

ON ERGODIC RELAXATION TIME IN THE THREE-DIMENSIONAL ISING MODEL

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We have studied the dynamical decay of the autocorrelation function of the 3D Ising model for different sizes $L = 20$ – 52 of spin cluster-cubes. The behaviour of the longest, ergodic relaxation time, τ_c , of a finite domain below the phase transition temperature T_c was mostly considered for two types of phase transition dynamics. A study of the scaling properties of τ_c demonstrates a negligible difference between the types of dynamics used, but a considerable difference for different boundary conditions. In contrast to the known result for periodic boundary conditions ($\tau_c \sim L^z \exp[\text{const}(Le^\nu)^2]$, where z and ν are the dynamical and correlation length exponents, respectively, and $\epsilon = 1 - T/T_c$), the ergodic relaxation time for open boundary conditions is proportional to $L^z \exp[\text{const}(Le^\nu)^{2k}]$ with coefficient k for lattices explored in this work slightly decreasing with L in between 1.65 and 1.58. This result implies that only the lattices of sizes close to or exceeding $L = 300$ with open boundary conditions might have ergodic relaxation times similar to those with periodic boundary conditions.

Keywords: Ising model, classical Monte Carlo simulations, finite size scaling, ergodic relaxation time

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1. Introduction

The static critical properties of the 3D Ising model are well-known, and the corresponding critical exponents are numerically well estimated both above and below the phase transition point. The tabulated values of static critical exponents might be found in comprehensive reviews [1–3]. The dependence of the dynamical properties of this model on finite size effects was studied numerically in Refs. [4–7] mostly above the phase transition point. In particular, the value of the so-called dynamical (or critical slowing down) exponent z for the 3D Ising model was obtained in a range 1.95–2.17 (see [7–9]) using different numerical techniques. Actually the discussion on the z value for systems belonging to the 3D Ising universality

class continues up to now (most recent data on z is limited to 2.017–2.10, see e. g. [10, 11]).

However, the most interesting results are expected to occur below the phase transition point, where the response functions and the relaxation times of the magnetization [12, 13] are extremely sensitive to finite-size effects. Thus, the problems dealing with occurrence of the so-called “ergodic relaxation time” [4], which is related to magnetization reversals of a spin cluster below the phase transition point, might still be of considerable interest.

In this paper we present the relaxation times of finite 3D clusters which were obtained by expansion of the autocorrelation function of the 3D Ising model. This function is obtained by a single flip Monte Carlo (MC) calculation for temperatures

below the phase transition point, $T < T_c$, for different cluster-cubes of sizes L^3 ranging from $L = 20$ to 52. The spin interaction energy is calculated using the usual Ising Hamiltonian $\mathcal{H} = -\sum_{ij} \sigma_i \sigma_j$ with spin variable $\sigma_i = \pm 1$ and the range of ferromagnetic interaction $J > 0$ restricted to the nearest neighbours (NN) only. Both periodic (PBC) and open boundary conditions (OBC) are employed. The magnitude of these relaxation times was shown [14] to be very different when PBC and OBC were employed: the system with PBC approaches thermodynamic equilibrium much faster. The lattices considered in Ref. [14] were quite small ($L < 28$). Therefore, here we expect that using a set of larger lattices might give the scaling relation for ergodic relaxation time with OBC much closer to that [4, 5] obtained with PBC. The study might show at least the approximate sizes of 3D Ising lattices for which the scaling relation for 3D Ising lattices with OBC and PBC might be the same.

