

Fluctuating Interfaces

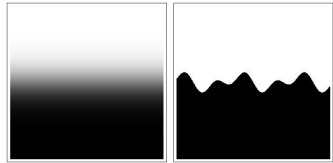
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Outline

- 1 Statistical Physics
 - microscopic theory
 - capillary wave theory
 - convolution approximation
- 2 Monte Carlo calculation
 - interface width
 - numerical results



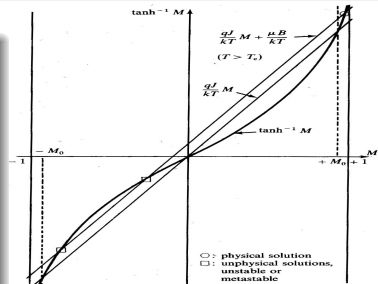
mean-field theory

MFT of the Ising-model

$$H = -J \sum_{\langle i,j \rangle} S_i S_j - \mu B \sum_i S_i$$

$$E_i = -J S_i \sum_j \langle S_j \rangle - \mu B S_i$$

$$\tanh^{-1} M = \frac{qJ}{kT} M + \frac{\mu B}{kT}$$



$$T_c = qJ/k$$

$$\frac{\mu B}{kT} = M \left(\frac{T - T_c}{T} \right) + \frac{1}{3} M^3$$

critical exponents depend on

- coefficient of M vanishes **linearly** at T_c ; ≥ 0 for $T \geq 0$
- coefficient of M^3 is **positive**

discrete Landau theory

- preserve the symmetry $H[\Phi_i] = H[-\Phi_i]$
- n.n. interaction $\sum_{i,\mu} \frac{1}{a^2} [\Phi(\mathbf{x}_i + \boldsymbol{\mu}) - \Phi(\mathbf{x}_i)]^2 = \sum_i (\partial\Phi(\mathbf{x}_i))^2$

$$H[\Phi_i] = a^D \sum_{i=1}^N \left[\frac{1}{2} (\partial\Phi_i)^2 + \frac{m^2(T)}{2} \Phi_i^2 + \frac{g}{4!} \Phi_i^4 \right]$$

- $Z = \int \prod_{i=1}^N d\Phi_i \exp \left(-H[\Phi_i] + \sum_i B_i \Phi_i \right), \quad B_i = \left. \frac{\partial H}{\partial \Phi_i} \right|_{\Phi_i = \Phi_{i0}}$
- Landau approximation: $W = \ln Z \approx -H[\Phi_{i0}] + \sum_i B_i \Phi_{i0}$

$$M_i = \frac{\partial W}{\partial B_i} = - \sum_j \left. \frac{\partial H}{\partial \Phi_j} \right|_{\Phi_{j0}} \frac{\partial \Phi_{j0}}{\partial B_i} + \Phi_{i0} + \sum_j B_j \frac{\partial \Phi_{j0}}{\partial B_i} = \Phi_{i0}$$

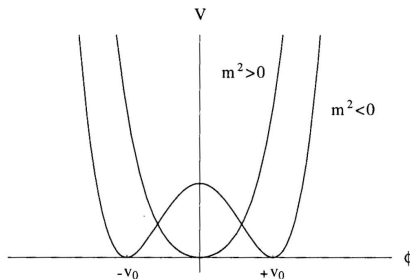
$$\Gamma(M_i) = M_i B_i - W = H(M_i), \quad B_i = \frac{\partial \Gamma}{\partial M_i}$$

continuum Landau theory

Landau free energy density

$$\mathcal{H}(\Phi(x)) = \frac{1}{2} (\partial\Phi(x))^2 + V(\Phi(x))$$

$$V(\Phi(x)) = \frac{g}{4!} \Phi^4 + \frac{m^2}{2} \Phi^2 + C$$



symmetric phase:

