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Random matrices theory elucidates the nonequilibrium critical phenomena

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The earlier times of the evolution of a magnetic system contain more information than we can imagine. Capturing correlation matrices built from different time evolutions of a simple testbed spin system, as the spin-1/2 and spin-1 Ising models, we analyzed the density of eigenvalues for different temperatures of the so called Wishart matrices. We observe a transition in the shape of the distribution that presents a gap of eigenvalues for temperatures lower than the critical temperature, or in its roundness, with a continuous migration to the Marchenko–Pastur law in the paramagnetic phase. We consider the analysis a promising method to be applied in other spin systems, with or without defined Hamiltonian, to characterize phase transitions. Our approach differs from the alternatives in literature since it uses the concept of magnetization matrix, not the spatial matrix of single spins.

Keywords: Random matrices; Time-dependent Monte Carlo simulations; Phase transitions and critical phenomena; Marchenko–Pastur law.

1. Introduction

The study of the phase transitions and critical[1,2] phenomena covers a considerable part of the investigations in Statistical Physics given its importance that goes beyond the physics of the so-called "natural" phenomena, approaching also the physics on the economy, society and biological systems.[3–5]

Studies about models' criticality are majorly concerned with their equilibrium regime or, if the systems do not have a defined Hamiltonian, such studies are performed in their steady state.

However, many authors have supported dynamic scaling laws for systems far from equilibrium via Monte Carlo (MC) simulations[6,7] in the context of short-time dynamics.

It indeed began with the analytical results of Janssen *et al.*[8] and the numerical simulations of Huse,[9] which demonstrated that the relaxation of the systems, initially at an infinite temperature ($m_0 \ll 1$), suddenly placed at critical temperature must follow a well-established protocol for magnetization:

$$m(t) = \begin{cases} m_0 t^{\theta} & \text{if } t < m_0^{z/x_0}, \\ t^{-\frac{\beta\nu}{z}} & \text{if } m_0^{z/x_0} < t < t_{\text{eq}}, \end{cases} \tag{1}$$

where $m(t) = \frac{1}{L^d}\sum_{i=1}^{L^d}\sigma_i(t)$ is the magnetization of the d-dimensional system, with $\sigma_i(t)$ the state of ith spin.

Here, t_{eq} is the equilibrium time, β and ν are static exponents, while z is the dynamic one. The new exponent $\theta = (x_0 - \frac{\beta}{\nu})/z$ governs the initial anomalous behavior of magnetization, where x_0 is known as the anomalous dimension of initial magnetization.

For systems starting from $m_0 = 1$, one does not observe the initial slip characterized by the exponent θ, but the power law behavior $m(t) \sim t^{-\frac{\beta\nu}{z}}$ directly occurs, followed by exponential decay at thermodynamic equilibrium. For $T > T_C$ or $T < T_C$, one must observe stretched exponential behavior for the magnetization.

In two-dimensional systems $\theta > 0$, and although the literature uses the term "initial slip" of magnetization, it assumes negative values, for example, in tricritical points.[10] One also observes similar behavior in nonequilibrium phase transitions of nonequilibrium models, the initial regime out of steady-state.[11–13]

Nevertheless, the topic deserves a better comprehension, and we would like to understand better how the earlier times of a spin system's evolution could respond to phase transitions of the systems. Based on this question, we intend to go beyond asking how the spectral properties of statistical mechanics systems can be affected by criticality out of equilibrium. More precisely, we would like to know if the traces of criticality in earlier times can influence the spectral properties of suitable correlation matrices defined on the systems.

Definitively, the question is fundamental since it explores if the spectral properties can capture nuances that are not only intrinsically linked to the steady-state of such systems.

In this case, what kind of correlation matrices are suitable to perform in this study? Fortunately, we will answer these points in this paper, showing a method that allows working with small systems compared with those traditionally used by extrapolating systems to a thermodynamic limit.

