About thermometers and temperature

M. Baldovin
Dipartimento di Fisica, Sapienza Università di Roma, p.le A. Moro 2, 00185 Roma, Italy
E-mail: marco.baldovin@roma1.infn.it

A. Puglisi, A. Sarracino
CNR-ISC and Dipartimento di Fisica, Sapienza Università di Roma, p.le A. Moro 2, 00185 Roma, Italy
E-mail: andrea.puglisi@roma1.infn.it, alessandro.sarracino@roma1.infn.it

A. Vulpiani
Dipartimento di Fisica, Sapienza Università di Roma and CNR-ISC, p.le A. Moro 2, 00185 Roma, Italy
Centro Interdisciplinare B. Segre, Accademia dei Lincei
E-mail: angelo.vulpiani@roma1.infn.it

Abstract. We discuss a class of mechanical models of thermometers and their minimal requirements to determine the temperature for systems out of the common scope of thermometry. In particular we consider: 1) anharmonic chains with long time of thermalization, such as the Fermi-Pasta-Ulam (FPU) model; 2) systems with long-range interactions where the equivalence of ensembles does not always hold; 3) systems featuring absolute negative temperatures. We show that for all the three classes of systems a mechanical thermometer model can be designed: a temporal average of a suitable mechanical observable of the thermometer is sufficient to get an estimate of the system’s temperature. Several interesting lessons are learnt from our numerical study: 1) the long thermalization times in FPU-like systems do not affect the thermometer, which is not coupled to normal modes but to a group of microscopic degrees of freedom; 2) a thermometer coupled to a long-range system measures its microcanonical temperature, even at values of the total energy where its canonical temperature would be very different; 3) a thermometer to read absolute negative temperatures must have a bounded total energy (as the system), otherwise it heavily perturbs the system changing the sign of its temperature. Our study shows that in order to work in a correct
way also in “non standard” cases, the proper model of thermometer must have a special functional form, e.g. the kinetic part cannot be quadratic.

1. Introduction

An instrument able to measure a system’s temperature must equilibrate with that system within an acceptable time and without perturbing it significantly. Among the system’s properties which are usually considered relevant for appropriate equilibration, one recognizes: 1) a reasonable (not mathematical) notion of ergodicity, 2) the possibility to take a small part of the system as a good representative of the whole system, and 3) thermalization, in a suitable time, among different parts of the system [1, 2].

As known, those requirements are satisfied by a widespread class of systems in condensed matter physics, a fact which explains why thermometers are common tools in everyday life and in scientific applications [3]. Statistical physics, however, has indicated a series of interesting systems where - for different reasons related to particular forms of the interactions or constraints on kinetic and potential energies - the fulfillment of the above simple requirements may be complicated.

Chains of weakly anharmonic oscillators are a paradigm of slow - or even not reached - equilibration: in this category the prototype system is the Fermi-Pasta-Ulam (FPU) chain, which played a seminal role in the history of chaos, numerical computation in physics [4, 5, 6], as well as in integrable systems [7], and, in addition, is widely used also in non equilibrium statistical mechanics, e.g. for the study of Fourier’s law [8]. In this system, roughly we can say that for any finite $N$, if the energy per particle $E/N$ is small enough, one can observe the proper statistical features only after a typical time $t_c$, which diverges as $N \to \infty$ and $E/N \to 0$, see [9]. Notwithstanding this well-established behavior, we remark here that for the purpose of defining a suitable thermometer we need the system to be already at equilibrium: our only requirement, therefore, is that the thermometer - a small perturbation which can be out-of-equilibrium at the instant of contact - exchanges energy with the system exploring, within an acceptable time, its statistical distribution.

A different complication originates from long-range interactions [10]: such a kind of forces prevent the usual argument which makes the interaction energy between a sub-system and the rest of the system negligible. As a result, canonical ensemble is not directly derived as the natural ensemble for small parts of a microcanonical one, and - conversely - equivalence of ensembles is no more
guaranteed [11]. A priori it is not obvious that the equilibration times are reasonably small, even in an optimistic scenario. The crucial question here is: what is the temperature read by a thermometer coupled to such a long-range system, at energies for which microcanonical and canonical ensembles predict different results?

