Introduction to Phase transitions and Critical phenomena

Hyunggyu Park (KIAS)

The 19th KIAS-APCTP Winter School on Statistical Physics
Postech, Pohang, Jan. 10-14, 201

Outline

0. Prologue

I. Patterns & Fractals

II. Scaling hypothesis

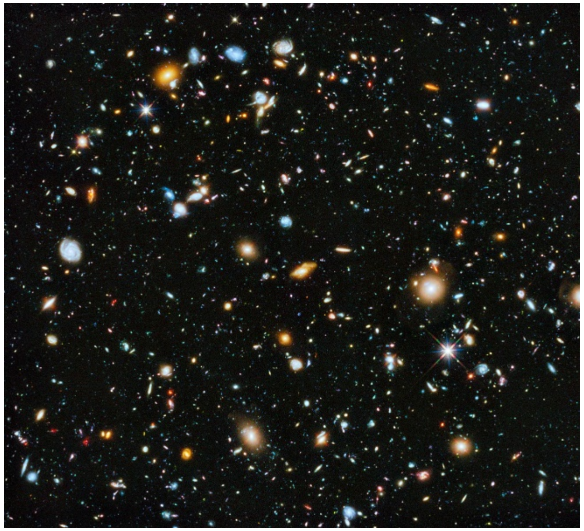
III. Renormalization group : JD Noh

IV. EQ and NEQ models (skipped)

V. Epilogue

Prolog

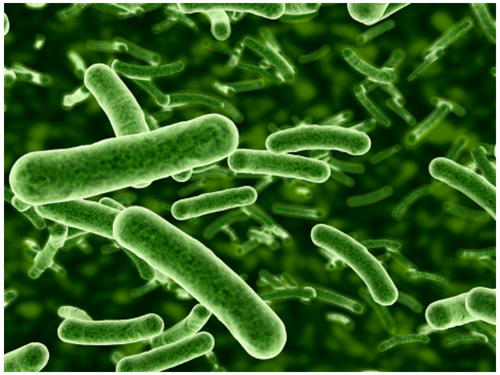
- **Physics of many-body dynamics**



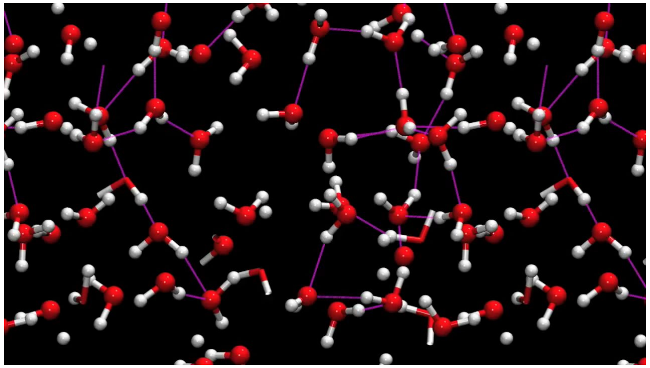
universe

nature

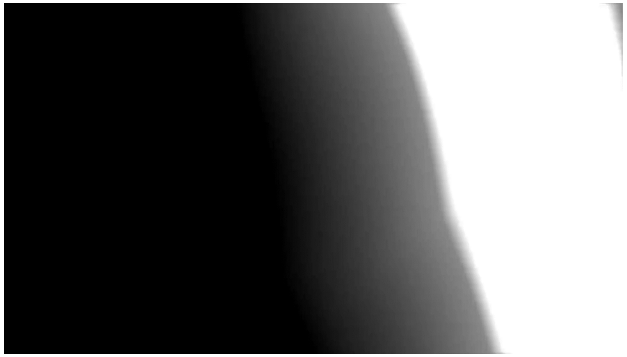
choco



bacteria

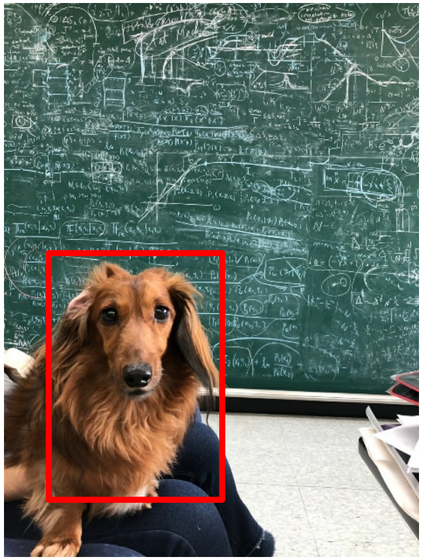


H_2O



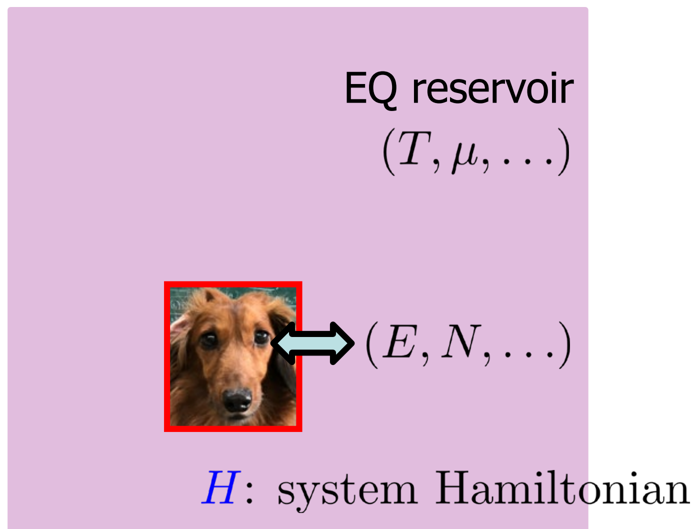
strings

- **Physics of subsystems of interest**



- **dimensional reduction**
  - *** trace/integrate out over uninteresting d.o.f.**
- **useful approximation**
  - *** simple/constant (EQ) reservoir**

    time-scale separation; huge reservoir wrt system



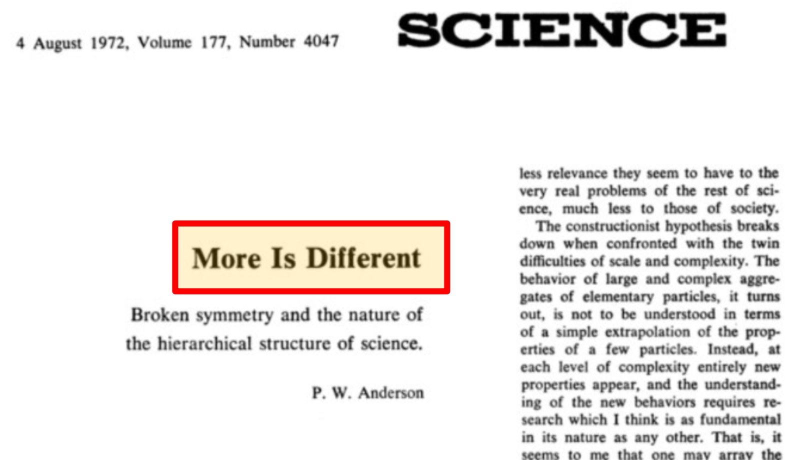
(weak coupling)

$\Rightarrow$ **stochastic/probabilistic**

Statistical mechanics

- **stochastic many-body dynamics**

  - $N=10^3 \sim 10^{23}$ (particles/agents/d.o.f.)



4 August 1972, Volume 177, Number 4047

SCIENCE

More Is Different

Broken symmetry and the nature of the hierarchical structure of science.

P. W. Anderson

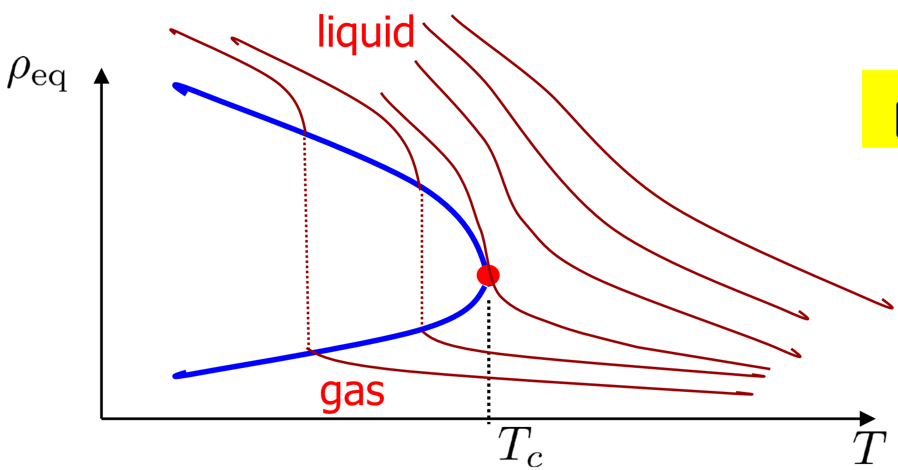
less relevance they seem to have to the very real problems of the rest of science, much less to those of society.
The constructionist hypothesis breaks down when confronted with the twin difficulties of scale and complexity. The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity entirely new properties appear, and the understanding of the new behaviors requires research which I think is as fundamental in its nature as any other. That is, it seems to me that one may array the

Emergence

  - How to describe/characterize complex dynamics(spatio-temporal patterns)?

