Effective field theory for interface delocalization transitions

R. Lipowsky, D. M. Kroll,* and R. K. P. Zia†
Sektion Physik der Ludwig-Maximilians-Universität München, D-8000 München 2, West Germany
(Received 4 January 1983)

Semi-infinite systems are considered which give rise to a delocalization transition of the interface between two coexisting phases. Since the interface position becomes a zero mode at the transition, interface fluctuations invalidate mean-field theory for space dimension $d \leqslant 3$. An effective field-theoretic model for this zero mode is obtained via the collective-coordinate method. Results for a simplified version of this model in $d=2$ and in $d=3$ are reported.

Recently, it has been found that interesting delocalization transitions can occur in semi-infinite systems with two coexisting phases.[1–16] At these transitions, the distance from the surface to the interface separating the coexisting phases diverges. Such behavior was first investigated in Ising-like systems[1–9] and has been observed in several binary fluids.[10,11] These transitions are usually referred to as wetting or pinning transitions. More recently, it was predicted[12] that such behavior can also occur when an ordered and a disordered phase coexist. In this case, there are additional critical surface phenomena[12–15] which apparently have been observed in the binary alloy Cu_3Au.[14,16] These transitions are referred to as surface induced disordering (SID) transitions.

Both wetting and SID have been investigated using various methods. First, they have been discussed in the framework of Landau or mean-field (MF) theory[1,6,8,12–14] where the mean interface position was found to diverge logarithmically. Secondly, they have been investigated for space dimension $d=2$ by using solid-on-solid (SOS) models for the interface coordinate.[3–5,15] Here, a power-law divergence for the mean interface position was found. In addition, a d-dimensional field-theoretic SOS model has been treated by renormalization-group methods.[7]

In this Communication, we show how one can derive effective interface models starting from an appropriate Ginzburg-Landau free-energy functional. MF theory is obtained as a saddle-point or "zero-loop" approximation. Expanding around the MF solution, we observe that *a zero mode emerges at the delocalization transition.* This zero mode is treated by the collective-coordinate method and an effective interface model is obtained. A simplified version of this model is analyzed using transfer-matrix methods for $d=2$ and a variational method for $d=3$. These results are discussed for SID. However, it is argued that they also apply to the wetting transition if an appropriate identification of the various scaling fields is made.

Consider a d-dimensional semi-infinite system described by the Ginzburg-Landau free-energy functional

$$F\{\phi\} = \int d^{d-1}\rho \int_0^\infty dz \left[\tfrac{1}{2}(\nabla\phi)^2 + f(\phi) + \delta(z) f_1(\phi) \right] \tag{1}$$

for the scalar field $\phi(\rho,z)$. z is the coordinate perpendicular to the $(d-1)$-dimensional surface and

$$f(\phi) = \tfrac{1}{2}a\phi^2 - \tfrac{1}{3}b\phi^3 + \tfrac{1}{4}c\phi^4 \; , \tag{1a}$$

$$f_1(\phi) = -h_1\phi + a_1\phi^2 \; . \tag{1b}$$

The MF theory for this model has been discussed previously.[12–14] For $a=a^*=2b^2/(9c)$, $h_1=0$, and $a_1 \geqslant \sqrt{a^*}$, critical surface phenomena occur.[12] There are two different types of transitions, namely, (O_2) for $a_1 > \sqrt{a^*}$ and $(\bar{s})$ for $a_1 = \sqrt{a^*}$. At both (O_2) and $(\bar{s})$, the MF order-parameter profile $M(z) = \langle \phi(\rho,z) \rangle$, has an interface at $z=\hat{l}$. For $(a,h_1) = (a^*,0)$, this interface is delocalized since $\hat{l}=\infty$. The way in which $\hat{l}$ goes to infinity is intimately related to the way in which the surface order parameter $M_1 \equiv M(z=0)$ tends to zero, since asymptotically