$$V(\Phi) = \frac{g}{4!} \Phi^4 + \frac{m^2}{2} \Phi^2$$

broken symmetry: $(-2m^2 \rightarrow m^2)$

$$V(\Phi) = \frac{g}{4!} (\Phi^2 - v_0^2)^2,$$

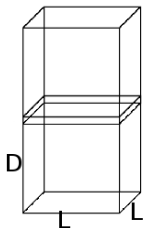
$$v_0 = \sqrt{3m^2/g}$$

boundary conditions

$$H[\Phi] = \int d^3x \mathcal{H}(\Phi(x)) = \int d^3x \left(\frac{1}{2} (\partial\Phi)^2 + V(\Phi) \right)$$

thermodynamic limit: $D \rightarrow \infty$

$$\frac{\delta H[\Phi]}{\delta \Phi_g} = -\partial^2 \Phi_g + V'(\Phi_g) = -\partial^2 \Phi_g + \frac{g}{3!} \Phi_g^3 - \frac{m^2}{2} \Phi_g = 0$$



periodic b.c. $\Phi_g(z \rightarrow \pm D/2 = \pm \infty) = v_0$

$$\Phi_g(z) = \pm v_0$$

antiperiodic b.c. $\Phi_g(z \rightarrow \pm D/2) = \pm v_0$

$$\Phi_g(z) = v_0 \tanh \left(\frac{m}{2} (z - h) \right) =: \Phi_K(z)$$

Φ^4 theory

- coarse graining

$$\Phi(x) = \frac{1}{N_B} \sum_{i \in B(x)} \langle S_i \rangle, \quad a < B < \xi$$

- free energy W

$$e^{-\beta W} = Z = \sum_{\{S_i\}} e^{-\beta \tilde{H}(\{S_i\})}$$

- energy $S[\Phi]$ of the configuration $\Phi(x)$

$$e^{-\beta H[\Phi]} = \sum_{\{S_i\}} e^{-\beta \tilde{H}(\{S_i\})} \delta \left(\frac{1}{N_B} \sum_{i \in B(x)} \langle S_i \rangle - \Phi(x) \right) = \sum_{\{\bar{S}\}} e^{-\beta \tilde{H}(\{S_i\})}$$

- free energy

$$e^{-\beta W} = \sum_{\{S^*\}} \sum_{\{\bar{S}\}} e^{-\beta \tilde{H}(\{S_i\})} = \sum_{\{S^*\}} e^{-\beta H[\Phi]} \approx \int \mathcal{D}\Phi e^{-\beta H[\Phi]}$$

generating functional

$$Z[J] = \int \mathcal{D}\Phi e^{-\beta H[\Phi]} e^{\beta \int d^3x J(x)\Phi(x)} = \int \mathcal{D}\Phi e^{-\beta H[\Phi, J]}$$
$$H[\Phi, J] = \int d^3x \left(\frac{1}{2} (\partial\Phi(x))^2 + V(\Phi(x)) - J(x)\Phi(x) \right)$$

$$\langle \Phi(x) \rangle_J := \Phi_c(x) = \frac{\int \mathcal{D}\Phi \Phi(x) e^{-\beta H[\Phi, J]}}{\int \mathcal{D}\Phi e^{-\beta H[\Phi, J]}} = \frac{1}{\beta Z} \frac{\delta}{\delta J(x)} Z[J]$$

- Legendre transformation

$$\Gamma[\Phi_c] = W[J] + \int d^3x J(x)\Phi_c(x)$$

$$\boxed{\left. \frac{\delta \Gamma[\Phi_c]}{\delta \Phi_c(x)} \right|_{J=0} = 0}$$

loop-expansion (J. Küster, 2001)

