Lecture 10: Beyond mean-field

Up to this moment, learning the basic concepts of the theory as scaling, universality, critical exponents, scaling laws, etc, we have seen in fact during exemplifications only mean-field results. So before the study of the Renormalization Group, is time to see some results also beyond mean-field. This is the aim of this Lecture.

1.) 1D Ising case:

a.) The thermodynamic potential:

The Hamiltonian, taking into account also external magnetic field becomes

(564) $\hat{H} = -J\sum_{i=1}^{N} S_i S_{i+1} - g\mu_B H \sum_{i=1}^{N} S_i \; ; \; S_i = \pm 1$

Hence the partition function becomes

(565) $Z = \mathrm{Tr}\, e^{-\beta\hat{H}} = \sum_{S_1 \dots S_N = \pm 1} e^{\beta[J\sum_i S_i S_{i+1} + \frac{1}{2}h\sum_i (S_i + S_{i+1})]} \; ; \; h = g\mu_B H$

Introducing the matrix $(S_i = \pm 1)$

(566) $W_{i,i+1} = e^{\beta J S_i S_{i+1} + \beta\frac{h}{2}(S_i + S_{i+1})}$, the partition function can be written as (periodic bondary conditions are used

(567) $Z = \sum_{S_1}\sum_{S_2}\dots\sum_{S_N} W_{S_1 S_2} W_{S_2 S_3} \dots W_{S_N S_1}$

But $\sum_{S_2} W_{S_1 S_2} W_{S_2 S_3} = M_{S_1 S_3}$ as a matrix product between the matrix $\hat{W}\cdot\hat{W}$. Furthermore

$\sum_{S_3} M_{S_1 S_3} \cdot W_{S_3 S_4} = N_{S_1 S_4}$ as a matrix product. Finally by multiplying all W matrices (whose number is N), the result will be

(568): $\sum_{S_1} W^N_{S_1 S_1} = \mathrm{Tr}\, W^N$;

Hence the partition function becomes

(569): $Z = \mathrm{Tr}(W^N)$; W is called tranfer matrix, and in the present case is a 2×2 matrix

(570): $W =$

$S_i \backslash S_{i+1}$	$+1$	-1
$+1$	W_{11}	W_{12}
-1	W_{21}	W_{22}

$W_{11} = e^{\beta J + \beta h}$; $W_{22} = e^{\beta J - \beta h}$

$W_{12} = W_{21} = e^{-\beta J}$

Consequently:

(571): $W = \begin{bmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{bmatrix}$ and its eigenvalues from $\mathrm{Det}[W - \lambda I] = 0$ become:

$$(e^{\beta(J+h)} - \lambda)(e^{\beta(J-h)} - \lambda) - e^{-2\beta J} = 0 \Rightarrow \lambda^2 - \lambda(e^{\beta(J+h)} + e^{+\beta(J-h)}) + (e^{2\beta J} - e^{-2\beta J}) = 0$$

We obtain (for eigenvalues):

(572): $\lambda^2 - 2\lambda e^{\beta J}\cosh\beta h + 2\sinh\beta J = 0$; hence $(\cosh^2 x = 1 + \sinh^2 x)$:

$$\lambda_{1,2} = \frac{1}{2}\left[2e^{\beta J}\cosh\beta h \pm \left\{4e^{2\beta J}\cosh^2\beta h - 8\sinh(2\beta J)\right\}^{1/2}\right] =$$

(573): $$= e^{\beta J}\left[\cosh(\beta h) \pm \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}\right] ;$$

Since now in self-representation W looks like

(574) $W = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$; so is diagonal, consequently:

(575) $W^N = \begin{pmatrix} \lambda_1^N & 0_N \\ 0 & \lambda_2^N \end{pmatrix}$; and we know that Tr not depends on the representation, we obtain from (569):

(576) $Z = \mathrm{Tr}(W^N) = \lambda_1^N + \lambda_2^N$; $\lambda_1 > \lambda_2$;

Now taking the thermodynamic limit $N \to \infty$ one has

(576) $\lambda_1^N + \lambda_2^N = \lambda_1^N \left(1 + \left(\frac{\lambda_2}{\lambda_1}\right)^N\right) \to \lambda_1^N$, since $\frac{\lambda_2}{\lambda_1} < 1$. Hence, in the thermodynamic limit

(577): $Z = \lambda_1^N = \left\{ e^{\beta J} \left[\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta J}} \right] \right\}^N$

Consequently, the thermodynamic potential (here free energy F) becomes:

(578): $\phi = -K_B T N \ln \left\{ e^{\beta J} \left[\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta J}} \right] \right\}$

By decomposing the logarithm, one obtains:

(579). $\phi = -NJ - K_B T N \ln \left[\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta J}} \right]$; $h \neq 0$

If one takes $h = 0$, $\cosh(\beta h) \to 1$, $\sinh(\beta h) \to 0$, we find under the logarithm

(580) $1 + e^{-2\beta J} = e^{-\beta J}(e^{+\beta J} + e^{-\beta J}) = 2 e^{-\beta J} \cosh(\beta J)$, and ϕ becomes

(581) $\phi = -NJ - K_B T N \ln 2 + NJ - K_B T N \ln[\cosh(\beta J)]$, hence

(582) $\phi = -K_B T N \ln 2 - K_B T N \ln(\cosh(\beta J))$; $h = 0$

b.) The magnetization:

We use (579), and $M = \frac{\partial \phi}{\partial H}$, and obtain ($h = \mu_B g H = \bar{\mu} H$; $\bar{\mu} = g \mu_B$)

$$M = \bar{\mu} \left[\frac{1}{\cosh\beta h + \sqrt{\sinh^2\beta h + e^{-4\beta J}}} \right] \cdot \left[\sinh\beta h + \frac{2 \sinh\beta h \cosh\beta h}{2\sqrt{\sinh^2\beta h + e^{-4\beta J}}} \right] =$$

(583)

$$= \bar{\mu} \frac{N \cdot \sinh(\beta h)}{\cancel{0 +} \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}} \text{ ; i.e.:}$$

(584): $M = \bar{\mu} N \frac{\sinh(\beta h)}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}}$; $h \neq 0$;

It can be seen that at $h = 0$ (and $T \neq 0$), $M = 0$, so there is not present ordered phase at nonzero temperatures. But if one takes at $h \neq 0$, $T \to 0$ one finds

(585) $M = \bar{\mu} N$; arbitrary h; which means that also at $h \to 0$, $M \neq 0$

Consequently

(586) $M = \bar{\mu} N$; $T = 0$; $h = 0$; so that one has ordered phase at $T = 0$, hence

(587) $\boxed{T_c = 0}$

For $\mathcal{J}=0$, because $\cosh^2 x = 1+\sinh^2 x$, one obtains the paramagnetic behavior for M, namely:

(588) $M_{para} = \bar{\mu} N \tanh(\beta h)$

which also provides for $h>0$, but arbitrary small value $M=\bar{\mu}N$ at $T=0$. Excepting $h=0$, where independent on T one has $M=0$ (also at $T=0$).