The third category of complication considered below is the one coming from systems with bounded energy: such a property - which is verified also in certain experiments [12] - implies a microcanonical entropy which is non-monotonous in the energy, and therefore a range of energies where the absolute temperature is negative [13, 14]. While negative temperatures do not entail any paradox for thermodynamics, their existence is strictly related to the bounded range of achievable energies. This means that coupling to such systems a normal thermometer (e.g. with kinetic energy of the usual kind $p^2/2m$) results in a catastrophic change of the state of the system which, necessarily, must transfer a very large amount of energy to the thermometer: in other words a normal thermometer, even very small, represents for those systems a huge perturbation. Experimental realization of systems with negative temperature is in fact conditioned on the ability of isolating the system from the rest of the world. In addition to such a sensitivity to external perturbations, in systems with negative absolute temperature the equipartition of energy is almost always broken [13], an evident further complication in designing a suitable thermometer.

In the present paper we propose a general model of “mechanical” thermometer which, with small adaptations, is able to measure temperature in examples of all the three classes mentioned above. Let us stress that the Hamiltonian of the proper thermometer must have some specific form, see Sec. 3.3. We enforce molecular dynamics simulations of the systems and the coupled thermometer, showing for the latter a dynamical evolution toward equilibration at the correct temperature. In all our numerical experiments a certain amount of noise in the measurements of temperature will be evident: we remark that the observables which we measure are estimators of the system’s temperature and for this reason are subject to statistical uncertainties, which of course cannot be considered as fluctuations of temperature [15]. We recall that a similar proposal of a mechanical thermometer was introduced in the - quite different - framework of aging systems with the aim of measuring the Fluctuation-Dissipation effective temperature [16, 17]. Another class of systems, again in the out-of-equilibrium realm, is constituted by granular fluids [18], where the problem of measuring temperature by means of probing a small sub-system has been studied in [19, 20].

The paper is organized in the following way. In Section 2 we discuss the classical
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definition of microcanonical temperature, we recall a precious formula allowing universal estimate of temperature through a dynamical measurement, and we present our model of a thermometer. In Section 3 we discuss numerical experiments where the thermometer is coupled to an FPU chain, a generalized Hamiltonian mean-field model (example of a system with long-range interactions), and finally with a model of coupled rotators with bounded kinetic energy, providing an example of system with negative temperatures. In Section 4 we draw our conclusions.

2. What temperature is and how to measure it

Many different types of efficient thermometers have been conceived, often involving rather sophisticate technologies [21]. The main aim of the present paper is to discuss the conceptual aspects behind the problem of measuring temperature. For this reason, of course, we do not claim to improve the practical and technical aspects of thermometry. A first conceptual prerequisite to propose a suitable candidate for a thermometer is a clear understanding of the concept of temperature.

2.1. Definitions of temperature

From the basic principles of the statistical mechanics we know how to define the microcanonical temperature $T$ in a system with Hamiltonian $H(Q, P)$:

$$\beta = \frac{1}{k_B T} = \frac{\partial}{\partial E} \ln \omega(E),$$

where

$$\omega(E) = \int \delta(E - H(Q, P))dQdP,$$

with $k_B$ the Boltzmann constant. Such a definition, although rather important, does not appear very useful for practical purposes. Measuring or computing the density in phase space is usually impossible. A possible alternative is to invoke the equipartition formula

$$\left\langle X_m \frac{\partial H}{\partial X_n} \right\rangle = \delta_{mn} k_B T,$$

where $\langle \cdots \rangle$ indicates the average with respect to the microcanonical measure. On the other hand - as discussed in [13] - such formula does not always hold in certain kinds of systems, for instance those with negative temperatures. The possible failure of Eq. (1) is mainly a consequence of bounded potential energy [13].
A precious help, for this task, is obtained following the approach introduced by Rugh [22, 23]. According to it, we can determine $\beta$ through the time average of a function:

$$\beta = \frac{1}{k_B T} = \langle \Phi(X) \rangle , \ X = (Q, P),$$

(2)

where

$$\Phi = \nabla \cdot \left( \frac{\nabla H}{||\nabla H||^2} \right).$$

Rugh’s approach is very elegant and rather relevant from a conceptual point of view. In fact,

- it gives us a definition of temperature for any kind of Hamiltonian system;
- formula (2) allows for computation of the temperature as a time average of an observable, e.g. from molecular dynamics simulations, and, at least in principle, in real experiments.

