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ϵ Expansion in Semi-infinite Ising Systems

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The Wilson-Fisher ϵ expansion is used to calculate critical exponents in a semi-infinite Ising model to first order in ϵ. It is found that potentials renormalize just as in the bulk, and all surface information is contained in the wave-function renormalization. ν is $\frac{1}{2}+\frac{1}{12}\epsilon$ and η is 0, just as in infinite systems. $\eta_\perp$ and $\eta_\parallel$ are, respectively, $1-\frac{1}{6}\epsilon$ and $2-\frac{1}{3}\epsilon$ and the surface gap exponent Δ_1 is $\frac{1}{2}-\frac{1}{12}\epsilon$ if scaling is assumed.

The Wilson renormalization procedure has been highly successful in calculating critical exponents in bulk or infinite systems.[1-3] In this paper we will outline a calculation of critical exponents in a semi-infinite Ising system using the ϵ expansion.[2,3] Particular emphasis will be placed on the calculation of the exponents $\eta_\parallel$ and $\eta_\perp$ introduced by Binder and Hohenberg[4] and the gap exponent Δ_1 introduced by Fisher.[5] The major purpose of this paper to to present results. Calculational details will appear in a subsequent publication.

We start with the standard S^4 Hamiltonian

$$\mathcal{H}=\tfrac{1}{2}b^2\sum_{\vec{x}}S^2(\vec{x})-\tfrac{1}{2}K\sum_{\vec{x}\vec{\delta}}S(\vec{x})S(\vec{x}+\vec{\delta})+u\sum S^4(\vec{x}), \tag{1}$$

where $\vec{x}=(x_\perp,x_1,\ldots,x_{d-1})\equiv(x_\perp,\vec{x}_\parallel)$ labels the sites on a semi-infinite cubic lattice and $\vec{\delta}$ is the nearest-neighbor position. $\vec{x}_\parallel$ is the $(d-1)$-dimensional vector parallel to the surface, and $x_\perp$ the component of $\vec{x}$ perpendicular to the surface. $x_\perp$ takes on values $1,2,3,\ldots$. All other components take on all positive and negative values. It is convenient to extend the sums in Eq. (1) to include the plane $x_\perp=0$ and to require that $S(0,\vec{x}_\parallel)$ be zero. Then $S(\vec{x})$ can be expressed as a Fourier sine integral

$$S(\vec{x})=\int_{-\pi}^{\pi}\frac{d^dp}{(2\pi)^d}\sigma(\vec{p})\exp(i\vec{p}_\parallel\cdot\vec{x}_\parallel)\sqrt{2}\,\sin p_\perp x_\perp, \tag{2}$$

where $\vec{p}=(p_\perp,\vec{p}_\parallel)$. [The $\sqrt{2}$ appearing in Eq. (2) puts $p_\perp$ and $\vec{p}_\parallel$ on an equal footing in the Hamiltonian below.] Following Wilson, we introduce a modified Hamiltonian in which $\vec{p}$ is restricted to a *unit cyl-*

inder D of radius 1 in the parallel direction and height 2 in the perpendicular direction:

$$\mathcal{H}=\frac{1}{2}\int\frac{d^dp}{(2\pi)^d}(r+p^2)\sigma(\vec{p})\sigma(-\nu\vec{p})+u\int_D\frac{d^dp_1\,d^dp_2\,d^dp_3\,d^dp_4}{(2\pi)^{3d}}\sigma(\vec{p}_1)\sigma(\vec{p}_2)\sigma(\vec{p}_3)\sigma(\vec{p}_4)\,\delta^d(\vec{p}_1,\vec{p}_2,\vec{p}_3,\vec{p}_4), \tag{3}$$

where $\nu\vec{p}=(-p_\perp,\vec{p}_\parallel)$,

$$\delta^d(\vec{p}_1,\vec{p}_2,\vec{p}_3,\vec{p}_4)=\delta^{d-1}(\vec{p}_{1\parallel}+\vec{p}_{2\parallel}+\vec{p}_{3\parallel}+\vec{p}_{4\parallel})\Delta(p_{1\perp},p_{2\perp},p_{3\perp},p_{4\perp}), \tag{4}$$

and

$$\Delta(p_{1\perp},p_{2\perp},p_{3\perp},p_{4\perp})=\frac{4}{2\pi}\sum_{x_\perp>0}\sin p_{1\perp}x_\perp\sin p_{2\perp}x_\perp\sin p_{3\perp}x_\perp\sin p_{4\perp}x_\perp. \tag{5}$$

