\pi}{\lambda_u}}\,2\pi\; I_0\left(\sqrt{\lambda_x^2+\lambda_y^2}\right)\right]^N, \tag{81}$$

the free energy associated with ψ

$$\bar{\phi}(\lambda_u,\lambda_v,\lambda_x,\lambda_y) = -\frac{\lambda_v^2}{4\lambda_u} - \frac{1}{2}\ln\pi + \frac{1}{2}\ln\lambda_u - \ln(2\pi) - \ln I_0\left(\sqrt{\lambda_x^2+\lambda_y^2}\right). \tag{82}$$

and finally the entropy

$$s(\varepsilon,v) = \frac{1}{2} + \frac{1}{2}\ln 2 + \frac{3}{2}\ln(2\pi) + \frac{1}{2}\ln\left(\varepsilon + J\frac{m^2}{2} - \frac{1}{2}v^2\right) - mB_{inv}(m) + \ln I_0(B_{inv}(m)), \tag{83}$$

where m satisfies the self-consistency equation

$$B_{inv}(m) = \frac{Jm}{2\varepsilon + Jm^2 - v^2}. \tag{84}$$

The entropy $s(\varepsilon)$ is obtained by maximizing with respect to v. It is immediate to see that this is obtained by putting $v = 0$ in Eqs. (83) and (84).

We thus find, as it could be argued on physical basis, that for a given energy ε the entropy is maximum when the average momentum v is equal to 0.