We notice that the use of Eq. (2) does not give particular advantages in systems with the usual form of the Hamiltonian, e.g. those with a quadratic kinetic part and a potential contribution, where equipartition formula is a valid and perhaps simpler alternative, see e.g. [24]. On the contrary, in systems with peculiar phase space structure, such that equipartition is not guaranteed, formula (2) becomes very important.

Let us now discuss another general-purpose way to define the temperature. In a large system whose Hamiltonian has the form:

$$H = \sum_{n=1}^{N} g(p_n) + V(q_1, ..., q_N),$$

it is easy to find the probability density function of the momentum with a generalized Maxwell-Boltzmann formula:

$$\rho(p) = \text{const.} e^{-\beta g(p)}.$$  

(3)

The previous result allows for a practical way to determine $\beta$ from a time average of a suitable function of $p$. The most common case is the familiar case $g(p) = p^2/(2m)$: $\beta^{-1} = \langle p^2/m \rangle$. The average $\langle \rangle$ here will be obtained through a double average in time and on the particles of the thermometers (or - for comparison - of the system). Remarkably Eq. (3) holds also for systems with negative temperature [13]. In the present paper we will use Eq. (3) as the starting point to measure temperature. Our
idea, however, is that the observer can measure observables only in the thermometer and not directly in the system. In the following we discuss how a thermometer can be modelled and coupled to the system of interest.

2.2. A minimal model for a thermometer

Our aim, here, is to introduce a very general setting for modelling the act of measuring temperature, from a dynamical point of view. In particular we need a mechanical model for a thermometer which can be adapted also to the three special cases considered in the rest of the paper. Our definitions are quite natural and do not reserve particular surprises.

We consider:

- a system with Hamiltonian $H_S(X)$ where $X \in \mathbb{R}^{N_S}$ denotes the system’s mechanical variables and in addition $N_S \gg 1$;
- a system (the “thermometer”) with Hamiltonian $H_T(Y)$ where $Y \in \mathbb{R}^{N_T}$ denotes the thermometer’s mechanical variables and $N_T \ll N_S$ ($N_T$ can be small, in principle).

The whole system therefore has the following Hamiltonian:

$$H_S(X) + H_T(Y) + \epsilon H_I(X,Y),$$

where we assume that the system weakly interacts with the thermometer i.e. $\epsilon \ll 1$. As possible interactions we consider

$$H_I = \sum_{i,j} V_{i,j}(q_i - Q_j),$$

where $\{q_i\} (i = 1, 2, .., N_T)$ denote the positions of the particles of the thermometer and $\{Q_j\} (j = 1, 2, .., N_S)$ the ones of the system. The particular forms of internal interactions and kinetic energies (for the system and for the thermometer) will be varied in the three numerical experiments explained below.

3. Numerical computations on different systems

We have put in evidence three classes of non-trivial systems (choices of $H_S$) where the possibility to measure temperature by coupling a thermometer is a priori challenged by some apparent complication.
• FPU-like systems. In such a class of models the validity of a fundamental assumption for the usual statistical mechanics (e.g. ergodicity) is not completely clear.
• Systems with long-range interactions. For these systems the equivalence of ensembles is not always guaranteed, resulting in a possibility of ambiguity for the expected value of temperature.
• Systems with negative temperature. Isolation is crucial for the survival of these systems, therefore the contact with a (standard) thermometer, even very small, could be dramatic. We will see that suitable thermometers exist also for this class.

