Chapter 1

Widom's scaling theory. Block-spin Kadanoff's transformation

1.1 Introduction

We have seen that as a given system approaches a critical point $T \to T_c^{\pm}$, the distance ξ over which the fluctuations of the order parameter are correlated becomes comparable to the size of the whole system L and the microscopic aspects of the system become irrelevant. This means that near a critical point the system has no longer characteristic lengths (a, L), besides ξ of course that becomes the only relevant length scale of the problem. We can therefore expect that if we "move" a little bit from a critical point $(t \sim 0)$, for example changing the temperature by a small amount, the free energy of the system as a function will not change its shape, hence it is invariant in form by a change of scale.

This hypothesis is also suggested by experimental data such as the ones shown by Guggenheim for the gas phase diagrams and the ones shown for ferromagnetic materials at different temperatures. Let us consider the experiment in Figure 1.2; we can see that data from different temperatures, if scaled properly, collapse into two (one for t < 0 and one for t > 0) unique curves. It is clearly illustrated in Figure 1.1. At the origin, the Widom's static scaling theory was introduced also to explain this collapse.

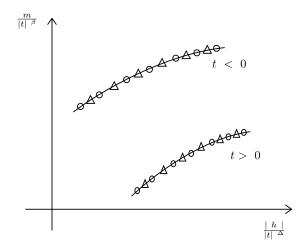


Figure 1.1: Scaled magnetization m is plotted against scaled magnetic field h.

Lecture 19.
Wednesday 18th
December, 2019.
Compiled: Friday
31st January, 2020.

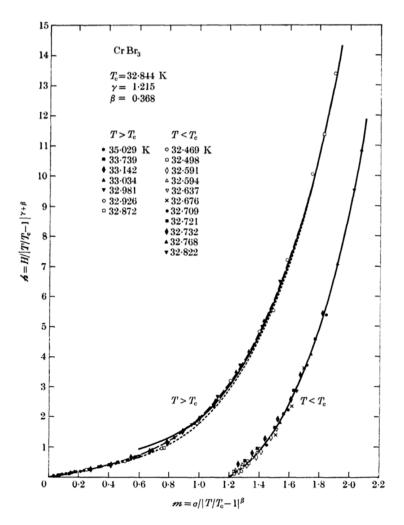


Figure 1.2: Scaled magnetic field h is plotted against scaled magnetization m for the insulating ferromagnet CrBr₃, using data from seven supercritical $(T > T_c)$ and from eleven subcritical $T < T_c$ isotherms. Here $\sigma \equiv M/M_0$. (1969)

1.2 Widom's static scaling theory

We have seen that when a phase transition occurs the free energy of the system is such that the response functions exhibit singularities, often in the form of divergences. To make a concrete example (but of course all our statements are completely general) if we consider a magnetic system we can suppose to write its free energy density as:

$$f(T,H) = f_r(T,H) + f_s(T,H)$$

where $t = (T - T_c)/T_c$ and $h = (H - H_c)/k_BT$, f_r is the "regular" part of the free energy (which does not significantly change near a critical point), while f_s is the "singular" one, which contains the non-analytic behaviour of the system near a critical point (i.e. $t \sim 0$ and $h \sim 0$).

Widom's static scaling hypothesis consists in assuming that the singular part f_s of the free energy is a generalized homogeneous function, i.e.:

$$f_s(\lambda^{p_1}t, \lambda^{p_2}h) = \lambda f_s(t, h)$$

Note that assuming that one thermodynamic potential is a generalized homogeneous function implies that all the other thermodynamic potentials are so.

Therefore, in order to properly define the scaling hypothesis, we should rely on the mathematical concept of homogeneous functions and now we discuss the main properties of such functions.

1.2.1 Homogeneous functions of one or more variables

Single variable

Let us begin with the definition of homogeneous function for a single variable r.

Definition 1: Homogeneous function

A function f(r) is said to be homogeneous in r if

$$f(\lambda r) = g(\lambda)f(r), \quad \forall \lambda \in \mathbb{R}$$
 (1.1)

where g is, for the moment, an unspecified function (we will shortly see that it has a precise form).

Example 1: Parabola $f(r) = Br^2$

An example of homogeneous function is

$$f(r) = Br^2$$

in fact

$$f(\lambda r) = B(\lambda r)^2 = \lambda^2 f(r)$$

and so in this case $g(\lambda) = \lambda^2$.

