Journal of Statistical Physics, Vol. 46, Nos. 3/4, 1987

Interfacial Free Energy of the Two-Dimensional Ising Model from the Renormalization Group

G. Bilalbegović[1] and N. M. Švrakić[1,2]

Received October 17, 1986

The interfacial free energy of a two-dimensional Ising model is calculated by using various renormalization group schemes. The results obtained are quantitatively consistent with known exact results. In addition, a general discussion of various drawbacks within different renormalization group approximations is given. The best result are obtained with the 4×4 finite cluster approximation, while the Migdal–Kadanoff approximation seems to be inherently unsuitable for calculation of interfacial properties.

KEY WORDS: Interfaces; interfacial free energy; Ising model; real-space renormalization.

1. INTRODUCTION

Phenomena associated with interfaces and surfaces in otherwise homogeneous physical/model systems have attracted considerable attention recently. In particular, it is known that two (or more) coexisting phases may undergo a variety of phase transitions associated with bulk, interface (surface), or coexistence instabilities.[1] This division reflects a widely accepted view that an inhomogeneous system consists of *bulk* and *interface* (surface) subsystems in strong interaction.[2] Consequently, one defines bulk and interfacial free energies, to be denoted f_b and f_i, respectively, which contain all information needed for thermodynamic description of the system. Thus, studies of inhomogeneous systems on this level of description focus on the calculation of free energies. But such calculations can often be difficult to perform.

Calculation of *bulk* free energy in various homogeneous systems has

[1] Institute of Physcis, 11001 Beograd, Yugoslavia.
[2] Present address: Department of Physics, Clarkson University, Potsdam, New York 13626.

0022-4715/87/0200-0777$05.00/0

been performed in a number of ways, including phenomenological approaches,[3] numerical methods,[4,5] and position-space renormalization-group (RG) methods.[6] The results obtained in such studies are believed to be quite accurate. On the other hand, calculations of *interfacial* free energies have not been nearly as successful. In particular, numerical simulations, such as the Monte Carlo method,[7,8] seem to be plagued by various finite-size effects,[9-11] phenomenological approaches are inadequate for description of transitions such as roughening,[12] and RG methods[13] are at best poorly developed in comparison with analogous bulk calculations.

The purpose of the present work is to analyze various position-space RG techniques[14] for the calculation of interfacial free energies. In what follows we shall concentrate on the Ising model of a ferromagnet with short-range interactions and try to develop a tractable, accurate RG method for calculation of the interfacial free energy. As will be shown below, such calculations are quite sensitive to details of the particular RG scheme employed and, indeed, some approaches often used in bulk calculations are not suitable for analogous interface problems.

We shall concentrate on three commonly used position-space RG schemes: (1) cumulant expansion,[15] (2) Migdal–Kadanoff approximation,[16] and (3) finite-cluster approximation.[15,17] These schemes have been successfully used in the past for calculation of bulk properties. Extension of such schemes to calculation of interfacial properties is not straightforward and can often lead to erroneous results. We shall discuss this problem as we proceed.

For definitness, let us consider a hypercubic, d-dimensional, Ising lattice of spins $S_i = \pm 1$ at each lattice site. We shall assume short-ranged, nearest neighbor ferromagntic interaction of strength J ($J<0$) between spins. It will be convenient to introduce dimensionless coupling constant $K = -J/k_B T$.

Now, in order to introduce the interface into the system, we can either (1) introduce periodic boundary conditions in $d-1$ directions and antiperiodic boundary conditions in one direction or (2) use the symmetry of the Ising bulk free energy under the change of sign of the coupling constant K and introduce a "seam" of defect couplings $K_d = -K$.[18] The defect ("seam") free energy is then precisely equal to the interfacial free energy. In what follows we shall use this second method to calculate the interfacial free energy.

For a d-dimensional system of N^d spins the dimensionless bulk free energy density is calculated from

$$f_b = \lim_{N \to \infty} N^{-d} \ln \operatorname{Tr} e^H = \lim_{N \to \infty} N^{-d} \ln Z \tag{1}$$

where the trace is taken over all spin configurations and the Hamiltonian H of the system is given by

$$H = \sum_{i,j} K_{ij} S_i S_j + N^d K_0 \tag{2}$$

In this expression the constant term K_0 is irrelevant for critical behavior, but is essential for calcultion of thermodynamic quantities. Note that expression (1) is independent of boundary conditions and/or the presence of the "seam."

