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# Bounds for Free Energy Derivatives Using Renormalization Group Methods

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The free energy of a thermodynamic system is known to be a concave function of the temperature. This fact is used, together with some results due to Fisher, to deduce bounds on the internal energy of the two-dimensional Ising model, given reasonably accurate upper and lower bounds on the free energy. These free energy bounds are derived from renormalization group transformations. Unfortunately, the numerical accuracy of the bounds on the internal energy is poor. The reasons for the failure are discussed.

**KEY WORDS:** Renormalization group; variational principles; convexity; bounds on free energy and internal energy; Ising model.

## 1. INTRODUCTION

Variational principles in statistical mechanics have been known for a long time (for a recent review see Girardeau and Mazo[(1)]). Recently, new methods, based on renormalization group transformations, have been developed.[(2–4)] These methods yield definite bounds on the free energy.

For the most part, however, these bounds have been used to justify a "best" set of recursion relations from which critical exponents can be estimated by standard renormalization group techniques (see Refs. 5 for reviews). Since the critical exponents characterize the behavior of various *derivatives* of the free energy, there are no reasons to believe that such approximate estimates should bear any particular relationship to the exact values.

In addition, recent work[(6–8)] has established that fully optimized variational approximations to renormalization groups suffer from major weak-

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nesses and problems. In particular, van Saarsloo *et al.*[6] argued that the optimal variational parameters can become nonanalytic at a fixed point, leading to nonanalytic recursion relations, which are against the fundamental spirit of the renormalization group. These singularities have been exhibited[8] explicitly for the Kadanoff approximation[2] to the square lattice Ising model.

These developments have to a large extent dashed the original hopes held for variational approximations to renormalization groups. Nevertheless, such methods do appear capable of generating fairly accurate bounds—both lower and upper—to the free energy. It is of interest to inquire whether anything rigorous and, one hopes, useful can be deduced from these bounds concerning the behavior of the derivatives of the exact free energy.

Since the free energy of a system is known[9] quite generally to be a concave function of physical variables, such as the temperature or the magnetic field, one might hope to bound some of its derivatives using the method of Fisher.[10] The aim of this paper is to test this possibility. Our argument is arranged as follows. In the next section, we summarize the relevant results of Fisher.[10] These are applied in Section 3 to deduce bounds for the internal energy of the Ising model on the square lattice from renormalization group upper[4] and lower[3] bounds to its free energy. A concluding discussion is given in Section 4. Unfortunately, the nature of the bounding functions results in rather disappointing results.

## 2. BOUNDS FOR THE DERIVATIVE OF A CONVEX FUNCTION

A continuous function $f(x)$ is *concave*[9] on an interval $[a, b]$ if

$$f[\lambda x_1 + (1-\lambda)x_0] \geqslant \lambda f(x_1) + (1-\lambda)f(x_0) \tag{2.1}$$

for all $x_0, x_1 \in [a, b]$ and all $\lambda \in [0, 1]$. For $\lambda \neq 0$, this can be rewritten as

$$\{f[x_0 + \lambda(x_1 - x_0)] - f(x_0)\}/\lambda \geqslant f(x_1) - f(x_0) \tag{2.2}$$

Taking the limit $\lambda \to 0$ with $x_0$ and $x_1$ fixed yields

$$f'(x_0) \equiv \left(\frac{df}{dx}\right)_{x=x_0} \geqslant \frac{f(x_1) - f(x_0)}{x_1 - x_0} \tag{2.3}$$

If we are now given bounding functions $f_U(x)$ and $f_L(x)$ for $f(x)$ such that

$$f_L(x) \leqslant f(x) \leqslant f_U(x) \tag{2.4}$$

then (2.3) immediately implies that

$$f'(x_0) \geqslant m_L(x_0; x_1) = [f_L(x_1) - f_U(x_0)]/(x_1 - x_0) \tag{2.5}$$

for all $x_1 > x_0$. The bound can be optimized by varying $x_1$ with $x_0$ fixed. Fisher[10] extended this analysis and showed that

$$f'(x_0) \leqslant m_U(x_0; x_2) = [f_U(x_0) - f_L(x_2)]/(x_0 - x_2) \qquad (2.6)$$

for all $x_2 < x_0$. Again varying $x_2$ with $x_0$ fixed allows the bound to be optimized.

