# Domain growth in the two-dimensional time-dependent Ginzburg-Landau model in the presence of a random magnetic field

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We present results of a numerical study of the two-dimensional time-dependent Ginzburg-Landau model with a random magnetic field. The growth of domains after a quench to low temperatures is investigated. Our results are, in general, consistent with the theories of Villain and of Grinstein and Fernandez. In particular, the predicted logarithmic growth is observed. The scaling behavior of the structure factor is also investigated. The zero-field scaling function closely agrees with the result of a theory of Ohta, Jasnow, and Kawasaki. For finite fields some evidence for the breakdown of scaling is obtained.

## I. INTRODUCTION

The random-field Ising model (RFIM) has been the subject of considerable research effort both theoretically and experimentally. As is typical of random systems, the free energy has numerous local minima in the phase space rendering the analysis of the equilibrium state and of the ordering characteristics rather difficult. It has only recently been established that the three-dimensional (d=3) RFIM is ordered at low temperatures for small field strengths.<sup>2,3</sup> Imbrie<sup>2</sup> has proved that in d=3 the ground state of the RFIM is ordered for small value of the random field. However, some doubts remained after that about whether the system orders at any finite temperature in three dimensions. Subsequently, Brickmont and Kupiainen,<sup>3</sup> inspired by the scaling arguments of Imry and Ma, 4 carried out renormalization-group calculations in the domain-wall representation of the system and settled the issue in favor of finite-temperature ordering in three dimensions in two dimensions the order is destroyed by the random-field induced roughening, for any nonzero field. Thus, the lower critical dimension for this model is now known to be 2.

The large number of metastable states present in the RFIM affects the dynamics of the system at low temperatures. The local clusters of random fields influence the formation of domains and subsequently slow down the evolution of these domains to the final equilibrium state. In this paper we consider the growth of unstable domains after the system is quenched from a high-temperature disordered state to a low-temperature state. The mecha-

nism of domain growth in the case of the pure model (zero field) with nonconserved dynamics is now thought to be well understood. Highly convoluted domains of ordered phase form in an early time regime after the quench. These domains then grow with time, the driving force being the reduction of their surface energy (and thus their curvature). The average size of the domains R(t) follows the well known Lifshitz-Allen-Cahn<sup>5</sup> (LAC) growth law  $R(t) \sim t^{1/2}$ . It is also found that at the late stages of evolution there is only one length scale in the system, namely the characteristic size of the domain R(t). Consequently, the structure factor satisfies a scaling relation. 6.7

In the presence of a random field the overall behavior of the domain growth is determined by the competition between the opposing tendencies of curvature driven growth and the roughening of the interfaces due to the random field. Although no detailed microscopic theory of the dynamics of the RFIM has been developed so far, a general picture of the growth can be given as follows:<sup>1,8-11</sup>, as in the pure model, convoluted domains form rapidly after quench. In an early time regime, the domains grow more slowly than in the case of zero field, due to the effects of the random field. This regime is followed by a late time regime in which the domain walls start getting pinned by the random field. This leads to a logarithmic growth characteristic of random systems. <sup>12</sup>

Experimentally, random-field models can be realized in diluted antiferromagnets in a uniform external field, <sup>13</sup> adsorbed monolayers on impure substrates, <sup>14</sup> binary liquid in gels, <sup>15</sup> frustrated antiferromagnets, <sup>16</sup> etc. Experi-

ments<sup>17</sup> on three-dimensional diluted antiferromagnets in a uniform magnetic field observe anomalously slow growth<sup>18</sup> following a temperature quench. Some aspects of the experiments may involve a novel kind of critical slowing down, <sup>19</sup> however. In a recent experiment<sup>20</sup> of growth kinetics of a chemisorbed overlayer in the presence of impurities [which is a model of RFIM (Ref. 14) in two dimensions] the results for the domain growth are interperted in terms of an effective power law where the effective exponent is always less than the LAC value of  $\frac{1}{2}$  and monotonically decreases with increasing impurity concentrations (i.e., field strengths).