It is known that the type of dynamics does not affect the static properties of the Ising model as long as the detailed balance principle is preserved. However, it is not obvious whether it affects the dynamical properties or not. There are some limitations on the choice of the MC algorithm dynamics [15], and it is often chosen on physical grounds rather than simple computational efficiency [16]. Therefore, here we use two types of single spin flip (or particle jump) dynamics for their mutual comparison. The first type considered here is the usual Glauber-type dynamics [17], when spin flip probability $\omega(E_i \rightarrow E_j) = 1/[1 + \exp(\Delta E/k_B T)]$ depends on a difference of energies $\Delta E = E_j - E_i$ after (E_j) and before (E_i) the local change of state. The second type is related to the fact that in some cases (e. g. considering barrier hopping in two minima potential characteristic for H-bond ferroelectrics, lattice-gas models with Kawasaki-type of dynamics or models with more than two states) the particle has no *a priori* knowledge of its final energy – the depth of minimum to which it is hopping. Then it is reasonable to assume the jump probability to be proportional just to $\exp(-E_i/k_B T)$, since the final energy might be important only when the particle overcomes the barrier, i. e. for the next jump of the particle. The fact that one has no knowledge of the final energy is more a philosophical question for a pure Ising spin flip ($\sigma_i \rightarrow -\sigma_i$), since then $E_i = -E_j = -J\sigma_i \sum_{\text{NN}} \sigma_{\text{NN}}$, where the sum is taken over

NN spins of spin i , and $\Delta E = 2E_i$ can be anticipated. For the pure Ising model we describe this dynamics by the probability $\omega(E_i \rightarrow E_j) = \exp[-(E_0 + \Delta E/2)/k_B T]$, with always existing barrier for hopping E_0 (equal to $6J$ in case of the 3D Ising model). In general, we assume this type of dynamics to be appropriate to describe the real experiment; therefore, further (to distinguish it from the Glauber one) we call it “experimental dynamics”.

Here we calculated the time-delayed autocorrelation function of magnetization, $\Psi = \frac{d}{dt} \langle (\sigma(t) - \langle \sigma \rangle)(\sigma(0) - \langle \sigma \rangle) \rangle$, where $\langle \sigma \rangle$ denotes spin average and $\sigma(t)$ time-dependent value of the spin variable. We register time dependence of spin operator and its variation over a chosen time range which is equal to the largest chosen correlation delay t_{max} . Then we collect the values of the time-delayed autocorrelation function at every MC step (MCS) for a set of delays ($0 < t < t_{\text{max}}$) and further move the time range of the system observing time evolution of this function. Eventually, the time-average of the correlation values is obtained and the autocorrelation function is normalized by L^3 . The dynamic susceptibilities might be calculated from this response functions by Fourier transform of $\Psi(t)$. To increase the speed of calculations we also used the n -fold algorithm approach [18].

With this approach we used to take 10^5 MCS/site for calculations resulting in shorter relaxation times (smaller L and higher $T < T_c$). For lattices with larger L and lower T we increased the calculations up to 2.5×10^5 MCS/site.

Performing the fitting of $\Psi(t)$ by exponential decays we have found that time dependence of the obtained autocorrelation function is best approximated by 4 relaxation times below and 2 relaxation times above T_c , i. e. $\Psi(t) = \sum_{\alpha} a_{\alpha} \exp(-t/\tau_{\alpha})$, where a_{α} denotes the amplitudes, and τ_{α} is the relaxation times, and summation over α is from 1 to 4 ($T < T_c$) and 2 ($T > T_c$). Due to different time scales of obtained relaxation times at $T < T_c$, we took just two longest relaxation times for further consideration: the longest one as ergodic (τ_e) and the second longest one as intrinsic (τ_i). The terms ergodic and intrinsic here and further are used as in Ref. [4]. The longest (ergodic) time, τ_e , is related to magnetization reversals of a finite system from one more or less uniform state to another through a non-uniform state with zero magnetization, and

these uniform states correspond to two minima of the free energy or two maxima of the magnetization distribution. The intrinsic time, τ_i , which is due to local fluctuations of magnetization, is the second by magnitude time on a time scale. The typical fitting procedure of time dependence of the calculated autocorrelation function by two longest relaxation times is demonstrated in Fig. 1.

