Pramana – J. Phys. (2022) 96:36
https://doi.org/10.1007/s12043-021-02284-w

Cross-over from microcanonical ensemble to canonical ensemble by using Gaussian ensemble for a long-range interacting spin chain

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MS received 27 April 2021; revised 1 October 2021; accepted 7 October 2021

Abstract. Contrary to the common thermodynamic systems, systems with long-range interaction may cause non-concavity of $s(\varepsilon)$ curves. In this paper, we propose a long-range interacting Ising chain in a staggered magnetic field model which has a non-concave entropy part. In this model, the first phase transition is accompanied by the phenomenon of temperature jump in microcanonical ensemble when proper magnetic field intensity is met, while this jump cannot be observed in canonical ensemble, which shows the non-equivalence of different ensembles. To exhibit the cross-over process from microcanonical to canonical, the cross-over phase transition properties are exhibited recently by putting the chain in thermal contact with an adjustable two-level heat reservoir. In this paper, we introduce a different method by employing Gaussian ensemble to show the cross-over process reversely, i.e., from canonical to microcanonical ensembles. As shown in this paper, by adjusting the parameters of the supporting parabolas in the Gaussian ensemble, one can observe the caloric curve of the system in any Gaussian ensemble.

Keywords. Long-range interaction; temperature jump; Gaussian ensemble.

PACS Nos **05.20.Gg; 05.50.+q; 05.70.Fh**

1. Introduction

If a d-dimensional two-body system with inter-particle potential decays as $V(r) \sim 1/r^{\alpha}$ at large distance, it is considered as a long-range system if $\alpha < d$, where $\alpha > 0$ [1,2]. It is interesting that the total energy of a whole long-range system cannot be considered as the sum of all the subsystem energy, which is known as non-additivity [1–3]. Long-range systems are rather common in nature. Classic examples are self-gravitational systems, ultracold trapped atoms and so on [3–8]. Differing from short-range systems, non-additivity leads to non-concavity of some thermodynamic functions, which causes a series of anomalous phenomena, such as temperature jump, negative heat capacity, etc. [3,4,9–34].

So far, the ensembles can be generally classified into eight types depending on the relation of the system with the environment [35–37]. Microcanonical ensemble is applied to analyse thermal systems with constant energy, and a physical quantity 'entropy' is introduced to help illustrate thermodynamic properties of systems in such ensembles [38–41]. Similarly, canonical ensemble is applied when systems meet constant temperature, and a physical quantity, 'free energy', is introduced [29]. These two kinds of ensembles were once thought to be equal because the equivalence of different ensembles is rigorously proven. Yet, only short-range interaction was considered, which means no concavity happens. In recent years, it was proven that non-equivalence occurs when the entropy function in microcanonical ensemble becomes non-concave [29].

In this paper, we propose a long-range interacting spin chain placed in a staggered magnetic field, and its entropy function is obtained using microcanonical approach. Additionally, a proper magnetic field intensity is chosen to guarantee that the phase transition is first-order, which means that the entropy function is non-concave around phase transition point. Therefore, non-equivalence occurs. By putting the Ising chain in thermal contact with a two-level heat reservoir, we can observe the intermediate states between the two ensembles. When the reservoir turns from infinitesimal to infinite, the cross-over from microcanonical ensemble to canonical ensemble occurs [29]. Additionally, in this paper, a different method is introduced to show the cross-over from canonical ensemble to microcanonical ensemble. A type of transition ensemble, also known as the Gaussian ensemble [42], is applied to give

Published online: 25 January 2022

an interpolation between canonical and microcanonical ensembles.

2. Non-equivalence of microcanonical ensemble and canonical ensemble

2.1 *Basic transformation*

For a clear illustration of Gaussian ensembles, the basic thermodynamic quantities are reviewed in this section. First, two different quantities, known as free energy and entropy, are deduced corresponding to canonical ensemble and microcanonical ensemble, respectively. Consequently, according to the LF transform, the two quantities are connected, and the condition of the LF transform is presented. We consider an N-particle system with microstates $\omega \in \Omega$, where Ω is the configuration space. In addition, let $h(\omega) = H(\omega)/N$ be the mean energy of the system. Thus, to characterise the thermodynamic properties in the canonical ensemble, the so-called thermodynamic free energy is introduced by