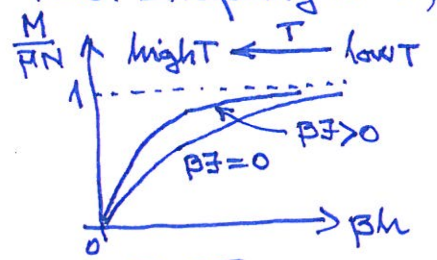


Fig 35:

If $\mathcal{J}>0$ appears, it provides a faster approach towards saturation. As $\beta\mathcal{J}\to\infty$, the M becomes a step function indicative of a singularity at $T=0$.

Critical exponent δ:

$M=\Delta \sim h^{1/\delta}$ at $t=0$ is the definition. For us $t=0$ means $T=0$ for which $M=$ constant. Hence

(589) $\boxed{\delta=\infty}$ This is indeed different from mean-field

Critical exponent β:

$M=\Delta\sim |t|^{\beta}$, $h=0$ is the definition. However $h=0$ provides in (584) $M=0$. So formally $\beta=0$ can be taken, but the reality is that there is no t domain for the variation of M. Consequently, β cannot be defined.

(590). β: cannot be defined

c.) The magnetic susceptibility:

By derivation in function of H of M given in (584) we can find the susceptibility. We obtain:

$$\chi = \frac{\partial M}{\partial H} = \bar{\mu}^2 N\beta \left[\frac{\cosh(\beta h)}{\sqrt{\sinh^2(\beta h)+e^{-4\beta\mathcal{J}}}} - \frac{1}{2}\sinh(\beta h)\frac{2\sinh(\beta h)\cosh(\beta h)}{\left[\sinh^2(\beta h)+e^{-4\beta\mathcal{J}}\right]^{3/2}}\right] =$$

(591)

$$= \bar{\mu}^2 N\beta \frac{\cosh(\beta h)}{\sqrt{\sinh^2(\beta h)+e^{-4\beta\mathcal{J}}}}\left[1-\frac{\sinh^2(\beta h)}{\sinh^2(\beta h)+e^{-4\beta\mathcal{J}}}\right]$$

Hence

(592) $\chi = \frac{\bar{\mu}^2 N}{k_B T}\frac{e^{-4\beta\mathcal{J}}\cosh(\beta h)}{\left[\sinh^2\beta h + e^{-4\beta\mathcal{J}}\right]^{3/2}}$; Now $h\to 0$ has to be taken: $\cosh(\beta h)\to 1$; $\sinh(\beta h)\to 0$, and we find:

(593) $\chi = \frac{\bar{\mu}^2 N}{k_B T} e^{+2\beta\mathcal{J}}$

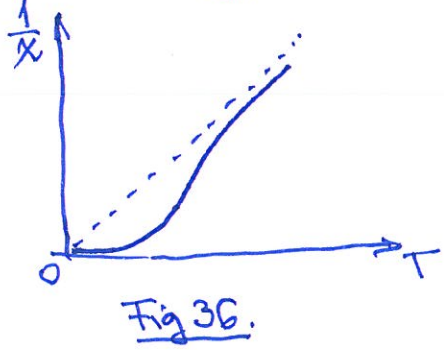


Fig 36.

As seen from Fig 36, for $T\gg 1$ the susceptibility is of $\frac{C}{T}$ Curie form, but as $T\to 0$ its dominant term becomes of $e^{+\frac{2\mathcal{J}}{k_B T}}$ form. We must note otherwise that the susceptibility diverges at $T\to T_c=0$.

In order to see what kind of divergence one has, let us deduce χ also by the fluctuation-dissipation result:

Let us take a Hamiltonian

(594) $\hat{H}' = -\sum_i J_i S_i S_{i+1}$; For $J_i = J$ this $\hat{H}'$ reproduces the starting Hamiltonian (564) at $h=0$.

Now the correlation function becomes

(595) $G(i,i+n) = \langle S_i S_{i+n} \rangle = \frac{1}{Z} Tr(S_i S_{i+n} e^{-\beta \hat{H}'})$; $\langle S_i \rangle = 0$ at $T \neq 0$.

where Z is the partition function. Hence, denoting $\beta J_i = \bar{J}_i$ one has

(596) $\langle S_i S_{i+n} \rangle = \frac{1}{Z} \sum_{\{S_i\}} S_i S_{i+n} e^{\sum_i \bar{J}_i S_i S_{i+1}}$

But one observes that $Z = \sum_{\{S_i\}} e^{\sum_i \bar{J}_i S_i S_{i+1}}$, and

$$\frac{\partial}{\partial \bar{J}_1}\frac{\partial}{\partial \bar{J}_2}\cdots\frac{\partial}{\partial \bar{J}_{i+n}} Z = \sum_{\{S_i\}} \frac{\partial}{\partial \bar{J}_1}\frac{\partial}{\partial \bar{J}_2}\cdots\frac{\partial}{\partial \bar{J}_{i+n}} e^{\sum_i \bar{J}_i S_i S_{i+1}} =$$

(597)
$$= \sum_{\{S_i\}} S_i \underbrace{S_{i+1}^2 S_{i+2}^2 \cdots S_{i+n-1}^2}_{=1 \text{ since } S_j^2 = 1} S_{i+n} e^{\sum_i \bar{J}_i S_i S_{i+1}} = \sum_{\{S_i\}} S_i S_{i+n} e^{\sum_i \bar{J}_i S_i S_{i+1}}$$

Hence

(598) $\langle S_i S_{i+n} \rangle = \frac{1}{Z} \frac{\partial}{\partial \bar{J}_1}\frac{\partial}{\partial \bar{J}_2}\cdots\frac{\partial}{\partial \bar{J}_n} Z$

But we know Z from (577). Taking in it $h=0$ we find

(599) $Z = \{e^{\beta J}[1 + e^{-2\beta J}]\}^N = [e^{\beta J} + e^{-\beta J}]^N = [2^N \cosh^N(\beta J)]$;

which for different J_i terms becomes

(600) $\boxed{Z = 2^N \prod_{i=1}^{N} \cosh(\beta J_i)}$; This is because in this case in (575) $W^N \to \prod_{i=1}^{N} W_i$; $\lambda_1^i = (e^{\beta J_i} + e^{-\beta J_i})$; $\lambda_2^i = (e^{\beta J_i} - e^{-\beta J_i})$ and $\lambda_2^i < \lambda_1^i$; $Tr \prod_i W_i = \prod_i \lambda_1^i + \prod_i \lambda_2^i$, the second term in the thermodynamic limit becomes zero.