Firstly, we know that spectral properties have a vital role in describing and characterizing physical systems from a general point of view. For example, in the context of random matrices, Wigner was the first to observe that the distribution of eigenvalues of symmetric/hermitian matrices, under well-behaved random entries,[14,15] could describe the energy spectra of the heavy atomic nucleus.

Some interesting contributions in the final of the 1980s and beginning of the early 1990s (see, for example Refs. 16 and 17) explored the relationship between critical properties of statistical mechanics models in equilibrium and density spectral of random matrices.

In an exciting application of random matrices, Stanley and collaborators,[18,19] using the known approach developed by Marchenko and Pastur,[20,21] showed that deviations from the bulk of spectra of random correlation matrices built with financial market assets are related to genuine correlations from Stock Market.

Interestingly, some authors investigated spectral properties of correlation matrices in near-equilibrium phase transitions.[22] In this case, they studied correlation matrices of the $N = L^2$ spins of the Ising model in the two-dimensional lattice under τ time steps of evolution to evidence the power-law spatial correlations at a phase transition display.

Similarly, the authors in Ref. 23 explored results in the steady-state for the correlation matrix of the asymmetric simple exclusion process. However, we believe that information about phase transitions in spin systems is still more "primitive" than we can imagine. The traces of the phase transition should reflect in properties of random matrices built from time evolutions simulated via MC simulations far from thermalization.

Thus, can we use alternative matrices differently from the ones considered in Refs. 22 and 23, i.e. considering the critical behavior far from equilibrium? In addition, can we use the spectral properties to determine the critical parameter of the spin model studied?

Our goal in this paper is to show that it is possible. The success of our approach is to use the correct matrix that considers magnetization time series and not a matrix of the individual spins.

Thus, using such matrix that captures the collective character of the system, we show that the density of eigenvalues presents an eigenvalues gap (Δ) intimately linked to the proximity of the critical system.

One performs that by first building a matrix M that stores a number N_{sample} of time series with N_{MC} MC steps. With this in hand, we show that the density of eigenvalues of the correlation magnetization matrix of the Ising model, built from M, presents a minimum strictly at its critical temperature, which corroborates the inflection point of the dispersion of eigenvalues.

In the following, we show how to define the magnetization matrix M for a correct analysis of the spectra for the localization of the critical parameter of the Ising model in the earlier times of evolution. In the sequence, we present our results, followed by a summary and our conclusions.

2. Marchenko–Pastur's Theorem and Magnetization Matrix

Here, we define the main object for our analysis, the magnetization matrix element m_{ij} that denotes the magnetization of the jth time series at the ith MC step of a system with $N = L^d$ spins. For simplicity, we used $d = 2$ (the minimal dimension to appear phase transition in the simple Ising model) in this work. Here $i = 1, \ldots, N_{\text{MC}}$

and $j = 1, \ldots, N_{\text{sample}}$. So the magnetization matrix M is $N_{\text{MC}} \times N_{\text{sample}}$. In order to analyze spectral properties, an interesting alternative is to consider not M but the square matrix $N_{\text{sample}} \times N_{\text{sample}}$:

$$G = \frac{1}{N_{\text{MC}}} M^T M,$$

such that $G_{ij} = \frac{1}{N_{\text{MC}}} \sum_{k=1}^{N_{\text{MC}}} m_{ki} m_{kj}$, known as the Wishart matrix.[24] At this point, instead of working with m_{ij}, it is more convenient to take the Matrix M^*, defining its elements by the standard variables:

$$m_{ij}^* = \frac{m_{ij} - \langle m_j \rangle}{\sqrt{\langle m_j^2 \rangle - \langle m_j \rangle^2}},$$

where

$$\langle m_j^k \rangle = \frac{1}{N_{\text{MC}}} \sum_{i=1}^{N_{\text{MC}}} m_{ij}^k.$$

