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COMMENT

# Surface transition and $\varepsilon$ expansion

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**Abstract.** We provide the first description of the surface transition that goes beyond mean-field theory and that develops a systematic $\varepsilon$-expansion method for this transition. The theory exhibits the emergence of $(d-1)$-dimensional physics with a complicated dependence on $c$ (the surface interaction parameter). A calculation is provided for the lowest correction to the shift in the critical temperature (from its mean-field value).

Surface effects on phase transitions are of considerable interest both theoretically and experimentally. A comprehensive review is given by Binder (1983). Using mean-field theory analysis, four phases can be identified according to the values of the temperature $t$ ($t \propto T - T_c^\infty$, where $T_c^\infty$ is the bulk transition temperature) and the surface interaction parameter $c$ (Binder 1983). These phases are as follows. When $c \leqslant 0$ the system orders at the bulk transition temperature $T_c^\infty$. For large values of $|c|$, i.e. $|c| \gg t^{1/2}$, the transition is called ordinary, while the special transition occurs at small values of $|c|$ where $|c| \ll t^{1/2}$. When $c > 0$ the surface orders spontaneously at a higher temperature $t = c^2$, while the bulk remains disordered. For large values of $c$, i.e. $c \gg t^{1/2}$, the latter yields the surface transition. Finally, as the temperature is further lowered (with $c > 0$) through the bulk critical temperature, the bulk also orders at the extraordinary transition.

Renormalisation group methods of field theory have been utilised to study semi-infinite (or infinite) systems in $d$ dimensions ($d = 4 - \varepsilon$) with a $(d-1)$-dimensional free surface (Lubensky and Rubin 1973, 1975, Bray and Moore 1977, Reeve and Guttman 1981, Diehl and Dietrich 1980, 1981a, b, 1983a, b, Diehl *et al* 1985). The most widely used model is a $d$-dimensional (infinite or semi-infinite) $N$-vector model with an additional surface term. This model has been applied to the study of the ordinary ($c \to -\infty$) and special ($c \to 0$) transitions. Calculations of scaling functions can be performed for arbitrary values of $c \leqslant 0$ and $t > 0$, providing the full crossover from the special to the ordinary transitions (Goldschmidt 1983, Goldschmidt and Jasnow 1984, Gompper 1984, Nemirovsky and Freed 1985a). In fact, the results are even valid for $c > 0$ in the symmetric phase as long as the system is not too close to the surface transition, i.e. for $c < t^{1/2}$.

As we approach this surface transition, the $\varepsilon$ expansion breaks down; the ratio of first-order corrections to zeroth-order ones is of order $(t - c^2)^{-1}$ which is becoming infinite so the series expansion becomes meaningless. Hence, the only currently available theory of the surface transition comes from mean-field theory which is inadequate to describe the strong fluctuations that are present near that transition. At the surface transition the ordered surface region is expected to be a slab of infinite extent in $(d-1)$ dimensions and of thickness given by $c^{-1}$ in the mean-field approximation. Properties of this critical slab exhibit the behaviour of the $(d-1)$-dimensional bulk, but they depend non-trivially on $c^{-1}$. This complicated $c$ dependence is of central interest. One of the difficulties cited above with $\varepsilon$ techniques for the surface transition arises because the theory is attempting to describe the $(d-1)$-dimensional physics of the critical slab with an inappropriate $d$-dimensional expansion, while direct $(d-1)$-dimensional calculations omit the essential $c$ dependence of the slab's properties.

The surface transition is a beautiful example of dimensional reduction, i.e. the emergence of $d'$-dimensional physics out of an underlying $d$-dimensional system. Recently, we have developed a formalism that is applicable to all problems where dimensional reduction occurs as some (internal or external) parameter of the model (like $c^{-1}$) becomes 'very small' (Nemirovsky and Freed 1985b). Then the presence of two small parameters, $c^{-1}$ and the coupling constant $u$, forms the basis for a new $\varepsilon$-expansion method designed to study the dimensional reduced $(d\rightarrow d-1)$ transitions and the non-trivial dependence of the critical slab properties on $c$.

