Interface Profiles in Field Theory

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Outline

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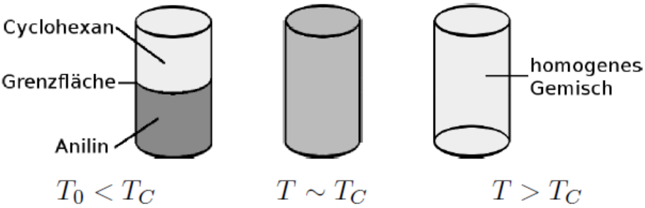
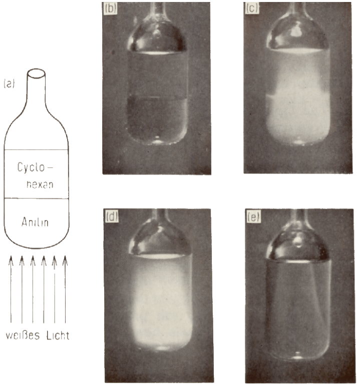
Criticality



- $T < T_c$: 2 phases separated by an interface
- $T \approx T_c$: Long range fluctuations (critical opalescence)
- $T > T_c$: One supercritical phase

Critical Opalescence



Order Parameter

Describe continuous phase transitions by a quantity which is

- nonzero in a phase of higher order ($T < T_c$)
- zero in the phase of higher symmetry

Example

- Ising model: $\phi(x) \sim a^{-D} \sum_{S_i \in W_a(x)} S_i$
- Binary fluid, constituents A and B:
  $\phi(x) = \rho_A(x) - \rho_B(x) - \left(\rho_{A,c}(x) - \rho_{B,c}(x)\right)$

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Energy Functional

Landau's idea:

- Thermodynamic potential as a functional of $\phi(x)$
- $\phi \to 0$ as $T \to T_c$
- Expand functional respecting the symmetries of the system

Ginzburg-Landau-Hamiltonian

$$\mathcal{H}(x) = \frac{1}{2}(\nabla\phi(x))^2 + \frac{\mu^2}{2}\phi(x)^2 + \frac{g}{4!}\phi(x)^4$$

- Symmetry: $\phi \to -\phi$
- Only interested in long wavelength fluctuation $\to$ neglect higher orders of derivatives

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Free Energy

- Interpretation of $H[\phi] = \int \mathrm{d}^D x \mathcal{H}(x)$ as a free energy
  $\rightarrow$ Minimize H
- Statistical physics: free energy via $F = -\beta^{-1} \ln(Z)$
- Landau-Theory is a mean field approximation, i.e. neglects fluctuations
- Incorporate fluctuations per $Z = \int \mathcal{D}\phi \; \exp\left(-H[\phi]\right)$ $(\beta = 1)$

ϕ^4-Theory

- Description of the critical system through a full-fledged euclidean ϕ^4-Theory
- Exploit the apparatus of QFT to calculate expectation values

Partition Function

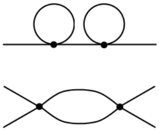
Moment-generating functional

$$Z[J] = \int \mathcal{D}\phi \;\; \exp\left(-H[\phi] + \int \mathrm{d}^D x \; J(x)\phi(x)\right)$$

Correlation functions:

$$\langle \phi(x_1)...\phi(x_n)\rangle = \frac{1}{Z[0]} \; \frac{\delta^n Z}{\delta J(x_1)...\delta J(x_n)}\bigg|_{J=0}$$

Wick's Theorem:
corresponding to diagrams
without 'vacuum-fluctuations'

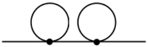


Free Energy

Cumulant-generating functional $W[J] = \ln(Z[J])$
Connected correlation functions:

$$\langle \phi(x_1)...\phi(x_n) \rangle_c = \left. \frac{\delta^n W}{\delta J(x_1)...\delta J(x_n)} \right|_{J=0}$$

Connected diagrams



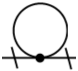
'+'

Gibbs' Free Energy

Generating functional $\Gamma[\phi_c] = W[J] - \int \mathrm{d}^D x \; J(x)\phi_c(x)$
with $\phi_c(x) = \frac{\delta W}{\delta \phi(x)}$

Proper vertices

$$\left.\frac{\delta^n \Gamma}{\delta\phi_c(x_1)...\delta\phi_c(x_n)}\right|_{\phi_c=\langle\phi\rangle}$$



