Convexity of the free energy in some real-space renormalization-group approximations

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Whereas the free energy for a spin system in a hierarchical lattice will be convex as a function of appropriate parameters (and thus the heat capacity positive, etc.), the same need not be true of a corresponding approximate real-space renormalization-group method applied to a Bravais lattice. Some examples are given which illustrate this point.

Various approximate real-space renormalization-group recursion relations are actually exact when applied to models on hierarchical lattices, as pointed out by Berker and Ostlund[1] and Bleher and Zalys.[2] In many cases it is known that the free energy ($+\ln Z$ divided by the number of lattice sites) for a spin system on such a lattice has a thermodynamic limit[3] f which is then necessarily a convex function of linear parameters[4] in the dimensionless Hamiltonian ($-\mathcal{H}/kT$). This means that various heat capacities, susceptibilities, etc., will be positive. In this paper we wish to point out that certain real-space renormalization-group approximations which are closely associated with hierarchical lattices in the manner just mentioned, but which involve modified schemes for obtaining the free energy, *need not* lead to a convex f, and in some cases direct calculations show that they do not.

The cluster methods of Niemeijer and van Leeuwen[5] belong to this latter category. Figure 1 shows the procedure for constructing the hierarchical lattice associated with their two-cluster approximation as applied to an Ising model on a triangular lattice. A set of $B=8$ bonds of the type shown in 1(a) are joined together as shown by the solid lines in 1(b), and two new "cell" spins (open circles) are added, along with a set of noniterated interactions (in the terminology of Ref. 3), indicated schematically by dashed lines, which correspond to the "majority rule" for determining the configuration of the cell spin in terms of that of its nearest neighbors. The cell spins then form the two ends of a "bond of order 1," eight of which are connected in the manner indicated in Fig. 1(b) to form a "bond of order 2," and so on, *ad infinitum*. The free energy f for an Ising model on the corresponding hierarchical lattice has the form of a convergent sum [Eq. (4.11) of Ref. 3]

$$f=\sum_{N=0}^{\infty} B^{-N}\psi_N \ . \tag{1}$$

However, when this procedure is used as an approximation for the triangular lattice,[5] the free energy $\bar{f}$ is given by (1) but with B replaced by

$$\bar{B}=b^d \ , \tag{2}$$

with $b=\sqrt{3}$ the change in linear scale and $d=2$ the dimensionality. Replacing $B=8$ with $\bar{B}=3$ in (1) has the effect, as one finds by direct numerical calculation, that the second derivative of $\bar{f}$ with respect to the dimensionless exchange interaction K ($=-J/kT$) is *negative* for K larger than approximately 1.12, corresponding to a violation of convexity resulting in a negative heat capacity at low temperatures. The singularities of f and $\bar{f}$ at the critical fixed point K^* are also quite different: The exponent α (corresponding to a singularity of the form $|K-K^*|^{2-\alpha}$) is -2.7910 for f and -0.5312 for $\bar{f}$.

Another example is provided by the methods of Martin and Tsallis,[6] a particular case being the lattice shown in Fig. 2, which should be interpreted in the same way as

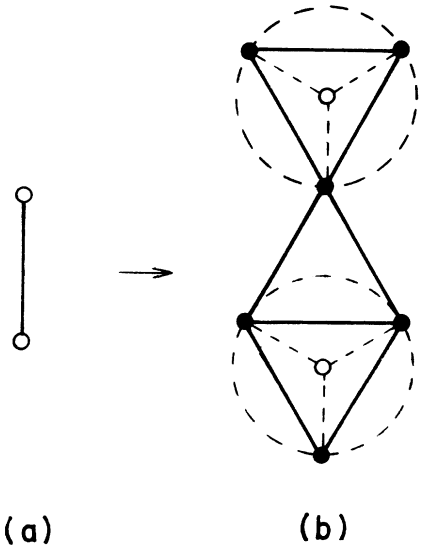

FIG. 1. Construction of hierarchical lattice corresponding to the two-cluster approximation of Ref. 5.

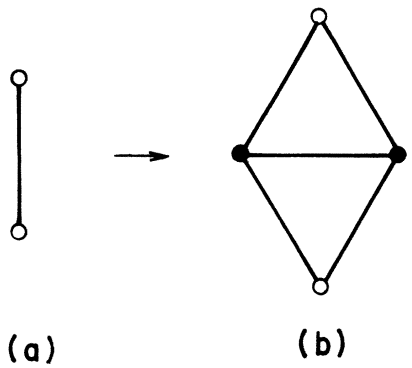

FIG. 2. Construction of hierarchical lattice corresponding to calculation in Ref. 6.

Fig. 1. While the aggregation number B for the hierarchical lattice is 5, $\bar{B}$ is 4 ($b=2$, $d=2$). The corresponding $\bar{f}$ for the Ising model fails to have a positive second derivative for K greater than about 1.13, and has a stronger singularity ($\alpha=-0.2973$) than does f ($\alpha=-0.6670$) for the hierarchical lattice; the latter, of course, is convex for all K.

A third example of a somewhat different kind is provided by the Kadanoff bond-shifting approximation[7] which, considered from the point of view of the associated hierarchical lattice [see Fig. 3(c) of Ref. 3 for the case of a square lattice], has a noniterated interaction depending on a parameter p. In this case the aggregation number B of the hierarchical lattice is equal to b^d, which means that $f=\bar{f}$ will be a convex function of the dimensionless exchange and magnetic field coupling *as long as p is held fixed.* Convexity will also be present in a case in which p is made a function of the order of the bonds (actually squares, cubes, etc.) assembled to construct the hierarchical lattice. However, this is quite different from making p a function of the dimensionless interactions which appear in the effective Hamiltonian at each stage of the recursion calculations. In the latter case there is no guarantee that the resulting free energy will be convex, and the presence or absence of convexity could well depend on how p is chosen, though we know of no cases in which convexity is actually violated if p is chosen as indicated in Ref. 7.

There are, of course, other real-space renormalization-group approximations which are not associated (in any obvious way) with hierarchical lattices. Convexity violations in one such scheme, that of a cumulant expansion, are pointed out in Ref. 8.

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