$$\hat{l} = -\frac{1}{\sqrt{a^*}} \ln(M_1/M_B^*) \; , \tag{2}$$

where M_B^* is the MF bulk order parameter for $a=a^*$. One has to distinguish two cases. Firstly, consider $h_1=0$ and infinitesimal $\delta a \equiv a - a^* < 0$. In this case, $M_1 \propto |\delta a|^{\beta_1}$ with $\beta_1 = \frac{1}{2}$ at (O_2) and $\beta_1 = \frac{1}{3}$ at $(\bar{s})$.[12] Secondly, consider $|\delta a| = 0$ and infinitesimal positive h_1. Then, $M_1 \propto h_1^{1/\delta_{1,1}}$, with[13]

$$1/\delta_{1,1} = \begin{cases} 1 & (O_2) \quad \text{(3a)} \\ \frac{1}{2} & (\bar{s}) \; . \quad \text{(3b)} \end{cases}$$

MF theory neglects fluctuations in the local position of the interface. In order to get some insight into the effect of these configurational fluctutations, one may expand around the MF profile:

$$\phi(\rho,z) = M(z) + \eta(\rho,z) \; . \tag{4}$$

The Gaussian fluctuations are obtained if (4) is inserted into (1) and the resulting functional is expanded up to second order in η. As a consequence, one is lead to consider the Schrödinger-type equation

$$\left[-\frac{d^2}{dz^2}+p^2+Q(z)\right]g_n(z)=(p^2+E_n)g_n(z) \quad , \qquad (5)$$

where p is a $(d-1)$-dimensional vector and

$$Q(z)=f''(M)=\dddot{M}(z)/\dot{M}(z) \quad . \qquad (5a)$$

The primes and the dots denote derivatives with respect to M and z, respectively. The eigenstates $g_n(z)$ have to fulfill the boundary condition

$$\frac{d}{dz}g_n(z)|_{z=0}=f_1''(M_1)g_n(0) \; . \qquad (6)$$

For infinitesimal $|\delta a|$ or h_1, the potential $Q(z)$ is almost flat apart from a well around $z=\hat{l}$. For $\hat{l}\to\infty$, the ground state $g_0(z)$ becomes proportional to $\dot{M}(z)$ and the corresponding energy E_0 tends to zero. Thus, *a zero mode emerges* in this limit. Since the energies of the excited states are separated from E_0 by a finite gap,[17] the leading contribution to the surface free energy f_s from the Gaussian fluctuations is

$$f_s^{(1)}=\frac{1}{2}\int\frac{d^{d-1}p}{(2\pi)^{d-1}}\ln(p^2+E_0) \propto \begin{cases}-E_0\ln(E_0), & d=3\\ E_0^{(d-1)/2}, & d<3 \; .\end{cases} \qquad (7)$$

A simple estimate of (7) may be obtained via a variational upper bound for E_0. This leads to

$$f_s^{(1)}\propto\begin{cases}|\delta a|\ln(|\delta a|), & d=3\\ |\delta a|^{(d-1)/2}, & d<3\end{cases} \qquad (8)$$

for $h_1=0$ both at (O_2) and at $(\bar{s})$. For $|\delta a|=0$, one finds

$$f_s^{(1)}\propto\begin{cases}h_1^x\ln(h_1), & d=3\\ h_1^{x(d-1)/2}, & d<3 \; ,\end{cases} \qquad (9)$$

with $x\equiv 1+1/\delta_{1,1}$ both at (O_2) and at $(\bar{s})$. These estimates of the "one-loop" contribution should be compared with the MF or zero-loop contribution $f_s^{(0)}\propto|\delta a|\ln(|\delta a|)$ for $h_1=0$ and $f_s^{(0)}\propto h_1^x$ for $|\delta a|=0$. Thus, for $d<3$, the Gaussian fluctuations invalidate the results of Landau theory while $d=3$ is obviously a boundary case.