Our general theory of dimensional reduction is utilised here for the first time to consider corrections to the mean-field description of the surface transition. A $d$-dimensional theory is used to evaluate a $c$-dependent effective free energy functional for the lowest mode of the order parameter (see below) with small corrections provided by higher modes. The effective functional corresponds to a system of infinite extent in $(d-1)$ dimensions which has the same internal symmetry as that of the original $d$-dimensional theory. This automatically implies that critical exponents are those of a bulk $(d-1)$ system in accordance with what many have argued (see, e.g., Bray and Moore 1977). However, critical amplitudes are calculated as non-trivial functions of $c$.

The effective free energy functional can be studied by various methods such as numerical ones, real space renormalisation group, $\varepsilon' = 4-d$ expansions, etc. Here we calculate the shift in the critical temperature to $O(\varepsilon')$ and evaluate the $c$ dependent $(d-1)$-dimensional effective free energy functional to lowest order. Consequently, this very interesting surface transition is now amenable to theoretical treatment that includes the important fluctuations which are absent in previous mean-field theories.

We start with the partition function $Z$ given by

$$Z=\int \mathrm{D}[\phi]\exp[-F\{\phi\}], \tag{1}$$

$$F\{\phi\}=\int_0^\infty \mathrm{d}z\int \mathrm{d}^{d-1}\rho\left(\phi(\boldsymbol{\rho},z)\tfrac{1}{2}[-\nabla^2+t_0-2c_0\delta(z)]\phi(\boldsymbol{\rho},z)+\frac{u_0}{4!}(\phi^2(\boldsymbol{\rho},z))^2\right), \tag{1a}$$

where $F$ is the $d$-space Landau free energy functional, $\phi(\boldsymbol{\rho},z)$ is the $N$ component order parameter, $\boldsymbol{\rho}$ is a $(d-1)$-dimensional vector perpendicular to the $(d-1)$-dimensional surface at $z=0$. The parameters $t_0 \propto T-T_c^\infty$, $u_0$ and $c_0$ are the bare temperature, coupling constant and surface interaction parameter, respectively.

The order parameter $\phi(\boldsymbol{k},z)$, where $\boldsymbol{k}$ is the Fourier variable conjugate to $\boldsymbol{\rho}$, can be expanded in normal modes as

$$\phi(\boldsymbol{k},z)=\phi_0(\boldsymbol{k})f_0(z)+\int_0^\infty \mathrm{d}\omega\,\phi_\omega(\boldsymbol{k})f_\omega(z), \tag{2}$$

where $\{f_\omega\}$ are the normalised eigenfunctions of the 'Hamiltonian' $H$ for a single particle in an attractive $\delta$ potential, i.e.

$$H = -\frac{d^2}{dz^2} - c_0\delta(z) \qquad Hf_\omega = E_\omega f_\omega. \tag{3}$$

Equation (3) is easily solved to obtain

$$f_0(z) = (2c)^{1/2}\exp(-cz) \qquad E_0 = -c^2 \tag{3a}$$

$$\begin{aligned} f_\omega(z) &= (4c)^{1/2}[\omega(\omega^2+1)^{-1/2}\cos\omega cz - (\omega^2+1)^{-1/2}\sin\omega cz] \\ E_\omega &= \omega^2c^2 \qquad \omega > 0. \end{aligned} \tag{3b}$$

The criterion for dimensional reduction is that the gap $E_1 - E_0$ to the lowest excited state grows unbounded as the length $c^{-1}$ that drives the dimensional reduction becomes 'small', so the lowest mode becomes dominant. Equation (3) shows this criterion to be satisfied for $c>0$. On the other hand, when $c<0$, equation (3) has a repulsive delta potential for the special and ordinary transitions. There are only continuum states, so no energy gap arises to produce a dimensional reduction to lower dimensional physics for these cases. The presence of the gap for $c>0$ implies that near the surface transition the lowest mode dominates, while higher ones only provide corrections.

