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Semi-infinite ϕ^4 systems: ε expansions for susceptibility exponents

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Abstract. The surface and local susceptibility exponents γ_1 and γ_{11} for semi-infinite ϕ^4, $O(n)$ systems are calculated to order $\varepsilon = 4-d$ at the ordinary bulk transition temperature. The results agree with the predictions of correlation function scaling.

1. Introduction

The study of bulk magnetic phase transitions in the presence of a surface has necessitated the definition of several extra exponents (Binder and Hohenberg 1972). We wish here to test certain relations between these surface exponents and the usual bulk exponents predicted by scaling theory.

If $G(\boldsymbol{X}, \boldsymbol{X}')$ is the correlation function for spins at sites $\boldsymbol{X}$ and $\boldsymbol{X}'$ of a lattice, then the exponents $\eta_\perp$ and $\eta_\parallel$ are defined by the relations

$$G(\boldsymbol{X}, \boldsymbol{X}') \sim \begin{cases} \dfrac{1}{|\boldsymbol{X}-\boldsymbol{X}'|}\, d-2+\eta_\parallel, & z, z' \text{ fixed}, |\boldsymbol{\rho}-\boldsymbol{\rho}'| \to \infty, \\ \dfrac{A(\theta)}{|\boldsymbol{X}-\boldsymbol{X}'|}\, d-2+\eta_\perp, & z' \text{ fixed}, |\boldsymbol{X}-\boldsymbol{X}'| \to \infty, \end{cases} \tag{1.1}$$

where

$$A(\theta) = \left[\cos^{-1}\left(\frac{z-z'}{|\boldsymbol{X}-\boldsymbol{X}'|}\right)\right]^{1-\tilde{\eta}}, \qquad \boldsymbol{X} = (\boldsymbol{\rho}, z).$$

All components of the $(d-1)$-dimensional vector $\boldsymbol{\rho}$ range from $-\infty$ to $+\infty$ and $0 \leqslant z < \infty$.

The general magnetic response function for the problem is $\chi(z, z')$, and is the change in the magnetisation at z due to a field variation at z':

$$\chi(z, z') = \sum_{\boldsymbol{\rho}'} G(\boldsymbol{X}, \boldsymbol{X}') = \sum_{\boldsymbol{\rho}-\boldsymbol{\rho}'} G(\boldsymbol{\rho}-\boldsymbol{\rho}', z, z') \tag{1.2}$$

by translational invariance in all directions other than the z direction. The critical exponents are for $t = T - T_c \to 0_+$ defined by

$$\chi(0, 0) = \chi_{11} \sim t^{-\gamma_{11}}, \tag{1.3a}$$

$$\chi(0) = \chi_1 = \sum_{z' \geqslant 0} \chi(0, z') \sim t^{-\gamma_1}, \tag{1.3b}$$

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$$\chi = \lim_{z\to\infty} \sum_{z'\geq 0} \chi(z, z') \sim t^{-\gamma}. \tag{1.3c}$$

The pioneering work on semi-infinite ϕ^4 systems within the renormalisation group framework was done by Lubensky and Rubin (1975a). To order $\varepsilon = 4-d$ they found

$$\eta_{\|} = 2-2\tilde{\eta} = 2-[(n+2)/(n+8)]\,\varepsilon \tag{1.4a}$$

and

$$\eta_{\perp} = 1-\tilde{\eta} = 1-\tfrac{1}{2}[(n+2)/(n+8)]\,\varepsilon \tag{1.4b}$$

where n is the number of components of the order parameter. As there appears to be only one correlation length in the problem, there is only one correlation length exponent, ν, which retains its bulk value, as does γ.

After defining appropriate surface and bulk free energies, Barber (1973) derived the relation

$$2\gamma_1 - \gamma_{11} = \gamma + \nu \tag{1.5}$$

while Binder and Hohenberg (1972), using correlation function scaling, found

$$\gamma_1 = \nu(2-\eta_{\perp}) \tag{1.6a}$$

and

$$\gamma_{11} = \nu(1-\eta_{\|}). \tag{1.6b}$$

Up to now there has been no direct test of the relations (1.6), and quoted results (Lubensky and Rubin 1975a, Bray and Moore 1977) have been obtained by inserting the expressions for $\eta_{\|}$ and $\eta_{\perp}$ from (1.4) into (1.6). It is our aim to test the relations (1.6) directly to first order in ε by a calculation from first principles of γ_1 and γ_{11}.

In addition to the above scaling results, Bray and Moore (1977) have argued, using renormalisation group analysis, that

$$\gamma_{11} = \nu - 1 \tag{1.7}$$

at the ordinary bulk transition temperature.

