

Ensemble inequivalence in long-range interacting systems

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Abstract: An important result we learn in the statistical physics course is that statistical ensembles are equivalent in the thermodynamic limit. However, a key assumption behind this result is that interactions in the system are short-range. When interactions are long-range, ensemble equivalence cannot be taken for granted. In this TFG, a simplified self-gravitating system is studied as an example of long-range interacting systems. By introducing the Thirring model, we will be able to see how negative specific heat appears in the microcanonical ensemble while in the canonical ensemble this region is replaced with an isothermal first-order phase transition.

I. INTRODUCTION

In the present work we are going to study a solvable model for long-range interacting systems, known as the Thirring Model. This toy model was introduced by Walter Thirring in 1969 [1], and reproduces some of the characteristic properties of self-gravitating systems, such as the presence of negative specific heat in the microcanonical ensemble. By introducing this model, Thirring was able to exemplify how ensemble inequivalence appears in long-range interacting systems by studying the behavior of a non-local potential in an isolated system and comparing it to a system in contact with a heat bath.

When we talk about long-range interactions, we are considering systems whose potential decays as a power law at large distances, $r^{-\alpha}$, and for which the total energy, E , grow superlinearly with volume, V , at constant density. Let be d the dimension of the system. E will grow linearly with volume, if and only if, $\alpha > d$, i.e., the system is extensive (size dependent thermodynamic variables are proportional to system size). In such case, we say that the interactions are *short-range*. On the contrary, if $\alpha \leq d$, E will grow superlinearly with volume, $E \propto V^{2-\alpha/d}$, which violates extensivity. In this case, we say that the interactions are *long-range* or *non-integrable*, just referring to the energy divergence [2].

Long/short-range interactions are intrinsically related to *additive* nature of systems. We say that a system is additive when dividing it into different subsystems, each with a certain energy, the total energy is comparable to the sum of the energies of each subsystem separately, while the interaction energy between subsystems is negligible. Additivity implies extensivity, thus non-extensivity implies non-additivity. Therefore, we can say that macroscopic systems with short-range interactions are additive, while systems with long-range interactions are non-additive [4].

Because of non-additivity, some striking properties may appear in equilibrium configurations, such as negative specific heat in the microcanonical ensemble, the violation of the usual Gibbs-Duhem equation or ensemble inequivalence (due to changes in the concavity of the thermodynamic potentials, for which non-additivity is re-

sponsible) [6].

The study on this work will be centered on a simplified model of a star (self-gravitating system). However, we can find some other examples of long-range interacting systems like plasmas, two-dimensional and geophysical fluids and spin systems [6].

II. ENSEMBLE INEQUIVALENCE IN LONG-RANGE INTERACTING SYSTEMS

A statistical ensemble consists of a collection of virtual replicas of the system under consideration from which averages are performed to obtain relevant information. The ensemble is characterized by the particular set of control parameters defining the macrostate of the replicas, thus defining the macrostate of the single system as well. Different ensembles then represent different physical conditions on the system, which are specified by the given set of control parameters. Whether the different ensembles can be regarded as equivalent or not depends on the system being examined, as we discuss below with an example.

A. Ensemble equivalence

Ensemble equivalence relies upon two important physical properties [2]:

1. In the thermodynamic limit, excluding critical points, the relative fluctuations of the thermodynamic parameters that are not held fixed vanish.
2. When a macroscopic physical state is realizable in an ensemble, it can be also realized in another ensemble.

Let us consider the microcanonical ensemble in which the system is isolated and assumed to have a fixed energy E , volume V and number of particles N . If this system is put in contact with a thermal bath that fixes its temperature T (thus the energy fluctuates) with the same V and N , the appropriate description of equilibrium states

is obtained in the canonical ensemble. Focusing on the second point above, if these two ensembles are equivalent it means that the system presents the same states when it is isolated as when it is thermalized with a bath. Below we describe a situation in which this is not the case.