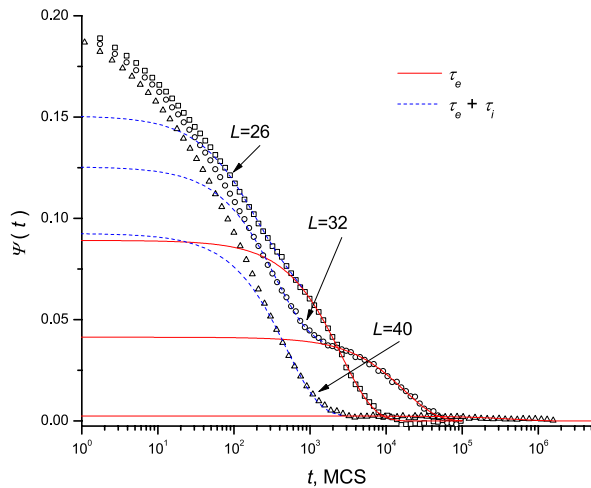


Fig. 1. Time dependences of the autocorrelation function for three lattice sizes and $k_B T/J = 4.41$ using OBC and “experimental” dynamics.

In Fig. 2(a) we present temperature dependences of ergodic relaxation time obtained using OBC for both Glauber and “experimental” dynamics and $L = 20–52$ lattices both above and below T_c . To show the difference in time scales of τ_e and τ_i , the intrinsic relaxation times are presented in Fig. 2(b). It should be noted that dependence of both times on L is different: τ_e exponentially increases, while τ_i saturates with increase of L . Their temperature dependences (Fig. 2) are also very different: below T_c with decrease of temperature, τ_e exponentially increases, while τ_i has a small rounded peak close to the phase transition point (implying some relation of this peak to $T_c(L)$). It should be noted that usually this peak is obtained at a bit higher values of temperature than the peak of susceptibility [12, 13]. In the inset to Fig. 2(a) the temperature dependence of ergodic relaxation time obtained using PBC is presented. As in the OBC case, this time also increases exponentially, but contrary to the behaviour of τ_e obtained

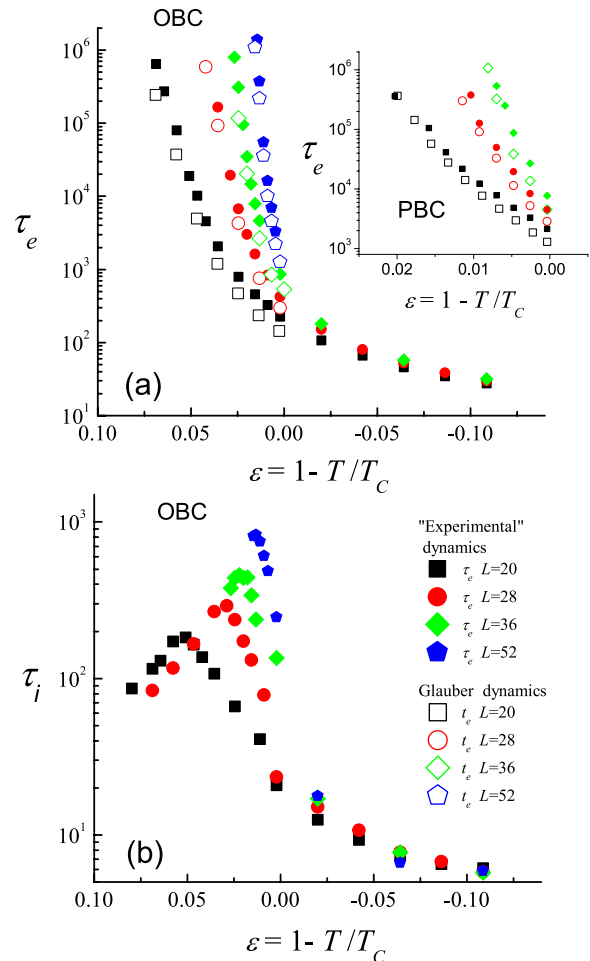


Fig. 2. (a) Temperature dependences of ergodic relaxation time using OBC and PBC (inset) and both types of dynamics. (b) Temperature dependences of intrinsic relaxation time using OBC and “experimental” dynamics.

with OBC the increase is much more drastical as should be for a system which approaches its thermodynamic limit much faster.