$$\varphi(\beta) = \lim_{N\to\infty} -\frac{1}{N}\ln Z_N(\beta), \tag{1}$$

where

$$Z_N(\beta) = \int_\Omega \mathrm{e}^{-\beta H(\omega)}\mathrm{d}\omega \tag{2}$$

is the partition function of this system. Here β denotes the inverse temperature $1/kT$, where k is the Boltzmann constant set to be 1. Note that $\varphi(\beta) = \beta f(\beta)$ where $\varphi(\beta)$ is the re-scaled free energy aimed at simplifying the proof process since it has no influence on concavity, while the formal free energy is $f(\beta)$. Consequently, we are able to define the microcanonical thermodynamic entropy function by utilising a familiar method at the limit

$$s(u) = \lim_{N\to\infty}\frac{1}{N}\ln\Omega(u), \tag{3}$$

where

$$\Omega(u) = \int_{\omega\in\Omega:h(\omega)=u}\mathrm{d}\omega = \int_\Omega \delta(h(\omega)-u)\mathrm{d}\omega \tag{4}$$

denotes the density of microstates, giving a statistical number of microstates ω which possesses the same energy corresponding to u. It is worth mentioning that the two functions of entropy and free energy are supposed to be correctly applied in the ensemble where they are defined: One is to characterise thermodynamic properties in an energy-fixed system (microcanonical), while the other is to demonstrate properties when the system is put in thermal contact with a huge, temperature-constant reservoir (canonical). Additionally, in order to show the dependence of these two functions, eq. (2) is modified by using parameter $\Omega(u)$

$$Z_N(\beta) = \int \Omega(u)\mathrm{e}^{-N\beta u}\mathrm{d}u. \tag{5}$$

Then imposing the Laplace's approximation on the integral, we obtain

$$Z_N(\beta) = \exp[-N\inf_u\{\beta u - s(u)\}]. \tag{6}$$

With this classic approximation in statistics, obviously one can use eq. (1) to obtain

$$\varphi(\beta) = s^*(u) = \inf_u\{\beta u - s(u)\}, \tag{7}$$

which indicates that $\varphi(\beta)$ fits the Legendre–Fenchel (LF) transform of $s(u)$. Notably, in convex analysis, it can be proved that $\varphi(\beta) = s^*(u)$ is always established under the condition of a concave, continuous function $\varphi(\beta)$, no matter whether $s(u)$ is concave or not. It implies that we can easily derive thermal quantities under canonical ensemble from a given entropy function in microcanonical ensemble, because $\varphi(\beta)$ is always concave. Incidentally, apart from the condition that $\varphi(\beta)$ is concave and continuous, its differentiability is also restricted, additionally, focussing on its converse process, which means to calculate $s(u)$ through an LF transform of $\varphi(\beta)$. For a concave $s(u)$ curve, it still follows the properties of the LF transform, that is, the equation $\varphi^*(\beta) = s^{**}(u)$ holds as we mentioned before. The problem is, however, different from a concave function of $\varphi(\beta)$. The entropy function $s(u)$ may not be concave, especially in long-range interacting systems. Thus, is $s^{**}(u)$ equal to $s(u)$? This will be qualitatively discussed in the next section.

2.2 *Gaussian approach*

To solve the equivalence of two ensembles, we introduce a significant concept, known as the supporting line. Assuming that there is a point A on the entropy curve, if a tangent exists at point A of $s(u)$ without any other intersection between $s(u)$ and this tangent, one accepts that s admits a supporting line at point A. Mathematically, we say that s admits a supporting line at A only if there exists β so that $s(v) \le s(u) + \beta(v-u)$ for all v, where u is the mean energy at A. From [43], equation $s(u) = s^{**}(u)$ holds if s satisfies the condition of a supporting line. Therefore, in this condition, one can conversely obtain the entropy function in canonical ensemble as well as show the equivalence of two ensembles.

However, if s does not admit a supporting line, we can show that $\varphi(\beta)$ keeps a constant, and non-differentiable point, which indicates a fixed temperature. That is, $s^{**}(u)$ invariably satisfies $s^{**}(u) \geq s(u)$ in this part, representing the non-equivalence of two ensembles.