B. Ensemble inequivalence - Negative specific heat

Ensemble inequivalence means that the experiments realized in a system described by a certain ensemble, may give different results compared to other similar experiments performed in another ensemble. In long-range interacting systems, ensemble equivalence does not always hold because of non-additivity [2]. One example of this inequivalence is materialized in systems that exhibit negative specific heat.

Let us consider the case of a star whose nuclear fuel is exhausted. When radiation energy is extracted from the star, it will contract and heat up. Thus, the star acts like a system with negative specific heat [1]. This behaviour can be understood with a simplified argument. We recall that the interaction in gravitating systems (in $d = 3$) goes as r^{-1} , so it is long-range.

According to the virial theorem, the kinetic energy K and the potential energy W of a self-gravitating system in a steady state are related to each other by

$$2K + W = 3PV, \quad (1)$$

where P is the pressure at the boundary of the system. If we consider the system large enough to assume that the boundary can be neglected, and that for an isothermal system $K = \frac{3}{2}NT$ (we use units in which the Boltzmann constant is $k_B = 1$), then the total energy will be [3]

$$E = K + W = -K = -\frac{3}{2}NT. \quad (2)$$

Therefore,

$$C_V = \frac{dE}{dT} = -\frac{3}{2}N < 0. \quad (3)$$

As we can see, the specific heat is negative. This means that, by losing heat the system grows hotter and continues to radiate energy. There is, however, a proof in statistical mechanics showing that specific heats are positive, so the above result could be seen as a paradox [3]. For a canonical ensemble in thermal equilibrium, the heat capacity is given by

$$C_V = \frac{d\langle E \rangle}{dT} = \beta^2(\langle E^2 \rangle - \langle E \rangle^2) > 0, \quad (4)$$

where $\langle E \rangle$ is the average energy. Since the specific heat is a measure of the fluctuations of energy, it must be positive [10]. Thirring then showed that the paradox is solved if one observes that negative specific heat can only be realized in systems with fixed energy and under certain conditions [1], in the microcanonical ensemble, where the canonical expression (4) does not necessarily apply.

III. THIRRING MODEL

Thirring realized that, for long-range interacting systems, the statistical ensembles are not necessarily equivalent. To analyze the problem, he introduced a model which is an exact solution for a [1] “somewhat artificial version of a star”. Phase transitions and ensemble inequivalence in Thirring’s model were studied in [6].

In this model we consider N particles of mass m enclosed in a volume V . The position and momentum of the i -th particle are denoted by x_i and p_i , respectively. The Hamiltonian of the system is $\mathcal{H} = K + W$, where the kinetic energy is

$$K = \sum_{i=1}^N \frac{p_i^2}{2m} \quad (5)$$

and the potential energy has the form

$$W = \sum_{i>j} w(x_i, x_j) \quad (6)$$

for which $w(x_i, x_j)$ specifies the interaction between particles. In this model, inside an interaction volume V_0 each particle has a constant, attractive interaction with the other particles and outside V_0 the particles are free, mimicking an “atmosphere”. By introducing the step function

$$\theta_{V_0}(x) = \begin{cases} 1 & \text{if } x \in V_0 \\ 0 & \text{if } x \notin V_0 \end{cases}, \quad (7)$$

such an interaction potential is given by

$$w(x_i, x_j) = -2\nu\theta_{V_0}(x_i)\theta_{V_0}(x_j), \quad (8)$$

where $\nu > 0$ is a coupling constant with units of energy. Just for clarifying that we are considering long-range interactions, notice that, being α the exponent in the power law, then $\alpha = 0$, which will be always lower than the dimension of the system. Using (8), the potential energy (6) is easily evaluated to $W = -\nu N_0(N_0 - 1)$, where N_0 is the number of particles inside the volume V_0 . Assuming a large number of particles, we simply take the potential energy as

$$W = -\nu N_0^2. \quad (9)$$

The potential energy (9) gives the system precisely the properties that interest us here. Since N_0 is a fraction of the total number of particles, with the potential energy (9) the total energy E behaves as $E \sim N^2$. Thus, the system is not additive [2, 4]. In particular, microcanonical and canonical ensembles are not equivalent for some range of parameters controlling the state of the system.

