

Near-Surface Long-Range Order at the Ordinary Transition

Uwe Ritschel and Peter Czerner

Fachbereich Physik, Universität GH Essen, 45117 Essen, FR Germany

(Received 28 February 1996)

We study the spatial dependence of the order parameter $m(z)$ near surface that reduces the tendency to order. Using scaling arguments and perturbative methods (ϵ expansion), we find that for $T \geq T_c^b$ a *small* surface magnetic field h_1 gives rise to a *macroscopic* length scale and an anomalous short-distance *increase* of $m(z)$, governed by the power law $m \sim z^\kappa$ (with $\kappa \equiv 1 - \eta_\perp^{\text{ord}} \approx 0.21$ for the $d = 3$ Ising model). This result is related to experiments where exponents of the ordinary transition were observed in Fe_3Al , while superstructure reflections revealed the existence of long-range order near the surface. [S0031-9007(96)01450-0]

PACS numbers: 75.40.Cx, 68.35.Rh, 75.30.Pd, 78.70.Ck

A prototypical system to study critical phenomena in restricted geometries is the semi-infinite Ising model, terminated by a plane surface and extending infinitely in the direction perpendicular to the surface (z direction) [1]. Spins located in the surface may experience interactions different from those in the bulk, for example, due to missing neighbors at a free surface or due to a strong coupling to an adjacent medium. In the framework of continuum field theory such as the ϕ^4 model, the surface influence is taken into account by additional fields such as the surface magnetic field h_1 and the local temperature perturbation c_0 at $z = 0$. The latter can be related to the surface enhancement of the spin-spin coupling in lattice models [2].

At the bulk critical temperature T_c^b , the tendency to order near the surface can be reduced ($c_0 > 0$) or increased ($c_0 < 0$), or, as a third possibility, the surface can be critical as well. As a result, each bulk universality class, in general, divides into several distinct surface universality classes, called ordinary ($c_0 \rightarrow \infty$), extraordinary ($c_0 \rightarrow -\infty$), and special transition ($c_0 = c_{\text{sp}}^*$).

Close to the surface, within the range of bulk correlation length $\xi \sim |\tau|^{-\nu}$, the singular behavior of thermodynamic quantities is markedly changed compared to the bulk. For $z \ll \xi$ the magnetization behaves as $\sim |\tau|^{\beta_1}$ when $\tau = (T - T_c^b)/T_c^b \rightarrow 0$ from below, with β_1 assuming characteristic values for special and ordinary transition, which are, in general, different from the bulk exponent β . (At the extraordinary transition the surface is already ordered at T_c^b .) Further, the correlation functions near the surface are characteristically modified. The correlation function for points within a plane parallel to the surface is given by $C(\rho) \sim \rho^{-(d-2+\eta_\parallel)}$, where $\rho \equiv |\mathbf{r}_\parallel - \mathbf{r}'_\parallel|$ and the anomalous dimension η_\parallel is related to β_1 by $\beta_1 = (\nu/2)(d - 2 + \eta_\parallel)$ [2]. Correlations in the z direction (and all other directions, except the parallel one) are governed by $C(z, z') \sim |z - z'|^{-(d-2+\eta_\perp)}$.

Some of the theoretical predictions [2–4] were found to be in excellent agreement with experiments carried out by Mailänder *et al.* [5,6]. In these experiments,

Fe_3Al was studied close to the DO_3 - B_2 transition by the scattering of evanescent waves generated by the total reflection of x rays at a $[1\bar{1}0]$ surface. The system was expected to belong to the universality class of the ordinary transition, and, indeed, the exponents measured were in remarkable agreement with theoretical predictions [5]. A somewhat disturbing feature was that superstructure reflections revealed the existence of unexpected long-range order (LRO) near the surface, reminiscent of the situation at the extraordinary transition. In the sequel it was demonstrated by Schmid [7] that in a similar situation (at the A_2 - B_2 transition in Fe_3Al) an effective ordering field h_1 in the surface can arise when the stoichiometry of the alloy is not ideal. Assuming that an h_1 is also present at the DO_3 - B_2 transition, the observed LRO can be explained, leaving unanswered the question, however, why exponents of the ordinary transition were measured despite the LRO. In the following we show that a *small* h_1 may generate a universal power-law growth of the order parameter near the surface and, as a result, a LRO considerably (and, in fact, infinitely) larger than expected from mean-field (MF) approximations, while the correlation function near the surface is still governed by the exponents of the ordinary transition.

