Phase Transitions: Scaling, Universality and Renormalization*

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*P.A.M. Dirac Proc. Roy. Soc. A 167 148 (1938) renormalization in classical electrodynamics.

"I might have thought that the new ideas were correct if they had not been so ugly" Dyson quoting Dirac on renormalization.

abstract

In present-day physics, the renormalization method, as developed by Kenneth G. Wilson, serves as the primary means for constructing the connections between theories at different length scales. This method is rooted in both particle physics and the theory of phase transitions. It was developed to supplement mean field theories like those developed by van der Waals and Maxwell, followed by Landau.

Sharp phase transitions are necessarily connected with singularities in statistical mechanics, which in turn require infinite systems for their realization. (I call this result the extended singularity theorem.) A discussion of this point apparently marked a 1937 meeting in Amsterdam celebrating van der Waals.

Mean field theories neither demand nor employ spatial infinities in their descriptions of phase transitions. Another theory is required that weds a breaking of internal symmetries with a proper description of spatial infinities. The renormalization (semi-)group provides such a wedding. Its nature is described. The major ideas surrounding this point of view are described including especially scaling, universality, and the development of connections among different theories.

Who am I?

A condensed matter theorist, with an interest in the history of science, who intends to talk about a subject closely related to condensed matter, but also to the philosophy of science and particle physics. I am not an expert in either of the latter subjects.

condensed matter physics: formulations clear (stat mech, Schrodinger equation, etc.) goal: explain amazing variety of nature. Nature = an Onion, exposed layer after layer. We hope to see mathematical and conceptual beauty arise from the mundane.

particle physics: simple results=masses, cross-sections goal: seek clear and final (!!) theoretic formulations based upon experiment and observations. Hope to see the mundane arise from the mathematical beauty of a single truth.

Connections in Condensed Matter Physics

Condensed matter physics relates the observable, often macroscopic, properties of liquids, gases, solids and all everyday materials to more microscopic theories, often the quantum theory of atoms and molecules. Since the macroscopic theories are themselves non-trivial, e.g. elasticity, hydrodynamics, the electrodynamics of materials, it follows that condensed matter physics is largely an exercise in connecting different kinds of theories.

Typically this connection involves different length scales

Size of molecule = 10^{-9} meter. Size of laboratory= 5 meter

One of the deepest aspects of this area of science is the existence of different thermodynamic phases, each with qualitatively different properties. E.g., freezing is a sudden qualitative change in which the material abruptly gains rigidity. How can this happen?

All thermodynamic behavior is based on statistical mechanics.

Connections in Particle Physics

Particle physics often wishes to relate its present, phenomenological, theory to a deeper (?!) theory at a much shorter or longer length scale. e.g. Connect the standard model to physics at a LHC, unification, or Planck scale.

Previously the search for a final theory has been impeded by ugliness or singularities arising at scales far from observation. These singularities show up directly as infinities in perturbation theory and indirectly as algebraic behavior ($1/|x-y|^p$) in a correlation function

I am going to follow condensed matter physics for the next parts of this talk, but particle physics and condensed matter physics are essentially similar.

Further Connections

Field Theory and Statistical Mechanics are closely connected. A Wick rotation $t \rightarrow i/(kT)$ will take you from one to the other.

Quantum Mechanics and Classical Mechanics are closely connected. Both employ Hamiltonians as basic generators of time development as do Field Theory and Statistical Mechanics.

All four have a dual structure in which terms in the Hamiltonian both describe measurable quantities and equally generate changes in development.

All four have the same structure: Poisson Bracket and Commutator, conjugate variables = p's and q's.

I shall talk mostly about statistical mechanics.

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STATISTICAL MECHANICS AND SINGULARITIES

Statistical mechanics (defined by Ludwig Boltzmann in 1870s) states that the probability for finding a equilibrium system in a volume element dγ about a position, γ, in phase (position and momentum) space is equal to dγ exp[-β(H{γ} -F)] . Here β is the inverse temperature, H{γ} the Hamiltonian or energy and F the free energy of the system. The latter is given by the normalization condition

$$\exp[-\beta F] = \int d\gamma \exp[-\beta H\{\gamma\}]$$

where the integral covers all the configurations of the system. Thus the free energy is proportional to a logarithm of a sum (or integral) of exponentials. For a system that is finite in extent, such a sum is always a smooth (real analytic) function of its arguments. Consequently phase transitions, which involve discontinuous changes as parameters like temperature or pressure are varied, can only be found in infinite systems.

…A phase transition appears as a sharp change in the form of thermodynamic functions, as you go from one kind of behavior to another. These sharp changes are mathematical singularities. A singularity will not happen in any finite system, as in a finite liquid. The singularity can (and does) happen in an infinite system. I call this result the extended singularity theorem. This theorem has been extensively used, but not really extensively discussed, in the previous literature.

It follows that any proper description of a phase transition requires a theory which makes an explicit use of the infinite size of the system. Most theories constructed before Wilson's renormalization group (1971) fail this test.

http://blogs.trb.com/news/local/longisland/politics/blog/2008/04/

swim in liquid water

abrupt change

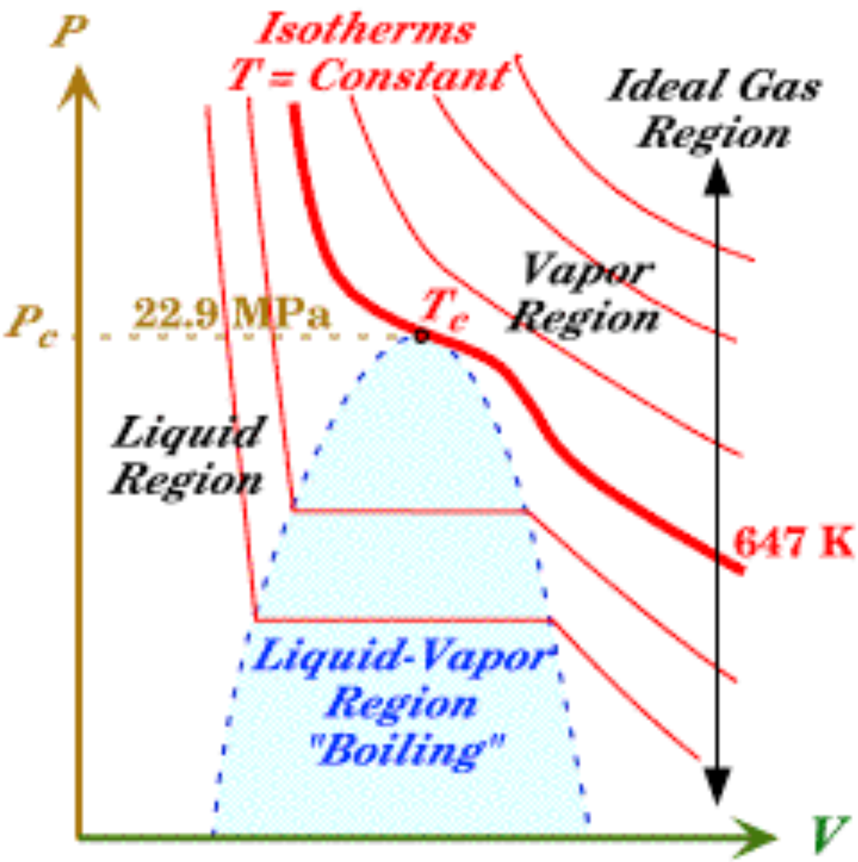
walk on soldi ice

http://azahar.files.wordpress.com/

History:

(1869) Thomas Andrews, experimentally studied the P-V diagram of CO_2. He discovered the critical point. His data look roughly like:

Phil. Trans. Roy. Soc. **159 p.** 575 (1869)



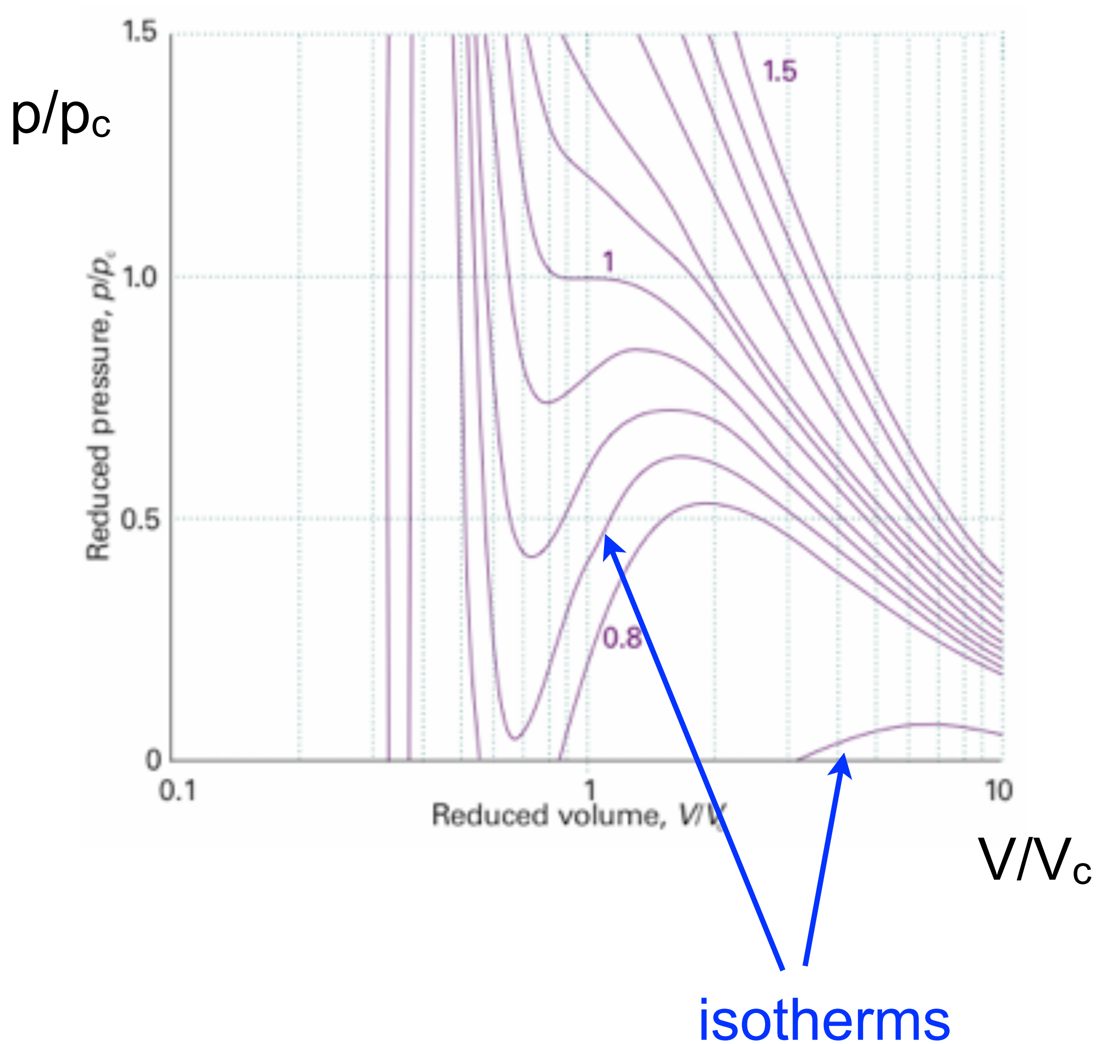
Cartoon is PVT plot for water, but CO_2 is similar, with a more accessible critical point.

Note qualitative changes.

- as boiling takes one from liquid to vapor
- as one passes from isotherm to isotherm through critical point

These qualitative changes are mathematical singularities.

In 1873 van der Waals derives an approximate equation of state for fluids:



Starts from pV=NkT, he gets cubic equation

$$(p+aN^2/V^2)(V-Nb)=NkT$$

Takes into account

- strong repulsive interaction via excluded volume (bN), and also
- attractive interactions via potential of mean force (aN^2/V^2), (accurate for long-ranged forces.)

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Sunday, April 18, 2010

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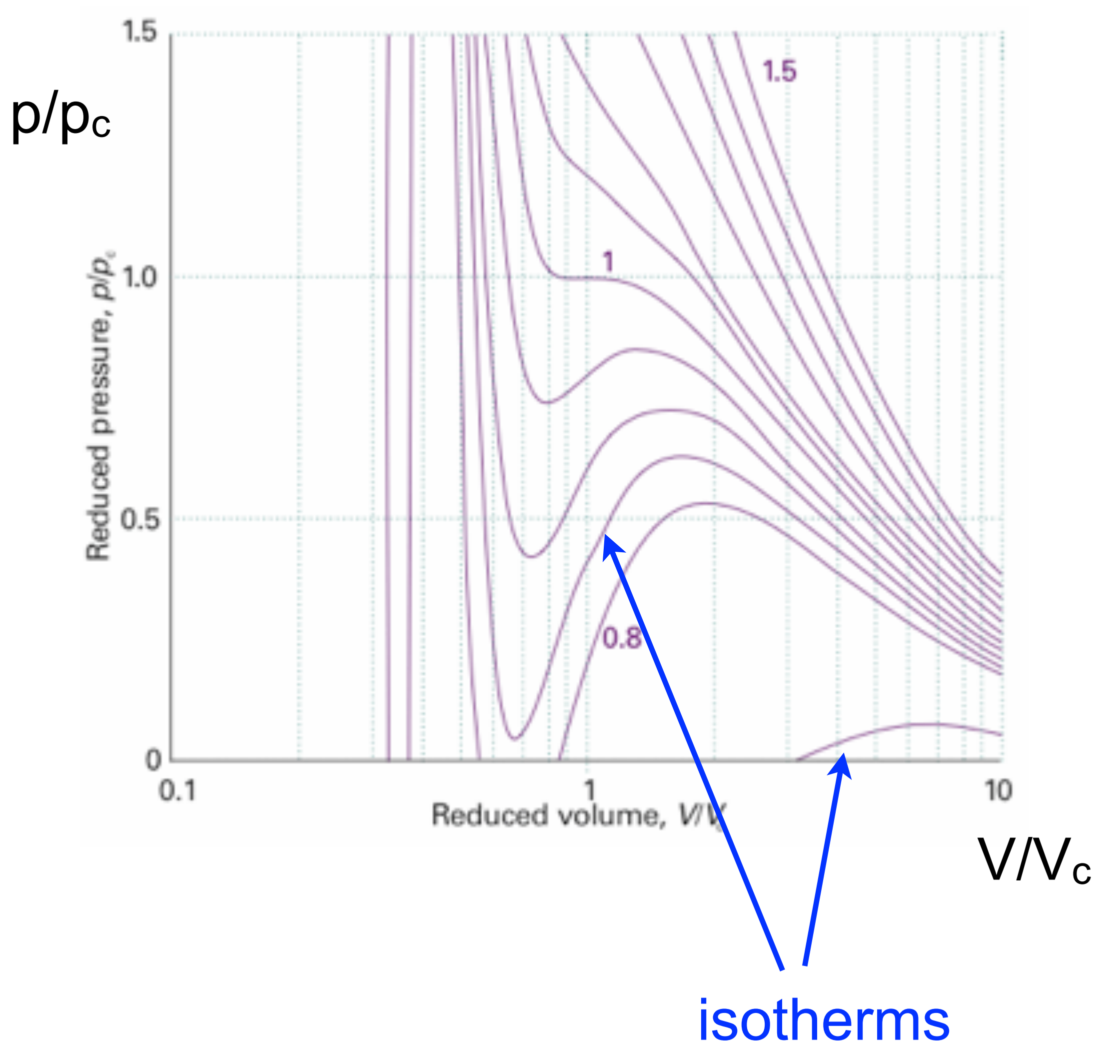