The renormalization procedure on the Hamiltonian (3) is essentially the same as for infinite systems. Let D_1 be the cylinder of radius b^{-1} in the $d-1$ parallel directions and of height $2b^{-1}$ in the perpendicular direction, and let $D_2=D-D_1$. Taking the trace over all $\sigma(\vec{p})$ with $\vec{p}\in D_2$, we obtain a new Hamiltonian, $\hat{\mathcal{H}}$, which is a function only of $\hat{\sigma}(\vec{p})\equiv\sigma(\vec{p})$ for $\vec{p}\in D_1$. $\hat{\mathcal{H}}$ is given to second order in u by

$$\begin{aligned}\hat{\mathcal{H}}[\hat{\sigma}(\vec{p})]=&\frac{1}{2}\int\frac{d^dp}{(2\pi)^d}[p^2+r+12uC_1(r)]\hat{\sigma}(\vec{p})\hat{\sigma}(-\nu\vec{p})-\frac{1}{2}\int\frac{d^dp_1}{(2\pi)^d}\int\frac{d^dp_2}{(2\pi)^d}v(\vec{p}_1,\vec{p}_2)\hat{\sigma}(\vec{p}_1)\hat{\sigma}(\vec{p}_2)\\&+[u-36u^2C_2(r)]\int\frac{d^dp_1\,d^dp_2\,d^dp_3\,d^dp_4}{(2\pi)^{3d}}\hat{\sigma}(\vec{p}_1)\hat{\sigma}(\vec{p}_2)\hat{\sigma}(\vec{p}_3)\hat{\sigma}(\vec{p}_4)\,\delta^d(\vec{p}_1,\vec{p}_2,\vec{p}_3,\vec{p}_4)\\&+\int\frac{d^dp_1\,d^dp_2\,d^dp_3\,d^dp_4}{(2\pi)^{4d}}v_4(\vec{p}_1,\vec{p}_2,\vec{p}_3,\vec{p}_4)\hat{\sigma}(\vec{p}_1)\hat{\sigma}(\vec{p}_2)\hat{\sigma}(\vec{p}_3)\hat{\sigma}(\vec{p}_4),\end{aligned} \tag{6}$$

where all explicit integrations are over D_1,

$$v(\vec{p},\vec{p}')=6u\,\delta^{d-1}(\vec{p}_\parallel+\vec{p}_\parallel')\int_{D_2}d^dp_3\frac{1}{p_3^2+r}[\delta(p_\perp+p_\perp'+2p_{3\perp})-\delta(p_\perp-p_\perp'+2p_{3\perp})], \tag{7}$$

and

$$C_1(r)=\int_{D_2}\frac{d^dp}{(2\pi)^d}\frac{1}{p^2+r},\quad C_2(r)=\int_{D_2}\frac{d^dp}{(2\pi)^d}\frac{1}{(p^2+r)^2}; \tag{8}$$

$v(\vec{p}_1,\vec{p}_2)$ is a nonlocal two-spin potential, and v_4 contains all four-spin interactions except for the $\vec{p}=0$ local part.

We now perform a series of three transformations on $\hat{\mathcal{H}}$ and $\hat{\sigma}$ to produce a new Hamiltonian $\mathcal{H}'$ and a new spin variable σ' such that $\mathcal{H}'(\sigma')$ looks as much as possible like the original Hamiltonian. The first transformation eliminates the nonlocal two-spin interaction from $\hat{\mathcal{H}}$. Let $\hat{\sigma}(\vec{p})=\hat{\sigma}'(\vec{p})+\delta\hat{\sigma}(\vec{p})$. If $\delta\hat{\sigma}(\vec{p})$ satisfies

$$\delta\hat{\sigma}(\vec{p})=\frac{1}{2p^2}\int_{D_1}\frac{d^dp'}{(2\pi)^d}v(\vec{p},\vec{p}')\hat{\sigma}(-\nu\vec{p}'), \tag{9}$$

then $\hat{\mathcal{H}}[\hat{\sigma}'(\vec{p})]$ contains no nonlocal two-spin interaction to first order in u. The second transformation takes $\vec{p}$ to $b\vec{p}$ so that integrations are over D rather than D_1. Finally, the third transformation renormalizes $\hat{\sigma}'$ so that the coefficient of the p^2 term is one half:

$$\hat{\sigma}'(b^{-1}\vec{p})=\zeta\sigma'(\vec{p}). \tag{10}$$

To order ϵ, ζ is $b^{1+d/2}$ which is the same as for an infinite system. The final transformed Hamiltonian has the same form as Eq. (3) with new potentials

$$r'=b^2[r+12uC_1(r)], \tag{11a}$$

$$u'=b^\epsilon[u-36u^2C_2(r)], \tag{11b}$$

where $\epsilon=4-d$. These are the same as the bulk renormalization equations.[2] Equation (11) yields a fixed-point value of u to first order in ϵ of $u^*=(2\pi^2/9)\epsilon$ and a coherence-length exponent ν equal to $\frac{1}{2}+\frac{1}{12}\epsilon$ which is the same as in infinite systems. Hence, there is a single divergent correlation length in a semi-infinite system which diverges in the same way as in an infinite system. This is consistent with previous assertions.[4,5,7-11] The nonlocal four-spin potential v_4 can be shown to be irrelevant[6] to first order in ϵ.