A very interesting property of an homogeneous functions is that, once its value in a point r_0 (i.e. $f(r_0)$) and the function $g(\lambda)$ are known, the entire f(r) can be reconstructed for all $r \in \mathbb{R}$; indeed, any r can be written in the form $r = \lambda r_0$ (of course with $\lambda = r/r_0$), so that

$$f(r) = f(\lambda r_0) = g(\lambda)f(r_0) \tag{1.2}$$

We now want to show that $g(\lambda)$ has a precise form.

Theorem 1

The function $g(\lambda)$ is not arbitrary, but it must be of the form

$$g(\lambda) = \lambda^p \tag{1.3}$$

where p is the degree of the homogeneity of the function.

Proof. From the definition of homogeneous function, for $\lambda, \mu \in \mathbb{R}$ we have on one hand that:

$$f(\lambda \mu r) = f(\lambda(\mu r)) = g(\lambda)f(\mu r) = g(\lambda)g(\mu)f(r)$$

on the other hand,

$$f((\lambda \mu)r) = g(\lambda \mu)f(r)$$

and so:

$$g(\lambda \mu) = g(\lambda)g(\mu)$$

If we now suppose g to be differentiable¹, then differentiating with respect to μ this last equation we get:

$$\frac{\partial}{\partial \mu}[g(\lambda \mu)] = \frac{\partial}{\partial \mu}[g(\lambda)g(\mu)] \quad \Rightarrow \lambda g'(\lambda \mu) = g(\lambda)g'(\mu)$$

¹Actually $g(\lambda)$ continuous is sufficient, but proof becomes more complicated.

Setting $\mu = 1$ and defining $p \equiv g'(\mu = 1)$, we have:

$$\lambda g'(\lambda) = g(\lambda)p \quad \Rightarrow \frac{g'(\lambda)}{g(\lambda)} = \frac{p}{\lambda}$$

which yields:

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}(\ln g(\lambda)) = \frac{p}{\lambda} \quad \Rightarrow \ln g(\lambda) = p \ln \lambda + c \quad \Rightarrow g(\lambda) = e^c \lambda^p$$

Now, $g'(\lambda) = pe^c \lambda^{p-1}$, so since g'(1) = p by definition we have $p = pe^c$ and thus c = 0. Therefore:

$$q(\lambda) = \lambda^p$$

A homogeneous function such that $g(\lambda) = \lambda^p$ is said to be homogeneous of degree p.

More variables

Let us now define homogeneous functions for more than only one variable. The function f(x, y) is a generalized homogeneous function if has as more general form

$$f(\lambda^a x, \lambda^b y) = \lambda f(x, y) \tag{1.4}$$

Remark. If we consider instead

$$f(\lambda^a x, \lambda^b y) = \lambda^p f(x, y)$$

we can always choose $\lambda^p \equiv s$ such that

$$f(s^{a/p}x, s^{b/p}y) = sf(x, y)$$

and choosing a' = a/p and b' = b/p we are back to (1.4). Hence, it is the most general form an homogeneous function can have.

Remark. Since λ is arbitrary, we can choose $\lambda = y^{-1/b}$, thus we get

$$f(x,y) = y^{1/b} f\left(\frac{x}{y^{a/b}}, 1\right)$$

in that way f depends on x and y only through the ratio $\frac{x}{y^{a/b}}$! Similarly, for x, one can choose $\lambda = x^{-1/a}$, obtaining

$$f(x,y) = x^{1/a} f\left(1, \frac{y}{x^{b/a}}\right)$$

Example 2

The function $f(x,y) = x^3 + y^7$ is an homogeneous one. Indeed, we have:

$$f(\lambda^{1/3}x, \lambda^{1/7}y) = \lambda x^3 + \lambda y^7 = \lambda f(x, y)$$

Instead, examples of non-homogeneous functions are:

$$f(x) = e^{-x}, \qquad f(x) = \log x$$

1.3 Widom's theory of static scaling

Close to the critical point, the singular part of the free energy does not change form by a change of the scale.

More precisely, given $t \equiv \frac{T-T_c}{T_c}$ and $h = \frac{H-H_c}{H_c}$ and the free energy density

$$f(T,H) = f_{ana}(T,H) + f_{sing}(t,h)$$

$$\tag{1.5}$$

where f_{ana} is an analytic term and f_{sing} diverges, has a singularity. Given that the scaling hypothesis is

$$f_s(\lambda^{p_1}t, \lambda^{p_2}h) = \lambda f_s(t, h), \quad \forall \lambda \in \mathbb{R}$$
 (1.6)

where p_1 and p_2 are the degrees of the homogeneity of the singular part of the free energy.

