$$C_{H=0} = \frac{\partial}{\partial T}\langle \mathcal{H} \rangle|_{H=0} =$$

$$= \frac{\partial}{\partial T}\left[\frac{1}{Z}\sum \mathcal{H} e^{-\beta\mathcal{H}}\right] =$$

$$= -\frac{1}{k_B T^2}\frac{\partial}{\partial \beta}\left[\frac{1}{Z}\sum \mathcal{H} e^{-\beta\mathcal{H}}\right] =$$

$$= -\frac{1}{k_B T^2}\left[\frac{1}{Z}\sum (-\mathcal{H}^2) e^{-\beta\mathcal{H}} + \right.$$

$$\left. + \frac{1}{Z^2}\left(\sum \mathcal{H} e^{-\beta\mathcal{H}}\right)^2\right]$$

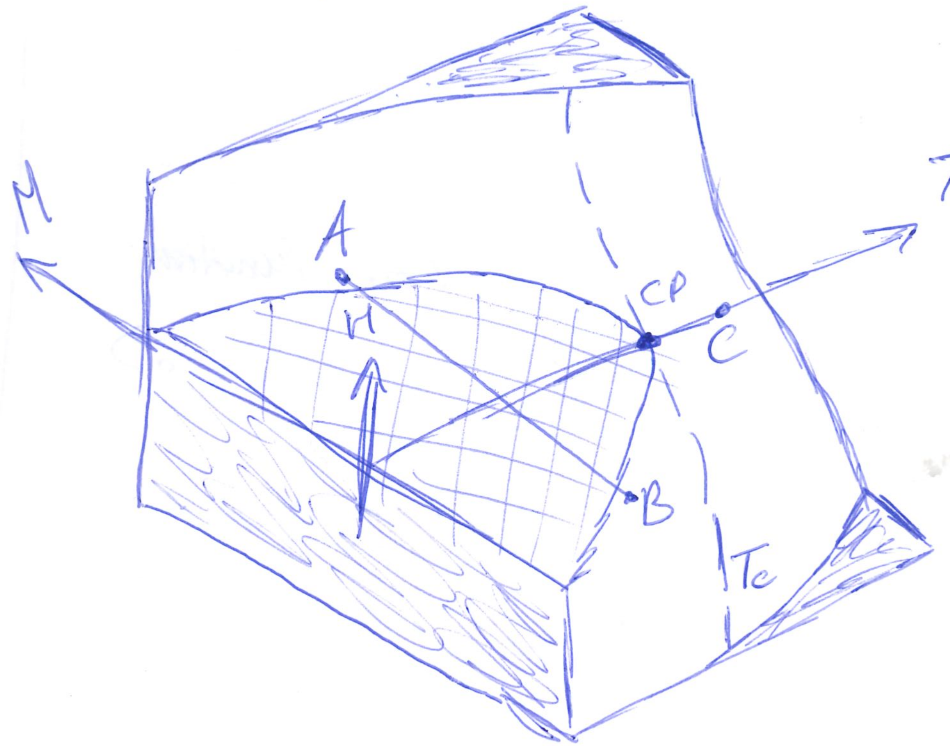
$$\Rightarrow \quad C_{H=0} = k_B\left[\langle(\beta\mathcal{H})^2\rangle - \langle\beta\mathcal{H}\rangle^2\right]$$

C_H can be calculated from energy fluctuations

2.2.6 Phase transition and critical phenomena

2.2.6.1) Correlation length, universality and critical exponents.

Phase diagram of a ferromagnet



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At critical point ($T=T_c$, $H=0$)

$$\left.\frac{\partial H}{\partial M}\right|_{T=T_c} = 0$$

$\Rightarrow$ Susceptibility $\chi = \left.\frac{\partial M}{\partial H}\right|_T$ is divergent

Relation to ~~Together with~~ the correlation function:

$$\tilde{\chi} = \frac{1}{N}\left.\frac{\partial M}{\partial H}\right|_T = \text{(Susceptibility pro Spin)}$$

$$= \beta \sum_j \left(\langle S_j S_0\rangle - \langle S_j\rangle\langle S_0\rangle\right)$$

