Thermodynamics of the 2-D Ising Model From a Random Path Sampling Method

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Thermodynamics of the 2-D Ising Model From a Random Path Sampling Method

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We explore the thermodynamics of the 2-D Ising model from a random path sampling method. We show how convergence of free energy and magnetization is obtained in a number of sweeps orders of magnitude below the number of total configurations. The effects of external parameters, such as magnetic field (H) and temperature (T) are accounted in a computationally simple way, allowing very detailed (H, T)-dependent calculations. The effects of more complex interactions can also be considered, particularly magnetovolume coupling, which has proven to be difficult to tackle using traditional approaches. We show its effect on magnetic entropy change (magnetocaloric effect) in this microscopic scenario. As magnetic refrigeration technology matures, the microscopic optimization of magnetovolume effects to enhance the magnetocaloric properties may become a valuable tool in the search of new magnetic refrigerants.

Index Terms—**Ferromagnetism, Ising model, magnetic refrigeration, magnetocaloric effect, thermodynamics.**

I. Introduction

THE Ising model is one of the most studied, if not the most studied, model in the whole of statistical physics. Proposed by Ernst Ising in 1924, it consists of spins, which are confined to the sites of a lattice and which may have only the values +1 or 1. These spins interact with their nearest neighbors on the lattice with interaction constant J. The well-known Hamiltonian is

$$\mathcal{H} = -\frac{1}{2}\sum_{\langle i,j \rangle}(J\ S_i \cdot S_j) - MH \tag{1}$$

where S_i and S_j are nearest-neighbor spins, M is the total magnetization of the system and H an external magnetic field. It took 20 years for an analytical solution to be found for zero-field infinite 2-D Ising model, by Onsager in 1944. It was shown that there occurs a second-order phase transition with divergences in the specific heat, susceptibility, and correlation length. Since then, other exact mathematical approaches have been employed in the study of this deceptively simple-looking model. While initially envisaged as a model for ferromagnetism, the Ising model has been applied in many topics, from gases to binary alloys [1], [2], biophysics [3], sociology [4], image analysis [5], and so on.

Exact solutions for finite Ising systems can be obtained by a simple summing of all possible spin configurations. This approach quickly becomes intractable since the number of possible spin configurations is 2^n, where n is the number of spins. As an example, even for the relatively small 5×5 lattice, there exist $\sim 3 \times 10^7$ possible spin configurations.

The Ising model has then been the object of the development of several methodologies to obtain approximate solutions, most notably Monte Carlo techniques, and in particular the Metropolis method [6]. Indeed, one would be hard-pressed to find a Monte Carlo textbook where the Ising model is not the first and main example of application. Very briefly, the Metropolis method is based on spin flipping attempts, with probability weighed by the Boltzmann factor of the resulting energy difference, $e^{(-\Delta E/(k_B T))}$, where ΔE will depend on an applied magnetic field (if any). Due to critical slowing down near the transition temperature, cluster models [7], [8] are usually applied. Clustered states result from the simple Metropolis sweeps since while the converged energy value might approach the correct value for a given (H, T), the resulting M may not, and can greatly vary. As the degeneracy of states (entropy) is not directly probed in Metropolis sweeps, in practical terms one can only artificially avoid cluster configurations. More recently, Wang and Landau [9] proposed an alternative Monte Carlo algorithm to estimate the density of states, applied to discrete (Ising-like) systems and later to continuous (Heisenberg-like) systems, and multiple variable-dependent density of states [10].

II. Methodology

A common practical detail of Metropolis-type or random walk Monte Carlo approaches to solve the Ising model is that for a given temperature T or field H value, an independent sweep is performed. Consequently, one rarely sees detailed thermodynamic characterization of (H, T)-dependent properties. We here explore the feasibility of employing a random path sampling method in the study of the 2-D Ising model, and discuss its advantages and disadvantages. As is well known, a naïve random sampling of spin configurations is not an effective way to obtain an approximate estimate of the degeneracy of energy and magnetization states. We then consider summing over states obtained from random path sampling from the fully ordered $+1$ to 1 magnetization states. At each step, a random spin in the $+1$ state is flipped, with a probability of 1. In principle, this would overcome the biased magnetization

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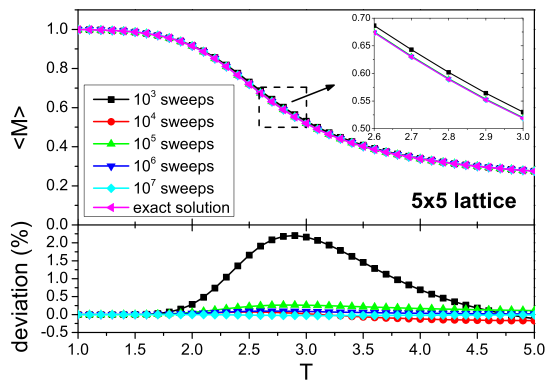

Fig. 1. T dependence of average absolute value of magnetization $\langle|M|\rangle$, of the 2-D Ising model with periodic boundary conditions, as described in text, for a square 5×5 lattice. Full symbols indicate results with varying numbers of sweeps, and the full symbols with dashed line the exact result. Bottom plot shows relative deviation to the exact result. Lines are eye-guides.

