Molecular Dynamics Study of Oscillators Spin Chain in Framework of Variable Interaction Range Model

M. Ati[a,*], C. Enachescu[b] and R. Bouamrane[c]

[a] *Faculty of Medicine, Université Oran 1 Ahmed Ben Bella, Oran, Algeria*
[b] *Faculty of Physics, Alexandru Ioan Cuza University, Iasi, Romania*
[c] *LEPM, Faculty of Physics, Université des Sciences et de la Technologie d'Oran Mohamed-Boudiaf USTO-MB, BP 1505, EL M'naouer, Oran, Algeria*

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Doi: 10.12693/APhysPolA.141.191 *e-mail: ati.moncef@univ-oran1.dz

We numerically study the thermodynamic critical behaviour of the one-dimensional ferromagnetic spin model with variable interaction ranges using molecular dynamics simulation. Our results suggest that the model presents an order to a disorder phase transition, if the range length parameter surpasses the threshold $\xi_c = 1.4$. As expected, the order parameter of the magnetization M respects the Hamiltonian mean field transition, which occurs at $\xi = 2$. We show that the evolution of the system temperature is independent of the number of neighbours spins L considered in the system.

topics: transition phase, molecular dynamics, interaction range, neighbours spins

1. Introduction

Since Onsager solved the two-dimensional Ising model [1, 2], the famous lattice composed of short-range interacting spins has been used as the main model to investigate the phase transition behaviour of interacting many-body systems [3–5]. It is known from the early stages of development of Ising models that a one-dimensional system does not show a phase transition if only short-range interactions are considered [6], and it presents a critical behaviour depending on the number of connections in the network, while a two-dimensional model with short-range interaction has a Berezinskii–Kosterlitz–Thouless phase transition [7, 8]. On the other hand, models with long-range interactions [9–12] justified when the potential energy decreases slowly with distance, are particularly interesting for possible applications in biology and physics [13].

In this paper we study the thermodynamic behaviour of the spin chain model in the absence of an external magnetic field, introducing the appropriate order parameter to analyze the characteristics of phase transition under a variable interactions length of spin neighbours L [14]. We describe how the thermodynamic properties [15], such as the heat capacity C_v or magnetization M, vary depending on the number of neighbors L connected in a spin chain network. Different methods, like the Monte Carlo simulation [16], have been proposed to investigate the thermodynamic properties of spin chain systems, but none of them explored the presence of an order to disorder critical temperature T_c as a function of the number of interacting neighbors L in the spin chain models [17, 18]. The present approach enriches other different approaches in which the spin chain has been explored from the short-range interaction limit to the long-range interaction coupling case spins. In such cases, the spin model is reduced to a Hamiltonian mean field (HMF) model [19], while we focus on the L variable, since all the spins of the chain interact equally. We perform classical molecular dynamics simulations, considering interacting linear spins located in the same plan, to investigate the behaviour of the system with variable order interactions [20].

2. Material and methods

2.1. The model

We consider a linear ferromagnetic spin S_i model with Hamiltonian

$$H = \frac{1}{2}\sum_{i=1}^{N} P_i^2 + \frac{J}{2L}\sum_{i=1}^{N}\sum_{j=i+1}^{i+L}\left(1-\cos\left(\theta_i-\theta_j\right)\right), \tag{1}$$

where

- J represents the coupling constant,
- L describes the number of nearest neighbors per unit,
- P_i is the term of the conjugate momentum,
- θ_i describes the angle of spin at site i.