Spin-spin correlation function:

$$G(|\underline{r}_j - \underline{r}_0|) = \langle S_j S_0\rangle - \langle S_j\rangle\langle S_0\rangle$$

$$\Rightarrow \tilde{\chi} = \beta \sum_j G(|\underline{r}_j - \underline{r}_0|)$$

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Correlation function is bound:

$$s_i \in \{-1,+1\} \Rightarrow s_i s_0 \in \{-1,+1\}$$

$$\Rightarrow |G(|\underline{r}_j - \underline{r}_0|)| \leq 1$$

Conclusion: Sum (or integral) can diverge only ~~when~~ when assymptotic decay of $G(r)$ as $r \to \infty$ is slow enough:

$$G(r) \sim r^{-p}$$

$$\Rightarrow \underset{\substack{\text{(sphere of}\\ \text{radius } R)}}{\int d^3r}\, r^{-p} \sim \int^R dr\, r^{2-p} \sim R^{3-p}$$

Conclusion: $G(r)$ decays slower than r^{-3} at the critical point

however for $T \neq T_c$ we have an exponential decay $G(r) \sim \exp(-r/\xi)$ with a correlation ~~line~~ length ξ.

Remark: Critical point is characterized by a long-range correlation.

Critical exponents

For a quantitative description of singularities at critical point we define critical exponents:

Magnetization (per Spin): $m(T, H=0) \sim |T-T_c|^{\beta}$

Susceptibility: $\bar{\chi}(T, H=0) \sim |T-T_c|^{-\gamma}$

Correlation function: $G(r, T=T_c) \sim r^{-(d-2+\eta)}$

Specific heat: $C_{H=0}(T) \sim |T-T_c|^{-\alpha}$

Correlation ~~time~~ length: $\xi(T, H=0) \sim |T-T_c|^{-\nu}$

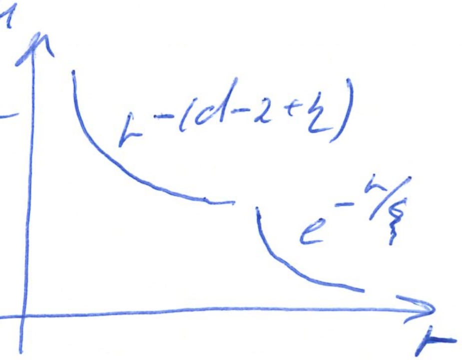
Magnetization: $m(T=T_c, H) \sim H^{1/\delta}$

and so on.

The defined exponents are not all independent, but related to each other through scaling relations.

Example:

$$\bar{\chi} \sim \int d^d r \, G(r, T) \sim \int_{r \lesssim \xi} d^d r \, r^{-(d-2+\eta)} \sim \xi^{2-\eta}$$



Temperature dependence:

$$\tau^{-\gamma} \sim \tau^{-\nu(2-\eta)} \quad \text{with } \tau = \frac{T-T_c}{T_c}$$

$$\Rightarrow \boxed{\gamma = (2-\eta)\nu}$$

Group renormalization theory shows:

There exist two independent critical exponents.

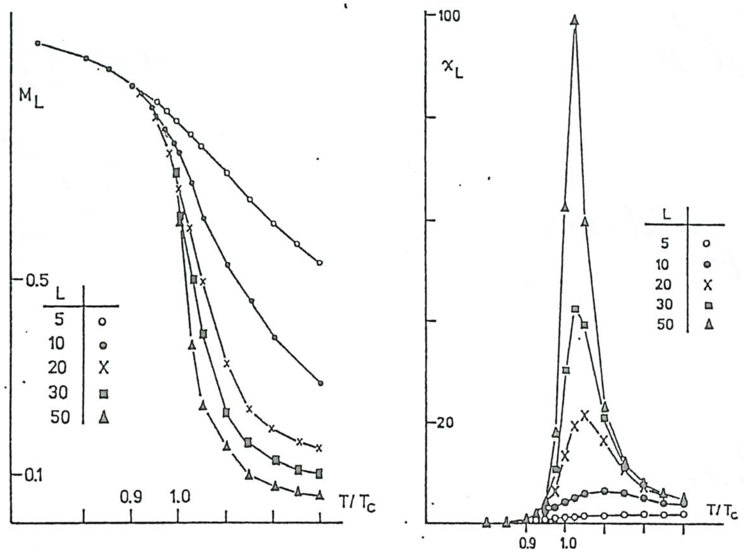


Fig. 3.9. Dependence of the magnetization and susceptibility on the linear lattice size L. The data shown are for the two-dimensional Ising model

2.2.6.2) Theory of small systems (Finite-size scaling)

In a finite system, thermodynamic quantities and correlation functions have no divergence or singularities, since state sum is an analytic function of a finite sum of exponential functions.