Thereby

$$G_{ij}^* = \frac{1}{N_{\text{MC}}} \sum_{k=1}^{N_{\text{MC}}} \frac{m_{ki} - \langle m_i \rangle}{\sqrt{\langle m_i^2 \rangle - \langle m_i \rangle^2}} \frac{m_{kj} - \langle m_j \rangle}{\sqrt{\langle m_j^2 \rangle - \langle m_j \rangle^2}} = \frac{\langle m_i m_j \rangle - \langle m_i \rangle \langle m_j \rangle}{\sigma_i \sigma_j}, \quad (2)$$

where $\langle m_i m_j \rangle = \frac{1}{N_{\text{MC}}} \sum_{k=1}^{N_{\text{MC}}} m_{ki} m_{kj}$ and $\sigma_i = \sqrt{\langle m_i^2 \rangle - \langle m_i \rangle^2}$. Analytically, if m_{ij}^* are uncorrelated random variables, the density of eigenvalues $\rho(\lambda)$ of the matrix $G^* = \frac{1}{N_{\text{MC}}} M^{*T} M^*$ follows the known Marchenko–Pastur (MP) distribution,[20] which for our case we write as:

$$\rho(\lambda) = \begin{cases} \frac{N_{\text{MC}}}{2\pi N_{\text{sample}}} \frac{\sqrt{(\lambda - \lambda_-)(\lambda_+ - \lambda)}}{\lambda} & \text{if } \lambda_- \leq \lambda \leq \lambda_+, \\ 0 & \text{otherwise,} \end{cases} \quad (3)$$

where

$$\lambda_\pm = 1 + \frac{N_{\text{sample}}}{N_{\text{MC}}} \pm 2\sqrt{\frac{N_{\text{sample}}}{N_{\text{MC}}}}.$$

Sure, in the case of m_{ij} is the average magnetization, we expect that for $T \gg T_c$ the density of eigenvalues $\rho^{\exp}(\lambda)$ obtained from computational simulations must follow $\rho(\lambda)$ in Eq. (3). The question is what happens when $T \approx T_C$. Moreover, it would be more interesting if the density $\rho^{\exp}(\lambda)$, the one obtained from computer simulations, should be used to obtain the critical parameter of spin models.

3. Results

We simulated different time evolutions of magnetization of the Ising model. We used $L = 100$, or $N = 10^4$ spins in this work, except when explicitly mentioned. Figure 1

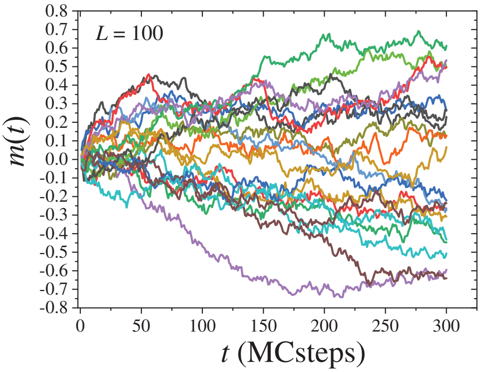


Fig. 1. An example of different time evolutions of magnetization of the two-dimensional spin-1/2 Ising model evolved according to Metropolis dynamics used to build the magnetization matrix M. The initial condition considers that spin states (+ or −) are equiprobable corresponding to $m_0 \approx 0$ ($T \to \infty$).

shows 20 different time series simulated at $T = T_C$ but starting from a random initial condition such that: $p(\uparrow) = p(\downarrow) = 1/2$ ($T \to \infty$).

Thus, for each temperature T, we simulated the Ising model, evolved according to Metropolis dynamics, building an ensemble $N_{\text{run}} = 1000$ square matrices G^*, built from rectangular matrices $N_{\text{sample}} \times N_{\text{MC}}$, with $N_{\text{sample}} = 100$ and $N_{\text{MC}} = 300$ MC

