INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE CENTRATOM TRIESTE

SMR/382- 40

WORKSHOP ON SPACE PHYSICS:
"Materials in Micorgravity"
27 February - 17 March 1989

"Phase Transitions and Critical Phenomena: An Introduction"

I. EGRY
German Aerospace Research Establishment, DLR
Köln - Proz
Federal Republic of Germany

PHASE TRANSITIONS AND CRITICAL PHENOMENA
AN INTRODUCTION

I. Egry
German Aerospace Research Establishment, DLR
Köln – Porz, FRG

Workshop on Space Physics
Materials in Microgravity
Trieste, 27.2.–17.3.1989

DFVLR

1.) INTRODUCTION

1.1) Statement of the Problem

"Every function describing a physical quantity is continuous, differentiable and analytical."

(Anonymous physicist)

"Thermodynamical functions at a phase transition are discontinuous or non-analytical".

(Ehrenfest)

DFVLR

1.2) Examples for Phase Transitions

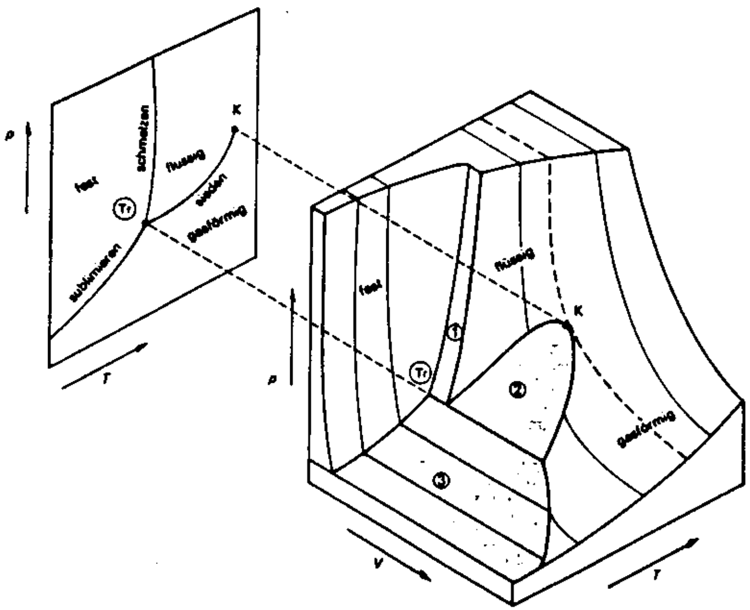
Phases	Transition	Order Parameter
vapour/liquid	condensation	density difference
liquid/liquid	phase separation	density difference
liquid/liquid	superfluidity	wave function
liquid/solid	melting	density difference
solid/solid	magnetic	magnetization
solid/solid	structural	displacement
solid/solid	order-disorder	order
solid/solid	superconductor	energy gap

DFVLR

1.3) Phase Diagram

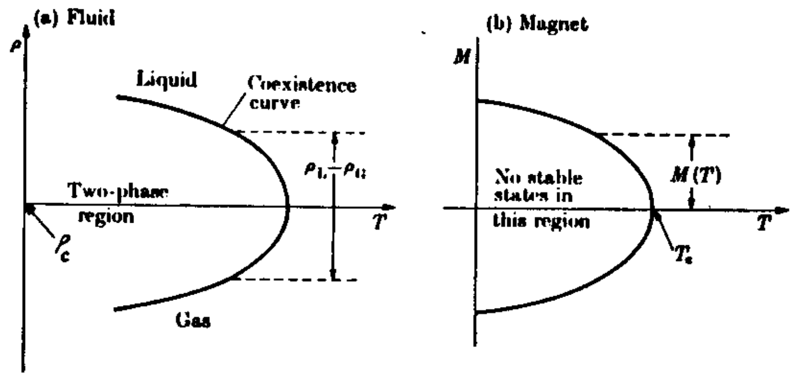
The Phase diagram defines the equilibrium states of a thermodynamic system.