- treelevel reproduces Landau theory

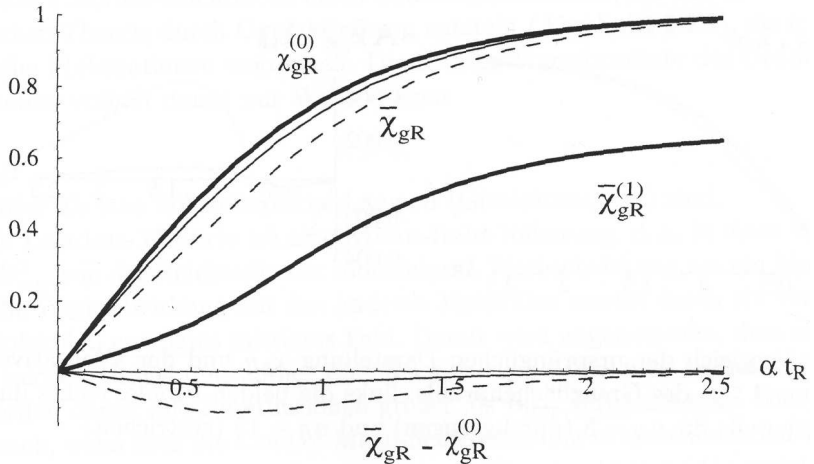
$$\chi_{gR}^{(0)}(t_R) = \tanh t_R = \tanh \left(\frac{m_R}{2}(z - h) \right)$$

- 1-loop order with local potential approximation

$$\begin{aligned} \Phi_{gR}(z) &= \sqrt{\frac{3m_R}{u_R}} \bar{\chi}_{gR}(z) \\ &= \sqrt{\frac{3m_R}{u_R}} A(u_R) \left\{ \chi_{gR}^{(0)}(\alpha(u_R)t_R) + \frac{u_R}{8\pi} \bar{\chi}_{gR}^{(1)}(\alpha(u_R)t_R) + \mathcal{O}(u_R^2) \right\} \end{aligned}$$

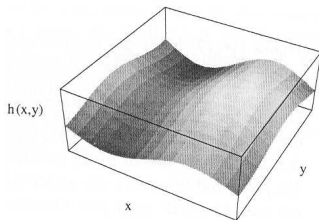
$$\begin{aligned} \bar{\chi}_{gR}^{(1)}(t_R) &= 2/9 \sinh t_R \cosh t_R - \left\{ 1/12 \operatorname{sech}^2 t_R \operatorname{artanh} \left(\sqrt{-1/2 + \sinh^2 t_R} (\sinh t_R)^{-1} \right) \right. \\ &\quad \left. - \sinh t_R \sqrt{-1/2 + \sinh^2 t_R} [2/9 - 1/2 \operatorname{sech}^2 t_R] \right\} \Theta(|t_R| - t_g) \end{aligned}$$

$$\alpha(u_R) = 1 + 1/12 \cdot u_R/(8\pi) + \mathcal{O}(u_R^2) \quad A(u_R) = 1 - 2/3 \cdot u_R/(8\pi) + \mathcal{O}(u_R^2)$$



- $a < \lambda < B_{\text{intr}} \sim \xi$
- long wave fluctuations still to be included
- width to be defined

capillary wave theory



- capillary wave free energy [Buff et al.]

$$\begin{aligned}\beta\mathcal{H} &= \sigma \int dx dy \left[\sqrt{1 + (\nabla h)^2} - 1 \right] \\ &\approx \frac{\sigma}{2} \int dx dy (\nabla h)^2\end{aligned}$$

- Gaussian distribution of the local interface position

$$\begin{aligned}P(h) &= \langle \delta(h(x,y) - h) \rangle = \frac{1}{\sqrt{2\pi} s} e^{-h^2/2s^2} \\ s^2 &= \langle h^2 \rangle = \frac{1}{2\pi\sigma} \int dq \frac{1}{q}\end{aligned}$$

- s^2 divergent for $q \rightarrow 0, \infty$
- introducing cutoff $\xi \sim B_{cw} < \lambda < L$

$$s^2 = \frac{1}{2\pi\sigma} \int_{2\pi/L}^{2\pi/B_{cw}} dq \frac{1}{q} = \frac{1}{2\pi\sigma} \ln \frac{L}{B_{cw}}$$

- capillary wave profile is sharp
 $\Phi_g(z - h(x,y)) = v_0 \operatorname{sgn}(z - h(x,y)) = \pm v_0$ für $z \gtrless h(x,y)$

$$\Phi_{cw}(z) = \int dh \Phi_g(z - h) P(h) = v_0 \operatorname{erf} \left(\frac{z}{\sqrt{2}s} \right)$$

