Title: Statistical Mechanics (PHYS 602) - Lecture 14

Date: Oct 16, 2009 10:30 AM

URL: http://pirsa.org/09100138

Abstract:

Periodization

- Early period: look at the whole phase diagram, glance at critical region. I talked about this in a previous part. During this period mean field theory was developed. — 1860 to 1937

- Period of unrest. focus on critical region. mean field theory is not working, what to do? Develop phenomenological theory. I'll talk about this now. — 1937 or 1963 to 1971

- The Revolution: Wilson put forward renormalization group theory of critical phenomena — 1971

- Afterward: various mathematical/theoretical expressions and extensions of theory. — 1971-now

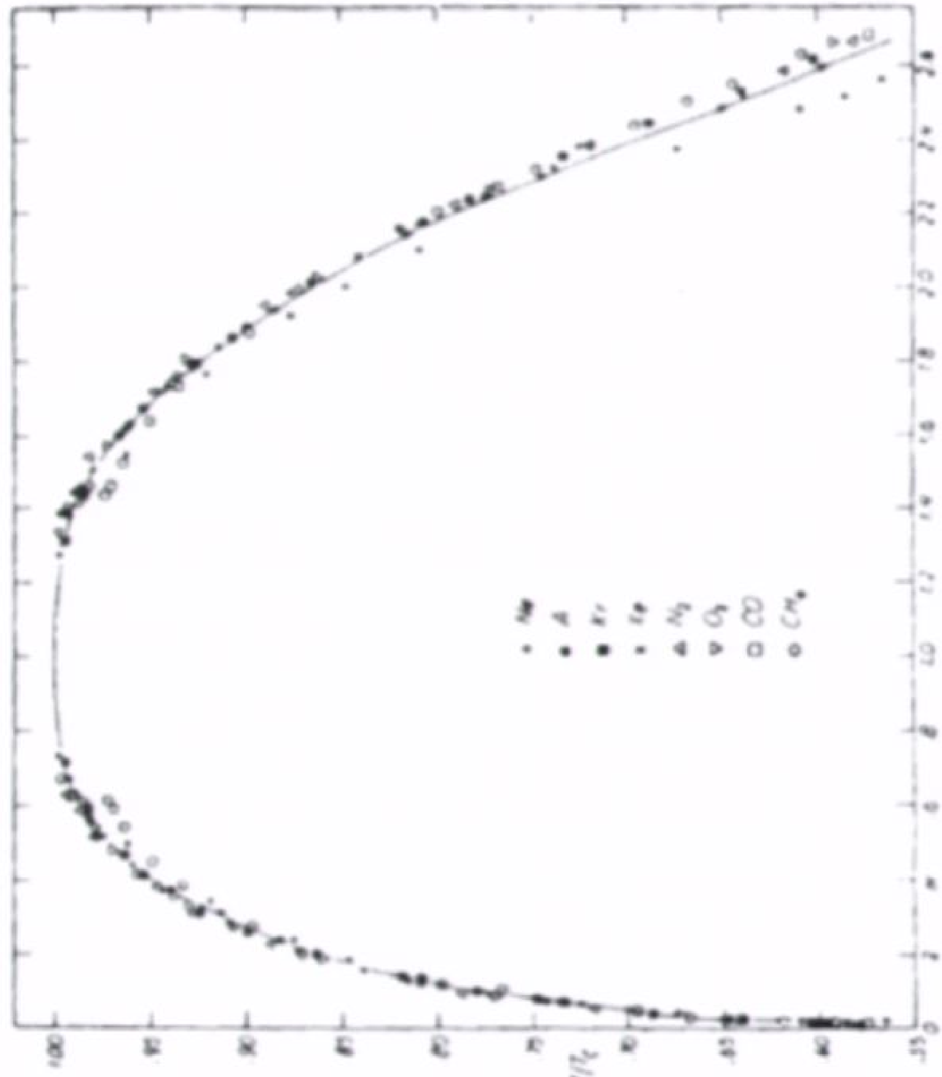
A worry?

Mean field theory gives $M \sim (T_c - T)^\beta$ and $\beta = 1/2$

This power is, however, wrong. Experiments are closer to

$$M \sim (T_c - T)^{1/3} \quad \text{in 3-D}$$

1880-1960: No one worries much about discrepancies



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

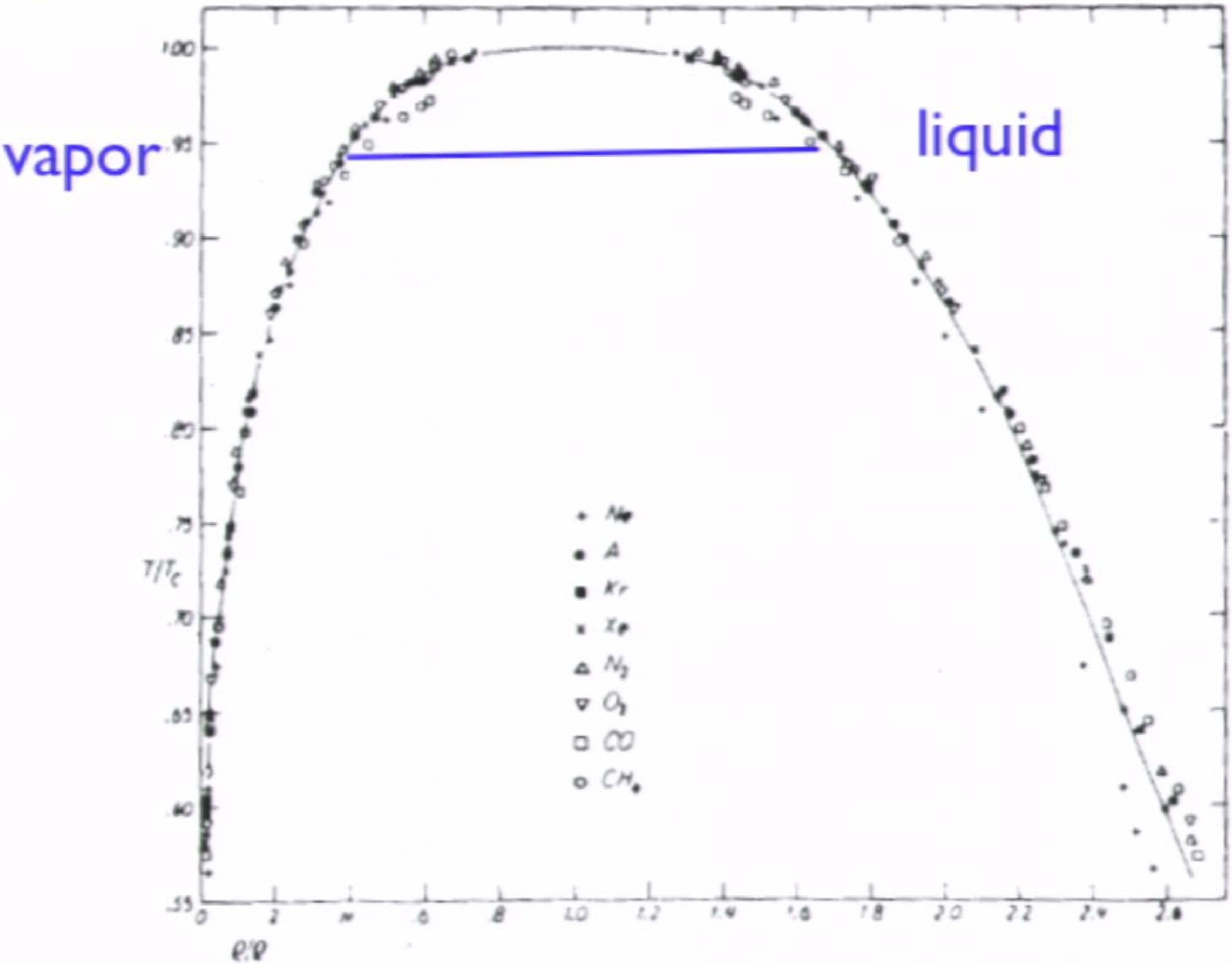


Figure 1.6 Reduced densities of coexisting liquid and gas phases for a number of simple molecular fluids (Guggenheim 1945). The experimental points support a law of corresponding states, but the universal curve is cubic rather than quadratic as required by van der Waals' theory.

Earlier Hints of Trouble

van der Waals had gotten something very much like $\beta = 1/3$ from analysis of Andrews data in the critical region. This worried him. He did not know what to do. He had no theory or model which gave anything like this. He believed that this was important, but he had no place to go with it.

Gugenheim was ignored.

Theoretical work

Onsager solution (1943) for 2D Ising model gives infinity in specific heat and order parameter index $\beta=1/8$ (Yang)--contradicts Landau theory which has $\beta=1/2$. Landau theory has jump in specific heat but no infinity.

Kings' College school (Cyril Domb, Martin Sykes, Michael Fisher, ... (1949-)) calculates indices using series expansion method. Gets values close to $\beta=1/8$ in two dimensions and $\beta=1/3$ in three and not the Landau\van der Waals value, $\beta=1/2$. They emphasize that mean field theory is incorrect.

Kramers recognizes that phase transitions require an infinite system. Mean field theory does not require an infinite system for its phase transitions.

Still Landau's no-fluctuation theory of phase transitions stands.

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Universality

Van der Waals and Uhlenbeck look for universal theory applying to entire phase diagram of many different fluids. This desire is misdirected. Experimental work on fluids shows that it is wrong. This conclusion also arises from theories of the Kirkwood school of physical chemists, which produces a non-universal theory of linked cluster expansion for fluids.

In the meantime, hints of another universality-- one near the critical point-- arises through work of Landau on mean field theory, which proves only partially correct, but also through the numerical work of the King's College School which sees different critical points on different lattices as quite alike. Brian Pippard brings this up in a more theoretical vein. These studies give hope of a universal behavior in critical region. Universality is a most attractive idea, drawing people to the subject.

Turbulence Work advances scaling ideas

drey Nikolaevich Kolmogorov

Kolmogorov theory (1941) uses a mean field argument to predict velocity in cascade of energy toward small scales.

Result: velocity difference at scale *r* behaves as

$$\delta v(r) \sim (r)^{1/3}$$

(N.B. One of first Scaling theories) Landau criticizes K's work for leaving out fluctuations. Kolmogorov modifies theory (1953) by assuming rather strong fluctuations in velocity. Landau & Lifshitz worry in print about Landau theory of phase transition.

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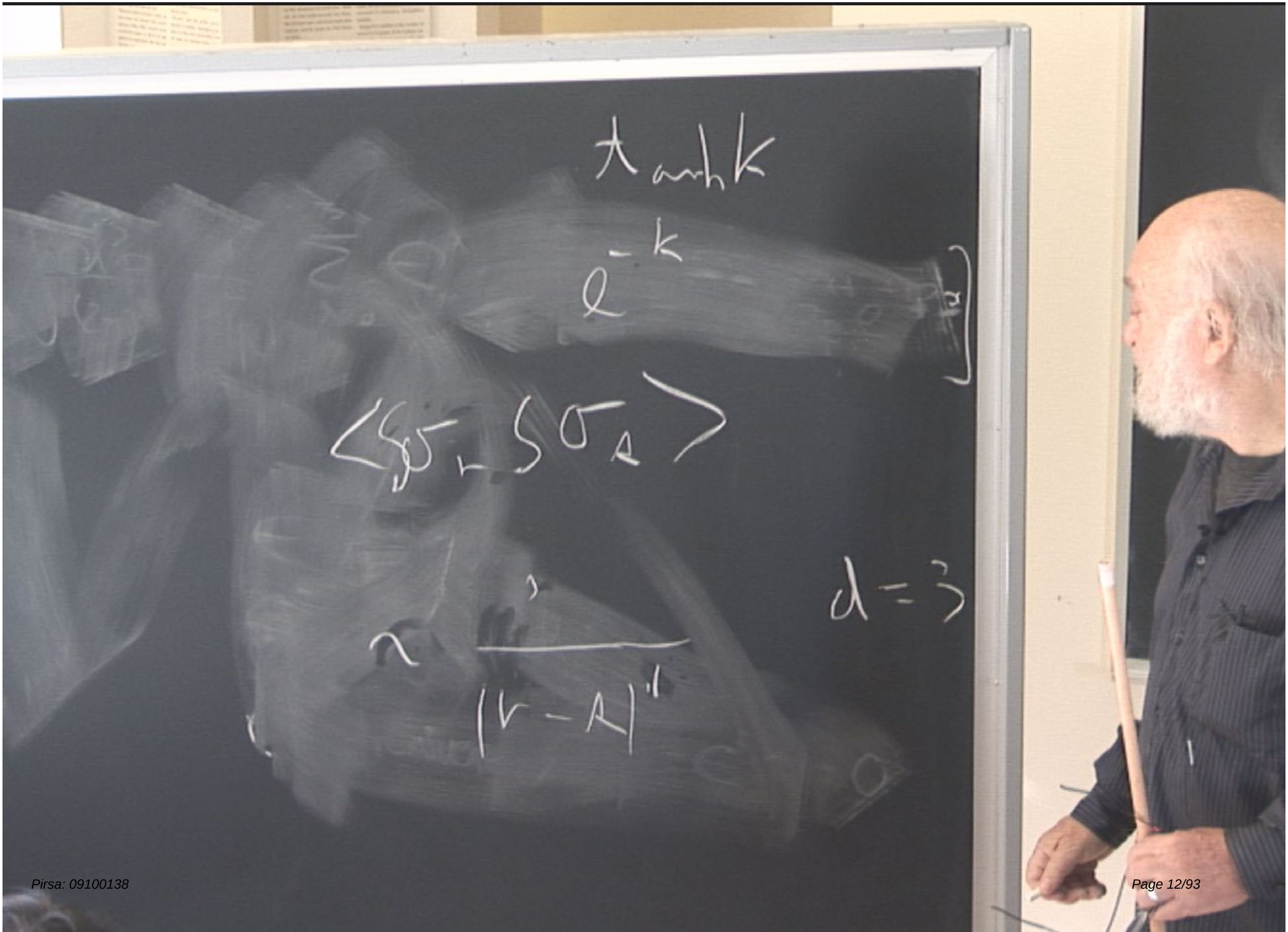
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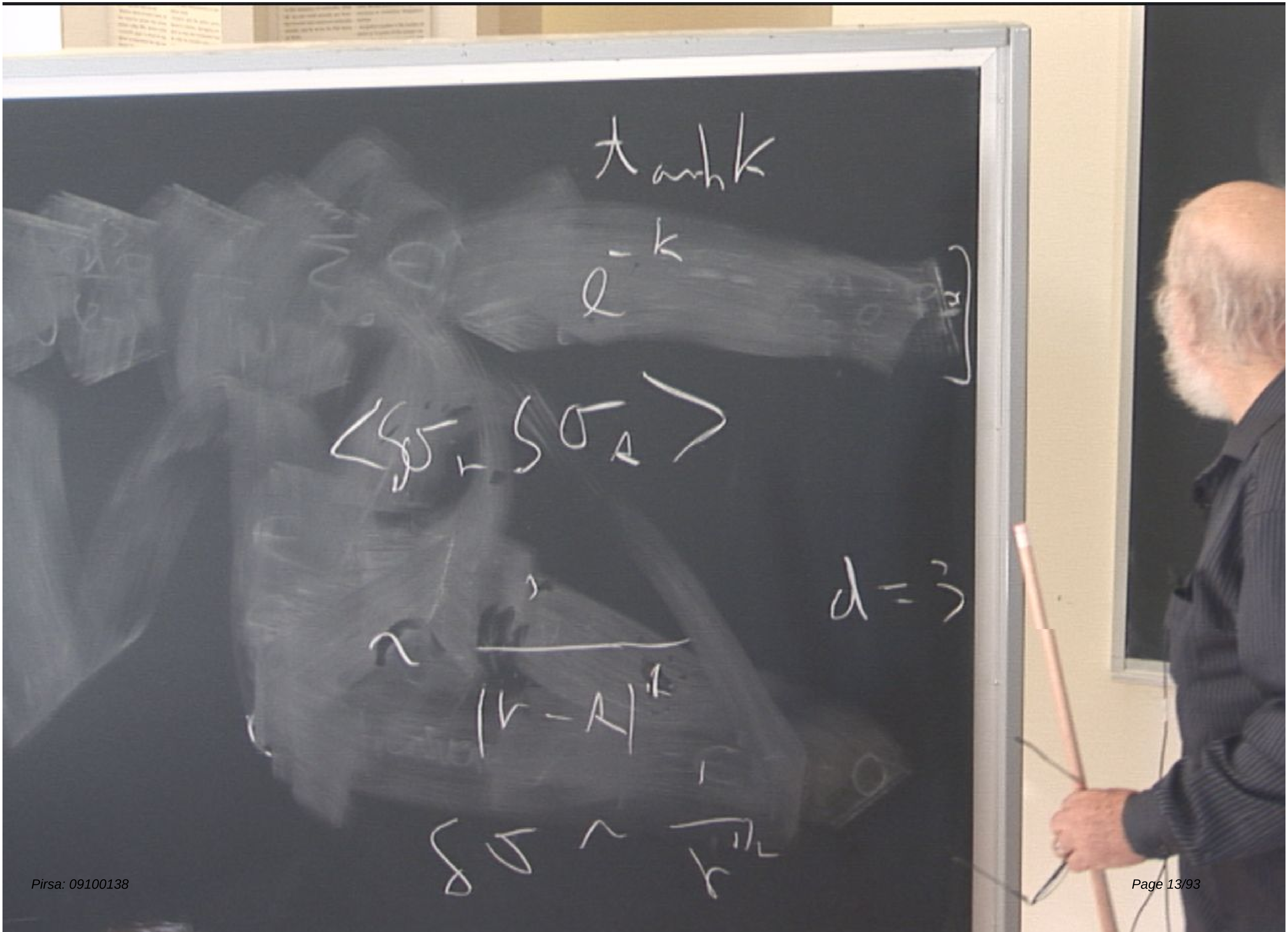
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More rumbles before the revolution