Our numerical simulations follow the usual Verlet algorithm, with time step chosen to be $5 \times 10^{-3}$, in order to keep relative energy fluctuations $< 10^{-4}$. In most of our numerical experiments we have applied the following protocol: 1) we have initialized the system in a typical thermal (equilibrium) state; 2) we have verified dynamically that the system is at equilibrium; 3) we have coupled the thermometer and 4) we have read the temperature averaging one or more observables (as discussed in Sec. 2.1), see captions of the figures for details. We underline that our numerical simulations are fully deterministic, i.e. without coupling with external reservoirs or thermostats.

3.1. FPU chain

Consider the usual FPU model, i.e. a chain of weakly non linear oscillators:

$$H_S = \sum_{i=1}^{N_S} \frac{P_i^2}{2M} + \sum_{i=1}^{N_S+1} \frac{1}{2}(Q_i - Q_{i-1})^2 + \sum_{i=1}^{N_S+1} \frac{\alpha}{3}(Q_i - Q_{i-1})^3 + \sum_{i=1}^{N_S+1} \frac{\beta}{4}(Q_i - Q_{i-1})^4$$

with $Q_0 = Q_{N_S+1} = 0$, $\alpha$ and $\beta$ positive constants, and

$$H_T = \sum_{i=0}^{N_T} \frac{P_i^2}{2m} + \sum_{i=1}^{N_T} (q_i - q_{i-1})^2$$

$$H_I = \sum_{i=1}^{N_T} \frac{1}{2}(Q_i - q_i)^2.$$

Many studies (see for instance [8, 5, 6] and references therein) give a strong evidence of the following scenario: starting with initial conditions very far from the equilibrium (typically the energy concentrated only on few low frequency normal modes), if the energy per particle $E/N$ is not large enough, the system is not able to reach the thermal equilibrium. More precisely for small values of $E/N$ one can
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reach thermal equilibrium only after a time very long which diverges as \( N \to \infty \) and \( E/N \to 0 \).

Following the previous results some authors considered the problem of the temperature in the FPU model, studying the features of the system interacting with a thermometer and a thermal bath. At variance with our model of thermometer, the authors of Refs. [25, 26] considered the cases where just one particle of the system interacts with the thermometer and, in addition, the initial conditions are typically very far from the thermal equilibrium. In such an approach, clearly in the tradition of studies on FPU, the main interest is for the possible presence of (very) long metastable behaviors whose relaxation times increase as \( E_S/N_S \) decreases.

![Figure 1. Measuring temperature in FPU chains. Evolution of \( \langle p^2/m \rangle \) for the system (black line) and the thermometer (red lines) after they have been connected, here \( \langle p^2/m \rangle \) is averaged also over all the components of the systems (or the thermometer). We consider the cases \( E_S/N_S = 2 \times 10^{-4} \) (left) and \( E_S/N_S = 10^{-2} \) (right). For the thermometer, both “instantaneous” averages over \( \Delta t = 500 \) time units and moving averages on a time window \( \tau = 25000 \) are shown. Parameters are \( \alpha = 1, \beta = 2, M = 1, N_S = 1000, N_T = 30, \epsilon = 0.01, \) and \( m = 0.2 \).

On the contrary here we are interested in a temperature measurement in a standard situation, i.e. checking the ability of a thermometer to thermalize with the system and bring information about its temperature. The initial conditions for the system and the thermometer used in our simulations are reported in the caption of Fig. 2. The results of our numerical simulations are reported in Fig. 1, where we show the evolution with time of the variance of the momentum distribution for the thermometer and in Fig. 2, where we compare such a variance with the variance of the chain’s momentum distribution. Let us note that in Fig. 2 the values of \( E_S/N_S \) vary from below the “critical” threshold (where one has weak chaos and the failure
of equipartition \cite{5,6}) to large energy per particle, for which the dynamics is in good agreement with the statistical mechanics prediction.

In Fig. 1 we see that the thermometer works rather well also at small energies (below the threshold), but the thermalization time is longer. Basically we can say that the weak ergodicity at low energy per particle does not produce particular problems and the thermometer works in the proper way. One can wonder about the origin, in our simulations, of the absence of the statistical anomalies observed in many numerical studies \cite{5,6}, e.g. the lack of equipartition with initial condition very far from equilibrium.