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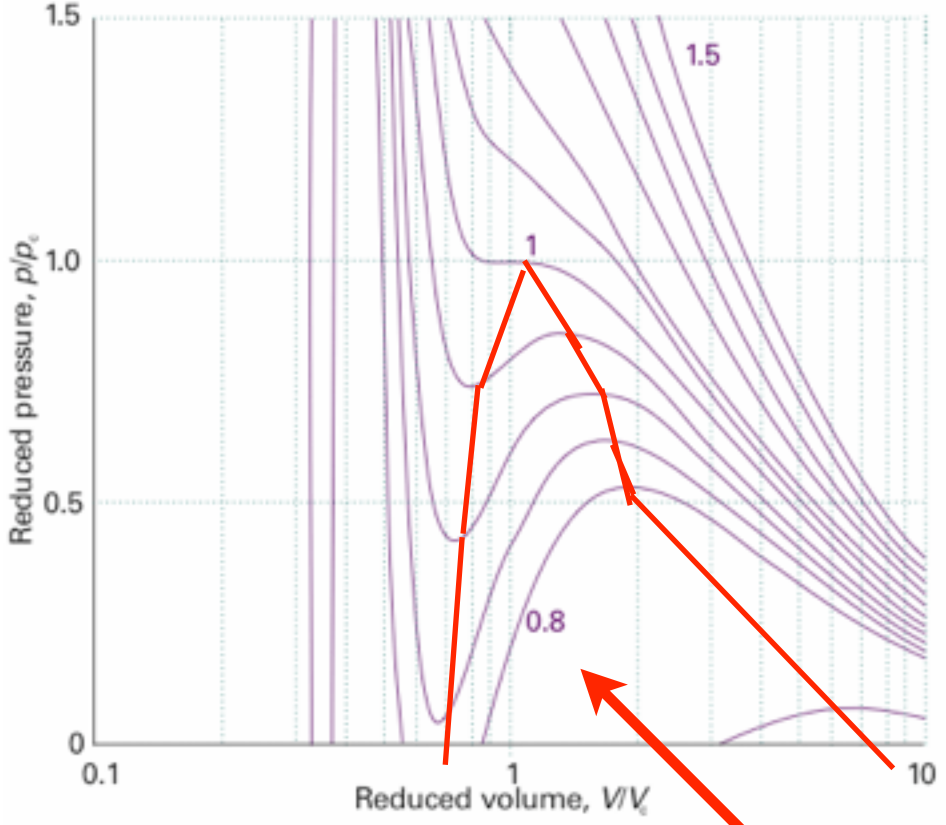
Note that there is here no reference to infinite size of system, no singularities and no phase transitions.

But van der Waals' result is not entirely stable.

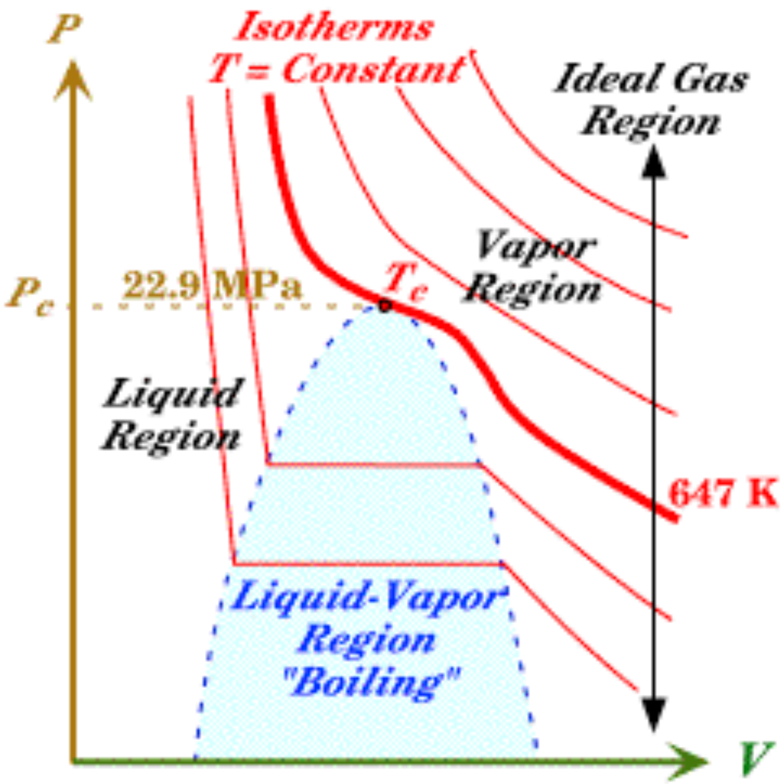


Red delimits region of absolute (mechanical) instability, where theory must be wrong.

(1875) Maxwell fixes up phase diagram

he puts in density jumps required by thermodynamics

J.C. Maxwell Nature, **10** 407 (1874),**11** 418 (1875).



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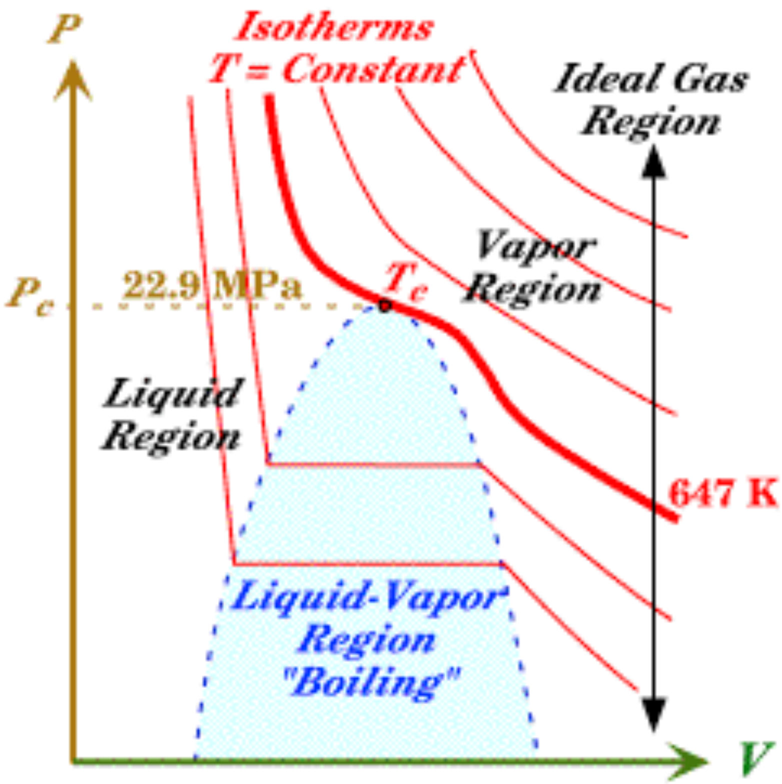


Cartoon P-V diagram for water but CO_2 is quite similar.