A. Microcanonical ensemble

The microcanonical ensemble corresponds to consider isolated systems, in which the control parameters are E ,

V and N . The thermodynamics of isolated systems follows from the microcanonical entropy

$$S(E) = \ln \Omega(E), \quad (10)$$

where $\Omega(E)$ is the number of microstates compatible with the energy E at fixed volume and number of particles. Here we compute $\Omega(E)$ as the number of microstates in phase space enclosed by a surface of energy E , so

$$\Omega(E) = \frac{1}{h^{3N} N!} \int d^{3N} x d^{3N} p \theta(E - \mathcal{H}), \quad (11)$$

where h is a constant and $\theta(x)$ is the Heaviside step function. Since a large number of particles is assumed, counting states on a thin energy shell in phase space or using the density of states leads to an equivalent entropy [5]. Carrying out the integration over momenta gives

$$\Omega(E) = \frac{1}{A_N N!} \int d^{3N} x \theta(E - W)(E - W)^{3N/2}, \quad (12)$$

where $A_N = (3N/2)!/(2m\pi/h^2)^{3N/2}$. To compute the remaining integral, we divide the total volume in two cells of volume V_0 and $V - V_0$ and take advantage from the fact that the potential energy is constant in each cell. Hence, instead of integrating over coordinates, we sum over the number of particles in the cells and take [1]

$$\frac{1}{N!} \int d^{3N} x \rightarrow \sum_{N_0} \frac{V_0^{N_0} (V - V_0)^{N - N_0}}{N_0! (N - N_0)!}, \quad (13)$$

which is obtained by using the binomial theorem. This procedure is exact if the integrand is constant for all particle configurations leading to the same number of particles N_0 . Using (13), the number of microstates (12) becomes

$$\Omega(E) = \frac{V_0^N}{A_N} \sum_{N_0=N_{\min}}^N \frac{(E + \nu N_0^2)^{3N/2} e^{\eta(N - N_0)}}{N_0! (N - N_0)!}, \quad (14)$$

where $\eta = \ln(V/V_0 - 1)$ is a reduced volume and a minimum value N_{\min} for N_0 is introduced to ensure that the condition $K = E + \nu N_0^2 > 0$ can be fulfilled for $E < 0$. By combining equations (10) and (14), we obtain

$$e^{S(E, \eta)} = \sum_{N_0=N_{\min}}^N e^{\hat{S}(E, \eta, N_0)}, \quad (15)$$

where the function $\hat{S}(E, \eta, N_0)$ can be identified from equation (14).

In order to evaluate the entropy $S(E, \eta)$ from equation (15), we approximate the sum by the single term for which $\hat{S}(E, \eta, N_0)$ reaches a maximum as a function of N_0 . This variational problem can be analyzed by introducing the reduced energy ε and the fraction of particles α defined by

$$E = \nu N^2 (\varepsilon - 1), \quad N_0 = N(1 - \alpha), \quad (16)$$

so the entropy per particle $s(\varepsilon, \eta) = S/N$ is obtained according to

$$s(\varepsilon, \eta) = \max_{\alpha} \hat{s}(\varepsilon, \eta, \alpha), \quad (17)$$

where $\hat{s} = \hat{S}/N$ is given by

$$\hat{s}(\varepsilon, \eta, \alpha) = \frac{3}{2} \ln(\varepsilon - 2\alpha + \alpha^2) - (1 - \alpha) \ln(1 - \alpha) - \alpha \ln \alpha + \alpha \eta. \quad (18)$$

To obtain the expression (18) we have used Stirling's approximation in (14) and for simplicity we have omitted constant terms which are not relevant for the variational problem. We highlight that the equation

$$\frac{\partial \hat{s}}{\partial \alpha} = -\frac{3(1 - \alpha)}{\varepsilon - 2\alpha + \alpha^2} + \ln\left(\frac{1 - \alpha}{\alpha}\right) + \eta = 0 \quad (19)$$

can have two solutions $\alpha = \bar{\alpha}$ for some values of ε and η , so the system exhibits first-order phase transitions in the microcanonical ensemble [6]. The variational problem (17) guarantees that $\bar{\alpha}$ is always the solution maximizing the entropy.