Most of the theoretical studies concerning inhomogeneous systems concentrated on the behavior at the fixed points $c_0 = \pm\infty$ and $c_0 = c_{\text{sp}}^*$, respectively. At T_c^b and for $h_1 = 0$ for both the ordinary and the special transition the order-parameter profiles are zero for all $z \geq 0$. At the extraordinary transition the surface is ordered, and the order decays as $z^{-\beta/\nu}$ with increasing distance from the surface [8], where, in the Ising case, $\beta/\nu \approx 0.52$ [9]. Concerning the effects of h_1 it was assumed for a long time [10], and recently also shown by rigorous arguments [11], that the case of strong h_1 and $c_0 > 0$ (the so-called normal transition) is equivalent to the extraordinary transition. The special transition was studied by Brezin and Leibler [12] and by Ciach and Diehl [13]. It was found that at the fixed point the scaling field h_1 gives rise to a length scale $l^{\text{sp}} \sim h_1^{-\nu/\Delta_1^{\text{sp}}}$. For $z \gg l^{\text{sp}}$

one finds that $m \sim z^{-\beta/\nu}$ as at the extraordinary transition. In the opposite limit, $z \ll l^{\text{sp}}$, the magnetization behaves as $m \sim m_1 z^{(\beta_1^{\text{sp}} - \beta)/\nu}$. Since $\beta_1^{\text{sp}} \leq \beta$, the order still decays, governed by a somewhat smaller exponent compared to large distances. For the Ising model $(\beta_1^{\text{sp}} - \beta)/\nu \simeq -0.15$ [9].

What do we expect if a *small* h_1 is applied in the presence of a *large* c_0 , i.e., close to the fixed point of the ordinary transition? In this situation the parameter c_0 is a so-called dangerous irrelevant variable [2,14], comparable to the ϕ^4 coupling constant g at and above the upper critical dimension $d^* = 4$, and, in general, must not be naively set to its fixed point value $c_0 = \infty$. Setting the bulk magnetic field $h = 0$, the remaining linear scaling fields at the ordinary transition are τ and $h_1 \equiv h_1/c_0$ [2,14,15]. Hence, the behavior of the magnetization under rescaling of distances should be described by

$$m(z, \tau, h_1) \sim b^{-\beta/\nu} m(zb^{-1}, \tau b^{1/\nu}, h_1 b^{y_1^{\text{ord}}}), \quad (1)$$

where the scaling dimension of h_1 is given by $y_1^{\text{ord}} = \Delta_1^{\text{ord}}/\nu = (d - \eta_{\parallel}^{\text{ord}})/2$ [2]. As usual, all quantities in (1) are made dimensionless with an appropriate power of the renormalization mass μ , and we set $\mu = 1$ afterwards.

Let us first discuss the profile for $h_1 = 0$. As mentioned above, for $\tau > 0$ we have $m = 0$ everywhere. For $\tau < 0$, on the other hand, the magnetization approaches its bulk value $m_b \sim |\tau|^\beta$ for $z \rightarrow \infty$. Close to the surface ($z \ll \xi$), the magnetization increases with a power law [16]. To see this from (1), we set $h_1 = 0$ and fix the arbitrary rescaling parameter b by setting it $\sim z$. Then the magnetization takes the scaling form

$$m(z, \tau) \sim z^{-\beta/\nu} \mathcal{M}_\tau(z/\xi). \quad (2)$$

Since we expect that $m(z \rightarrow 0) \sim m_1$ [17] and know that $m_1 \sim |\tau|^{\beta_1^{\text{ord}}}$, we conclude for the short-distance form of the scaling function $\mathcal{M}_\tau(\xi) \sim \xi^{\beta_1^{\text{ord}}/\nu}$, and, in turn, the behavior of m is given $m(z, \tau) \sim |\tau|^{\beta_1^{\text{ord}}} z^{(\beta_1^{\text{ord}} - \beta)/\nu}$ [16].

