A Simple Description of Geometric-Cluster Distributions in Zero-Field Ising Model

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The Ising model of ferromagnetism has been a useful tool in studying phase transition phenomena of atomic nuclei[1]. The clustering processes that occur in the Ising system bear a close similarity to the clustering of nucleons in the liquid-vapor phase transition of nuclei. Geometric clusters that form on the Ising lattice are the simplest clusters to visualize. These clusters are formed when spins of the same direction are connected in a group to their nearest neighbours. Assuming that the clusters are formed independent of each other (ideal gas), summing over their abundances produces the total gas pressure and leads to the construction of the phase diagram. Unfortunately, geometric clusters exhibit non-ideal behavior (predominantly excluded volume) that precludes them from being useful at high temperatures. Non-ideal effects become dramatic near the critical temperature. For this reason other more complex clustering algorithms are employed to remedy the problem (Coniglio-Klein clusters) at the cost of the simplicity of the geometric Ising clusters.

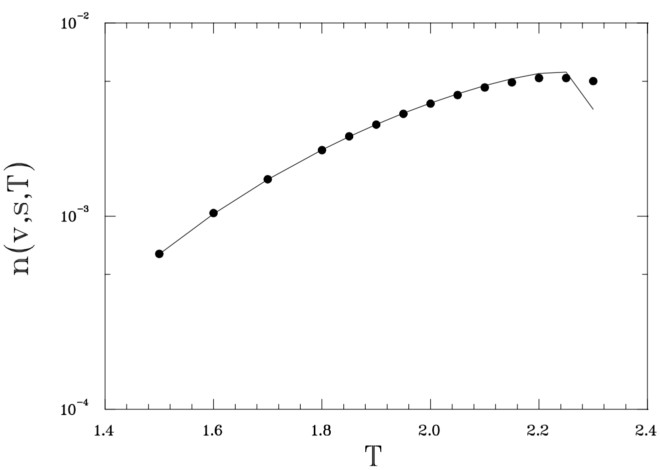

FIG. 1: An example of 2D geometric-cluster temperature distribution for $v = 2$ and $s = 6$ (solid circles). The line represents theoretical description.

We have investigated how geometric clusters might be used to still recover thermodynamic observables in the Ising model. Intuitively one would expect that the distribution of geometric clusters is directly related to the mean-field thermodynamics of the Ising model. Exactly what this relation should be may be intelligently guessed and tested. Our efforts lead to the following general expression for the geometric-cluster distribution of the Ising model:

$$n(v,s) = \frac{1}{L^2}\exp\left(-\frac{F_s}{T}\right)\exp\left(\frac{\Delta\bar{F_v}}{T}\right)V_{free} \qquad (1)$$

In (1) L is the lattice box size; v and s mean volume and surface of a cluster. F_s is the surface free energy of a cluster. $\Delta\bar{F_v}$ represents the cluster mean-field volume free energy above the ground state due to excluded volume effects on the lattice. V_{free} is the fractional volume available to form clusters of a given type, and T is temperature. Below the critical temperature Eq.1 may be put in a form analytic in 2D:

$$n(v,s) = g(v,s)\exp\left(-\frac{cs}{T} + v_{ex}\frac{\Delta F_I}{T}\right)\left(1-\sum v\right) \qquad (2)$$

where g is the cluster combinatorial factor, $c = 2$ is the surface energy coefficient; v_{ex}, numerically equal to the sum of volume and surface of a cluster, accounts for the number of sites that a given cluster excludes from the lattice; F_I is the Ising free energy per spin of the lattice; $\sum v$ means the average fractional volume occupied by all the clusters which is related to spontaneous magnetization.

Fig.1 shows an example of how (2) works. Slight imperfections around the critical temperature are believed to be due to insufficient approximation to V_{free} by $\sum v$ of the infinite lattice

REFERENCES

[1] C.M. Mader, A. Chappars, J.B. Elliott, L.G. Moretto, L. Phair, G.J. Wozniak. LBNL-47575.