    * still too many d.o.f $\rightarrow$ dyn. eqs. of a few coarse-grained quantities.

      (ex: local density $\rho(\vec{x}, T, \mu; t)$)



phase transition

* 1st order , 2nd order

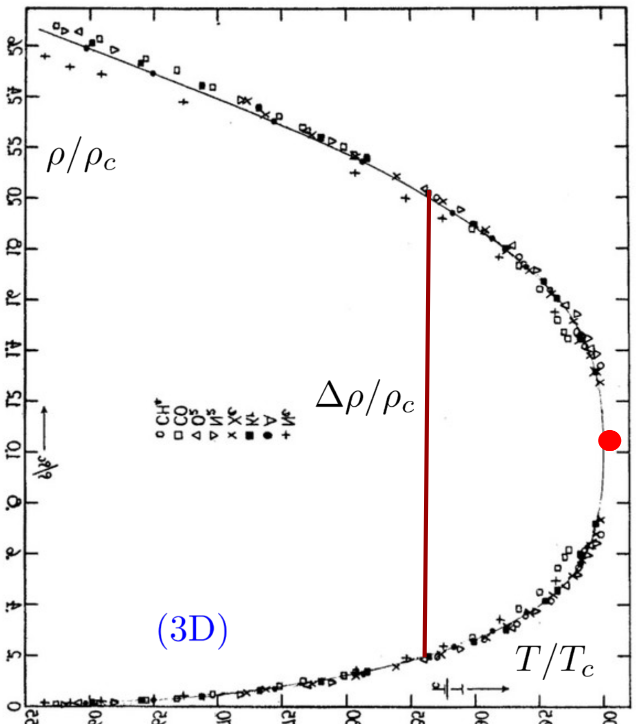
critical point (T_c, ρ_c, μ_c)

Scaling and Universality

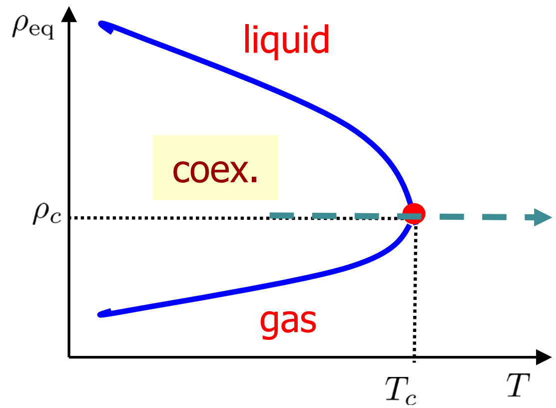
mathematical singularity $(N = \infty)$

Finite-size-scaling

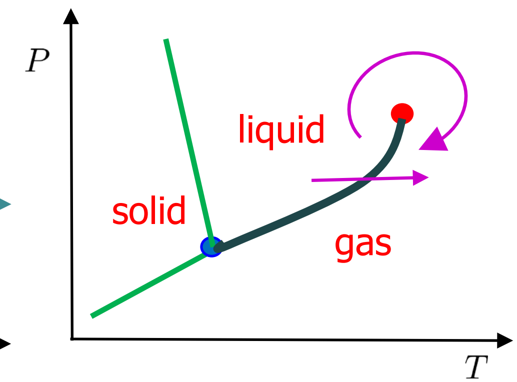
- **Laws of corresponding states**



[Guggenheim 1945]



Phase diagram



- **universal scaling curve**

$$\frac{1}{2}\Delta\rho/\rho_c \simeq \frac{7}{4}(1-T/T_c)^{1/3} \quad \equiv a(1-T/T_c)^{\beta}$$

* **universal over other systems**

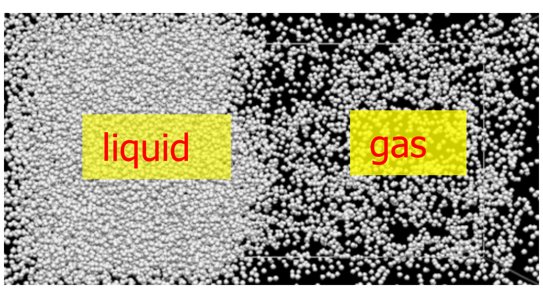
3D Ising magnet: $\beta \simeq 0.3264$, $a \simeq 1.692$ (sc)

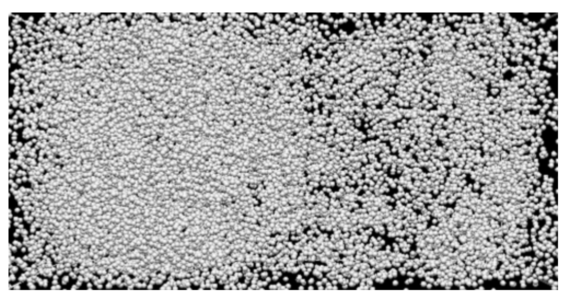
(universal critical exponents/non-universal metric factor)

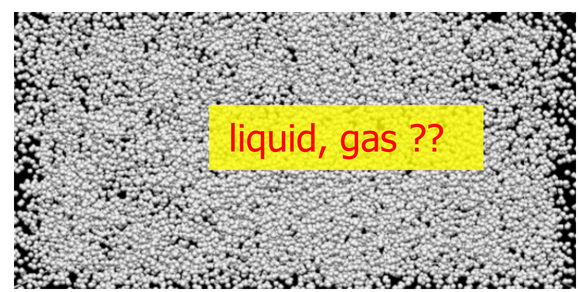
- **correlation function ?** $G(\vec{x},\vec{y}) = \langle \rho(\vec{x})\rho(\vec{y})\rangle_{\rm eq}$

- **typical patterns**

(LJ MD) [Watanabe/Ito/Hu 2012]





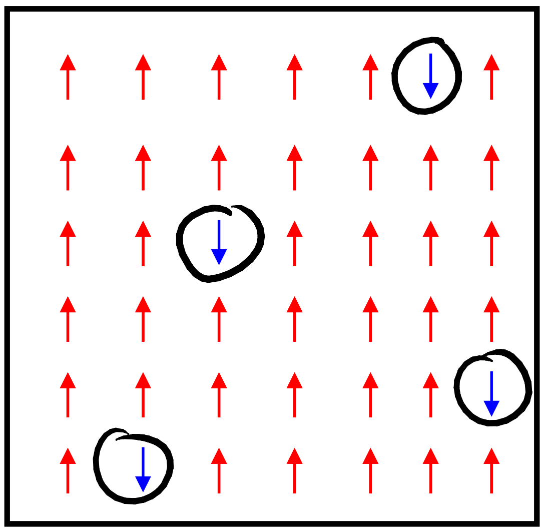


● Magnetic system (EQ)

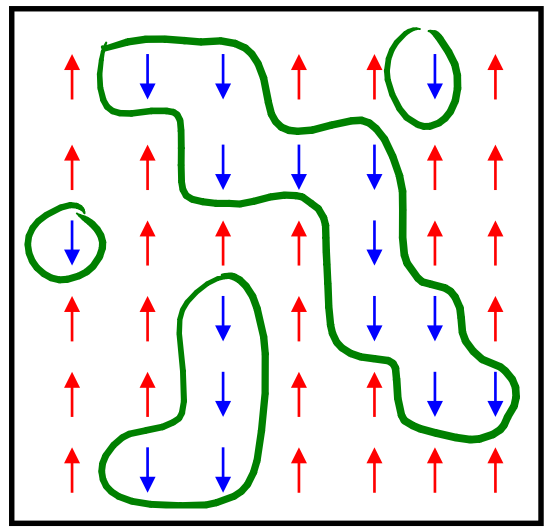
- ferromagnetic Ising model

$$\mathcal{H} = -J\sum_{\langle i,j\rangle} S_i S_j - H\sum_i S_i \quad (S_i = \uparrow(+), \downarrow(-))$$