Let us note that in the FPU system at low energy the normal modes are almost decoupled. Nevertheless starting from a typical equilibrium initial condition (as in our computation), for \( N_S \gg 1 \), non-negligible fluctuations of the energy of a subregion can be observed and therefore an exchange of energy between the system and the thermometer can be realized: in particular, the thermometer is able to work in the proper way. We can say that our results are in agreement with those of Khinchin on the pure role of the details of the dynamics for the time average of global quantities in high dimensional systems: thanks to this “practical ergodicity” the thermometer is able to behave in the proper way also at low energy \cite{27}.

Figure 2. Measuring temperature in the FPU chains. \( \langle p^2/m \rangle \) as a function of \( \langle P^2/M \rangle \). The parameters are as in Fig. 1, \( E_S/N_S = 2 \times 10^{-4}, 10^{-2}, 0.1 \) and 1, and \( E_T/N_T = 2 \times 10^{-5} \) at \( t = 0 \).
3.2. Long-range systems

Usually statistical mechanics considers systems with short range interactions. Such a class of systems is physically rather important (e.g. gases or liquids) and, in addition, it can be treated mathematically showing, in a rigorous way, many relevant
properties, e.g. the existence of a thermodynamic limit and the equivalences of the ensembles in the limit of very large systems.

On the other hand there are systems with long-range interactions, which are very important for instance in fluid dynamics, laser and plasma physics, and astrophysics \[\text{[11]}\]. In addition, in the presence of long-range interactions one can have a failure of the equivalence of the ensembles, which means that the results obtained in the microcanonical and in the canonical ensembles can be different also in the thermodynamic limit.

An interesting case of long-range interacting system in which canonical and microcanonical ensembles are not equivalent is the Generalized Hamiltonian Mean Field model (GHMF), introduced in \[\text{[28]}\]. The system is described by \(N_S\) angular positions \(\theta_i \in [-\pi, \pi)\), \(i = 1, \ldots, N_S\) and their conjugate momenta \(P_i\). The Hamiltonian of the system can be written as:

\[
H_S = \sum_{i=1}^{N_S} \frac{P_i^2}{2} + N_S \frac{J}{2} (1 - \mu^2) + N_S \frac{K}{4} (1 - \mu^4),
\]

where

\[
\mu = \sqrt{\mu_x^2 + \mu_y^2}, \quad \mu_x = \sum_{i=1}^{N_S} \cos \theta_i, \quad \mu_y = \sum_{i=1}^{N_S} \sin \theta_i,
\]

and \(K\) and \(J\) are positive constants. In our simulations one particle was always anchored in the origin by a restoring force, in order to prevent rigorous conservation of the total momentum.

Since the positions are angular variables, it is rather natural to introduce our thermometer with the same features, i.e.:

\[
H_T = \sum_{i=0}^{N_T} \frac{P_i^2}{2m} + \sum_{i=1}^{N_T} m \gamma^2 [1 - \cos(\phi_i - \phi_{i-1})],
\]

with \(\gamma\) a positive constant. Finally, we choose an interaction term such that the forces between the particles are periodic in \(\phi_i - \theta_i\):

\[
H_I = \sum_{i=1}^{N_T} [1 - \cos(\phi_i - \theta_i)].
\]

As mentioned above, the system (4) in a range of values of \(E_S/N_S\) shows a statistical behavior which is quite different from the usual one. Namely, \(E_S/N_S\) is a nonmonotonic function of the temperature and the results obtained with the
canonical and microcanonical ensembles are different, even for $N_S \gg 1$. In Fig. 3 we show the time evolution of the variance of the single-particle distribution of momentum for the system and for the thermometer. In Fig. 4 the time-averaged values of those observables are shown for a wide range of energies, demonstrating an overall agreement with the microcanonical expectation, also for the temperature read by the thermometer.