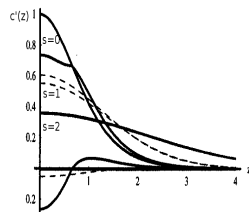
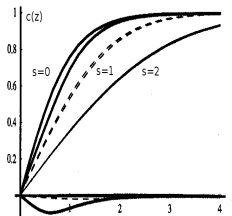
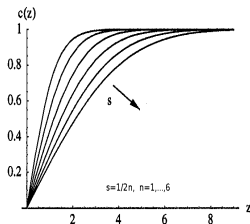
- macroscopic width $w^2 \sim s^2 \sim \ln L$

convolution approximation (M. Müller, 2004)



$$c(z) = \Phi_g(z) * P(z) = \int dh \Phi_g(z - h) P(h)$$

- rescaling: $v_0 = 1$, $\frac{1}{2}m_{RZ} \rightarrow z$, $\frac{1}{2}m_{RS} \rightarrow s$



- $s \rightarrow \infty$ leads to capillary wave theory

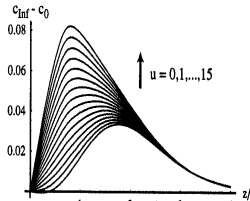
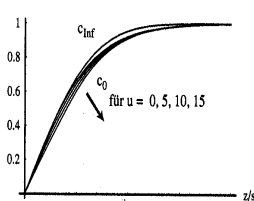
$$\Phi_g(z - h) = \text{sgn}(z - h)$$

$$c(z) \xrightarrow{s \rightarrow \infty} \text{sgn}(z) * \mathcal{N}(0, s^2) = \text{erf}\left(\frac{z}{\sqrt{2}s}\right)$$

- $s \rightarrow 0$ leads to intrinsic interface profile

$$P(h) = \frac{1}{\sqrt{2\pi}s} e^{-h^2/2s^2} \xrightarrow{s \rightarrow 0} \delta(h)$$

$$c(z) \xrightarrow{s \rightarrow 0} \Phi_g(z)$$



$$c_{\text{Inf}}(z) := \text{erf}\left(\frac{1}{\sqrt{2}} \frac{z}{s}\right)$$

$$c_0(z) := \Phi_g\left(\sqrt{\frac{\pi^2 - 6}{6}} \frac{z}{s}\right)$$

interface width

definiton

$$w^2 = \frac{\int dz z^2 c'(z)}{\int dz c'(z)}$$

$$w_{ca}^2 = w_{int}^2 + w_{cw}^2 = \frac{\pi^2}{3} \xi^2 + \frac{1}{2\pi\sigma} \ln \frac{L}{B_{cw}}$$

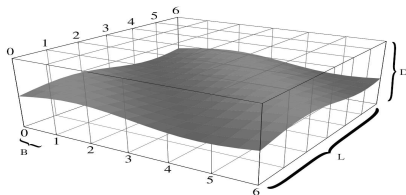
- temperature independent form

$$\hat{w}_{ca}^2 = \left(\frac{w}{2\xi} \right)^2 = \hat{w}_{int}^2 + \hat{w}_{cw}^2 = \frac{\pi^2}{12} + \hat{A}_{cw} \log_2 \frac{\hat{L}}{\hat{B}_{cw}}$$

$$\hat{L} = L/2\xi, \quad \hat{B}_{cw} = B_{cw}/2\xi, \quad \hat{A}_{cw} = \ln 2 / 8\pi\sigma\xi^2 = 0.265(2)$$

Monte Carlo

The following calculations have been done by Melanie Müller (2004).