As in previous computations [4, 5], we also tried to scale the ergodic relaxation time below the phase transition point using scaling argument $x = L\epsilon^\nu$, where $\epsilon = 1 - T/T_c$ and ν is the critical exponent of the correlation length which for the 3D Ising model has the value in between 0.62 and 0.63 (see [19, 20] and references therein). Assuming $z = 2$ and $\nu = 0.625$ and using PBC we obtain that τ_e is proportional to $L^z \exp(\text{const } x^2)$ (see Fig. 3(a)), i. e. the same result which was obtained [4–6] from calculations of interface free energy between two coexisting magnetization domains. It should be noted that our results do not depend on a type of dynamics used. At the same time the

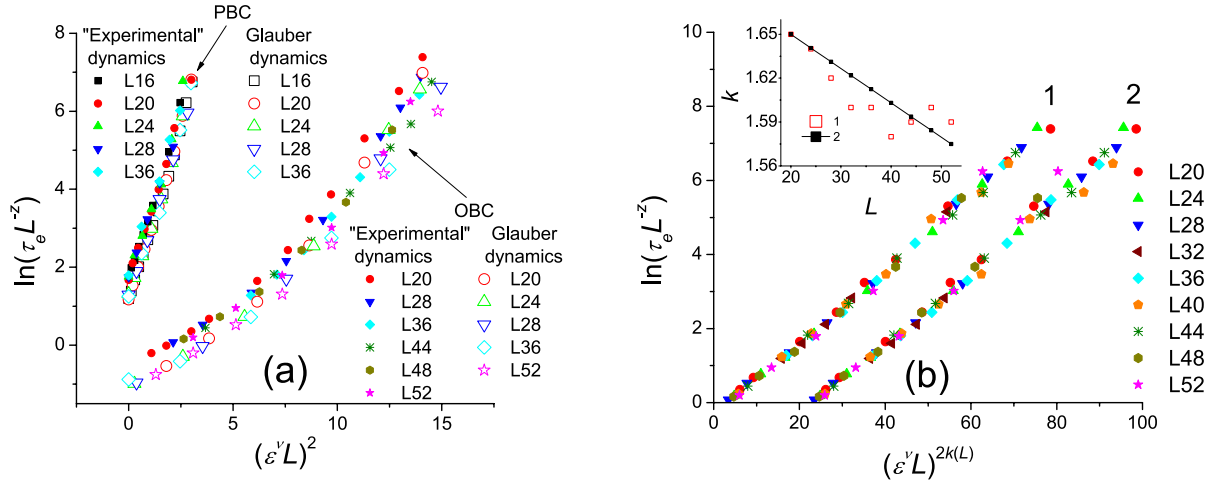


Fig. 3. (a) Ergodic relaxation time τ_e as a function of $(L\epsilon^\nu)^2$ obtained from calculation of the autocorrelation function for $L = 20\text{--}52$ using OBC and PBC for two types of dynamics. (b) Scaling 1: τ_e obtained using OBC linearized with values of parameter $k(L)$ given by grey open squares (red in an electronic version) in the inset; scaling 2: the same linearized with values from the $k(L)$ line (black squares in inset). For clarity, the data of scaling 2 is shifted by 20 along the horizontal axis.

function $\ln(L^{-z} \tau_e)$ obtained using OBC demonstrates nonlinearity with respect to x^2 and in an interval of lattice sizes studied here ($L = 20\text{--}52$) linearizes only with respect to $x^{2k(L)}$ with $k \approx 1.65\text{--}1.58$. Again, this result does not change for both types of dynamics used.