The interfacial free energy density is obtained from[19,20]

$$f_i = \lim_{N \to \infty} N^{-(d-1)} [\ln Z(+-) - \ln Z(++)] \tag{3}$$

where $Z(++)$ $[Z(+-)]$ denotes the partition function of the system with periodic (antiperiodic) boundary conditions. If the interface is introduced into a system via a "seem" of defect bonds, then the interfacial free energy density is calculated from

$$f_i = \lim_{N \to \infty} N^{-(d-1)} [\ln Z(K, K_d = -K) - \ln Z(K, K_d = K)] \tag{4}$$

In this paper we shall concentrate on the calculation of f_i via a position-space RG method. We first make a few remarks that we shall need below. It is useful to known the behavior of f_i in various limits. In particular, we need the behavior of f_i in the limit $T \to 0$ and $T \to T_c$. It is easy to show that[18,21]

$$f_i \sim -2K \qquad \text{as} \quad T \to 0 \quad (\text{or } K \to \infty) \tag{5}$$

and[22]

$$f_i \sim \text{const} \times (K - K_c)^{\mu} \qquad \text{as} \quad T \to T_c \quad (\text{or } K \to K_c) \tag{6}$$

where the exponent μ is determined by Widom's scaling law from $\mu = (d-1)\nu$. The above forms (5) and (6) are valid for arbitrary dimension d of the system. The exponent μ has value $\mu = 1$ (for $d = 2$) and $\mu \approx 1.26$ (for $d = 3$).

Calculation of the exponent μ within RG follows from the behavior of the RG recursion relations in the vicinity of the critical point. Thus, the behavior (6) of f_i ultimately depends on the accuracy of *bulk* recursion relations.

On the other hand, the low-temperature behavior (5) of f_i depends on the global behavior of RG flows and is thus very sensitive to the particular form of RG approximation chosen in the calculation (see below).

After these lengthy, but necessary, preliminary remarks let us concentrate on a particular renormalization procedure for calculation of f_i. Suppose that we have developed an RG scheme that gives us certain recursion relations, i.e., the functional dependence of new (rescaled) coupling constants on those of the original system. Then, in principle we have

$$K' = R(K), \qquad K_0' = R_0(K, K_0) \tag{7}$$

The bulk free energy density, as defined by (1), follows from[17]

$$f_b = \lim_{n \to \infty} b^{-nd} K_0^{(n)} \tag{8a}$$

which gives

$$f_b[K, K_0] = \sum_{n=0}^{M-1} b^{-d(n+1)} r_b[K^{(n)}, K_0^{(n)}] + b^{-dM} f_b[K^{(M)}, K_0^{(M)}] \tag{8b}$$

where M is the number of renormalization iterations, b is the rescaling factor, and r_b is a constant-term contribution to the free energy, which comes from the integration of short-wavelength fluctuations. Note that the last factor in (8b) vanishes in the limit $M \to \infty$.

In a similar manner, the interfacial free energy density is obtained from

$$f_i[K, K_0] = \sum_{n=0}^{M-1} b^{-(d-1)(n+1)} r_i[K^{(n)}, K_0^{(n)}] + b^{-(d-1)M} f_i[K^{(M)}, K_0^{(M)}] \tag{9}$$

which, after some algebra, gives

$$f_i = \lim_{n \to \infty} (-2K^{(n)}/b^{n(d-1)}) \tag{10}$$

where $K^{(n)}$ is the nth iterate of the bulk coupling constant K. Observe that, since the calculation is performed for $T < T_c$ (or $K > K_c$), all flows will go to infinity, i.e., $\lim_{n \to \infty} K^{(n)} = \infty$. It is clear now that if we want to obtain correct low-temperature behavior of f_i as given by (5) from the expression (10), then the low-temperature limit of the RG recursion relations must be[23]

$$K' = b^{(d-1)} K + O(e^{-K}) \tag{11}$$

If this condition is not met, then the limit (5) will not be correctly obtained within the RG group. In particular, within the Migdal–Kadanoff approximation to the RG one can show that

$$K' = b^{(d-1)} K - 0.5 \ln b + O(e^{-K}) \tag{12}$$

so that, as $T \to 0$,

$$f_i \sim -2K + (\ln b \cdot b^{-(d-1)})/(1 - b^{(d-1)}) \tag{13}$$

We have performed several versions of cumulant,[13,15] Migdal–Kadanoff,[14,16] and finite-cluster[15,17] approximations to the RG equations. We now take them in order.

