Ground Work towards Understanding COMPLEXITY

An Introduction to Critical Phenomena

Y.M. WONG

LAFAYETTE COLLEGE

3/2/2012

Q: Mechanisms/Origins of power law?

Fractional Time or Frequency *Power Law*:

$$\frac{1}{t^{1-\alpha}} = \sum_{n=0}^{\infty} a_n e^{i\omega_n t} \;\; meaningful?$$

Mandelbrolt says No.

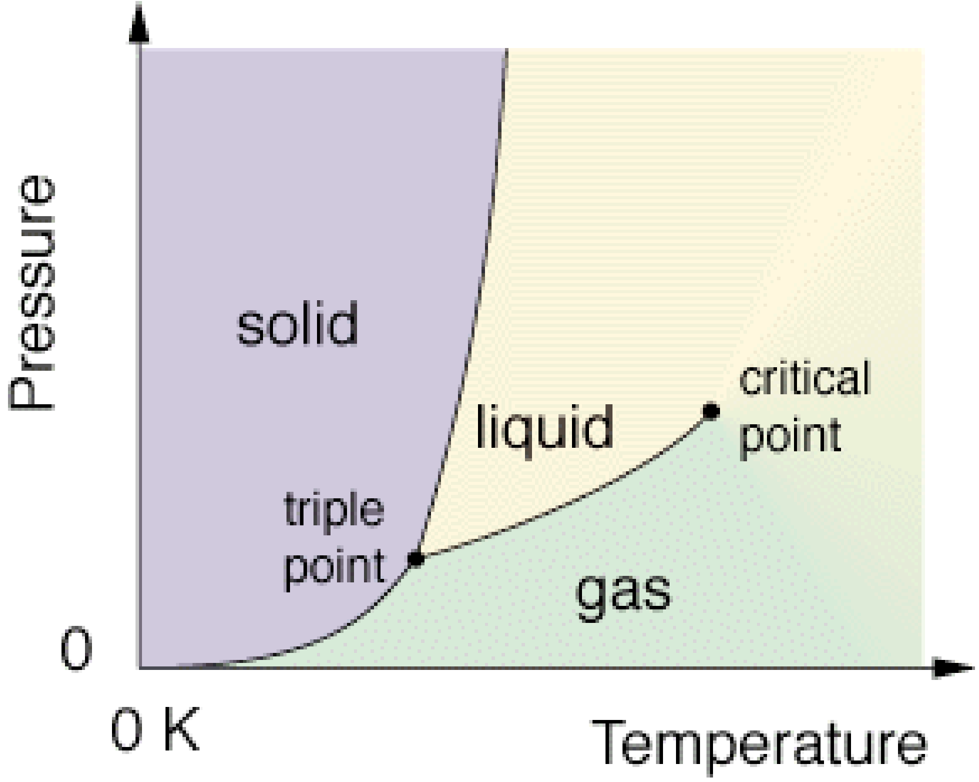
$$\frac{1}{t^{1-\alpha}} \to \int_0^{\infty} dt e^{-st} \frac{1}{t^{1-\alpha}} = \Gamma(\alpha) \frac{1}{s^{\alpha}}$$

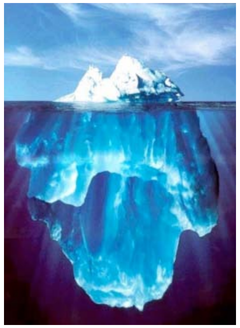
Agenda

- Phase diagrams: Simple and Complicated
- Ideal to non ideal gas law: van der Waals
- Weiss Mean Field Theory of ferromagnetism
- Landau: Unified Variational Field Theory
- Homogeneous Functions

