

Core Method of Numerical Calculation of Vector Models Density of States

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Abstract

This article presents a new method for the numerical calculation of the density of states in vector models. The method is based on quasi-Markov random walks in the state space of vector models and is multi-spin. An exhaustive enumeration of all cluster states for each of the $2L$ states of the boundary of length L makes it possible to obtain a local distribution of configurations, and such a piecewise method allows one to approximately calculate the entire state space. The method is designed to calculate the degeneracy rate G , the interaction energy E , and the magnetization M for any given lattice geometry, knowing which Gibbs approach can be used in order to calculate the partition function and thermodynamic averages.

1 Introduction

The models under consideration should be studied from different points of view [3].

To study the behavior of spin systems, you need to know magnetic susceptibility, heat capacity and entropy.

According to the definition, magnetic susceptibility characterizes the connection between the magnetization of the magnetic system and the external field:

$$\chi(T)|_{h \rightarrow 0} = \frac{\partial \langle M \rangle(T)}{\partial h} \quad (1)$$

In this case, the average magnetization at a given temperature

$$\langle M \rangle(T) |_{h \rightarrow 0} = \frac{1}{Z} \sum_i M_i \exp \left[-\frac{E_i + hM_i}{k_B T} \right] \quad (2)$$

a statistical amount

$$Z = \sum_i \exp \left[-\frac{E_i + hM_i}{k_B T} \right] \quad (3)$$

Combining equations (2) and (3) we get

$$\chi(T)|_{h \rightarrow 0} = \frac{\partial \langle M \rangle}{\partial h} \Big|_{h \rightarrow 0} = \frac{\partial}{\partial h} \frac{\sum_i M_i \exp \left[-\frac{E_i + hM_i}{k_B T} \right]}{\sum_i \exp \left[-\frac{E_i + hM_i}{k_B T} \right]} \Big|_{h \rightarrow 0} \quad (4)$$

For convenience, you can enter an abbreviation:

$$\beta = \frac{1}{k_B T}.$$

Because

$$\left(\frac{u}{v} \right)' = \frac{u'v - v'u}{v^2} \quad (5)$$

Imagine the numerator and denominator as:

$$\begin{aligned} u &= \sum M_i \exp [-\beta(E_i + hM_i)] \\ v &= \sum \exp [-\beta(E_i + hM_i)] \end{aligned} \quad (6)$$

and their derivatives:

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$$u' = \frac{\partial u}{\partial h} = \beta \sum M_i^2 \exp[-\beta(E_i + hM_i)] \quad (7)$$

$$v' = \frac{\partial v}{\partial h} = \beta \sum M_i \exp[-\beta(E_i + hM_i)],$$

this implies

$$\chi(T)|_{h \rightarrow 0} = \frac{\beta(M_i^2 \exp \sum [-\beta(E_i + hM_i)]) \exp \sum [-\beta(E_i + hM_i)]}{(\sum \exp[-\beta(E_i + hM_i)])^2} - \frac{\beta(M_i \exp[-\beta(E_i + hM_i)])^2}{(\sum \exp[-\beta(E_i + hM_i)])^2} =$$

$$\beta \left(\frac{(\sum M_i^2 \exp[-\beta(E_i + hM_i)])}{(\sum \exp[-\beta(E_i + hM_i)])} - \left(\frac{(M_i \exp[-\beta(E_i + hM_i)])}{(\sum \exp[-\beta(E_i + hM_i)])} \right)^2 \right)$$

$$\chi(T)|_{h \rightarrow 0} = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_B T} \quad (8)$$

In turn, the heat capacity

$$C(T) = \frac{\partial \langle E \rangle(T)}{\partial T} = \frac{\partial \beta}{\partial T} \frac{\partial \langle E \rangle(T)}{\partial \beta}, \quad (9)$$

where the average energy at a given temperature is

$$\langle E \rangle(T) = \frac{\sum E_i \exp[-\beta E_i]}{\sum \exp[-\beta E_i]} \quad (10)$$