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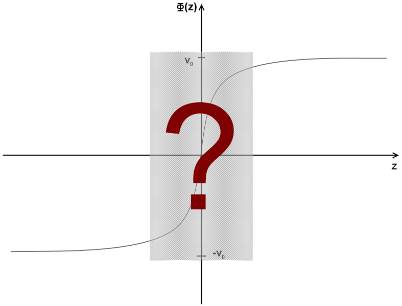
Field Expectation Value

Since $\phi_c(x)|_{J=0} = \langle \phi(x) \rangle$ and $\frac{\delta \Gamma}{\delta \phi_c(x)} = -J(x)$

$$\Rightarrow \left. \frac{\delta \Gamma}{\delta \phi_c(x)} \right|_{\phi_c(x) = \langle \phi(x) \rangle} = 0$$

- Analogon to Euler-Lagrange-Equations allowing for fluctuations
- Solve differential equation $\rightarrow$ get $\langle \phi(x) \rangle$

Starting Point



$$\phi \to \pm v_0 \text{ as } z \to \pm\infty$$

Van der Waals' Ansatz

Free energy density given by

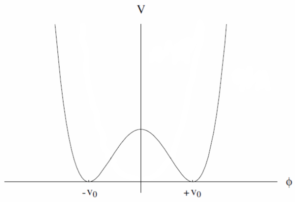
$$\mathcal{H} = \frac{1}{2}\left(\phi'(z)\right)^2 + V\left(\phi(z)\right)$$

- First term: Energy corresponding to fluctuations
- Second term: Potential stationary at equilibrium values of ϕ

Double-Well-Potential

$$V(\phi) = -\frac{m_0^2}{4}\phi^2 + \frac{g_0}{4!}\phi^4 \left(+ \frac{g_0 v_0^4}{4!} \right)$$

with $v_0^2 = \frac{3m_0^2}{g_0}$



$\rightarrow$ ϕ^4-Theory in a phase of broken symmetry

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Cahn-Hilliard-Profile

'Classical' equation of motion: $\frac{\delta \mathcal{H}}{\delta \phi} = 0$

- $-\nabla^2 \phi(x) - \frac{m_0^2}{2}\phi(x) + \frac{g_0}{3!}\phi^3(x) = 0$
- Cahn-Hilliard-Profile

$$\phi(x) = v_0 \tanh\left(\frac{m_0}{2}(z-a)\right)$$

- Free parameter a: Interface position

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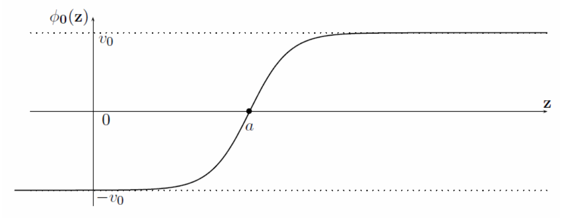
Intrinsic Profile

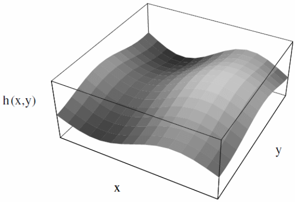


- MFA provides intrinsic interface structure
- Only fluctuations $\lambda < \xi = m^{-1}$ are taken into account by CH-Profile

Long-Range Fluctuations

Complementing the intrinsic profile: Capillary Waves

- Interface as a sharp discontinuity between phases
- Deformations against interfacial tension σ (and gravity)



CW-Hamiltonian

Energy of deviations h from the plane (disregarding gravity):

$$H = \sigma \int \mathrm{d}x\,\mathrm{d}y\, \left[\sqrt{1 + (\nabla h(x,y))^2} - 1\right]$$

- Interested in long-range fluctuations ($\lambda > \xi$)
  $\Rightarrow (\nabla h)^2$ is small
- Expansion yields:

$$H[h] \approx \frac{\sigma}{2} \int \mathrm{d}x\,\mathrm{d}y\, (\nabla h)^2$$

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Free Field Theory

- Periodic boundary conditions on $[0, L] \times [0, L]$
- 2D-Field Theory via

$$Z = \int \mathcal{D}h \, \exp\left(-H[h]\right)$$

- Propagator $\propto \frac{1}{k^2}$
- Interface width:

$$\langle h^2 \rangle = \frac{1}{2\pi\sigma} \int \mathrm{d}q \, \frac{1}{q}$$

Cut-Offs

$$\langle h^2 \rangle = \frac{1}{2\pi\sigma} \int \mathrm{d}q \, \frac{1}{q}$$

is IR- and UV-divergent!