- blocking $L \times L \times D \rightarrow B \times B \times D$

high-pass filter $\lambda < B$

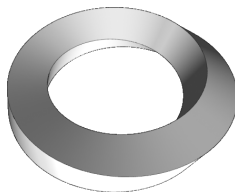
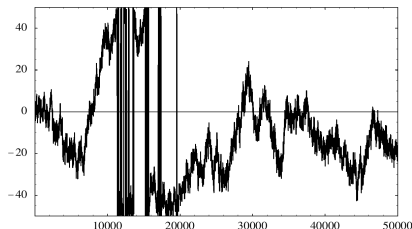
low-pass filter $\lambda > B$

- $w^2 = w_{int}^2 + A_{cw} \log_2 \frac{B}{B_{cw}} + A_{cw} \log_2 \frac{L}{B}$

- local block profile

$$m_i^B(z) = \frac{1}{B^2} \sum_{x,y \in \text{block } i} S(x,y,z)$$

local interface position by boundary shift

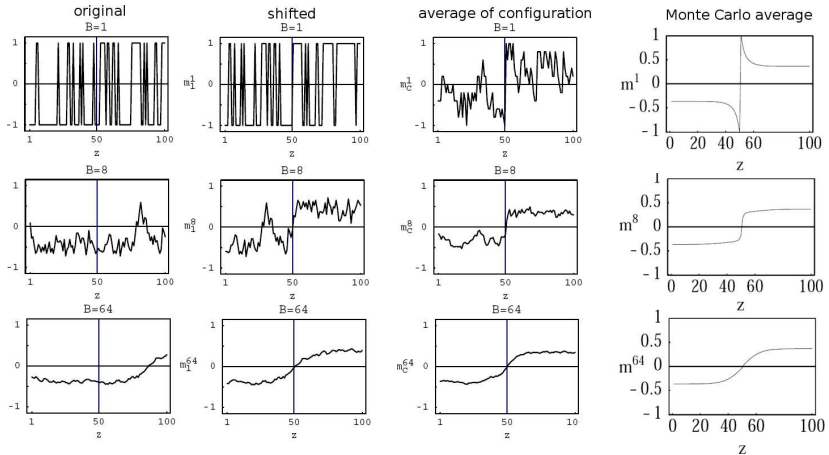


$$m_{tot} = \sum_{z=1} m_i^B(z) \quad \text{for b.c. at } t_{AP} = -\frac{D}{2}$$

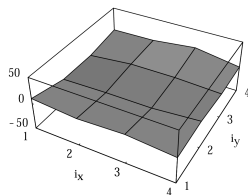
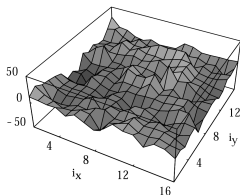
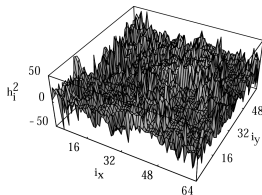
$$m_{tot} := \sum_{z=1}^D m_i^B(z) - \sum_{z=1}^{t_{AP} + \frac{D}{2}} 2 \cdot m_i^B(z)$$

$$M_{tot}(h_i) = \max\{|m_{tot}(t_{AP})|, \quad t_{AP} = -\frac{D}{2}, \dots, \frac{D}{2} - 1\}$$

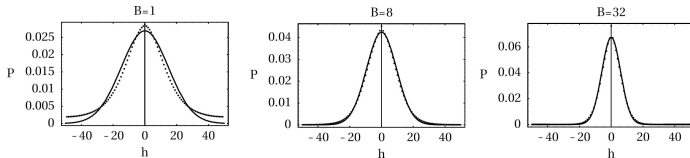
(local) magnetisation profile



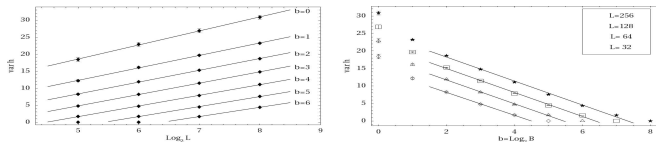
capillary waves



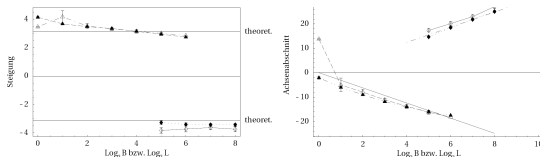
- expect Gaussian distribution with $\text{var}(h) = \frac{\ln 2}{2\pi\sigma} \log_2 \frac{L}{B}$
- slope $= \pm \frac{\ln 2}{2\pi\sigma} = \pm 3.1(1)$
- axis intercept $= \frac{\ln 2}{2\pi\sigma} \log_2 X, \quad X = L, B$