Remark. The exponents p_1 and p_2 are not specified by the hypothesis but they will depend on the critical exponents.

Remark. Since f_s is a generalized homogeneous function, it is always possible to choose λ to eliminate one dependence.

For example, one can choose $\lambda = h^{-1/p_2}$ to obtain

$$f_s(t,h) = h^{1/p_2} f_s(h^{-p_1/p_2}t,1)$$
(1.7)

where

$$\Delta \equiv \frac{p_1}{p_2} \tag{1.8}$$

is called the gap exponent.

Now, let us see how this simple hypothesis allow us, by simple differential calculus, to obtain relations between the thermodynamic critical exponents.

1.3.1 Scaling of the magnetization

Let us start from the scaling hypothesis

$$f_s(\lambda^{p_1}t, \lambda^{p_2}h) = \lambda f_s(t, h) \tag{1.9}$$

Since M is the 1^{st} derivative of f with respect to H, let us derive (1.9) with respect to h

$$\lambda^{p_2} \frac{\partial f_s}{\partial h} (\lambda^{p_1} t, \lambda^{p_2} h) = \lambda \frac{\partial f_s}{\partial h}$$
 (1.10)

$$\Rightarrow \lambda^{p_2} M_s(\lambda^{p_1} t, \lambda^{p_2} h) = \lambda M_s(t, h) \tag{1.11}$$

On the other hand, we know that, for h=0 and $t\to 0^-$, $M_s(t)\sim (-t)^{\beta}$. Putting h=0 in (1.11)

$$M_s(t,0) = \lambda^{p_2-1} M_s(\lambda^{p_1} t, 0) \tag{1.12}$$

Since λ is arbitrary, we can eliminate the dependence on t by choosing

$$\lambda^{p_1} t = -1 \quad \Rightarrow \lambda = (t)^{-1/p_1} \tag{1.13}$$

hence,

$$M_s(t,0) = -(t)^{\frac{1-p_2}{p_1}} M_s(-1,0)$$
(1.14)

Obtaining the 1^{st} relation:

$$\beta = \frac{1 - p_2}{p_1} \tag{1.15}$$

Exponent δ

At $T = T_c$ (t = 0) we have

$$M_s \stackrel{h \to 0^+}{\sim} h^{1/\delta}$$
 (1.16)

$$\Rightarrow M_s(0,h) = \lambda^{p_2-1} M_s(0,\lambda^{p_2}h) \tag{1.17}$$

Now, we want

$$\lambda^{p_1} h = 1 \quad \Rightarrow \lambda = h^{-1/p_2} \tag{1.18}$$

$$\Rightarrow M_s(0,h) = h^{\frac{1-p_2}{p_2}} M_s(0,1) \tag{1.19}$$

Since $M_s \sim h^{1/\delta}$, we get the 2^{nd} relation:

$$\delta = \frac{p_2}{1 - p_2} \tag{1.20}$$

By getting p_1 and p_2 from the two relations we have

$$p_1 = \frac{1}{\beta(\delta+1)}, \quad p_2 = \frac{\delta}{\delta+1} \tag{1.21}$$

and in particular the gap exponent is

$$\frac{p_2}{p_1} \equiv \Delta = \beta \delta \tag{1.22}$$

1.3.2 Equation of state

We can also predict the scaling form of the equation of state and explain the collapse of the experimental data. Let us start from

$$M_s(t,h) = \lambda^{p_2-1} M_s(\lambda^{p_1} t, \lambda^{p_2} h)$$
(1.23)

and choose $\lambda = |t|^{-1/p_1}$.

We have

$$M_s(t,h) = |t|^{\frac{1-p_2}{p_1}} M_s(\frac{t}{|t|}, \frac{h}{|t|^{\Delta}})$$
 (1.24)

Since $\beta = \frac{1-p_2}{p_1}$, $\delta = \frac{p_2}{p_1}$ we have

$$\frac{M_s(t,h)}{|t|^{\beta}} = M_s(\frac{t}{|t|}, \frac{h}{|t|^{\Delta}})$$
(1.25)

We define the scaled magnetization as

$$\bar{m} \equiv |t|^{-\beta} M(t, h) \tag{1.26}$$

and the scaled magnetic field as

$$\bar{h} \equiv |t|^{-\Delta} h(t, M) \tag{1.27}$$

Hence, the equation (1.25) becomes

$$\bar{m} = F_{\pm}(\bar{h}) \tag{1.28}$$

universal curves!