Similar to magnetic susceptibility, the abbreviation is introduced:

$$\beta = \frac{1}{k_B T}$$

$$u = \sum E_i \exp\left[-\frac{E_i}{k_B T}\right] = \sum E_i \exp[-\beta E_i] \quad (11)$$

$$v = \sum \exp\left[-\frac{E_i}{k_B T}\right] = \sum \exp[-\beta E_i]$$

and their derivatives:

$$C(T) = \left(-\beta^2 - \frac{-E_i^2 \exp[-\beta E_i] \sum \exp[-\beta E_i]}{(\sum \exp[-\beta E_i])^2} - \frac{-E_i \exp[-\beta E_i] \sum E_i \exp[-\beta E_i]}{(\sum \exp[-\beta E_i])^2} \right)$$

$$= \beta^2 \left(\frac{\sum E_i^2 \exp[-\beta E_i]}{\sum \exp[-\beta E_i]} - \left(\frac{\sum E_i \exp[-\beta E_i]}{\sum \exp[-\beta E_i]} \right)^2 \right)$$

$$C(T) = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2}. \quad (12)$$

If we represent the multiplicity of degeneracy of states as a function of the energy $G(E)$, then the entropy for a given energy level, according to the Boltzmann definition, is given by $S(E) = k_B \ln G(E)$. Entropy can be considered as a thermodynamic quantity that determines the measure of energy dissipation in the system and is given by the relation

$$S(T) = \frac{U - F}{k_B T} = \ln Z + \frac{\langle E \rangle(T)}{k_B T} \quad (13)$$

where U is the internal energy of the system, $F = U - k_B \ln Z$ is the Helmholtz free energy. In equation (10), $\langle E \rangle(T)$ is the Gibbs thermodynamic averaging for the energy level. Similarly, the distribution of the energy level of entropy can be obtained:

$$\langle S \rangle = \frac{\sum_i G(E_i) \ln G(E_i) \exp\left[\frac{-E_i}{k_B T}\right]}{\sum G(E_i) \exp\left[\frac{-E_i}{k_B T}\right]} \quad (14)$$

2 A Brief Presentation of the Method and the Results of the Software Product. Visualization of Results

2.1 Theoretical Component of the Method

For vector models of Ising spins, the interaction energy is usually given by the Hamiltonian of the form

$$E = - \sum_{\langle i, j \rangle} J_{ij} S_i S_j, \quad (15)$$

where S_i is «spins», or one-component vectors whose components take the values either «+1» or «-1», and J_{ij} is a constant of exchange interaction, usually takes the value «+1» for ferromagnets, t. e. if the vectors S_i and S_j are co-directed, then this corresponds to a minimum of energy, «-1» is an antiferromagnet, where the antiparallel orientation of vectors leads to minimization of energy. The magnetization of the N spin Ising system is calculated by the formula:

$$M = \sum_{i=1}^N S_i \quad (16)$$

Ising spins are placed in space, for example, in a lattice - a metal model, or randomly for modeling amorphous structures.

To solve the problem of thermodynamics of the system of interacting Ising spins (calculate the heat capacity, magnetization, magnetic susceptibility, and other statistical characteristics as a function of temperature), you need to

know how many states G (configurations) will have given values of E, M . Thus, we are interested in Any given system geometry that has only three global numbers G, E, M . In total there will be 2^N states.

Even in the interaction model of the nearest environment, there are serious computational problems associated with an exponentially rapid increase in the number of possible configurations. For example, for a system of Ising spins on a three-dimensional pyrochlore lattice with 16 nodes there will be 2^{16} configurations.

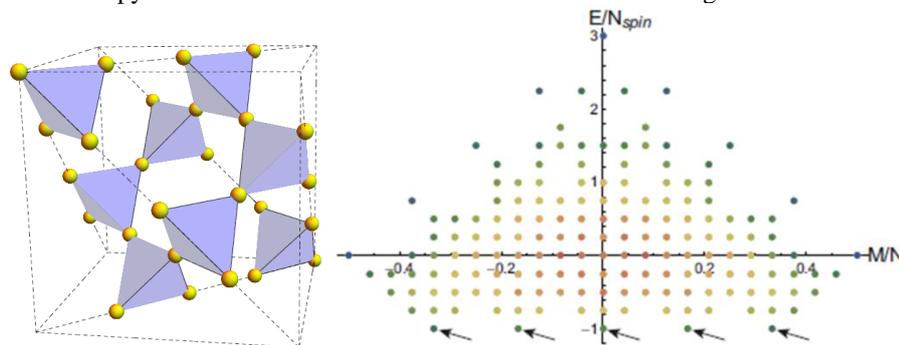


Figure 1: Structure of the pyrochlore lattice (left) [1]. The state space of the Ising spin system with the interaction of the nearest environment on the pyrochlore lattice obtained by the method of exhaustive enumeration (right) [2] histogram G, E, M .