Each spin S_i interacts equally with all other S_j spins on every side of the chain. The spins are co-planar and can rotate with an angle $\theta_i = (-\pi, \pi)$ around the z-axis in the absence of the external magnetic field H. In fact, the limit case of $L = \frac{N}{2}$ in each side corresponds to the HMF with global interactions between all spins of the model [21, 22], while $L \to 1$ in both sides is the nearest neighbour case. In (1) we consider $J > 0$ for the ferromagnetic model. We are interested in studying different regimes in the model, from a short-range regime ($L = 1$) to the limit of a fully coupled HMF regime [23] in order to numerically explore the thermodynamic behaviour, such as the heat capacity, magnetization, and the Binder cumulant. In the following, we shall introduce a dilution variable denoted as ξ, which can be continuously shifted from the short-range interaction model to the case of the long-range interaction model. The parameter ξ is given by [24]

$$\xi = \frac{\log(N_L)}{\log(N)}, \tag{2}$$

where

- N_L is the total number of links in the system,
- N represents the system size.

The normalization constant L corresponds to the number of links per unit [23], it is imposed by the variable ξ and defined by the relation

$$L = \frac{2^{2-\xi}\,(N-1)^{\xi}}{N}. \tag{3}$$

For $\xi = 1$ the model is a linear chain with only nearest neighbors (a single coupling link per unit is set on each side). On the other hand, $\xi = 2$ corresponds to the full coupled spins regime (the HMF case, see (1)).

2.2. Simulation

2.2.1. Molecular dynamics equations

Using a classical method of molecular dynamics process, we study the interactions of a variable range on one-dimensional N spin chain, using the equations of motion derived from (1) [25]

$$\tau_i = -\frac{\partial H}{\partial \theta_i}, \tag{4}$$

where τ_i represent the torque on the spin i and is given by

$$\tau_i = -\frac{J}{2L}\sum_{i=1}^{N}\sum_{j=i+1}^{i+L}\sin(\theta_i - \theta_j). \tag{5}$$

The dynamics of each spin S_i $(i = 1, \ldots, N)$ in the chain obeys the following equation of motion

$$I\,\ddot{\theta}_i = \tau_i - \gamma\,\dot{\theta}_i + R_i(t), \tag{6}$$

where

- γ represents the rotational friction coefficient,
- $\ddot{\theta}_i$ and $\dot{\theta}_i$ are the second and first-time derivatives of the orientation moments of spins.

In the initial state, all the spins respect the ferromagnetic condition and are parallel oriented with $\theta_i = 0$ and $\dot{\theta}_i = 0$ at $t = 0$, as in the steady state given by (1). Symmetrically, the other important condition of simulation implies an introduction of a term of generating an angular velocity $\dot{\theta}$ attached to each spin S_i. This is represented by our approach to the Langevin thermostat, which adds random forces to the system according to (6). We have used random numbers given by a Gaussian distribution with zero mean and the variance scaled by [20]

$$\sqrt{\frac{2k_{\mathrm{B}}T\,\gamma I}{\delta t}} \tag{7}$$

According to (7) the random force R_i can be written as

$$R_i(t) = G_i\sqrt{\frac{2k_{\mathrm{B}}T\,\gamma I}{\delta t}} \tag{8}$$

where G_i is uniformly distributed in the range $-1 \to 1$, while the temperature T in units of $\frac{NJ}{k_{\mathrm{B}}}$, where k_{B} is the Boltzmann constant, I is the moment of inertia, and γ represents the friction parameter.

We would like to mention that, when the system is in contact with a Langevin bath, the chain of spins is set on an out of equilibrium state, so its energy will decrease with time. The friction parameter γ controls the damping force characterized by the fluctuation–dissipation state, and stabilizes the rotation of the spin chain for various values of temperature T. The numerical equation of motion of the model becomes

$$\ddot{\theta}_i = -\frac{J}{2L}\sum_{i=1}^{N}\sum_{j=i+1}^{i+L}\sin(\theta_i - \theta_j) - \dot{\theta}_i + R_i(t). \tag{9}$$