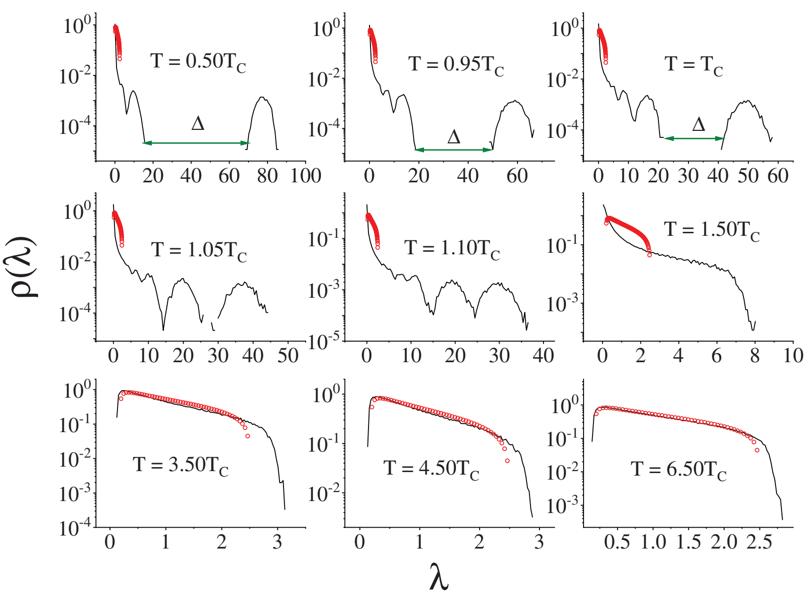


Fig. 2. The density of eigenvalues from an ensemble of $N_{\text{run}} = 1000$ matrices G^*, built from rectangular matrices M^* of dimension $N_{\text{sample}} \times N_{\text{MC}}$, where their columns correspond to $N_{\text{sample}} = 100$ different time evolutions of magnetizations of $N_{\text{MC}} = 300$ MC steps of the Ising model via Metropolis dynamics. Gaps of eigenvalues disappear for $T > T_C$. One observes Marchenko–Pastur law (red points) when T is large enough, i.e. $p(+) \approx p(-) \approx 1/2$).

steps, except when explicitly mentioned. Thus we calculated the density of eigenvalues $\rho_{\exp}(\lambda)$ for each temperature as shown in Fig. 2. In all cases, we subdivided the interval into 100 subintervals to build the histograms.

We can observe that for $T < T_C$, a gap of eigenvalues characterizes the density of eigenvalues. This gap occurs until the proximity of T_C. For $T = 1.05T_C$ the gap almost disappears, which entirely happens for $T = 1.10T_C$. Thus, we observe a migration in the density of eigenvalues as T increases. The Marchenko–Pastur law described by Eq. (3) (red points in Fig. 2) fits the density of eigenvalues for large T as can be observed, for example, for $T = 6.5T_C$.

An important computational detail is that the density of eigenvalues does not present qualitative differences for a different number of MC steps, or even for different system sizes as observed in Figs. 3(a) and 3(b), respectively.

Although the density of eigenvalues changes with temperature and the gap after T_C disappears, we would like to obtain a more precise parameter to localize the critical temperature of the system quantitatively. A natural choice is to compute the moments of the density of eigenvalues:

$$\langle \lambda^k \rangle = \int_{-\infty}^{\infty} \lambda^k \rho_{\exp}(\lambda) d\lambda,$$

where we analyze $\langle \lambda \rangle$ and $\mathrm{var}(\lambda) = \langle \lambda^2 \rangle - \langle \lambda \rangle^2$ as function of T which is shown in Figs. 4(a) and 4(b). We observe an interesting minimal value of $\langle \lambda \rangle$ (Fig. 4(a)) exactly at $T = T_C$, showing this amount captures the evolution of the density of eigenvalues and the gap of the eigenvalues that appears for $T \leq T_C$. This minimal seems to occur at $T = T_C$ independently on N_{sample}, keeping constant the ratio $Q = \frac{N_{\text{sample}}}{N_{\text{MC}}}$. Figure 4(b) shows that at $T = T_C$ we have a corresponding inflection point. It is also interesting to observe that for $T \gg T_C$, $\langle \lambda \rangle$ approaches the average value predicted by MP law (green dashed line) as expected (see Fig. 4(a)). We find