Then, P. Curie, Ann. Chem. Phys. 5, 289 (1895). P. Weiss, J. Phys. 6, 661 (1907). use very similar mean field theory arguments to derive properties of paramagnetic to ferromagnetic transition. This is followed by a host of mean field calculations mostly used to describe many different kinds of phase transitions, with many different kinds of order.

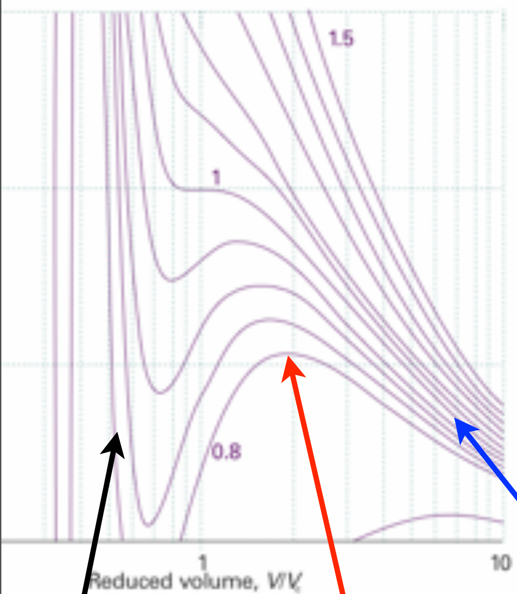
Sunday, April 18, 2010

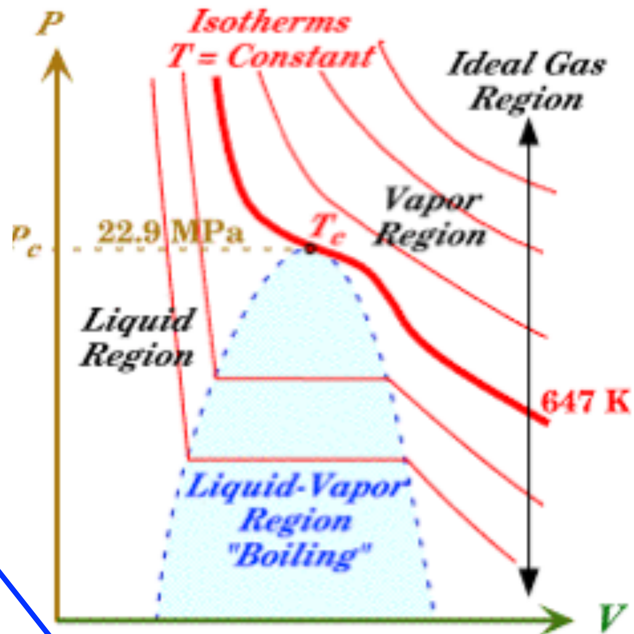
fast forward to 1937 at statistical mechanics conference in Amsterdam for van der Waals centennial

P. Debye, G. Uhlenbeck, H. Kramers present ….

stat mech theory
van der Waals

Maxwell &
experiment





Kramers* chairs a session. He knows extended singularity theorem, i.e. that for finite N picture on the right (with singularities!) is incompatible with statistical mechanics of finite system. Picture on left is incompatible with thermodynamics.

liquid region: little theory

mixed state region: instabilities

vapor region: expansions from statistical mechanics

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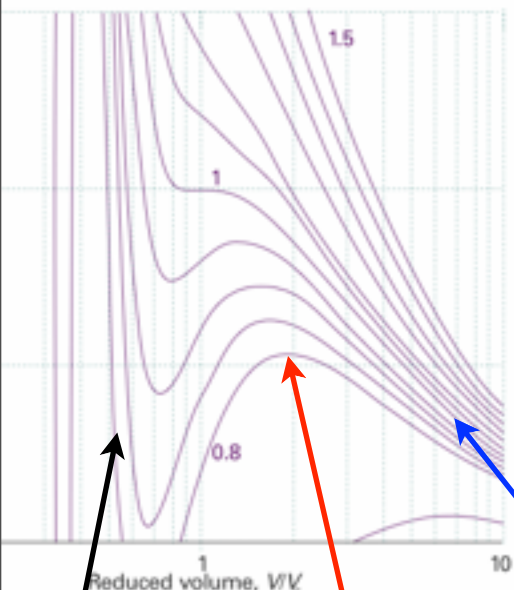

Maxwell &
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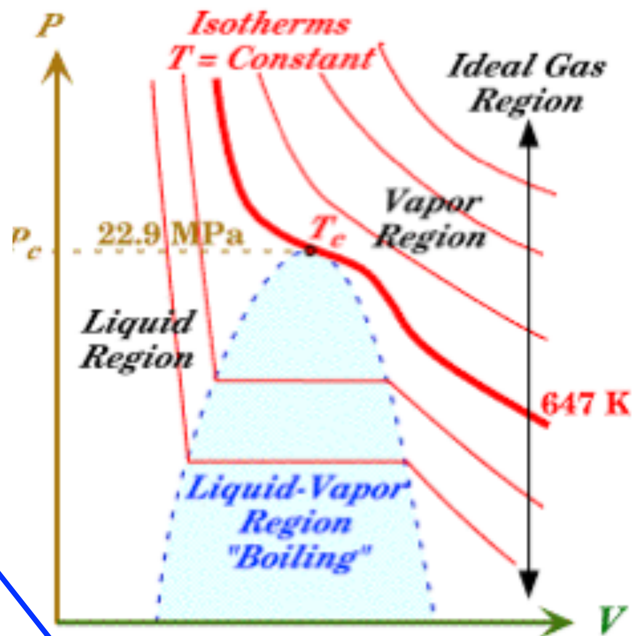

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This is wrong answer, liquids are described by statistical mechanics.