Numerical studies of domain growth in RFIM have been carried out so far by using a Monte Carlo simulation on discrete spin stochastic dynamics.  $^{21-24}$  The behavior  $^{10}$   $R(t) \sim \ln^2 t$  valid at intermediate times has been checked by Chowdhury and Stauffer  $^{21}$  and by Pytte and Fernandez.  $^{22}$  An early-time small-field theory by Grant and Gunton  $^{11}$  has also been checked to some extent by Gawlinski et al.  $^{23}$  The authors of Ref. 23 also found that the self-similar scaling for the structure factor breaks down for long times. Anderson  $^{24}$  has carried out a detailed simulation of RFIM in two dimensions and has carefully analyzed the validity of several theoretical arguments.  $^{8-11}$  His calculations strongly support the late-time theories of Villain  $^9$  and Grinstein-Fernandez.  $^{10}$ 

In this paper we have considered the continuous version of the RFIM with relaxation dynamics, which is often used in theoretical calculations. 1 Specifically, we have analyzed, by direct numerical solution, the nonlinear Langevin dynamics of the two-dimensional  $\phi^4$ model in the presence of a Gaussian random external magnetic field. The Langevin dynamics model has been previously<sup>25</sup> used to study growth kinetics in pure models. Here, we find a strong correspondence between the coarse-grained model and the kinetic Ising model in the presence of randomness, i.e., a random magnetic field. These calculations thus serve as a test of the validity of the time-dependent Ginzburg-Landau model in the analysis of complicated random systems. This is notable, since analytical calculation of the dynamics of random systems quite often start from the coarse-grained model. Our results for the time dependence of the domain size demonstrate the existence of various time regimes in this growth. For a suitable value of the field strength, we have obtained clear evidence for the logarithmic growth predicted by Villain<sup>9</sup> and Grinstein and Fernandez. <sup>10</sup>

We have also investigated the scaling behavior of the structure factor. In the case of the pure model, the form of the scaling function seems to be well described by a theory of Ohta, Jasnow, and Kawasaki<sup>6</sup> (OJK) at low temperatures. This theory has been previously checked by a Monte Carlo simulation of the discrete Ising model. Our results for the scaling function obtained by a direct numerical solution of the underlying Langevin dynamics constitute a strong check of the theoretical predictions. We have obtained good agreement with the OJK theory in the absence of the field. In the presence of the random field, scaling behavior has been predicted to break down in two dimensions, 11 due to the absence of long-range order in two dimensions. Evidence for the

breakdown was obtained in a Monte Carlo study of the discrete RFIM.<sup>23</sup> Our results for the Langevin model also provide some evidence for a breakdown of scaling for large-field strengths and for small wave numbers.

The rest of the paper is organized as follows. In Sec. II, we describe the model and the method of numerical calculations. In Sec. III, we present our main results about the growth law and the scaling functions. We conclude with a brief summary in Sec. IV.

# II. MODEL AND THE METHOD OF CALCULATION

We consider a Ginzburg-Landau-type free-energy functional in the presence of a random magnetic field as follows:

$$F[\phi] = \frac{1}{2} \int d\mathbf{r} \left[ -b\phi^2 + \frac{u}{2}\phi^4 + \frac{u}{2}\phi^4 + K|\nabla\phi|^2 - 2H(\mathbf{r})\phi \right],$$
(2.1)

where b, u, and K are phenomenological positive parameters and the random magnetic field  $H(\mathbf{r})$  is assumed to have Gaussian distribution with a zero mean and variance given by

$$\langle H(\mathbf{r})H(\mathbf{r}')\rangle = H^2\delta(\mathbf{r}-\mathbf{r}')$$
 (2.2)

The dynamics are governed by a Langevin equation appropriate for a model with a nonconserved order parameter, i.e.,

$$\frac{\partial \phi}{\partial \tau} = -\Gamma \frac{\delta F}{\delta \phi} + \eta , \qquad (2.3)$$

where  $\tau$  denotes the time,  $\Gamma$  is a kinetic coefficient, and  $\eta(\mathbf{r},\tau)$  is a Gaussian noise term satisfying

$$\langle \eta(\mathbf{r},\tau)\eta(\mathbf{r}',\tau')\rangle = 2\Gamma k_B T\delta(\mathbf{r},\mathbf{r}')\delta(\tau-\tau')$$
 (2.4)