2. Calculation of the exponents

In the momentum representation the Hamiltonian density is (Lubensky and Rubin 1975a)

$$H = \tfrac{1}{2}\int \mathrm{d}\boldsymbol{q}(m^2+q^2)\phi_i(\boldsymbol{q})\phi_i(\nu\boldsymbol{q}) + \frac{g_0}{4!}\frac{1}{8}\sum_{\{\varepsilon_i=\pm1\}} \varepsilon_1\varepsilon_2\varepsilon_3\varepsilon_4$$
$$\times \int \Big(\prod_i \mathrm{d}\boldsymbol{q}_i\Big)\phi_i(\boldsymbol{q}_1)\phi_i(\boldsymbol{q}_2)\phi_j(\boldsymbol{q}_3)\phi_j(\boldsymbol{q}_4) \times \delta\Big(\sum_i p_i\Big)\,\delta\Big(\sum_i \varepsilon_i k_i\Big) \tag{2.1}$$

where $\boldsymbol{q} = (\boldsymbol{p}, k)$, $\boldsymbol{p}$ being a $(d-1)$-dimensional vector, $\nu\boldsymbol{q} = (-\boldsymbol{p}, k)$ and the Fourier expansion functions are

$$\Psi_q(\boldsymbol{X}) = \sqrt{2}\,\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{\rho}} \sin(kz+\theta). \tag{2.2}$$

The repeated indices on the ϕ fields are summed from 1 to n, and from now on only the case where the spin interaction strength in the surface is the same as in the bulk will be considered, namely $\theta = k$ (see Lubensky and Rubin (1975a)). The mass squared is to be identified with t.

We wish to develop ε expansions for the response functions of the systems defined by H, using renormalisation of vertex functions by minimal subtraction of poles in ε (Amit 1978).

The propagator for the system is

$$G_p^{(0)}(k_1, k_2) = [\delta(\boldsymbol{q}_1 - \nu \boldsymbol{q}_2) - \delta(\boldsymbol{q}_1 + \boldsymbol{q}_2)]/2(m^2 + q_1^2) \tag{2.3}$$

where $\boldsymbol{q}_1 = (\boldsymbol{p}, k_1)$ and $\boldsymbol{q}_2 = (\boldsymbol{p}, k_2)$.

The mean field response function $\chi^{\mathrm{MF}}(z, z')$ is the Fourier inverse of $G_0^{(0)}(k_1, k_2)$, that is

$$\chi^{\mathrm{MF}}(z_1, z_2) = -(1/2m)(\mathrm{e}^{-m(z_1+z_2+2)} - \mathrm{e}^{-m|z_1-z_2|}) \tag{2.4}$$

and consequently in the free field limit

$$\chi_{11}^{\mathrm{MF}} = 1/(1+m), \tag{2.5a}$$

$$\chi_1^{\mathrm{MF}} = 1/m(1+m) \tag{2.5b}$$

$$\chi^{\mathrm{MF}} = 1/m^2, \tag{2.5c}$$

giving $\gamma_{11}^{\mathrm{MF}} = -\frac{1}{2}$, $\gamma_1^{\mathrm{MF}} = \frac{1}{2}$ and $\gamma = 1$ for the ordinary bulk transition at $m^2 = 0$. (For a full account of the mean field theory, see Lubensky and Rubin (1975b).)

The two-point vertex function $\Gamma_p^{(2)}(k_1, k_2)$ is the inverse of the Green function, that is,

$$\int \mathrm{d}k \Gamma_p^{(2)}(k_1, k) G_p^{(2)}(k, k_2) = [\delta(k_1 - k_2) - \delta(k_1 + k_2)]/2 \tag{2.6a}$$

which is the momentum space version of

$$\sum_{z' \geq 0} \Gamma_p^{(2)}(z_1, z') G_p^{(2)}(z', z_2) = \delta_{z_1 z_2}. \tag{2.6b}$$

To calculate $\chi(z_1, z_2)$ to first order in ε requires that we find $\Gamma^{(2)}$ to order g_0 for finite mass and zero external momentum.

Using the normal diagrammatic expansion up to one loop and gleaning the necessary multi-dimensional integrals from Amit (1978) gives

$$\begin{aligned}\Gamma_p^{(2)}(k_1, k_2) = {} & (k_1^2 + m^2)[\delta(k_1 - k_2) - \delta(k_1 + k_2)]/2 \\ & - \frac{n+2}{3} \frac{g_0}{2} \frac{1}{4} \Gamma\left(\frac{d}{2}\right) \Gamma\left(1 - \frac{d}{2}\right) (m^2)^{d/2-1} [\delta(k_1 - k_2) - \delta(k_1 + k_2)] \\ & - \frac{n+2}{3} g_0 \left(\int \frac{\mathrm{d}^{d-1} p}{p^2 + m^2 + \mu_+^2} - \int \frac{\mathrm{d}^{d-1} p}{p^2 + m^2 + \mu_-^2} \right)\end{aligned} \tag{2.7}$$

where $\mu_\pm = (k_1 \pm k_2)/2$.