US NBS conference 1965 helps people recognize that 'critical phenomena' is a subject .

Focus changes: Don't look at the entire phase diagram, examine only the region near the critical point.

Get a whole host of new experiments,

embrace a new phenomenology,

Significant earlier work: Voronel' et. al (1960) specific heat of near-critical Argon.

superfluid transition helium, Kellers PhD thesis (1960) Stanford.

In each case, mean field theory says specific heat should remain finite but have a discontinuous jump at critical point. Data suggests an infinity at critical point.

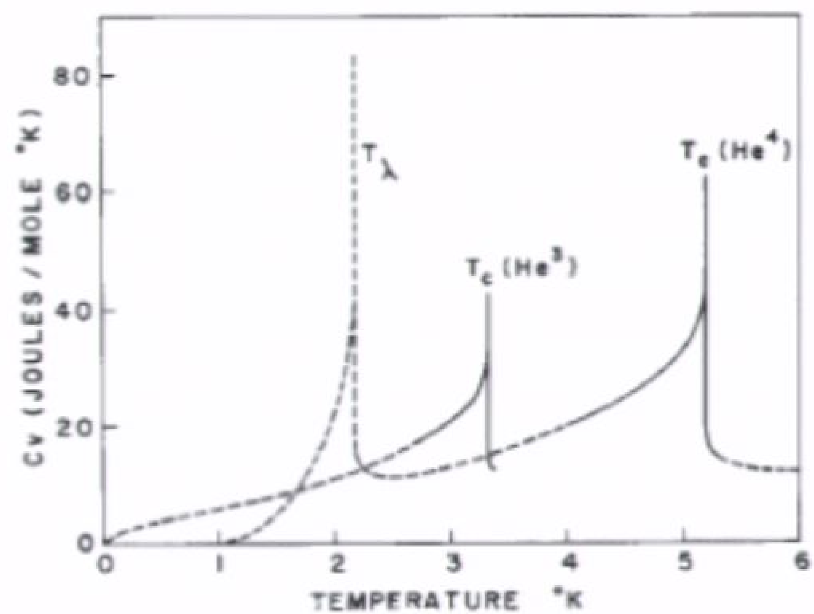

FIGURE 1. C_v of He³ and He⁴ at their respective critical den is plotted as a function of temperature. The solid curves are the present work.

Moldover and Little (1966)

Toward the revolution

The phenomenology

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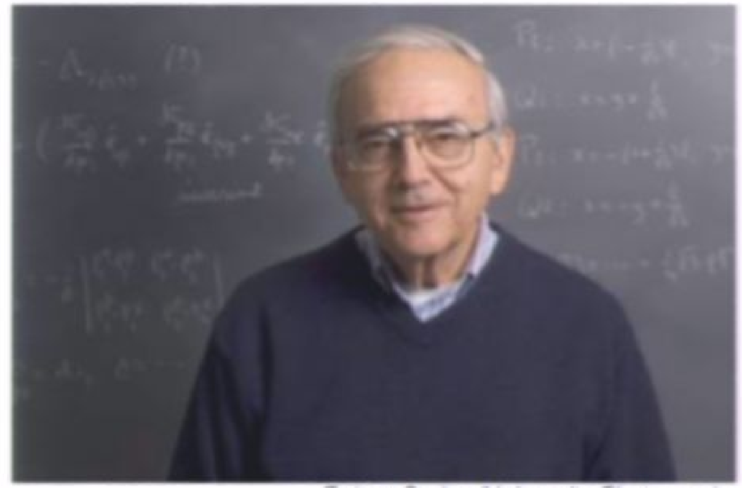


Robert Barker/University Photography
Professor Benjamin Widom in his office in Baker Lab.

Widom 1965: scaling result $F(t,h)=F_{ns} + t^{d\nu} f^{*}(h/t^{\Delta})$:

He focuses attention on scaling near critical point. In this region, averages and fluctuations have a characteristic size, for example

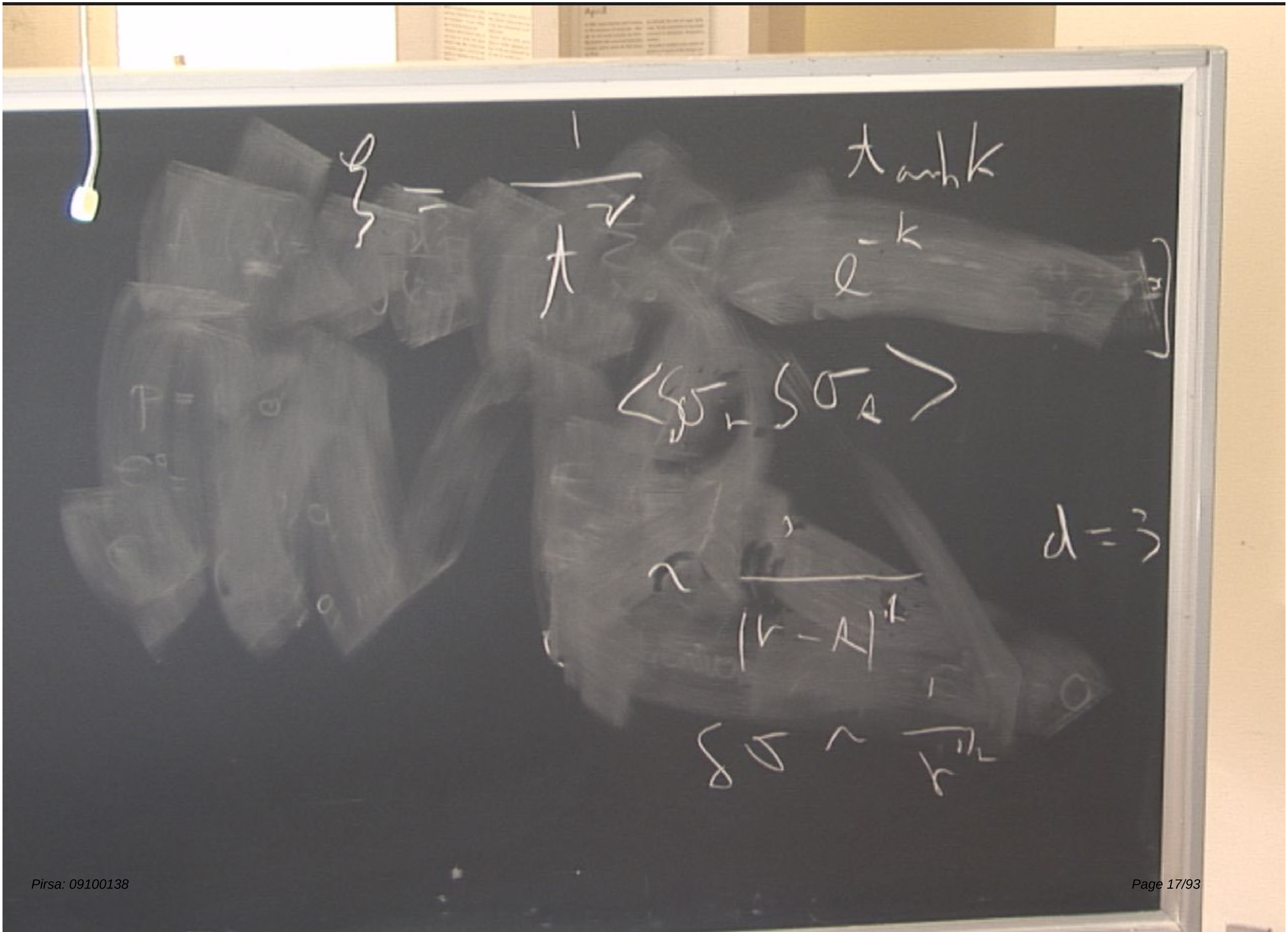
free energy ~ (coherence length)$^{-d}$, i.e. there is a free energy of kT per coherence volume

magnetization ~ $(-t)^{\beta}$ when h=0

magnetization ~ $(h)^{1/\delta}$ when t=0 implies h ~ $(-t)^{\beta\delta}$ implies $\Delta=\beta\delta$