Both (2.5) and (2.6) are valid for any bounds $f_L$ and $f_U$—no additional assumptions on these functions are necessary. If $f_L(x)$ is continuous and at least once differentiable, then it is straightforward to show that the optimum bounds occur when $x_1$ and $x_2$ satisfy the equations

$$f_L'(x_2) = m(x_0; x_2), \qquad f_L'(x_1) = m_L(x_0; x_1) \qquad (2.7)$$

provided $x_2 < x_0$ and $x_1 > x_0$.

## 3. BOUNDS FOR THE INTERNAL ENERGY OF THE TWO-DIMENSIONAL ISING MODEL

As a test of the possible significance of Fisher's results when combined with renormalization group bounds for the free energy, we shall now consider the two-dimensional Ising model on the square lattice. The upper bound is that constructed by Barber.[4] Explicitly, if $K = \beta J$, $f_U(K)$ is defined by

$$f_U(K) = \sum_{l=0}^{\infty} 4^{-l-1} g(K_l) \qquad (3.1)$$

where

$$g(K) = -\ln(6 + 2\cosh 4K) \qquad (3.2)$$

and

$$K_{l+1} = 2K_l h(e^{-4K_l}), \qquad K_0 = K \qquad (3.3)$$

with

$$h(x) = (1 + 2x)/(1 + 6x + x^2) \qquad (3.4)$$

This function is plotted in Fig. 1 for $0 < K \leqslant 1.6$. The lower bound is supplied by the Kadanoff one-hypercube approximation[2] and optimized by the algorithm OPTVAR,[8] which makes use of control theory methods.[11] This function is also exhibited in Fig. 1, where both bounds are compared with the exact free energy.[12] For convenience a factor of $k_B T$ is absorbed into the definition of $f$ to make it dimensionless. It is significant that both bounds become exact for both weak and strong coupling. This seems to be quite a common feature of bounds derived from renormalization group approximations.

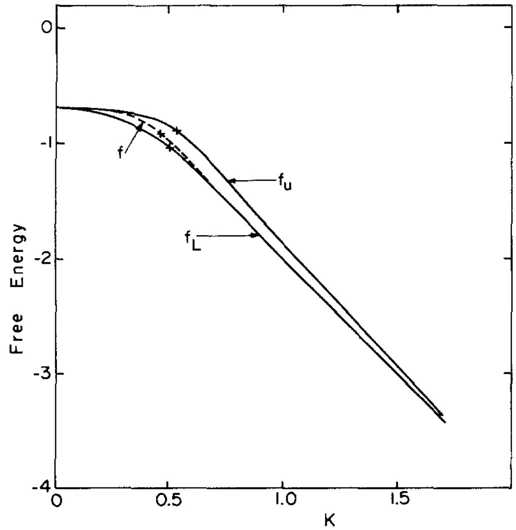


Fig. 1. The upper $f_U(K)$ and lower $f_L(K)$ bounds to the exact free energy $f(K)$ (broken curve) of the two-dimensional Ising model on the square lattice used in this paper. The crosses mark the nonanalytic points of each function.

We also note that both bounds are nonanalytic; the singular points are[4,8] $K = K_{c,U} \simeq 0.5187$ for $f_U(K)$ and $K = K_{c,L} \simeq 0.4785$ for $f_L(K)$. The second derivative of $f_U(K)$ actually diverges at $K_{c,U}$ as

$$f''(K) \sim |K - K_{c,U}|^{-\alpha_U} \tag{3.5}$$

with $\alpha_U \simeq 0.012$. The second derivatives of $f_L(K)$ is, however, cusped, varying as

$$f_L''(K) \sim f_L''(K_{c,L}) + A|K - K_{c,L}|^{-\alpha_L} + \cdots \tag{3.6}$$

with $\alpha_L \simeq -0.19$. The negative exponent $\alpha_L$ is to be expected in a fully optimized bound of the Kadanoff type and is one of the weaknesses of such approximations.[6]

Since the evaluation of $f_L(K)$ is reasonably difficult even given the efficiency of OPTVAR,[8] we did not attempt to optimize the derivative bounds $m_L$ and $m_U$ continuously. Rather, $f_L(K)$ was evaluated using OPTVAR at 32 select points ranging from $K = 0$ to $K = 2$ and clustered more densely near $K = K_{c,L} \sim 0.48$. Above $K = 2$, as is apparent from Fig. 2, $f_L(K)$ is numerically indistinguishable from the exact free energy, which in this regime is well-approximated by