From (600) one has

(601) $\frac{\partial Z}{\partial \bar{J}_1} = [\sinh(\bar{J}_1)][2^N \prod_{i=2}^{N} \cosh(\bar{J}_i)] = \frac{\sinh(\bar{J}_1)}{\cosh(\bar{J}_1)} \underbrace{[2^N \prod_{i=1}^{N} \cosh(\bar{J}_i)]}_{Z} = Z \tanh \bar{J}_1$

similarly

(602) $\frac{\partial^2 Z}{\partial \bar{J}_2 \partial \bar{J}_1} = Z \tanh \bar{J}_1 \tanh \bar{J}_2$; and in the same way

(603) $\frac{\partial}{\partial \bar{J}_1} \cdot \frac{\partial}{\partial \bar{J}_2} \cdots \frac{\partial}{\partial \bar{J}_n} Z = Z \prod_{i=1}^{n} \tanh \bar{J}_i$. This introduced in (598) and taking into account that Z simplifies at the end, and $\bar{J}_i = \bar{J} = \beta J$ in our case:

(604) $\boxed{G(i,i+n) = \langle S_i S_{i+n} \rangle = \tanh^n(\beta J)}$

Since $\tanh x|_{x \to \infty} = 1$, it turns out that for $T \to 0$ one has

(605) $\lim_{n \to \infty} G(i,i+n)|_{T=0} = 1$; So long-range order is present in the system at $T=0$, hence indeed $T_c = 0$ is a phase transition point.

Furthermore, (605) is no more valid at an arbitrary small, but $T \neq 0$ temperature:

(606) $\lim_{n\to\infty} G(i,i+n)\Big|_{T>0} = 0$

This means that in 1D Ising case the $T=0$ ferromagnetism is unstable in fact, and an arbitrary small energy perturbation from outside will destroy it.

The advantage that one has $G(i,i+n)$ is that we can express now the correlation length. Indeed, if one measures the distance in lattice spacing units, $r = na$; $a=1 \Rightarrow r=n$, one has from (604)

(607). $G(r) = \tanh^r(\beta J)$

Since $G(r) = \exp\left[-\frac{r}{\xi}\right]$ should be present, where ξ is the correlation length, we transcribe (607) as follows:

(608) $G(r) = \tanh^r(\beta J) = \exp\left[\ln(\tanh^r(\beta J))\right] = \exp\left[-r \ln\frac{1}{\tanh(\beta J)}\right] =$

$= \exp\left[-\frac{r}{\xi}\right]$; $\xi = \frac{1}{\ln\coth(\beta J)}$; note: $\coth x = \frac{1}{\tanh x}$

Now we work a littlebit on the ξ expression in the $T \to 0$ limit where $\beta J \to \infty$. In this limit

(609) $\coth x\Big|_{x\to\infty} = 1 + 2e^{-2x} + \dots$ hence

(610) $\xi = \frac{1}{\ln\coth(\beta J)} \cong \frac{1}{\ln\left[1+2e^{-2\beta J}\right]}$; But now $y = 2e^{-2\beta J} \ll 1$, and $\ln(1+y)\Big|_{y\to 0} = y + \dots$ consequently

(611) $\xi \cong \frac{1}{2e^{-2\beta J}} = \frac{1}{2}e^{2\frac{J}{k_BT}}$, hence

(612) $\boxed{\xi \sim e^{\frac{2J}{k_BT}}\ ;\ T \to T_c}$; Hence, as seen, $\xi \sim t^{-\nu}$ do not holds, and instead of the power-function divergence, one has an exponential divergence of the form

(613) $\xi \sim e^{\frac{2J}{t}}$; $t = (T - T_c)$; $\Rightarrow$ Severe critical exponents and scaling laws must be used (Lecture 5, pg 10).

Now we turn back to the susceptibility. From the fluctuation dissipation result (see (502), from Lecture 8.)

(614) $\chi = \sum_{ij} \chi_{ij}$; $\chi_{ij} = \frac{1}{k_BT} G_M(i,j)$; Here $G_M(i,j) = \langle M_i M_j \rangle$; $M_i = \bar{\mu} S_i$ where $\bar{\mu} = g\mu_B$

Consequently:

(615) $\chi = \frac{\bar{\mu}^2}{k_BT}\sum_{i,j=1}^{N} \langle S_i S_j \rangle = \frac{\bar{\mu}^2}{k_BT}\sum_{i,j=1}^{N} v^{|i-j|}$; $v = \tanh(\beta J)$; (see (604))

Since $i=j$ it happens N times, this case provides $Nv^0 = N$, one has

(616) $\chi = \frac{\bar{\mu}^2}{k_BT}\left[N + \sum_{\substack{i,j=1 \\ i\neq j}}^{N} v^{|i-j|}\right]$

And simply we have to count that a fixed $|i-j| = n \in [1, N-1]$ how many times occurs.