therefore scaling for free energy

and "magic" relations e.g. $2-\alpha = d\nu$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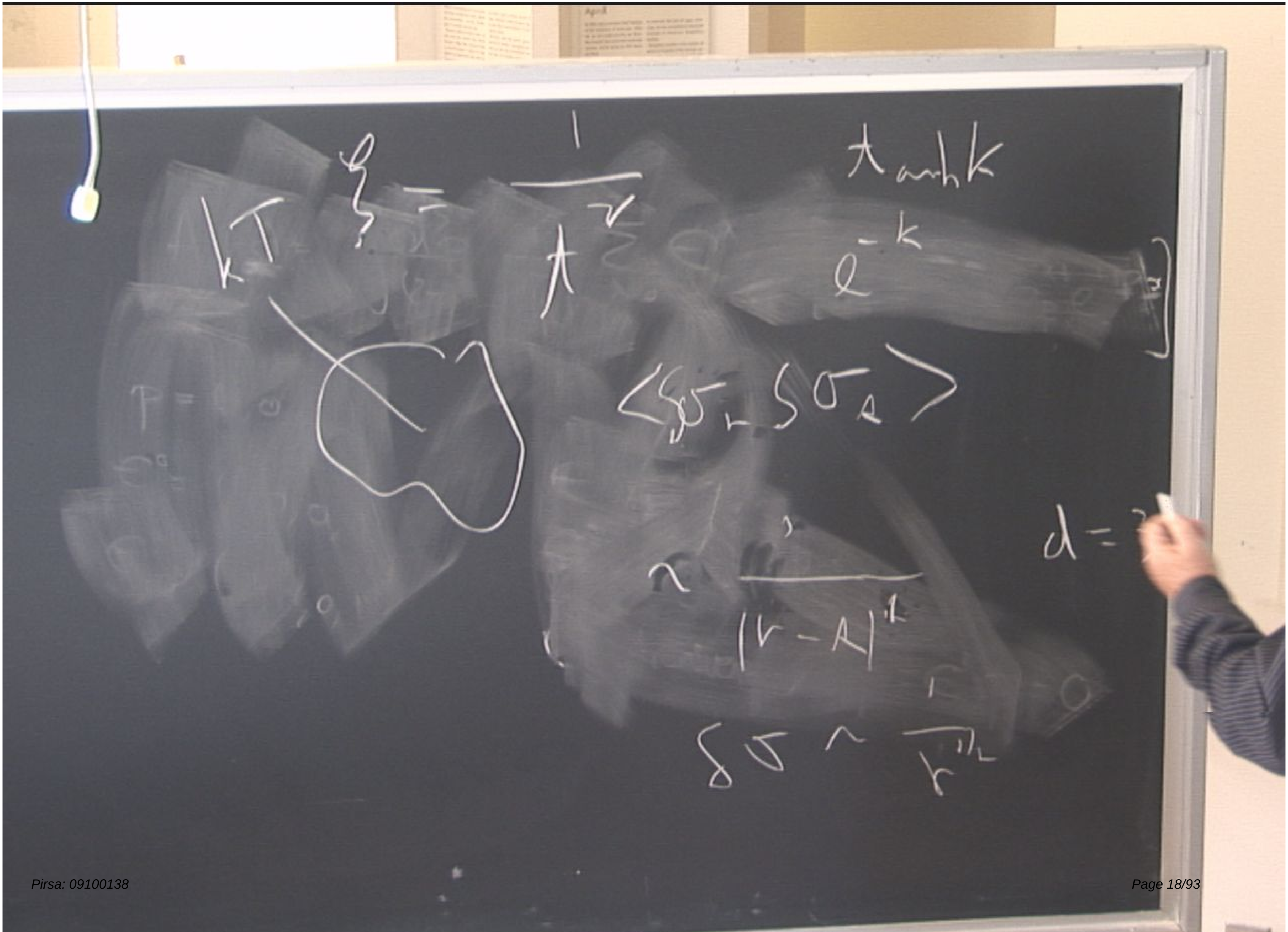
kT
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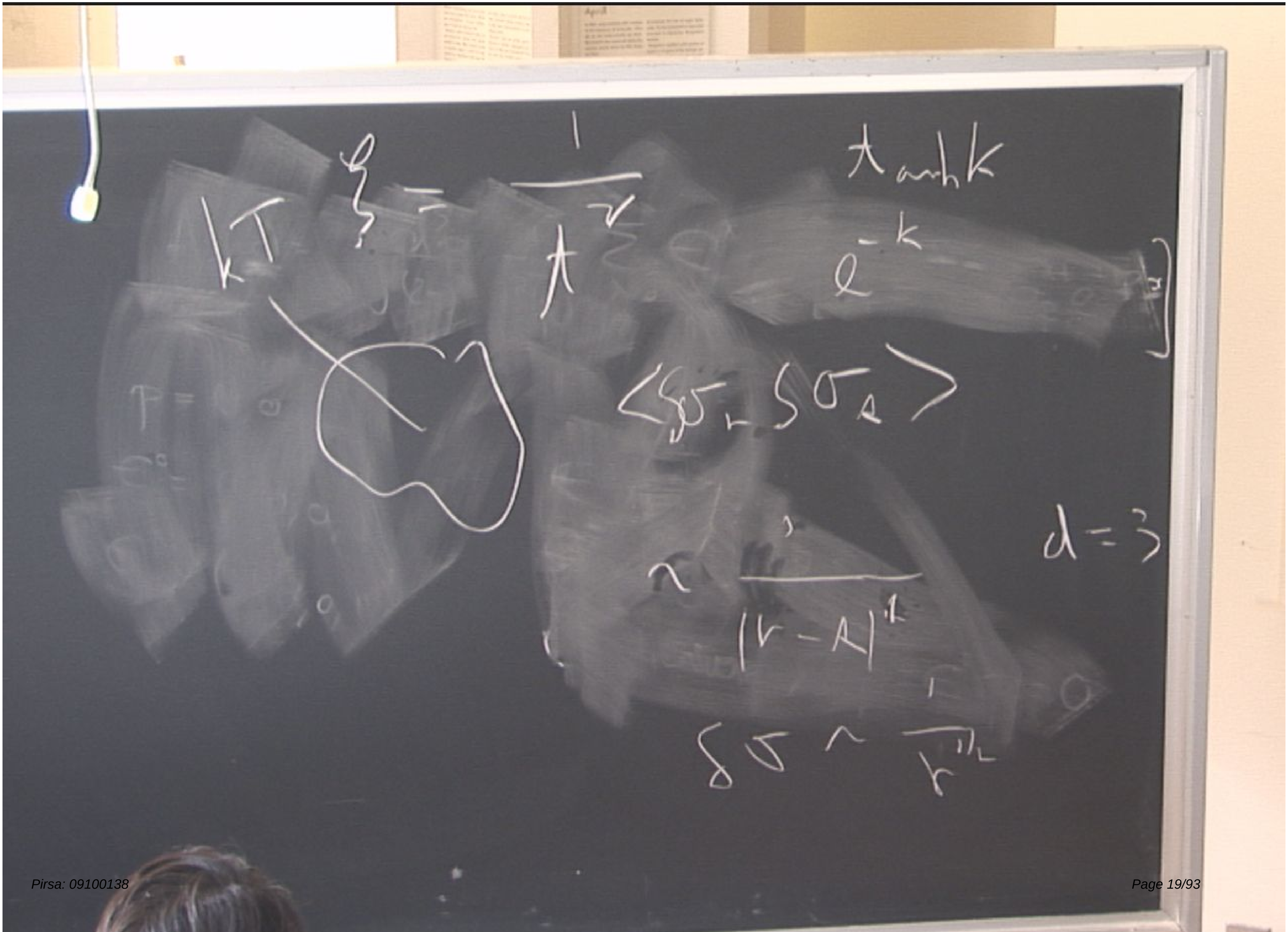
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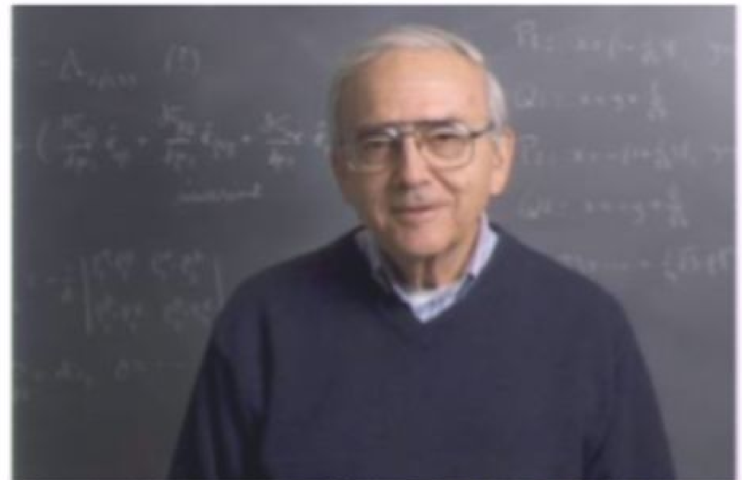

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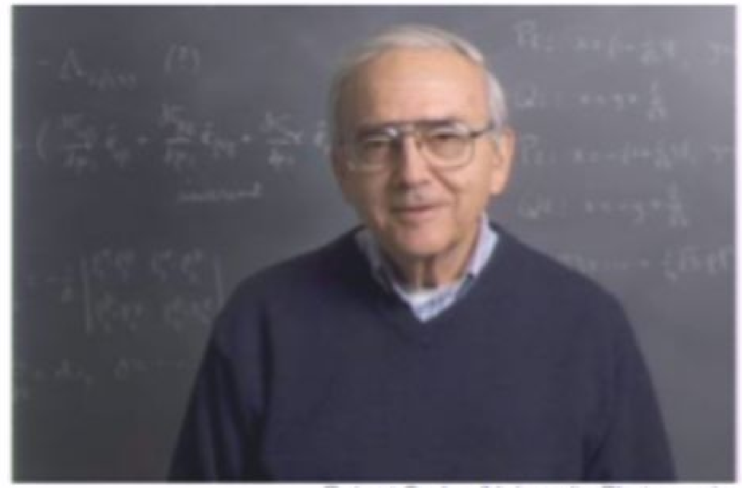

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additional phenomenology

Pokrovsky & Patashinskii study correlation functions, build upon Widom's work

They have scaling ideas $\sigma(r) \sim 1/r^x$
orders of magnitude from field theory gives
$< \sigma(r_1)\ \sigma(r_2) \ldots\ \sigma(r_m) > \sim 1/r^{mx}$
1964, 1966: This is a good idea but produces a partially wrong answer $x \neq 3/2$. (It is actually close to 1/2.)

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Kadanoff (1966) .....

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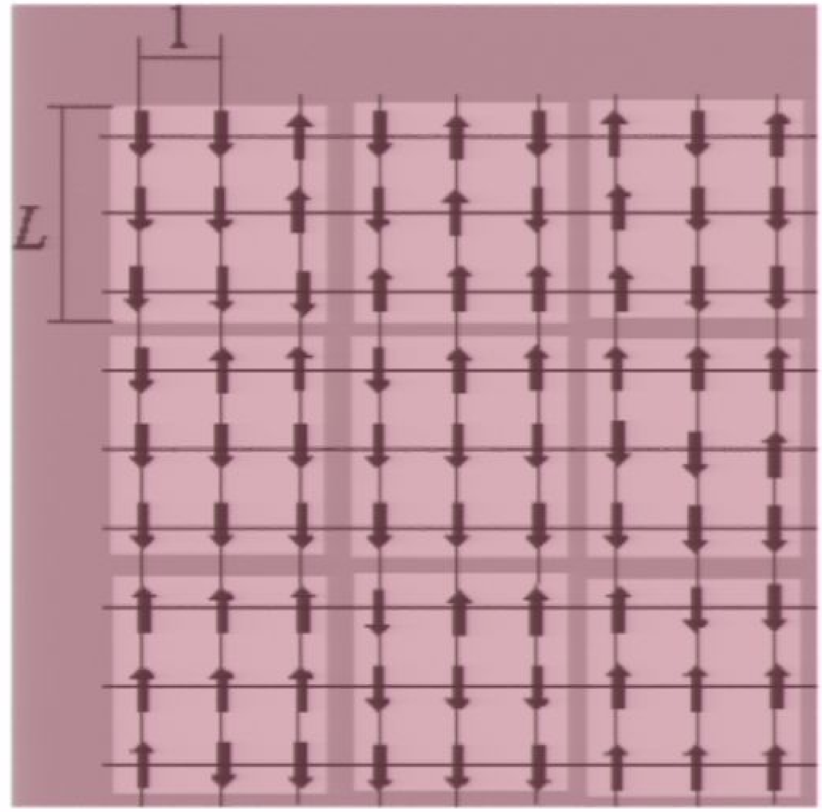
Kadanoff (1966) .....

Kadanoff 1966 Less is the same, too.

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

Answer: There are new effective values of (T-Tc)=t, magnetic field=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. This approach justifies the phenomenology of Widom and provides the outlines of a theory which might give the correlation functions of Pataskinskii & Pokrovsky.

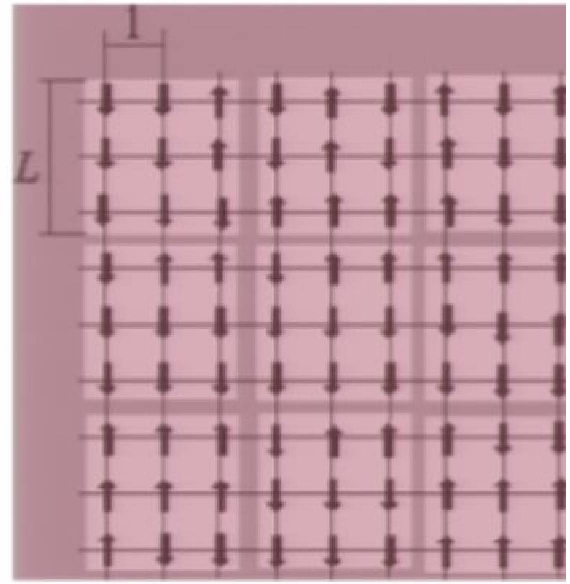


fewer degrees of freedom produces "block renormalization"

Renormalization for Ising model in any dimension; reprise

$Z = \text{Trace}_{\{\sigma\}} \exp(W_K\{\sigma\})$

Each box in the picture has in it a variable called μ_R, where the R's are a set of new lattice sites with nearest neighbor separation 3a. Each new variable is tied to an old ones via a renormalization matrix $G\{\mu, \sigma\} = \prod_R g(\mu_R, \{\sigma\})$ where g couples the μ_R to the σ's in the corresponding box. We take each μ_R to be ± 1 and define g so that, $\Sigma_\mu\, g(\mu,\{s\}) = 1$.



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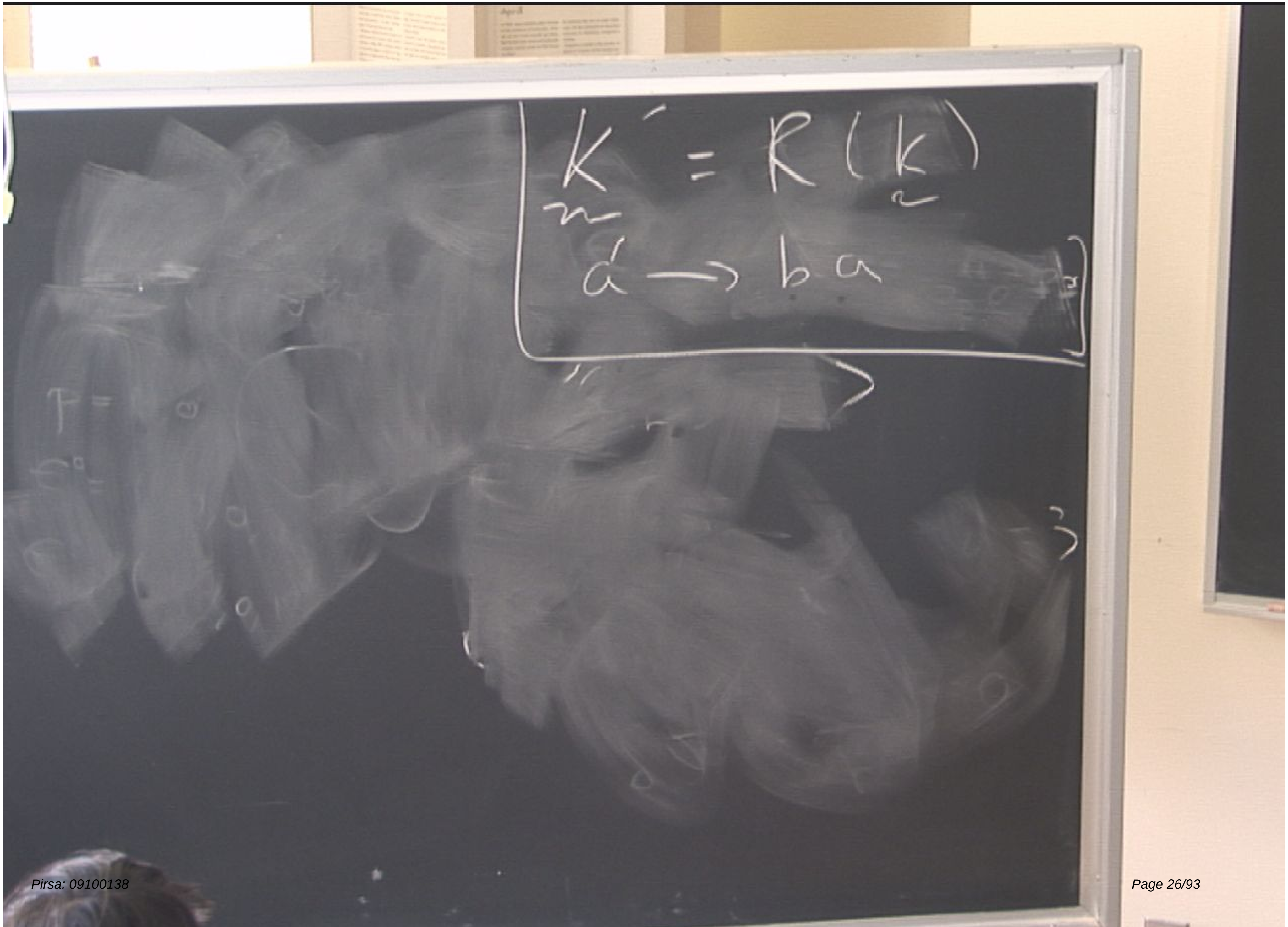
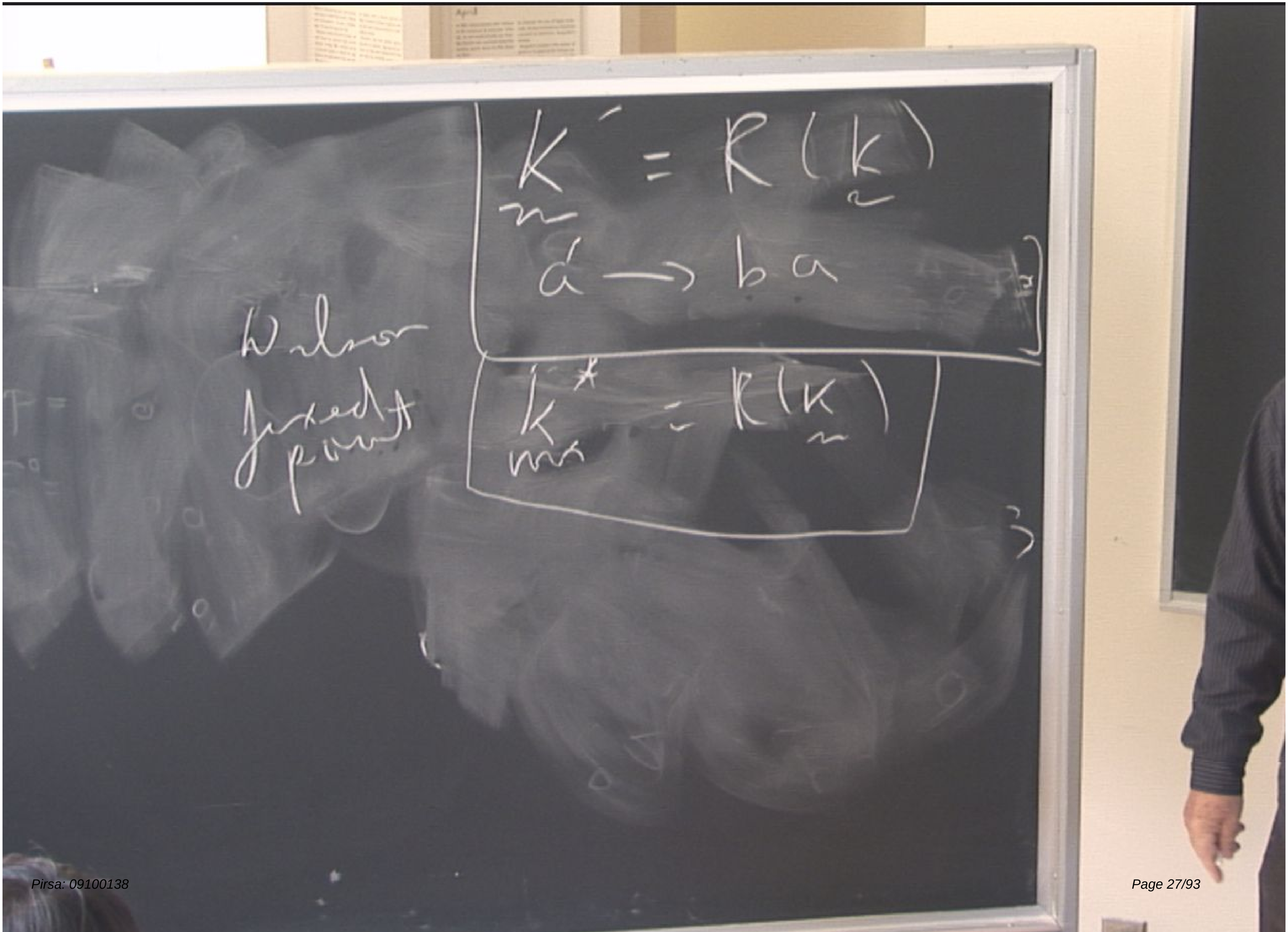