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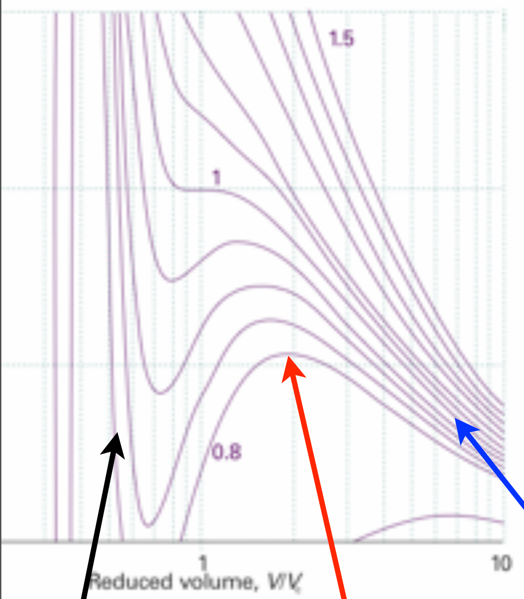

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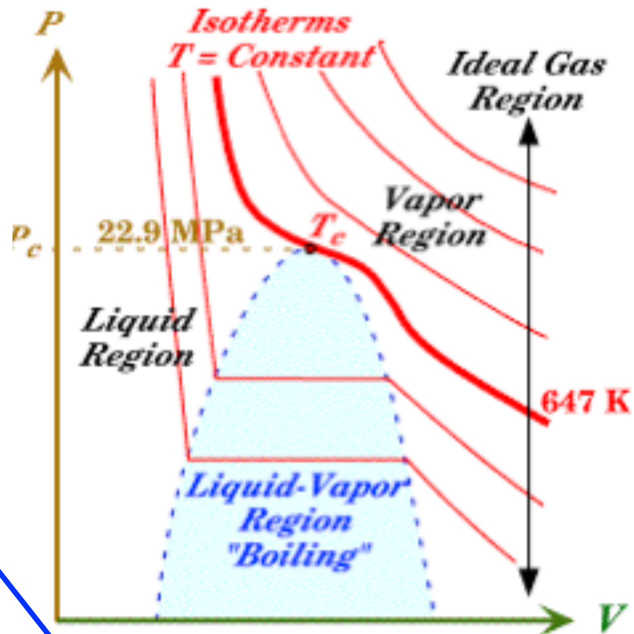

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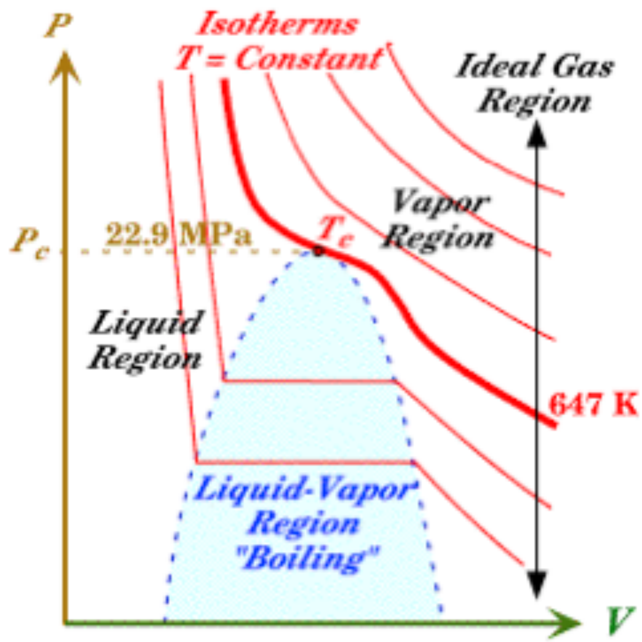
* "Kramers introduced the idea of renormalization" T. Veltman

Sunday, April 18, 2010

Application to Phase Transitions: today's view

- thermodynamic phase transitions involve singularities, and infinities arising (almost always) from unbounded numbers of particles
- these infinities appear in thermodynamic derivatives which is caused by a coherence length (correlation length) that diverges*
- in practice coherence length describes spatial extent of fluctuations that look like regions of two phases intermixed, e.g. drops of vapor in liquid or drops of liquid in vapor.

* This divergence makes extended similarity theorem work



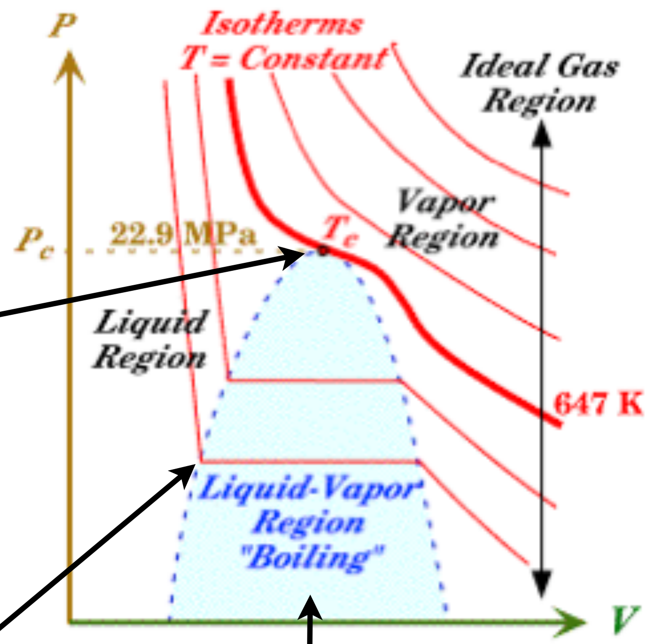
statistical mechanics does mostly fail, but not in liquid region--- rather in boiling region.

The approximate theories of stat mech (e.g. MFT's) must be improved near critical point.

theories available in 1937 all fail near critical point.

Application to Phase Transitions: today's view..., continued

Finite size of real systems cuts off infinities, for example, in the derivative of density with respect to pressure, at some very large value.



Finite size of real systems produces small regions of rounding here rather than sharp corners

statistical mechanics mostly fails in boiling region.

Additional Information about fluctuations

Even as far back as 1937, there was evidence of divergent fluctuations near the critical point, as evidenced by critical opalescence. As a clear fluid is brought near the critical point, it becomes cloudy.

Smoluchowski (1908) and then Einstein (1910) argued that fluctuations in density in the fluid produced scattering and that these fluctuations would diverge at the critical point causing a divergence in the compressibility of the fluid.

A little later, Ornstein and Zernike (1914,1916) argued that it was not the magnitude of the local fluctuations which would diverge near criticality. Instead the typical size of the fluctuation region, the coherence length, ξ, would diverge as the critical point was approached. That divergence would produce the infinity in the susceptibility. Specifically the divergence would appear in a correlation function

$$\langle [\rho(\mathbf{x})-\langle\rho\rangle]\,[\rho(\mathbf{y})-\langle\rho\rangle] \rangle = (1/|\mathbf{x}-\mathbf{y}|)\,\exp(\,-\xi|\mathbf{x}-\mathbf{y}|)$$

How could these divergences occur? Mean field theory does roughly predicts them, but its detailed predictions are incorrect.

Specific descriptors of critical region:

look for dependence on $t = T - T_c$, $h = p - p_c$

quantity	formula	value (MFT)	value* d=2	value d=3
compressibility (opalescence)	$t^{-\gamma}$	$\gamma = 1$	15/8	1.33
coherence length, ξ	$a\, t^{-\nu}$	$\nu = 0.5$	1	0.62
jump in density	$(-t)^{\beta}$	$\beta = ½$	1/8	0.34
density dependence on pressure	$\rho - \rho_c \sim h^{1/\delta}$	$\delta = 3$	15	4.3

* Onsager solution, Ising model

Mean Field Theory's application to electrodynamics of continuous media

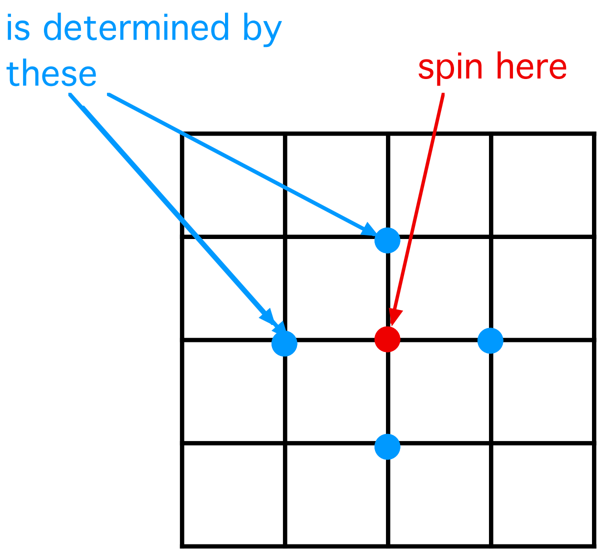
In van der Waals MFT, a particle is affected by the average field produced by particles around it.   A good and accurate example of MFT is the electrodynamics of continuous media: described by **E,D,B,H** fields.