Here  $k_B$  is the Boltzmann constant and T is the temperature. Equation (2.3) [together with Eq. (2.1)] can be put in a relatively simpler form:

$$\frac{\partial \psi}{\partial t} = \theta(\psi - \psi^3) + \nabla^2 \psi + h\tilde{h}(\mathbf{r}) + \sqrt{\epsilon} \xi(\mathbf{r}, t)$$
 (2.5)

with

$$\langle \widetilde{h}(\mathbf{r})\widetilde{h}(\mathbf{r}')\rangle = \delta(\mathbf{r} - \mathbf{r}')$$
, (2.6)

$$\langle \xi(\mathbf{r},t)\xi(\mathbf{r}',t')\rangle = \delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$$
, (2.7)

and the new variables are

$$\theta = b/K$$
,  $\epsilon = 2k_B T u/bK$ ,  $t = \Gamma K \tau$ ,  
 $\psi = (u/b)^{1/2} \phi$ , and  $h = (u/b)^{1/2} H/K$ . (2.8)

We point out that  $\epsilon$  represents the dimensionless temperatures and h is the dimensionless field strength. In the limit  $\theta \to \infty$ , Eq. (2.5) directly reduces to the discrete spin RFIM. The opposite limit,  $\theta \to 0$ , is known as the "displacive limit" in the case of the pure model. <sup>27,28</sup> The phase diagram of this model in the absence of an external field has been studied by various numerical methods <sup>25,27,29</sup> and the critical line joining the discrete Ising and the displacive regimes has been mapped out. The

critical properties have been found to be in the same universality class as the discrete Ising model. The none-quilibrium properties of the discrete and the continuous models have also been found to be in the same universality class, which, as stated before, is characterized by the LAC curvature driven growth. In view of the aforementioned, we would also expect the growth characteristics of the continuous and discrete models to be similar in the presence of the random field.

We have integrated the dynamic equation (2.5), by using a finite difference scheme for both the spatial and temporal derivatives. The spatial discretization is achieved by replacing the continuous space of position vectors r by a square lattice with  $128^2$  sites and lattice space  $\delta r = 1$ . We have used a first-order Euler scheme to integrate Eq. (2.5):

$$\psi(r,t+\Delta t) = \psi(r,t) + \Delta t \frac{\partial \psi}{\partial t} . \qquad (2.9)$$

For the time step  $\Delta t$  we have tried several values of convergence and finally chose  $\Delta t = 0.02$ . We have found that further reductions in  $\Delta t$  does not affect the measured quantities appreciably. For example, a reduction of  $\Delta t$  by a factor of 2 yields the same domain size as for  $\Delta t = 0.02$ , considering the statistical errors of the data, which is about 5%. Since the random external field is static, the Gaussian random variables  $\bar{h}$  are generated at the beginning of each run according to (2.6) and this configuration of h remains fixed for the duration of the run. The initial configuration of  $\psi(r,t)$  should have the characteristics of a high-temperature state and is chosen to be a random uniform distribution in the interval (-1,1). For the final state of the quench we have chosen ( $\theta=2$ ,  $\epsilon=0.7$ ), a point well into the ordered region of the zero-field phase diagram. 25,27,29 Our results are averaged over 100 runs for each value of the field strength.

We have focused on the following quantities: the pair correlation function

$$g(\mathbf{r},t) = \langle \psi(0,t)\psi(\mathbf{r},t) \rangle , \qquad (2.10)$$

and its Fourier transform, the nonequilibrium structure factor  $s(\mathbf{k},t)$ . We have performed circular averages on both  $g(\mathbf{r},t)$  and  $s(\mathbf{k},t)$ . We will denote the circularly averaged quantities by G(r,t) and S(k,t), respectively. A length scale associated with the average domains size can be defined in a variety of ways. We have considered the following lengths. From S(k,t) one can define<sup>23,24</sup>

$$R_m^2(t) = S(0,t) \tag{2.11}$$

and

$$R_k^2(t) = \left[ \frac{\sum_{k} k^2 S(k, t)}{\sum_{k} S(k, t)} \right]^{-1} . \tag{2.12}$$

Using G(r,t) one can also define<sup>30</sup> a length scale  $R_g$  as the value of r for which G(r,t) is half its value at the origin at time t, i.e.,

$$G(R_g,t) = \frac{1}{2}G(0,t)$$
 (2.13)

We have calculated  $R_g$  by fitting the four points of G(r,t) closest to G(0,t)/2 to a cubic polynomial. We have computed all three lengths  $R_m$ ,  $R_k$ , and  $R_g$ . Although all these measures of domain sizes behave in the same qualitative fashion, we have found that the statistical error in  $R_g$  is always much less than those in the other two lengths. In view of this, we will discuss our results here in terms of  $R_g$  only. In the rest of this article R(t) will stand for  $R_g$ .