We now turn to the case $\tau = 0$ and $h_1 \neq 0$. This is the situation we are actually interested in and which is important for understanding the experimental results of Ref. [5]. In this case, the scaling form derived from (1) is

$$m(z, h_1) \sim z^{-\beta/\nu} \mathcal{M}_{h_1}(zh_1^{1/y_1^{\text{ord}}}). \quad (3)$$

First of all, we notice from (3) that the scaling field h_1 gives rise to a length scale $l^{\text{ord}} \sim h_1^{-1/y_1^{\text{ord}}}$ quite comparable to the situation near the special transition discussed above. In order to find the short-distance behavior of $\mathcal{M}_{h_1}(\xi)$ we have to recall that the surface is paramagnetic at the ordinary transition [10], and m_1 will respond *linearly* to h_1 [18]. Arguing again that $m(z \rightarrow 0) \sim m_1$, we now find that $\mathcal{M}_{h_1}(\xi) \sim \xi^{y_1^{\text{ord}}}$ for $\xi \ll 1$, and, in turn, with the scaling relation $\eta_{\perp} = (\eta_{\parallel} + \eta)/2$

[2], the short-distance behavior is given by

$$m(z, h_1) \sim h_1 z^{\kappa} \quad \text{with } \kappa \equiv y_1^{\text{ord}} - \beta/\nu = 1 - \eta_{\perp}^{\text{ord}}. \quad (4)$$

In the opposite limit, $z \gg l^{\text{ord}}$, the magnetization approaches the bulk equilibrium value zero as $\sim z^{-\beta/\nu}$.

Equation (4) is the central result of this Letter. It states that the magnetization even at (or slightly above) T_c^b in the presence of a surface field h_1 shows a power-law increase reminiscent of the situation below T_c^b . The short-distance exponent κ defined in (4) is zero in MF theory. Below d^* , however, as for the Ising system in $d = 3$, it is nonzero and positive. Taking the literature values for the surface exponents from Refs. [2] and [9], one obtains $\kappa \simeq 0.21$, which implies a rapid growth of LRO with increasing z .

The *spatial* variation of the magnetization discussed above strongly resembles the *time* dependence of the magnetization in relaxational processes at the critical point. If a system with nonconserved order parameter (model A) is quenched from a high-temperature initial state to the critical point, with a small initial magnetization $m^{(i)}$, the order parameter behaves as $m \sim m^{(i)} t^{\theta}$ [19], where the short-time exponent θ is proportional to the difference between the scaling dimensions of initial and equilibrium magnetization [20]. Like the exponent κ in (4), the exponent θ vanishes in MF theory, but becomes positive below d^* .

There is also heuristic argument for the growth of LRO near the surface. As stated above, h_1 generates a surface magnetization $m_1 \sim h_1$. Regions (on macroscopic scales) close to the surface will respond to this magnetization by ordering as well. How strong this influence is depends on two factors. First, it is proportional to the correlated area in a plane parallel to the surface in a distance z . While in the surface, correlations are suppressed; close to the surface the effective correlation length in directions parallel to the surface, ξ_{\parallel} , grows as $\sim z$. Second, for small h_1 (and thus small surface magnetization) it depends linearly on the probability that a given spin orientation "survives" in a distance z from the surface. The latter is governed by the *perpendicular* correlation function $C(z) \sim z^{-(d-2+\eta_{\perp}^{\text{ord}})}$. Taking the factors together, we obtain

$$m(z) \sim h_1 C(z) \xi_{\parallel}^{d-1} = h_1 z^{1-\eta_{\perp}^{\text{ord}}}. \quad (5)$$

Qualitatively speaking, the surface, when carrying a small m_1 , induces a much larger magnetization in the adjacent layers, which are much more susceptible and respond with a magnetization $m(z) \gg m_1$. This effect is not observed on the MF level since there the increase of the correlated surface area is *exactly* compensated by the decay of the perpendicular correlations.

In order to corroborate our scaling analysis and the heuristic arguments from above, we carried out a one-loop calculation for the ϕ^4 model employing the ϵ expansion. Expanded in powers of the coupling constant,

the magnetization can be written in the form $m = m^{(0)} + gm^{(1)} + \mathcal{O}(g^2)$, where $m^{(0)}$ is the well known MF solution [10,21] and $m^{(1)}$ is the one-loop term. The latter was calculated exactly for arbitrary c_0 and h_1 in Refs. [12] and [13]. However, the improvement by means of the renormalization group was done at (or in the vicinity of) the special transition in these references. As a consequence, the anomalous short-distance behavior at the ordinary transition was missed.