Taking periodic boundary conditions all $|i-j|=n$ distances for $n=1,2,\dots N-1$ appear N times (we simply move the starting point to each site. Furthermore, since in $|i-j|$ the indices can be interchanged a factor 2 appears. Hence

(617) $$\chi = \frac{\bar{\mu}^2}{K_BT}\left[N+2N\sum_{n=1}^{N-1} v^n\right] = \frac{\bar{\mu}^2 N}{K_BT}\left[1+2\sum_{n=1}^{N-1} v^n\right]$$

But we know that

(618). $$\sum_{n=0}^{N-1} = \frac{1-v^N}{1-v} \Rightarrow \sum_{n=1}^{N-1} v^n = \sum_{n=0}^{N-1} v^n - 1 = \frac{1-v^N}{1-v} - 1 = \frac{v-v^N}{1-v}$$

Taking the thermodynamic limit $N\to\infty$; $v^N\to 0$, since at $T\neq 0$, from (615) one has $v<1$. Consequently

(619) $$\chi = \frac{\bar{\mu}^2 N}{K_BT}\left[1+2\frac{v}{1-v}\right] = \frac{\bar{\mu}^2 N}{K_BT}\cdot\frac{1+v}{1-v}$$; $v = \tanh(\beta J)$; but

(620) $$\frac{1+v}{1-v} = \frac{1+\tanh x}{1-\tanh x} = \frac{1+\frac{\sinh x}{\cosh x}}{1-\frac{\sinh x}{\cosh x}} = \frac{\cosh x + \sinh x}{\cosh x - \sinh x} = \frac{\frac{e^x+e^{-x}}{2}+\frac{e^x-e^{-x}}{2}}{\frac{e^x+e^{-x}}{2}-\frac{e^x-e^{-x}}{2}} = e^{2x}; \ x=\beta J$$

and $\tanh x = \frac{\sinh x}{\cosh x}$; $\cosh x = \frac{e^x+e^{-x}}{2}$; $\sinh x = \frac{e^x-e^{-x}}{2}$;

Introducing this result back in (619) we obtain

(621) $$\chi = \frac{\bar{\mu}^2 N}{K_BT} e^{2\beta J}$$; which is identical to (593).

So for $T\to T_c$; $\chi \sim e^{2\beta J} \sim \xi \sim \xi^1$; (see (612)), hence the critical exponent defined in severe conditions:

(622) $$\boxed{\gamma = 1}$$

d.) Specific heat:

Since $C = T\frac{\partial S}{\partial T}$ one must calculate first the entropy $S = -\frac{\partial\phi}{\partial T}$; we finds from (582):

$$S = -\frac{\partial\phi}{\partial T} = K_BN\ln 2 + K_BN\ln[\cosh(\beta J)] + K_BTN\frac{\sinh(\beta J)}{\cosh(\beta J)}\left(-\frac{J}{K_B}\cdot\frac{1}{T^2}\right) =$$

(623) $$= K_BN\ln[2\cosh(\beta J)] - \frac{NJ}{T}\tanh(\beta J).$$

Now the specific heat

(624) $$C = T\frac{\partial S}{\partial T} = T\left\{\underbrace{\tanh(\beta J)\left(-\frac{J}{K_BT^2}\right)K_BN + \frac{NJ}{T^2}\tanh(\beta J)}_{=0} - \frac{NJ}{T}\frac{1}{\cosh^2\beta J}\left(-\frac{J}{K_BT^2}\right)\right\}$$

(625) $$\boxed{C = K_BN\frac{(\beta J)^2}{\cosh^2(\beta J)}}$$

Plotting (625) we find a maximum in the specific heat. But this has nothing to do with a phase transition. The maximum is a Schottky-anomaly which is specific for the systems with a well defined excitacion energy (in our case $2J$ in order to flip an Ising spin). The maximum in (625) appears at $\beta J = 2.07\dots$, hence $K_BT \sim 2J$. Indeed $\frac{\partial C}{\partial T}$ has the expression:

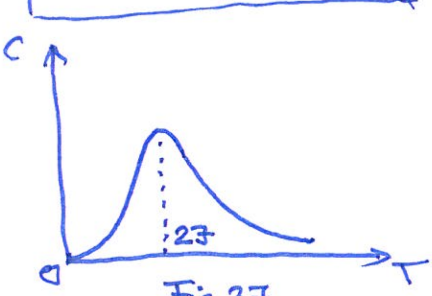


Fig 37.

(626): $\frac{\partial C}{\partial T} = \left[\beta J \tanh \beta J - 2\right] \frac{\left(\frac{J}{k_B}\right)^2 \frac{1}{T^3}}{\cosh^2 \beta J} = 0 \Rightarrow \tanh \beta J = \frac{2}{\beta J} \Rightarrow \beta J = 2.07$

In order to deduce the critical exponent of the specific heat one observes from (625) that for $T \to T_c = 0$ one has

(627) $C \sim \frac{1}{\cosh^2 \frac{J}{k_B T}} \sim \frac{1}{e^{\frac{2J}{k_B T}}} \sim e^{-\frac{2J}{k_B T}} \sim \xi^{-1}$; see (611)

Consequently, because $c \sim \xi^{\bar{\alpha}}$ is the $\bar{\alpha}$ definition (see (264), lecture 5) it results

(628) $\boxed{\bar{\alpha} = -1}$

e) Critical exponent η:

The definition of η is $G(r) \sim \frac{1}{r^{d-2+\eta}}$; $t=0$; (i.e. $T=T_c$).
Since in our case, see (605), one has $G(r)=1=$ const. for $T=T_c=0$ which that $\eta=1$ must hold in order to obtain

(629) $d-2+\eta=0$; $d=1 \Rightarrow G(\vec{r}) = \text{const}$

Consequently:

(629) $\boxed{\eta = 1}$; (i.e. far from the Ornstein-Zernike behavior.)

Collecting all critical exponents one has:

(630) $\bar{\alpha} = -1$; $\bar{\gamma} = 1$; $\eta = 1$; $\delta = \infty$

The severe critical exponents satisfy the scaling laws in severe form (Lecture 5, pg. 10):

(631)
Josephson: $\bar{\alpha} = -d \Rightarrow -1 = -1$ ✓
Fisher: $2-\eta = \bar{\gamma} \Rightarrow 2-1 = 1 \Rightarrow 1 = 1$ ✓
First B-G: $2-\eta = d\frac{\delta-1}{\delta+1} \Rightarrow 2-1=1 \Rightarrow 1=1$ ✓

In (631) all scaling laws are satisfied, and this must be so because here an exact solution is described.

II. 2D Ising case: a.) Set up of the partition function:

The Hamiltonian now in the absence of the external magnetic field becomes

(632) $H = -J \sum_{k,l=1}^{L} \left[S_{kl} S_{k,l+1} + S_{kl} S_{k+1,l} \right]$; $S_{kl} = \pm 1$

where our square 2D lattice has $N = L \times L$ sites. The k and l indices denote the spin position in x and y directions. The partition function becomes

(633) $Z = \sum_{\{S_{kl}\}} e^{-\beta \hat{H}} = \sum_{\{S_{kl}\}} e^{\beta J \sum_{k,l} \left[S_{kl} S_{k,l+1} + S_{k,l} S_{k+1,l} \right]}$

The sum

(634) $\sum_{\{S_{kl}\}} = \sum_{S_{1,1}} \sum_{S_{1,2}} \dots \sum_{S_{L,L}}$; gives 2^N terms.