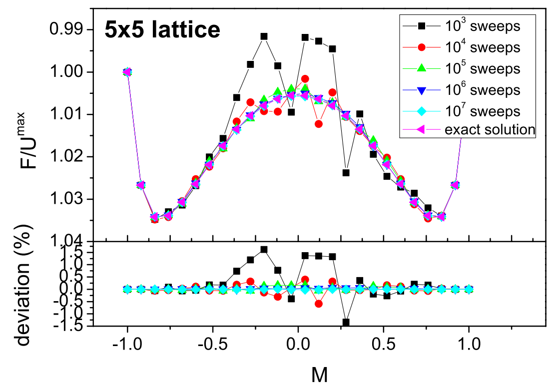

Fig. 2. Normalized free energy dependence on magnetization, of the 2-D Ising model with periodic boundary conditions, as described in text, for a square 5×5 lattice. Full symbols indicate results with varying numbers of sweeps, and the full symbols with dashed line the exact result. Bottom plot shows relative deviation to the exact result. Lines are eye-guides.

sampling of purely random configurations, and would lead to faster convergence. Prior to each sweep, a shuffled list of spin position numbers is generated. Spin flips are then performed sequentially following this list. Contrary to purely random spin flipping attempts, repetitions are then avoided. These would lead to considerable performance issues, particularly for large systems. Also, the configuration energy is determined via the energy difference due to a spin flip, as usually done in the Metropolis method. This is naturally much faster compared with the computationally heavy full sum required to determine the energy of a random spin configuration. With a sufficient number of sweeps, an estimate of individual energy and magnetization states is obtained, together with their degeneracy. As H and T affect energy values and not magnetization or entropy of a given spin configuration, the most time consuming part of the methodology (counting energy and magnetization states and their degeneracy) is performed only once, and then the partition function is re-evaluated for each (H, T) value, and so consequently all relevant thermodynamic variables and their (H, T) dependence.

III. Convergence in a 5×5 Lattice

As the initial object of this method, we consider the 5×5 square Ising lattice with periodic boundary conditions, and compare the convergence of the random path sampling method to the exact result obtained from full configuration summing. This system size is generally considered to be a practical limit for simple configuration summing, which was indeed the case observed in this paper. Fig. 1 shows the obtained average of the absolute magnetization, $\langle|M|\rangle$, for a varying number of sweeps at zero field.

We note that for even a comparatively small number of sweeps ($\sim 10^4$) good convergence ($<0.2\%$) is reached. We can also evaluate the convergence of the calculations via the free energy, $F = U - TS$, where U is the internal energy, and S the entropy of the system. Fig. 2 shows the normalized free energy values obtained for varying sweep values, compared with the exact result, for a given $T < T_C$.

From the free energy, one can estimate the non-average M value, from its T-dependent minimum. As observed in Fig. 2, the small relative change of free energy throughout the magnetization range requires more accurate convergence, particularly for $T \sim T_C$. Nevertheless, for ($\sim 10^6$–10^7) sweeps we obtain a good estimate of the free energy minima magnetization values, as compared with the exact result (not shown). Fig. 3 shows the evolution of the average absolute magnetization value under zero applied field, for system sizes up to 8×8, with convergence $\leq 0.1\%$, compared with either the exact solution or calculations with larger number of sweeps.

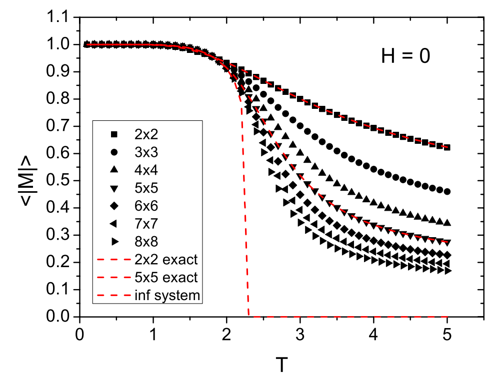

Fig. 3. Average of absolute magnetization of the 2-D Ising model with periodic boundary conditions, as described in text. Solid symbols are approximate results from random path sampling, while dashed lines indicate the exact solutions of the 2×2, 5×5, and infinite lattices.