K' = R(k)
a' → b a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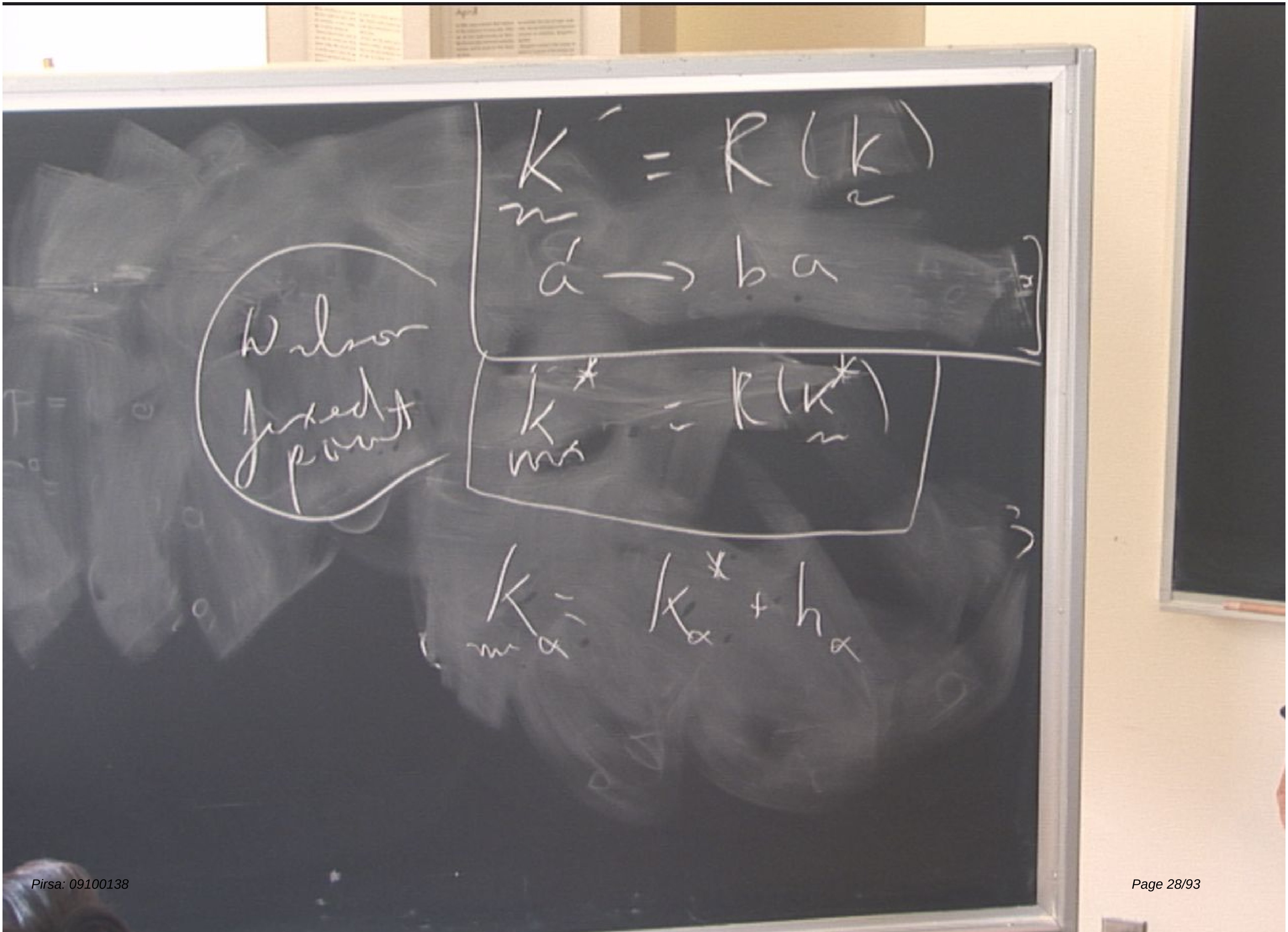
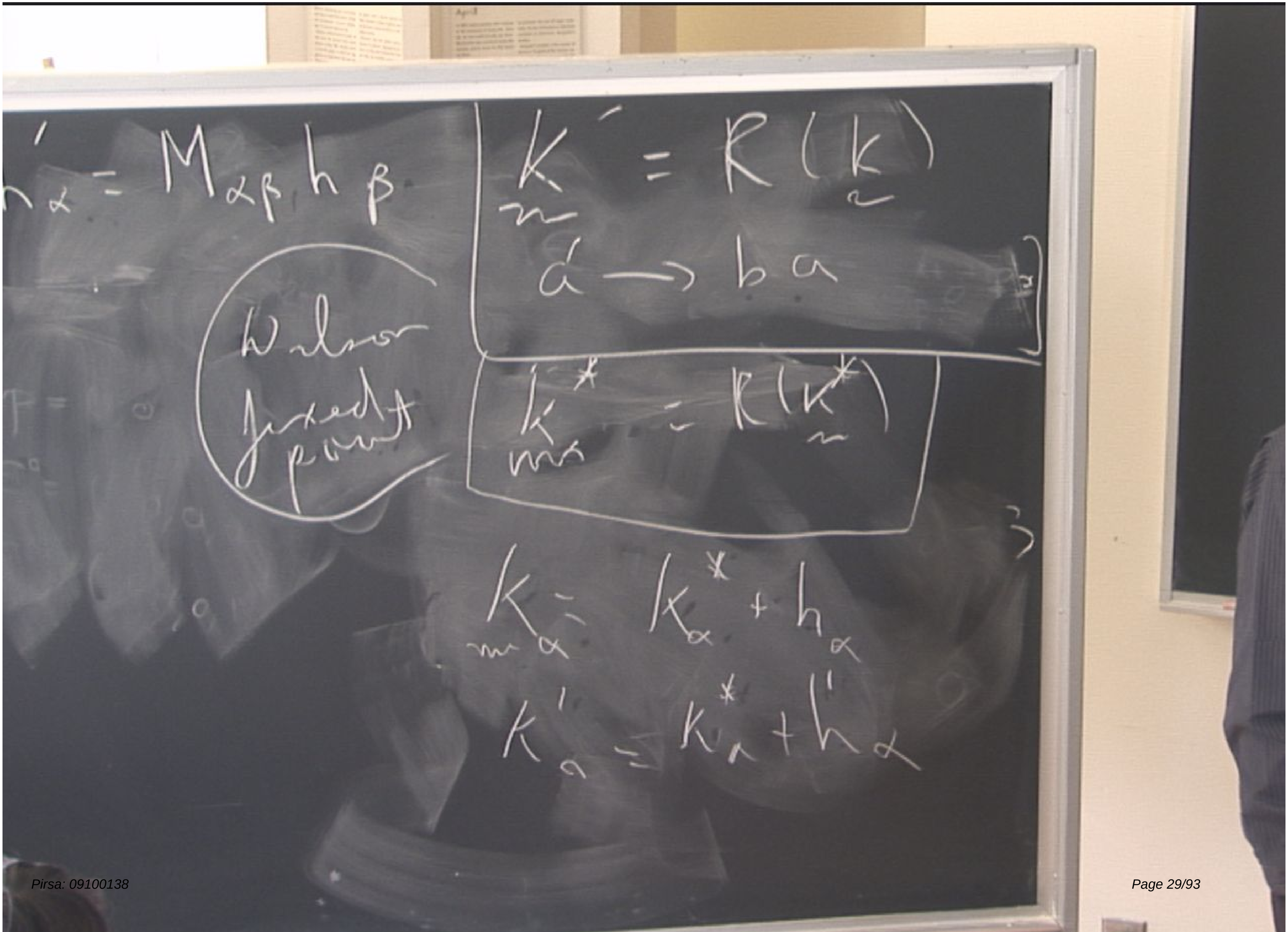

K' = R(K)
a → ba
Wilson
fixed point
K* = R(K*)
K = K* + h


$h'_\alpha = M_{\alpha\beta} h_\beta$
$K' = R(K)$
$a \to ba$
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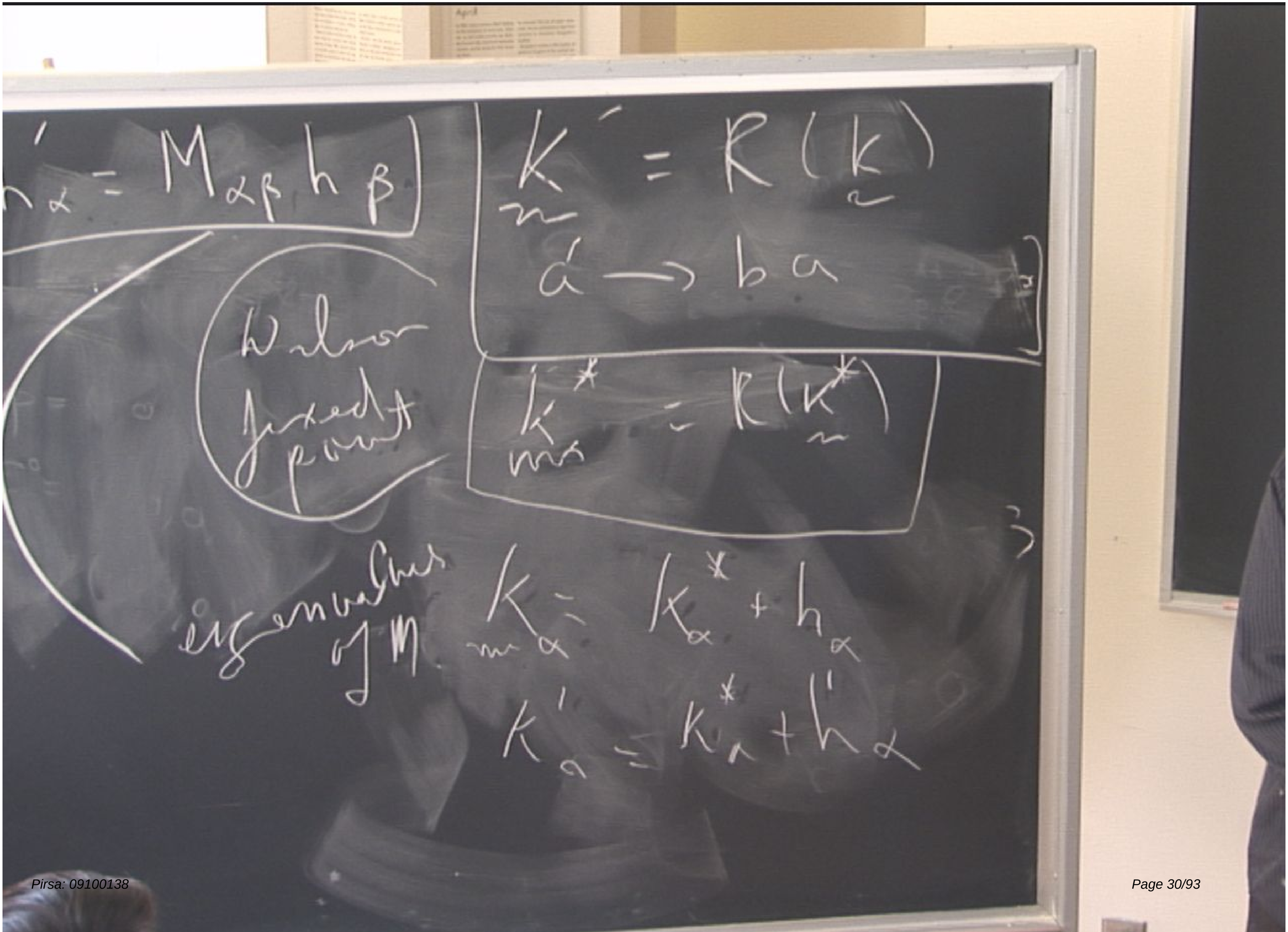
$K^* = R(K^*)$
$K_\alpha = K^*_\alpha + h_\alpha$
$K'_\alpha = K^*_\alpha + h'_\alpha$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Other Renormalizations

coherence length: $\xi = \xi_0 \, a \, t^{-\nu}$ 2d Ising has $\nu=1$; 3d has $\nu \approx 0.64$....