The free energy functional (1$a$) can be rewritten in terms of normal modes as

$$\begin{aligned} F\{\phi\} = {}&\tfrac{1}{2}\int dk\,\phi_0(\boldsymbol{k})(k^2+\mathring{t}_0)\phi_0(-\boldsymbol{k}) + \tfrac{1}{2}\int dk\int_0^\infty d\omega_1\int_0^\infty d\omega_2\,\phi_{\omega_1}(\boldsymbol{k}) \\ &\times[k^2+\mathring{t}_0+(E_{\omega_1}-E_0)]\phi_{\omega_2}(-\boldsymbol{k})\delta(\omega_1+\omega_2) \\ &+\frac{u_0c_0}{4!}\int dk_1\,dk_2\,dk_3\,dk_4\,(2\pi)^{d-1}\delta(\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3+\boldsymbol{k}_4) \\ &\times\sum_{\omega_1,\omega_2,\omega_3,\omega_4}\phi_{\omega_1}(\boldsymbol{k}_1)\phi_{\omega_2}(\boldsymbol{k}_2)\phi_{\omega_3}(\boldsymbol{k}_3)\phi_{\omega_4}(\boldsymbol{k}_4)S_{\omega_1\omega_2\omega_3\omega_4}, \end{aligned} \tag{4}$$

where $k^2 = |\boldsymbol{k}|^2$, $\mathring{t}_0 = t_0 + E_0 = t_0 - c_0^2$, the tensor $S_{\omega_1\omega_2\omega_3\omega_4}$ is given by

$$S_{\omega_1\omega_2\omega_3\omega_4} = c_0^{-1}\int_0^\infty dz f_{\omega_1}(z)f_{\omega_2}(z)f_{\omega_3}(z)f_{\omega_4}(z) \tag{4a}$$

and $\int dk$ stands for $\int d^{d-1}k/(2\pi)^{d-1}$. The $\omega>0$ modes can be integrated out using techniques we have recently discussed (Nemirovsky and Freed 1985b). The effective field theory for the $\phi_0(\boldsymbol{k})$ mode contains all diagrams with lowest mode external legs and a sum over all $\omega>0$ modes as internal lines. Feynman rules are easily derived from (4). A consistent $\varepsilon$-expansion procedure emerges by use of the formal scheme $\mathring{t}_0 \sim u_0c_0$ as described by us for finite size scaling (Nemirovsky and Freed 1985b, c). Analogous techniques have been utilised to study finite temperature field theories close to the transition (Ginsparg 1980).

The first contribution $\delta\mathring{t}_0$ to the quadratic term in $\phi_0(\boldsymbol{k})$ of equation (4) is calculated to be

$$\begin{aligned} \delta\mathring{t}_0 &= u_0c_0[\tfrac{1}{6}(N+2)]\int_0^\infty d\omega\int dk\,S_{00\omega\omega}[k^2+\mathring{t}_0+(E_\omega-E_0)]^{-1} \\ &= u_0[\tfrac{1}{6}(N+2)]\int_0^\infty dz\,f_0^2(z)\int dk\,G'(\boldsymbol{k},z,z), \end{aligned} \tag{5}$$

where $G'(\mathbf{k}, z, z')$ is the subtracted propagator that contains all modes but the lowest:

$$G'(\mathbf{k}, z, z') = G(\mathbf{k}, z, z') - 2c_0 \exp[-c_0(z+z')](k^2 + \mathring{t}_0)^{-1} \quad (6a)$$

$$G(\mathbf{k}, z, z') = (2p)^{-1}\{\exp(-p|z-z'|) + [(p-c_0)(p+c_0)^{-1}] \exp[-c_0(z+z')]\}$$
$$p = (k^2 + t_0)^{1/2}. \quad (6b)$$

The shifted critical temperature $T_B = T_B(t_0, c_0, u_0)$ given by $T_B = \mathring{t}_0 + \delta\mathring{t}_0$ can be obtained with the aid of equations (3$a$), (5) and (6) after some algebra. $T_B$ is renormalised by the usual $d$-dimensional bulk counter-terms, so the renormalised shifted temperature $T$ is given by

$$T(t, c, u) = T_B(Z_t t, Z_c c, [(2\pi)^d / S_d] Z_u u), \quad (7)$$

where the factor $(2\pi)^d/S_d$, with $S_d$ the surface of a unit sphere in $d$ space, is introduced for convenience and where the renormalisation constants $Z_t$, $Z_c$ and $Z_u$ are obtained from the $d$ space renormalisations as (Goldschmidt 1983, Nemirovsky and Freed 1985a)

$$Z_t = 1 + [\tfrac{1}{6}(N+2)]u + O(u^2) \qquad Z_c = 1 + [\tfrac{1}{6}(N+2)]u + O(u^2) \quad (7a)$$