1.3.3 Magnetic susceptibility

Compute $\frac{\partial^2}{\partial h^2}$ of the scaling hypothesis

$$f_s(\lambda^{p_1}t, \lambda^{p_2}h) = \lambda f_s(t, h) \tag{1.29}$$

From equation (1.25) we have

$$\lambda^{2p_2} \chi_T(\lambda^{p_1} t, \lambda^{p_2} h) = \lambda \chi_T(t, h) \tag{1.30}$$

Exponent γ

Consider h = 0, $t \to 0^-$ (for example). Let $\lambda = -t^{-1/p_1}$, from equation (1.25)

$$\chi_T(t,0) = (-t)^{-\frac{2p_2-1}{p_1}} \chi_T(-1,0)$$
(1.31)

and since

$$\chi_T(t,0) \stackrel{t \to 0^-}{\sim} (-t)^{-\gamma_-} \tag{1.32}$$

we get

$$\gamma_{-} = \frac{2p_2 - 1}{p_1} = \beta(\delta - 1) \tag{1.33}$$

Remark. For $t \to 0^+$, we have $\lambda = t^{1/p_1}$ and we get

$$\gamma_{-} = \gamma_{+} \equiv \gamma = \beta(\delta - 1) \tag{1.34}$$

relation between exponents!

1.3.4 Scaling of the specific heat

Starting again from

$$f_s(\lambda^{p_1}t, \lambda^{p_2}h) = \lambda f_s(t, h) \tag{1.35}$$

and compute $\frac{\partial^2}{\partial t^2}$ of both side, we get

$$\lambda^{2p_1}c_h(\lambda^{p_1}t,\lambda^{p_2}h) = \lambda c_H(t,h) \tag{1.36}$$

For h=0 and $t\to 0^-$, we have $\lambda=(-t)^{-1/p_1}$ which implies

$$-t^{-2}c_H(-1,0) = -t^{-1/p_1}c_H(t,0)$$
(1.37)

and since

$$c_H(t,0) \stackrel{t \to 0^-}{\sim} t^{-\alpha_-} \tag{1.38}$$

we get

$$\alpha_{-} = 2 - \frac{1}{p_1} \tag{1.39}$$

Also in this case it is easy to show that

$$\alpha_{-} = \alpha_{+} \tag{1.40}$$

Moreover, by inserting in (1.39) the relation $p_1 = \frac{1}{\beta(\delta+1)}$ one gets the Griffith relation

$$\alpha + \beta(\delta + 1) = 2 \tag{1.41}$$

Moreover, by combining Griffith with the relation $\gamma = \beta(\delta - 1)$ one get the Rushbrooke relation

$$\alpha + 2\beta + \gamma = 2 \tag{1.42}$$

Remark. By using these hypothesis you can get equalities. All the inequality that you have in thermodynamics becames equalities. (lesson)

1.3.5 Second form of the static scaling hypothesis

$$f_s(\lambda^{p_1}t, \lambda^{p_2}h) = \lambda f_s(t, h) \tag{1.43}$$

The relation $\lambda = t^{-1/p_1}$ implies

$$f_s(1, t^{-p_2/p_1}h) = t^{-1/p_1}f_s(t, h)$$
(1.44)

Since $\Delta = \frac{p_2}{p_1}$ and $\alpha = 2 - \frac{1}{p_1}$, one gets

$$f_s(t,h) = t^{2-\alpha} f_s(1, \frac{h}{t^{\Delta}}) \tag{1.45}$$

that is the 2^{nd} scaling form of the free-energy.

1.4 Kadanoff's block spin and scaling of the correlation function

Widom's theory refers only to the free energy of the system. Moreover it do, not fully explain how the scaling hypothesis derives by ξ being the only relevant length of the system.

The first argument on this point was given 1966 by Kadonoff. The Kadonoff's intuition was: the divergence of ξ implies a relation between the coupling constants of a \mathcal{H}_{eff} and the length scales over which m is defined.

