ISS 0029-3865

CBPF-NF-035/83

# COMMENT ON "CONVEXITY OF THE FREE ENERGY IN SOME REAL-SPACE RENORMALIZATION-GROUP APPROXIMATIONS"

by

Constantino TSALLIS

Centro Brasileiro de Pesquisas Físicas - CBPF/CNPq
Rua Dr. Xavier Sigaud, 150
22290 - Rio de Janeiro, RJ , Brasil

ABSTRACT

We comment on a recent paper by Kaufman and Griffiths which induces to think that certain types of real-space renormalization group are not able to preserve standard thermodynamic convexity properties. We point out this is not the case for at least one of those types, if form-invariance (under uniform translation of the energy scale) of a central equation is demanded.

Key-words: Real-space renormalization group; Specific heat; Ising and Potts models; Bravais and hierarchical lattices.

In a recent paper Kaufman and Griffiths [1] have analysed certain types of real-space renormalization group (RG) frameworks [2-4] which intend to approximately describe d-dimensional Bravais lattices. These RG's are commonly said to be exact for the associated hierarchical lattices [5] (at least as long as they concern systems which are classical, in the sense that all relevant commutators vanish). Three interesting questions can be raised around the exactness of these RG's: (i) do they provide the exact critical exponent $\nu$? ; (ii) assuming a hyperscaling law $2 - \alpha = d_f \nu$ ($\alpha \equiv$ specific heat critical exponent), what is the dimensionality $d_f$ to be put therein?; (iii) are the standard thermodynamic convexity properties (such as positivity of the specific heat) satisfied?.

Although Kaufman and Griffiths [1] do not state it explicitely, their paper tends to reinforce the common belief that the answer to question (i) is "yes" (at least for the RG presented in Ref. 3 and references therein); consequently [6] the exact $\nu$ for the q-state Potts ferromagnet ($q = 2$ recovers the Ising model) in let us say the standard $b = 2$ Wheatstone-bridge hierarchical lattice (see Fig. 2 of Ref. 1) will be given by

$$\nu = \ln 2 / \ln \frac{8 + 13\sqrt{q} + 5q}{8 + 7\sqrt{q} + q} \qquad (1)$$

With respect to question (ii), Kaufman and Griffiths remarks [1] (see also Ref. 7 and references therein) are consistent (at least for the RG of Ref. 3) with the answer $d_f = \ln B/\ln b$, where B is the aggregation number, and b the change in linear scale ($d_f$ is the fractal intrinsic dimension discussed in Ref. 8 and references therein); $d_f$ equals $\ell n5/\ell n2$ for Fig. 2 of Ref. 1, and therefore the Potts ferromagnet exact $\alpha$ for the associated hierarchical lattice is given by $\alpha = 2 - (\ell n5/\ell n2)\nu$, with $\nu$ given by Eq. (1).

Finally, with respect to question (iii), Kaufman and Griffiths[1] induce a sceptical view of the capability of the above mentioned RG's to reproduce the correct thermodynamical convexity properties. We want to point out, and this is the main purpose of the present Comment, that we see no fundamental reason preventing such RG's (at least the type used in Ref. 3) from recovering, for instance, positive specific heats. More than that, we have shown how this can be done in Ref. 9 (Ising ferromagnet in d = 3, 4 like hierarchical lattices; see Figs. 2-4 therein) and Ref. 10 (Potts ferromagnet in d= 2 like hierarchical lattices, including that of Fig. 2 of Ref. 1; see Fig. 2(b) in Ref. 10). In both cases the specific heat is positive for all finite temperatures. The procedure is very simple indeed, and can be recalled as follows.

The adimensional free energy f associated with the whole lattice scales, within the RG, according to

$$f(K) = b^{-d} f(K') + g(K) \qquad (2)$$

where K and K' respectively are the original and renormalized adimensional two-body coupling constants of the model and g(K) is the standard background term (see Refs. 2,3,9,10 and references therein). On the other hand, at the graphs (cells) level, the preserval of the partition function imposes

$$\underset{\{\sigma_i\}}{\mathrm{Tr}}\ e^{\mathcal{H}(K;\sigma_1,\sigma_2;\{\sigma_i\})} = e^{\mathcal{H}'(K';\sigma_1,\sigma_2)+K_0'} \tag{3}$$

