IV) Beyond mean-field: fluctuations and scaling

→ Fluctuation correction to the saddle point

Back to our Ising functional; $B = 0$:

$$\beta \mathcal{R}[m(\vec{r})] = \int d\vec{r} \left[\frac{a_2}{2} m^2(\vec{r}) + \frac{a_4}{4} m^4(\vec{r}) + b\left(\vec{\nabla} m\right)^2 \right]$$

and we account for small fluctuations around the most probable profile: $\delta m = m - m^*$

$$\frac{\delta \mathcal{R}}{\delta m(\vec{r})} = 0 \quad \text{for} \quad m^*(\vec{r}) \quad : a_2\, m(\vec{r}) + a_4\, m^3(\vec{r}) - b\, \nabla^2 m = 0$$

$$\frac{\delta^2 \beta\mathcal{R}}{\delta m(\vec{r})\delta m(\vec{r}\,')} = \delta(\vec{r}-\vec{r}\,')\left(a_2 + 3a_4\, m^2 - b\, \nabla^2\right) \equiv K(\vec{r},\vec{r}\,')$$

$$\Rightarrow \beta \mathcal{R}[m(\vec{r})] \simeq \frac{1}{2}\int d\vec{r}\, d\vec{r}\,'\, K(\vec{r},\vec{r}\,')\, \delta m(\vec{r})\, \delta m(\vec{r}\,') + h.o.t$$

We thus restrict to gaussian fluctuations; note that the kernel K may be viewed as a matrix [remember the advice: "be wise, discretize"], symmetric

$$Z = \exp(-\beta \mathcal{R}[m^*]) \underbrace{\int \mathcal{D}m(\vec{r}) \exp\left\{-\frac{1}{2}\int d\vec{r}\, d\vec{r}\,'\, K(\vec{r},\vec{r}\,')\, \delta m(\vec{r})\, \delta m(\vec{r}\,')\right\}}_{\frac{1}{\sqrt{\det K}}}$$

$$\Rightarrow F = \underbrace{\mathcal{R}[m^*]}_{\underbrace{F_{s.p.}}_{\text{mean-field}}} + \frac{1}{2} kT \underbrace{\log \det K}_{\mathrm{Tr} \log K}$$

In a homogeneous system, $K(\vec{r},\vec{r}\,') = K(\vec{r}-\vec{r}\,')$ is invariant by translation ($\sim$ circulant matrix): diagonalized by a basis of plane waves → go to Fourier.

Imagine indeed K is a circulant matrix

$$\hat{K}(\vec{q}) = \sum_j K_{ij}\, e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)}$$ does not depend on i, hence notation

this also means $$\sum_j K_{ij}\, e^{-i\vec{q}\cdot\vec{r}_j} = \underbrace{\hat{K}(\vec{q})}_{\text{eigenvalue}}\, \underbrace{e^{-i\vec{q}\cdot\vec{r}_i}}_{\text{eigenvector}}$$ eigenvector, one for each $\vec{q}$, (and $\vec{q}$ discretized)

Here:
$$\begin{aligned}
\hat{K}(\vec{q}) &= \int d\vec{r}\,'\, K(\vec{r},\vec{r}\,') \exp\left[i\vec{q}\cdot(\vec{r}-\vec{r}\,')\right] \\
&= \int d\vec{r}\,'\, \delta(\vec{r}-\vec{r}\,')\left(a_2 + 3a_4 m^2 - b\nabla^2\right) e^{i\vec{q}(\vec{r}-\vec{r}\,')} \\
&= \int d\vec{r}\,'\, \delta(\vec{r}-\vec{r}\,')\left(a_2 + 3a_4 m^2 + b q^2\right) e^{i\vec{q}(\vec{r}-\vec{r}\,')} \\
&= a_2 + 3a_4 m^2 + b q^2 \equiv b\left(\xi^{-2} + q^2\right)
\end{aligned}$$

We need here to remember: $\vec{q} = \frac{2\pi}{L}(n_x, n_y, n_z)$ say in a 3d cubix box

$$\mathrm{Tr} \Leftrightarrow \sum_{\vec{q}} \Leftrightarrow \sum_{n_x, n_y, n_z} \Leftrightarrow L^3 \int \frac{d\vec{q}}{(2\pi)^3} \Leftrightarrow V \int \frac{d\vec{q}}{(2\pi)^d} \text{ in general}$$

$$\Rightarrow \boxed{F = F_{s.p.} + \frac{1}{2} kTV \int \frac{d\vec{q}}{(2\pi)^d} \log\left(\xi^{-2} + q^2\right) \cancel{\beta}} \rightarrow \text{omited}$$