Fields produced externally to material are **D,H**

Fields **E,B** include, in addition, averaged effects of charges and currents within material**.**

This kind of mean field theory is usually very accurate because electrodynamics includes long-ranged forces and many charges.   It fails in nanoscopic materials.

A simple example of a statistical system: Ising Model



according to Lee and Yang, this model can represent the liquid-gas phase transition

Defined by a lattice and "spin" variables $\sigma_r = \pm 1$ on that lattice. These represent two different densities in a fluid. The usual Hamiltonian is

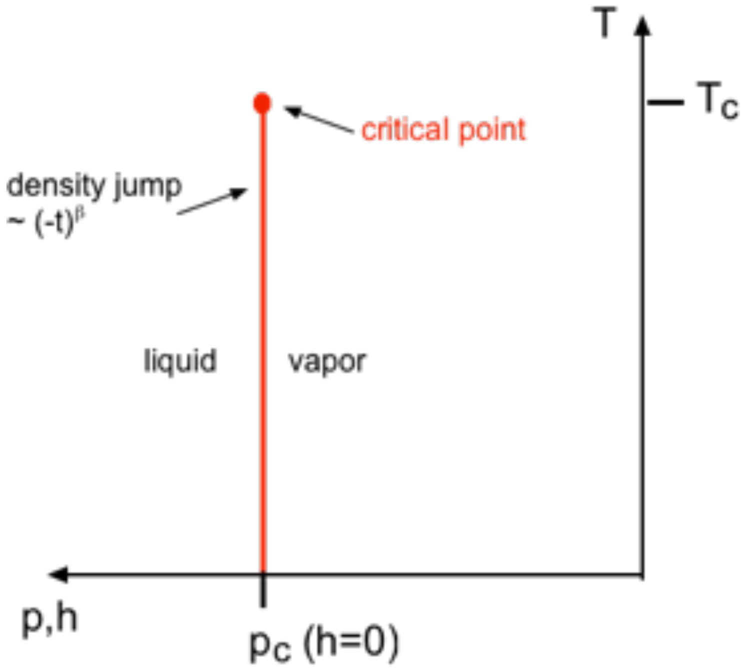
$$-\beta\mathcal{H} = K\sum_{nn}\sigma_r\sigma_s + h\sum_r \sigma_r$$

K=-J/(kT) is attraction between regions of equal density

$h = (p-p_c)/kT$ controls average density

$$-\beta\, F = \ln\left(\sum_{\{c\}} \exp[-\beta H\{c\}]\right)$$

Note that phase space integral is replaced by sum in this description.



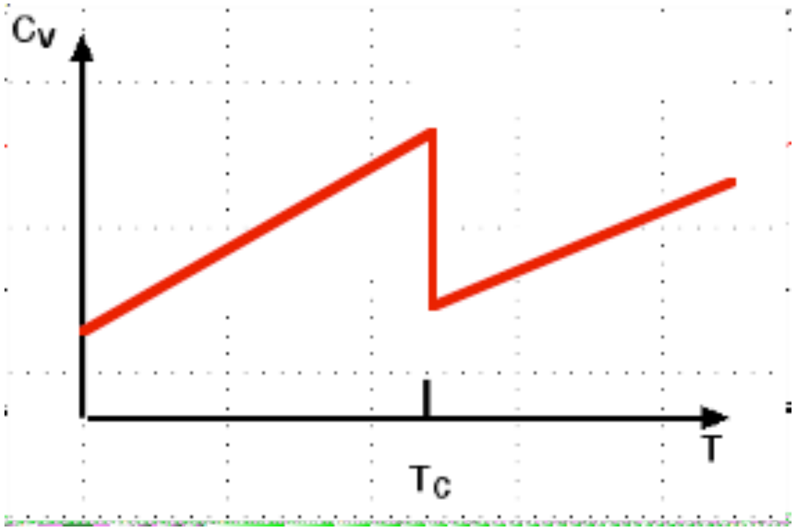
This model can have an ordering in which similar values of density variables, σ_r, attract one another. High average density is liquid, low density is vapor. The density jumps and the σ_r 's flip in sign as h crosses zero, the line of first order phase transitions.

Mean Field Theory is useless in predicting phase transitions and ordering over long distances

It predicts transitions in one-dimensional systems with finite-range interactions at non-zero temperatures.. (In fact, these transitions never occur.)

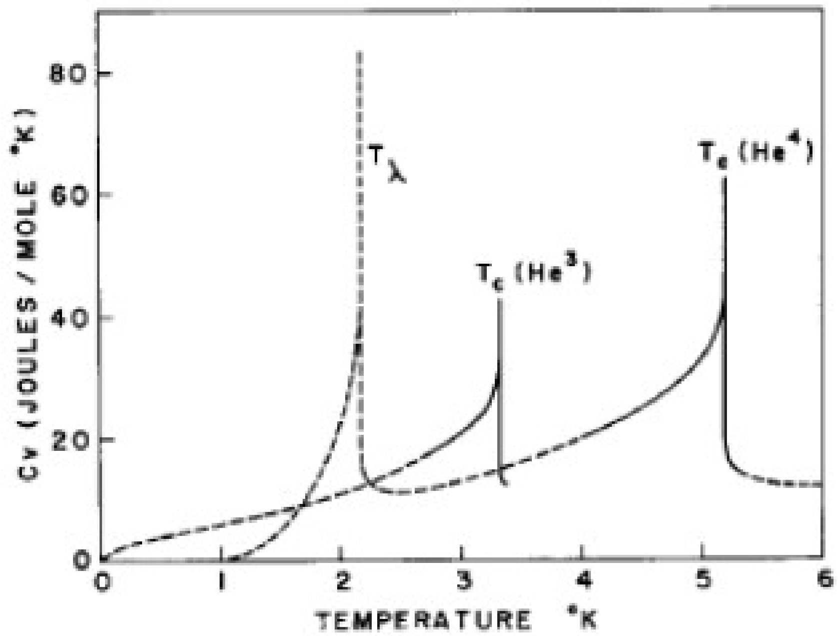
It predicts average order and transitions in two dimensions for Ising models, XY models, and Heisenberg models at non-zero temperatures. In these cases. there are respectively transitions plus order ($<\sigma_{\mathbf{r}}> \neq 0$), transitions but no average order ($<\sigma_{\mathbf{r}}>=0$), and no transitions or ordering.