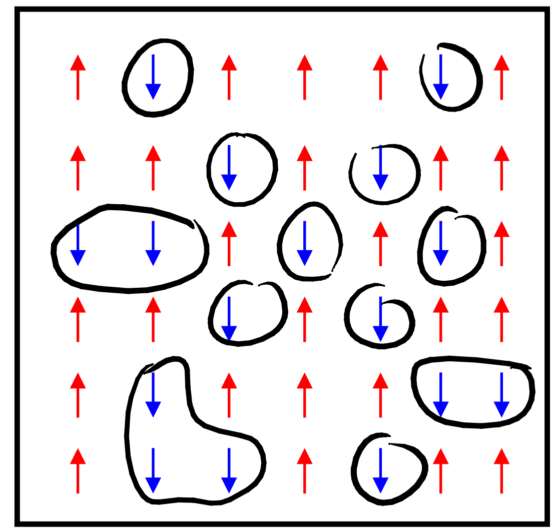
[Z_2-symmetric ground states] $\qquad (H=0\text{: } Z_2\text{-symmetry})$



low T $|m| \lesssim 1$



$T = T_c$ $\quad m = 0$

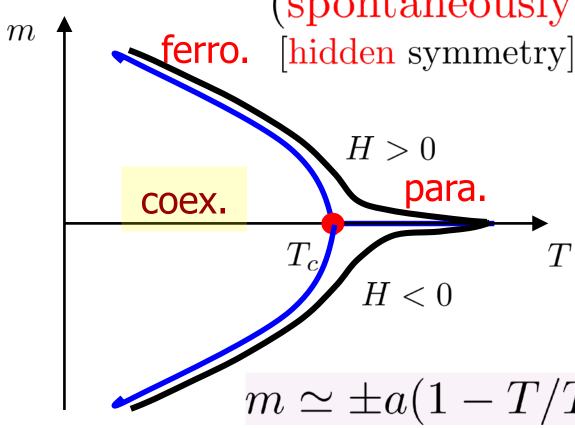


high T $\quad m = 0$

[magnetization $m = \langle S\rangle$ in EQ]

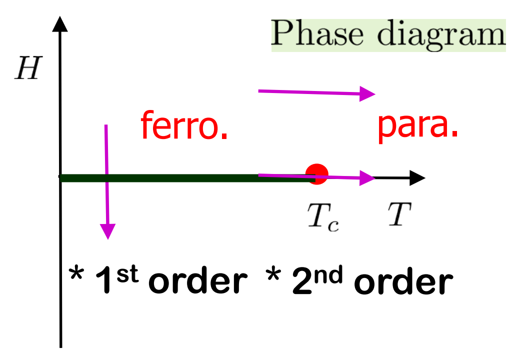
(spontaneously broken symmetry)

[hidden symmetry]



$m \simeq \pm a(1 - T/T_c)^\beta$

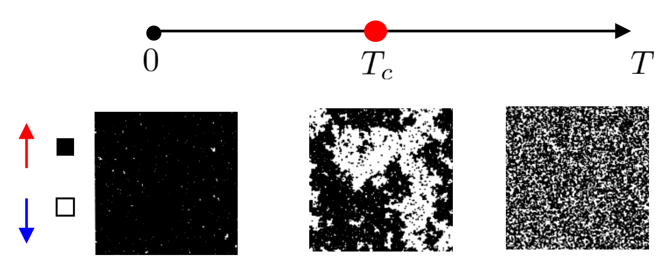
Phase diagram



* 1st order * 2nd order

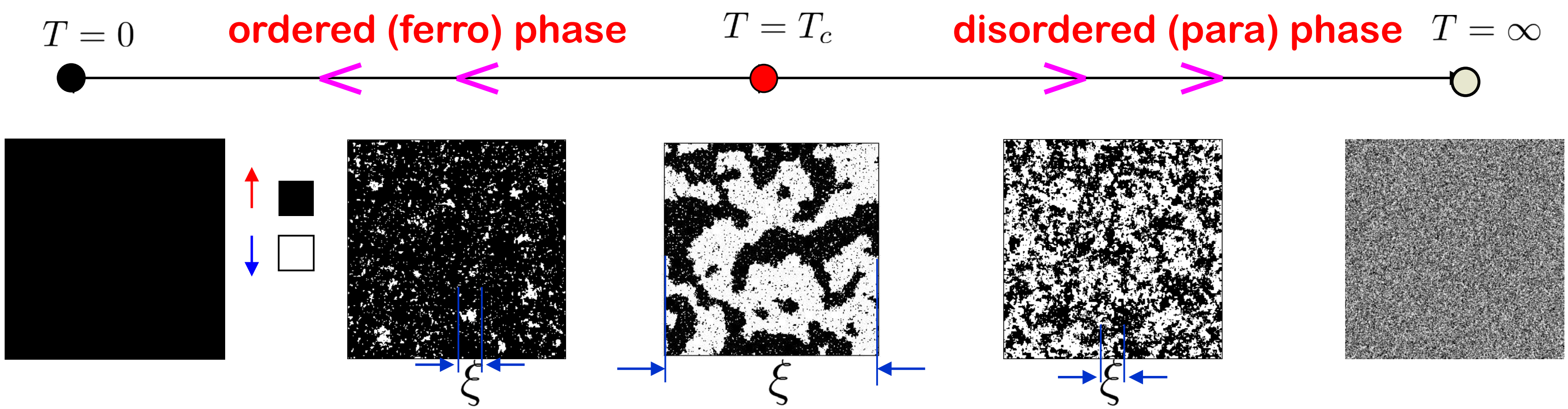
- typical patterns

(2nd order)



2D: $\beta = 1/8,\ a = [4\sqrt{2}(-\ln(\sqrt{2}-1))]^{1/8}$ (sq) $\quad$ 3D: $\beta \simeq 0.3264,\ a \simeq 1.692$ (sc) $\quad$ 4D$^+$: $\beta = 1/2,\ a = \sqrt{3}$ (hc) [MF]

- EQ spatial patterns



*** Key question: What is "phase" ?**

- How to classify seeming different patterns into a few groups (phases)?

Zoom out (coarsening) for scale transformation (RGT) ⟹ approaching a fixed point

- Stable f.p. represents phase & unstable f.p. represents critical point (fractal).
- Characteristics of f.p. patterns?? ⟹ fractal dimensions

*** How to determine fractal dimensions?** [a set of fractal dimensions]

$$A(\ell)=\sum_{w(\ell)}\mathcal{O}_A \ (\mathcal{O}_A\text{: local observable like } S_i,\ S_iS_j,\ \ldots;\ w(\ell)\text{: window of linear size } \ell)$$

$$\sim \ell^{d_{\rm A}} \text{ for large } \ell \quad (d_{\rm A}\text{: fractal dimension of object 'A'})$$

- Critical patterns are (nontrivial) fractals. $P(s_A)\sim s^{-d_A}$ [no typical scale] [self-similar]

*** Is it useful to know fractal dimensions?**

- Critical exponents are simply related to fractal dimensions. $d_A=y_H,\, d_L=y_T$

History of scaling & critical phenomena

1822 Cagniard de la Tour found a special point of alcohol/water
[Faraday1845: disliquefying point] [Mendeleev1861: absolute boiling point]
1869 Andrews liquid-gas transition CO_2 molecules ("critical" point/phenomena)
1873 van der Waals MF equation for liquid-gas transitions [Maxwell1874]
1900 Verschaffelt 3D experiment (?) $(\beta \simeq 0.3434, \delta = 4.259)$
1907 Curie-Weiss MF theory for magnetic systems $(\beta = 1/2, \alpha = 0(\text{jump}), \gamma = 1, \delta = 3)$

vs Gibbs /Peierls
» fluctuation

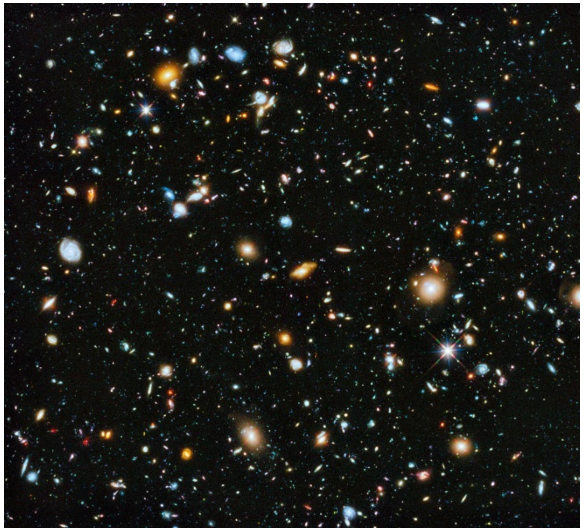
1937 Landau: order parameter, symmetry breaking, free energy functional
1941 Kolmogorov turbulence energy cascade scaling
1944 Onsager exact solution of 2D Ising model [+1949/Yang1952] $(\beta = 1/8, \alpha = 0(\log), \gamma = 7/4, \delta = 15)$
1945 1st BOOM time for universality; $(\beta \simeq 1/3\ (3\text{D}), \ldots)$
many experiments [Guggenheim1945], series expansion [Domb/Fisher/Sykes1959], …