Now $(m^2)^{d/2-1}$ is expanded as $m^2(1 - \frac{1}{2}\varepsilon \ln m^2)$ and $\Gamma(d/2)\Gamma(1 - d/2) = -(2/\varepsilon)[1 + \mathrm{O}(\varepsilon^2)]$ to give the finite (pole in ε subtracted) part of $\Gamma^{(2)}$ as

$$\Gamma_{\mathrm{R}}^{(2)} = \{k_1^2 + m^2 - m^2[(n+2)/12] g \ln m^2\}[\delta(k_1 - k_2) - \delta(k_1 + k_2)]/2 - T(k_1, k_2, m) \tag{2.8}$$

where T is the last term in (2.7) and g is the renormalised coupling constant. The renormalised Green function is

$$G_{\mathrm{R}}^{(2)}(k_1, k_2) = \frac{1}{k_1^2+m^2}\frac{1}{k_2^2+m^2}\Gamma_{\mathrm{R}}^{(2)} \tag{2.9}$$

and we can fix g at the fixed-point value $g^* = 6/(n+8)\varepsilon$ by noting that the bulk terms in the expansion (2.7) above agree with those found by Amit (1978) for the bulk ϕ^4 theory.

So at the fixed point we have

$$G_{\mathrm{R}}^{(2)}(k_1, k_2) = \left[\frac{1}{k_1^2+m^2} - \frac{m^2}{2}\left(\frac{n+2}{n+8}\right)\varepsilon \ln m^2 \frac{1}{k_1^2+m^2}\frac{1}{k_2^2+m^2}\right]$$
$$\times[\delta(k_1-k_2)-\delta(k_1+k_2)]/2 - T^*(k_1, k_2, m)\frac{1}{k_1^2+m^2}\frac{1}{k_2^2+m^2}. \tag{2.10}$$

This expression can now be Fourier inverted to give

$$\chi(z_1, z_2) = \frac{2}{(2\pi)^2}\int_{-\infty}^{\infty} \mathrm{d}k_1\, \mathrm{d}k_2 G_{\mathrm{R}}^{(2)}(k_1, k_2) \sin k_1 z_1' \sin k_2 z_2' \tag{2.11}$$

where $z_1' = z_1 + 1$ etc.

The first term of (2.10) in (2.11) gives just $\chi^{\mathrm{MF}}(z_1, z_2)$ (equation (2.4)), and the second term is readily evaluated by the method of contours as

$$\chi_2(z_1, z_2) = -\frac{m^2}{2}\left(\frac{n+2}{n+8}\right)\varepsilon \ln m^2 \frac{2}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k \frac{\sin kz_1' \sin kz_2'}{(k^2+m^2)^2} \tag{2.12}$$
$$= \frac{1}{8}\left(\frac{n+2}{n+8}\right)\varepsilon \ln m^2 \{\mathrm{e}^{-m(z_1+z_2+2)}[(z_1+z_2+2)+m^{-1}]$$
$$-\mathrm{e}^{-m|z_1-z_2|}(|z_1-z_2|+m^{-1})\}. \tag{2.13}$$

The last term is the inverse Fourier transform $\chi_3(z_1, z_2)$ of

$$\left(\frac{n+2}{n+8}\right)^{\varepsilon}\left(\int \frac{\mathrm{d}^{d-1}p}{p^2+\mu_+^2+m^2} - \int \frac{\mathrm{d}^{d-1}p}{p^2+\mu_-^2+m^2}\right)\frac{1}{k_1^2+m^2}\frac{1}{k_2^2+m^2}$$

that is,

$$\chi_3(z_1, z_2) = \left(\frac{n+2}{n+8}\right)\varepsilon \frac{2}{(2\pi)^2}\int \mathrm{d}k_1\, \mathrm{d}k_2 \frac{\sin k_1 z_1' \sin k_2 z_2'}{(k_1^2+m^2)(k_2^2+m^2)}$$
$$\times \frac{\pi}{2}\left(\frac{(\mu_+^2+m^2)^{1/2}-(\mu_-^2+m^2)^{1/2}}{(m^2+k_1^2)(m^2+k_2^2)}\right), \tag{2.14}$$