Mean Field Theory is Useless near Critical Point: Look at heat capacity, C_v



Mean Field Theory=

discontinuous but finite jump at T_c



Moldover and Little see singular result, probably going to infinity

The physics is in fluctuations

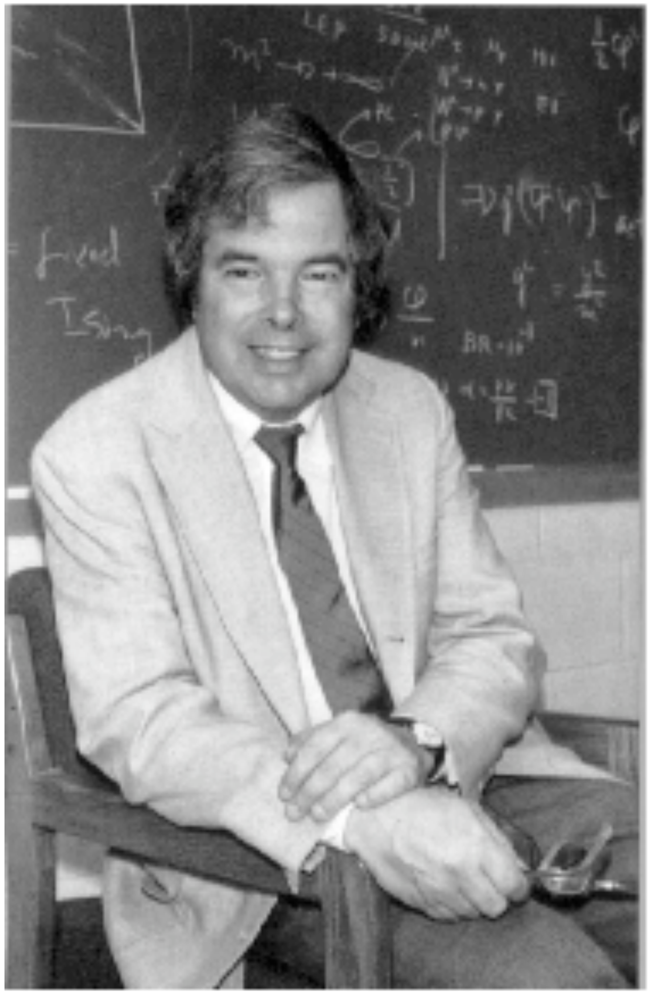
which extend over an indefinite range at critical point. t and h limit range of fluctuations to finite value, called the correlation length,ξ. How can we convert this fact into a theory?

At the singularities these fluctuations are droplets of fluid which have all different scales from the microscopic to as large as you want. Away from singularity correlation length serves to cut off the largest-scale fluctuations. These droplets are regions of density different from that of the surrounding fluid.

The Renormalization Revolution:

precursors:

- Onsager solves d=2 Ising model. His results disagree with mean field theory.
- King's College School (Cyril Domb, Martin Sykes, Michael Fisher) do expansions in K and exp(-K) and find mean field theory critical indices are wrong.
- Patashnskii & Pokrovsky look at correlations in fluctuations
- Benjamin Widom gets scaling and phenomenology right
- Kadanoff suggests partial direction of argument



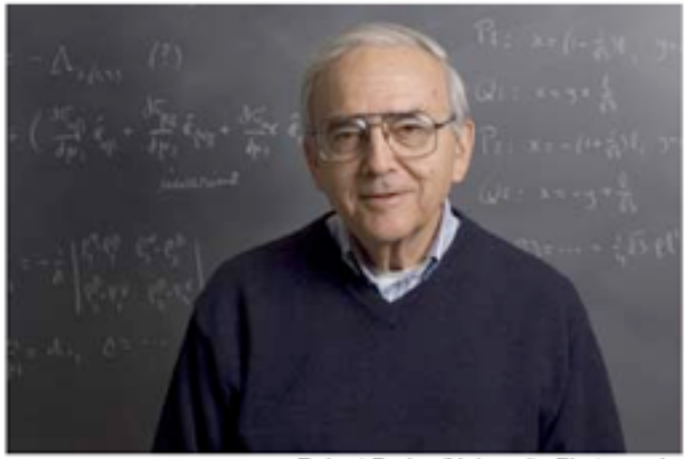
Kenneth G. Wilson synthesizes new theory

Toward the revolution

The phenomenology

Ben Widom noticed the most significant scaling properties of critical phenomena, but did not detail where they might have come from.

B. Widom, J. Chem. Phys. **43** 3892 and 3896 (1965).



Robert Barker/University Photography

Professor Benjamin Widom in his office in Baker Lab.

Widom's results

in terms of $t=T-T_c$ $h=p-p_c$

Widom 1965: scaling result He focuses attention on scaling near critical point. In this region, averages and fluctuations have a characteristic size, for example density jump ~ $(-t)^\beta$ when h=0

density minus critical density ~ $(h)^{1/\delta}$ when t=0

Therefore, Widom argues there is a characteristic size for h, which is

$h^* \sim (-t)^{\beta\,\delta} = (-t)^\Delta$ with $\Delta=\beta\,\delta$

so that density minus critical density = $(-t)^\beta g(h/t^\Delta)$

therefore, using a little thermodynamics, scaling for free energy is

$F(t,h)= V\, t^{\beta+\Delta} f^*(h/t^\Delta)+ F_{non\text{-}singular}$: (V is volume of system)

Further he says singular term in free energy given by excitations of size of coherence length with kT per excitation. They fill all space, giving

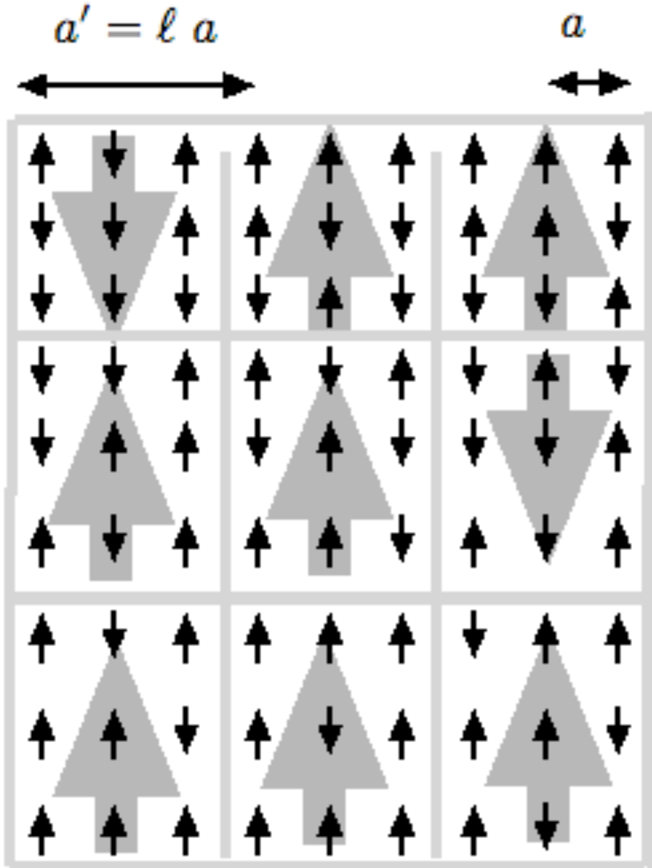
$F - F_{non\text{-}singular} \sim$ (Volume of system)/ $\xi^d \sim Vt^{d\nu}$

Therefore "magic" relations, e.g. $\beta + \Delta = d\,\nu$

Block Scaling 1966

Kadanoff considers invariance properties of critical point and asks how description might change if one replaced a block of spins by a single spin, thus changing the length scale and having fewer degrees of freedom.