- Lower cut-off: $\frac{2\pi}{L}$ since $\lambda \leq L$
- Upper cut-off: $\frac{2\pi}{B_{cw}}$ since small fluctuations where excluded
- Intrinsic and capillary wave profile should be complementary: $B_{cw} \sim \xi$

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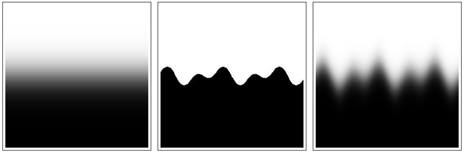
Convolution Approximation

- Intrinsic profile: $\phi(z)$
- Propability to find interface at h: $P(h)$
- Emerging profile:

$$m(z) = \int \mathrm{d}h \, \phi(z-h)P(h)$$



Interface Width

Müller, 2004: Define the width by

$$w^2 = \frac{\int \mathrm{d}z\, z^2 m'(z)}{\int \mathrm{d}z\, m'(z)}$$

It follows:

$$w^2 = w_{int}^2 + w_{cw}^2$$

$$w^2 = \text{const.} \cdot \xi^2 + \frac{1}{2\pi\sigma} \ln\left(\frac{L}{\text{const.} \cdot \xi}\right)$$

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Convolution Approximation

- CW introduce a dependence on L
- Profile is infinitely smeared out for $L \to \infty$
- Distinction between intrinsic profile and capillary waves seems artificial
- All the more the introduction of cut-offs

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Holistic Approach

- Start from ϕ^4-Theory

$$\mathcal{H}(\phi) = \frac{1}{2}\left(\nabla\phi(x)\right)^2 - \frac{m_0^2}{4}\phi^2 + \frac{g_0}{4!}\phi^4$$

- Fluctuations about CH-Profile

$$\phi_0^{(a)}(z) = v_0 \tanh\left(\frac{z-a}{2\xi}\right)$$

$$Z = \int \mathcal{D}\varphi \, \exp\left(-H[\phi_0 + \varphi]\right)$$

- $\varphi(x)$ obeys periodic boundary conditions

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Hamiltonian

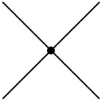
$$\mathcal{H}(\phi_0+\varphi) = \mathcal{H}(\phi_0) + \underbrace{\frac{1}{2}\varphi(x)K\varphi(x)}_{\text{gaussian}} + \underbrace{\frac{g_0}{3!}\phi_0(x)\varphi^3(x) + \frac{g_0}{4!}\varphi^4(x)}_{\text{interaction}}$$

with the fluctuation operator

$$K = -\Delta - \frac{m_0^2}{2} + \frac{g_0}{2}\phi_0^2(x)$$

Two interaction vertices

$\sim g_0\phi_0(x)$



$\sim g_0$

Interface Translations

For

$$\phi_0^{(a+\varepsilon)} = \phi_0^{(a)} + \delta\varphi^{(\varepsilon)}$$

obeying

$$\left.\frac{\delta H}{\delta\phi}\right|_{\phi=\phi_0^{(a+\varepsilon)}} = 0$$

it follows

$$K\,\delta\varphi^{(\varepsilon)} = 0$$

$\rightarrow \delta\varphi^{(\varepsilon)}$ is an eigenvector to eigenvalue 0

- Gaussian part (0^{th} order) of the partition functional would diverge:

$$\int \mathcal{D}\varphi \; \exp\left(-\int \frac{1}{2} \mathrm{d}^D x \varphi(x) K \varphi(x)\right) = (\det K)^{-\frac{1}{2}}$$

- Choosing an interface position breaks translational invariance
- Interface has to be fixed to examine its properties

Method of Collective Coordinates

- Separate interface translation from interesting fluctuations
- $\{f_m\}$ ONB in function space
  $\rightarrow \varphi = \sum_m c_m f_m$
- Write measure $\mathcal{D}\varphi \sim \prod_m \mathrm{d}c_m$
- Transform to ONB containing $\delta\varphi^{(\varepsilon)}$
  $\rightarrow \mathcal{D}\varphi \sim \mathrm{d}a \prod \mathrm{d}c'_m$

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Separation of Fluctuations

$$\int \mathcal{D}\varphi \;\rightarrow\; \int \mathrm{d}a \underbrace{\int \prod_m \mathrm{d}c'_m}_{\int_{N_\perp} \mathcal{D}\varphi}$$