The number of sweeps used to obtain the data shown in Fig. 3 range from 10^3, corresponding to the 2×2 lattice, up to 10^9 for the 8×8 lattice. Convergence is typically reached in a number of sweeps orders of magnitude below the 2^n number of states, $\sim\sqrt{2^n}$. This tendency requires further investigation for larger system sizes and also in the case of more complex interactions.

We explore detailed (H, T)-dependent calculations in a larger 8×8 lattice, which in practical terms is intractable by a simple summing of states, due to the $\sim 2 \times 10^{19}$ possible spin configurations. As described earlier, we take advantage of the reduced time required to calculate the (H, T)-dependent

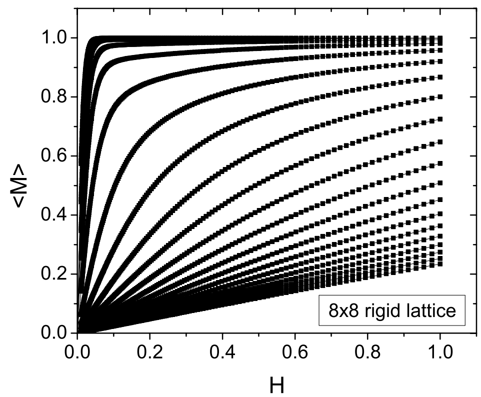

Fig. 4. Field-dependent isothermal average magnetization of the 8×8 Ising model in a square lattice with periodic boundary conditions, for T above and below T_C.

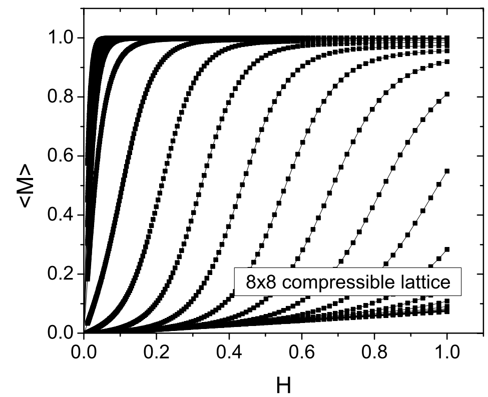

Fig. 5. Field-dependent isothermal magnetization of an 8×8 Ising spin system in a compressible homogeneous square lattice with periodic boundary conditions, with magnetovolume interactions as described in text.

partition function, as these external parameters do not alter the magnetization and degeneracy values obtained from the random sampling sweeps.

IV. Field and Temperature Dependence in a 8×8 Lattice

Fig. 4 shows the average magnetization value, $\langle M \rangle$, of the 8×8 lattice, and its (H, T) dependence. T values are taken both above and below T_C.

We observe a typical ferromagnetic behavior, quickly approaching saturation in the ferromagnetic phase, and an approximately linear behavior for high temperatures. As we are analyzing average magnetization values, as opposed to average absolute magnetization, the symmetry of the Ising model leads to null average magnetization values at zero field (no spontaneous magnetization). In the ferromagnetic phase, a low field value quickly counterbalances this. For larger system sizes, this effect becomes less noticeable. The free energy minimum magnetization does show spontaneous magnetization, and presents also a typical ferromagnetic behavior (not shown), but available magnetization values are limited due to the size of the system. While in this paper, we focus on magnetization properties, a detailed analysis of the effect of H and T on other properties, such as specific heat, energy, and so on, is readily obtainable.

In Section V, we study the field-induced magnetic entropy change (ΔS_M), of the 2-D Ising model. We consider both the magnetization data of the rigid system (Fig. 4) and the effects of magnetovolume coupling, considering J to be dependent on the distance between spins, and including an elastic term in the Hamiltonian, as first suggested in [11]. Even using modern Monte Carlo methods, the compressible Ising model has been shown to be a difficult problem to tackle, particularly due to convergence problems, related to potential non-ergodicity [12].

V. Magnetocaloric Effect in a Compressible 8×8 Lattice

Magnetic refrigeration is an efficient and ecologically friendly technology that is poised to replace current vapor-compression-based refrigerators [13]. Since the discovery of the giant magnetocaloric effect [14], as a result from coupled magnetic and volume/structural transitions, many modern magnetic refrigerant materials present strong magnetovolume coupling. Finding new giant magnetocaloric materials or optimizing their magnetovolume coupling through composition changes has been for the most part empirically based, since theories that account for these effects are typically phenomenological in nature [15]–[17]. A microscopic methodology that considers magnetovolume coupling and assesses its effect on magnetocaloric properties may become a valuable tool in the search of new magnetic refrigerants, particularly when using compositional/structural-dependent parameters that can be obtained from readily available density functional theory methods.