2.2.2. Numerical simulation

The simulations presented here start from an initial chain with ferromagnetic configuration, with $\dot{\theta}_i(0) = 0$ for all particles in the system. Then we integrate $\ddot{\theta}_i$ from (9) according to the velocity. During the simulation, the trajectory of the system is calculated by integrating the equations of motions [26, 27]. The temporal evolution of our system is described by the laws of classical mechanics. The time increment for numerical integration of the dynamical equations is set according to velocity Stormer–Verlet method [25]

$$\theta_i(t+\delta t) = \theta_i(t) + \dot{\theta}_i(t)\,\delta t + \frac{\tau_i(t)}{2I}\,\delta t^2, \tag{10}$$

$$\dot{\theta}_i(t+\delta t) = \dot{\theta}_i(t) + \frac{\tau_i(t)}{2I}\,\delta t. \tag{11}$$

The temperature values are inferred from the average values of the rotational kinetic energy (equipartition theorem), in a sufficiently long molecular dynamics run. For the numerical simulation of the ferromagnetic spin chain, we use an algorithm with the Langevin thermostat carried out at a range of bath temperature $T = (0.2, 0.6)$, considering several sizes of the system and time step $\delta t = 0.005$ under the periodic boundary condition, with a computed time equal to 1000 000 MD steps. We use the coupling strength $J = 1$. At every temperature a parallel initial condition for S_i is considered. To investigate the thermodynamic behaviours for various interaction range states in our model, we compute the torque τ_i and the interaction field between each spin S_i at every molecular dynamics step for every diluted parameter $\xi \in (1, 2)$. Finally, averages are performed for all measured quantities, such as the heat capacity C_v, magnetization M and the Binder cumulant U_B measured after a 50000 MD steps, where the steady equilibrium is achieved[†].

The heat capacity C_v for a given configuration of various interaction ranges is computed from the energy system as

$$C_v = \frac{1}{k_{\mathrm{B}} T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right). \tag{12}$$

In order to understand the order-disorder behaviour of the system near to T_c in terms of the phase transition, we measure the order parameter using the magnetization average $\langle M \rangle$ of the system via the following equations

$$M_x = \frac{1}{N} \sum_{i}^{N} \cos(\theta_i), \tag{13}$$

$$M_y = \frac{1}{N} \sum_{i}^{N} \sin(\theta_i), \tag{14}$$

$$M_{xy} = \sqrt{M_x^2 + M_y^2}. \tag{15}$$

The average equilibrium magnetization $\langle M \rangle$ of the spin chain is calculated by

$$\langle M \rangle = \frac{1}{t_{\mathrm{simulation}}} \int_0^{t_{\mathrm{simulation}}} \mathrm{d}t \, M_{xy}(t). \tag{16}$$

In order to confirm whether the variable interactions from the short-range to the long-range of a linear spin system present a thermodynamical critical behaviour, we should check the critical temperature with the Binder cumulant method [28]. It is usually defined as [29]

$$U_B = 1 - \tfrac{1}{3} \frac{\langle M^4 \rangle}{\langle M^2 \rangle^2}, \tag{17}$$

where M^2 and M^4 are the thermal averages of the second and fourth moments of the magnetization defined by (16).

[†]1 (one) MD is accomplished when the equation of rotation has been integrated once for all spins in the model.

3. Results and discussion

To study the thermodynamic behaviour of the variable interaction range of linear spin S_i systems defined by (1)–(4), we have numerically integrated (11). We used the Stormer–Verlet method [25] for various sizes of oscillator spins. The simulation step size δt was selected to be 0.005 for a total of 1000 000 MD steps. To minimize all statistical fluctuations, we average the data over the final 50000-time steps for every chain size with a unit inertia term ($I = 1$). Independent numerical simulations were needed to study the thermodynamic critical behaviour for various ξ where, as stated above, ξ corresponds to the key interaction parameter to change the model from a short to long-range interaction regime by connecting each spin to L neighbors in each side according to a power law given by (2) and (3). The evolution of the number of links as a function of the system size is presented in Fig. 1 for two different values of ξ.