3.3. Systems with negative temperature

In the present subsection we use the following Hamiltonian

$$H_S = \sum_{i=1}^{N_S} (1 - \cos P_i) + \frac{J}{2N_S} \sum_{i,j=1}^{N_S} (1 - \cos(\theta_i - \theta_j)) + K \sum_{i=1}^{N_S} (1 - \cos(\theta_i - \theta_{i-1})) \quad (8)$$

with $\theta_0 = 0$. We decided to use the above system for the following reasons:

- In the limit $J = 0$, we have the model discussed in [13], showing absolute negative temperatures; it also corresponds to the model used to interpret the experiments in [12];
- For $K = 0$, one has a generalization of the GHMF model [28].

Let us open a short parenthesis on the above system. For the FPU system, the “natural” variables are the normal modes, which, even in a statistical analysis, may show regular behavior and are able to remember for a very long time the initial conditions: therefore the approach to the equipartition can be, if any, very slow. However, even if the normal modes are almost decoupled, when one looks at “local” variables $\{q_n, p_n\}$, basically one recovers the correct features predicted by statistical mechanics. On the contrary, for the chain of (generalized) rotators in Eq. (8) with $J = 0$ at large energy the normal modes, i.e. the carriers of the energy, are the local variables $\{\theta_n, P_n\}$ themselves, and therefore exchange of energy among the subsystems is strongly depressed [29]. Therefore in order to avoid non ergodic behavior, or more likely, very slow exchange of energy, a small non local interaction contribution has been introduced (the term with $J$). Such a term has the mere aim of avoiding long living metastable situations. Let us also note that for this model, using a large deviation approach, one can obtain an analytical prediction for the behavior of $\beta$ as a function of $E/N$. The results of our computations are reported in the Appendix.

It is useful to recall an argument to show that the coupling of the system $\mathcal{A}$ at negative temperature with a system $\mathcal{B}$ which can have only positive temperature
always produces a system with final positive temperature. Indeed, at the initial time
the total entropy is
\[ S_I = S^A(E_A) + S^B(E_B), \]  
while, after the coupling, it will be
\[ S_F = S^A(E'_A) + S^B(E'_B), \]  
where \( E'_A + E'_B = E_A + E_B \) and, within our assumptions, \( E'_A \) is determined by the
equilibrium condition that \( S_F \) takes the maximum possible value \([1]\), i.e.
\[ \beta_A = \frac{\partial S^A(E'_A)}{\partial E'_A} = \beta_B = \frac{\partial S^B(E'_B)}{\partial E'_B}. \]  

Since \( \beta_B \) is positive for every value of \( E'_B \), the final common temperature must also
be positive. The above result helps to understand why it is not common to observe
negative temperatures. Therefore using as thermometer a “standard” system with
only positive \( \beta \) as those used for the FPU system, the thermometer cannot work.

In Fig. 5 we show schematically the mechanism for the energy transfer.

![Figure 5. Entropy of the system \( S_s(E) \) (left panel), and of the thermometer
\( S_T(E) \) (right panel), as a function of \( E \). At initial time the system’s energy \( E'_S \)
corresponds to a negative temperature, \( T_I < 0 \); after the thermalization, due to
the coupling with the “standard” thermometer, the system’s temperature must
be necessarily positive, and a huge transfer of energy from the system to the
thermometer occurs, in such a way that \( E'_S + E'_I \approx E'_S + E'_T \).](image)

We have checked this argument using the “standard” thermometer with
Hamiltonian given by Eq. (6) and the following interaction Hamiltonian
\[ H_I = \sum_{i=1}^{N_T} [1 - \cos(\phi_i - \theta_i)]. \]  

(12)
Figure 6. Inverse temperature $\beta$ as a function of time, for the system (8) and the “usual” thermometer (6) (with $m = 1$). In the left (right) panel the $\beta$ corresponding to the initial energy is negative (positive). $\beta(t)$ of the system is computed from a fit on the single particle momentum p.d.f.: we consider the histogram of the measured momenta from time $t$ to time $t + \Delta t$, with $\Delta t = 50000$ in this case, and we get the value of $\beta$ from the slope of $\log[\rho(p)]$, as explained in Ref. [13]. Thermometer’s inverse temperature has been determined, as usual, by $\beta = \langle p^2/m \rangle^{-1}$. Parameters: $N_S = 1000$, $N_T = 30$, $K = \gamma = 0.5$, $J = 0.05 \epsilon = 0.1$.