Actually, first we explored the autocorrelation functions and τ_e s of smaller OBC lattices, $L = 16\text{--}28$, and obtained the scaling with $k = 1.6$ [14]. Of course, this could be the artifact of using too small a lattice. Since the PBC results for finite lattices approach the asymptotic thermodynamic equilibrium much faster, the idea was to see if the coefficient k stays constant or decreases with increase of a lattice size (implying that for very large lattices the properties of the lattice with OBC might be closer to those with PBC). Unfortunately, due to lack of computational resources we could not perform a systematic study of how the scaling relation changes as the data for smaller L values are excluded from the analysis. Nevertheless, we managed to make the calculations up to $L = 52$ and noticed that the best scaling of results for $20\text{--}52$ lattices is obtained for the set of $k(L)$ values shown by open square symbols in the inset of Fig. 3(b) (scaling set 1). To evaluate what might be the approximate size of the OBC lattice, when ergodic relaxation scales as in the PBC case (with $k = 1$), we performed the scaling of data points for all available lattices up to $L = 52$ assuming the linear $k(L)$ dependence as shown by the line

of black squares in the inset to Fig. 3(b). The scaling given by the scaling set 2 is quite satisfying. The linear $k(L)$ dependence might be approximated by the line $k \approx 1.705 - 0.0025L$ which gives $L \approx 300$ as the minimal OBC lattice for which the ergodic time might scale similarly as the PBC.

It should be noted that the indirect way to find the scaling properties of ergodic time from calculation of interface tension was proposed by Binder [4–6]. He has shown that τ_e is inversely proportional to the magnetization distribution function $P(\langle\sigma\rangle)$ at its minimum, $\langle\sigma\rangle \approx 0$, and can be expressed as $\tau_e \sim L^z \exp(2L^{D-1}F/k_B T)$, where F is the free energy of interface tension, and $F/k_B T \sim \xi^{-(D-1)}$ close to T_c . This expression for the 2D case was later corroborated by direct Monte Carlo calculations of the autocorrelation function using PBC [21]. The function $F(\epsilon)$ was obtained from Monte Carlo calculations of $P(0)$ distribution, and for the 3D Ising model with PBC $F/k_B T \approx 1.01\epsilon^{2\nu}$, where $2\nu = 1.26$ [6]. Using OBC, strong nonlinearity in the semi-log plot of $P(0)$ versus L^2 was noticed [5], but $F(\epsilon)$ dependence was not obtained.

To compare with the results obtained from calculation of the autocorrelation function, we also performed the calculation of magnetization distribution at $T < T_c$ and obtained the expression for interface tension. Our results obtained using both Glauber and “experimental” dynamics and PBC were very similar to those obtained

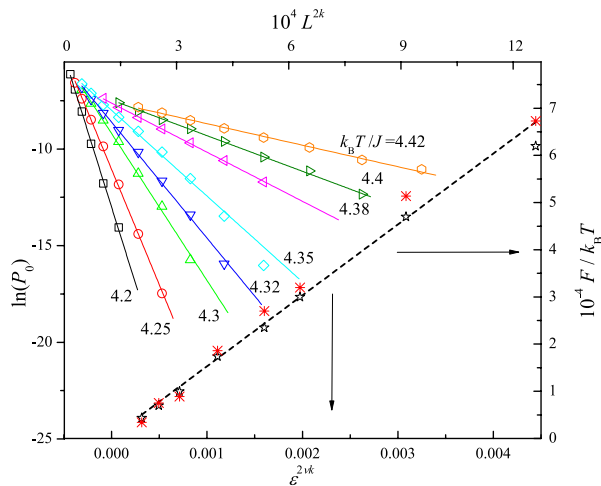


Fig. 4. The results of calculation of interface tension with “experimental” dynamics using OBC: the straight lines $\ln P(0)$ as a function of L^{2k} (with $k = 1.6$) for different values of $T < T_c$ (left) and the surface tension $F/k_B T$ as a function of ϵ^{2vk} (right) obtained from the slopes of lines in the left (black stars) and from extrapolation of two surface tension functions with respect to $\ln L/L^{3.2}$ (red asterisks). The dashed line is a guide to the eye.