1965 Modern theory starts with scaling [Widom1965], block (real-space) RG [Kadanoff1966]
1971 Wilson RG transformations (systematic workable tool to calculate critical exponents, fixed point)
1972 Baxter exact solution of 2D 8-vertex model (Yang-Baxter or star-triangular relation) [Yang1968]
1975 Mandelbrot fractal; self-similarity and fractal dimension [Weierstrass1872, Cantor1883, ..]
2nd BOOM time for EQ critical phenomena; universality classes, upper/lower critical dimensions, …
1984 Conformal invariance for 2D EQ critical phenomena [Belavin/Polyakov/Zamolodchikov1984]

1978- general scaling invariant phenomena; Feigenbaum's chaos(1978), DLA(1981), growth(1985), SOC (1987), polymer (1972), non-EQ critical phenomena, dynamic critical scaling, …

Patterns & Fractals

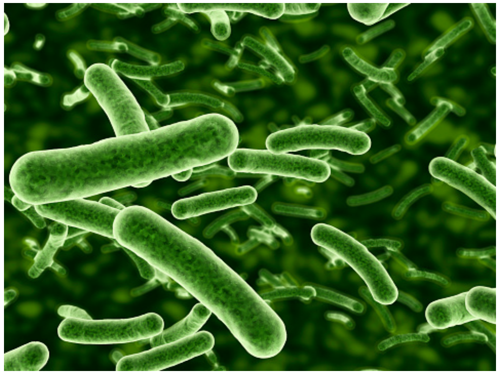
- **Patterns**



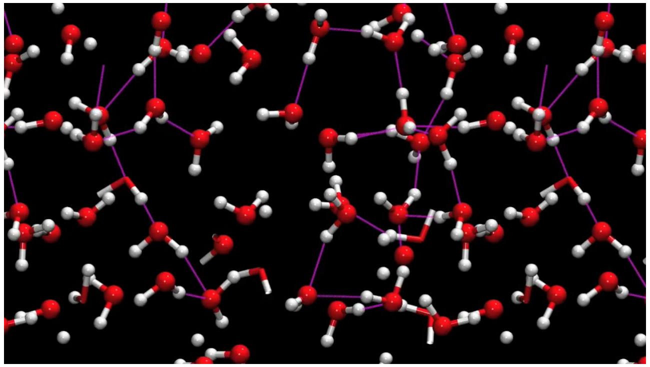
universe

nature

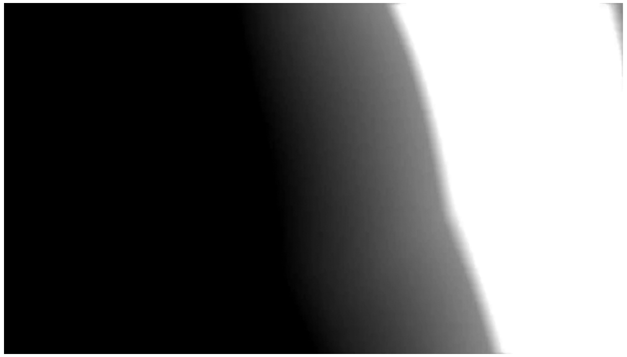
choco



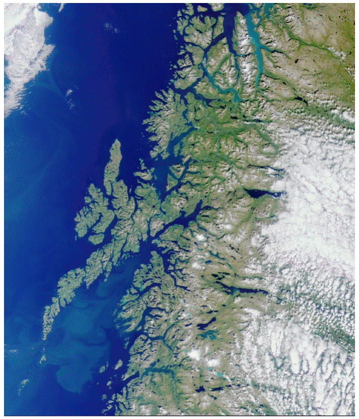
bacteria



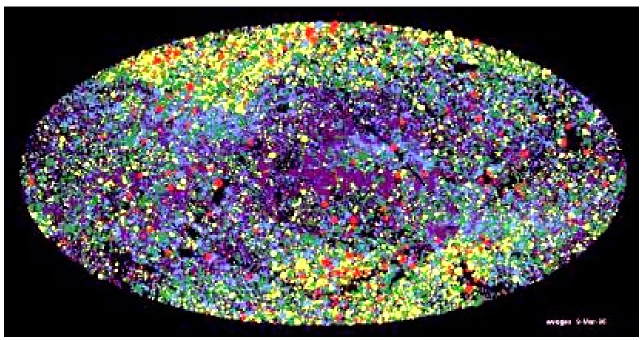
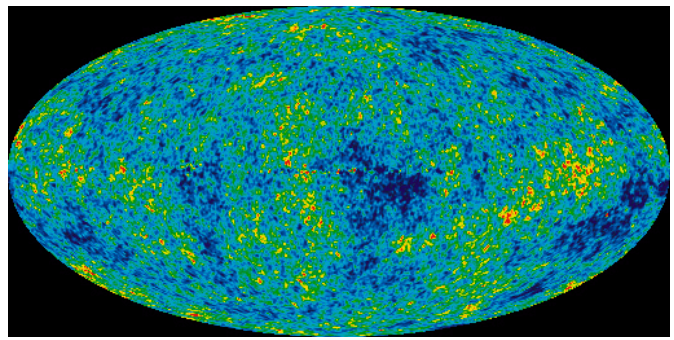
H_2O

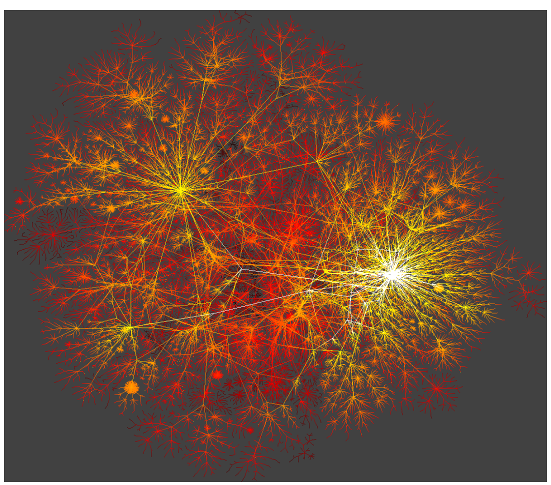
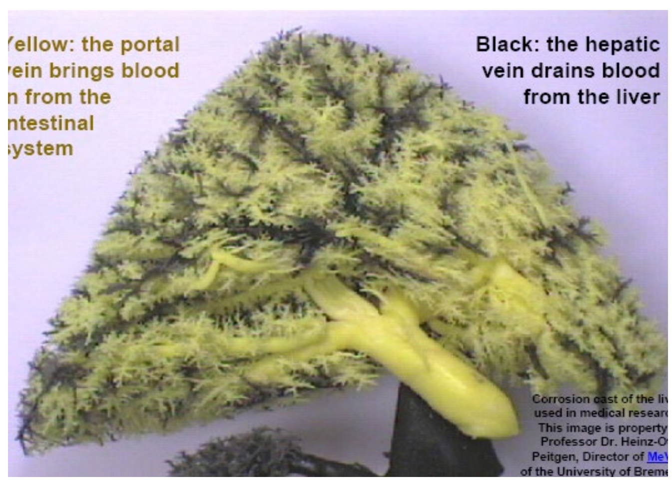
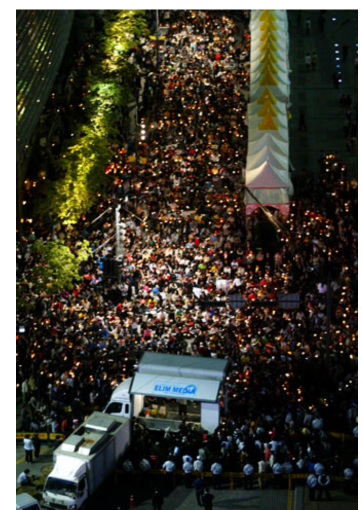