Figure 7. Inverse temperature $\beta$ as a function of time, for the system (8) and the thermometer (13), both measured by the distribution fitting procedure explained in Fig 6. In the left (right) panel the $\beta$ corresponding to the initial energy is negative (positive). Parameters as in Fig. 6.

Figure 6 shows the scenario predicted by the previous simple thermodynamic arguments: in the left plot we see how starting from a situation at negative temperature we have an energy flux from the system to the thermometer. The amount of the exchanged energy is huge even if the size of the thermometer is small (and its coupling $\epsilon \ll 1$) and the final state of the system must be very different
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from the initial one. Therefore we can say that the thermometer acts as a “vampire” producing a qualitative change in the system.

On the contrary using a proper thermometer able to measure even negative temperature, i.e. one with Hamiltonian

$$H_T = \sum_{i=0}^{N_T} (1 - \cos p_i) + \sum_{i=1}^{N_T} \gamma [1 - \cos(\phi_i - \phi_{i-1})]$$  (13)

a correct measurement is achieved, see Fig. 7.

4. Conclusions

We have discussed the meaning of temperature and the issue of defining a proper model thermometer in non standard cases, featuring systems with long-range interactions or bounded phase space. Starting from the generalized Maxwell-Boltzmann distribution, allowing one to measure the temperature as a time average for Hamiltonian systems with a generic form of the kinetic part, we have considered different mechanical models for a thermometer. First, we have studied the case of FPU-like chains, showing that, even in the presence of weak ergodicty at low energy, at equilibrium a thermometer coupled to the system measures the proper temperature. Second, we have considered the generalized Hamiltonian mean field model, characterized by long-range interactions. In this case, we have introduced a model thermometer with angular variables and we have shown that it efficiently determines the system temperature. Finally, we have addressed the interesting issue of the measurement of temperature in systems with a bounded phase space, where such a quantity can take on negative values. For these systems we have shown that, in order to measure in a correct way the system’s temperature, one has to introduce a suitable model thermometer, with a negative temperature scale.

Appendix: Equilibrium properties of a “hybrid” system for $\beta < 0$

Let us consider the system described by the Hamiltonian

$$H = \sum_{i=1}^{N} (1 - \cos p_i) + NJ \left[ 1 - \left( \frac{1}{N} \sum_{i=1}^{N} \cos \theta_i \right)^2 - \left( \frac{1}{N} \sum_{i=1}^{N} \sin \theta_i \right)^2 \right]$$

$$+ K \sum_{i=1}^{N} [1 - \cos(\theta_{i+1} - \theta_i)]$$  (14)
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with \( (\theta_{N+1} \equiv \theta_1) \). In order to determine its equilibrium properties we need to find the canonical equipartition function \( Z(\beta, N) \), and then to compute the free energy per particle through the limit \( -\beta f(\beta) = \lim_{N \to \infty} \log Z/N \).

\( Z(\beta, N) \) can be factorized into two terms:

- a kinetic part,
  \[
  Z_K(\beta, N) = \int_{-\pi}^{\pi} dp_1...dp_N \exp \left[ -\beta \sum_{i=1}^{N} (1 - \cos p_i) \right]; \quad (15)
  \]

- a configurational one,
  \[
  Z_C(\beta, N) = e^{-\beta JN/2} \int_{-\pi}^{\pi} d\theta_1...d\theta_N \exp \left[ \frac{\beta J}{2N} \left( \sum_{i=1}^{N} \cos \theta_i \right)^2 + \frac{\beta J}{2N} \left( \sum_{i=1}^{N} \sin \theta_i \right)^2 \right]
  \]
  \[
  \times \exp \left[ -\beta K \sum_{i=0}^{N} (1 - \cos(\theta_{i+1} - \theta_i)) \right]. \quad (16)
  \]