Separation works because of translational invariance of H

- a is called a collective coordinate
- Done by an 'insertion of 1':

$$1 = \int \mathrm{d}c_0(a)\, \delta\left(c_0(a)\right)$$

with $c_0(a) = \left(\varphi^{(a)}, \delta\varphi^{(\varepsilon)}\right)$

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Modified Theory

$$Z_\perp[J] = \int_{N_\perp} \mathcal{D}\varphi \;\exp\left(-H + \int \mathrm{d}^D x\; J(x)\varphi(x)\right)$$

$$\Downarrow$$

$$Z_\perp[J] = \mathcal{N} \exp\left\{-\int \mathrm{d}^D x \left[\frac{g_0}{3!}\phi_0(x)\left(\frac{\delta}{\delta J(x)}\right)^3 + \frac{g_0}{4!}\left(\frac{\delta}{\delta J(x)}\right)^4\right]\right\} \cdot$$

$$\cdot \exp\left\{\frac{1}{2}\int \mathrm{d}^D x\, \mathrm{d}^D y\; J(x) K'^{-1}(x,y) J(y)\right\}$$

with $K'^{-1}(x,y)$ the kernel of the inverse to $K' = K|_{N_\perp}$

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1-Loop-Order

- Loop-expansion gives

$$\langle \varphi(x) \rangle_\perp \quad =$$

$$= \quad -\frac{g_0}{2} \int \mathrm{d}^D x' \; K'^{-1}(x, x') K'^{-1}(x', x') \phi_0(x')$$

- Alternative: Solve $\left.\frac{\delta \Gamma}{\delta \phi_c(x)}\right|_{\phi_c(x) = \langle \phi(x) \rangle} = 0$ to this order

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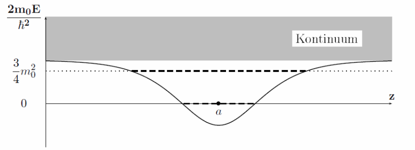
Spectrum of K

$$K = \underbrace{-\left(\partial_x^2 + \partial_y^2\right)}_{\text{free particle in 2D}} + \underbrace{\left[-\partial_z^2 - \frac{m_0^2}{2} + \frac{g_0}{2} v_0^2 \tanh^2\left(\frac{m_0}{2} z\right)\right]}_{\text{particle in potential}}$$

- 'Free particle' spectrum determined by boundary conditions
- 'Particle in potential'-spectrum is also known:



Boundary Conditions of the 'Free' Operator

Köpf, 2008: Periodic boundary conditions

- Eigenfunctions $\chi_{\vec{n}} \propto \exp(i\frac{2\pi}{L}\vec{n}\vec{x})$ with $\vec{n} \in \mathcal{Z}^2$
- Zero-mode exists
  $\Rightarrow$ combines to zero-mode of K

Drees, 2010: Fixed boundary conditions

- $\phi(0, y, z) = \phi(L, y, z) = \phi(x, 0, z) = \phi(x, L, z) = v_0 \tanh\left(\frac{m_0}{2}z\right)$
- Eigenfunctions $\chi_{\vec{n}} \propto \sin\left(\frac{n_1\pi}{L}x\right)\sin\left(\frac{n_2\pi}{L}y\right)$ with $\vec{n} \in \mathcal{N}^2\backslash\{0\}$
- No zero-mode! Interface is fixed

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Calculation of K^{-1}

Representation in terms of eigenvalues and -functions:

$$K^{-1} = \sum\!\!\!\!\!\!\int_{\lambda} \Psi_\lambda(x)\Psi^*_\lambda(x)\,\frac{1}{\lambda}$$

while $K\Psi_\lambda(x) = \lambda\Psi_\lambda(x)$

- Periodic boundary conditions: Exclude $\lambda = 0$
- Calculation amounts to evaluation of infinite series and divergent integrals ($\rightarrow$ renormalization)

Periodic Boundary Conditions

Profile calculation done to 1-loop-order
solving $\frac{\delta\Gamma}{\delta\phi_c(x)}\Big|_{\langle\phi(x)\rangle} = 0$ by variation of parameters with

$$K'^{-1} = C_0 + (C_2 + C_3)\,\mathrm{sech}^2\left(\frac{m_0}{2}z\right) +$$

$$+ (C_1 + C_4 - C_2)\,\mathrm{sech}^4\left(\frac{m_0}{2}z\right)$$

Boundary Conditions and K^{-1}

$$C_0 = \frac{1}{2\pi}\int \mathrm{d}p \sum_{\vec{n}} \frac{1}{4\pi^2 n^2 + (m_0^2 + p^2)L^2}$$

$$C_1 = \frac{3m_0}{8}\sum_{\vec{n}\neq 0} \frac{1}{4\pi^2 n^2}$$

$$C_2 = \frac{3m_0}{4}\sum_{\vec{n}} \frac{1}{4\pi^2 n^2 + \frac{3}{4}m_0^2 L^2}$$