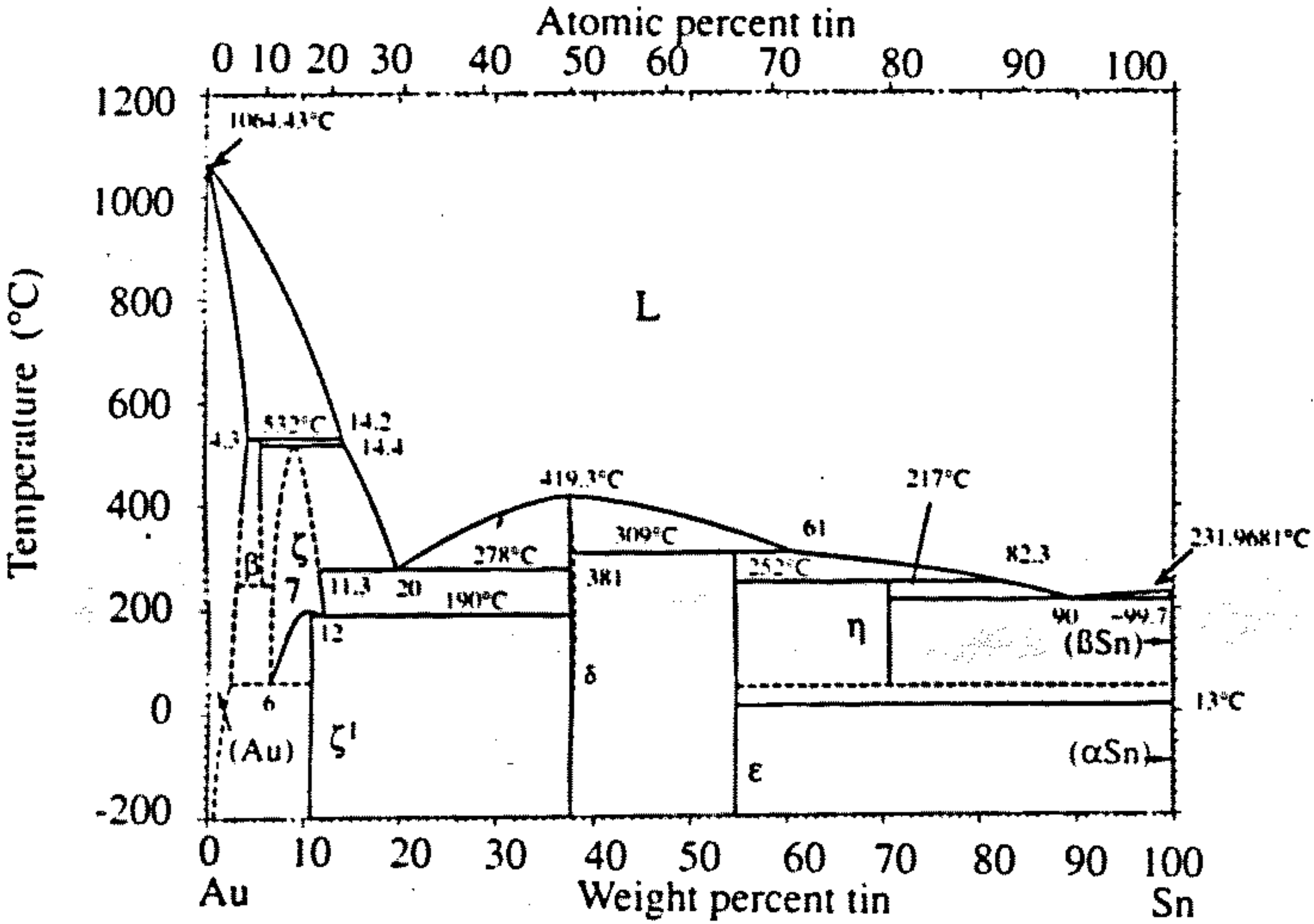
- Next time:
  - Correlation function of Ornstein-Zernike
  - Scaling hypothesis of Widom
  - Block Renormalization of Kadanoff