Near the critical point: $\xi \gg a$

$\Rightarrow$ Correlation ~~time~~ length ξ is only relevant ~~time~~ length scale (in limit $N \to \infty$)

Ansatz (for example for susceptibility)

$$\boxed{\chi(\tau, L) = \tau^{-\gamma}\, \Omega\left(\frac{L}{\xi}\right)}$$

scaling function

with L - linear system size (e.g. $N = L^d$)

Properties of scaling function Ω:

(i) For $L \to \infty$ we should obtain the behavior of an infinite system.

$\Rightarrow \Omega(x) \to$ const, for $x \to \infty$

(ii) For $T = T_c$, χ must remain finite (for $L < \infty$)

$\Rightarrow \lim_{\tau \to 0} \chi(\tau, L)$ is independent of τ $\quad \frac{L^{\gamma/\nu}}{\xi^{\gamma/\nu}}$

$\Rightarrow \Omega(x) \sim x^{\gamma/\nu}$

This means $\boxed{\chi(\tau=0, L) \sim L^{\gamma/\nu}}$

Conclusion: The (seeming) drawback of simulations, which can handle only systems of finite size, ~~will~~ is transformed into an advantage through the finite-size scaling.

2.2.6.3) 1D Ising model

Partition function ~~state sum~~:

$$Z(s_0, s_{N+1}) = \sum_{s_1 \dots s_N} e^{K \sum_{i=0}^{N} s_i s_{i+1}} =$$

$$= \sum_{s_1 \dots s_N} e^{K s_0 s_1} e^{K s_1 s_2} \dots e^{K s_N s_{N+1}}$$

with $K = \beta J$

Matrix representation:

$$\begin{pmatrix} Z_{++} & Z_{+-} \\ Z_{-+} & Z_{--} \end{pmatrix} = T^{N+1}$$

with the transfer matrix:

$$T = \begin{pmatrix} e^{K} & e^{-K} \\ e^{-K} & e^{K} \end{pmatrix}$$

Eigen-values and eigen vectors:

$$\det(T - \lambda I) = 0$$

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$$\det\begin{pmatrix} e^K-\lambda & e^{-K} \\ e^{-K} & e^K-\lambda \end{pmatrix} = (e^K-\lambda)^2 - e^{-2K} = 0$$

$$\Rightarrow \lambda_{1,2} = e^K \pm e^{-K}$$

$$\boxed{\lambda_1 = 2\cosh K, \quad \lambda_2 = 2\sinh K}$$

$$\begin{pmatrix} e^K-\lambda_i & e^{-K} \\ e^{-K} & e^K-\lambda_i \end{pmatrix} \underline{v}_i = 0$$

$$\Rightarrow \underline{v}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}; \quad \underline{v}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Transformation matrix U:

$$U^{-1} T U = D = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

$$\Rightarrow U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}; \quad U^{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

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Back to the ~~state sum~~ partition function:

$$T^{N+1} = U \underbrace{U^{-1} T U}_{D} \underbrace{U^{-1} T}_{D} \dots T U U^{-1} =$$

$$= U D^{N+1} U^{-1} =$$

$$= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} \lambda_1^{N+1} & 0 \\ 0 & \lambda_2^{N+1} \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} =$$

$$= \frac{1}{2}\begin{pmatrix} \lambda_1^{N+1} + \lambda_2^{N+1} & \lambda_1^{N+1} - \lambda_2^{N+1} \\ \lambda_1^{N+1} - \lambda_2^{N+1} & \lambda_1^{N+1} + \lambda_2^{N+1} \end{pmatrix}$$

For $N \gg 1$ (thermodynamic limit)

$Z_{ij} = \frac{1}{2}\lambda_1^{N+1}$ (independent of constraints)

Free energy per Spin:

$$f = \frac{F}{N} = -k_B T \ln \lambda_1$$

$$\boxed{f = -k_B T \ln(2\cosh K)}$$