$\xi = \xi'$ $\quad\quad \xi_0 \, a \, t^{-\nu} = \xi_0 \, a' \, (t')^{-\nu}$

so $\nu = 1/x$

number of lattice sites: $N = \Omega / a^d$ $\quad N' = \Omega / a'^d$

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Free energy: $F = ... + N f_c(t) = F' = ... + N' fc(t')$

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Specific heat: $C = d^2F/dt^2 \sim t^{dx-2} = t^{-\alpha}$ form of singularity determined by x

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Fields: Relevant, Irrelevant, marginal, ...

a field is a number multiplying a possible term in the Hamiltonian

there are a few relevant fields: like t,h, K_0, which grow at larger length scales, completely dominate large-scale behavior

there are many irrelevant fields: they have |b|<1, don't play a role at large scales

there can be but usually are not marginal fields. they have |b|=1 and produce a continuously varying behavior at critical point

Universality: marginal variables are rare, mostly problems fall into a few universality classes. All problems in a given class have the same fixed point and the same critical and near-critical behavior.

Universality classes:
Ising ferromagnets+all single-axis ferromagnets + all long-gas phase transitions (Z2 symmetry)
Heisenberg Model ferromagnet (U3 symmetry)
superconductor, superfluid, easy plane ferromagnet (U2 symmetry).

Particle Physics RG before Wilson

idea: masses, coupling constants, etc. in Hamiltonian description of problem different from observed masses, coupling constants, etc. . They change with distance scale as particles are "dressed" by effects of the interaction.

A good phenomenological idea, used in quantum electrodynamics but not really crucial to particle physics.

Not used in statistical physics.

Renormalization

Transformations: $a \dashrightarrow 3a = a'$ $W_K\{\sigma\} \dashrightarrow W_{K'}\{\mu\}$ $Z' = Z$ $\mathbf{K}' = R(\mathbf{K})$

Scale Invariance at the critical point: --> $K_c = R(K_c)$

Temperature Deviation: $K = K_c + t$ $K' = K_c + t'$

critical point: if $t=0$ then $t'=0$

coexistence (ordered) region: if $(t<0, h=0)$ then $(t'<0, h'=0)$

disordered region $(t>0, h=0)$ goes into disordered region $(t'>0, h=0)$

if t is small, $t'=bt$. $b=(a'/a)^x$ defines $x=x_t$ = critical index for temperature. b>1 implies motion away from critical point

near critical point, $h'=b_h h$ $\ln b_h = x_h \ln (a'/a)$ defines x_h which then describes renormalization of magnetic field.

b's can be found through a numerical calculation.

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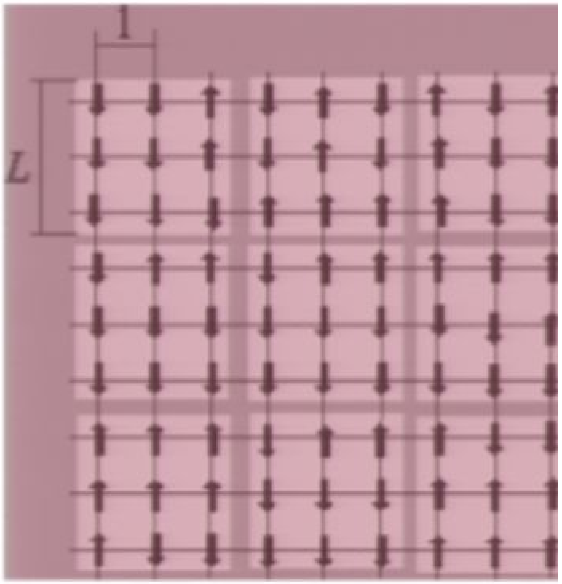

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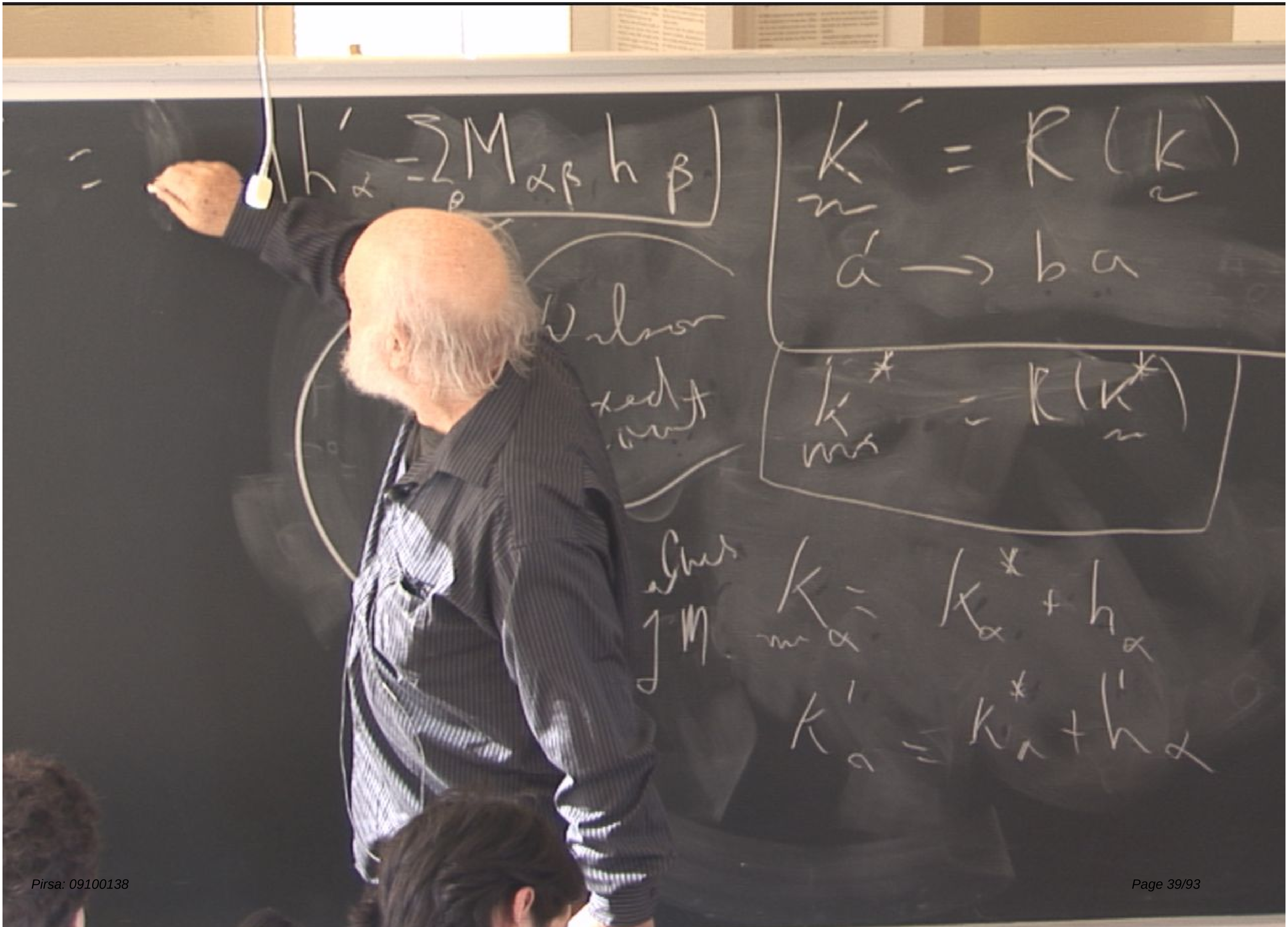

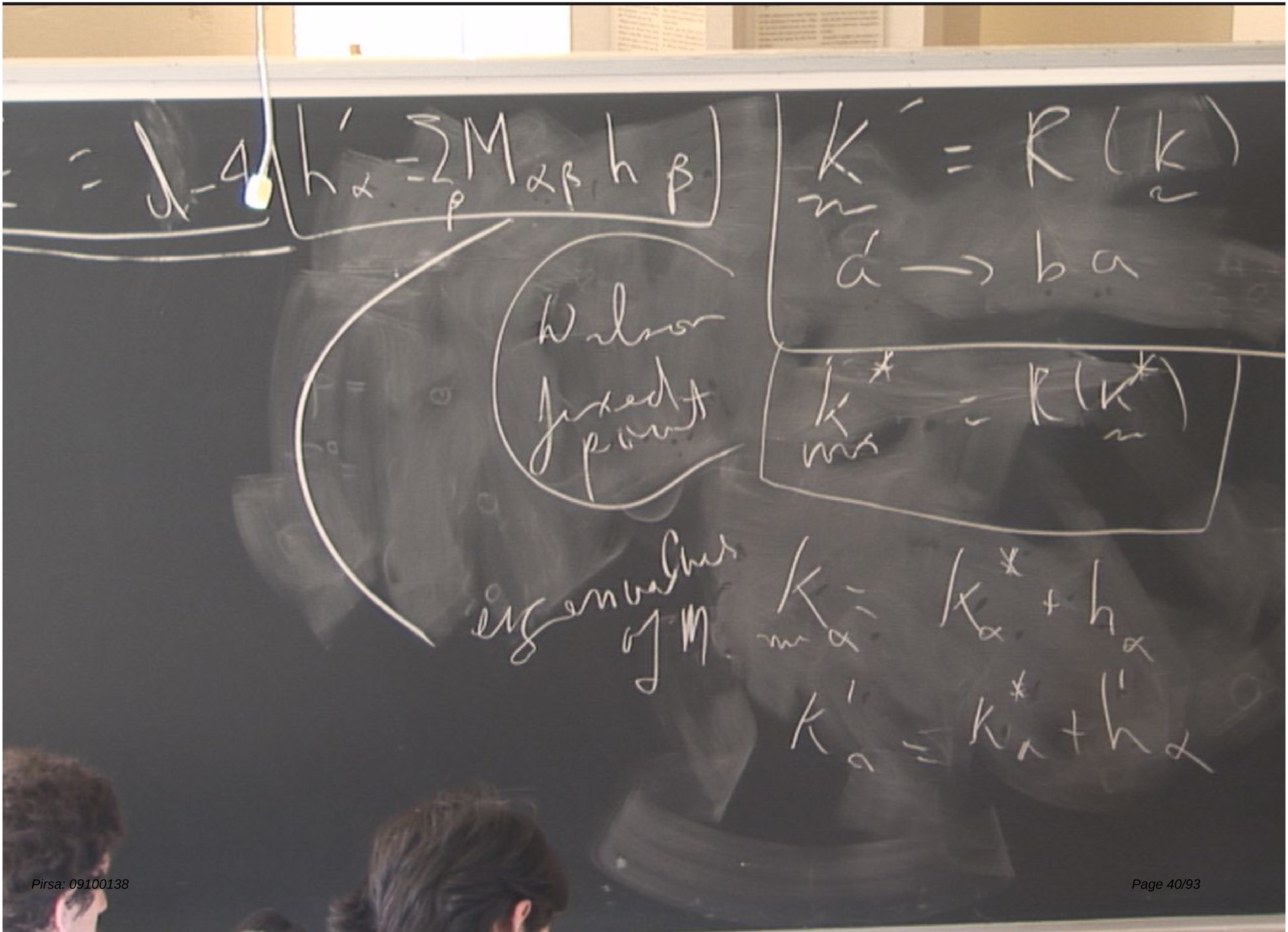
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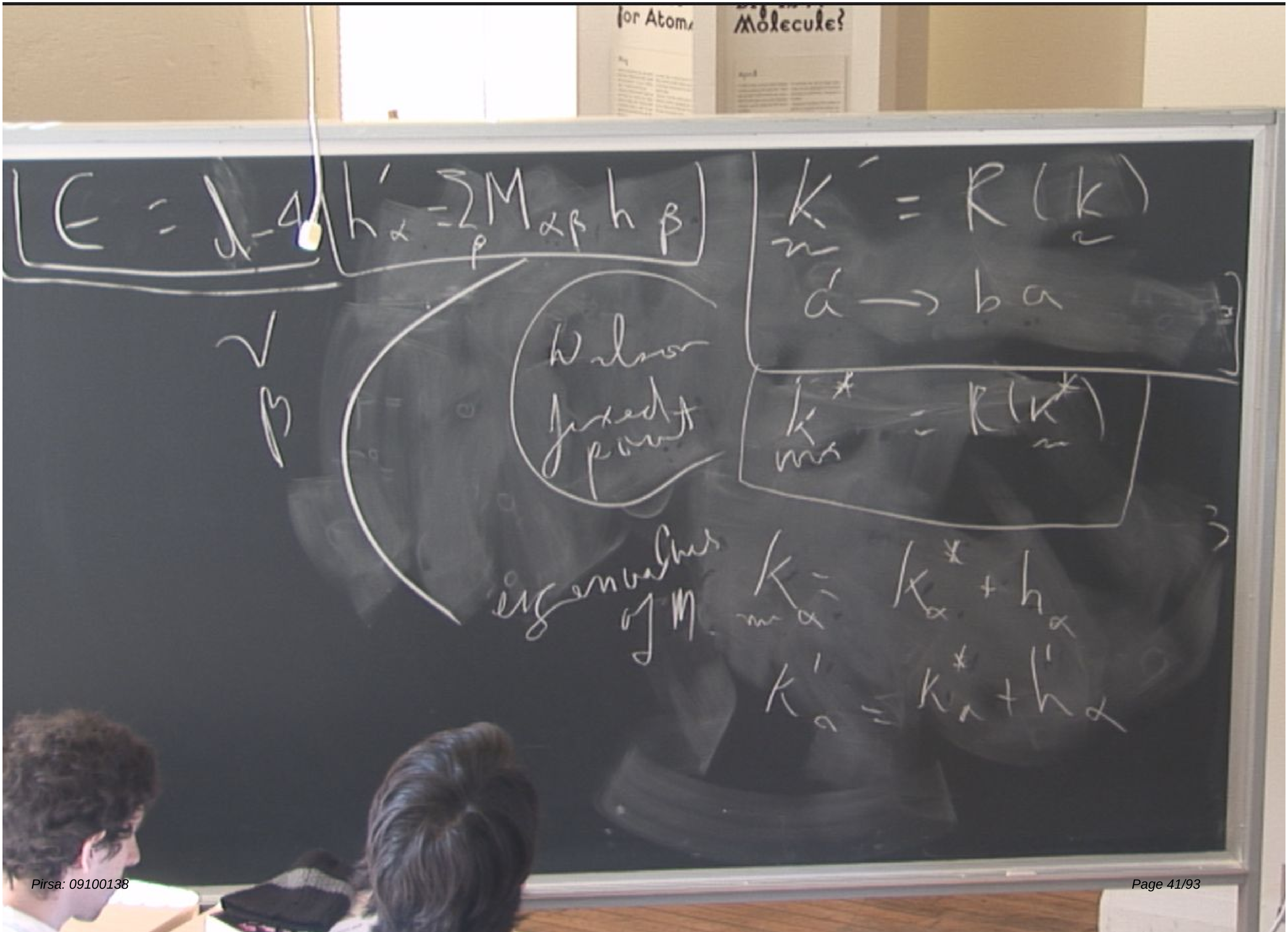
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ii. One cannot be sure about what parts of theory are right, what parts wrong.

iii. cannot determine universality classes from theory

iv. Does not provide lots of indication of what one should do to make the next step.