Phase Transition and Critical Phenomena





AuSn Phase Diagram: Application



The Ising(-Lenz) Model (1925)

$$\hat{H} = -J\sum_{nn}\sigma_r\sigma_s - \mu H_{applied}\sum_r \sigma_r$$

where

$\hat{H}$ ~ *energy Hamiltonian*

σ_r ~ *spin at* r^{th} *site*

μ ~ *magnetic moment*

$H_{applied}$ ~ *applied magnetc field*

J ~ *nearest neighbour coupling*

$$-\frac{H}{T} = K\sum_{nn}\sigma_r\sigma_s + h\sum_r \sigma_r$$

Single Spin Ising Model

$$-\frac{E(\sigma)}{T} = h\sigma \textit{ where } \sigma = \pm 1$$

$$\textit{The famous Boltzmann factor}: p(E) \propto e^{-\beta E} \textit{ where } \beta \equiv \frac{1}{k_B T} = \frac{1}{T}$$

$$\textit{and} \text{ the Partition function: Z} \equiv \sum_{\{\sigma\}} e^{-\beta E}$$

$$\textit{or } p(E) = \frac{e^{-\beta E}}{Z} = \frac{e^{h\sigma}}{Z}$$

$$p(\sigma = +1) = e^{h} / Z \text{ and } p(\sigma = -1) = e^{-h} / Z$$

$$Z = e^{h} + e^{-h} = 2\cosh(h)$$

$$< \sigma > = ? = \frac{1}{Z} \sum_{\sigma = \pm 1} \sigma e^{-\beta E(\sigma)} = \frac{e^{h} - e^{-h}}{e^{h} + e^{-h}} = \tanh(h)$$

The Power Of Partition Function, Z

the "magnetic" Partition function: $Z \equiv \sum_{\{\sigma\}} e^{-\beta E} \equiv e^{-\beta G}$

where G(T,H) is the "Gibbs" potential;

$Let\ Z = 2\cosh(h)$

$$<\sigma>=\sum_{\sigma}\sigma\, p(E(\sigma)) = \sum_{\sigma}\sigma\left(\frac{e^{h\sigma}}{Z}\right) = \frac{1}{Z}\frac{\partial}{\partial h}\sum_{\sigma}e^{h\sigma}$$

$$<\sigma>=\frac{\partial}{\partial h}\ln\ Z = -\beta\frac{\partial}{\partial h}G(t,h)$$

$Therefore <\sigma>= \tanh(h)$

$Helmholtz\ Free\ Energy: A(T,V) = U - TS$

$Enthalpy: E(S,P) = U + PV$

$Z\ or\ G\ or\ A\ etc \Rightarrow\Rightarrow$ Literally ALL thermodynamics

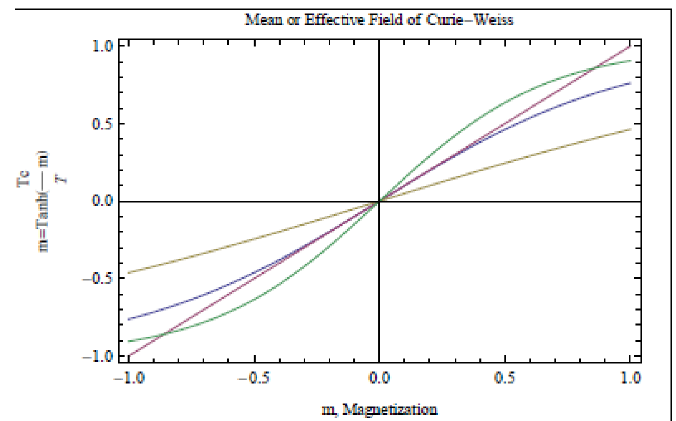
Weiss N spins Model Mean Field Theory (1907)

$$-\frac{H_r}{T} = \sigma_r \left[h(r) + K \sum_{s\ nnn} \sigma_s \right]$$

$h(r)$ is an external field

$K \sum_{s\ nnn} \sigma_s$

is a fluctuating or time dependent (coupling) field



Introduction of an "effective" field: $h_{eff}(r)$

$$h_{eff}(r) = h(r) + K \sum_{s\ nnn} < \sigma_s >$$

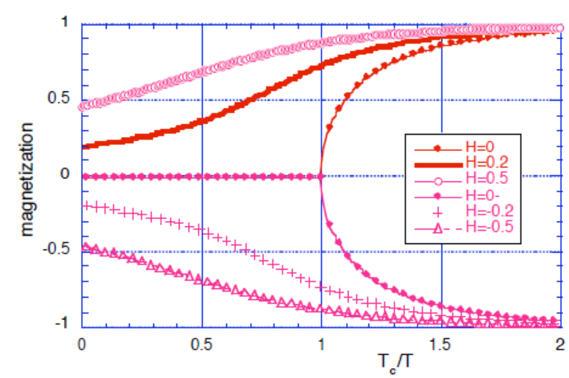
Then σ_r sees this effective field only:

$$<\sigma_r> = \tanh(h_{eff}(r))$$

For constant H, with magnetization $\sim <\sigma>$

$$m = \tanh(h + Kz\ m) \equiv \tanh\left[h + \frac{T_c}{T} m \right]$$

where z is the number of nearest neighbors



order parameter in mean field transition

Critical Exponent near Tc

$T \to T_c$, m=$<\sigma>$ is very small,

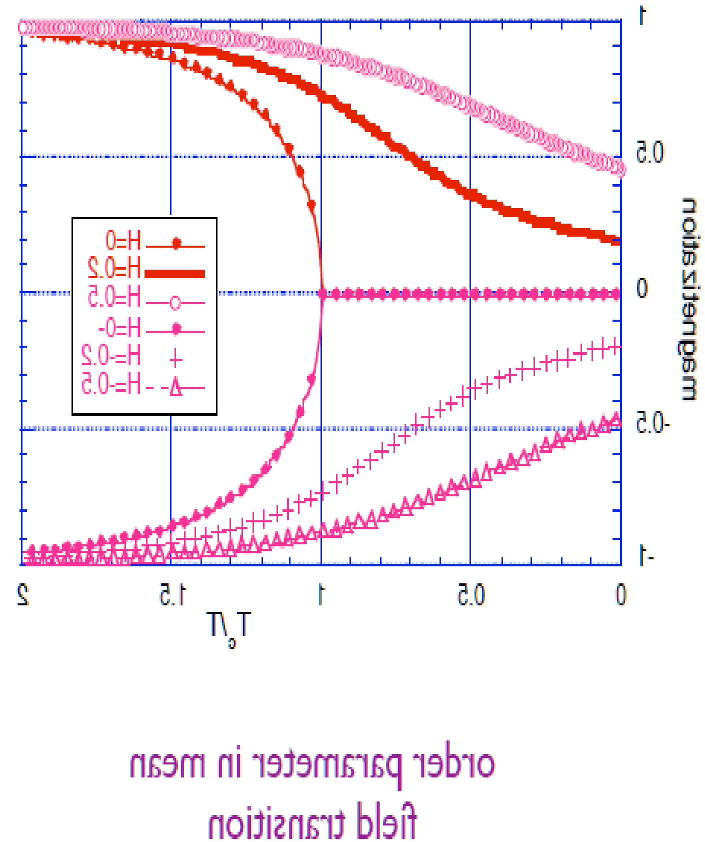
power series expansion about m=0:

$$(\text{T-T}_c)m \sim h - \frac{1}{3}m^3 \Rightarrow$$

$$m = 0 \ or$$

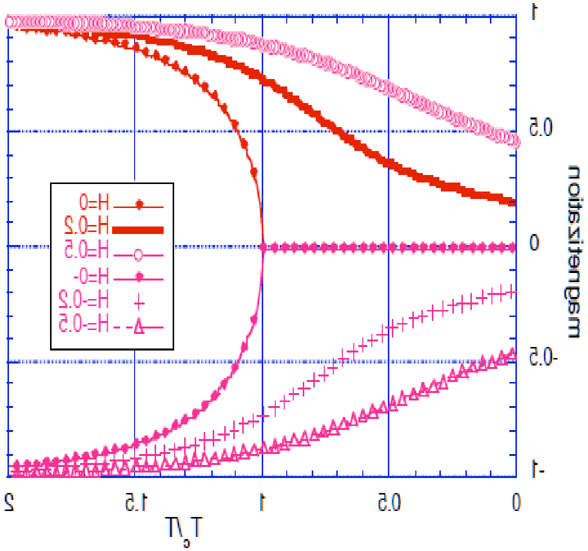
$$T - T_c = -\frac{1}{3}m^2 < 0 \Rightarrow$$

$$m = \pm(T_c - T)^{\beta} \quad with \quad \beta = 1/2$$



Critical Exponent near Tc

1. M=<σ> is the Order Parameter
2. Jump of m when T<Tc and H=0
3. Jump disappears as T-> Tc from below
4. Similar to van der Waals' liquid-gas MFT or
5. Universal for many more systems:
   1. Superconductivity
   2. Liquid crystal
   3. Ferroelectric
6. β=1/2 origin understood
7. It disagrees with experimental value of 1/3
8. BUT No body cared for a long time



order parameter in mean field transition

Liquid Gas Phase Diagram

- van der Waals: (1873)
- Different simple liquids-gas transitions have very similar thermodynamic properties.
- Derives a mean field theory (MFT) of liquid.
- Universal!