- Gaussian distribution with $\text{var}(h) = \frac{\ln 2}{2\pi\sigma} \log_2 \frac{L}{B}$, $B_{cw} \sim (5-7)\xi$

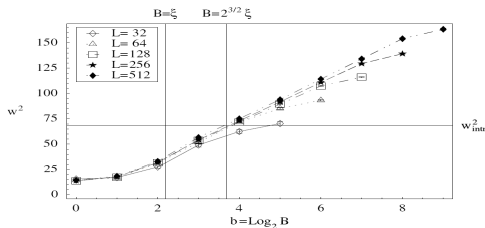


- slope $= \pm \frac{\ln 2}{2\pi\sigma} = \pm 3.1(1)$, axis intercept $= \frac{\ln 2}{2\pi\sigma} \log_2 X$

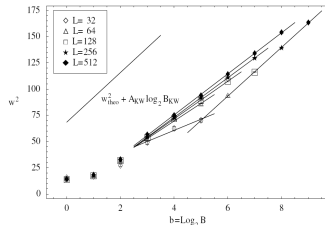


convolution approximation

$$w^2 = c_{intr} \xi^2 + A_{cw} \log_2 \frac{B}{B_{cw}}$$



- ✓ characteristic width w^2 ,
L-independent
- ✓ $w^2 \propto \log_2 B$

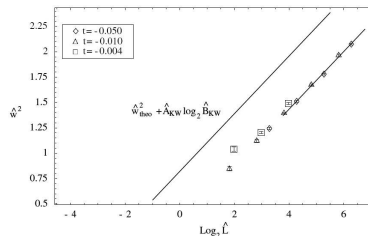
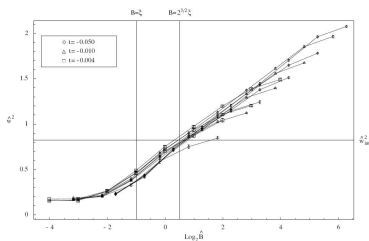


- w_{const}^2 much too small
- w^2 grows for $B < \xi$
- no intrinsic width
- estimate B_{intr}

$$B_{intr} \sim 2^{3/2} \sim 2.8\xi$$

temperature independent

$$\hat{w}^2 = \left(\frac{w}{2\xi} \right)^2 = \frac{c_{intr}}{4} + \hat{A}_{cw} \log_2 \frac{\hat{B}}{\hat{B}_{cw}}$$



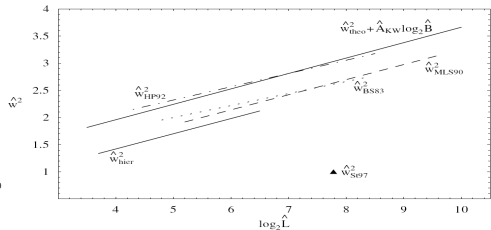
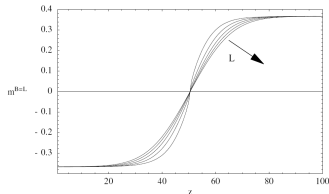
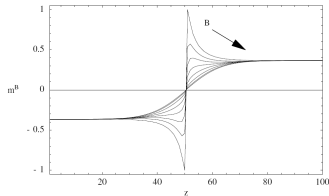
$$\frac{c_{intr}}{4} = \pi^2/12 = 0.822$$

$$\hat{A}_{cw} = \frac{c_{cw} \ln 2}{8\pi\sigma\xi^2} = 0.284(9)$$

$$\hat{w}_{B < L}^2 = 0.57(1) + 0.26(3) \log_2 \hat{B}$$

$$\hat{w}_{B = L}^2 = 0.30(4) + 0.28(1) \log_2 \hat{L}$$

conclusion



- description on two length scales
 $a < \lambda < B_{intr} \sim \xi \sim B_{cw} < \lambda < l$
- interface width shows universal behaviour
- simulation consistent with convolution approximation
- intrinsic regime: ϕ^4 -theory