There is an upper cutoff: $q < 1/a$, as a signature of the underlying lattice

Define $t \equiv \frac{T - T_c}{T_c}$, we have seen that

$$\xi^{-2} \propto |t|, \quad \text{at mean-field level} \quad (\text{ie } \nu = 1/2)$$

We also know that $F_{s.p.}$, the mean-field term, yields $\alpha = 0$ (*) for specific heat

$$C \equiv -T \left.\frac{\partial^2 F}{\partial T^2}\right|_B$$

and since $\partial_T F$ does not exhibit any singularity, what matters for the singular contribution to C is

$$C_{sing} = -k_B \frac{\partial^2 \beta F}{\partial t^2}$$

The fluctuation terms thus give a correction to c in

$$\int \frac{d\vec{q}}{(2\pi)^d} \frac{1}{(\xi^{-2} + q^2)^2}$$

integral convergent at small q but is in q^{d-5}, hence diverges for $d > 4$, converges $d < 4$

the integral has dimension $(\text{length})^{4-d}$, changes behaviour at $d = 4$

$d > 4$: diverges at large $q \sim \frac{1}{a}$, hence $\propto a^{4-d}$

$d < 4$: converges at large q (also at small q) and q can be rescaled by $\xi^{-1} \Rightarrow \propto \xi^{4-d}$

Thus for $\boxed{d > 4}$, the correction is finite and does not alter the mean-field conclusion.

For $\boxed{d < 4}$, the correction $\to \infty$ for $T \to T_c$ (since $\xi \to \infty$): the approach is not self-consistent, mean-fied is invalid; fluctuations destroy mean-field prediction

(*) $a_2 m^* + a_4 (m^*)^3 = 0$; $a_4 m^{*2} = -a_2$

$$F_{s.p} = \frac{1}{2} a_2 (m^*)^2 + \frac{1}{4} a_4 (m^*)^4 \propto \frac{(a_2)^2}{a_4} \quad \text{and } a_2 = \tilde{a}_2 \times (T - T_c) = \tilde{a}_2 T_c t$$

$$\propto t^2 \quad \text{for } t < 0$$

$$C^{m.f}_{sing} = 0 \quad T > T_c$$

$$\propto \tilde{a}_2^2 / a_4 \quad T < T_c$$

→ **Ginzberg criterion:**

$$\frac{C_{\text{fluct correction}}}{C_{\text{mean-field}}} \propto \xi^{4-d} = \left(\frac{\xi}{\xi_G}\right)^{4-d} \quad ; \quad \xi_G \equiv \text{Ginzberg length}$$

In some systems, ξ_G is very large, and $\xi \lll \xi_G$ except very close to T_c. For superconductors in particular, we have $\xi \simeq \xi_G$ for $|t| < 10^{-16}$, which is beyond reach → we will thus see mean-field critical exponents in such a system. This behavior is exceptional. Usually, ξ_G is microscopic, and mean-field behavior is not observed.

→ Summary on fluctuations

For the Ising model, $d=4$ corresponds / defines the upper critical dimension, d_u (for other models, d_u may be ≠t from 4).

- $d > d_u$: mean-field critical exponents are exact (but non universal quantities, such as T_c, are not)
- $d_{lower} < d < d_u$: fluctuations are strong enough to invalidate mean-field, but not sufficient to destroy order.

  ↳ 1 for discrete
  2 for continuous symmetry
- $d < d_{lower}$: fluctuations destroy the ordered phase

→ Scattering and fluctuations: experimental aspects

Scattering exp probe fluctuations at a scale $\lambda \propto 1/k$

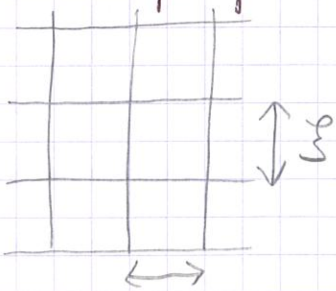
Scattering light ⟷ positional order (atomic density)
e^- ⟷ charge " (charge ")
neutrons ⟷ magnetic "

Chandler 7.5

The key object is the structure factor $S(\vec{k}) = \frac{1}{N}\left\langle \sum_{i,j} e^{i\vec{k}\cdot(\vec{r_i}-\vec{r_j})} \right\rangle$

→ Beyond mean-field: the scaling hypothesis

Scaling arguments can be very powerful. For instance, we found a fluctuation correction to the mean-field free energy in $VkT\int d\vec{q}\,\ln\left[\xi^{-2}+q^2\right] \propto V\,kT/\xi^d$



Partition indeed the system in boxes of size ξ, and assume $\xi \gg a$ (microscopic length). The different boxes are uncorrelated and by extensivity

$$F_{fluct} \propto \frac{V}{\xi^d}\,\underbrace{F_{1box}}_{kT\,f(t,B),\ \text{regular}}$$