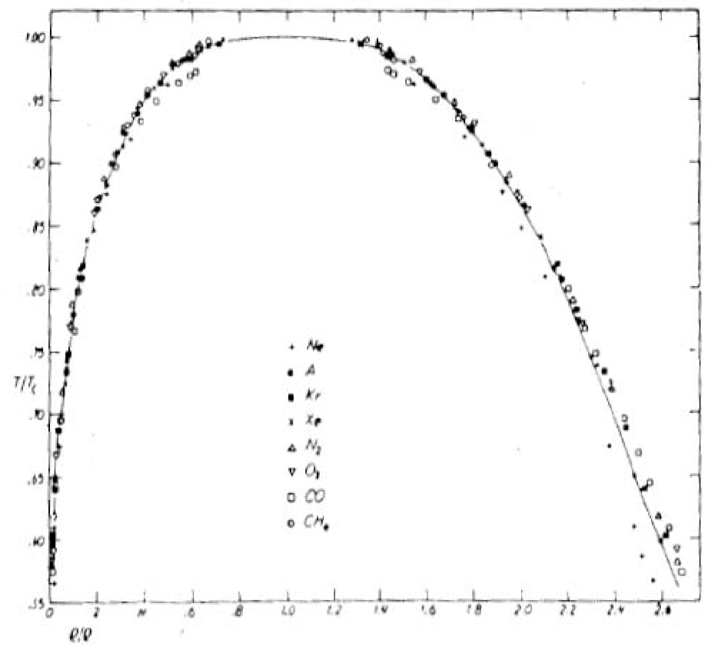


Figure 1.6 Reduced densities of coexisting liquid and gas phases for a number of simple molecular fluids (Guggenheim 1945). The experimental points support a law of corresponding states, but the universal curve is cubic rather than quadratic as required by van der Waals' theory.

•Order parameter: density versus Temperature
in liquid gas phase transition.
After E. A. Guggenheim J. Chem. Phys. **13 253 (1945)**

MFT of Liquid Gas Critical Indices

van der Waals $MFT \Rightarrow$

- $P = Nk_BT / V$
- Exclude volume effect: $V \rightarrow V - bN$
- Reduced pressure effect: $p \rightarrow p - a(N/V)^2$
- $p = \dfrac{NkT}{V - bN} - a\left(\dfrac{N}{V}\right)^2$

$$\frac{\rho}{\rho_c} - 1 \sim \left(1 - \frac{T}{T_c}\right)^{\beta} \quad \text{with } \beta = 1/2$$