To express the cross-over process, here we invoke one kind of generalised ensembles – Gaussian ensemble – by adding an extra term on microstate numbers in the partition integral, $\exp(-N\gamma h^2(\omega))$. Thus, the partition function is given by

$$Z_{N,\gamma}(\alpha) = \int_\Omega \mathrm{e}^{-N\alpha h(\omega) - N\gamma h^2(\omega))}\mathrm{d}\omega. \tag{8}$$

Consequently, the corresponding free energy is

$$\varphi_\gamma(\alpha) = \lim_{N\to\infty} -\frac{1}{N}\ln Z_{N,\gamma}(\alpha). \tag{9}$$

Note that we use α to represent the inverse temperature here. Now, imposing a familiar modified LF transform, one gets

$$\varphi_\gamma(\alpha) = \inf_u\{\alpha u - s(u) + \gamma u^2\}. \tag{10}$$

Clearly, here we can substitute s by $s_\gamma(u) = s(u) - \gamma u^2$ and $\alpha = s'_\gamma(u) = s'(u) - 2\gamma u$. Therefore, according to the theory of supporting lines, the equivalence happens when s_γ meets

$$s_\gamma(v) \leq s_\gamma(u) + \alpha(v-u) \tag{11}$$

at point A. In such a case, the actual entropy curve needs to meet

$$s(v) \leq s(u) + \alpha(v-u) + \gamma(v^2 - u^2). \tag{12}$$

From this equation, its geometric interpretation is more specific: supporting parabolas, which possess the identical concept of supporting lines. By adjusting the value of γ, which is also known as the width of the parabola, it expresses different tangent intervals. Hence, with $\gamma \to \infty$, the result of the modified LF transform of free energy recovers the non-concave entropy $s(u)$ in the microcanonical ensemble.

3. Long-range spin chain model in Gaussian ensemble

Here, we propose a long-range interacting spin chain model of N particles which is placed in a staggered magnetic field [22]

$$H = -\sum_{i=1}^{N/2}\frac{K}{2}S_i + \sum_{i=\frac{N}{2}+1}^{N}\frac{K}{2}S_i - \frac{J}{2N}\left(\sum_{i=1}^{N}S_i\right)^2, \tag{13}$$

where $K < 0$ and $J > 0$. The first two terms in the right denote the interaction between spins and magnetic field. The third term represents a long-range interaction called

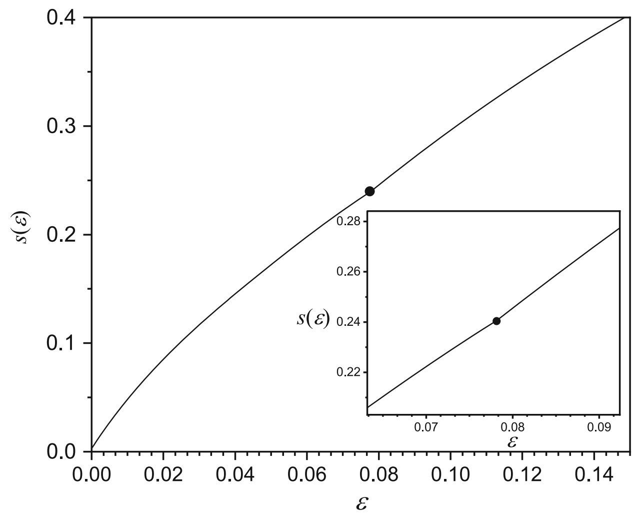

Figure 1. s–ε curve when $K = -0.97$ in microcanonical ensemble. $s(\varepsilon)$ is partly non-concave around the first-order phase transition point.

Curie–Weiss Hamiltonian [44]. As a known conclusion, if $|K| > J$, the system always remains unmagnetised, independent of any temperature value. When $|K| < J$, with increase of temperature from absolute zero, the system undergoes a phase transition from the ferromagnetic state to the unmagnetised state. More precisely, the value of K determines if this phase transition is first-order or second-order.