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Particle Physics RG before Wilson

idea: masses, coupling constants, etc. in Hamiltonian description of problem different from observed masses, coupling constants, etc.. They change with distance scale as particles are "dressed" by effects of the interaction.

A good phenomenological idea, used in quantum electrodynamics but not really crucial to particle physics.

Not used in statistical physics.

The Renormalization Revolution:

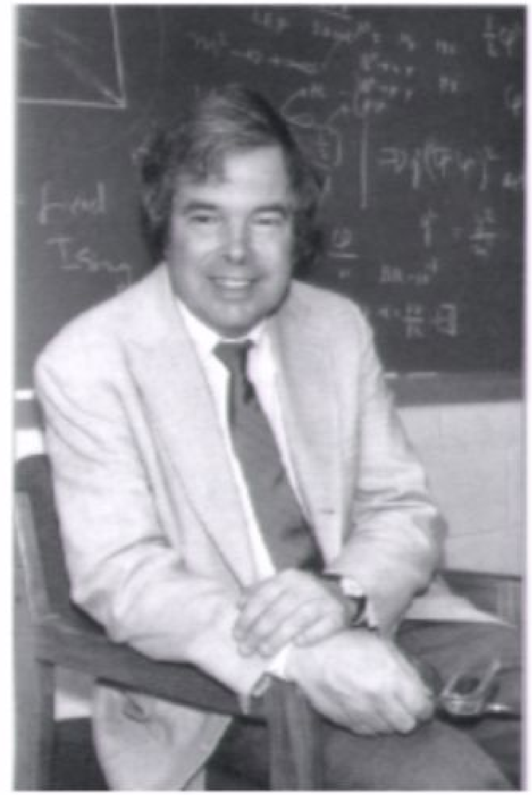
Wilson converts a phenomenology into a calculational method.

- Instead of using a few fields (T-Tc, h), he conceptualizes the use of a whole host of fields $K' = R(K)$
- Adds concept of fixed point $K_c = R(K_c)$
- He considers repeated transformations

This then provides a method which can be used by many people for many real calculations. The most notable is the epsilon (4-d) expansion of Wilson and Fisher.

This theory permits one to calculate everything people wanted to know at the time and fully matches experiments.

Everything in critical phenomena seems to be explained.



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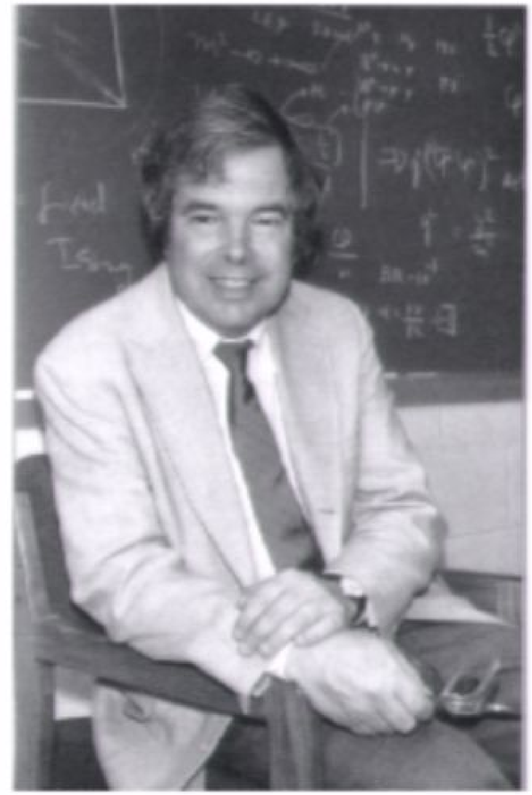

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The Crucial Ideas-for the revolution

Ideas:

- Criticality: recognized as a subject in itself
- Scaling: Behavior has invariance as length scale is changed
- Universality: Expect that critical phenomena problems can be divided into different "universality classes"
- Running Couplings: Depend on scale. Cf. standard model based on effective couplings of Landau & others.
- effective fields of all sorts: Running couplings are but one example of this.
- Fixed Point: Singularities when couplings stop running. K. Wilson
- Renormalization Group: K. Wilson (1971), calculational method based on ideas above.

Each Item, except RG, is a "consensus" product of many minds

The Outcome of Revolution

Excellent quantitative and qualitative understanding of phase transitions in all dimensions. Information about

- **Universality Classes**

All problems divided into “Universality Classes” based upon dimension, symmetry of order parameter, ...

Different Universality Classes have different critical behavior

e.g. Ising model, ferromagnet, liquid-gas are in same class

XYZ model, with a 3-component spin, is in different class

To get properties of a particular universality class you need only solve one, perhaps very simplified, problem in that class.

moral: theorists should study simplified models. They are close to the problems we wish to understand

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Conceptual Advances

First order phase transition represent a choice among several available states or phases. This choice is made by the entire thermodynamic system.

Critical phenomena are the vacillations in decision making as the system chooses its phase.

Information is transferred from place to place via local values of the order parameter.

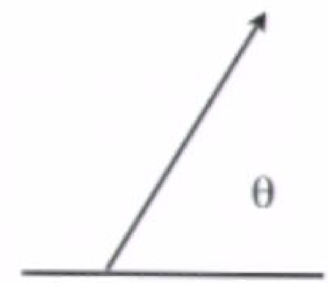
There are natural thermodynamic variables to describe the process. The system is best described using these variable.

Each variable obeys a simple scaling.

Next: After the Revolution:

2D XY model-
Kosterlitz & Thouless (1973)

$\mathbf{S}$= (cos θ, sin θ).



The XY model is a set of two-dimensional spins, described by an angle θ and a nearest neighbor coupling

K cos ($\theta - \theta'$).

There is an elegant description in terms of free charges and monopoles with electromagnetic interactions between them.

This work is also important because it is a successful calculation involving topological excitations. Milestone.

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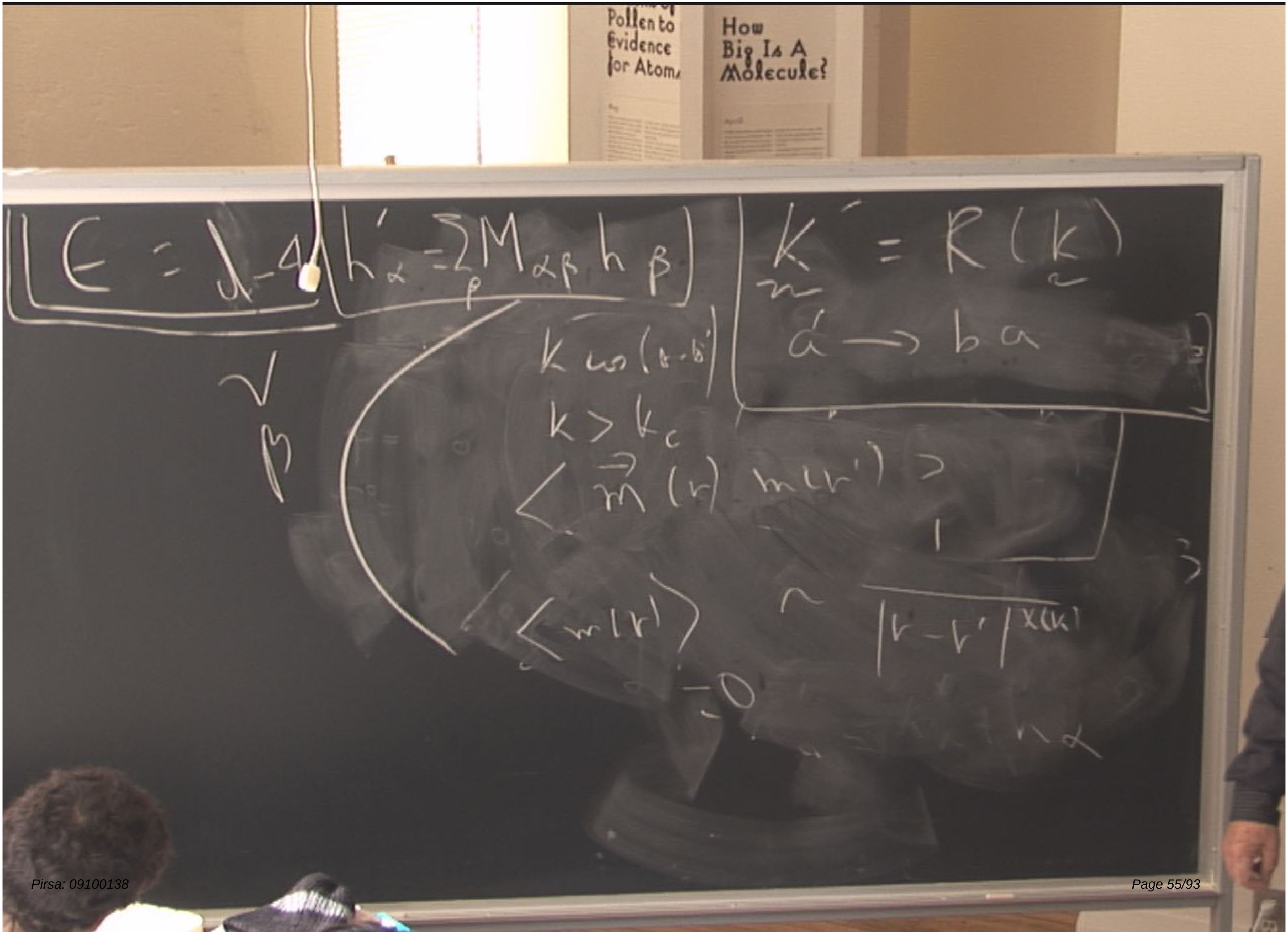
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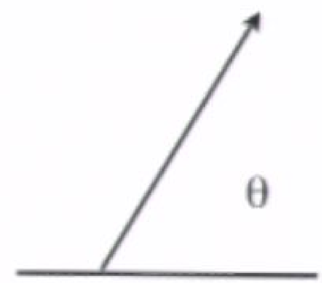

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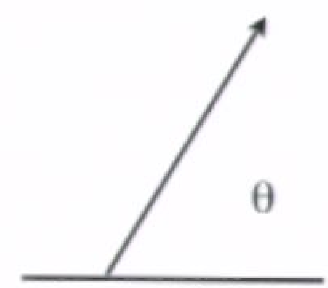

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The RG point of view is Fully Absorbed into Particle Physics

Running coupling constants help define the standard model.

The model is extrapolated back to when weak, electromagnetic and strong interactions are all equal.

Asymptotic freedom--weakening of strong interactions at small distances--permits high energy calculations. Gross, Wilczek, Politzer (1973).

Coulomb gas: B. Nienhuis (~1985)

Nienhuis extended this approach to give a description of correlation functions in terms of a screened coulomb gas (and magnetic monopoles) for many kinds of critical phenomena problems in two dimensions. The list includes:

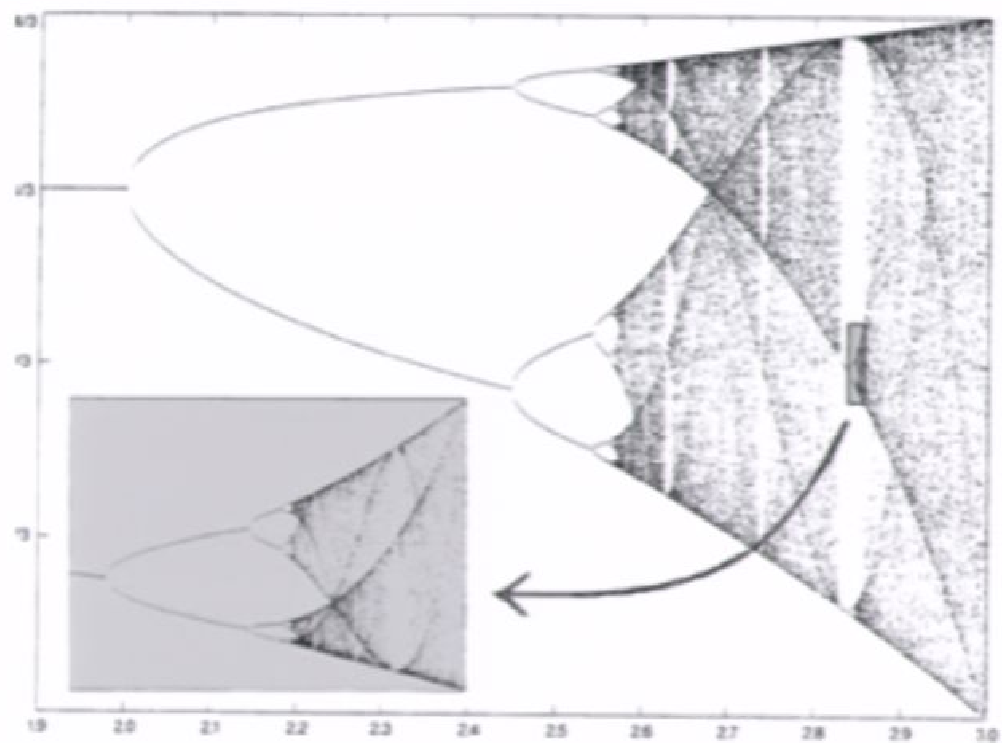
- q-state Potts models (spin takes on q values)
- O_n models (n-component vectors)

These models permit generalizations in which behavior varies continuously with q or n.