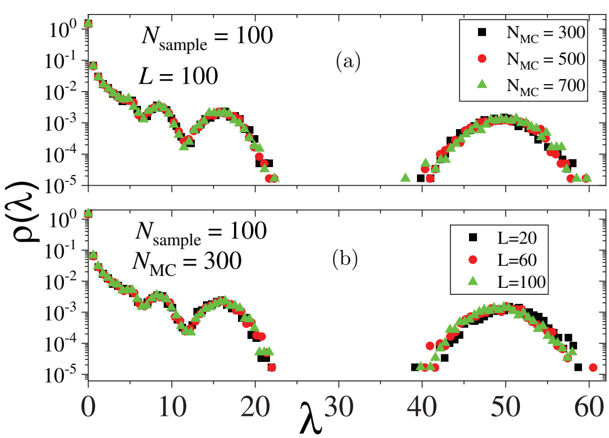
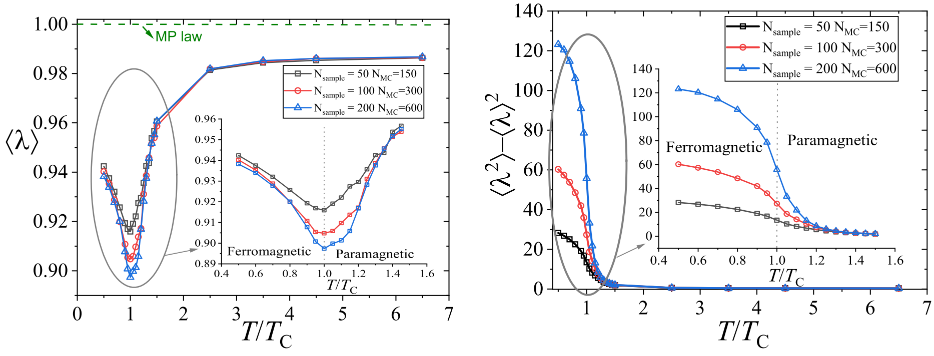


Fig. 3. Density of eigenvalues for a different number of MC steps (N_{MC}) and size lattices (L), respectively, in (a) and (b). We also observe that such a pattern remains even for small values of these quantities.



(a) (b)

Fig. 4. (a) Average eigenvalue of matrix G^* as a function of temperature. The minimal value corresponds to phase transition point. It is interesting to observe that for $T \gg T_C$, such average approaches to the value from Marchenko-Pastur law (green dashed line) as expected (b) Dispersion of eigenvalue. The inflection point occurs strictly at the same critical temperature. For $T \gg T_C$, we also observe that variance approaches the value expected for the MP law: $\mathrm{var}(\lambda) = 1/3$.

for example $\langle\lambda\rangle \approx 0.987$ for $T = 6.5\,T_C$ against $\langle\lambda\rangle = 1$ that is the exact value, or the first moment of the distribution so defined by Eq. (1). Fig. (4)(b) also shows that for $T \gg T_C$, $\langle\lambda^2\rangle - \langle\lambda\rangle^2$ approaches the MP distribution variance. We find $\mathrm{var}(\lambda) = 0.375$ also for $T = 6.5\,T_C$ in comparison with the exact value $Q = \frac{N_{\mathrm{sample}}}{N_{\mathrm{MC}}} = 1/3$.

Understanding the nuances of the correlations leading to such behavior is interesting. We performed histograms of correlations of magnetization (Eq. (2)) for the Ising model for $N_{\mathrm{sample}} = 100$, which results in 4050 values of correlation. In our simulations, as before, we prepared our system at a high temperature ($m_0 \approx 0$) and studied its relaxation at different temperatures.

The magnetization has a growth trend over the different evolutions when the system suddenly quenches to a temperature $T = \frac{1}{2}T_C$. This tendency of ordering generates correlations between the different evolutions corroborated by Fig. 5(a), where considerable negative or positive correlations occur depending on the initial configuration.