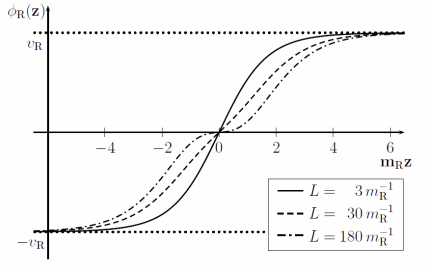
$$C_3 = -3m_0^2 \int \mathrm{d}p \underbrace{\frac{1}{2\pi(4p^4 + 5p^2 m_0^2 + m_0^4)}}_{} \sum_{\vec{n}} \frac{m_0^2 + p^2}{4\pi^2 n^2 + (m_0^2 + p^2)L^2}$$

$$C_4 = \frac{9m_0^4}{4}\int \mathrm{d}p\, \mathcal{N}_p^2 \sum_{\vec{n}} \frac{1}{4\pi^2 n^2 + (m_0^2 + p^2)L^2}$$

Solution after renormalization:

$$\langle \phi_R(z) \rangle = v_R \left\{ \tanh\left(\frac{m_R}{2} z\right) + \right.$$

$$\left. -\frac{g_R}{8\pi m_R} \left[\frac{1}{2} [\alpha + \ln(m_R L)] \tanh\left(\frac{m_R}{2} z\right) - \eta \left(\frac{m_R}{2} z\right) \right] \mathrm{sech}^2\left(\frac{m_R}{2} z\right) \right\}$$



Interface Width

Width given by resulting profile:

$$w^2 = \left(\text{const. incl. } w_{int}^2\right) + \text{const.} \cdot \ln\left(m_R L\right)$$

- Includes results of the convolution approximation
- Especially L-dependence endorses the capillary wave picture

Fixed Boundary Conditions

- Expression of K^{-1} in terms of sums already given by Drees
- Even though no zero-modes: Those sums might bring further complications
- The (numerical?) evaluation has yet to be done

$$K^{-1} = \sum_{\substack{n_1,n_2>0\\ m_1,m_2>0}} A_{n_1,2m_1-1} A_{n_2,2m_2-1} \cdot$$

$$\cdot \sin\left(\frac{(2m_1-1)\pi}{L} x_1\right) \sin\left(\frac{(2m_2-1)\pi}{L} x_2\right) M_{n_1,n_2}$$

with $A_{n_i,2m_i-1} = \frac{4n_i^2}{(2m_i-1)(4n_i^2-(2m_i-1)^2)\pi}$

$$M_{n_1,n_2} = \frac{4}{L^2}\left\{\frac{3m_0}{8}\frac{L^2}{\pi^2\vec{n}^2}\operatorname{sech}^4\left(\frac{m_0}{2}z\right) + \right.$$
$$+\frac{3m_0}{4}\frac{1}{\frac{\pi^2\vec{n}^2}{L^2}+\frac{3}{4}m_0^2}\tanh^2\left(\frac{m_0}{2}z\right)\operatorname{sech}^2\left(\frac{m_0}{2}z\right) +$$
$$\left. + \int \mathrm{d}p \, \frac{1}{\frac{\pi^2\vec{n}^2}{L^2}+m_0^2+p^2}\left|\Psi_{\lambda_p}(z)\right|^2 \right\}$$

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Resume

- The convolution approximation and ϕ^4-theory deliver consistent results
- In the latter different difficulties concerning boundary conditions arise
- Next task: Find the profile for fixed boundary conditions

Thank you for your attention!

Resources

- M. Köpf, Rauhigkeit von Grenzflächen in der Ising-Universalitätsklasse, Diploma Thesis (2008)
- M. Köpf and G. Münster, Interfacial roughening in field theory, J. Stat. Phys. 132 (2008) 417
- B. Drees, Intrinsische Fluktuationen und Rauigkeit kritischer Grenzflächen, Diploma Thesis (2010)
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- M. Müller and G. Münster, Profile and width of rough interfaces, J. Stat. Phys. 118 (2005) 669.