Introducing the reduced temperature $\tau = T/\nu N$ and employing the relation $1/T = \partial S/\partial E$, one obtains the microcanonical temperature as

$$\frac{1}{\tau} = \frac{\partial}{\partial \varepsilon} s(\varepsilon, \eta) = \frac{\partial}{\partial \varepsilon} \hat{s}(\varepsilon, \eta, \bar{\alpha}), \quad (20)$$

where $\bar{\alpha}$ maximizes the entropy according to (17). From (18) and (20) we explicitly get

$$\frac{3}{2} \tau = \varepsilon - 2\bar{\alpha} + \bar{\alpha}^2. \quad (21)$$

Notice that the above equation is simply $K = E - W$ expressed in terms of the reduced variables. Notice also that since $E \sim N^2$ and $S \sim N$, the temperature scales as $T \sim N$ in such a way that the kinetic energy behaves as $K \sim N^2$ as well. This is a typical scaling of long-range interacting systems [2] and, in particular, of more accurate models of a self-gravitating gas [7–9]. Expression (21) allows us to represent the microcanonical temperature of the Thirring model as a function of the energy. From this curve one can infer the sign of the heat capacity.

B. Canonical ensemble

In the canonical ensemble the system is assumed to be in thermal equilibrium with a thermostat a temperature T at fixed V and N . The thermodynamics of the system in this case follows from the free energy

$$F(T) = -T \ln Z(T), \quad (22)$$

where $Z(T)$ is the canonical partition function given by

$$Z(T) = \frac{1}{h^{3N} N!} \int d^{3N} x d^{3N} p e^{-\beta \mathcal{H}} \quad (23)$$