The MF solution that satisfies the boundary condition $\partial_z m - cm|_{z=0} = h_1$ at the surface is given by

$$m^{(0)}(z) = \sqrt{\frac{12}{g}} \frac{1}{\tilde{z}} \quad (6a)$$

with

$$\tilde{z} \equiv z + z_+ \quad \text{and} \quad z_+^{-1} = \frac{(c_0^2 + 4h_1\sqrt{g/12})^{1/2} - c_0}{2}, \quad (6b)$$

which holds for general c_0 and h_1 . Close to the ordinary transition (large c_0) the mean-field length scale becomes $z_+ \approx l^{\text{ord}} = (12/g)^{1/2} c_0/h_1$. As expected from (4), there is no anomalous short-distance behavior on the MF level. The profile has its maximum value at $z = 0$, and for $z \gg l^{\text{ord}}$ the profile decays as $\sim z^{-\beta/\nu}$ with the MF value $\beta/\nu = 1$.

The one-loop term $m^{(1)}$ is given by [13,22]

$$m^{(1)}(z) = -\frac{1}{2} \int_0^\infty dz' C(0; z, z') m^{(0)}(z') \int_p C(p; z', z'), \quad (7)$$

where $m^{(0)}(z)$ is the zero-loop (MF) profile (6a) and $\int_p \equiv (2\pi)^{1-d} \int d^{d-1}p$. The propagator $C(p; z, z')$ is Fourier transformed with respect to the spatial coordinates parallel to the surface. It can be calculated exactly [12,13], and the somewhat lengthy results will be omitted here. The integrations in (7) necessary to obtain the full scaling function \mathcal{M}_{h_1} are complicated and can only be carried out numerically. However, it is straightforward to extract the divergent terms, poles $\sim 1/\epsilon$ in dimensional regularization, and the short-distance singularities $\sim \log z$, which, when exponentiated, give rise to power laws modified compared to the MF theory. Collecting these terms, $m^{(1)}$ is given by (7) with

$$\begin{aligned} \int_p C(p; z, z) &= \frac{K_{d-1}}{2} \tilde{z}^{-2+\epsilon} \int_1^\infty dk \\ &\times k^{1-\epsilon} \left[e^{-2k} (e^{2kl^{\text{ord}}/\tilde{z}} - 1) \right. \\ &\times \left. \left(1 + \frac{3}{k} + \frac{3}{k^2} \right)^2 - \frac{3}{k^2} \right] \\ &+ \text{finite}, \end{aligned} \quad (8)$$

where $K_d \equiv 2/[(4\pi)^{d/2} \Gamma(d/2)]$ and “finite” stands for terms which are finite for $\epsilon \rightarrow 0$ and $z \rightarrow 0$. Terms of $\mathcal{O}(1/c_0)$ are also omitted in (8). The zero-momentum

propagator $C(0, z, z')$ appearing in (7) (for $c_0 \rightarrow \infty$) takes the simple form

$$C(0, z, z') = \frac{1}{5} \frac{1}{\tilde{z}^2 \tilde{z}'^2} (\tilde{z}^5_{<} - \tilde{z}'^5_{>}), \quad (9)$$

where $< (>)$ denotes the smaller (larger) of \tilde{z} and \tilde{z}' .

Further analysis shows that the UV divergences can be absorbed in the standard fashion by renormalization of the coupling constant $K_d g_0 = u(1 + 3u/2\epsilon + \mathcal{O}(u^2))$ and of the scaling field $h_{1,0} = h_1(1 - u/4\epsilon + \mathcal{O}(u^2))$ [2]. After this, the coupling constant is set to its fixed point value $u^* = 2\epsilon/3$. Eventually, after exponentiation of logarithms, we find the asymptotic power laws

$$m(z, h_1) \sim \begin{cases} z^{-1+\epsilon/2} & \text{for } z \gg l^{\text{ord}}, \\ h_1 z^{\epsilon/6} & \text{for } z \ll l^{\text{ord}}. \end{cases} \quad (10)$$

As expected, the decay of the profile for $z \gg l^{\text{ord}}$ is governed by the one-loop result $\beta/\nu = 1 - \epsilon/2$. The short-distance behavior is consistent with our scaling analysis; in first order ϵ expansion $\kappa = 1 - \eta_\perp^{\text{ord}} = \epsilon/6$ [2].