We should then compare this contribution to the mean-field $F_{m\text{-}f} = F_{s.p} \propto t^2$ (we found $\alpha = 0$)

Mean-field holds provided $t^2 \gg \xi^{-d} \propto t^{\nu d}$ (with $\nu = 1/2$) $\propto t^{d/2}$

$$\Rightarrow \quad d/2 > 2 \qquad \text{ie} \qquad d > d_{upper} = 4$$

We now explore further the consequences of having ξ large (close to a 2^{nd} order transition)

Consider the free energy density of magnetic system (its singular contribution)

$$f_{sing} = -\frac{\ln Z}{V} = \frac{1}{\xi^d}\,f\left(t, B, \frac{a}{\xi}\right)$$

only depends on dimensionless quantities

Microscopic details matter, through a. Yet, for T close enough to T_c, ξ very large and those details should become irrelevant, $\frac{a}{\xi} \to 0$ and $\tilde{f}$ should be well behaved in this limit. Hence

$$f_{sing} = \frac{1}{\xi^d}\,\tilde{f}(t, B)$$

Next assumption: the info can be compressed down to a form where every q^{ty} is expressed on its relevant scale. For B, this scale is m^δ with $m \propto |t|^\beta$, hence

$$f_{sing} = \frac{1}{\xi^d}\,g\left(\frac{B}{|t|^{\beta\delta}}\right)$$

↳ For the equation of state of liquids, or ρ vs T, see Guggenheim's plot.

Consequences

We can assume that $g(0)$ is finite, since $B=0$ well behaved. Then

$$f_{sing} \propto \xi^{-d} \propto |t|^{\nu d} \quad \text{and also} \propto |t|^{2-\alpha}$$

$$\nu d = 2 - \alpha$$

Likewise : $\chi \propto |t|^{-\gamma} \propto \dfrac{\partial^2 f}{\partial B^2} \propto \xi^{-d} |t|^{-2\beta\delta}$

$$\Rightarrow -\gamma = \nu d - 2\beta\delta$$

These are scaling relations, true for all universality classes. Among the 6 exponents $\alpha, \beta, \gamma, \delta, \eta, \nu$, only 2 are independent. We can also show

$$(1+\delta)\beta = \nu d \quad \rightarrow \quad m = -\partial_B f \propto \xi^{-d} |t|^{-\beta\delta} \propto |t|^{+\beta} \text{ at } B=0$$

$$\nu d \quad - \beta\delta = \beta$$

At this point, we only have 3 scaling relations: we miss one, following from correlat. funct.

→ An interesting prediction for the correlation length We know that $\xi \propto |t|^{-\nu}$ for $B=0$.

What about ξ for $B \neq 0$ but $T = T_c$, that should diverge for $B \to 0$?

Scaling ansatz :

$$\xi = |t|^{-\nu} \varphi\left(B/|t|^{\beta\delta}\right) \rightarrow \text{called the gap exponent}$$

$$= B^{-\nu/\beta\delta} \tilde{\varphi}\left(\frac{B}{|t|^{\beta\delta}}\right) \qquad \text{ie } \varphi(x) \equiv x^{-\nu/\beta\delta} \tilde{\varphi}(x)$$

The value of ξ is finite for $B \neq 0$ and $t = 0$, thus

$\xi \propto B^{-\nu/\beta\delta}$ @T_c. Diverges when $B \to 0$, as expected

From Onsager 2d solution $\dfrac{\nu}{\beta\delta} = \dfrac{1}{\frac{1}{8}15} = \dfrac{8}{15} \simeq 0{,}53$, non-trivial result.

NB Mathematically speaking, we are playing here with homogeneous functions, s.t.

$$f(\lambda^a x, \lambda^b y) = \lambda f(x,y) \overset{\lambda = x^{-1/a}}{\Longrightarrow} f(x,y) = x^{1/a} f(1, y\, x^{-b/a})$$

For instance : $\xi = \quad \varphi(t, B) = |t|^{-\nu} \tilde{\varphi}\left(\dfrac{B}{|t|^{\beta\delta}}\right)$

thus here $a = -1/\nu$, $b/a = \beta\delta$

which are the homogeneity indices of the function φ

→ Finite-size scaling : turning a drawback into an advantage

Computer simulations are always with a finite-size system (L), and close to T_c, $L \ll \xi$ necessarily → pb for studying a bulk property.

Solution? A bona fide scaling assumption : close to T_c, the only relevant length is ξ.

Consider $\chi(t, L)$ at $B = 0$. We know that $\chi(t, \infty) \propto |t|^{-\gamma}$, but $\chi(t,L)$?