by Binder [6], i. e. $\ln P(0)$ was linear with respect to L^2 , and $F/k_B T \sim \epsilon^{2\nu}$. The same tendency was found analysing the $P(0)$ distributions of Ref. [20]. Using OBC, however, the logarithm of $P(0)$ showed linear dependence only with respect to L^{2k} (see straight lines in Fig. 4, left). The surface tension function $F/k_B T$ in the OBC case was calculated using two fitting procedures (see [6]): linearization of $\ln P(0)$ vs L^{2k} and extrapolation of two surface tension functions ($\ln P(0)/L^{2k}$ and $\ln[P(\langle\sigma_{\max}\rangle)/P(0)]/L^{2k}$) linear in $\ln L/L^{2k}$ to the unique F value by fitting an appropriate value of k . The latter procedure was possible to best perform for $k \approx 1.6$, since for this value the functions were linearized and easily extrapolated. The interface tension function $F/k_B T$ obtained by both fitting procedures as a function of $\epsilon^{2\nu k}$ is presented in Fig. 4 and data points fall into a similar line: $F/k_B T = 0.15\epsilon^{2\nu k}$.

It should be noted that $k = 1.6 \approx 1/\nu$ and correspondingly $2k\nu \approx 2$ for the 3D Ising model. Thus, our results using OBC, obtained from direct calculation of autocorrelation functions as well as from calculation of magnetization distribution, indicate that interface tension and correspondingly the ergodic time in the OBC case for lattices up to $L = 52$

are very weakly dependent on correlation length exponent. At the same time, the scaling properties of ergodic time for both types of dynamics used, despite obvious difference in absolute time scales, are very similar.

In conclusion, in order to explore the behaviour of ergodic relaxation time, related to magnetization reversals of a spin cluster below the phase transition point, we have studied the autocorrelation function of the 3D ferromagnetic Ising model for cluster-cubes of linear sizes $L = 20\text{--}52$. We used the Monte Carlo single flip technique and two phase transition dynamics. We also used OBC and PBC. Performing the scaling of ergodic relaxation times, we have shown that results do not depend on the type of dynamics, but are very different if PBC or OBC are used. By increasing the size of a lattice, we tried to find how the results obtained with OBC approach those obtained with PBC. Our results imply that the ergodic relaxation time obtained with OBC might be described by the same relation as that with PBC [4, 5] only when lattices exceed the sizes $L > 300$.

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APIE ERGODINĘ RELAKSACIJOS TRUKMĘ TRIMAČIAME ISINGO MODELyje

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Santrauka

Tyrėme trimačio Isingo modelio autokoreliacijos funkcijos slopimo dinamiką skirtingų dydžių (kraštinės ilgis $L = 20$ – 52) kubiniams sukinių klasteriams. Ilgiausios – ergodinės relaksacijos trukmės τ_c elgsena baigtinio dydžio domene, žemesnėse nei fazinio virsmo T_c temperatūrose, buvo tiriama dviem fazinių virsmų dinamikos būdais. Trukmės τ_c skaliavimo savybių analizė parodė tik nedidelius skirtumus naudojant skirtingą fazinių virsmų dinamiką, tačiau pastebėti gana akivaizdūs pokyčiai naudojant kitokias kraštines sąlygas.

Skirtingai nuo žinomo rezultato, gauto naudojant periodines kraštines sąlygas $\tau_c \sim L^z \exp[\text{const}(L^\nu)^2]$, ergodinė relaksacijos trukmė, kai kraštinės sąlygos yra atviros, yra proporcinga $L^z \exp[\text{const}(L^\nu)^{2k}]$, o koeficientas k mažėja nuo 1,65 iki 1,58, didėjant gardelės dydžiui nuo $L = 20$ iki $L = 52$. Čia z ir ν yra atitinkamai krizinės dinaminė ir koreliacijos ilgio eksponentės, o $\epsilon = 1 - T/T_c$. Daroma išvada, kad ergodinės relaksacijos trukmės esant atviroms ir periodinėms kraštinėms sąlygoms bus panašios, kai gardelių kraštinių ilgiai bus ne mažesni nei $L = 300$.