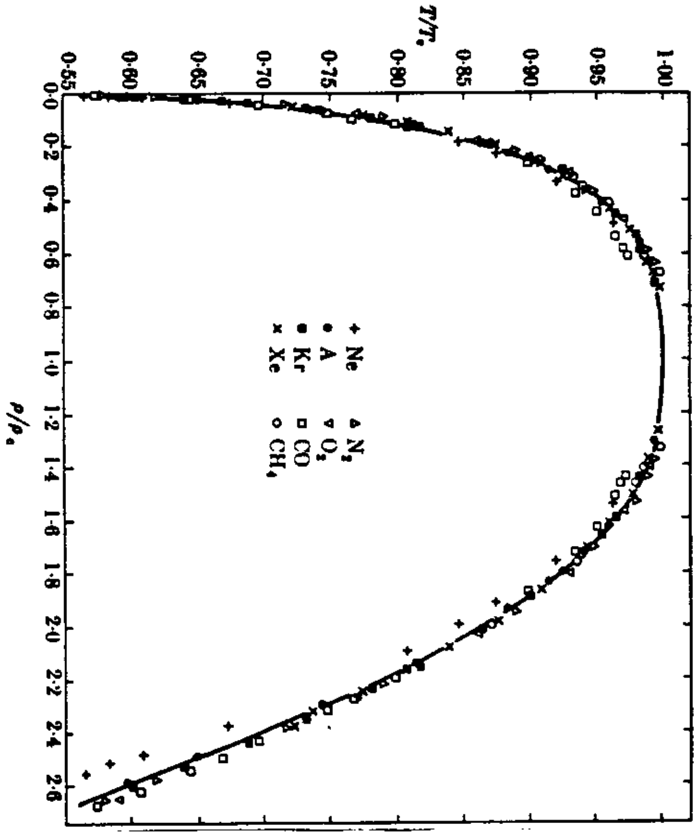
In particular, *phases*, *coexistence curves* and *critical points* are defined.