In calculating the partition function we observe the following:

(635)
$\cosh x = \frac{e^x + e^{-x}}{2}$; $\Rightarrow e^x = \cosh x + \sinh x$
$\sinh x = \frac{e^x - e^{-x}}{2}$; $\Rightarrow e^{-x} = \cosh x - \sinh x$
$\Rightarrow$
$e^x = \cosh x \left[1 + \tanh x\right]$
$e^{-x} = \cosh x \left[1 - \tanh x\right]$

So if one has $\alpha = \pm 1$, then we can write

(635) $e^{\alpha z} = (\cosh z)[1 + \alpha \tanh z]$

In our case $\alpha = S_{k\ell} S_{k,\ell+1}$, (or $S_{k\ell} S_{k+1,\ell}$), and $z = \beta J$, so one has

(636) $e^{\beta J S_{k\ell} S_{k,\ell+1}} = [\cosh(\beta J)][1 + S_{k\ell} S_{k,\ell+1} \tanh(\beta J)]$; etc.

Consequently, by denoting

(637) $x = \tanh(\beta J)$; and taking into account that

$\tanh^2 z = \frac{\sinh^2 z}{\cosh^2 z} = \frac{\cosh^2 z - 1}{\cosh^2 z} \Rightarrow \cosh^2 z = \frac{1}{1 - x^2}$

(638) $Z = \left[\frac{1}{1-x^2}\right]^{\frac{N_H}{2}} \sum_{\{S_{k\ell}\}} \prod_{k,\ell=1}^{L} (1 + x S_{k\ell} S_{k,\ell+1})(1 + x S_{k\ell} S_{k+1,\ell})$

where

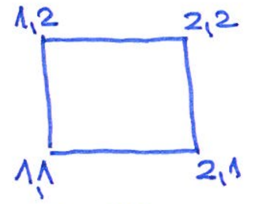
(639) $N_H = 2N$ is the number of terms from the Hamiltonian

Consequently, the partition function becomes

(640) $Z = (1-x^2)^{-N} \cdot \mathcal{S}$; $\mathcal{S} = \sum_{\{S_{k\ell}\}} \prod_{k,\ell=1}^{L} (1 + x S_{k\ell} S_{k,\ell+1})(1 + x S_{k\ell} S_{k+1,\ell})$

$x = \tanh(\beta J)$

Now we must effectuate the product from $\mathcal{S}$. Since $S_{ij} = \pm 1$, only those terms survive which all have all $S_{k\ell}$ at even power (i.e. closed loops in the lattice containing the spins), eg



$= (S_{1,2} S_{2,2} \cdot x)(S_{2,2} S_{2,1} \cdot x)(S_{2,1} S_{1,1} \cdot x)(S_{1,1} S_{1,2} \cdot x) =$

$= S_{1,2}^2 S_{2,2}^2 S_{2,1}^2 S_{1,1}^2 \cdot x^4$

Fig 38.

These nonzero terms (as x^4 in Fig 38) will have the same value for all 2^N contributions of the $\sum_{\{S_{k\ell}\}}$ sum in $\mathcal{S}$. Furthermore, each bond provides an x, so

(641) $\mathcal{S} = 2^N \sum_r x^r g_r$

where g_r is the number of closed loops containing r bonds in the system, each loop being considered only once.

b.) Counting the closed loops:

Now the difficult problem is to count the loops. The main difficulty is caused by the fact that for fixe r, we have also: 1°) self intersecting loops, and 2°) not connected (disjoint) loops (i.e. build up from non-touching parts.

1° Self intersection: For example a closed loop with 1 self intersection (Fig 39a) can be obtained in 3 ways, namely Fig 39, b, c, d. But if one associates a sign to each loop by introducing a phase factor to each bond $\exp[i\frac{\phi}{2}]$ when ϕ schows in which direction (relative to the previous bond) the bond starts ($\phi = 0, +\frac{\pi}{2}, -\frac{\pi}{2}$) (see Fig 40), then

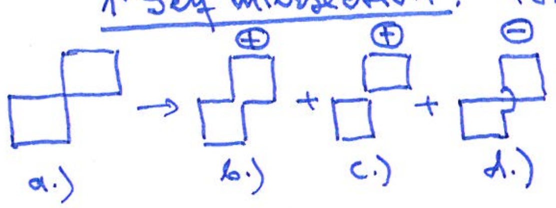


Fig 39

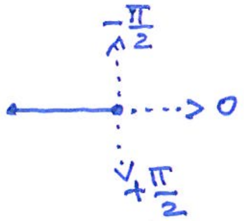


Fig 40: The ϕ values

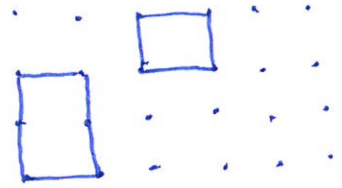


Fig 41: Disjoint closed loop for $r=10$

$$\prod_{\substack{\text{whole}\\ \text{closed}\\ \text{loop}}} e^{i\frac{\phi_i}{2}} = (-1)^{\nu+1} \qquad (642)$$

holds, where ν = number of self intersection points

2° Disjoint closed loops:

Fig 41 shows a disjoint closed loop for the fixed $r=10$ bonds. In this case (642) becomes for s disjoint terms in the closed loop

$$(-1)^{n+s} \quad ; \; n=\sum_{i=1}^{s} \nu_i \qquad (643)$$

where n becomes the number of total self intersections.

Let denote by f_{r_1} the expression:

$$(644) \quad f_{r_1} = \sum e^{\frac{i}{2}\sum_{\alpha=1}^{r_1}\phi_\alpha}$$

where r_1 is the number of bonds over a closed, now single (not disjoint), loop, then sum over loop with fixed r_1.

Now if one has pair of bonds ($s=2$) as in Fig 41, their contribution in the sum counting the closed loops will be

$$(645) \quad \frac{1}{2!}\sum_{r_1+r_2=r} f_{r_1} f_{r_2} \; ;$$

where $1/2!$ (i.e. $1/s!$) takes into account the fact that the same pair of loops is obtained when r_1 and r_2 are interchanged.