We have just seen that potentials in a semi-infinite system renormalize in exactly the same way as potentials in a bulk system, at least to first order in ϵ. All information about the surface is lumped into the wave-function renormalization. In bulk systems, wave-function renormalization is characterized completely by a single number ζ. In the semi-infinite system, ζ becomes an operator $\zeta(\vec{p}\vec{p}')$ resulting from transformations one and three, given by

$$\zeta(\vec{p},\vec{p}') = \zeta[(2\pi)^d \delta(\vec{p}-\vec{p}') + (1/2p^2)v(-\nu\vec{p},\vec{p}')]. \tag{12}$$

At the fixed point, the correlation function $\Gamma^*(\vec{p}\vec{p}') = \langle\sigma(\vec{p})\sigma(\vec{p}')\rangle$ satisfies

$$\Gamma^*(\vec{p},\vec{p}') = \int \frac{d^dp_1}{(2\pi)^d}\int\frac{d^dp_2}{(2\pi)^d}\,\zeta^*(\vec{p},\vec{p}_1)\zeta^*(\vec{p}',\vec{p}_2)\Gamma^*(b\vec{p}_1,b\vec{p}_2), \tag{13}$$

where the star indicates the fixed-point values of $\zeta(\vec{p}\vec{p}')$ and $\Gamma(\vec{p}\vec{p}')$. The solution to Eq. (13) for $d=4-\epsilon$ to first order in ϵ is

$$\Gamma^*(\vec{p}\vec{p}') = \Gamma_0^*(\vec{p}\vec{p}') + \frac{1}{pp'}(2\pi)^{d-1}\delta^{d-1}(\vec{p}_\parallel,\vec{p}_\parallel{}')\gamma^*(\vec{p},\vec{p}'), \tag{14}$$

where $p=(p_\perp{}^2+p_\parallel{}^2)^{1/2}$, $\Gamma_0^*(\vec{p}\vec{p}')$ is the Gaussian fixed-point function

$$\Gamma_0^*(\vec{p}\vec{p}') = \frac{(2\pi)^d}{2}\frac{1}{p^2}[\delta(\vec{p}+\vec{p}') - \delta(\vec{p}+\nu\vec{p}')], \tag{15}$$

and

$$\gamma^*(\vec{p}\vec{p}') = \frac{3}{4\pi^2}u^*\frac{1}{pp'}\left\{(p_\perp+p_\perp{}')\tan^{-1}\frac{2}{p_\perp+p_\perp{}'} - (p_\perp-p_\perp{}')\tan^{-1}\frac{2}{p_\perp-p_\perp{}'}\right\}. \tag{16}$$

It should be stressed that the factors of 2 appearing in $\tan^{-1}$ in Eq. (16) result from reflections off of the surface and are unrelated to any cutoff. Fourier transformation of Eq. (14) yields the spatial correlation function

$$\Gamma^*(\vec{x},\vec{x}') = \Gamma_0^*(\vec{x},\vec{x}') + \Gamma_1^*(\vec{x},\vec{x}'), \tag{17}$$

where Γ_0^* is the Gaussian half-space propagator,

$$\Gamma_0^*(\vec{x},\vec{x}') = \frac{\Gamma(\frac{1}{2}d-1)}{4\pi^{d/2}}\left(\frac{1}{|\vec{x}-\vec{x}'|^{d-2}} - \frac{1}{|\vec{x}-\nu\vec{x}'|^{d-2}}\right), \tag{18}$$

and

$$\Gamma_1(\vec{x},\vec{x}') = \frac{3u^*}{8\pi^3\rho}\{J_+(x_\perp-x_\perp{}'+i\rho,x_\perp{}') - J_-(x_\perp+x_\perp{}'+i\rho,x_\perp{}') + J_+(x_\perp{}'-x_\perp+i\rho,x_\perp) - J_-(x_\perp+x_\perp{}'+i\rho,x_\perp) - J_+(x_\perp+x_\perp{}'+i\rho,0) + J_-(x_\perp x_\perp{}'+i\rho,0)\}, \tag{19}$$

where $\rho = |\vec{x}_\parallel - \vec{x}_\parallel{}'|$ and

$$J_\pm(\eta,x_\perp) = \mathrm{Re}\int_0^2 dy\int_0^\infty (dp_\perp/2\pi)[\exp(ip_\perp\eta)\exp(-yx_\perp)/(y\pm 2ip_\perp)]. \tag{20}$$