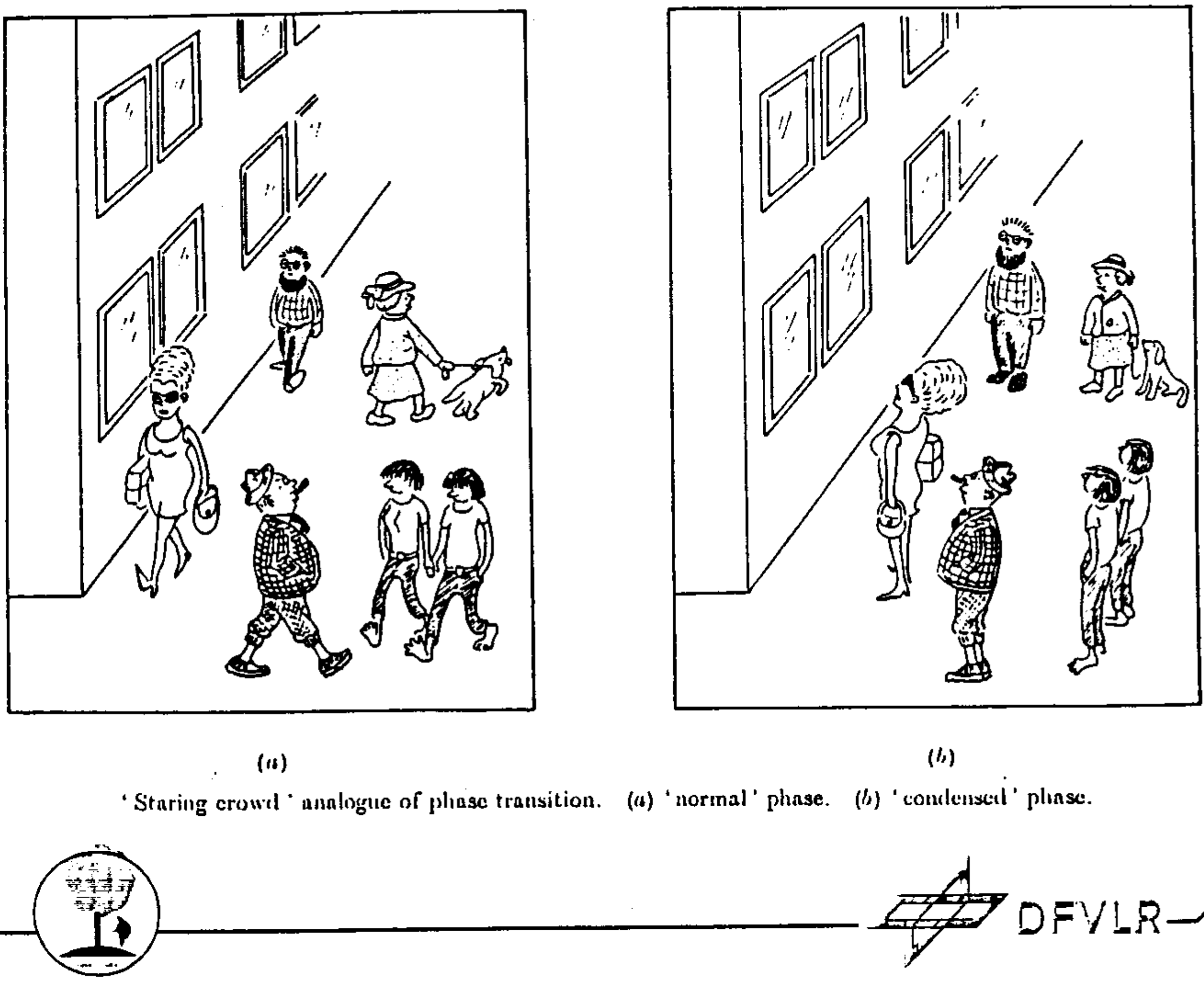


1.4) Properties of Phase Transitions

- **Long Range Order**
  range of order ≫ interaction range
- **Order Parameter**
  = 0 in the unordered phase, ≠ 0 in the ordered phase
- **Collective Behaviour**
  correlation extends over macroscopic portion of sample
- **Universality**
  Different systems behave similarly near the critical point ⇒ definition of universality classes







(a) (b)

'Staring crowd' analogue of phase transition. (a) 'normal' phase. (b) 'condensed' phase.

2.) THEORY

2.1) Models

The simplest models are *Spin Models* for magnetic phase transitions.

All degrees of freedom (lattice vibrations, electronic,..) are suppressed, only spin variables are retained.

ISING - MODEL

$$\mathscr{H} = -\frac{1}{2} \sum J_{ij} S_i^z S_j^z$$

HEISENBERG - MODEL

$$\mathscr{H} = -\frac{1}{2} \sum J_{ij} \underline{S}_i \underline{S}_j$$

Important Parameters:

- **Range of Interaction J_{ij}**
- **Lattice Dimensionality d**
- **Spin Dimensionality D**

Due to Universality, most Systems can be mapped onto Spin Models

⇒ *Pseudospin Models*

2.2) Model Hamiltonians

Special cases of the model Hamiltonian The parameter D is the spin dimensionality. After Stanley and Lee (1970).

D	*Hamiltonian*	*Name*	*System*
1	$\mathscr{H} = -J \sum_{\langle ij \rangle} S_{iz}S_{jz}$	Ising model	one-component fluid; binary alloy, mixture
2	$\mathscr{H} = -J \sum_{\langle ij \rangle} (S_{ix}S_{jx} + S_{iy}S_{jy})$	plane rotator model (Vaks-Larkin model)	λ-transition in a Bose fluid
3	$\mathscr{H} = -J \sum_{\langle ij \rangle} (S_{ix}S_{jx} + S_{iy}S_{jy} + S_{iz}S_{jz})$	classical Heisenberg model	ferromagnet; antiferromagnet
⋮			
∞	$\mathscr{H} = -J \sum_{\langle ij \rangle} \left(\sum_{n=1}^{\infty} S_{in}S_{jn} \right)$	spherical model	none

Some of the cases in which the model Hamiltonian is exactly soluble. Here the notation n.n. *stands for nearest-neighbour interactions only. A blank indicates that the system has not yet been solved. D and d denote the spin and lattice dimensionality respectively. After Stanley and Lee* (1970)

D	*d* = 1	*d* = 2	*d* = 3	*d* > 3
1	all *H*; both n.n. and $1/r^{d+\varepsilon}$	*H* = 0; n.n.	—	—
2	*H* = 0; n.n.	—	—	—
3	*H* = 0; n.n.	—	—	—
⋮				
∞	all *H*; both n.n. and $1/r^{d+\varepsilon}$	all *H*; both n.n. and $1/r^{d+\varepsilon}$	all *H*; both n.n. and $1/r^{d+\varepsilon}$	only critical-point exponents are known exactly

2.3) Mean Field Approximation (MFA)