A more detailed account concerning the behavior of the magnetization in between the asymptotic regimes of Eq. (10) will be given elsewhere. A qualitative preview on the form of the scaling function $\mathcal{M}_{h_1}(\zeta) \equiv \zeta^{-\beta/\nu} \mathcal{M}_{h_1}(\zeta)$ [see Eq.(3)] is shown in Fig. 1, where the asymptotic power laws are quantitatively correct but the crossover is described by a simple substitute for the scaling function. Regarding the crossover between ordinary ($h_1 = 0$) and the extraordinary (or normal) transition ($h_1 = \infty$), the following scenario should hold. While at the ordinary transition $m(z)$ vanishes everywhere, for $h_1 \neq 0$ the magnetization increases as $\sim z^\kappa$ up to $z \approx l^{\text{ord}} \sim h_1^{-1/y_1^{\text{ord}}}$ ($1/y_1^{\text{ord}} \approx 1.36$ for the Ising model) and thereafter crosses over to the long-distance form given in (10). When h_1 becomes larger, the short-distance increase is steeper and l^{ord} shrinks. For $h_1 \rightarrow \infty$ we have $l^{\text{ord}} \rightarrow 0$, and one finds $m \sim z^{-\beta/\nu}$ for all (macroscopic) distances, the result at the extraordinary transition. Largely analogous results—monotonous behavior at the fixed points and profiles with one extremum in the crossover regime—were found by Mikheev and Fisher for energy density of the two-dimension Ising model [23].

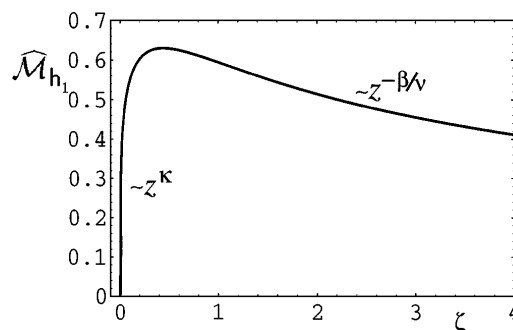


FIG. 1. Qualitative shape of the scaling function $\mathcal{M}_{h_1}(\zeta) = \zeta^{-\beta/\nu} \mathcal{M}_{h_1}(\zeta)$ of the magnetization. More details are described in the text.

Also, other quantities exhibit a crossover behavior similar to the one described in the previous paragraph for $m(z)$. As an example, consider the correlation function $C(\rho, z)$ for points in a plane parallel to the surface in a distance ρ from each other. The respective structure function was measured in the experiment by Mailänder *et al.* [5]. When $\rho \gg z$ the behavior of $C(\rho, z)$ is governed by surface exponents, by the ones of the ordinary transition for $z \ll l^{\text{ord}}$ and by the ones of the extraordinary (or normal) transition for $z \gg l^{\text{ord}}$, with a crossover at $z \approx l^{\text{ord}}$.

In conclusion, we studied the effects of a small surface magnetic field in the vicinity of a surface that disfavors order. Our main result is that, for $T \gtrsim T_c$, the order parameter exhibits an anomalous short-distance behavior in the form of a power-law increase $m \sim h_1 z^{1-\eta_{\perp}^{\text{ord}}}$ for $z \lesssim l^{\text{ord}}$, implying a much larger magnetization density (long-range order) in this regime than could be expected from mean-field theory. As a consequence, as at the extraordinary transition, one has to expect superstructure reflections in scattering experiments that are sensitive to the near-surface behavior of $m(z)$ (such as one reported in Ref. [5]). However, the correlation function in directions parallel to the surface (and thus the structure function) is still governed by the exponents of the *ordinary* transition in the near-surface regime $z \lesssim l^{\text{ord}}$. Thus, assuming that there exists a small ordering field h_1 in the system studied by Mailänder *et al.* [5], our scenario gives a plausible explanation for the experimental findings. The possible significance of our result for other experiments, such as the one recently carried out by Desai, Peach, and Franck [24], remains to be explored in the future.

We thank H. W. Diehl, S. Dietrich, E. Eisenriegler, and R. Leidl for useful discussions and hints to the literature. This work was supported in part by the Deutsche Forschungsgemeinschaft through Sonderforschungsbereich 237.