2.2 Brief Introduction of the Method

The essence of the proposed method is to get one random configuration from the 2^N space; this is quite easy to do; we simply set random values of the vector component S_i . One configuration corresponds to one point in the histogram of fig. 1 (right). Select the nucleus (region) of closely spaced spins. We carry out an exhaustive enumeration for each of the 2^L states of the boundary, where L is the number of spins on the boundary and each configuration of the nucleus from 2^N and we obtain local numbers g, e, m taking into account the interaction with the boundaries.

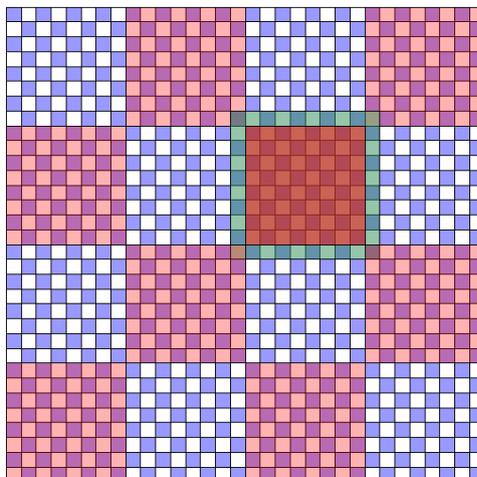


Figure 2: Schematic representation of the Core (cluster) method.

If the core contains 4×4 spins, then there will be a total of 65,536 kernel configurations for one configuration. However, not all of them will have the same values of E_i, M_k , since in systems with the interaction of the nearest environment, degeneracy in E and M is essential. It is possible to use any geometry of the kernel.

We find on the histogram of fig. 1 (on the right), the point with these coordinates corresponding to each value of E_i and M_k is added to the value of g_i that exists at this point g . Thus, we must go through each point in this projection of the histogram, along the horizontal and vertical axes. You may need to make several passes.

The absence of new points E_i, M_k in the process of full coverage of the projection of the histogram can be selected as a criterion for stopping the numerical calculation. After stopping, we will need to normalize G . There are several ways of normalization. For example:

The sum of all histogram columns is 2^N

The sum of the histogram columns with the given value E_i, M_k is the binomial coefficient $B = \binom{N}{\frac{1-M_k}{2}}$.

If we know the degeneracy of one or several points, for example, when all the spins are «up» or all «down» in an antiferromagnet, we can control the normalization of these points.

Knowing the numbers G , E , M , we can use the Gibbs approach to calculate the partition function and thermodynamic averages.

To test our method, a software product was implemented, the algorithm of which is presented below.

2.3 Algorithm for the Implementation of a Software Product

We fill the double array with all kernel variants (each spin value takes the value -1 or $+1$), where L is the linear size of the core. Then we display an array of a kernel of size $L \times L$, write it into a file. Next, we find and return the numbers of configurations with minimal energy and magnetization. We determine the nearest neighbors of all spins and return the energy of the system. We define the point for building the kernel and derive it. We define the periodicity condition and output the array of the kernel.

Set the boundaries of the nucleus and determine the boundary conditions. Calculate and return the magnetization of the entire system. Find the interaction energy of spins inside the nucleus without taking into account the boundaries, where n is the linear size of the system, N is the number of spins in the system, L is the linear size of the nucleus, N_{bound} is the number of spins on the boundary, N_{core} is the number of spins in the core, allconfig is the number of all configurations - maximum number of neighbors of each particle, E_{max} - maximum number of system energy, M_{max} - maximum number of system magnetization, dE and dM - system energy without core energy / without core magnetization, E_{core} and M_{core} - core energy / magnetization, E_{tot} and M_{tot} - total energy / magnetization of the whole system, spins - array in which the values of spins are stored (± 1), bound is the array in which the boundaries are stored, core is the array in which the core is stored, e is the array in which the core energy is stored, m -array in which the core magnetization is stored, b is the double array (allconfig size on N_{core}) with all kernel variants (± 1), gem is the array in which EM and g are stored (E and M are array indices, and g is the value of these indices).

In the next stage, creating an array with all the configurations and display the indexes of the system spins. We prepare the starting configuration, that is, we scatter $+1$ or -1 values throughout the system. Calculate and derive the energy and magnetization of the system. We determine the interaction of the spins with the boundary, then sum up with what was calculated without considering the boundary and obtaining the energy.