Feigenbaum: Analyzes Route to Chaos (1978)

Feigenbaum used RG, Universality, and Scaling concepts to investigate the period doubling route to chaos via the discrete equation

$x(t+1) = r\, x(t)\, (1-x(t))$



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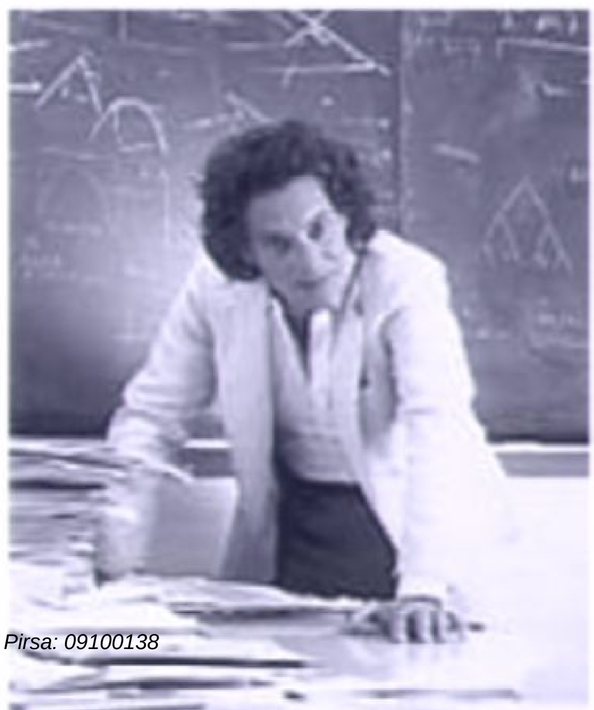

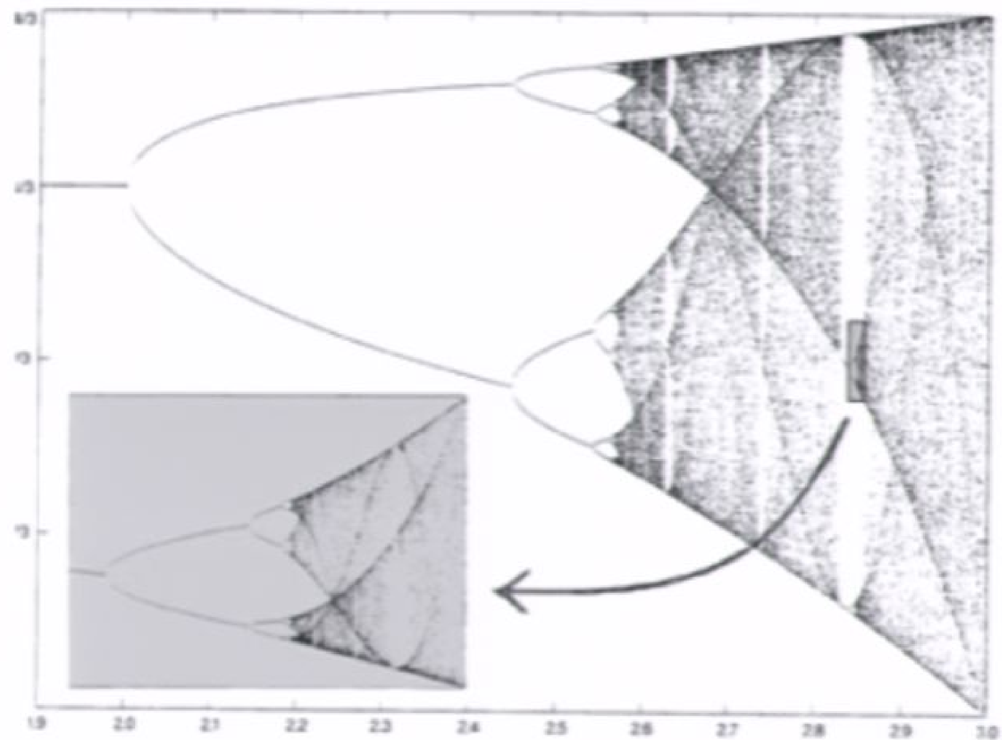

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Operator Product Expansion: Wilson, Kadanoff

Local operators proved particularly interesting
Products of nearby operators O(R+r/2)O(R-r/2)
can be expanded in terms of the local operators at R.

$$O_\alpha(R+r/2)O_\beta(R+r/2)$$
$$= \sum_\gamma A_{\alpha\beta\gamma}(r)O_\gamma(R)$$

This operator product expansion particularly suggests that the operators obey a kind of algebra. Working from the algebra, something deeper might be found.

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Onsager solution of 2-D Ising model is free fermion theory

Revolutionary Period:
The connection: Wilson & Fisher (1972) use Ginzburg Landau free energy formulation plus path integral formulation of quantum mechanics to describe critical phenomena theory as a close relative of quantum field theory.

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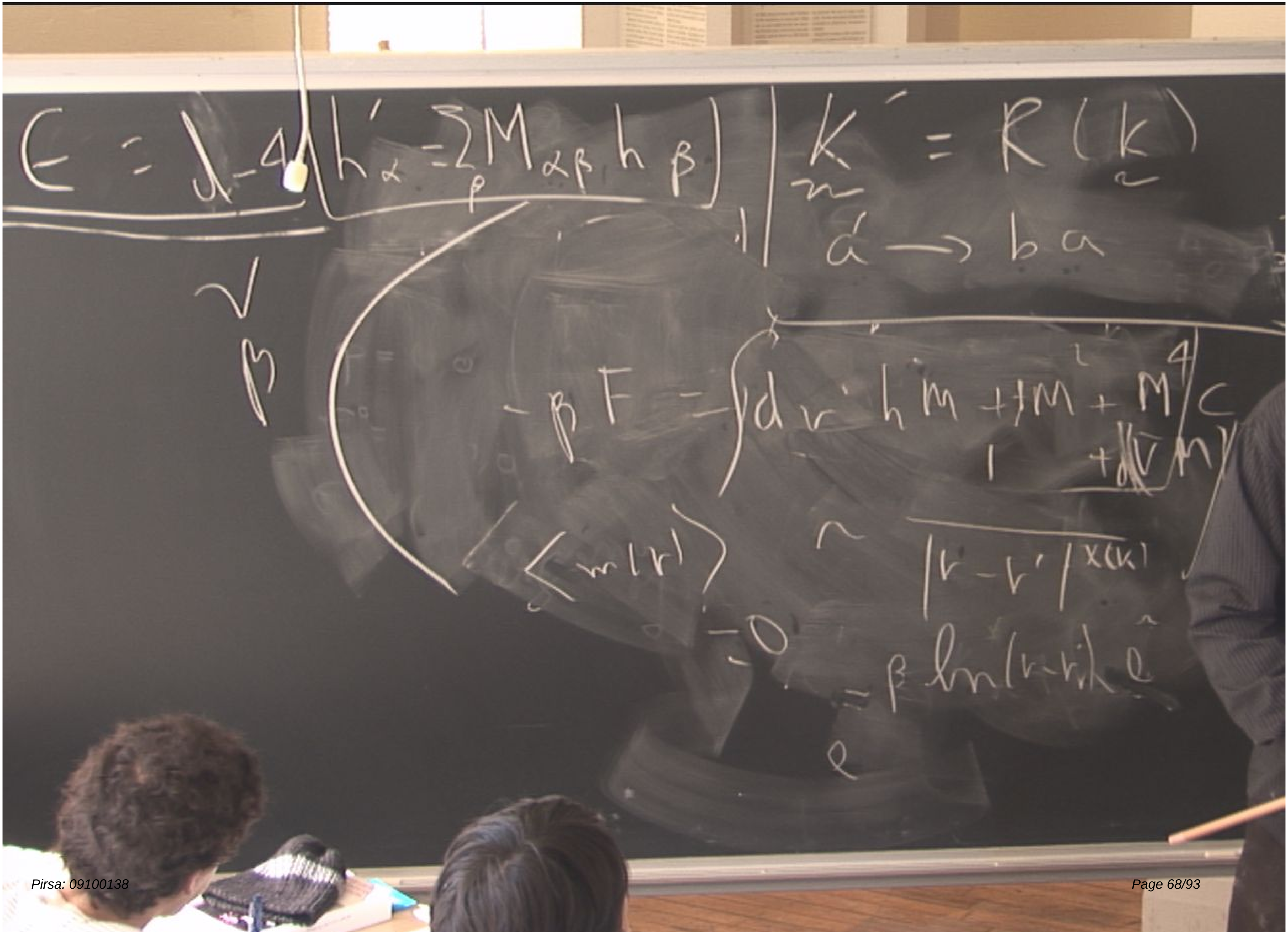
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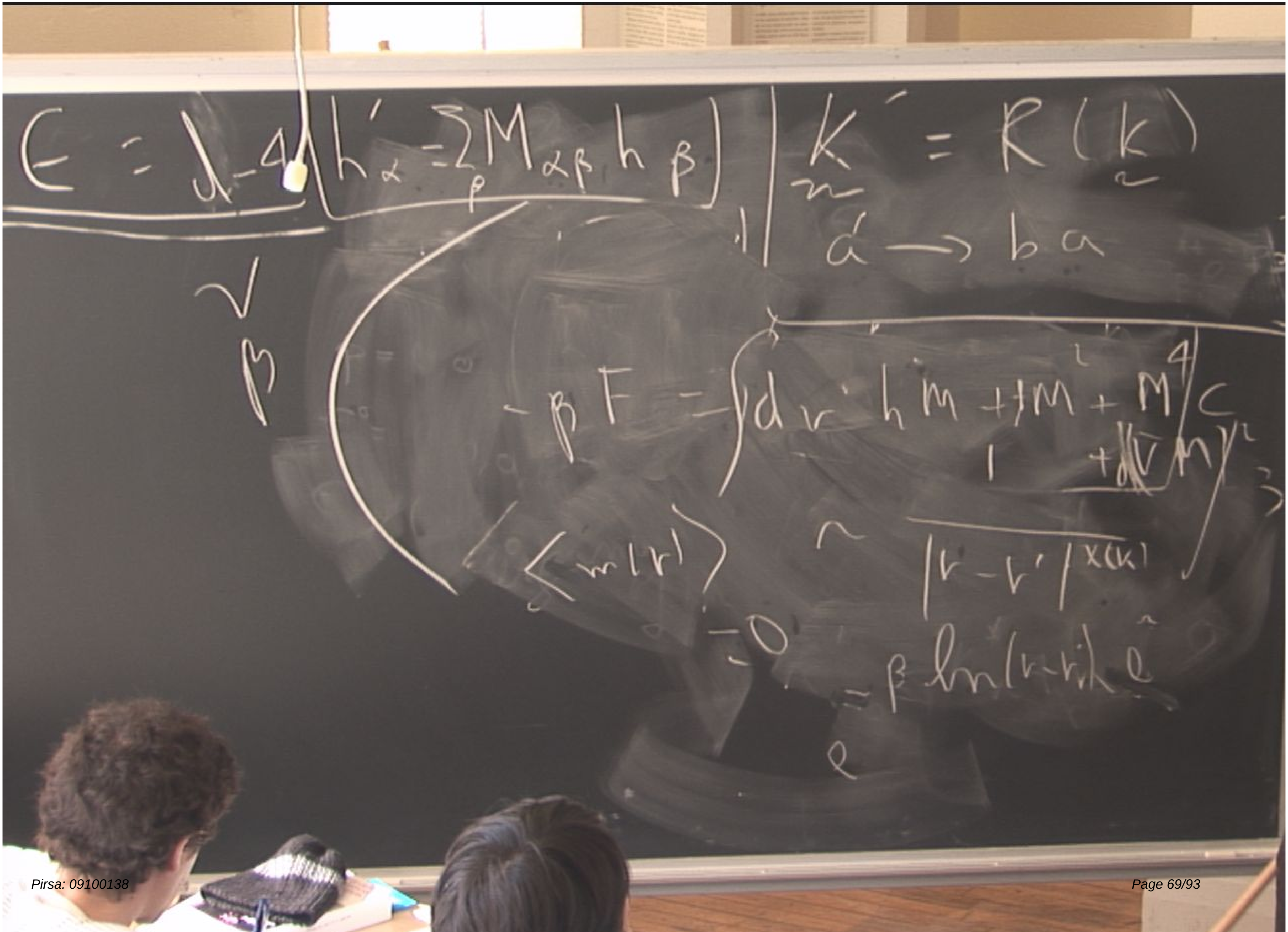

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After the Revolution:
New Ideas-mostly for d=2

- XY model- Kosterlitz & Thouless
- Coulomb gas: B. Nienhuis
- Conformal Field Theory: A. Polykov
- Quantum Gravity: B. Duplantier
- SLE: Oded Schramm

Conformal Field Theory: I

A. Polyakov emphasized that there is a special form of field theory which holds at critical points, i.e. places in which there is full scale invariance. In two dimensions this is super-special because the invariance includes all kinds of conformal (angle preserving) transformations which can then be studied through the use of complex variable methods.

Space distortions are based upon stress tensor operators, with the Virasoro algebra being the algebra of local stress tensor densities. Just as spinors, vectors and tensors are derived as representations of the rotation group algebra, equally the local operators of critical phenomena have properties, including critical indices, derivable from the fact that they are representations of the Virasoro algebra.

Continuously varying families of solutions are generated in this fashion

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Friedan Qiu & Shenker (1984) showed that unitarity, a quality of all field theories representing possible quantum processes, limits the domain of field theories to include all the known critical 2-D models, e.g. q=2,3, 4 Potts models, but not others (e.g q=1.5).

Further we get a quite different algebra for each model.

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Compared to general situations, all the familiar statistical mechanical models are all degenerate and truncated, and permit considerable calculation of correlation functions.

Further conformal transformation permit the calculation of correlations in all kinds of shapes from just a few shapes: plane, half-plane, interior of circle.