$$f(K) \simeq -2K + O(e^{-4K}) \tag{3.7}$$

The bounds (2.5) and (2.6) were then optimized over these points. The

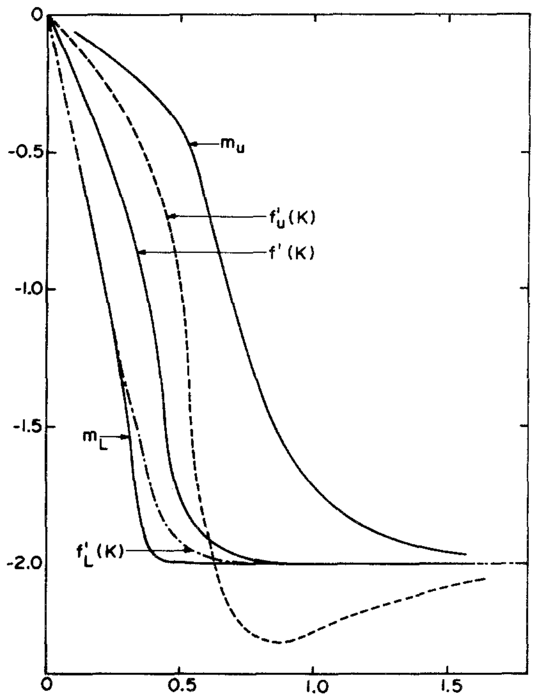


Fig. 2. Plot of the upper $m_U$ and lower $m_L$ bounds on the internal energy derived from Fisher's results (see text). For comparison the exact internal energy $f'(K)$ and the derivatives $f_U'(K)$ (broken curve) and $f_L'$ (chain curve) of the free energy bounds are also shown.

resulting optimum bounds are plotted in Fig. 2. For comparison, we also show the exact internal energy and the derivatives of $f_L(K)$ and $f_U(K)$. Somewhat surprisingly, $f_U'(K)$ is not strictly monotonic, implying that $f_U(K)$ is not a concave function. We do not know whether this is true of other renormalization group approximations.

## 4. DISCUSSION

Unfortunately, as is evident from Fig. 2, the Fisher bounds (2.5) and (2.6) are not very good. Indeed, the derivatives $f_L'$ and $f_U'$ of the free energy bounds provide better *numerical* approximations to the exact internal energy. This is especially so in the critical region where $f'(K)$ varies most rapidly. The reason for this failure is not difficult to locate: $f_L(K)$ is monotone decreasing and thus for $K_0 \gtrsim 0.4$, the value of $K_2$ for which $m_L(K_0, K_2)$ is optimum is pushed out to infinity. This results in little sensitivity.

Better bounds could undoubtedly be obtained, given better bounds for the free energy. Some improvement could be achieved fairly readily. For example, $f_U(K)$, which, as noted earlier, is not concave, could be replaced by its concave envelope. Similarly, the fact that $f_U(K) = -2K + O(1)$ as $K \to \infty$ could be incorporated. However, such modifications are unlikely to significantly improve the accuracy, particularly in the critical region. It is, however, dubious whether one could actually construct sufficiently worthwhile bounds to apply the Fisher results without also actually deriving rather accurate approximations to $f'(K)$ and $f''(K)$. This would almost certainly be the case if renormalization group methods are used. Any improvement must involve an improvement in the recursion relations in the vicinity of the fixed point and hence improved estimates of the exponents.

## REFERENCES

1. M. D. Girardeau and R. M. Mazo, *Adv. Chem. Phys.* **24**:187 (1973).
2. L. P. Kadanoff, *Phys. Rev. Lett.* **34**:1005 (1975).
3. L. P. Kadanoff, A. Houghton, and M. C. Yalabik, *J. Stat. Phys.* **14**:171 (1976).
4. M. N. Barber, *J. Phys. A* **10**:1187 (1977).
5. M. N. Barber, *Phys. Repts.* **29C**:1 (1977); P. Pfeuty and G. Toulouse, *Introduction to the Renormalization Group and to Critical Phenomena* (Wiley, 1977); D. J. Wallace and R. K. P. Zia, *Rep. Prog. Phys.* **41**:1 (1978); and other references cited in these.
6. W. van Saarloo, J. M. J. van Leeuwen, and A. M. M. Pruisken, *Physica* **92A**:323 (1978).
7. M. P. M. den Nijs and H. J. F. Knops, *Physica* **93A**:441 (1978).
8. M. N. Barber, *J. Comp. Phys.*, in press.
9. D. Ruelle, *Statistical Mechanics* (Benjamin, New York, 1969).
10. M. E. Fisher, *J. Chem. Phys.* **42**:3852 (1965).
11. M. N. Barber, *J. Phys. A* **10**:1721 (1977).
12. L. Onsager, *Phys. Rev.* **65**:117 (1944).