strings





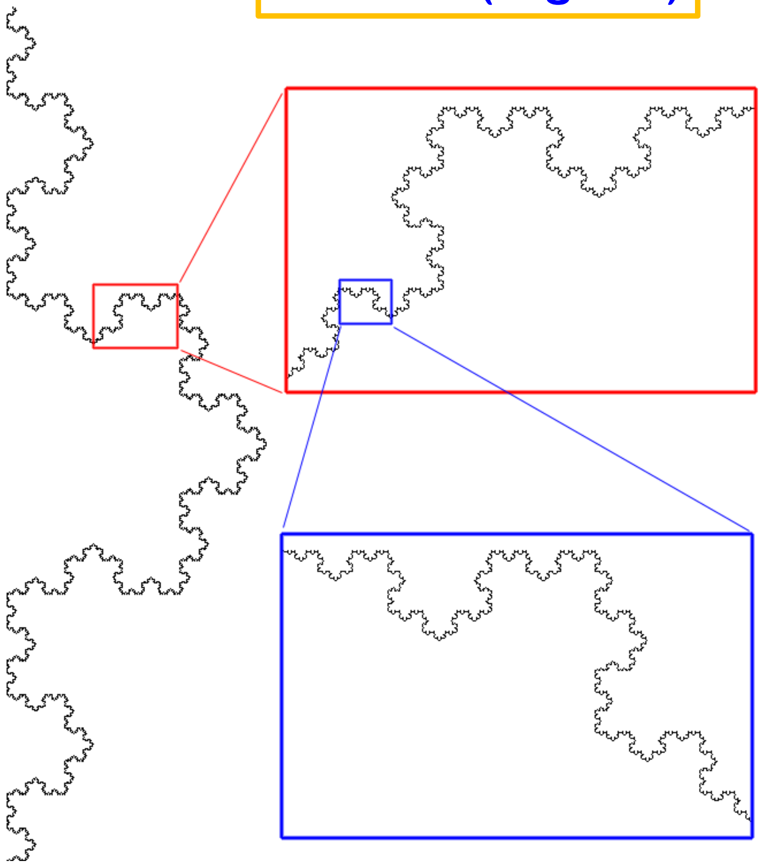





ellow: the portal
ein brings blood
n from the
ntestinal
ystem
Black: the hepatic
vein drains blood
from the liver


- **Fractals**

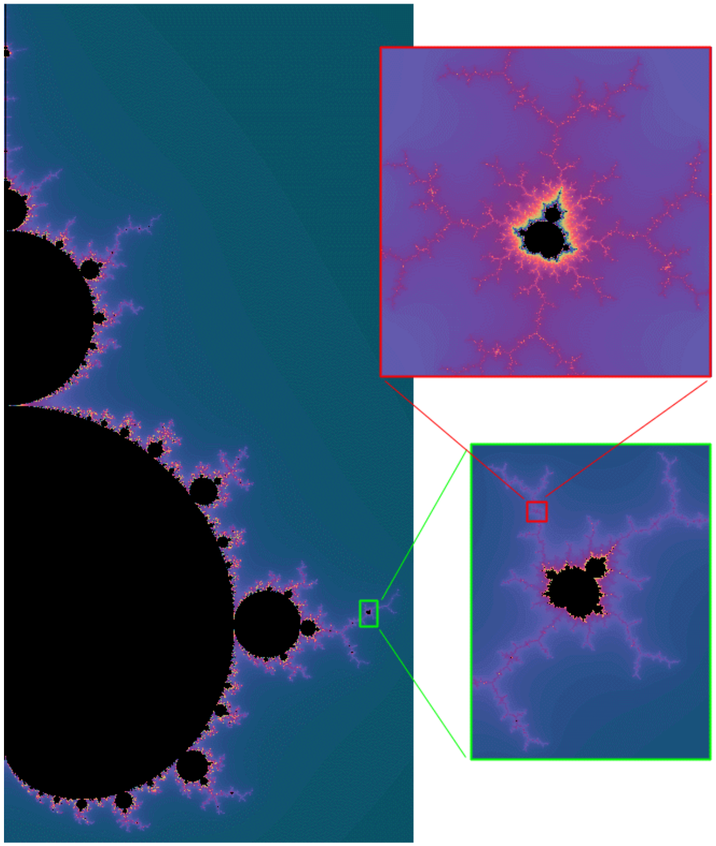
  - Self-similarity in zooming in or out.

➢ exact (regular)



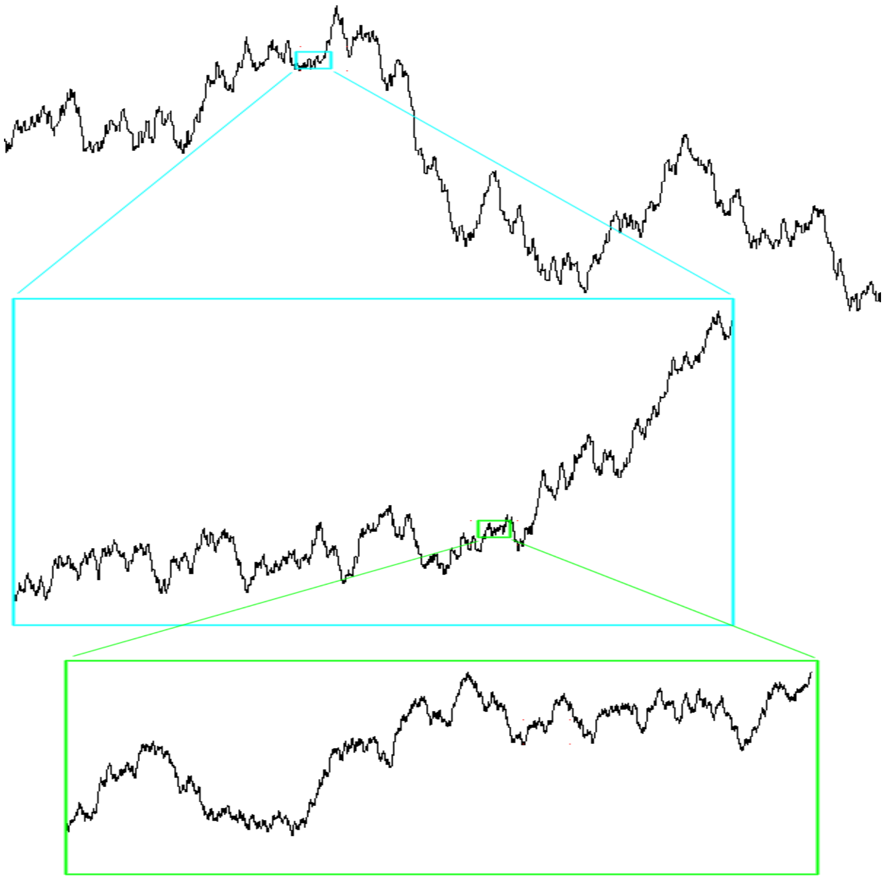
[Koch curve]

➢ approximate

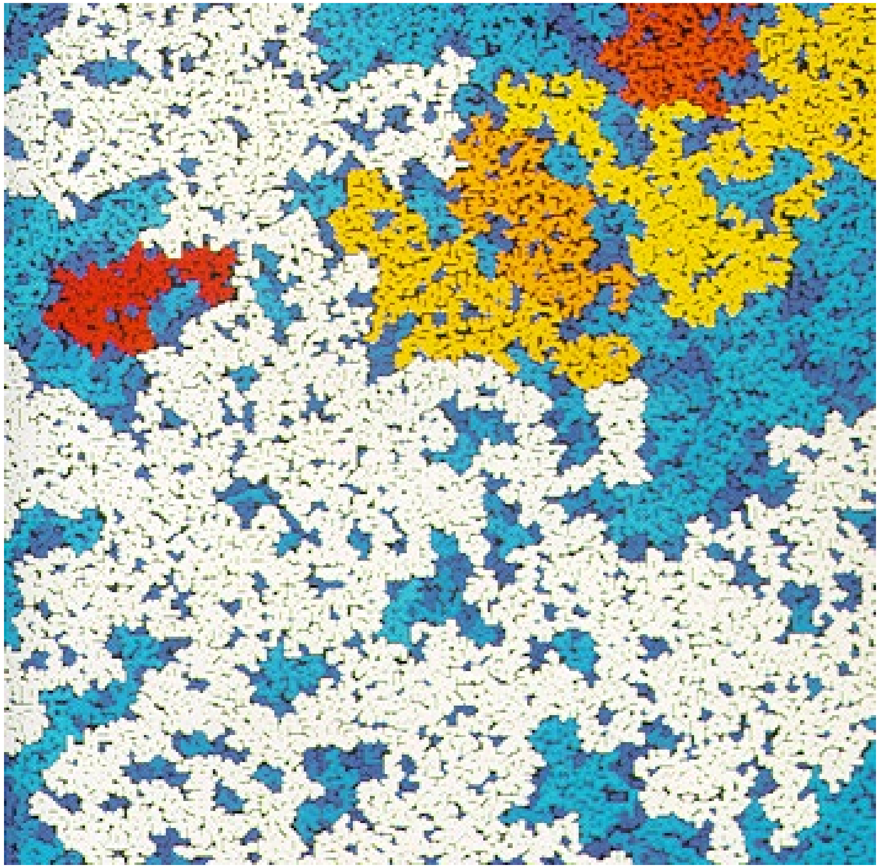


[Mandelbrot set]

➢ **statistical**



[time series]