We will that Kadanoff's intuition is correct. However, the relation found by Kadanoff is an approximation of the one proposed later by the theory of renormalization.

Remark. How can we relate the coupling costant of the two hamiltonian. This is the idea of the renormalization group. (lesson)

1.4.1 Kadanoff's argument

It is based on a coarse-grained operation on the system and two basic assumptions.

Coarse graining operation

Let us start from the Hamiltonian

$$-\beta \mathcal{H}_{\Omega} = k \sum_{\langle ij \rangle} \sigma_i \sigma_j + h \sum_i \sigma_i \tag{1.46}$$

with

$$\sigma_i = \pm 1, \quad k \equiv \frac{J}{k_B T}, \quad h \equiv \frac{H}{k_B T}$$
 (1.47)

Given xi we know that, for distances $r < \xi$, the spins are correlated.

Let partition the system into blocks of size la (a is the lattice unit length while l is a adimensional scale) such that

$$r \ll \xi \quad \Rightarrow a \ll la \ll \xi(t)$$
 (1.48)

The coarse-graining procedure consits in substituting the spins σ_i in a block of length la with a superspin or block spin S_I .

The transformation chosen by Kadanoff was the following

$$S_I \equiv \frac{1}{|m_l|} \frac{1}{l^D} \sum_{i \in I} \sigma_i \tag{1.49}$$

where m_l is the average magnetization of the *I*-esim block

$$m_l \equiv \frac{1}{l^D} \sum_{i \in I} \sigma_i \tag{1.50}$$

with the sum that is over all the sites with a given cell.

Remark. The division by $|m_l|$ in equation (1.49) is crucial because it rescales the new variables S_I to have the original values ± 1 (rescaling of the fields).

1^{st} crucial assumption

The frist assumption is that the Hamiltonian of the new system \mathcal{H}_l is equal in form to \mathcal{H}_{Ω} , the original one:

$$-\beta \mathcal{H}_{l} = k_{l} \sum_{\langle I,I \rangle}^{N_{b}} S_{I} S_{J} + h_{l} \sum_{I=1}^{N_{b}} S_{I}$$
 (1.51)

Remark. This assumption is in general wrong!

Only the coupling constants k_l and h_l can change by the transformation. Note that the number of block spins N_l is given by $N_l = \frac{N}{lD}$.

How you measure in the new system the lengths? the correlations lengths. Before we have changed the size of the system. We have increased the ruler, so the number is smaller now. It seems stupid but it is fundamental. An important point is: the new system has a lattice length equal to la, hence in the new system all the lengths will be measured in units of la. In particular

$$\xi_l = \frac{\xi}{l} \tag{1.52}$$

that is ξ_l has a numerical value smaller than the one measured in the original lattice.

What does it mean? Since $\xi_l < \xi$ the system described by \mathcal{H}_l is more distant from the critical point than the original $\mathcal{H}(\sigma_i)$! We should expect $t_l > t$.

Similarly, h_l will be such that

$$h\sum_{i}\sigma_{i} = h\sum_{I}\sum_{i\in\sigma_{i}}\sigma_{i} = h\sum_{I}|m_{l}|^{D}S_{I} = \underbrace{h|m_{l}|^{D}}_{h_{I}}\sum_{I}S_{I} \equiv h_{l}\sum_{I}S_{I}$$
(1.53)

giving

$$h_l = |m_l| l^D h (1.54)$$

Since \mathcal{H}_l is equal in form to \mathcal{H} , so it is Z_l and hence the free energies per spins satisfy the equation

$$N_l f_s(t_l, h_l) = N f_s(t, h) \tag{1.55}$$

Hence,

$$\Rightarrow f_s(t_l, h_l) = l^D f_s(t, h) \tag{1.56}$$

Note that the homogeneity condition is recovered with $\lambda \equiv l^D$. We now should ask how t and h change under the block spin transformation.