From the last section, to obtain the specific caloric curves in Gaussian ensemble, an analytical result of the system should be given in microcanonical ensemble. Suppose that there are N_-^L down spins in the left half of the system and N_+^R in the right half of the system. Hence, the compliance number U and the magnetisation M of the model are given by $U = N_-^L + N_+^R$ and $M = 2(N_+^R - N_-^L)$, respectively. Then the number of microstates is

$$\Omega = \binom{U/2}{N_+^R}\binom{U/2}{N_-^L}. \tag{14}$$

Let $u = U/N$, $m = M/N$. The energy per spin is $\varepsilon = (E/N) + (J/2)$. Applying the Stirling's approximation, then the entropy per spin is calculated by

$$\begin{aligned} s(\varepsilon, m) = &-\frac{1}{2}\left(u + \frac{m}{2}\right)\ln\left(u + \frac{m}{2}\right) \\ &-\frac{1}{2}\left(1 - u - \frac{m}{2}\right)\ln\left(1 - u - \frac{m}{2}\right) \\ &-\frac{1}{2}\left(u - \frac{m}{2}\right)\ln\left(u - \frac{m}{2}\right) \\ &-\frac{1}{2}\left(1 - u + \frac{m}{2}\right)\ln\left(1 - u + \frac{m}{2}\right), \end{aligned} \tag{15}$$

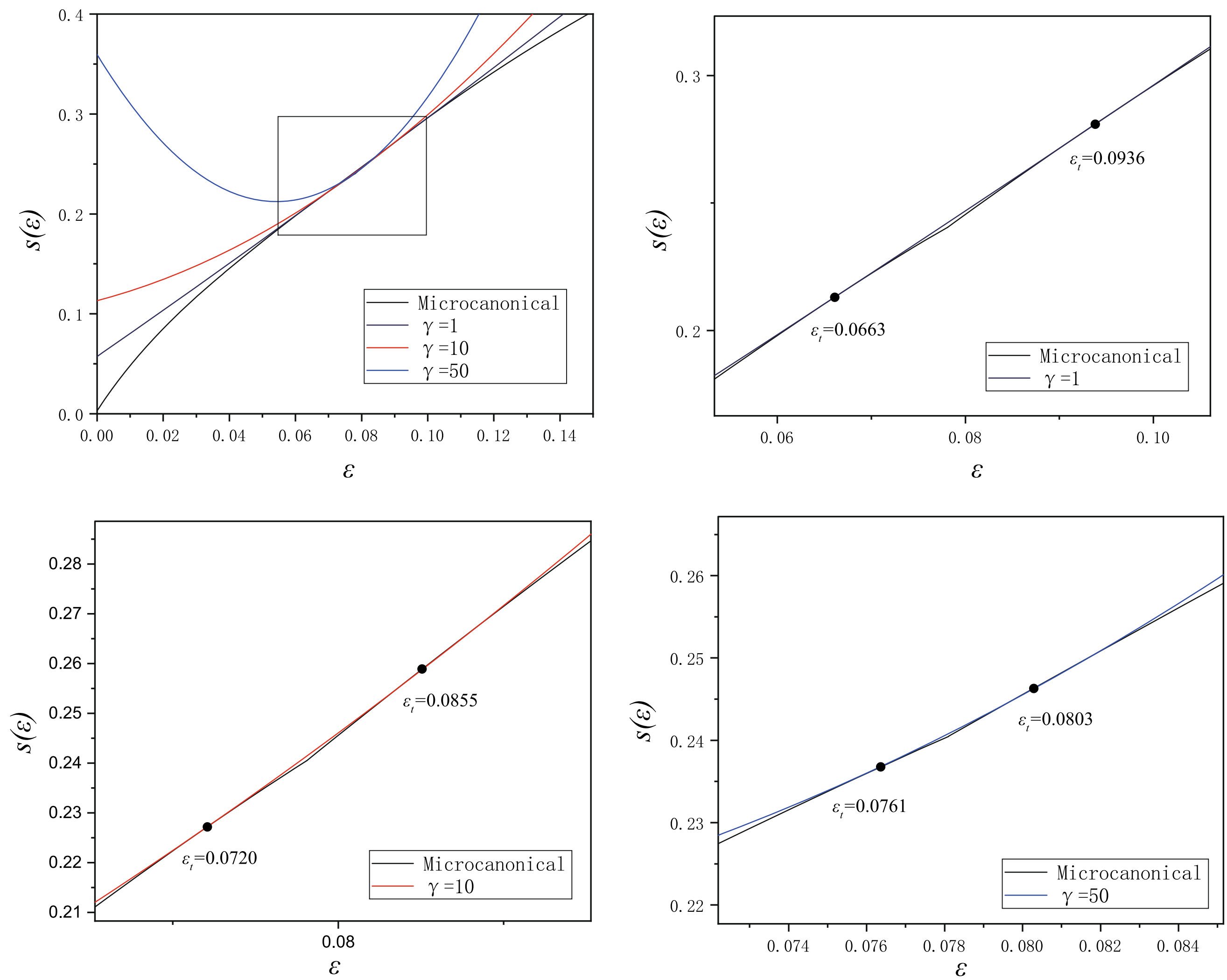

Figure 2. Supporting parabolas with different values of γ. The figure in the upper left draws a general picture, and the rest of the figures exhibit details around the tangent points. Tangent points are marked by black points, and their energy ε_t is shown in figures.