Figure 2a–c shows the heat capacity C_v for a various dilution parameters (interaction range of oscillators in the ferromagnetic spin chain) $\xi = 1.3$, $\xi = 1.4$, $\xi = 1.6$ and for $N = 20$ to 640, assuming the periodic boundary conditions and considering a system temperature variation from 0.2 to 0.6. It was found that after excitation of the system at $t = 0$ the characteristic of the heat capacity C_v varies with the number of spin neighbors L when the dilution parameter ξ changes from 1 to 2. The result shows that the critical behaviour of the heat capacity C_v is obvious when the range parameter surpasses $\xi = 1.4$ (see Fig. 2b).

Figure 2d shows the variation of C_v with temperature T for different system sizes in the case of the globally interacting system ($\xi = 2$). We notice that the C_v curves cross at $T \approx 0.50$ for all system sizes.

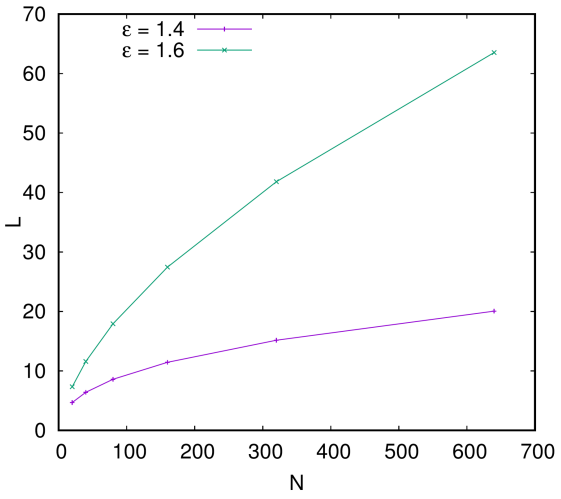

Fig. 1. Variation of the number of links (L) as a function of system (N) sizes for ξ equal to 1.4 and 1.6.

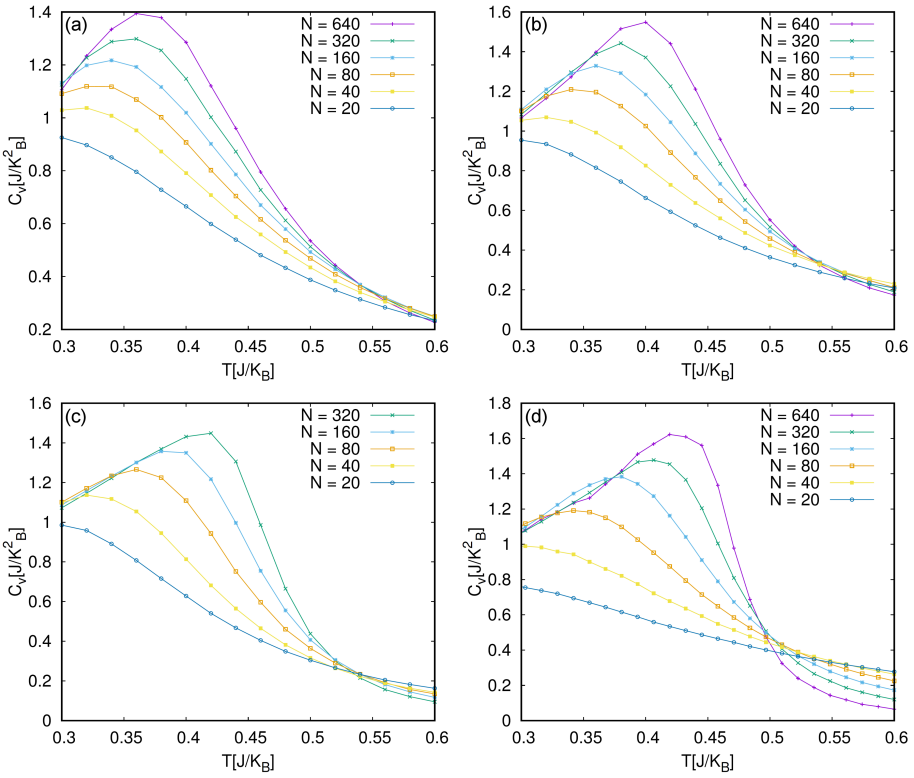

Fig. 2. Heat capacity for a variable-range ξ interaction values, i.e., (a) $\xi = 1.3$, (b) $\xi = 1.4$, (c) $\xi = 1.6$, (d) $\xi = 2$ full coupling (HMF model).