As both $x_\perp$ and $x_\perp{}'$ go into the bulk, i.e., $x_\perp, x_\perp{}' \to\infty$ with $x_\perp - x_\perp{}'$ finite, $\Gamma_0^*(xx')$ becomes the bulk Gaussian (or mean field) propagator[4,9] $(1/4\pi^2)|\vec{x}-\vec{x}'|^{-d+2}$, and Γ_1^* dies off as

$$\frac{1}{(x_\perp+x_\perp{}')^2}\ln\frac{x_\perp+x_\perp{}'}{|\vec{x}-\vec{x}'|}.$$

Hence, the fixed-point correlation function in the bulk becomes the same as for infinite systems with $\eta=0$ to first order in ϵ. Note, however, that the effect of the surface dies off very slowly at the fixed point. This corroborates results obtained by high-temperature expansions.[4]

Two other limits are of interest. In the first, $\vec{x}'$ is fixed on the surface and $\vec{x}$ goes to infinity in the bulk at an angle θ to the normal to the surface. In this case, Γ^* behaves like

$$\Gamma^*(\vec{x},\vec{x}') \sim A(\theta)/|\vec{x}-\vec{x}'|^{d-2+\eta_\perp}. \tag{21}$$

By comparing $|\vec{x}-\vec{x}'|^{-3}\ln|\vec{x}-\vec{x}'|$ terms in Eqs.

(19) and (21), we obtain

$$\eta_\perp = (1 - \tfrac{1}{6}\epsilon). \qquad (22)$$

In the Gaussian limit, $A(\theta)$ is $\pi^{-2}\cos\theta$. Corrections to $A(\theta)$ to order ϵ can be obtained from $|\vec{x} - \vec{x}'|^{-3}$ terms in Eq. (21). They will be presented in a more detailed subsequent publication. In the second limit of interest, both $\vec{x}$ and $\vec{x}'$ are on the surface and

$$\Gamma^*(\vec{x}, \vec{x}') \sim B/\rho^{d-2+\eta_\parallel}. \qquad (23)$$

Again comparing $\rho^{-4}\ln\rho$ terms in Eqs. (19) and (23), we obtain

$$\eta_\parallel = (2 - \tfrac{1}{3}\epsilon). \qquad (24)$$

These are to be compared with the mean-field and spherical-model[8] values of $\eta_\parallel = 2$ and $\eta_\perp = 1$.[12-14] They are consistent with the numerical calculations of Binder and Hohenberg[4] on the three-dimensional Ising model in which $\eta_\parallel$ and $\eta_\perp$ are less than their mean-field values.

Using the scaling relation derived by Binder and Hohenberg,[4] we can calculate the exponent γ_1 governing the variation of the surface magnetization m_s with bulk magnetic field h, $\chi_1 = \partial m_s/\partial h \sim t^{-\gamma_1}$, where $t = |T - T_c|$:

$$\gamma_1 = \nu(2 - \eta_\perp) = \tfrac{1}{2} + \tfrac{1}{6}\epsilon. \qquad (25)$$

γ_1 can also be calculated from a scaling form for the surface free energy[5,9,10]

$$F^\times(t, h_s, h) = |t|^{2-\alpha^\times} Q^\times(h_s/t^{\Delta_1}, h/t^{\Delta}), \qquad (26)$$

where h_s is the surface magnetic field, $\alpha^\times = \alpha + \nu$ is the surface specific-heat exponent, and $\Delta = \beta + \gamma = \beta\delta$ and Δ_1 are, respectively, the bulk and surface gap exponents. We have

$$\chi_1 = \partial^2 F/\partial h_s \partial h \sim |t|^{-\gamma_1},$$

where

$$\gamma_1 = \Delta_1 + \nu - \beta. \qquad (27)$$

Comparing Eqs. (25) and (27), we obtain

$$\Delta_1 = \tfrac{1}{2} - \tfrac{1}{12}\epsilon. \qquad (28)$$

Extrapolation of this result to $\epsilon = 1$ gives $\Delta_1 = 0.416$. Binder and Hohenberg[4,9] estimate γ_1 for the three-dimensional Ising model to be about $\frac{7}{8}$ from high-temperature expansions. This gives $\Delta_1 \gtrsim 0.5$ in disagreement with our result evaluated at $\epsilon = 1$. Clearly, near $d = 3$, ϵ^2 terms are important. At the moment, it is difficult to estimate the magnitude of these higher order terms within the context of the ϵ expansion. If we terminate the ϵ expansion for $\eta_\perp$ at ϵ^2 and write $\eta_\perp = 1 - \frac{1}{6}\epsilon + c\epsilon^2$ and equate this to 0.64 for $\epsilon = 1$, we find $c \sim -0.2$. A coefficient of ϵ^2 of this size is perfectly reasonable within the ϵ expansion.

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