where $\mathcal{H}$ and $\mathcal{H}'$ respectively are the adimensional Hamiltonians corresponding to the original (Fig. 2(b) of Ref. 1) and renormalized (Fig. 2(a) of Ref. 1) graphs; $\sigma_1$ and $\sigma_2$ are the random variables associated with the terminal nodes of the two-rooted graphs (open circles of Fig. 2 of Ref. 1), and $\{\sigma_i\}$ are those associated with the internal nodes of the original graph (full circles in Fig. 2(b) of Ref. 1); $K_0'$ is the additive term that has to be added in order to exactly preserve the cell partition function. This equation completely determines $K' = K'(K)$ and $K_0' = K_0'(K)$. We introduce now a proportionality factor $D(K)$ (to be determined) through the relation

$$g(K) = D(K)K_0'(K) \tag{4}$$

Let us now analyse what happens if we shift the zero-energy point by adding an arbitrary constant $\lambda$ to the energy associated with each single bond: $f$ transforms according to $f(K) \to f(K) + \lambda dK$, and consequently Eq. (2) implies

$$g(K) \to g(K) + \lambda d\left[K - b^{-d}K'(K)\right] \tag{5}$$

At the cell level, Eq. (3) implies

$$K_0'(K) \to K_0'(K) + \lambda\left[b^{d_f}K - K'(K)\right] \tag{6}$$

If we impose now that Eq. (4) remains form-invariant under uniform translation of the energy scale (i.e., D(K) does not change with $\lambda$), in a similar way the Maxwell equations are form-invariant under the Lorentz transformation, it immediately follows that

$$D(K) = \frac{d\,[b^d K - K'(K)]}{b^d\,[b^{d_f} K - K'(K)]} \tag{7}$$

This equation closes the operational procedure as (together with Eq. (4)) it provides g(K), which (together with the recursive relation (2)) enables the calculation of quantities such as the specific heat. If we are studying the hierarchical lattice, then d is replaced by $d_f$, therefore $D = d_f/b^{d_f}$ is a purely topological number. If we are interested in an approximation for the d-dimensional Bravais lattice, then D(K) contains both topological and thermal informations; typically D(K) smoothly decreases from a finite value to a smaller finite value when K increases from zero to infinity.

Although less analyzed than herein, the whole procedure is illustrated in detail in Refs. 9 and 10. The consequences of the apparently inocuous form-invariance hypothesis concerning Eq. (4) are quite instructive indeed: specific heats presenting (within similar frameworks but which do not allow for appropriate K-dependence of D) strongly negative values for large regions of K, automatically (without introducing any adjustable parameter) become positive for all finite temperatures. In addition to that, the procedure provides (at least for the cases we are aware of) a specific heat high-tem perature expansion which contains an enlarging set of exact (for the d-dimensional Bravais lattice) terms if both b and B (associated with the corresponding hierarchical lattices) increase in such a way that $d_f = \ell n B/\ell n b \rightarrow d$.

Useful discussions with A.O. Caride are acknowledged with pleasure.

REFERENCES

[1] M. Kaufman and R.B. Griffiths, Phys. Rev. B 28, 3864 (1983)

[2] Th. Niemeijer and J.M.J. van Leeuwen, in "Phase Transitions and Critical Phenomena", edited by C. Domb and M.S. Green (Academic Press, New York, 1976), vol. 6, p. 470

[3] H.O. Martin and C. Tsallis, J. Phys. C 14, 5645 (1981)

[4] L.P. Kadanoff, Phys. Rev. Lett. 34, 1005 (1975); L.P. Kadanoff, A. Houghton and M.C. Yalabik, J. Stat. Phys. 14, 171 (1976)

[5] A.N. Berker and S. Ostlund, J. Phys. C 12, 4961 (1979); P.M. Bleher and E. Zalys, Commun. Math. Phys. 67, 17 (1979)

[6] C. Tsallis and S.V.F. Levy, Phys. Rev. Lett. 47, 950 (1981)

[7] R.B. Griffiths and M. Kaufman, Phys. Rev. B 26, 5022 (1982)

[8] J.R. Melrose, J. Phys. A 16, 3077 (1983)

[9] H.O. Martin and C. Tsallis, Z. Phys. B 44, 325 (1981)

[10] H.O. Martin and C. Tsallis, J. Phys. C 16, 2787 (1983)