As stated before, our interest here also lies in the scaling behavior. We have calculated the scaling function in the form

$$F(x) = \frac{S(k,t)}{R^2(t)} , \qquad (2.14)$$

where x = kR(t). We discuss our results in Sec. III.

#### III. RESULTS

We first present our result for the zero-field case. We have carried out the calculation of R(t) in this case as a check on our method against know results. As seen in Fig. 1, we obtain a clear LAC growth as expected. Figure 2 shows our results for the zero-field scaling function in comparison with the prediction of OJK. As can be seen from Fig. 2, we obtain fairly good scaling and the scaling curve is rather well described by the OJK theory.

Before we discuss our results for finite-field strengths, let us briefly restate the various predictions on the none-quilibrium behavior of the RFIM: in an early-time regime, Grinstein and Fernandez<sup>10</sup> have predicted a logarithm-square time dependence for the average domain size

$$R(t) \sim \left[\frac{T}{2H}\right]^2 \ln^2 t \ . \tag{3.1}$$

Grant and Gunton have also developed an early-time theory for small-field strengths. They predict<sup>11</sup>

$$R(t) \sim t^{1/2} [1 - H^2 a \ln(t/b)]^{1/2}$$
, (3.2)

where a and b are field-independent constants. At later

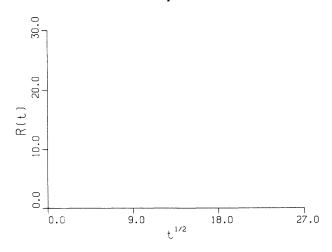


FIG. 1. R(t) vs  $t^{1/2}$  in the absence of a random field. The Lifshitz-Allen-Cahn law is well satisfied.

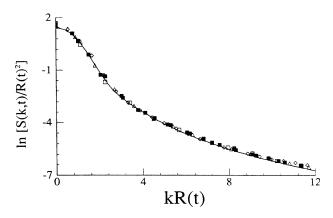


FIG. 2. Zero-field scaling function for different times after quench. The solid line is the theoretical prediction of Ohta, Jasnow, and Kawasaki (Ref. 6). The symbols are as follows:  $\Diamond t = 100$ ,  $\blacksquare t = 200$ ,  $\Delta t = 300$ , t = 400, and  $\Box t = 500$ .

times, Villain<sup>9</sup> and Grinstein and Fernandez<sup>10</sup> have predicted a logarithmic time dependence

$$R(t) \sim \frac{1}{h^2} \ln t \ . \tag{3.3}$$

We emphasize that the boundaries between the various time regimes are expected to shift towards early times as the field strength is increased. This is evident from the fact that as h is increased, the retarding effects of the random field on the curvature driven growth will start becoming effective at smaller domain sizes, i.e., at earlier times.

We now discuss our results for finite fields. In Fig. 3 we show R(t) as a function of  $\ln t$  for h=0.2, 0.4, 0.6, and 0.8. We obtain a clear logarithmic growth for h=0.4. We note that although this time regime is not as clearly visible for h=0.2, it extends down to relatively early times for h=0.4. Thus, the expected shift of the boundaries of the time regimes appears to be rather rapid. This tendency continues as h is increased further. As can be seen from Fig. 3, the  $\ln t$  region seems to shift to early times as h is increased from 0.4 to 0.8. For early times and for small-field strengths our results are con-

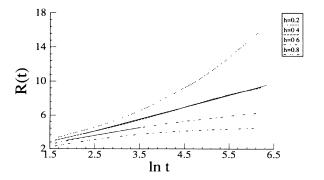


FIG. 3. R(t) vs.  $\ln t$  for several field strengths. For  $h = -0.4 \ln t$  behavior is seen over the whole time range. For other values of the field strengths,  $\ln t$  behavior is seen over limited time regimes, as discussed in the text.