and since we are only interested in the small-m behaviour of this integral we can put $m^2 = 0$ in the denominator of the integrand. The result (evaluated in the Appendix) is

$$\chi_3(z_1, z_2) = \left(\frac{n+2}{n+8}\right)\frac{\varepsilon}{4m}\Big\{\mathrm{e}^{-m(z_1'+z_2')}[E_1(2mz_1') + \mathrm{Ei}(2mz_1') - E_1(mz_1')]$$
$$+\mathrm{e}^{-m(z_2-z_1)}E_1(mz_1') + \mathrm{e}^{m(z_2-z_1)}E_1(2mz_2') - \mathrm{e}^{m(z_1'+z_2')}E_1(2mz_2')\Big\},$$
$$z_2 > z_1, \tag{2.15}$$

where Ei and E_1 are the exponential integral functions defined in Abramowitz and Stegun (1964).

The total response function is to first order

$$\chi(z_1, z_2) = \chi^{\mathrm{MF}}(z_1, z_2) + \chi_2(z_1, z_2) + \chi_3(z_1, z_2). \tag{2.16}$$

It is now straightforward to put $z_1 = z_2$ in (2.16) and expand the exponential integral functions for small argument to obtain

$$\chi_{11} = 1 - m - \left(\frac{n+2}{n+8}\right)\frac{\varepsilon}{4} m \ln m^2 + \left(\frac{n+2}{n+8}\right)\frac{\varepsilon}{2} m \ln m^2, \tag{2.17}$$

which on exponentiation gives

$$\gamma_{11} = -\frac{1}{2} + \left(\frac{n+2}{n+8}\right)\frac{\varepsilon}{4}. \tag{2.18}$$

Putting $z_1 = 1$ and summing over z_2 in the limit of m^2 small gives

$$\chi_1 = \frac{1}{m} - \frac{1}{4}\left(\frac{n+2}{n+8}\right)\frac{\varepsilon}{4}\frac{1}{m}\ln m^2 - \frac{1}{4}\left(\frac{n+2}{n+8}\right)\frac{\varepsilon}{4}\frac{1}{m}\ln m^2,$$

implying that

$$\gamma_1 = \frac{1}{2} + \left(\frac{n+2}{n+8}\right)\frac{\varepsilon}{2}. \tag{2.19}$$

3. Conclusions

The results for γ_1 and γ_{11} of the previous section together with the values for $\eta_\parallel$ and $\eta_\perp$ obtained by Lubensky and Rubin (1975a) satisfy the scaling relations (1.5) and (1.6) to order ε, and consequently they also agree with the conjectured exact result (1.6). Although series expansions for the Ising model ($n = 1$) would appear to agree with (1.6) (see Whittington *et al* (1979) for the most recent study), results for the $n = 0$, $d = 2$ case (the self-avoiding walk attached to a surface) do not (Barber *et al* 1978, Enting and Guttmann 1980). It would be of some interest then to test the proposition that $\gamma_{11} = \nu - 1$ to second order in ε.

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Appendix

The integral

$$\chi_3(z_1, z_2) = \left(\frac{n+2}{n+8}\right)\varepsilon\frac{1}{4\pi}\int \mathrm{d}k_1\,\mathrm{d}k_2\,\frac{\sin k_1 z_1' \sin k_2 z_2'}{(k_1^2+m^2)(k_2^2+m^2)}(|\mu_+| - |\mu_-|) \tag{A1}$$

can be simplified by writing

$$|\mu_+| = \frac{2}{\pi} \lim_{L\to\infty} \mu_\pm \tan^{-1}\left(\frac{L}{\mu_\pm}\right) = \frac{2}{\pi}\mu_\pm^2 \int_\infty^\infty \frac{dx}{x^2+\mu_\pm^2} \tag{A2}$$

and changing the order of integration so that

$$\chi_3(z_1, z_2) = \frac{1}{4\pi}\left(\frac{n+2}{n+8}\right)\varepsilon \int_0^\infty dx \int_{-\infty}^\infty dk_1 \frac{\sin k_1 z_1'}{k_1^2+m^2} I_1(k_1, x, z_2) \tag{A3}$$

where

$$I_1(k_1, x, z_2) = \int_{-\infty}^\infty dk_2 \frac{\sin k_2 z_2}{k_2^2+m^2} \frac{(k_1+k_2)^2}{x^2+(k_1^2+k_2^2)}. \tag{A4}$$

This and the subsequent integral over k_2 can be done by the method of contours, leaving only the real integral over the x variable, which is readily evaluated directly. The result is the expression (2.15) for χ_3.

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