The kinetic contribution to \( f(\beta) \) can be easily computed from (15) in terms of the Modified Bessel Functions of the first kind, as in Ref. [13]; one gets

\[
-\beta f_K(\beta) \equiv \lim_{N \to \infty} \frac{1}{N} \log Z_K = -\beta + \log (2\pi I_0(\beta)).
\]

The strategy to determine the configurational part has been outlined in Ref. [28], where a model with a similar interacting potential has been extensively studied. The result for \( \beta > 0 \) is

\[
-\beta f_C(\beta) \equiv \lim_{N \to \infty} \frac{1}{N} \log Z_C = -\beta K - \beta J - \min_{m \geq 0} \left( \frac{m^2}{2\beta J} - \log[\lambda(m, K\beta)] \right) \quad (17)
\]

where \( \lambda(z, \alpha) \) is the maximum eigenvalue of the symmetric integral operator

\[
(T_{z,\alpha} \psi)(\theta) = \int_{-\pi}^{\pi} d\theta' \exp \left[ \frac{1}{2} z (\cos \theta + \cos \theta') + \alpha \cos(\theta - \theta') \right] \psi(\theta'). \quad (18)
\]

In the following we will explicitly derive the case \( \beta < 0 \), with the same strategy which has been used in Ref. [28] for \( \beta > 0 \).
Figure 8. Equilibrium behaviour of the system (8). Analytical solution (solid line) and simulations with $N = 200$ (circles) are compared, for $K = 0.5, J = 0.05$.

From Eq. (16), by mean of a standard Hubbard-Stratonovich transformation, we get

$$Z_C(\beta, N) = \frac{N e^{-\beta J N/2}}{2\pi |\beta| J} \int d\rho_x d\rho_y \exp \left[ -\frac{N}{2|\beta| J} (\rho_x^2 + \rho_y^2) - N \beta K \right] \times$$

$$\times \int_{-\pi}^\pi d\theta_1 \ldots d\theta_N \exp \left[ i \sum_{j=1}^N (\rho_x \cos \theta_j + \rho_y \sin \theta_j) + \beta K \sum_{j=1}^N \cos(\theta_{j+1} - \theta_j) \right] =$$

$$= \frac{N e^{-\beta J N/2}}{2\pi |\beta| J} \int_0^\infty d\rho \int_{-\pi}^\pi d\phi \rho \exp \left[ -N \frac{\rho^2}{2|\beta| J} - N \beta K \right] \times$$

$$\times \int_{-\pi}^\pi d\theta_1 \ldots d\theta_N \exp \left[ i\rho \sum_{j=1}^N \cos(\theta_j - \phi) + \beta K \sum_{j=1}^N \cos(\theta_{j+1} - \theta_j) \right], \quad (19)$$

where we have introduced “polar” coordinates for the plane $(\rho_x, \rho_y)$. Now we shift all the integration variables $\{\theta_j\}$ by an angle $\phi$, then we can rewrite the last term in a symmetric fashion and recover the functional form of the integral operator $T$ introduced above, so that

$$Z_C(\beta, N) \approx \frac{N e^{-\beta J N/2}}{2|\beta| J} \int_0^\infty d\rho \exp \left[ -N \frac{\rho^2}{2|\beta| J} - N \beta K \right] Tr \left[ T_{i\rho, \beta K}^N \right]. \quad (20)$$

(reminding $\theta_1 \equiv \theta_{N+1}$). The last equality holds in thermodynamical limit, $N \gg 1$. Note that since $T_{i\rho, \beta K}$ is not an hermitian operator, its eigenvalues will be in general
complex numbers: therefore $\lambda(z, \alpha)$ has to be defined, in this case, as the eigenvalue with the maximum modulus. Finally, one can use steepest-descent method to reduce the calculation of the integral to a minimization problem, that can be solved numerically.

In Fig. 8 we compare our analytical prediction for the curve $\beta(E)$ with computer simulations of the system at equilibrium, finding an excellent agreement.

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