From the above discussion, it follows that the dominant fluctuations are due to the emerging zero mode. In a different context, a zero mode has been handled via the collective-coordinate method.[18] As a result, the drumhead model has been obtained.[18,19] Here, we follow a similar strategy: We introduce the collective coordinate $\zeta(\rho)$ via the ansatz

$$\phi(\rho,z)=M(z-\zeta(\rho)) \quad . \qquad (10)$$

In terms of $\zeta(\rho)$, the local interface position is given by

$$l(\rho)=\hat{l}+\zeta(\rho) \quad , \qquad (11)$$

where $\hat{l}$ is the MF interface position [compare (2)]. If (10) is inserted into (1), a straightforward calculation yields

$$F\{\zeta\}=\int d^{d-1}\rho[\tfrac{1}{2}\sigma(\nabla\zeta)^2+V(\zeta)+W(\zeta,\nabla\zeta)] \quad , \qquad (12)$$

with the surface tension

$$\sigma=\int_{M_1}^{M_B}dm\,[2f(m)-2f(M_B)]^{1/2} \qquad (12a)$$

and

$$V(\zeta)=\int_{M(-\zeta)}^{M_B}dm\,[2f(m)-2f(M_B)]^{1/2}+f_1(M(-\zeta)) \quad , \qquad (12b)$$

$$W(\zeta,\nabla\zeta)=-\tfrac{1}{2}(\nabla\zeta)^2\times\int_{M_1}^{M(-\zeta)}dm\,[2f(m)-2f(M_B)]^{1/2} \quad , \qquad (12c)$$

where M_B is the MF value for the bulk order parameter. In this Communication, we focus attention on the nongradient interaction term $V(\zeta)$. There is no *a priori* justification for ignoring the last term in (12) since naive power counting indicates that the gradient-interaction term $W(\zeta,\nabla\zeta)$ is a marginal operator (for $d=3$). However, the essential physics obtained from the MF analysis of (1) is contained in $V(\zeta)$ (see below). The influence of the term $W(\zeta,\nabla\zeta)$ will be discussed elsewhere.

We are particularly interested in the form of $V(\zeta)$ near the transitions (O_2) and $(\bar{s})$, where $|\delta a|=0$ and $h_1=0$. Therefore we expand $V(\zeta)$ in powers of $|\delta a|$ and h_1, respectively. In the leading term of this expansion, we transform from $\zeta(\rho)$ to the interface position $l(\rho)=\hat{l}+\zeta(\rho)$ and insert the asymptotic form (2) for $\hat{l}$. In this way, we obtain

$$V(l)=Ae^{-3\sqrt{a^*}l}+B(a_1-\sqrt{a^*})e^{-2\sqrt{a^*}l}-Ch_1e^{-\sqrt{a^*}l}+D|\delta a|\sqrt{a^*}l \quad , \qquad (13)$$

with $A,B,C,D>0$. The effective free-energy functional thus reduces to

$$F\{l\}=\int d^{d-1}\rho[\tfrac{1}{2}(\nabla l)^2+V(\sigma^{-1/2}l)] \quad , \qquad (14)$$

where $V(x)$ is given by (13) and a factor $\sigma^{1/2}$ has been absorbed in the field variable l for convenience. It should not be forgotten that, in principle, we still have a restriction $l>0$ in (14). This is due to the semi-infinite geometry of the original model (1) $(z>0)$. However, since the potential $V(l)$ is very repulsive for negative l, it appears permissible to ignore this restriction.

First, we apply MF theory to model (14) and determine $\langle l \rangle$ from $\partial V/\partial l|_{\langle l \rangle}=0$. It turns out that at both (O_2) and at $(\bar{s})$ all critical properties, which have been obtained in the MF theory for the original model (1),[12,13] are recovered. This feature provides some justification for the fact that we retained only the leading terms of the expansion for $V(l)$ in powers of $|\delta a|$ and h_1.