For general r this means

$$(646) \quad \frac{1}{s!}\sum_{r_1+r_2+\dots+r_s=r} f_{r_1} f_{r_2} \dots f_{r_s} \; ;$$

Now in order to find correctly the loop sign in Fig 39, we must compensate $(-1)^s$ from (643) by a $(-1)^s$ in (646) (i.e. $n=1$ in (643) to provide sign $-$ in Fig 39, and $n=0$, sign $+$ in Fig 39). Taking into account that r goes to ∞ in the thermodynamic limit (and s as well) and $x^r = x^{r_1+r_2+\dots+r_s}$ can be written in (641), we has

$$(647) \quad \mathfrak{S} = 2^N \sum_{s=0}^{\infty} (-1)^s \frac{1}{s!} \sum_{r_1,r_2,\dots r_s=1}^{\infty} x^{r_1+r_2+\dots+r_s} f_{r_1} f_{r_2} \dots f_{r_s}$$

But since

$$(648) \quad \sum_{r_1,r_2,\dots r_s} x^{r_1+r_2+\dots+r_s} f_{r_1} f_{r_2} \dots f_{r_s} = \left(\sum_{r=1}^{\infty} x^r f_r\right)^s$$

We find

$$(649) \quad \boxed{\mathfrak{S} = 2^N \exp\left[-\sum_{r=1}^{\infty} x^r f_r\right]}$$

where now the advantage in comparison to (641) is that f_r describe individual (not disjoint) closed loops with r bonds. f_r counts the closed loops of this type with fixed r, but also associates to each closed loop the sign $\exp\left[\frac{i}{2}\sum_{\alpha=1}^{r}\phi_\alpha\right]$. A bond double crossing is not allowed.

c.) The calculation of f_r.

The number f_r can be expressed as

$$(650) \quad f_r = \frac{1}{2r}\sum_{k_0,l_0,\alpha_0} W_r(k_0,l_0,\alpha_0) \; ;$$

where $W_r(k_0,l_0,\alpha_0)$ is the sum over all loops leaving the point k_0,l_0,α_0 (i.e. in the direction α_0 from k_0,l_0) and turning back to the starting point after r steps (bonds.). $\sum W_r$ contains each loop $2r$ times since it can be traversed in two opposite directions, and can be assigned to each of its r starting points.

Now let us take the matrix $\tilde{\Lambda}$ which connects $\tilde{W}_{r+1}$ to $\tilde{W}_r$:

(651) $\tilde{W}_{r+1} = \tilde{\Lambda} \cdot \tilde{W}_r$, i.e: $W_{r+1}(k,l,\alpha) = \sum_{k',l',\alpha'} \Lambda(k,l,\alpha; k',l',\alpha') W_r(k',l',\alpha')$

Since $\tilde{\Lambda}$ increases with one the r value, $\tilde{\Lambda}^r = \underbrace{\tilde{\Lambda} \cdot \tilde{\Lambda} \cdots \tilde{\Lambda}}_{r\text{-times}}$ provides $\sum_{k_0,l_0,\alpha_0} W_r(k_0,l_0,\alpha_0)$; (see the right side of (650)), but only if $\tilde{\Lambda}^r$ is taken with the same indices in left and right arguments (i.e. we have a closed curve. Hence

(652) $\mathrm{Tr}\, \tilde{\Lambda}^r = \sum_{k_0,l_0,\alpha_0} W_r(k_0,l_0,\alpha_0)$, which introduced in (650) gives

(653) $f_r = \frac{1}{2r} \mathrm{Tr}\, \tilde{\Lambda}^r = \frac{1}{2r} \sum_i \lambda_i^r$; This is because the Tr not depends on the representation, and in self-representation has only the eigenvalues along the diagonal. Going back now to (649)

(654) $\mathfrak{S} = 2^N \exp\left[-\frac{1}{2} \sum_i \sum_{r=1}^{\infty} \frac{(x\lambda_i)^r}{r}\right]$; But $-\ln(1-z) = \sum_{r=1}^{\infty} \frac{z^r}{r}$, (655), hence

(655) $$\mathfrak{S} = 2^N \exp\left[\frac{1}{2} \sum_i \ln(1 - x\lambda_i)\right] = 2^N \exp\left[\sum_i \ln\sqrt{1-x\lambda_i}\right] =$$
$$= 2^N \exp\left[\ln\left\{\prod_i \sqrt{1-x\lambda_i}\right\}\right] = 2^N \prod_i \sqrt{1-x\lambda_i}$$; One has now

the explicite expression of $\mathfrak{S}$, namely:

(656) $\boxed{\mathfrak{S} = 2^N \prod_i \sqrt{1-x\lambda_i}}$ where λ_i are the eigenvalues of the matrix $\tilde{\Lambda}$.

d.) The eigenvalues λ_i :

The $W_{r+1}(k,l,\alpha)$, $\alpha = 1,2,3,4$ can be expressed in function of $W_r(k',l',\alpha')$ (i.e. (651)) as follows

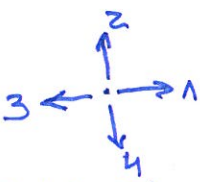


Fig 42: The possible α directions

$$W_{r+1}(k,l,1) = W_r(k-1,l,1) + W_r(k,l-1,2)\, e^{-i\frac{\pi}{4}} + W_r(k,l+1,4)\, e^{i\frac{\pi}{4}};$$
$$W_{r+1}(k,l,2) = W_r(k,l-1,2) + W_r(k-1,l,1) \cdot e^{+i\frac{\pi}{4}} + W_r(k+1,l,3)\, e^{-i\frac{\pi}{4}};$$
$$W_{r+1}(k,l,3) = W_r(k+1,l,3) + W_r(k,l-1,2)\, e^{i\frac{\pi}{4}} + W_r(k,l+1,4)\, e^{-i\frac{\pi}{4}};$$
$$W_{r+1}(k,l,4) = W_r(k,l+1,4) + W_r(k-1,l,1)\, e^{-i\frac{\pi}{4}} + W(k+1,l,3)\, e^{i\frac{\pi}{4}} \quad (657)$$

The construction method of the equations (657) is quite simple (k is x coordinate and l is y coordinate): taking for example th first row: the point $k,l,1$ can be reached by taking the last $(r+1)$th step from the left $(k-1)$, from below $(l-1)$, or from above $(l+1)$, but not from the right (in this case a bond is 2 times considered, which is forbidden, see explanations at (649)). The coefficients of W_r are the $e^{\frac{i}{2}\theta}$ factors (W_r direction in comparison to the W_{r+1} direction.).