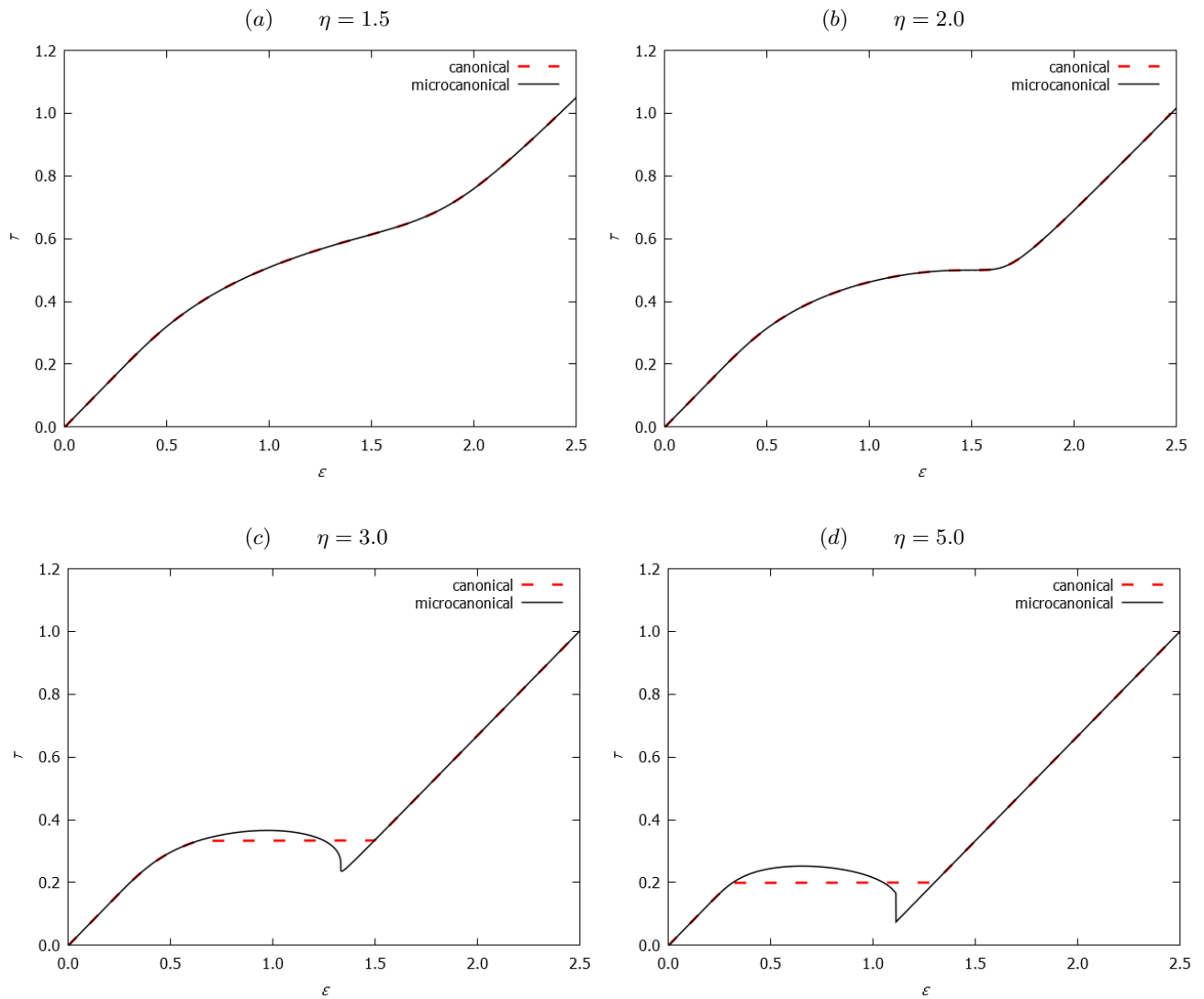


FIG. 1: Graphical representation of the caloric curves in both microcanonical and canonical ensembles for different values of the reduced volume η . Four different intervals can be seen in the figure. In the first interval (a) we can see how ensembles are equivalent, while for a certain value of η we reach the canonical critical point (b) for which the slope in the canonical representation starts to become negative (c) and, therefore, negative specific heat appears. Finally, for a certain η value the tangent starts to become vertical for the microcanonical representation, causing a jump in the reduced temperature axis (d).

with $\beta = 1/T$. The evaluation of this partition function proceeds in a similar way to the microcanonical case. Integration over momenta and replacing the integration over positions according to (13) yields

$$Z(T) = \frac{V_0^N}{\lambda_T^{3N}} \sum_{N_0=0}^N \frac{e^{\beta\nu N_0^2 + \eta(N-N_0)}}{N_0!(N-N_0)!}, \quad (24)$$

where $\lambda_T = h/(2\pi mT)^{1/2}$ is the thermal wavelength and we have used (9) to express the potential energy. From equations (22) and (24) we get

$$e^{-\beta F(T,\eta)} = \sum_{N_0=0}^N e^{-\beta \hat{F}(T,\eta,N_0)}, \quad (25)$$

where $\hat{F}(T,\eta,N_0)$ can be identified from (24) and we will approximate the sum by the single term for which this quantity reaches a minimum. In the canonical ensemble we also consider the reduced temperature τ and the fraction of particles α defined by

$$T = \nu N \tau, \quad N_0 = N(1 - \alpha). \quad (26)$$

However, here they have a meaning different from the microcanonical case; τ is now a control parameter and we will take $\alpha = \bar{\alpha}$ minimizing the free energy for given τ and η .