2. CUMULANT EXPANSION

We have used a first-order cumulant expansion approximation to the RG equations for 2×2, 3×3, and 4×4 basic blocks.[24] This is illustrated in Fig. 1. In spite of the seeming simplicity of this approach, the first-order expansion turns out to be well suited for our calculation. Recursion relations are generally given by

$$K' = K \sum_i \langle S \rangle_i^2 \tag{14a}$$

where $\langle S \rangle_i$ is the average of the spin on the edge of the basic block. In the case when we use 2×2 approximation $\langle S \rangle_i$ is given by[25]

$$\langle S \rangle_i = (e^{4K} + p)/(e^{4K} + 6 + e^{-4K}) \qquad (i = 1, 2) \tag{14b}$$

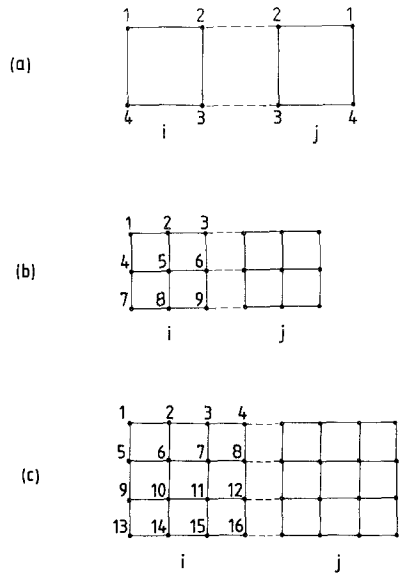

Fig. 1. Three basic blocks used in the cumulant expansion approximation: (a) 2×2, (b) 3×3, and (c) 4×4 cells.

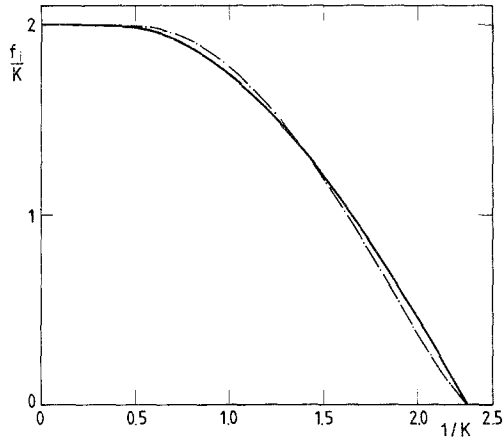

Fig. 2. Interfacial free energy for the first-order cumulant expansion with cell 2×2 and $p=4\sqrt{2}-3$ (see text). (—) The exact result[18]; (–·–) the result of the RG calculation.

Similar, but lengthier expressions can be written for 3×3 and 4×4 basic blocks. Note that in (14b) we have used the parameter p as a variable parameter, which enables us to chose the projection rule at will. In particular, if $p=2$, we have majority rule.[13] In our calculation we have chosen $p=4\sqrt{2}-3$, since this value reproduces the critical point K_c of the planar Ising model exactly.

Our results for cumulant expansion methods are shown in Figs. 2–4. One can clearly see that the results are quantitatively similar. For reasons

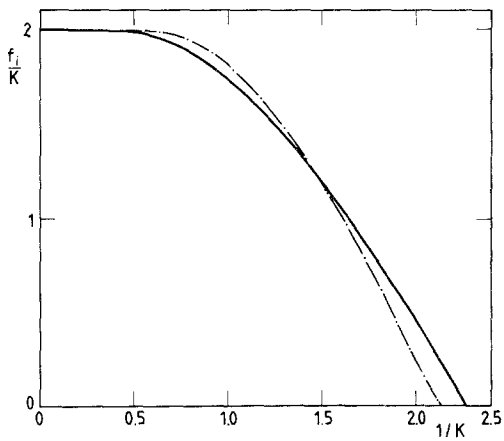

Fig. 3. Interfacial free energy for the first-order cumulant expansion with cell 3×3 and majority rule projection operator. (—) The exact result[18]; (–·–) the result of the RG calculation.