Now we Fourier transform (657) by

(658) $$W_r(p,q,\alpha) = \sum_{k,l=0}^{L} e^{-\frac{2\pi i}{L}(pk+ql)} W_r(k,l,\alpha)$$

Hence multiplying (657) by $\exp[-\frac{2\pi i}{L}(pk+ql)]$ and suming over $\sum_{kl=0}^{L}$ we obtain :

$$W_{r+1}(p,q,1) = W_r(p,q,1)e^{-\frac{2\pi i}{L}p} + W_r(p,q,2)e^{-\frac{2\pi i}{L}q - i\frac{\pi}{4}} + 0 + W_r(p,q,4)e^{+\frac{2\pi i}{L}p + i\frac{\pi}{4}},$$

$$W_{r+1}(p,q,2) = W_r(p,q,1)e^{-\frac{2\pi i}{L}p + i\frac{\pi}{4}} + W_r(p,q,2)e^{-\frac{2\pi i}{L}q} + W_r(p,q,3)e^{+\frac{2\pi i}{L}p - i\frac{\pi}{4}} + 0,$$

(659) $$W_{r+1}(p,q,3) = 0 + W_r(p,q,2)e^{-\frac{2\pi i}{L}q + i\frac{\pi}{4}} + W_r(p,q,3)e^{+\frac{2\pi i}{L}p} + W_r(p,q,4)e^{+\frac{2\pi i}{L}q - i\frac{\pi}{4}},$$

$$W_{r+1}(p,q,4) = W_r(p,q,1)e^{-\frac{2\pi i}{L}p - i\frac{\pi}{4}} + 0 + W_r(p,q,3)e^{+\frac{2\pi i}{L}p + i\frac{\pi}{4}} + W_r(p,q,4)e^{+\frac{2\pi i}{L}q};$$

The huge advantage of (659) is that one has only (p,q) present in it. So we can write $\tilde{\Lambda}$ from (651) only as a 4×4 matrix, only dependent on the directions α at fixed p,q. Denoting: $\varepsilon = \exp[2\pi i/L]$; $z = \exp[i\pi/4]$, we have

(660) $$\hat{\Lambda} = \Lambda_{\alpha\alpha'} = \begin{bmatrix} \varepsilon^{-p} & z^{-1}\varepsilon^{-q} & 0 & z\varepsilon^{q} \\ z\varepsilon^{-p} & \varepsilon^{-q} & z^{-1}\varepsilon^{p} & 0 \\ 0 & z\varepsilon^{-q} & \varepsilon^{p} & z^{-1}\varepsilon^{q} \\ z^{-1}\varepsilon^{-p} & 0 & z\varepsilon^{p} & \varepsilon^{q} \end{bmatrix};$$

Now in order to find (656) one writes

$$\prod_i \sqrt{1-x\lambda_i} = \prod_p \prod_q \prod_\alpha \sqrt{1-x\lambda_{p,q,\alpha}} = \left[\prod_p\prod_q\prod_\alpha (1-x\lambda_{p,q,\alpha})\right]^{1/2} \quad (661)$$

But

(662) $$\prod_{\alpha=1}^{4}(1-x\lambda_{p,q,\alpha}) = \mathrm{Det}\big[\underbrace{\mathbb{1}-x\hat{\Lambda}}_{\tilde{V}}\big];$$ where $\mathbb{1}$ is the 4×4 unity matrix, and $\hat{\Lambda}$ is in (660)

But

(662) $$\tilde{V} = \begin{bmatrix} 1-x\varepsilon^{-p} & xz^{-1}\varepsilon^{-q} & 0 & zxe^{q} \\ xz\varepsilon^{-p} & 1-x\varepsilon^{-q} & xz^{-1}\varepsilon^{p} & 0 \\ 0 & xz\varepsilon^{-q} & 1-x\varepsilon^{p} & xz^{-1}\varepsilon^{q} \\ xz^{-1}\varepsilon^{-p} & 0 & xz\varepsilon^{p} & 1-x\varepsilon^{p} \end{bmatrix} = \mathbb{1} - x\hat{\Lambda}$$

One finds: $(z^4=-1)$:

$$\mathrm{Det}\tilde{V} = (1+x^2-2xC(p))(1+x^2-2xC(q)) - 4x^2[C(q)-x][C(p)-x] + 4x^4 =$$

(663) $$= (1+x^2)^2 - 2x(1-x^2)(C(p)+C(q))$$

where

(664) $$C(p) = \frac{\varepsilon^{p}+\varepsilon^{-p}}{2} = \cos\frac{2\pi p}{L}; \quad C(q) = \frac{\varepsilon^{q}+\varepsilon^{-q}}{2} = \cos\frac{2\pi q}{L}$$

Consequently, using (656) and (640), one has

(665) $$\mathfrak{S} = 2^N \prod_{p,q=0}^{L} \left[(1+x^2)^2 - 2x(1-x^2)\left(\cos\frac{2\pi p}{L} + \cos\frac{2\pi q}{L}\right)\right]^{1/2}$$ and the partition function becomes

(666) $$\boxed{\begin{aligned} Z &= 2^N(1-x^2)^{-N}\prod_{p,q=0}^{L}\left[(1+x^2)^2 - 2x(1-x^2)\left(\cos\frac{2\pi p}{L} + \cos\frac{2\pi q}{L}\right)\right]^{1/2} \\ x &= \tanh(\beta J). \end{aligned}}$$

The thermodinamic potential $\Phi = -k_B T \ln Z$ (here is the free energy)

(667) $$\boxed{\begin{aligned} \Phi = &-k_B T N \ln 2 + k_B T N \ln(1-x^2) \\ &- \frac{1}{2}k_B T \sum_{p,q=0}^{L} \ln\left[(1+x^2)^2 - 2x(1-x^2)\left(\cos\frac{2\pi p}{L} + \cos\frac{2\pi q}{L}\right)\right]; \end{aligned}}$$

or in the thermodinamic limit $\sum_p \to \frac{\Lambda}{2\pi}\int_0^{2\pi} d\omega$; $\frac{2\pi p}{L} \to \omega$, we have

(668) $$\Phi = N k_B T \ln\frac{1-x^2}{2} - \frac{k_B T N}{8\pi^2}\int_0^{2\pi} d\omega_1 \int_0^{2\pi} d\omega_2 \ln\left[(1+x^2)^2 - 2x(1-x^2)(\cos\omega_1 + \cos\omega_2)\right].$$

The critical temperature T_c.