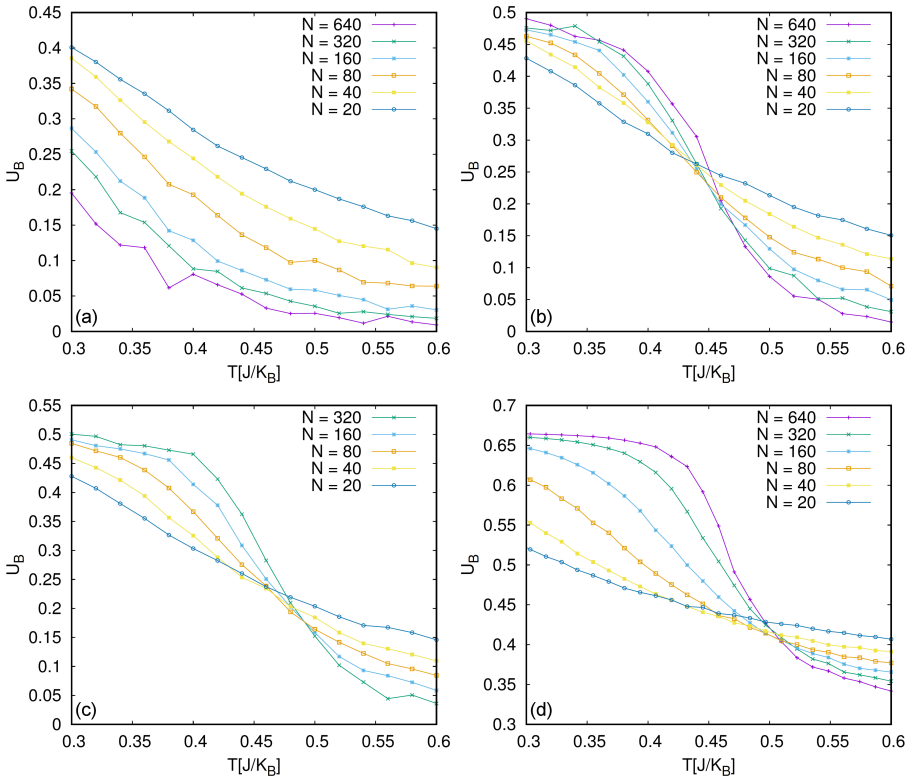

Fig. 3. Binder cumulant for variable-range ξ values, i.e., (a) $\xi = 1.3$, (b) $\xi = 1.4$, (c) $\xi = 1.6$, (d) (d) $\xi = 2$ full coupling (HMF model).