Consider Ising Model in an external field:

$$\mathcal{H} = -\frac{1}{2}\sum_{i,j} v_{ij}\mu_i\mu_j - \sum_i \mu_i B$$

without interaction: $v_{ij} = 0 \quad \Rightarrow \quad \mu = \langle\mu_i\rangle = \frac{\mu_B}{kT} B$

with interaction: $v_{ij} \neq 0$

Replace one of the Operators by its mean Value (⇔MFA)

$$\frac{1}{2}\sum_{i,j} V_{ij}\ \mu_i\ \mu_j \quad \rightarrow \quad \sum_{i,j} V_{ij}\ \langle\mu_j\rangle\ \mu_i$$

$$\mathcal{H}^{eff} = -\sum_i \mu_i\ (B + \sum_j V_{ij}\ \langle\mu_j\rangle) = -\sum_i \mu_i\ B_i^{eff}$$

$$\langle\mu_i\rangle = \frac{\mu_B}{kT} B_i^{eff} = \frac{\mu_B}{kT}(B + \sum_j V_{ij}\langle\mu_j\rangle)$$

$$\langle\mu_i\rangle = \mu = \frac{\mu_B}{kT}(B + V_0\mu)$$

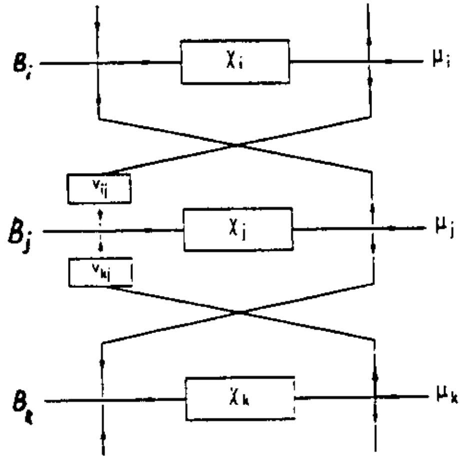
This yields:

$$\mu = \frac{\mu_B}{k\ (T - T_c)}\ B \qquad \text{(Curie – Weiss law)}$$

$$V_0 = \sum_j V_{ij} \qquad kT_c = \mu_B V_0$$

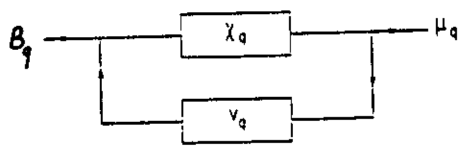
The MFA as a Network Theory

$$\langle\mu_i\rangle = \chi_i\,(B_i + \sum_j V_{ij}\langle\mu_j\rangle)$$



or, after diagonalization:

$$\langle\mu_q\rangle = \chi_q\,(B_q + V_q\,\langle\mu_q\rangle)$$



This is a feed-back loop !

2.4) Landau Theory

Second Order Phase Transitions

Expand free energy in powers of order parameter:

$$F = F(T, M) = F_0(T) + F_2(T) M^2 + F_4(T) M^4 + ...$$

Due to symmetry $M \rightarrow -M$ only even powers of M.

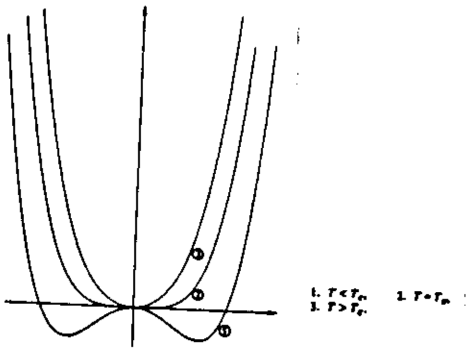
Equlibrium value of M determined by: $\frac{\partial F}{\partial M} = 0$

$M = 0$ shall be solution for $T > T_c$
$M \neq 0$ shall be solution for $T < T_c$

$$F(T, M) = a(T - T_c) M^2 + bM^4$$

Solution for $T < T_c$:

$$M_S^2 = -\frac{F_2}{2F_4} = \frac{a(T_c - T)}{2b} \quad \text{with} \quad F(T, M_S) = -\frac{a^2 (T_c - T)^2}{4b}$$



DFVLR

2.5) Critical Exponents

Critical Exponents describe the non-analytical behaviour near the critical point.