$$Experiment \Rightarrow \beta = 1/3$$

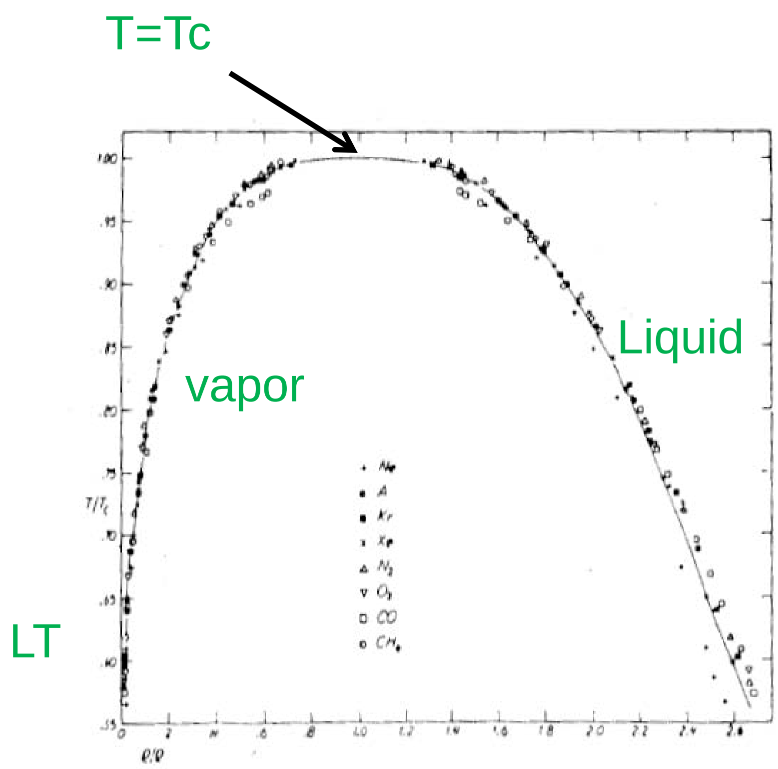


Figure 1.6 Reduced densities of coexisting liquid and gas phases for a number of simple molecular fluids (Guggenheim 1945). The experimental points support a law of corresponding states, but the universal curve is cubic rather than quadratic as required by van der Waals' theory.

Landau (~1937) Order Parameter, Generalized

- Phase transitions were manifestations of a Broken Symmetry
- Order parameter to measure the extent of symmetry breaking
    - fluid density, magnetization
- New Spatial dependence term implicates
    - Correlation (scattering experiments) and Dimensionality

A Variational Field $\phi(r,t)$ theory *Near Tc*:

- $F[\phi] \equiv \int d^3\vec{r}\left[a + h\phi + \frac{b}{2}\phi^2 + \frac{c}{4}\phi^4 + \frac{\gamma}{6}\phi^6 + p[\nabla\phi(r,t)]^2\right]$

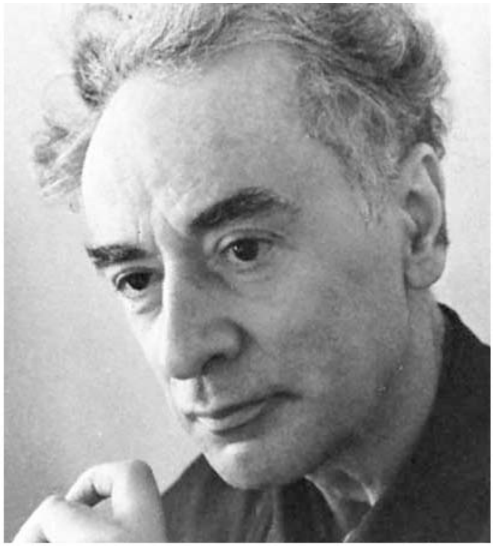
$h = external\ field$

$b \sim T - T_c$, the temperature parameter

- $\frac{\delta F[\phi]}{\delta\phi} \equiv 0 \Rightarrow MFT$

- A recipe for kinetic phase transition:

$$\frac{d\phi[t]}{dt} \equiv -\frac{\delta}{\delta t}F[\phi(r,t)] + \epsilon\eta(t,t')$$



Homogeneous Function

Some simple algebra

[1] Homogeneous function of 1 variable: f(x)

$\mathrm{f(r)} \rightarrow \ \mathrm{f}(\lambda \mathrm{x}) \equiv \mathrm{g}(\lambda)\mathrm{f(x)} \Rightarrow g(\lambda) = \lambda^{p}$

where λ is arbitray scaling factor, and p is the "degree of homogeniety".

Example: f(x)=ax^2

Proof :

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

$$g(\lambda) g(\mu) = g(\lambda\mu) \Leftrightarrow g(\lambda) = \lambda^{p}$$

[2] Homogeneous function of 2 variable: f(x,y)=$x^2 + y^2$

$$f(\lambda x, \lambda y) = \lambda^{p} f(x, y) \Leftrightarrow F(z = x/y) \equiv f(x/y, 1) = y^{-p} f(x, y) \Leftrightarrow$$

$$f(x, y) = y^{p} F(x/y) = x^{p} H(y/x)$$