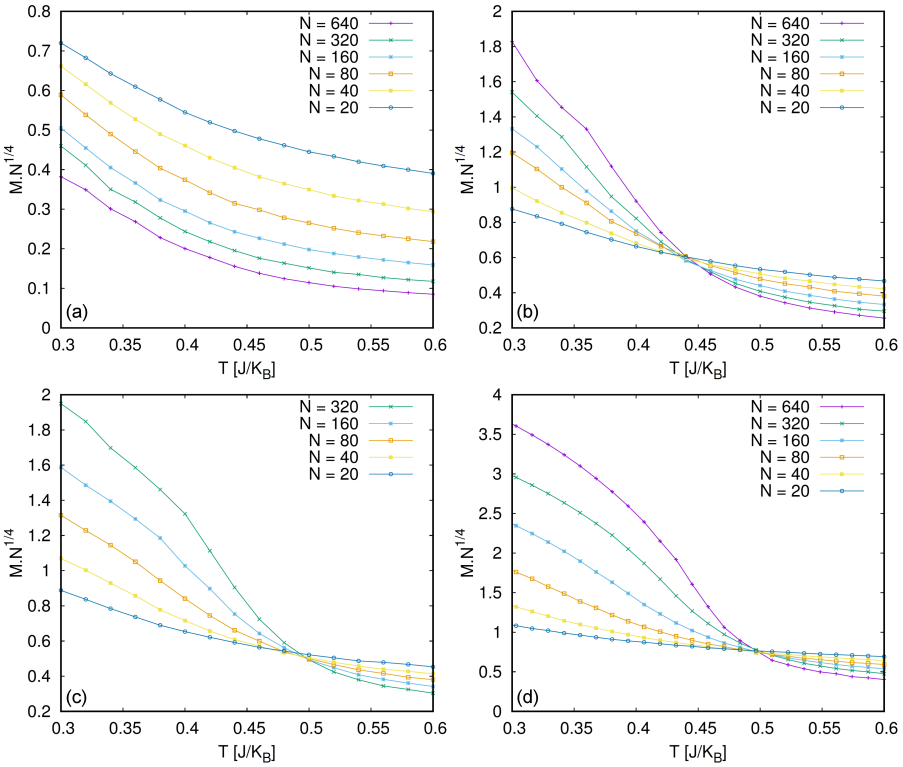

Fig. 4. Scaling order parameter for a variable-range ξ values, i.e., (a) $\xi = 1.3$, (b) $\xi = 1.4$, (c) $\xi = 1.6$, (d) $\xi = 2$ full coupling (HMF model).

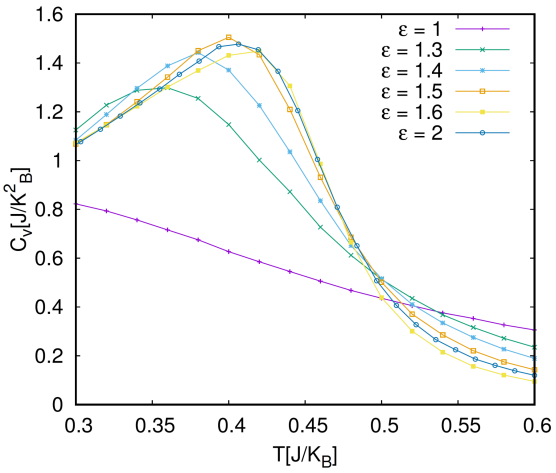

Fig. 5. Heat capacity C_v for a spin chain size $N = 320$ under several length of spins neighbors.

Moreover, the peak of C_v approaches the analytic transition for the fully coupled HMF model studied by Antoni et al. [30] as indicated by the following equation

$$T_c = \frac{J}{2k_{\mathrm{B}}}. \tag{18}$$

To investigate the Binder cumulant in our model, we first measure the magnetization M for each size N and compute its value according to (17) for different interaction ranges from $\xi = 1$ to 2. In Fig. 3a–d, we have presented the Binder cumulant method. We notice that the results cross at a similar T_c value for large interaction range $\xi \geq 1.4$, which confirms the findings obtained via previous results for C_v (see Fig. 3c and d). Figure 3a and b shows that there is no Binder cumulant cross point that would indicate a critical behaviour.

In this study, our main finding is the presence of a critical interaction range for the thermodynamic behaviour of a ferromagnetic linear spin chain, beyond which T_c disappears even when the interaction range parameter ξ is below than 1.4. The finite-size scaling [31, 32] of magnetization parameter shown in Fig. 4a–d is an important tool for analyzing the results of our molecular dynamics simulation. This method shows a clear cross point around $T_c \simeq 0.5$ which becomes sharper as L increases, with eventually only a discernible cross point of all curves at a large diluted value of $\xi = 1.4$. We note that the spin chain has a single critical interaction range length at $\xi = 1.4$. This indicates that the disappearance of the order-disorder parameter state is observed with the occurrence of an almost perfect phase transition characterized by $\xi = 1.4$.