The function under the logaritm in ϕ from (667) is

(669) $f(x) = (1+x^2)^2 - 2x(1-x^2)\cdot a$; $a = \left(\cos\frac{2\pi p}{L} + \cos\frac{2\pi q}{L}\right)$; $a \le 2$

has the form (see Fig. 43). If a increases $f(x_c) \to 0$, and exactly for $a=2$ touches the $0x$ axis. Then, for $a=2$ one has from (669):

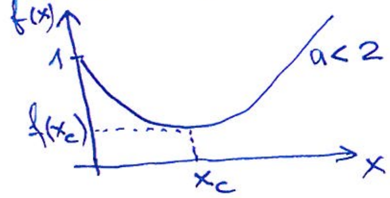


Fig 43.

$\underbrace{(1+x^2)^2 - 4x(1-x^2)}_{(x^2+2x-1)^2} = 0$; (670)

Thus: $x^2+2x-1=0 \Rightarrow x_{1,2} = -1 \pm \sqrt{2}$ (671)

Since $J>0 \Rightarrow$ one needs $x>0$, hence

(672) $\tanh \beta_c J = \sqrt{2}-1$; is the expression of the critical temperature

This gives

(673) $k_B T_c = \dfrac{J}{\ln \frac{1}{\sqrt{\sqrt{2}-1}}} = 2.269185..J$

Specific heat.

Around T_c in (668) one expands $\cos w = 1 - \frac{w^2}{2} + \dots$ and finds the integral part of ϕ as

(674) $\phi \sim \int_0^{2\pi}\int_0^{2\pi} \ln\left[F(x) + x(1-x^2)(w_1^2+w_2^2)\right] dw_1 dw_2$; $F(x) = (1+x^2)^2 - 4x(1-x^2)$

Now $F(x)$ Taylor expanded around x_c gives

(675) $F(x) = F(x_c) + (x-x_c)\frac{\partial F(x)}{\partial x}\Big|_{x=x_c} + \frac{(x-x_c)^2}{2}\cdot\frac{\partial^2 F}{\partial x^2}\Big|_{x=x_c} + \dots$

But as Fig 43 shows $\partial F/\partial x\,|_{x=x_c} = 0$, hence $F(x)$ becomes:

(676) $F(x) = F(x_c) + \frac{1}{2}(x-x_c)^2 \frac{\partial^2 F}{\partial x^2} + \dots$; $(x-x_c)^2 \sim t^2$, hence

around T_c:

(677) $\phi \approx \int_0^{2\pi}\int_0^{2\pi} dw_1 dw_2 \ln\left[C_1 t^2 + C_2(w_1^2+w_2^2)\right]$; for the singular term

This gives

(678) $\phi \approx C_1 + C_2 (T-T_c)^2 \ln|T-T_c|$;

And from here $C \sim \frac{\partial^2 \phi}{\partial T^2}$ one find for the specific heat

(679) $C \sim -2T_c \ln|T-T_c|$. The thermodynamic potential is continuous, but the specific heat has a logaritmic divergence, so

(680) $\boxed{\alpha = 0}$

The magnetization:

Has the expression

(681) $m = \frac{M}{N} = \left[1 - \frac{1}{\sinh^4(2\beta J)}\right]^{1/8}$;

From here $\sinh(2\beta J) = 1\,|_{T=T_c}$ (682)

But

$\sinh(2\beta J) = 2\sinh\beta J\cosh\beta J =$
$= 2\tanh\beta J\cosh^2\beta J = \frac{2\tanh\beta J}{1-\tanh^2\beta J} = 1$

gives T_c, i.e $x = \tanh\beta J$, the equation $x^2+2x-1=0$ is reobtained (see (671)) which provides back the known T_c.

The function $G(T) = 1 - \sinh^{-4}(2\beta J)$ expanded around T_c gives

(682) $G(T) = G(T_c) + (T-T_c)\frac{\partial G}{\partial T}\Big|_{T=T_c}$; and since $G(T_c) = 0 \Rightarrow G(T) \sim t\,|_{T\to T_c}$

hence $m \sim t^{1/8} \Rightarrow$

(683) $\boxed{\beta = \frac{1}{8}}$

For other exponents: $\gamma = \frac{7}{4}$; $\delta = 15$; $\nu = 1$; $\eta = \frac{1}{4}$ (correlation function and field dependence is needed to deduce them.

(See annex.)

The η critical exponent:

If one has the fluctuation of the $S_{k\ell}$ spin denoted as $\Delta S_{k\ell}$, then the correlation function

(690) $\langle \Delta S_{k\ell} \Delta S_{mn} \rangle \sim \left[(k-m)^2 + (\ell-n)^2\right]^{-1/8}$; $T = T_c$

But $r = \sqrt{(k-m)^2 + (\ell-n)^2}$, so

$$\langle \Delta S(\vec{r}_i) \Delta S(\vec{r}_j) \rangle \sim \frac{1}{r^{1/4}}; \quad r = |\vec{r}_i - \vec{r}_j|$$

Since $G(\vec{r}) \sim \frac{1}{r^{d-2+\eta}}$, and $d = 2 \Rightarrow \eta = \frac{1}{4}$, consequently

(691) $\boxed{\eta = \frac{1}{4}}$

The ν critical exponent:

Outside of T_c, the correlation function is of the form ($K = \beta J$):

(692) $G(\vec{r}) \sim (K_c - K) \exp\left[-\frac{r}{\xi}\right]$; $\xi = \frac{1}{4(K_c - K)}$; (close to T_c) $T > T_c$

Consequently

(693) $\xi = \frac{1}{4J\left(\frac{1}{k_B T_c} - \frac{1}{k_B T}\right)} = \frac{1}{\frac{4J}{k_B} \frac{T - T_c}{T_c T}} \Rightarrow \xi \sim \frac{1}{t} = t^{-1}$; $\xi \sim t^{-\nu}$ is the ν definition, hence

(694) $\boxed{\nu = 1}$

Magnetic susceptibility:

Close to the T_c value the susceptibility behaves as

(695) $\chi \approx \frac{N\bar{\mu}^2}{k_B T} \begin{cases} C_+ \cdot t^{-7/4}; & t > 0 \\ C_- \cdot |t|^{-7/4}; & t < 0 \end{cases}$; where $t = \frac{T - T_c}{T_c}$; The two constants $C_+ \approx 0.9625$; $C_- \approx 0.02554$; so $\frac{C_+}{C_-} = 37.69$; (the mean-field value is 2)

Because $\chi \sim |t|^{-\gamma}$ defines the γ exponent, one has

(696) $\boxed{\gamma = \frac{7}{4}}$