Scaling assumption: $\dfrac{\chi(t,L)}{\chi(t,\infty)}$ = dimensionless function of t and L

$$= \varphi\left(\frac{L}{\xi_\infty(t)}\right) \quad ; \quad \xi_\infty(t) \propto |t|^{-\nu}$$

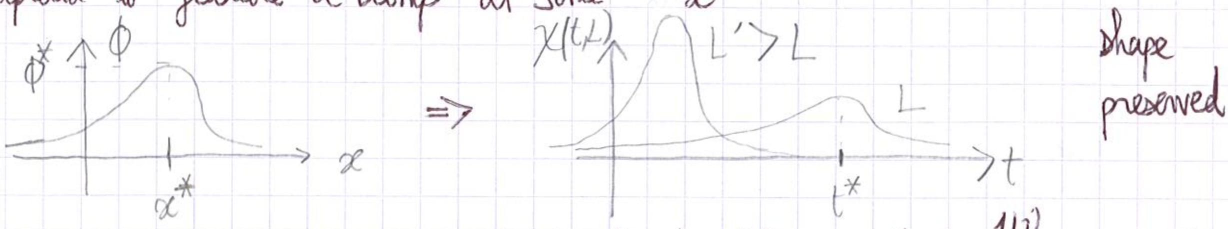
$$\Rightarrow \chi(t,L) = |t|^{-\gamma}\,\varphi(L|t|^{\nu})$$
$$= L^{\gamma/\nu}\,\psi(L|t|^{\nu}) \qquad \varphi(x) = x^{\gamma/\nu}\,\psi(x)$$

We have been a bit sloppy with sign of t, and one should distinguish $t<0$ from $t>0$.
To include both $t>0$ and $t<0$ in a relevant expression, we write

$$\boxed{\chi(t,L) = L^{\gamma/\nu}\,\phi(t\,L^{1/\nu})}$$

Because $\chi(t,\infty) \propto |t|^{-\gamma}$, we have $\phi(x) \propto |x|^{-\gamma}$ for $x \to \infty$ or $-\infty$

ϕ is expected to feature a bump at some x^*

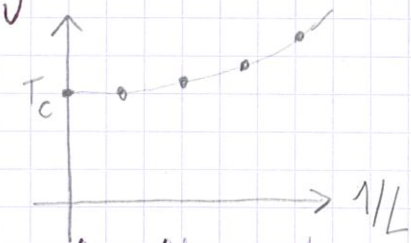


Bump of $\chi(t,L)$ at $t^* = x^*\,L^{-1/\nu} \xrightarrow[L\to\infty]{} 0$

Height " " $\propto L^{\gamma/\nu}$

In practice, we plot $\chi(T,L)$ vs T. Look at $T^{(L)}_{bump}$ vs L

$$T^{(L)}_{bump} = T_c + a\,L^{-1/\nu}$$



Once T_c is found, we get ν from this plot, and γ/ν from the height of χ (its maximum value, vs L).

Criticality is not encoded in $\varphi(0)$ nor $\varphi(\infty)$ but some $\varphi(x^*)$ where x^* is the max of ϕ

→ Correlation functions and self-similarity

Scaling ansatz: $G(\vec{r},t) = \xi^a\,g(r/\xi) = r^a\,h(r/\xi)$

that we can rewrite, from the known behavior at T_c:

$$G(\vec{r},t) = \frac{1}{r^{d-2+\eta}}\,g\left(\frac{r}{\xi}\right) \quad ; \quad g(0) \text{ finite}$$

system is self-similar, up to scale ξ (of critical opalescence).

At T_c: scale invariance / self-similarity ie $G(\lambda r) = \lambda^a\,G(r)$

Meaning: if a snapshot of a critical system is blown up by a factor λ, then apart from a change of contrast (multiplication by λ^a), the new snapshot is statistically equivalent to original. Hallmark of fractal geometry

We now have the final scaling relation, from $\chi \propto \int G(\vec{r})\, d\vec{r}$

$$\int d\vec{r}\, G(\vec{r}) = \int d\vec{r}\, \frac{1}{\xi^{d-2+\eta}}\, g(r/\xi) \propto \frac{\xi^d}{\xi^{d-2+\eta}} \propto \xi^{2-\eta} \propto |t|^{\nu(\eta-2)}$$

$$\propto |t|^{-\gamma}$$

$$\Rightarrow \gamma = \nu(2-\eta)$$

Check with ⊗ Onsager solution in 2d: $\frac{7}{4} = 1\left(2-\frac{1}{4}\right)$

⊗ mean-field: $1 = \frac{1}{2}(2-0)$