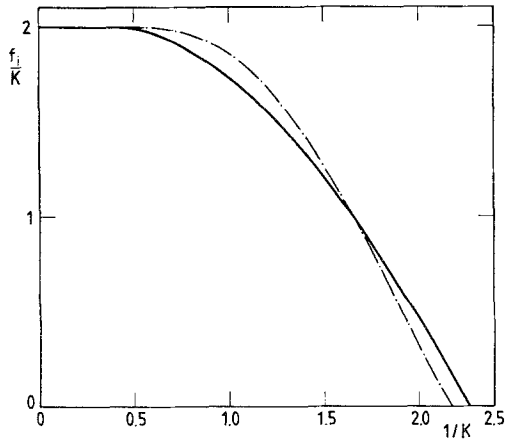

Fig. 4. Interfacial free energy for the first-order cumulant expansion with cell 4×4 and majority rule projection operator. (—) The exact result[18]; (-·-) the result of the RG calculation.

we do not quite understand, this simple first-order approximation yields good quantitative results. Our belief is that this is not entirely fortuitous.

3. MIGDAL–KADANOFF APPROXIMATION

Calculation of f_i via the Migdal–Kadanoff approximation suffers from the basic drawback that the low-temperature limit of the recursion relations does not have property (11), but behaves as (12), thus giving

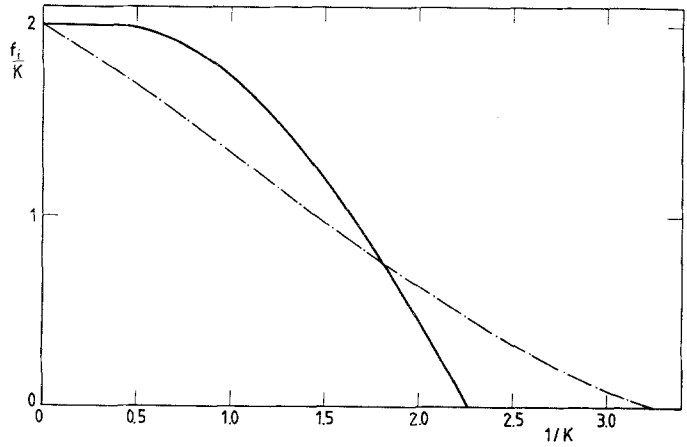

Fig. 5. Interfacial free energy for the RG Migdal–Kadanoff approximation. (—) The exact result[18]; (-·-) the result of the RG calcultion.

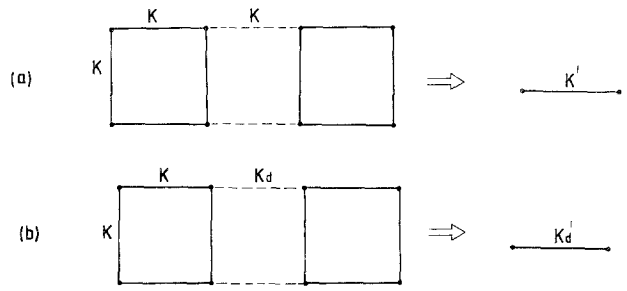

Fig. 6. Clusters 2×4 for (a) bulk and (b) defect in the finite-cluster approximation.

erroneous $T \to 0$ limiting behavior of the interfacial free energy (13). This is clearly visible in Fig. 5, where we have shown results of our Migdal–Kadanoff calculation for $b = 2$. This feature was noted earlier by Oliveira *et al.*,[13] who performed the Kadanoff lower-bound approximation. The explanation for this behavior in our Migdal–Kadanoff calculation is simple. This approximation is ultimately a reduction of the problem to 1d decimation and such a procedure picks up a $\ln b$ entropic term of the 1d Ising model.

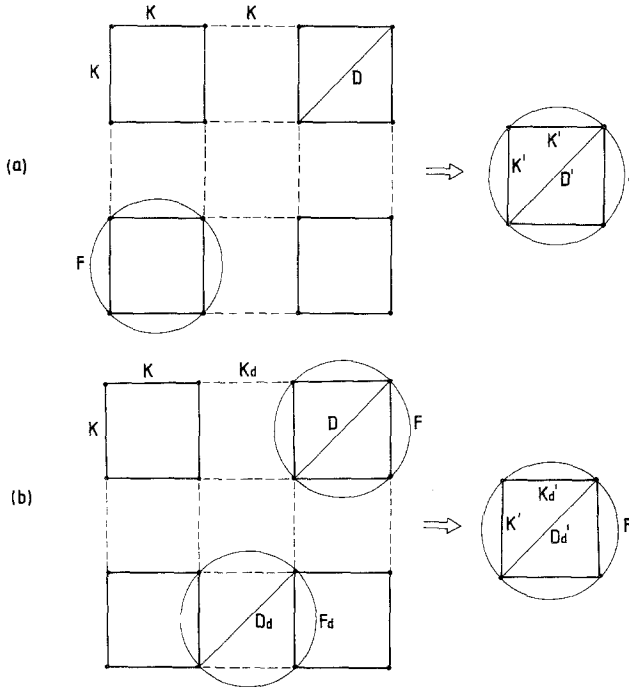

Fig. 7. Clusters 4×4 for (a) bulk and (b) defect in the finite-cluster approximation.