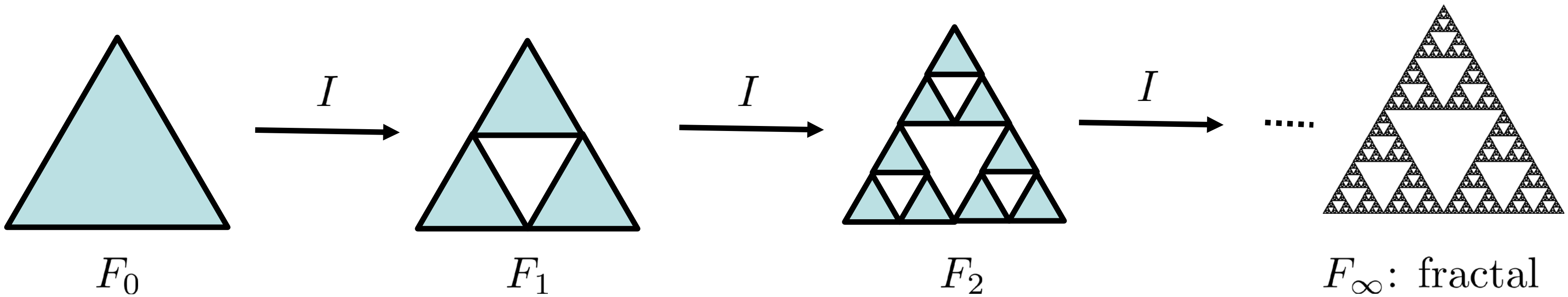


[spatial critical pattern]

- Fractal constructions and dimensions

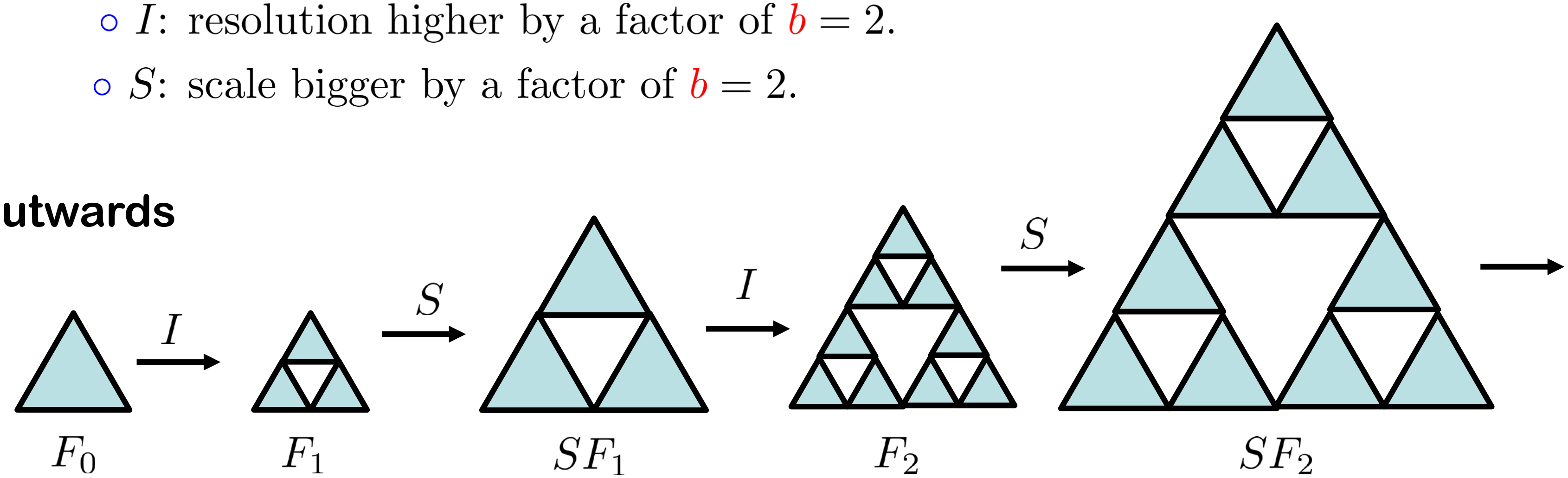
* inwards

[Sierpinsky gasket]



- ○ I: resolution higher by a factor of $b = 2$.
- ○ S: scale bigger by a factor of $b = 2$.

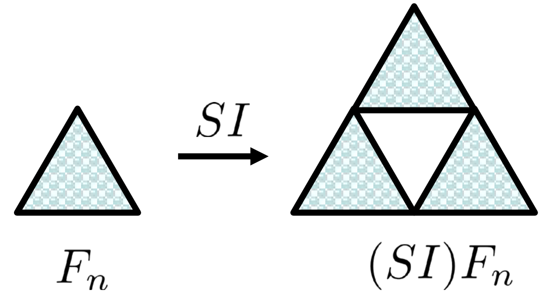
* outwards



- same resolution but large size (correlation length ξ is b times bigger)

¶ RG transformation $\equiv (SI)^{-1}$ (move away from the critical (fractal) pattern)

* definition of fractal dimension



– $b^{d_A^{(n)}} \equiv \dfrac{A((SI)F_n)}{A(F_n)}$ with $A(F_n) = \sum_{F_n} \mathcal{O}_A$

$d_A = \lim_{n\to\infty} d_A^{(n)}$

$A(\ell) \sim \ell^{d_A}$

○ example: (1) Sierpinsky gasket ($b = 2$)

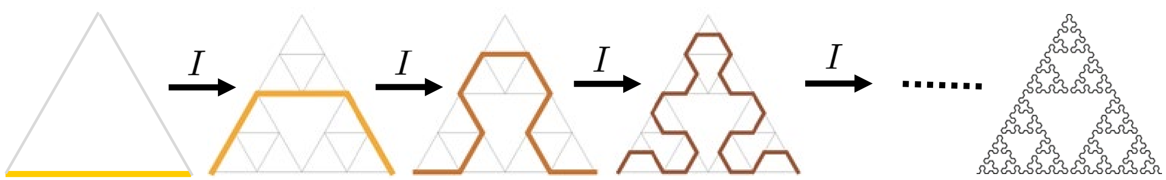
- length: $2^{d_L} = 3 \Rightarrow d_L = \ln 3/\ln 2$
- filled area: $2^{d_A} = 3 \Rightarrow d_A = \ln 3/\ln 2$

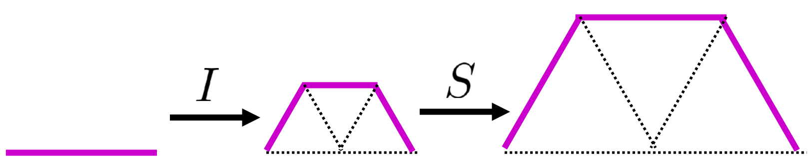
vacant area: $2^{d_V^{(n)}} = 2^2(1 + \frac{1}{4}(\frac{3}{4})^n + \cdots)$

$\Rightarrow d_V = 2$ (correction-to-scaling)

$(A(\ell) = \ell^{d_A}, V(\ell) = \ell^2 - \ell^{d_A})$

(2) Sierpinsky-arrow head





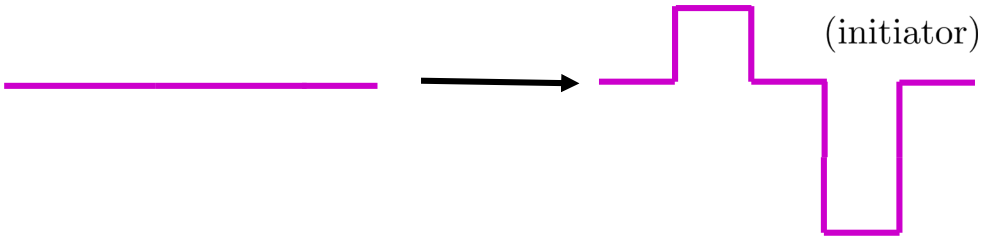
($b = 2$)

- length: $2^{d_L} = 3 \Rightarrow d_L = \ln 3/\ln 2$

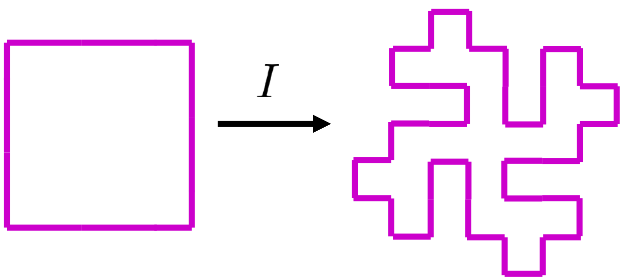
(correction-to-scaling)

- area above line (A_a) and below line (A_b): $d_{A_a} = d_{A_b} = 2$
- $B = 3A_a - 2A_b$: $d_B = i\pi/\ln 2$ (marginal) [relevant/irrelevant]

(3) quadratic Koch islands [[Project 1]]



$(b = 5)$



$\xrightarrow{S}$

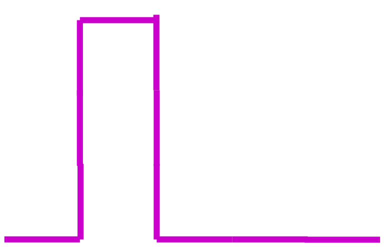
- length: $5^{d_L} = 11 \Rightarrow d_L = \ln 11 / \ln 5$
- area: 6 different types of elementary squares classified by # of enclosed line segments

$\Rightarrow$ 2 relevant, 1 marginal, 3 irrelevant d_{a_i}

* corresponding geometric objects ??