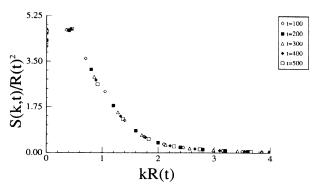


FIG. 4. Scaling function for h = 0.4. Deviation from scaling is seen only at late times and for small values of the scaling variable kR(t).

sistent with both Eqs. (3.1) and (3.2) over a limited interval. However, the rather sensitive dependence of the boundaries of the time regimes on the field strength make it rather difficult to analyze the field dependence of the growth and compare with the predictions of in (3.1) and (3.3). In two dimensions the domains have been predicted to reach only a finite size in equilibrium. Although the finite duration of our simulations prevents us from making a definitive analysis of this, one can nevertheless see some qualitative evidence for this behavior in Fig. 3 as well for field strengths h > 0.4.

We now turn to the scaling behavior. In Figs. 4 and 5 we show the scaling function data for h = 0.4 and h = 0.8. We have included the zero-field scaling curve in Fig. 5 for comparison. From Figs. 4 and 5 we can see that, for the times we have considered and for the range of wave numbers that were available in our system, the time dependence of the scaling function is fairly weak, except at very small values of the scaling variable for h = 0.8. The scatter in F(x) for small x may be taken as a signal of the breakdown of scaling. If one defines the domain size R(t) in terms of S(0,t) as in Eq. (2.11), then by definition the scaling function F(x) would be identi-

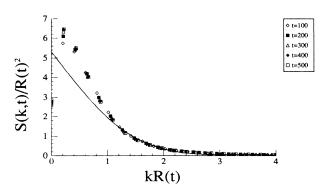


FIG. 5. Scaling function for h = 0.8. The solid line is the scaling function in the absence of the magnetic field which is included for comparison. In this case also, deviation from scaling is seen only at late times and for small values of the scaling variable kR(t), although the deviations are larger than those for h = 0.4. Note that for small values of the scaling variable the scaling function in the presence of the field lines above that in the absence of the field.

cally equal to unity for x = 0 (i.e., k = 0) and the scatter seen at x = 0 in Figs. 4 and 5 would disappear. Thus, it seems clear that the breakdown of scaling seen in this study is somewhat weaker than that seen in simulation of kinetic Ising models.<sup>23</sup> Since the Langevin model with a random field is a "soft-spin" version of the RFIM, the occurrence of a nonuniversal behavior, such as the breakdown of scaling, may show up at different length scales in these two models. Much larger lattice sizes will be required to probe the scaling functions accurately in order to settle this issue. Further investigations are necessary to understand other points such as the significance of the fact that for small values of x the scaling function data lie increasingly above the zero-field curve as the field strength is increased.

#### IV. CONCLUSIONS

We have investigated the domain growth in a continuum version of the RFIM with Langevin dynamics. Our results are consistent with the theories of Villain and Grinstein and Fernandez and in this respect agree well with some of the previous simulations on the discrete RFIM. We have also investigated the scaling behavior of the structure factor. For the pure model we made a direct numerical check with the theory of Ohta et al. and obtained good agreement. For finite-field strengths, we have obtained some indication of the predicted breakdown and scaling and pointed out the need for further theoretical and numerical analysis in this respect.

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<sup>&</sup>lt;sup>1</sup>For a recent review, see T. Natterman and J. Villain, Phase Transition 11, 5 (1988); T. Natterman and P. Rujan (unpublished).

<sup>&</sup>lt;sup>2</sup>J. Z. Imbrie, Phys. Rev. Lett. **53**, 1747 (1984); Commun. Math. Phys. **98**, 145 (1985).

<sup>&</sup>lt;sup>3</sup>J. Brickmont and A. Kupiainen, Phys. Rev. Lett. **59**, 1829 (1987); Commun. Math. Phys. **116**, 539 (1988).

<sup>&</sup>lt;sup>4</sup>Y. Imry and S. K. Ma, Phys. Rev. Lett. **35**, 1399 (1975).

<sup>&</sup>lt;sup>5</sup>I. M. Lifshitz, Zh. Eksp. Teor. Fiz. **42**, 1354 (1962) [Sov. Phys.—JETP **15**, 939 (1962)]; S. M. Allen and J. W. Cahn, Acta Metall. **27**, 1085 (1979).

<sup>&</sup>lt;sup>6</sup>T. Ohta, D. Jasnow, and K. Kawasaki, Phys. Rev. Lett. 49, 1223 (1982).