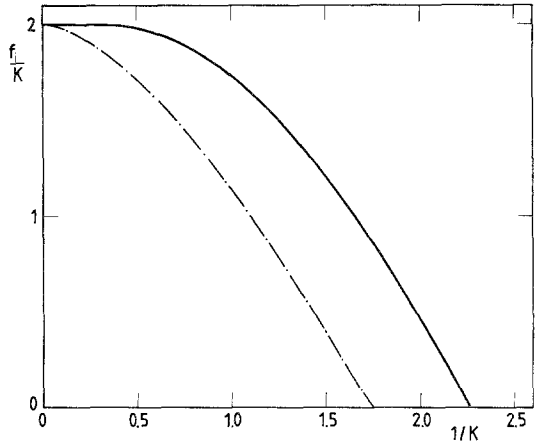

Fig. 8. Interfacial free energy for 2×4 cluster approximation and majority rule projection operator. (—) The exact result[18]; (–·–) the result of the RG calculation.

4. FINITE-CLUSTER APPROXIMATION

This kind of approximation was earlier used for calculation of bulk[6] and surface[17] free energies. Our 4×4 cluster approach is intended as a complementary calculation of f_i. We have used clusters 2×4 and 4×4, shown in Figs. 6 and 7. For the 2×4 cluster the situation is simple, since the subspace of interactions is closed under repeated RG applications. However, in this case, one again encounters the problem of erroneous low-temperature asymptotic behavior (Fig. 8). This can be remedied by a dif-

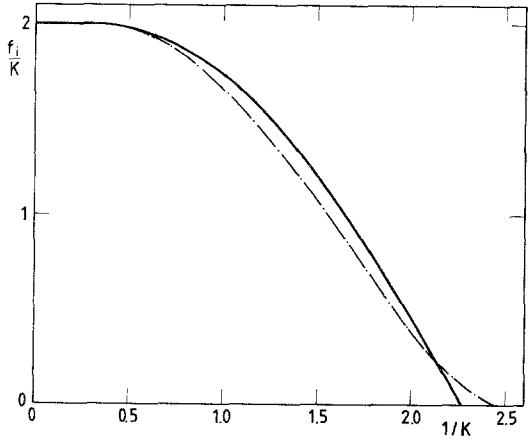

Fig. 9. Interfacial free energy for 2×4 cluster approximation and M1 projection operator (see text). (—) The exact result[18]; (–·–) the result of the RG calculation.

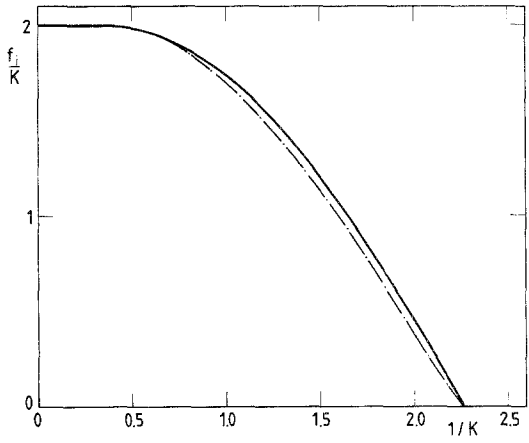

Fig. 10. Interfacial free energy for 4×4 cluster approximation with majority rule projection operator and $\alpha = 1.217$ (see text). (—) The exact result[18]; (-·-) the result of the RG calculation.

ferent choice of projection rule (called rule M1[26]). The resulting free energy is shown in Fig. 9. Finally, the 4×4 cluster calculation is performed with free boundary conditions and by the use of the Ursell cluster expansion.[17] In this case, however, one generates interactions beyond nearest neighbors (diagonal and four-spin interactions). It is reasonable to expect that the 4×4 cluster should be best suited for calculation on planar, square lattice, since it reflects the geometry of the lattice. We have encountered difficulties with generated diagonal interactions D. How is one to include them in the interfacial free energy (10)? We do not have a definitive answer to this question. One obvious choice is to write

$$f_i = \lim_{n \to \infty} [(-2K^{(n)} - \alpha D^{(n)})/2^n] \tag{15}$$

instead of (10), where α is a variable parameter chosen in such a way that the low-temperature behavior (5) of f_i is preserved. We have numerically determined $\alpha = 1.217$. With such a choice of α our results agree quite well with the exact f_i. This is shown in Fig. 10. In this calcultion it seems essential to match $T = 0$ and $T = T_c$ behavior correctly in order to obtain good results over the whole temperature interval.