The next step is to calculate the energy and magnetization for all configurations by iterating through all configurations. Next, fill the core with spins, which correspond to the configuration. We consider the magnetization and energy of the system without taking into account the interaction with the boundaries. We consider the energy of interaction of spins with the boundary and record the energy of the nucleus. We write in the gem energy and magnetization of the nucleus and then we find the configuration with the minimum energy and magnetization and write the core with the minimum energy and magnetization into a common system. Output to file: energy and magnetization of the nucleus; energy and magnetization of the system with a new core; E M and g .

2.4. Calculated Density of States

According to the results of calculations, the following histograms were constructed with a grid size of 4×4 (Fig. 3) and 5×5 (Fig. 4)

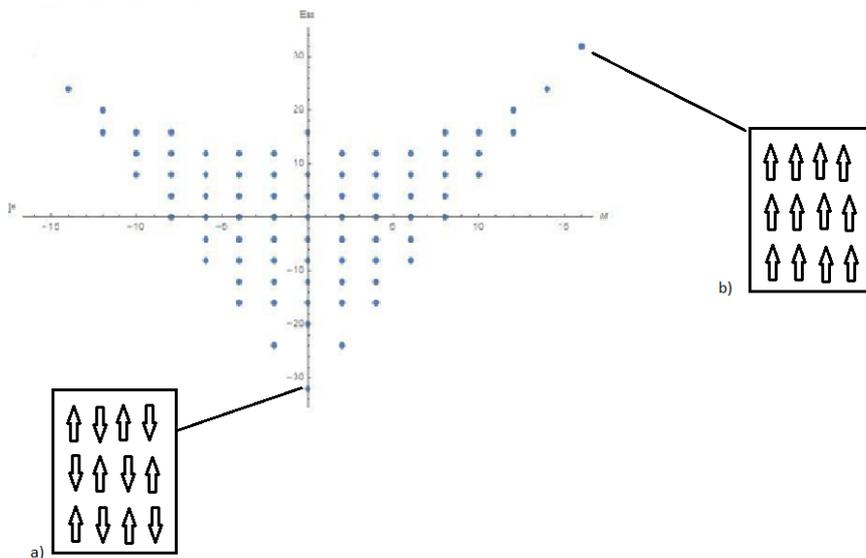


Figure 3: Two-dimensional representation of DOS for systems of 4×4 . a) one of two possible configurations with minimum energy ($E=-32$, $M=0$), b) configuration with maximum energy ($E=32$, $M=16$)

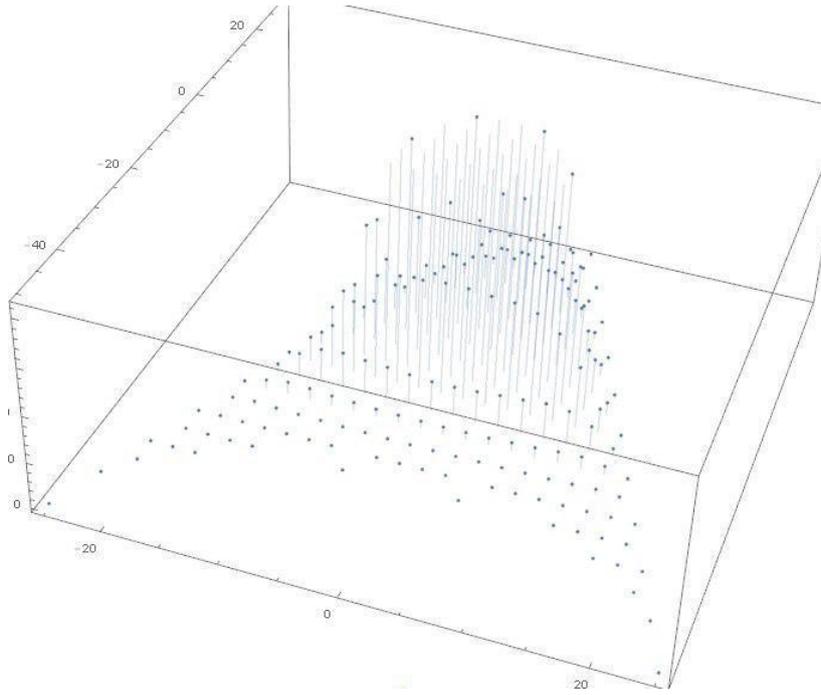


Figure 4: DOS 3D view for 5x5 systems

3 Conclusion

The obtained approximate solutions by the cluster method of numerical calculation of the density of states of vector models exhaustively repeat the exact solution in relation to E and M. The accuracy of the calculations is controlled by comparing the values of the multiplicity of degenerations G obtained approximately and the exact values.

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