Definition: λ is critical exponent of f(x) at x=0, if:

$$\lambda = \lim_{x \to 0} \frac{\ln |f(x)|}{\ln x}$$

Example: $f(x) = x^\lambda \qquad \lambda \in \mathbb{R}$

Usually, $x = \frac{|T - T_c|}{T_c}$ **(reduced temperature)**

Some Critical Exponents

f(x)	Fluid	Magnet
Specific Heat	$c_v \sim x^{-\alpha}$	$c_H \sim x^{-\alpha}$
Susceptibility	$\kappa_T \sim x^{-\gamma}$	$\chi \sim x^{-\gamma}$
Order Parameter	$\lvert\rho_n - \rho_g\rvert \sim x^\beta$	$M_s \sim x^\beta$
Ordering Field	$\lvert p - p_c\rvert \sim \lvert\rho - \rho_c\rvert^\delta$	$H \sim M^\delta$

DFVLR

Landau Theory - Critical Exponents

$$M^2 = \frac{a\,(T_c - T)}{2b} \Rightarrow M \sim (T_c - T)^{1/2} \qquad \beta = 1/2$$

$$H = \left.\frac{\partial F}{\partial M}\right|_{T = T_c} = 4bM^3 \qquad \delta = 3$$

$$\chi^{-1} = \frac{\partial H}{\partial M} = 2a\,(T - T_c) + 12bM^2$$

$$T > T_c \Leftrightarrow M = 0 \Leftrightarrow \chi^{-1} = 2a(T - T_c) \qquad \gamma = 1$$

$$T < T_c \Leftrightarrow M \neq 0 \Leftrightarrow \chi^{-1} = 4a(T - T_c) \qquad \gamma = 1$$

$$c = -T\,\frac{\partial^2 F}{\partial T^2}$$

$$T > T_c \Leftrightarrow M = 0 \Leftrightarrow F = 0 \Leftrightarrow c = 0 \qquad \alpha = 0$$

$$T < T_c \Leftrightarrow M^2 = \frac{a(T_c - T)}{2b} \Leftrightarrow c = T\,\frac{a^2}{2b} \qquad \alpha = 0$$

The Specific Heat is discontinuous at $T = T_c$

$$\Delta c = \frac{T_c a^2}{2b}$$

DFVLR

Beziehung	$C_H \sim t^{-\alpha}$	$M_s \sim t^{\beta}$	$\chi \sim t^{-\gamma}$	$H_i \sim M^{\delta}$	$\xi \sim t^{-\nu}$	$\chi \sim k^{-(2-\eta)}$
Exponent	α	β	γ	δ	ν	η
Landau-Theorie	0[1])	$\frac{1}{2}$	1	3	$\frac{1}{2}$	0
2d-Ising[3])	0[2])	$\frac{1}{8}$	$\frac{7}{4}$	15	1	$\frac{1}{4}$
$n = 1$ 3d-Ising[4])	0,1100 ±0,0024	0,325 ±0,001	1,2402 ±0,0009	4,816 ±0,015	0,6300 ±0,0008	0,0315 ±0,0025
$n = 2$ 3d-XY[4])	−0,0079 ±0,0030	0,3454 ±0,0015	1,3160 ±0,0012	4,810 ±0,021	0,6693 ±0,0010	0,0335 ±0,0025
$n = 3$ 3d-Heisenberg[4])	−0,1162 ±0,003	0,3646 ±0,0012	1,3866 ±0,0012	4,803 ±0,016	0,7054 ±0,0011	0,0340 ±0,0025
$n = \infty$ 3d-Sphärisches Modell[5])	−1	$\frac{1}{2}$	2	5	1	0

SCALING LAWS

$$2\,(\beta - 1) + \alpha + \gamma = 0 \qquad \beta\,(\delta - 1) - \gamma = 0$$

DFVLR

2.6) Landau Theory
First Order Phase Transitions

The Order Parameter changes discontinuously at a First Order Phase Transition.

⇒ Modify Power Expansion of Free Energy:

$$F(T,M) = a\,(T - T_0)\,M^2 - bM^4 + cM^6$$

Note: $T_0 \neq T_c$, $b > 0$, $c > 0$

Extrema are given by

$$\frac{\partial F}{\partial M} = 0 = 2M\,\{a(T - T_0) - 2bM^2 + 3cM^4\}$$

⇒ Minima:

$$M = 0 \qquad T > T_0$$

$$M^2 = \frac{b + \sqrt{b^2 - 3ac(T - T_0)}}{3c} \qquad T < T_1$$

$$T_1 = T_0 + \frac{b^2}{3ac}$$

T_c **is defined by** $F(T_c, 0) = F(T_c, M^2)$

$$T_0 < T_c = T_0 + \frac{b^2}{4ac} < T_1$$

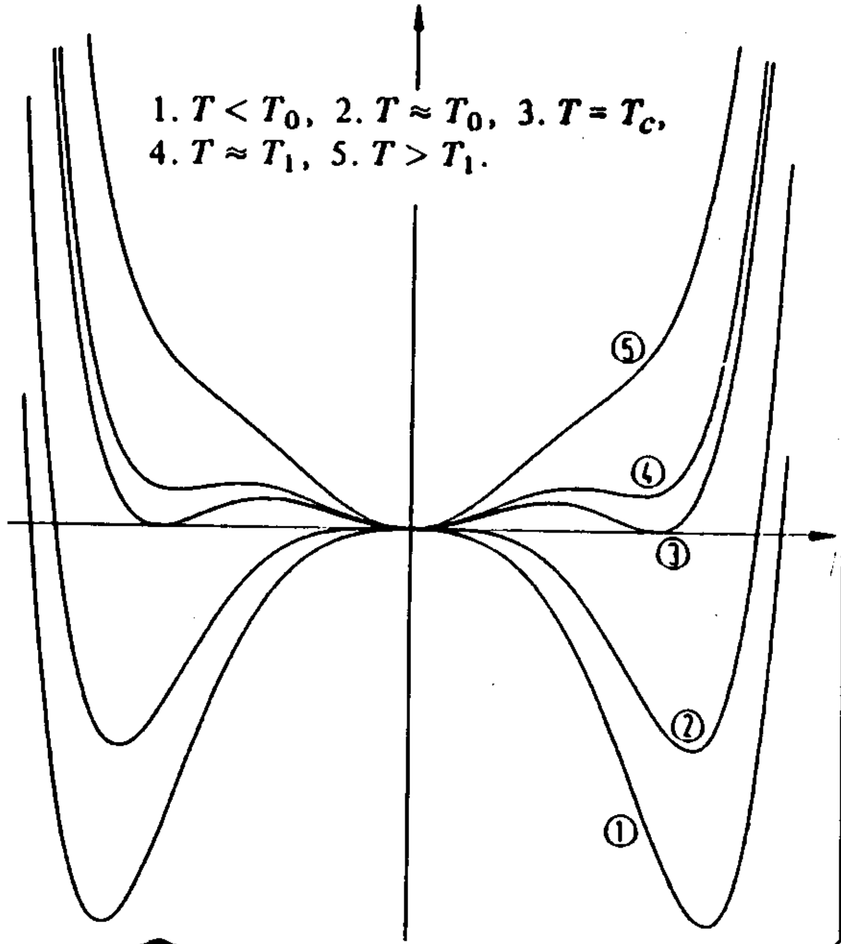
For $T_0 < T < T_1$ **Metastable Phases exist.**

At $T = T_c$ **the Order Parameter changes discontinuously.**

DFVLR

Landau Theory

Free Energy at a First Order Phase Transition



DFVLR

3.) CONCLUSION

3.1) Summary

- Phase transitions are drastic changes in the state of matter either discontinuously (1st order transition) or continuously, but non-analytically (2nd order).
- Phase change is characterized by the onset of long range order described by an order parameter.
- Near the critical point, universality classes can be defined, according to the values of the critical exponents.
- Classical theories (MFA, Landau) are qualitatively correct, (they satisfy scaling laws) but quantitatively wrong.
- Theory of phase transitions deals only with equilibrium phenomena, temporal evolution (dynamics) is not considered.

DFVLR

3.2) Bibliography

1. D. Beysens, J. Straub, D.J. Turner
   Phase Transitions and Near-Critical Phenomena
   In: Fluid Sciences and Material Science in Space, H.U. Walter ed.
2. H.E. Stanley
   Introduction to Phase Transitions and Critical Phenomena
   Clarendon Press Oxford 1971
3. M.E. Fisher
   The Theory of Equilibrium Critical Phenomena
   Repts. Prog. Phys.30, 615, (1967)
4. J.D. Gunton, M. San Miguel, P.S. Sahni
   The Dynamics of First Order Phase Transitions
   Phase Transitions, Vol.8 Domb and Green eds., Academic Press London
5. R.D. Mattuck, B. Johansson
   Quantum Field Theory of Phase Transitions in Fermi Systems
   Adv. Physics 17, 509, (1968)
6. H. Thomas
   Phase Transitions, Soft Modes, and Critical Fluctuations
   IEEE Trans. Magns, 5, 874, (1969)

DFVLR