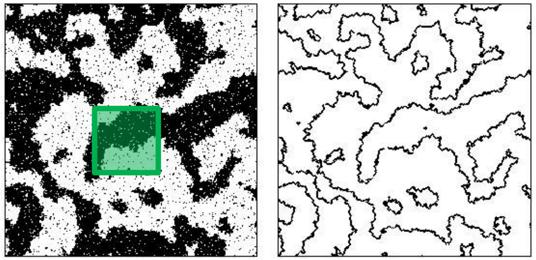
* full correction-to-scaling for enclosed area ??

- What about different initiator ??



(Is it universal ??)

- Fractal dimensions of Ising critical patterns



* magnetization

– $M(\ell) = \sum_{w(\ell)} \langle S_i \rangle \simeq a\ \ell^{d_A} + \langle S_i \rangle \ell^d$ $\quad (d_A < d)$

$A(\ell) \sim \ell^{d_A}$

$m(\ell) \simeq a\ \ell^{-d+d_A} = a\ \ell^{-x_A}$ $\quad$ (x_A: scaling dimension)

$(x_A + d_A = d)$

Finite-size-scaling

* energy

– $E(\ell) = \sum_{w(\ell)} \langle S_i S_j \rangle \simeq b\ \ell^{d_L} + \langle S_i S_j \rangle \ell^d$

$e(\ell) \simeq b\ \ell^{-d+d_L} + \langle S_i S_j \rangle = \boxed{b\ \ell^{-x_L}} + \boxed{\langle S_i S_j \rangle}$ (regular part) (singular part) $\quad (x_L + d_L = d)$

- 2D Ising: $d_A = \frac{15}{8}$, $d_L = 1$ (relevant)
- all others are $d_\beta < 0$ (irrelevant) $\quad$ [# of intersection points; $d_{\text{int}} = -2$]

- **Universality of complex patterns**

  - pattern classification by fractal dimensions after RGT (zooming out)

    [infinite # of fractal dimensions including all irrelevant ones]

  - fractal dimensions do not depend on details of system Hamiltonians or dynamic evolution rules (phenomenological).

→ **universality classes**

↑

- equilibrium critical systems:
  symmetry, embedding dimensions, disorder,...

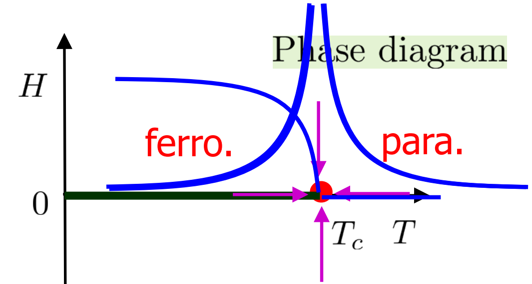
(symmetry between ground states in the ordered phase)

2d equilibrium critical patterns:
almost complete list is known by conformal field theory.

- Non-equilibrium critical systems:
  + dynamic conservation law, boundary condition, ensemble dependence, SOC, ...

Scaling hypothesis

- **critical (scaling) exponents of Ising model**



* **themodynamic quantities**

- $H = 0 \ (h = 0)$ line: $C \sim |t|^{-\alpha}, \ m \sim (-t)^{\beta}, \ \chi \sim |t|^{-\gamma}$
- $T = T_c \ (t = 0)$ line: $m \sim \pm |h|^{1/\delta}$ $\longrightarrow$ $(\alpha, \beta, \gamma, \delta, \cdots)$

⋆ $t = (T - T_c)/T_c$ (reduced temp.)
$h = H - H_c = H$

* **correlation function and length**

$$G_H(r) = \langle S(0)S(r)\rangle - \langle S(0)\rangle\langle S(r)\rangle \sim \frac{e^{-r/\xi}}{r^{d-2+\eta}}, \quad \xi \sim |t|^{-\nu} \longrightarrow (\eta, \nu, \cdots)$$

- **universality and scaling relations**

* a set of critical exponents is independent of details of Hamiltonians, such as further-neighboring interactions, embedding lattice structures, anisotropy, and etc.

$\longrightarrow$ **universality classes**

$\longrightarrow$ Fundamental properties like symmetry, disorder emerge in scaling exponents.

* scaling relations $\alpha + 2\beta + \gamma = 2, \ \ \gamma = \beta(\delta - 1), \ \ d\nu = 2 - \alpha$ (hyperscaling), $\cdots$,

$\longrightarrow$ **deeper level of emergent scaling behavior exists!**

- **Homogeneity postulate for free energy** [Widom 1965]

$$f(t,h) = f_{\rm sing}(t,h) + f_{\rm reg}(t,h)$$

$$\boxed{f_{\rm sing}(t,h) = b^{-d} f_{\rm sing}(b^{y_T} t, b^{y_H} h)}$$

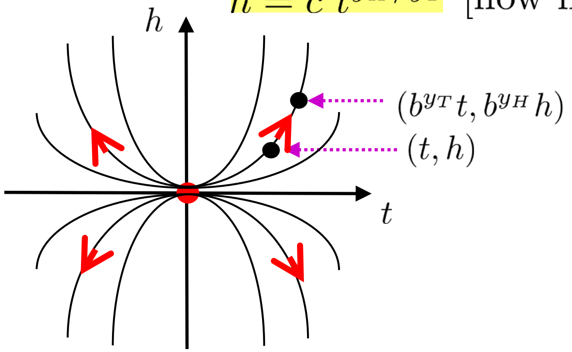
⋆ $t = (T - T_c)/T_c$ (reduced temp.)
$h = H - H_c = H$

(b: arbitrary constant)

(y_T: thermal exponent, y_H: field exponent)

($f_{\rm sing}$: generalized homogeneous function)

$h = c\, t^{y_H/y_T}$ [flow lines]



- $m = \left(\dfrac{\partial f}{\partial h}\right)_t \rightarrow m_{\rm s}(t,h) = b^{-d+y_H} m_{\rm s}(b^{y_T} t, b^{y_H} h)$

  ○ $m_{\rm s}(t,0) = b^{-d+y_H} m_{\rm s}(b^{y_T} t, 0)$

  $b = (-t)^{-\frac{1}{y_T}}$ $\quad = (-t)^{(d-y_H)/y_T} m_{\rm s}(-1,0)$

  $\sim (-t)^{\beta}$ $\quad [\beta = (d - y_H)/y_T]$

  ⋆ $m_{\rm r}(t,0) \sim (-t)^n$ (subdominant)

  ○ $m_{\rm s}(0,h) \sim |h|^{1/\delta}$ $[\delta = y_H/(d - y_H)]$

  $b = |h|^{-\frac{1}{y_H}}$

- $\chi = \left(\dfrac{\partial^2 f}{\partial h^2}\right)_t \sim |t|^{-\gamma}$ $\quad [\gamma = (-d + 2y_H)/y_T]$