Introducing the reduced free energies $\varphi(\tau,\eta) = \beta F/N$ and $\hat{\varphi}(\tau,\eta,\alpha) = \beta \hat{F}/N$, according to (25), the variational

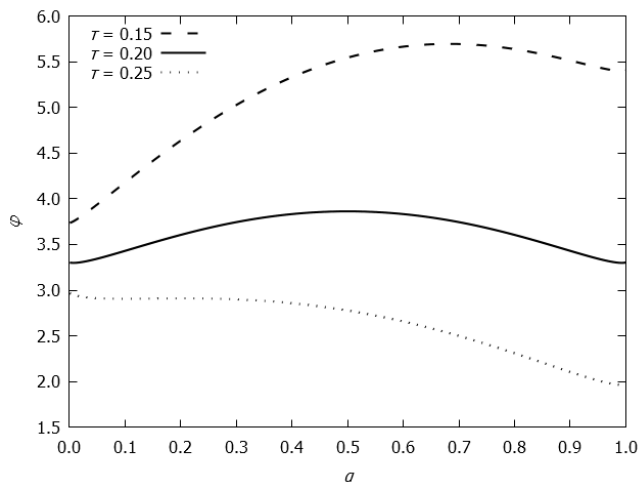


FIG. 2: Graphical representation of the reduced free energy, φ , depending on the fraction of particles, α , for a constant value of the reduced volume, $\eta = 5.0$, and different values of the reduced temperature, τ .

problem in the canonical ensemble can be stated as

$$\varphi(\tau, \eta) = \min_{\alpha} \hat{\varphi}(\tau, \eta, \alpha), \quad (27)$$

where

$$\hat{\varphi}(\tau, \eta, \alpha) = -\frac{1}{\tau}(1-\alpha)^2 - \frac{3}{2} \ln\left(\frac{3\tau}{2}\right) + (1-\alpha) \ln(1-\alpha) + \alpha \ln \alpha - \eta\alpha. \quad (28)$$

Expression (28) is obtained from (24) omitting, for simplicity, irrelevant constant terms. Since the equation

$$\frac{\partial \hat{\varphi}}{\partial \alpha} = \frac{2}{\tau}(1-\alpha) - \ln\left(\frac{1-\alpha}{\alpha}\right) - \eta = 0 \quad (29)$$

can have two solutions $\bar{\alpha}$ for some values of τ and η , the system also undergoes first-order phase transitions in the canonical ensemble. Among these solutions we choose $\bar{\alpha}$ that minimizes the free energy according to (27). Furthermore, to represent the caloric curve in the canonical ensemble, we have to compute the mean energy $\bar{\varepsilon}$ as a function of τ . From the relation $\bar{E} = \partial(\beta F)/\partial\beta$, in terms

of the reduced variables we obtain

$$\bar{\varepsilon} = \frac{3\tau}{2} + 2\bar{\alpha} - \bar{\alpha}^2. \quad (30)$$

C. Microcanonical and canonical caloric curves

From the representation of the caloric curves for the microcanonical and canonical ensembles (Fig. 1), we can see that above a certain η value, the representation of both ensembles is no longer equivalent. Considering that the specific heat is the relation between energy and temperature, a negative slope will mean a negative specific heat. As can be seen in figure (c), in the canonical representation there is a jump in the energy, evidencing a first order phase transition.

By plotting the reduced free energy in front of the fraction of particles (Fig. 2), we can see the behavior of the two free energy minima. Considering that for $\eta = 5.0$, the transition line in the canonical ensemble appears for $\tau \simeq 0.2$ (as we can see in (d)), by taking values of τ below the transition line we will see the dominance of one of the two minima (equilibrium value) over the other (metastable minimum). As we increase the value of τ the two minima reach the same value (transition line), until for higher values, the dominance is reversed.

IV. CONCLUSIONS

We have studied a simplified model of a self-gravitating system by using the Thirring's model. We have studied the thermodynamics in the microcanonical and canonical ensembles. By maximizing the entropy per particle (18) in the microcanonical ensemble and minimizing the reduced free energy (28) in the canonical one, we have been able to plot the reduced temperature depending on the reduced energy, which have allowed us to see states with negative specific heat in the microcanonical ensemble. In the canonical ensemble these states are replaced by an isothermal first-order phase transition, leading to ensemble inequivalence. Therefore, we have analyzed an example of a long-range interacting system for which ensemble equivalence does not hold.

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