However, when the system quenches to a temperature $T = T_C$ (Fig. 5(b)), we have that correlation distribution seems to be uniformly distributed by showing exactly an intermediate situation, presenting a kind of "indetermination" which characterizes the spontaneous breaking of symmetry.

The system becomes uncorrelated (no novelty) when the relaxation occurs from a high temperature $T = \frac{13}{2}T_C$ (Fig. 5(c)).

Such results also suggest that the spectral properties of matrix G capture the critical behavior described by Eq. (1).

Finally, to show the strength of our method, we also performed simulations for the two-dimensional spin-1 Ising model, i.e. the Blume–Capel model for zero anisotropy: $H = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j$, with $\sigma_i = 0, \pm 1$. Using $T_C = 1.69378$ (see Ref. 25). In this case, we

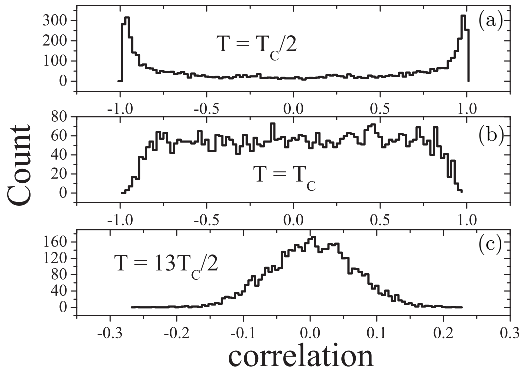


Fig. 5. Histograms of the correlations between different time evolutions for the Ising. Such study was performed for three different temperatures, starting from random initial configurations. (a) $T = T_C/2$, (b) $T = T_C$ and (c) $T = 6T_C/5$, showing strong correlation, indetermination and decorrelation, respectively.

also used our standard set of parameters: $L = 100$, $N_{\rm MC} = 300$ MC steps, $N_{\rm sample} = 100$, considering an ensemble of $N_{\rm run} = 1000$ square matrices.

Figures 6(a) and 6(b) show that the method also works for this model, exhibiting the inflection point for the dispersion and the minimum of the average eigenvalue occurs exactly at the critical temperature of the model as occurred for spin-1/2 Ising model.

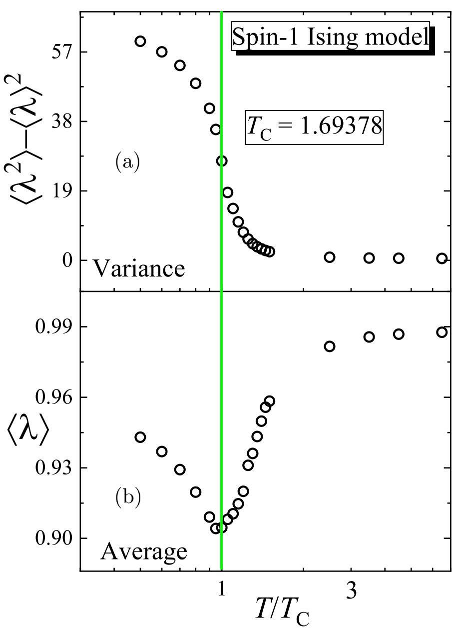


Fig. 6. (a) Dispersion of eigenvalues of matrix G^* for the spin-1 Ising model. The inflection point strictly occurs at the critical temperature ($T_C \approx 1.694$). (b) The minimal value of the average eigenvalue for this model occurs precisely at the same T_C, as can be observed.

4. Conclusions

These results corroborate that the spectrum of correlation matrices built from the time series of magnetization of the spin-1/2 and spin-1 Ising model in the earlier times of the evolution can precisely identify the critical temperature of the models.

The moments of the density of eigenvalues seem to be suitable amounts to perform that. The method is promising and deserves an exploration of other spin systems in interdisciplinary areas of physics[26,27] where phase transitions in Ising-like models often need to be determined. It includes many models, such as cellular automata, agent-based modeling and voter models, among many others, only to cite a few.

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