In Fig. 5 we plot the heat capacity as a function of system temperature T for various interaction range length L ($\xi = 1$, 1.3, 1.4, 1.5, 1.6 and 2). We note that the critical behaviour of our model is less obvious as L increases and that it eventually goes to

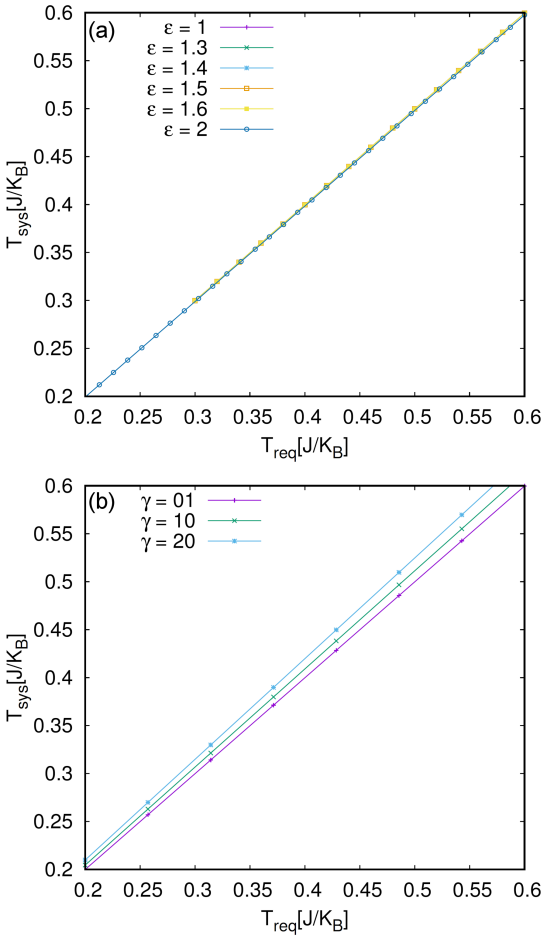

Fig. 6. Behavior of the simulated system temperature (T_{sys}) as function of desired temperature (T_{req}) (a) under varing number of nearest neighbors (L) and (b) under different friction γ values. The different lines represent temperature of the system calculated from the equipartition of the energy equation and the dotted line represents the required temperature (Langevin bath temperature).

real transition from order to disorder parameter at a sufficiently long interaction range. This indicates that for a ferromagnetic linear spin chain, the critical interaction range L_c exists. We can clearly see that the critical value $\xi_c = 1.4$ is well obtained.

In Fig. 6a and b, we have traced the system temperature as a function of the required temperature (bath temperature of simulation) for various interaction ranges $\xi = 1$, 1.3, 1.4, 1.5, 1.6 (Fig. 6a) and under different friction parameter $\gamma = 1$, 10, 20 (Fig. 6b). The temperature results obtained with various ξ and $\gamma = 1$ show that there is no dependence between the calculated temperature of the system and the number of neighbors L. However, as shown in Fig. 6b, there exists a clear dependence between the calculated temperature and the friction factor γ. At the lower damping regime $\gamma = 1$, the calculated temperature of the system does not reach the temperature of the bath.

4. Conclusions

We have studied by the molecular dynamics technique the influence of the number of neighbors spin L on the thermodynamic critical behaviour of ferromagnetic oscillators spins in one dimension with different ranges of interactions. We introduced the parameter ξ, which allows to switch the number of links L from a linear chain with nearest neighbors coupling characterized by $\xi = 1$, to a full coupling configuration with $\xi = 2$ (HMF) model [30]. We identified two main regions. In the first region, for $\xi < 1.4$, the model has a one-dimensional nearest neighbors behaviour and thus does not display any critical temperature T_c, as our numerical simulations showed. In the second region, $\xi_c \geq 1.4$, on the contrary — the model presents the quasi-long-range order state and we can observe the mean field phase transition T_c of the magnetization at 0.5 for $\xi = 2$, identical to that of the Hamiltonian mean field model [30, 33]. In addition, we show numerically that the systems temperature is affected by the friction parameter γ, which seems to be size-independent of the number L of spin neighbors.

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