Next, consider $d-1=1$. In this case, the field-theoretic model defined by (13) and (14) is one-dimensional and can be easily treated by transfer-matrix methods.[3-5,15] For $h_1=0$, the delocalization transition occurs at $|\delta a|=0$. For $|\delta a|=0$, it occurs at a finite surface field h_1^*. As a result, one obtains for the surface free energy,

$$f_s \propto \begin{cases} |\delta a|^{2-\alpha_s}, & h_1=0 \ , \quad (15) \\ \delta h_1^{1+1/\delta_{1,1}}, & |\delta a|=0 \ , \quad (16) \end{cases}$$

with $\alpha_s=\frac{4}{3}$, $1/\delta_{1,1}=1$, and $\delta h_1 \equiv h_1-h_1^*$. For the mean distance $\langle l \rangle$ of the interface from the surface, one finds

$$\langle l \rangle \propto \begin{cases} |\delta a|^{\beta_s}, & h_1=0 \ , \quad (17) \\ \delta h_1^{1/\delta_{s,1}}, & |\delta a|=0 \ , \quad (18) \end{cases}$$

with $\beta_s=-\frac{1}{3}$ and $1/\delta_{s,1}=-1$. Note that only two of the four surface exponents defined above are independent. This follows from general scaling considerations discussed previously.[13]

Finally, we discuss (14) for $d-1=2$ using a variational method. This method has been applied previously to the roughening transition[20] and to multilayer adsorption.[21,22] In this method, one introduces two variational parameters L and μ^2 via the Gaussian functional

$$F_0\{l\}=\int d^{d-1}\rho\left[\tfrac{1}{2}(\nabla l)^2+\tfrac{1}{2}\mu^2(l-L)^2\right] \ . \quad (19)$$

L and μ^2 are determined self-consistently in such a way that the difference between the free energy of model (14) and the free energy of (19) becomes minimal. As a result, we find

$$\langle l \rangle = L \propto -\ln(|\delta a|) \ , \quad (20)$$

$$f_s \propto -|\delta a|\ln(|\delta a|) \ , \quad (21)$$

for $h_1=0$ both at (O_2) and at $(\bar{s})$. Thus the MF results are recovered in this case. In contrast, for $|\delta a|=0$ and $h_1>0$, an additional phase boundary not present in MF theory is found. This new phase boundary is given by a critical value τ_c of the parameter $\tau \equiv (a^*/\sigma)^{1/2}$, where σ is the surface tension (12a). At (O_2), $\tau_c=2\sqrt{\pi}$, whereas $\tau_c=2(2\pi/3)^{1/2}$ at $(\bar{s})$.[23] As a consequence, the interface behaves differently for large surface tension $(\tau<\tau_c)$ and for small surface tension $(\tau>\tau_c)$, since

$$\langle l \rangle \propto \begin{cases} -\ln(h_1), & \tau<\tau_c, \quad h_1 \to 0 \quad (22) \\ (\tau_c-\tau)^{-1}, & \tau \to \tau_c-0, \quad h_1>0 \quad (23) \end{cases}$$

whereas $\langle l \rangle = \infty$ for $\tau \geq \tau_c$. Thus an interface with a large surface tension is pinned by a finite surface field h_1, while an interface with a small surface tension is delocalized even in the presence of a finite h_1. The surface free energy is found to behave as

$$f_s \propto \begin{cases} h_1^{1+1/\delta_{1,1}}, & \tau<\tau_c, \quad h_1 \to 0 \ , \quad (24) \\ (\tau_c-\tau)\exp\left(-\dfrac{|\text{const}|}{\tau_c-\tau}\right), & \tau \to \tau_c-0, \quad h_1>0 \ . \quad (25) \end{cases}$$

Note that an essential singularity similar to (25) has been obtained previously.[7] The surface exponent in (24) is

$$1+1/\delta_{1,1}=\begin{cases} 2\left(1-\dfrac{\tau^2}{4\pi}\right)^{-1} & (O_2) \\ \dfrac{3}{2}\left(1-\dfrac{3\tau^2}{8\pi}\right)^{-1} & (\bar{s}) \ . \end{cases}$$

The variational approach just described is equivalent to the leading term of a cumulant expansion for the generating functional $\Gamma\{\langle l \rangle\}$ of vertex functions. A full treatment of the problem requires an investigation of the higher-order terms in the cumulant expansion. This may be done using a field-theoretic renormalization procedure similar to that used in Ref. 7. Work in this direction is in progress.