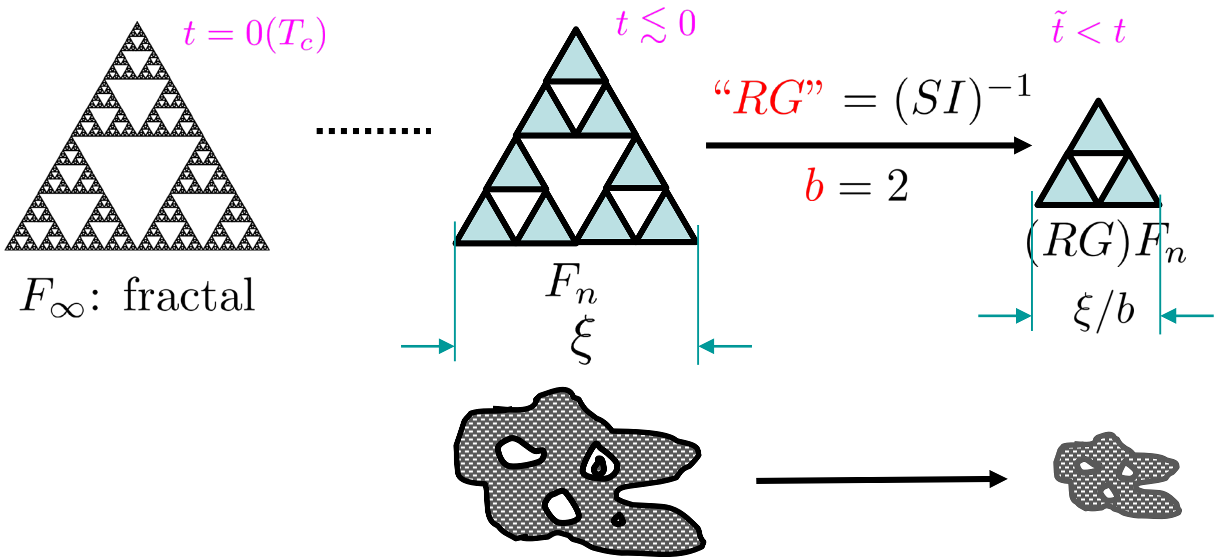
- $C_H = \left(\dfrac{\partial^2 f}{\partial t^2}\right)_h \sim |t|^{-\alpha}$ $\quad [\alpha = (-d + 2y_T)/y_T]$

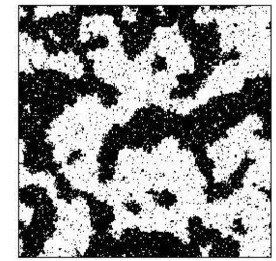
* **scaling relations are satisfied with** $\alpha + 2\beta + \gamma = 2, \quad \gamma = \beta(\delta - 1)$.

* **only two independent exponents** (y_T, y_H) $\qquad [d\nu = 2 - \alpha$: hyperscaling ??]

- **Geometric perspective (block spin formulation)** [Kadanoff 1966]

- **Typical off-critical patterns are NOT fractals, but can be characterized as a "fractal" constructed up to finite order.**





- RG: coarsening + shrinking scale (zoom out)

[or linear combination]

$\star$ $(t,h) \overset{\mathrm{RG}}{\to} (\tilde{t},\tilde{h})$ - assume $\tilde{t} = g_t(b)t$ and $\tilde{h} = g_h(b)h$ near criticality.

- should have $g(b_1 b_2) = g(b_1)g(b_2)$ $\rightarrow$ $g_\alpha(b) = b^{y_\alpha}$ [power law]

$\rightarrow$ $\tilde{t} = b^{y_T} t$ and $\tilde{h} = b^{y_T} h$ & $F(t,h) = F(\tilde{t},\tilde{h})$ $\rightarrow$ $f(t,h) = b^{-d} f(\tilde{t},\tilde{h})$

[Widom postulate]

- correlation length: $\xi(t,h) = b^1 \xi(b^{y_T} t, b^{y_H} h)$ $\rightarrow$ $\xi(t,0) \sim |t|^{-\nu}$ $[\nu = 1/y_T]$

$b = (-t)^{-\frac{1}{y_T}}$ $d\nu = 2 - \alpha$ (hyperscaling)

- correlation length: $\xi(t,h) = b^1 \xi(b^{y_T} t, b^{y_H} h)$ $\rightarrow$ $\xi(t,0) \sim |t|^{-\nu}$ $[\nu = 1/y_T]$

(hyperscaling)

- correlation function:

$\star$ $FDT:\ \chi(t,h) = \int dr\ G_H(t,h,r)$

$$= \left(\frac{\partial^2 f}{\partial h^2}\right)_t = b^{-d+2y_H} \chi(b^{y_T} t, b^{y_H} h)$$

$$= b^{-d+2y_H} \int dr\ G_H(b^{y_T} t, b^{y_H} h, r)$$

$$= b^{-2d+2y_H} \int dr\ G_H(b^{y_T} t, b^{y_H} h, b^{-1} r)$$

$\star$ tempting to say $\quad G_H(t,h,r) = b^{-2x_H} G_H(b^{y_T} t, b^{y_H} h, b^{-1} r) \quad (x_H + y_H = d)$

$$\rightarrow \quad \underbrace{G_H(0,0,r) = r^{-2x_H}}_{b=r} G_H(0,0,1) \sim \frac{1}{r^{d-2+\eta}}, \quad [d-2+\eta = 2(d-y_H)]$$

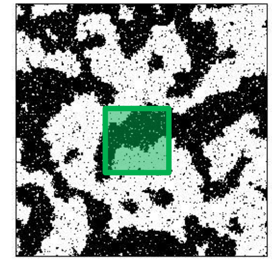
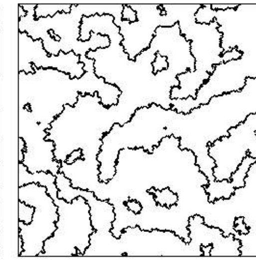
(hyperscaling)

$$\underbrace{G_H(t,0,r) = |t|^{-2x_H/y_T}}_{b=|t|^{-\frac{1}{y_T}}} G_H(\pm 1, 0, r|t|^{1/y_T}) \sim \exp[-ar|t|^{1/y_T}]$$

$$\sim \exp[-r/\xi] \rightarrow \xi \sim |t|^{-1/y_T}$$

$\star$ hyperscaling is fragile and broken in MFT.

- Fractal dimensions of Ising critical patterns

$A(\ell) \sim \ell^{d_A}$

* magnetization

– $M(\ell) = \sum_{w(\ell)} \langle S_i \rangle \simeq a\ \ell^{d_A} + \langle S_i \rangle \ell^d \qquad (d_A < d)$

$m(\ell) \simeq a\ \ell^{-d+d_A} = a\ \ell^{-x_A} \qquad (x_A\text{: scaling dimension})$

$(x_A + d_A = d)$

* energy

Finite-size-scaling

– $E(\ell) = \sum_{w(\ell)} \langle S_i S_j \rangle \simeq b\ \ell^{d_L} + \langle S_i S_j \rangle \ell^d$

$e(\ell) \simeq b\ \ell^{-d+d_L} + \langle S_i S_j \rangle = \boxed{b\ \ell^{-x_L}} + \boxed{\langle S_i S_j \rangle}$ (regular part) (singular part) $\qquad (x_L + d_L = d)$

- 2D Ising: $d_A = \frac{15}{8}$, $d_L = 1$ (relevant)
- all others are $d_\alpha = 0$ (marginal) or $d_\beta < 0$ (irrelevant)

- critical inside window $w(\ell)$ for $\ell \lesssim \xi(t,0) \sim |t|^{-1/y_T} \Rightarrow \quad \ell^{y_T}|t| \lesssim \mathcal{O}(1)$

  – $\xi(t,0) = b^1 \xi(b^{y_T} t, 0) = \ell^1 \xi(\ell^{y_T} t, 0) \sim \ell \quad \text{for} \quad \ell^{y_T}|t| \lesssim \mathcal{O}(1)$

- $m_s(t,0) = b^{-d+y_H} m_s(b^{y_T} t, 0) = \ell^{-d+y_H} m_s(\ell^{y_T} t, 0) \sim \ell^{-d+y_H} \longrightarrow d_A = y_H$

- $e_s(t,0) = \left(\frac{\partial f_s}{\partial t}\right) = b^{-d+y_T} e_s(b^{y_T}, 0) = \ell^{-d+y_T} e_s(\ell^{y_T} t, 0) \sim \ell^{-d+y_T}$

  $\longrightarrow d_L = y_T$

- **extensions**

  - **universal scaling function & amplitude ratios**

  - **all scaling fields with finite-size and irrelevant scalings**

$$f_{\text{sing}}(u_t, u_h, L^{-1}, u_1, \cdots) = b^{-d} f_{\text{sing}}(b^{y_t} u_t, b^{y_h} u_h, bL^{-1}, b^{y_{ir,1}} u_1, \cdots)$$

[exact with correct scaling eigenfields]

- critical line, FSS theory, Fisher renormalization, ...

  - **Mean field theory**

- Landau-Ginzburg functional, upper critical dimension, networks,
  hyperscaling violation, various FSS, ...

  - **critical phases**

- XY model, clock model, antiferromagnetic models, 8-vertex model, ...

[marginal operator]

  - **conformal invariance**

- conformal chage, universal FSS amplitudes, integrable systems, ...

[Coulomb gas method, algebraic(coordinate) Bethe ansatz]

Epilogue

- Phase & transitions: emergent property of many-body systems
- Critical phenomena and scaling: universal
- Macroscopic behavior reveals microscopic symmetry.
- Thermodynamic scaling is governed by geometric scaling: fractal dimensions.
- Universality classes in NEQ critical phenomena ?
- …