5. CONCLUSIONS

In conclusion, we have studied various position-space RG approximations to the calculation of interfacial free energies. Our study

indicates that with little effort one can obtain quite quantitative results for f_i, both in the critical and noncritical region. We hope that our conclusions regarding this kind of calculation, and in particular the general discussion at the beginning of this article, should also be applicable to 3d models.

ACKNOWLEDGMENT

This research has been supported in part by the U.S. National Science Foundation under grant DMR–86–01208, and by the Donors of the Petroleum Research Fund, administered by the American Chemical Society, under grant ACS–PRF–18175–G6. This financial assistance is gratefully acknowledged.

REFERENCES

1. M. Wortis, in *Fundamtental Problems in Statistical Mechanics VI*, D. Cohen, ed. (North-Holland, Amsterdam, 1985), p. 87.
2. R. B. Griffiths, in *Phase Transitions in Surface Films*, J. G. Dash and J. Ruvals, eds. (Plenum Press, New York, 1980), p. 1.
3. L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon, London, 1959).
4. C. Domb and M. S. Green, eds., *Phase Transitions and Critical Phenomena*, Vol. 3 (Academic Press, London, 1974).
5. K. Binder, in *Phase Transitions and Critical Phenomena*, Vol. 8, C. Domb and J. L. Lebowitz, eds. (Academic Press, London, 1983), p. 1.
6. M. Nauenberg and . Nienhuis, *Phys. Rev. Lett.* **33**:1598 (1974).
7. K. Binder, *Phys. Rev. A* **25**:1699 (1982).
8. E. Bürkner and D. Stauffer, *Z. Phys. B* **53**:241 (1983).
9. K. K. Mon and D. Jasnow, *Phys. Rev. A* **30**:670 (1984).
10. K. K. Mon and D. Jasnow, *Phys. Rev. A* **31**:4008 (1985).
11. D. B. Abraham and N. M. Švrakić, *Phys. Rev. Lett.* **56**:1172 (1986).
12. J. D. Weeks, in *Ordering in Strongly Fluctuating Condensed Matter Systems*, T. Riste, ed. (Plenum Press, New York, 1980), p. 293.
13. M. J. de Oliveira, D. Furman, and R. B. Griffiths, *Phys. Rev. Lett.* **40**:977 (1978).
14. T. W. Burkhardt and J. M. J. van Leeuwen, eds., *Real-Space Renormalization* (Springer-Verlag, Berlin, 1982).
15. T. Niemeyer and J. M. J. van Leeuwen, *Physica* **71**:17 (1974).
16. L. P. Kadanoff, *Ann. Pys.* (N.Y.) **100**:359 (1976).
17. N. M. Švrakić, R. Pandit, and M. Wortis, *Phys. Rev. B* **22**:1286 (1980).
18. L. Onsager, *Phys. Rev.* **65**:117 (1944).
19. D. B. Abraham, *Phys. Rev. Lett.* **44**:1165 (1980).
20. D. B. Abraham, *J. Phys. A* **14**:L369 (1981).
21. J. D. Weeks, G. H. Gilmer, and H. J. Leamy, *Phys. Rev. Lett.* **31**:549 (1973).
22. B. Widom, in *Phase Transitions and Critical Phenomena*, Vol. 2, C. Domb and M. S. Green, eds. (Academic Press, London, 1972), p. 79.
23. W. Klein, D. J. Wallace, and R. K. Zia, *Phys. Rev. Lett.* **37**:639 (1976).
24. S. Hsu and J. D. Gunton, *Phys. Rev. B* **15**:2688 (1977).
25. N. M. Švrakić, *J. Phys. A* **16**:L171 (1983).
26. T. W. Burkhardt and E. Eisenriegler, *Phys. Rev. B* **16**:3213 (1977).