At this point, it is appropriate to discuss the relationship of SID and wetting. It is shown in a separate publication[15] that both types of transitions are closely related: (O_2) is related to the critical wetting transition (CW), whereas $(\bar{s})$ is related to the wetting tricritical point. This relationship is most clearly discussed in terms of the relevant scaling fields. For instance, consider (O_2) and CW. At both transitions, there are two relevant scaling fields: At (O_2) one has the linear fields $u_1 \propto |\delta a|$ and $u_2 \propto \delta h_1$.[13] At CW, one has $v_1 \propto |T-T_W|$ and $v_2 \propto H$, where T_W is the wetting transition temperature and H is the bulk magnetic field.[8] It can be shown[15] that both transitions exhibit the same scaling behavior if one makes the identification $u_1 \sim v_2$ and $u_2 \sim v_1$. As a consequence, one may translate all critical properties of (O_2) into critical properties of CW and vice versa. For example, the results (16) and (18) imply $f_s \propto |T-T_W|^2$ and $\langle l \rangle \propto |T-T_W|^{-1}$, which are just the exact results of Abraham.[2] In the present context, the correspondence between SID and wetting implies that the effective interface model (14) also applies for wetting provided one makes the abovementioned identification of the scaling fields.

Note added in proof. After the completion of this work, we received a report of work prior to publication, by E. Brezin, B. Halperin, and S. Leibler, on this subject restricted to $|\delta a|=0$.

ACKNOWLEDGMENTS

It is a pleasure to thank H. W. Diehl, W. Speth, and H. Wagner for stimulating discussions and helpful comments. One of us (R.K.P.Z.) acknowledges receipt of an Alexander von Humboldt Fellowship.

---

*Permanent address: Institut für Festkörperforschung, Kernforschungsanlage Jülich, 5170 Jülich, West Germany.
†Permanent address: Physics Department, Virginia Polytechnic Institute and State University, Blacksburg, Va. 24061.

[1] J. W. Cahn, J. Chem. Phys. 66, 3667 (1977).
[2] D. B Abraham, Phys. Rev. Lett. 44, 1165 (1980).
[3] D. M. Kroll, Z. Phys. B 41, 345 (1981).
[4] T. Burkhardt, J. Phys. A 14, L63 (1981).
[5] J. M. J. van Leeuwen and H. J. Hilhorst, Physica (Utrecht) 107A, 319 (1981).
[6] R. Pandit, M. Schick, and M. Wortis, Phys. Rev. B 26, 5112 (1982).
[7] D. M. Kroll and R. Lipowsky, Phys. Rev. B 26, 5289 (1982).
[8] H. Nakanishi and M. E. Fisher, Phys. Rev. Lett. 49, 1565 (1982).
[9] Long-range pinning forces in $d=2$ have been considered by D. M. Kroll and R. Lipowsky (unpublished).
[10] O'D. Kwon *et al.*, Phys. Rev. Lett. 48, 185 (1982).
[11] D. W. Pohl and W. I. Goldburg, Phys. Rev. Lett. 48, 1111 (1982).
[12] R. Lipowsky, Phys. Rev. Lett. 49, 1575 (1982).
[13] R. Lipowsky (unpublished).
[14] R. Lipowsky and W. Speth (unpublished).
[15] D. M. Kroll and R. Lipowsky (unpublished).
[16] V. S. Sundaram *et al.*, Phys. Rev. Lett. 31, 1136 (1973).
[17] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Vol. 2, p. 1650.
[18] H. W. Diehl, D. M. Kroll, and H. Wagner, Z. Phys. B 36, 329 (1980).
[19] D. J. Wallace and R. K. P. Zia, Phys. Rev. Lett. 43, 808 (1979).
[20] Y. Saito, Z. Phys. B 32, 75 (1978).
[21] J. D. Weeks, Phys. Rev. B 26, 3998 (1982).
[22] D. M. Kroll (unpublished).
[23] At (O_2), the first term of $V(l)$ in (13) has been ignored since the role of the repulsive part of this potential is played by the second term.