-
- [1] For reviews on surface critical phenomena, see K. Binder, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J.L. Lebowitz (Academic Press, London, 1983), Vol. 8, and Ref. [2].
- [2] H. W. Diehl, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J.L. Lebowitz (Academic Press, London, 1986), Vol. 10.
- [3] H. W. Diehl and S. Dietrich, *Z. Phys. B* **42**, 65 (1981); **43**, 281(E) (1981).
- [4] S. Dietrich and H. Wagner, *Phys. Rev. Lett.* **51**, 1469 (1983); *Z. Phys. B* **56**, 207 (1984).
- [5] X. Mailänder, H. Dosch, J. Peisl, and R. L. Johnson, *Phys. Rev. Lett.* **64**, 2527 (1990).

- [6] For a review of the experimental work, see H. Dosch, in *Critical Phenomena at Surfaces and Interfaces*, edited by G. Höhler and E. A. Niekisch, Springer tracts in Modern Physics (Springer, Berlin, 1992).
- [7] F. Schmid, *Z. Phys. B* **91**, 77 (1993).
- [8] From the power-law decay $m \sim z^{-\beta/\nu}$ at the extraordinary transition, it appears that the magnetization diverges when going towards the surface. One has to bear in mind, however, that the power law is only valid for distances much larger than microscopic scales. Upon approaching the surface, the magnetization would depart from the power law and assume a finite value in the surface.
- [9] C. Ruge, S. Dunkelmann, and F. Wagner, *Phys. Rev. Lett.* **69**, 2465 (1992).
- [10] A. J. Bray and M. A. Moore, *J. Phys. A* **10**, 1927 (1977).
- [11] H. W. Diehl and T. W. Burkhardt, *Phys. Rev. B* **50**, 3894 (1994).
- [12] E. Brézin and S. Leibler, *Phys. Rev. B* **27**, 594 (1983).
- [13] A. Ciach and H. W. Diehl (unpublished).
- [14] H. W. Diehl, G. Gompper, and W. Speth, *Phys. Rev. B* **31**, 5841 (1985).
- [15] The correct scaling field at the ordinary transition is actually h_1/c_0^y , where the exponent $y = 1$ in MF theory but $\neq 1$ in general. It is discussed in detail in Ref. [2] that, in the framework of the loop expansion, one does not capture the deviation from the MF value in this exponent, while, e.g., the z dependence of expectation values is reproduced correctly. For details, we refer to Refs. [2] and [14].
- [16] G. Gompper, *Z. Phys. B* **56**, 217 (1984).
- [17] This is in accord with, and actually motivated by, the field-theoretical short-distance expansion [see K. Symanzik, *Nucl. Phys.* **B190(FS3)**, 1 (1981); H. W. Diehl and S. Dietrich, *Z. Phys. B* **42**, 65 (1981)], where field operators near a boundary are expressed in terms of boundary operators multiplied by c -number functions.
- [18] The relation $m_1 \sim h_1$ seems to be inconsistent with the definition of the surface exponent δ_{11} via $m_1 \sim h_1^{1/\delta_{11}}$ and the result $\delta_{11}^{\text{ord}} \approx 0.6$ for the Ising model [2]. One has to bear in mind, however, that δ_{11}^{ord} governs the leading singular behavior of m_1 which is weaker here than the linear dependence on h_1 [10].
- [19] H. K. Janssen, B. Schaub, and B. Schmittmann, *Z. Phys. B* **73**, 539 (1989).
- [20] H. W. Diehl and U. Ritschel, *J. Stat. Phys.* **73**, 1 (1993); U. Ritschel and H. W. Diehl, *Phys. Rev. E* **51**, 5392 (1995); *Nucl. Phys.* **B464**, 512 (1996).
- [21] T. C. Lubensky and M. H. Rubin, *Phys. Rev. B* **12**, 3885 (1975).
- [22] M. Smock and H. W. Diehl, *Phys. Rev. B* **47**, 5841 (1993).
- [23] L. V. Mikheev and M. S. Fisher, *Phys. Rev. B* **49**, 378 (1994).
- [24] N. S. Desai, S. Peach, and C. Franck, *Phys. Rev. E* **52**, 4129 (1995).