where u satisfies

$$\varepsilon = Ku + \frac{J}{2}(1 - m^2). \tag{16}$$

From eq. (15), it is an entropy function corresponding to m and ε. Therefore, from the second law of thermodynamics, the equilibrium state of each fixed energy is obtained by finding the maximum $s(m)$ corresponding to m. Then we can derive the caloric curve of the system by calculating every equilibrium state at different energy values. The $s(\varepsilon)$–ε curve is shown in figure 1.

Consequently, one can introduce supporting parabolas to exhibit the $s(\varepsilon)$–ε curves in Gaussian ensemble corresponding to a series of values of γ, which is shown in figure 2. As mentioned above, if a point on $s(\varepsilon)$–ε curve admits a supporting parabola, the equivalence happens at this point. Clearly, values of γ determine the width of the supporting parabolas. The microcanonical result is recovered only when $\gamma \to \infty$ because $s(\varepsilon)$ has a corner at phase transition point. With γ decreasing, the width of the supporting parabolas becomes flatter, which means the horizontal distance between the two tangent points becomes larger. It denotes that the transition-energy gap in T–ε increases. As $\gamma \to 0$, the supporting parabolas turn to supporting lines gradually, leading to a canonical result.

Then, from the equation

$$\frac{\partial s}{\partial \varepsilon} = \frac{1}{T}, \tag{17}$$

one obtains the caloric curves in Gaussian ensemble corresponding to a series of γ, as well as in canonical ensemble and microcanonical ensemble. It is given in figure 3.

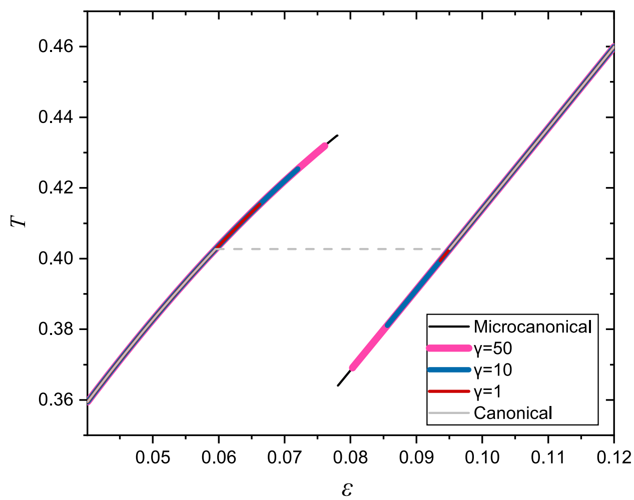

Figure 3. The caloric curves of our long-range system in different Gaussian ensemble of γ. The result of the canonical ensemble can be reproduced by setting $\gamma \to 0$.

4. Summary

In this paper, a long-range interacting Ising chain model is proposed. Previously, the cross-over process of this model from microcanonical ensemble to canonical ensemble is observed by adding an adjustable two-level reservoir [29]. However, in this paper, a different method is introduced to exhibit the cross-over process reversely. The entropy function of the system $s(\varepsilon)$ in microcanonical ensemble is calculated, and the property of non-concavity is also exhibited while the magnetic field intensity is fitting, which means non-equivalence happens. In such a case, by imposing the Gaussian ensemble, we interpolate transition ensemble between microcanonical and canonical ensembles, helping to observe the cross-over process. When $\gamma \to 0$, the results in the canonical ensemble are covered, while it turns to microcanonical when $\gamma \to \infty$.

Acknowledgements

This work was jointly supported by the Educational Reform and Research Foundation of Southeast University under Grant 2019-074 and the Physical Education Foundation of Higher Education Steering Committee of the Ministry of Education.

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