We then consider a compressible Ising lattice, where the magnetic exchange factor J is dependent on the distance between nearest-neighbors, and a quadratic volume energy term. The Hamiltonian is then

$$\mathcal{H} = -\frac{1}{2}\sum_{\langle i,j \rangle}\left[J\ S_i \cdot S_j - K(d_{i,j} - d_{\text{eq}})^2\right] - MH \qquad (2)$$

where $d_{i,j}$ is the distance between nearest neighbors, d_{eq} is the equilibrium distance, and K is a proportionality constant. We consider J to be linearly dependent on $d_{i,j}$, and the system to be homogeneous, with discrete available $d_{i,j}$ (and consequently J) values. The relation between volume and magnetic energy imposes changes on J throughout the (H, T) phase space. As an example of the possible results obtained by this methodology, Fig. 5 shows the $\langle M \rangle$ dependence on (H, T) for the compressible system (2), where $K = 0.030$; available J values range from -1.8 to 2, in steps of 0.025, and the minimum volume energy corresponds to $J = -1.8$. Since changing J values does not affect the possible magnetization and entropy states, the partition function is simply re-evaluated for each considered J value, with no need to repeat the random sampling sweeps.

Fig. 5 shows metamagnetic-type behavior in the compressible lattice, as the isothermal magnetization values present field-induced inflections. As the observed average J values becomes implicitly dependent on $\langle M \rangle$, both H and T induce the compression/expansion of the lattice. The relatively sharp

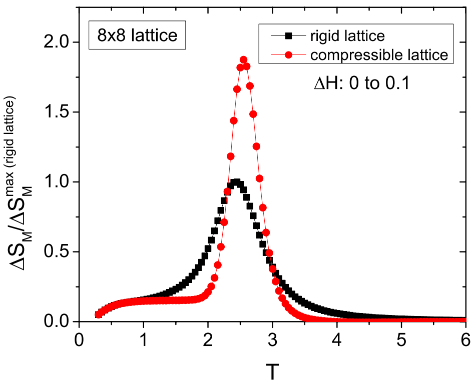

Fig. 6. Normalized field-induced (0–0.1) magnetic entropy change of a rigid (solid squares) and compressible (solid circles) Ising spin system in an 8×8 square lattice with periodic boundary conditions, as described in text. T units are those of the $J = 1$ scale.

field-induced transitions observed in Fig. 5 coincide with volume (and consequently J value) changes. Isothermal magnetic entropy change can be obtained from the data shown in Figs. 4 and 5, for the rigid and compressible lattice, respectively, as shown in Fig. 6, for an applied H change of 0.1.

Fig. 6 shows how the considered magnetovolume coupling affects the magnetic entropy change, in this case leading to a maximum ΔS_M value that is approximately double of the corresponding rigid lattice for this field change value. This results from the complex balance between the lattice and magnetic energies, and external parameters. This result opens the way to the study of the potentially rich phase diagram of the (H, T)-dependent compressible Ising model. It is important to note that the microscopic parameters required in (2) can be calculated by density functional theory (DFT) calculations of a given magnetic system, particularly via the use of packages that estimate J via the method of Liechtenstein *et al.* [18], such as SPR-KKR [19] and openmx [20]. It is then possible to explore the optimization of the magnetocaloric properties of real materials, particularly their magnetovolume coupling through a combined DFT/Monte Carlo approach, where magnetovolume coupling effects are taken into account in both methods. By taking advantage of the massive parallelization possibilities of this method, the study of larger systems or more complex interactions are within reach, particularly through GPU acceleration [21].

VI. Conclusion

We have presented a method based on random sampling of spin configurations and have shown it to lead to accurate estimates of the energy and entropy of the 2-D Ising model, in a number of sweeps orders of magnitude below the total number of possible configurations. We considered simple square systems with periodic boundary conditions, up to 8×8 size. Detailed analysis of the (H, T)-dependent thermodynamic properties is achievable, as the change of external parameters does not require the re-evaluation of magnetization or entropy. We consider the homogeneous compressible Ising model, and show how the field-induced magnetic entropy change (magnetocaloric effect) can be greatly affected by magnetocaloric coupling, in this microscopic scenario. This paper opens the possibility of quantifying and optimizing microscopic parameters of real materials, in a combination with DFT calculations. This methodology may prove to be very useful in the optimization and search for new magnetocaloric materials for magnetic refrigeration applications.

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