<sup>&</sup>lt;sup>7</sup>J. D. Gunton, M. San Miguel, and P. S. Sahni, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Adademic, New York, 1983), Vol. 8.

<sup>&</sup>lt;sup>8</sup>R. Bruinsma and G. Aeppli, Phys. Rev. Lett. 52, 1543 (1984).

<sup>&</sup>lt;sup>9</sup>J. Villain, Phys. Rev. Lett. **52**, 1543 (1984).

<sup>&</sup>lt;sup>10</sup>G. Grinstein and J. F. Fernandez, Phys. Rev. B 29, 6389 (1984).

<sup>&</sup>lt;sup>11</sup>M. Grant and J. D. Gunton, Phys. Rev. B 29, 6266 (1984); 35, 4922 (1987).

<sup>&</sup>lt;sup>12</sup>D. A. Huse and C. L. Henley, Phys. Rev. Lett. **54**, 2708 (1985).

<sup>&</sup>lt;sup>13</sup>S. Fishman and A. Aharony, J. Phys. C **12**, L729 (1979); J. Cardy, Phys. Rev. B **29**, 505 (1984).

<sup>&</sup>lt;sup>14</sup>J. Villain, J. Phys. (Paris) Lett. 43, 551 (1982); 43, 808 (1982).

<sup>&</sup>lt;sup>15</sup>P. G. de Gennes, J. Phys. Chem. **88**, 6469 (1984).

<sup>&</sup>lt;sup>16</sup>J. F. Fernandez, Europhys. Lett. 5, 129 (1988).

<sup>17</sup>D. P. Belanger, A. R. King, and V. Jaccarino, Phys. Rev. B
31, 4538 (1985); H. Yoshizawa, R. A. Cowley, G. Shirane, and
R. J. Birgeneau, *ibid.* 31, 4548 (1985); D. P. Belanger, Phase Transition 11, 53 (1988).

<sup>&</sup>lt;sup>18</sup>T. Natterman and I. Vilfan, Phys. Rev. Lett. **61**, 223 (1988).

<sup>&</sup>lt;sup>19</sup>J. Villain, J. Phys. (Paris) **46**, 1843 (1985); D. S. Fisher, Phys. Rev. Lett. **56**, 416 (1986).

<sup>&</sup>lt;sup>20</sup>J. K. Zuo, G. C. Wang, and T. M. Lu, Phys. Rev. Lett. 60, 1053 (1988).

<sup>&</sup>lt;sup>21</sup>D. Chowdury and D. Stauffer, Z. Phys. B **60**, 249 (1985).

<sup>&</sup>lt;sup>22</sup>E. Pytte and J. F. Fernandez, Phys. Rev. B 31, 616 (1985).

<sup>&</sup>lt;sup>23</sup>E. T. Gawlinski, K. Kaski, M. Grant, and J. D. Gunton, Phys. Rev. Lett. 53, 2266 (1984); E. T. Gawlinski, S. Kumar, M. Grant, J. D. Gunton, and K. Kaski, Phys. Rev. B 32, 1575 (1985).

<sup>&</sup>lt;sup>24</sup>S. R. Anderson, Phys. Rev. B 36, 8435 (1987).

<sup>&</sup>lt;sup>25</sup>O. T. Valls and G. F. Mazenko, Phys. Rev. B 34, 7941 (1986).

<sup>&</sup>lt;sup>26</sup>K. Kaski, M. C. Yalabik, J. D. Gunton, and P. S. Sahni, Phys. Rev. B 28, 5263 (1983); S. Kumar, J. D. Gunton, and K. Kaski, *ibid.* 35, 8517 (1987).

<sup>&</sup>lt;sup>27</sup>A. Milchev, D. W. Heerman, and K. Binder, J. Stat. Phys. 44, 749 (1986).

<sup>&</sup>lt;sup>28</sup>A. Milchev, K. Binder, and D. W. Heerman, Z. Phys. B 63, 521 (1986).

<sup>&</sup>lt;sup>29</sup>R. Toral and A. Chakrabarti, Phys. Rev. B (to be published).

<sup>&</sup>lt;sup>30</sup>A. Chakrabarti, J. B. Collins, and J. D. Gunton, Phys. Rev. B 38, 6894 (1988).