and

$$Z_u = 1 + O(u).$$

Then $T$ is found to be

$$T(t, c, u) = t - c^2 + c^2\{u[\tfrac{1}{6}(N+2)](-\tfrac{1}{2}\ln c^2 + 3) + O(u^{3/2})\} \quad (8)$$

and the $c$ dependent effective free energy functional is given to lowest order by

$$F_{\text{eff}}\{\phi_0\} = \tfrac{1}{2} \int \mathrm{d}k\, \phi_0(\mathbf{k})(k^2 + T)\phi_0(-\mathbf{k})$$
$$+ \frac{uc}{4!} \int \mathrm{d}k_1\, \mathrm{d}k_2\, \mathrm{d}k_3\, \mathrm{d}k_4\, (2\pi)^{d-1} \delta^{d-1}(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4)$$
$$\times \phi_0(\mathbf{k}_1)\phi_0(\mathbf{k}_2)\phi_0(\mathbf{k}_3)\phi_0(\mathbf{k}_4) + \ldots. \quad (9)$$

This effective free energy functional (9) has the same form as that of an $O(N)\phi^4$ field theory in $(d-1)$ dimensions, but equation (8) shows that it has a non-trivial $c$ dependence. Equation (9) can be studied by various methods (numerical ones, real space renormalisation group, $\varepsilon' = 4-(d-1)$ expansions, etc). For definitiveness we utilised $\varepsilon'$ expansions (though corrections from $\phi_0^6$ and higher terms may be relevant for $d=3$ and $d'=2$). At the fixed point $u^* = 6\varepsilon'/(N+8)$ the shifted temperature $T$ of (8) becomes

$$T(t, c, u^*) = t - c^2 + \varepsilon' c^2\{[(N+2)/(N+8)](-\tfrac{1}{2}\ln c^2 + 3) + O((\varepsilon')^{1/2})\}$$
$$= t - c^a + \varepsilon' c^2\{3[(N+2)/(N+8)] + O((\varepsilon')^{1/2})\}$$
$$a = 2 + \tfrac{1}{2}[(N+2)/(N+8)]\varepsilon' + O(\varepsilon'^{3/2})$$

displaying the non-trivial $c$ dependence emerging along with the expected $(d-1)$-dimensional physics.

This comment is the first description of how to go beyond mean-field theory with systematic $\varepsilon$-expansion methods for the surface transition. The dimensional reduction occurring for the surface transition is thus demonstrated to parallel that driven by finite dimensions for the system (finite size scaling). A central difference for the surface transition is the fact that the dominant mode is not homogeneous, while our previous treatment of dimensional reduction in finite size scaling (Nemirovsky and Freed 1985b) using periodic boundary conditions involves a homogeneous dominant mode. Both problems result in $(d-1)$-dimensional physics, but with an essential (e.g. power law) dependence on the confining lergth scale.


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## References


Binder K 1983 *Critical Behavior at Surfaces* vol 8, ed C Domb and J Lebowitz (New York: Academic) p 1
Bray A J and Moore M A 1977 *J. Phys. A: Math. Gen.* **10** 1927
Diehl H W and Dietrich S 1980 *Phys. Lett.* **80A** 408
—— 1981a *Z. Phys.* B **42** 65
—— 1981b *Phys. Rev.* B **24** 2878
—— 1983a *Phys. Rev.* B **27** 2937
—— 1983b *Z. Phys.* B **50** 117
Diehl H W, Gompper G and Speth W 1985 *Phys. Rev.* B to be published
Ginsparg P 1980 *Nucl. Phys.* B **170** [FS1] 388
Goldschmidt Y 1983 *Phys. Rev.* B **28** 4052
Goldschmidt Y and Jasnow D 1984 *Phys. Rev.* B **29** 3990
Gompper G 1984 *Z. Phys.* B **56** 217
Lubensky T C and Rubin M H 1973 *Phys. Rev. Lett.* **31** 1469
—— 1975 *Phys. Rev.* B **11** 4533
Nemirovsky A M and Freed K F 1985a *Phys. Rev.* B **31** 3161
—— 1985b *Phys. Rev. Lett.* submitted
—— 1985c *J. Phys. A: Math. Gen.* **18** to be published
Reeve J and Guttmann A J 1981 *J. Phys. A: Math. Gen.* **14** 3351