Answer: There are new effective values of $(T-T_c)=t$, $(p-p_c)=h$, and free energy per spin K_0. These describe the system just as well as the old values. Fewer degrees of freedom imply new couplings, but no change at all in the physics. This result incorporates both scale-invariance and universality.



$$N' = N/\ell^d$$

$$h' = h\ \ell^{y_h}$$

$$t' = t\ \ell^{y_t}$$

The physics is in fluctuations

which extend over an indefinite range at critical point. t and h limit range (called the correlation length,ξ) to finite value

As renormalization is done, the lattice constant assumes a new value a´=ℓ a

The new deviation from the critical temperature is $t' = t\ \ell^{y_t}$

The new pressure variable is $h' = h\ \ell^{y_h}$

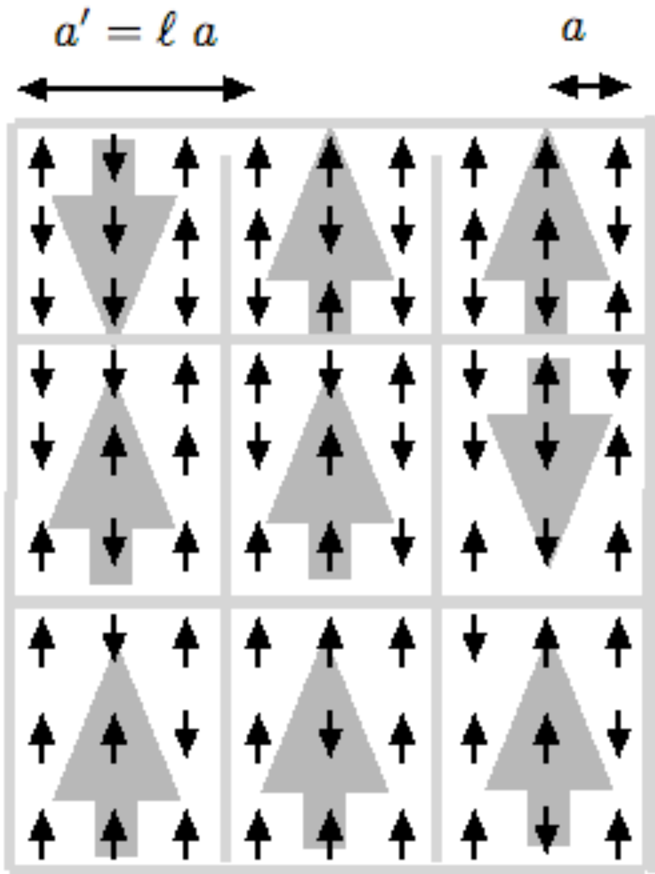
but the coherence length is just the same.

Since the length scale is irrelevant h and t must appear in the combination $h/t^{y_h/y_t}$ while the coherence length appears as $a/t^{1/y_t}$ which is invariant. The demand that the ℓ cancels out of all physical results produces the phenomenology of Widom.

So in 1966 Kadanoff produces a heuristic and incomplete theory

But it does describe scaling

Now there is a five year pause while the field tries to figure out what to do next



fewer degrees of freedom produces "block renormalization"

Wilson 1971 produces complete theory

Wilson's changes:

• He consider all possible couplings.   So you don't have to guess which couplings to use. The scale change produces a closed algebra of couplings.

• He considers a succession of renormalizations, not just one. So you don't have to guess where a big scale change will take you. You simply follow result of renormalizations.*

• After many renormalizations you eventually reach a fixed point where the couplings stop changing. Each fixed point can be considered to be its own separate physical theory.

* See also earlier work, e.g. Gell-man and Low

Types of Fixed Points

- continue changes in length scale until we reach limits of system (finite system) or
- continue changes in length scale until we reach a situation in which coupling change no more (infinite system)
- The latter is called a fixed point and describes phases

There are three kinds fixed points:

strong coupling: K,h go to infinity describes e.g. liquid phase

weak coupling: K, h go to zero describes e.g. vapor phase

critical: K set to K_c h set to zero, critical point

The different in destinations encode different behavior.

Different symmetries and spatial dimensions produce different fixed points.

Franz Wegner: At a particular fixed point there is a list of couplings.

We use eigenvalue analysis to pick out the linear combinations of couplings which have a simple change under the renormalization analysis:

$$K'_\mu = K_\mu \ \ell^{y_\mu}$$

These couplings appear in the near-critical Hamiltonian in the form of a linear variation about the fixed point Hamiltonian. $\mathcal{H}^*$

$$\mathcal{H}^* = \mathcal{H}^* + \sum_\mu \int d\mathbf{r} \ K_\mu O_\mu(\mathbf{r})$$

Here the $O_\mu(\mathbf{r})$ describes the local density of some fluctuating quantity, like σ_r. This particular one is conjugate to the coupling K_μ

If the coupling scales with an index y_μ, then the local operator, *O,* scales with an index $x_\mu = d - y_\mu$.

Franz Wegner & LPK: The couplings may be classified by the values of y_μ.

• If $Re(y_\mu) > 0$ then the coupling grows as we renormalize. The operator is called relevant and the coupling must be set to zero if we are the have a critical behavior at that fixed point.

If $Re(y_\mu) < 0$ then the coupling shrinks to zero as we renormalize. The operator is called irrelevant. As we renormalize, it goes away and has no effect on that universality class.

If $y_\mu = 0$ then the coupling remains constant as we renormalize. The operator is called marginal and may give us a fixed point which has some continuous variation with a parameter. Usually the is no marginal operator and the universality class remains isolated.

Universality

Start from view of microscopic system(s). We want to understand macroscopic behavior near critical point.

1. Adjust relevant couplings so system is near critical
2. Do renormalizations, lots of them, approach macroscopic behavior
3. Notice that irrelevant couplings have renormalized almost to zero. System approaches one of a few distinct fixed points.

Very different starting points reduce to a few distinct fixed points. Different starting systems fall in a few classes called Universality Classes depending upon their eventual fixed point. Each member of universality class has identical critical behavior.

Universality Classes

Ising model universality class:

- ferromagnet with easy axes
- liquid gas phase transition

XY model universality class:

- magnet with easy plane of magnetization
- normal fluid to superfluid transition
- in (d=2) also solid to liquid transition

Renormalization Group produces big change

old way: start with ensemble (like canonical ensemble) find averages

new way: start with ensemble calculate new ensemble.

after many renormalizations, find fixed point

- at weak coupling fixed point: find averages
- at critical fixed point: find scalings
- at strong coupling fixed point: find theory of nontrivial behavior, e.g. elasticity, acoustics, ferromagnetism, superconductor. Connect theories on different length scales.

Extended Singularity

Each universality class shows a connection between a microscopic internal symmetry (e.g. Ising model's up & down) or (rotation in a plane) and the topological properties of a large hunk of space, much larger than the range of the forces. It shows thermodynamic singularities, correlation functions which fall off algebraically, internal parameters, e.g. coherence length =inverse particle mass that have singular behavior.

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This connection between macroscopic and microscopic is interesting and quite beautiful.

So I disagree with Dirac, who said that renormalization is ugly. If you believe in a world of rich physics, and of many different theories, renormalization provides a quite elegant connection among theories.

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