2^{st} crucial assumption

The second assumption is

$$\begin{cases} t_l = t l^{Y_t} \\ h_l = h l^{Y_h} \end{cases} \tag{1.57}$$

where Y_t , Y_h are scaling exponents and are unknown! Inserting (1.57) in the free energy equation one obtains

$$f_s(t,h) = l^{-D} f_s(t l^{Y_t}, h l^{Y_h})$$
(1.58)

As the parameter λ , in Widom also l can be chosen such that

$$l = |t|^{-1/Y_t} (1.59)$$

so

$$f_s(t,h) = |t|^{D/Y_t} f_s(1,h|t|^{-Y_h/Y_t})$$
(1.60)

Therefore,

$$\Delta = \frac{Y_h}{Y_t} \tag{1.61}$$

Remark. By comparing with the Widom's scaling

$$f_s(t,h) \sim t^{2-\alpha} f_s\left(1, \frac{h}{t^{\Delta}}\right)$$
 (1.62)

we get the new relation

$$2 - \alpha = \frac{D}{Y_t} \tag{1.63}$$

1.5 Kadanoff's argument applied to the two-point correlation

Let us compute the two-point correlation function for the block spins

$$G_{IJ}(\vec{\mathbf{r}}_l, t_l) \equiv \langle S_I S_J \rangle - \langle S_I \rangle \langle S_J \rangle \tag{1.64}$$

Since

$$h_l = h|m_l|l^D \quad \Rightarrow |m_l| = \frac{h_l l^{-D}}{h} \tag{1.65}$$

and using $h_l = h l^{Y_h}$, we obtain

$$|m_l| = l^{\frac{1}{h} - D} \tag{1.66}$$

Since

$$S_I = \frac{1}{|m_l|} \frac{1}{l^D} \sum_{i \in I} \sigma_i \tag{1.67}$$

we have

$$G_{IJ}(\vec{\mathbf{r}}_{l}, t_{l}) = \langle S_{I}S_{J} \rangle - \langle S_{I} \rangle \langle S_{J} \rangle$$

$$= \frac{1}{l^{2(Y_{h} - D)}l^{2D}} \sum_{i \in I} \sum_{j \in J} \left[\underbrace{\langle \sigma_{i}\sigma_{j} \rangle - \langle \sigma_{i} \rangle \langle \sigma_{j} \rangle}_{(a)} \right]$$

$$= \frac{l^{D}l^{D}}{l^{2(Y_{h} - D)}l^{2D}} [\langle \sigma_{i}\sigma_{j} \rangle - \langle \sigma_{i} \rangle \langle \sigma_{j} \rangle]$$
(1.68)

in fact (a) we have made the assumption that since $la \ll \xi$, G_{ij} inside a block is fairly constant

Remark.

$$|\vec{\mathbf{r}}_l| = \frac{\vec{\mathbf{r}}}{l} \tag{1.69}$$

Hence,

$$G_{IJ}(\vec{\mathbf{r}}_l, t_l) = l^{2(D-Y_h)} G_{ij}(\vec{\mathbf{r}}, t)$$
 (1.70)

If one includes also the h dependence:

$$G_{IJ}\left(\frac{\vec{\mathbf{r}}}{l}, tl^{Y_t}, hl^{Y_h}\right) = l^{2(D-Y_h)}G_{ij}(\vec{\mathbf{r}}, t, h)$$

$$\tag{1.71}$$

By choosing $l = t^{-1/Y_t}$ one gets

$$G(\vec{\mathbf{r}}, t, h) = t^{\frac{2(D - Y_h)}{Y_t}} G(\vec{\mathbf{r}}t^{1/Y_t}, 1, ht^{-Y_h/Y_t})$$
(1.72)

Since we are interested at large length scale in proximiti of $T = T_c$, we can choose $|\vec{\mathbf{r}}|$ such that

$$|\vec{\mathbf{r}}|t^{1/Y_t} = 1 \quad \Rightarrow t = |\vec{\mathbf{r}}|^{-Y_t} \tag{1.73}$$

Hence, inserting in (1.72)

$$G(\vec{\mathbf{r}}, t, h) = |\vec{\mathbf{r}}|^{-2(D - Y_h)} F_G(ht^{-Y_h/Y_t})$$
(1.74)

where

$$F_G(ht^{-Y_h/Y_t}) \equiv G(1, ht^{-Y_h/Y_t}, 1)$$
 (1.75)

Remembering the power law behaviour of G in proximity of the critical point, i.e. $G \sim |\vec{\mathbf{r}}|^{2-D-\eta}$ and $\xi \sim t^{-\nu}$. Finally we get

$$\nu = \frac{1}{Y_t}, \quad 2(D - Y_h) = D - 2 + \eta \tag{1.76}$$

Hence, we obtain the hyperscaling relation

$$\Rightarrow 2 - \alpha = \nu D \tag{1.77}$$