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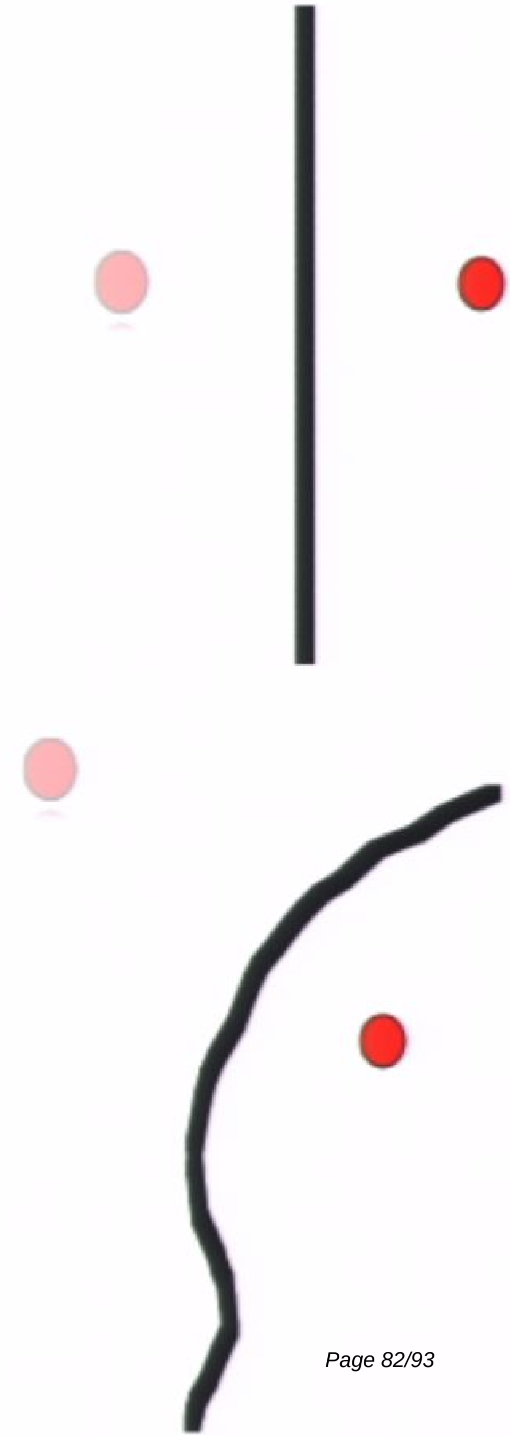
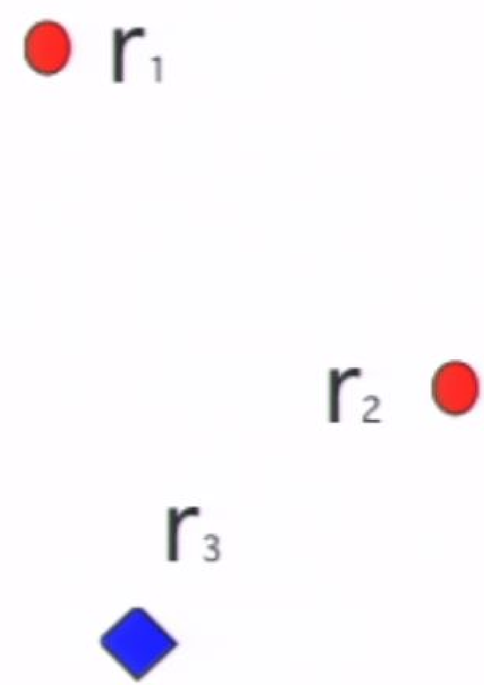


Many Exact Calculations



find correlation of two spins
(local magnetization densities)
and a local energy density

$$< \sigma(r_1)\sigma(r_2)\epsilon(r_3) > \quad = C{r_{12}}^{x_\epsilon - 2x}(r_{23}r_{13})^{-x_\epsilon}$$

For Ising model, x=1/8

and x_ϵ = 1

Quantum Gravity:

The next step beyond scale invariance is no scale at all. One can formulate "quantum gravity theory" as a classical theory in which one sums over all possible metrics on a given space.

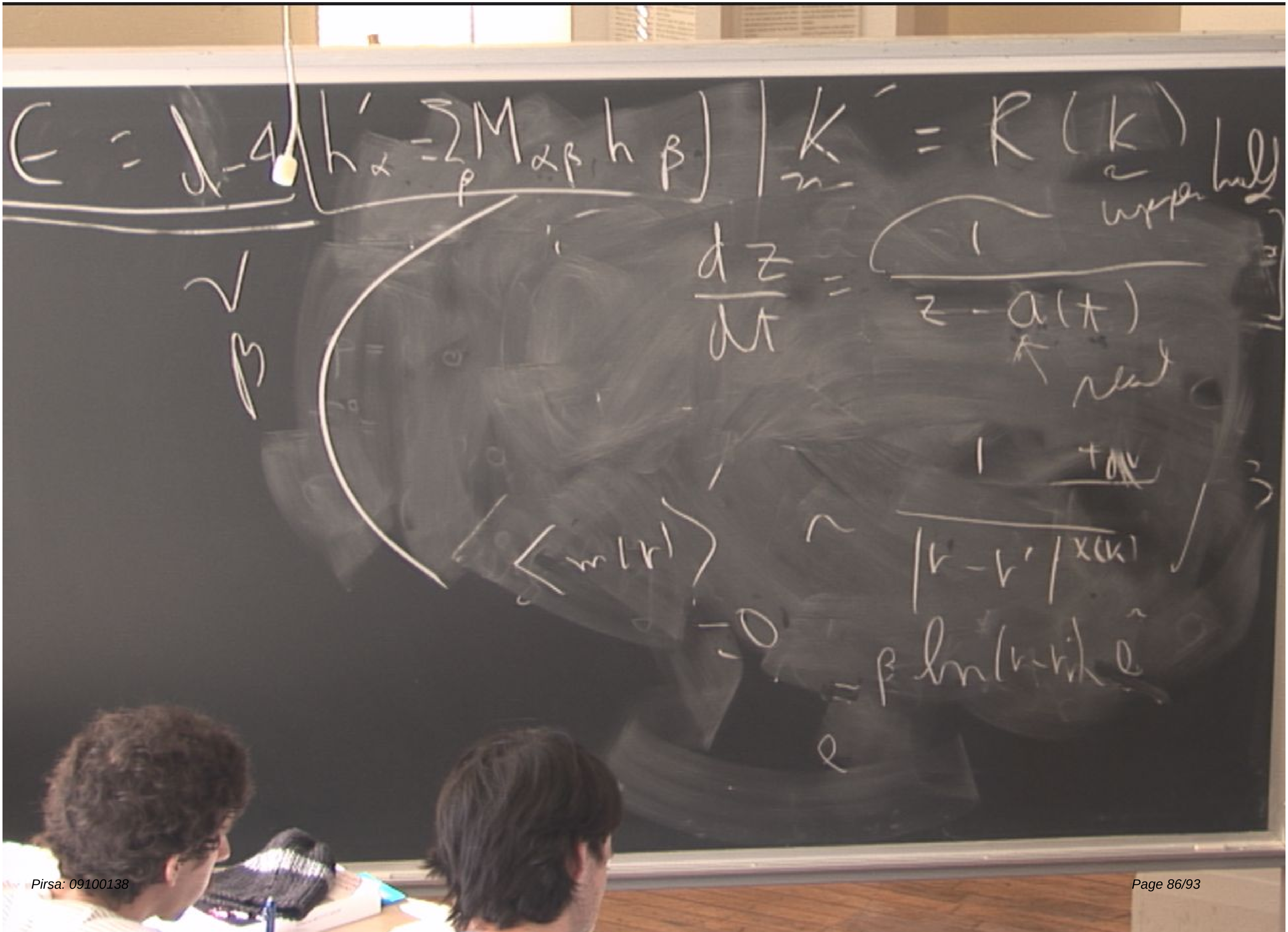
In two dimensions, there are no physical degrees of freedom in gravity theory, and the summation can be carried out exactly. (Gross & Migdal, Douglas & Shenker, Brezin & Kazakov.) In addition to being a solvable gravity model, this approach offers a good start for critical problems. For example B. Duplantier carried out a calculation in which he calculated the spectrum of electric fields in the neighborhood

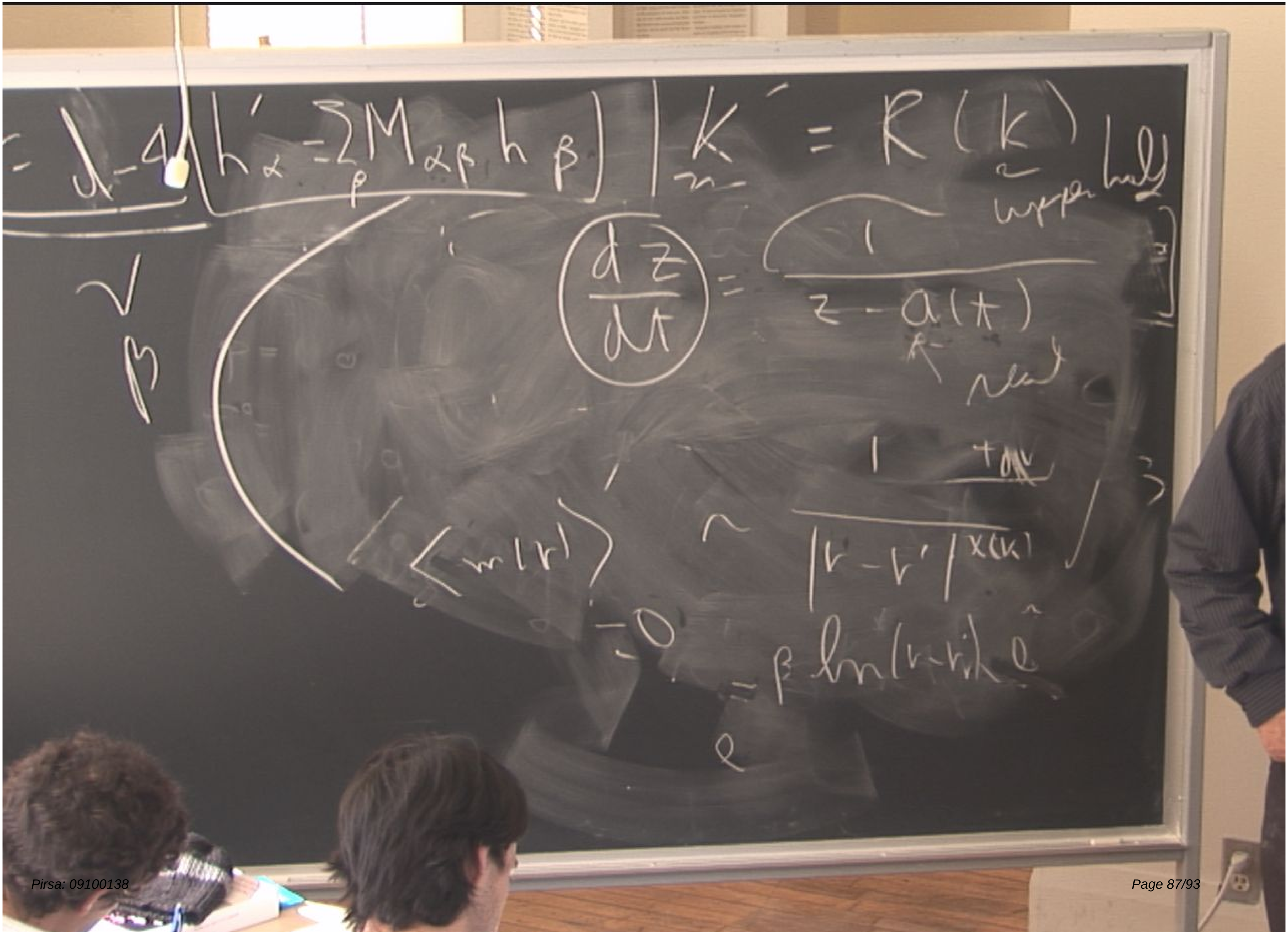
SLE=Schramm-Loewner-Evolution

Conformal field theory took us to a point at which we could formulate critical phenomena problems on surfaces of various shapes. The most recent area of progress arises from work of Oded Schramm, who combined the complex analytic techniques of Loewner with methods of modern mathematical probability theory to gain new insight into the shapes which arise in critical phenomena.

Oded Schramm

O. Schramm, Israel J. Math. 118 (2000), 221--288.


E = d - 4 [h'α - Σβ Mαβ hβ]
K' = R(K)
dz/dt = 1/(z - a(t))
real
~ 1/|r - r'|^x(k)
β ln(r - r')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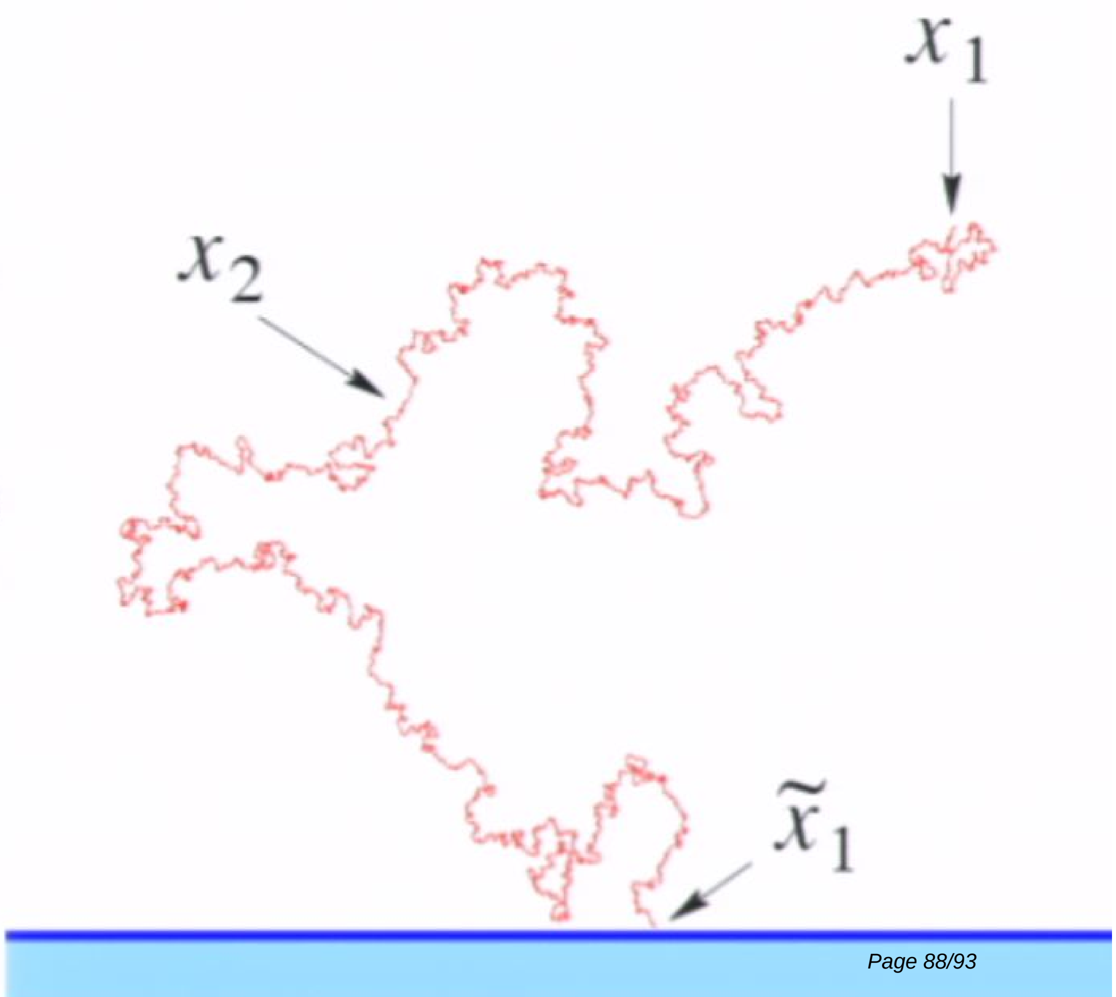
From Schramm to Critical Shapes

The work of the 20th. Century on critical phenomena was centered on thermodynamics, and correlation functions.

We depicted but did not calculate the shapes of the correlated fractal clusters arising in critical situations. Schramm provided a constructive technique, involving a differential equation, for making the ensemble of such clusters at critical points.

SAW in half plane - 1,000,000 steps



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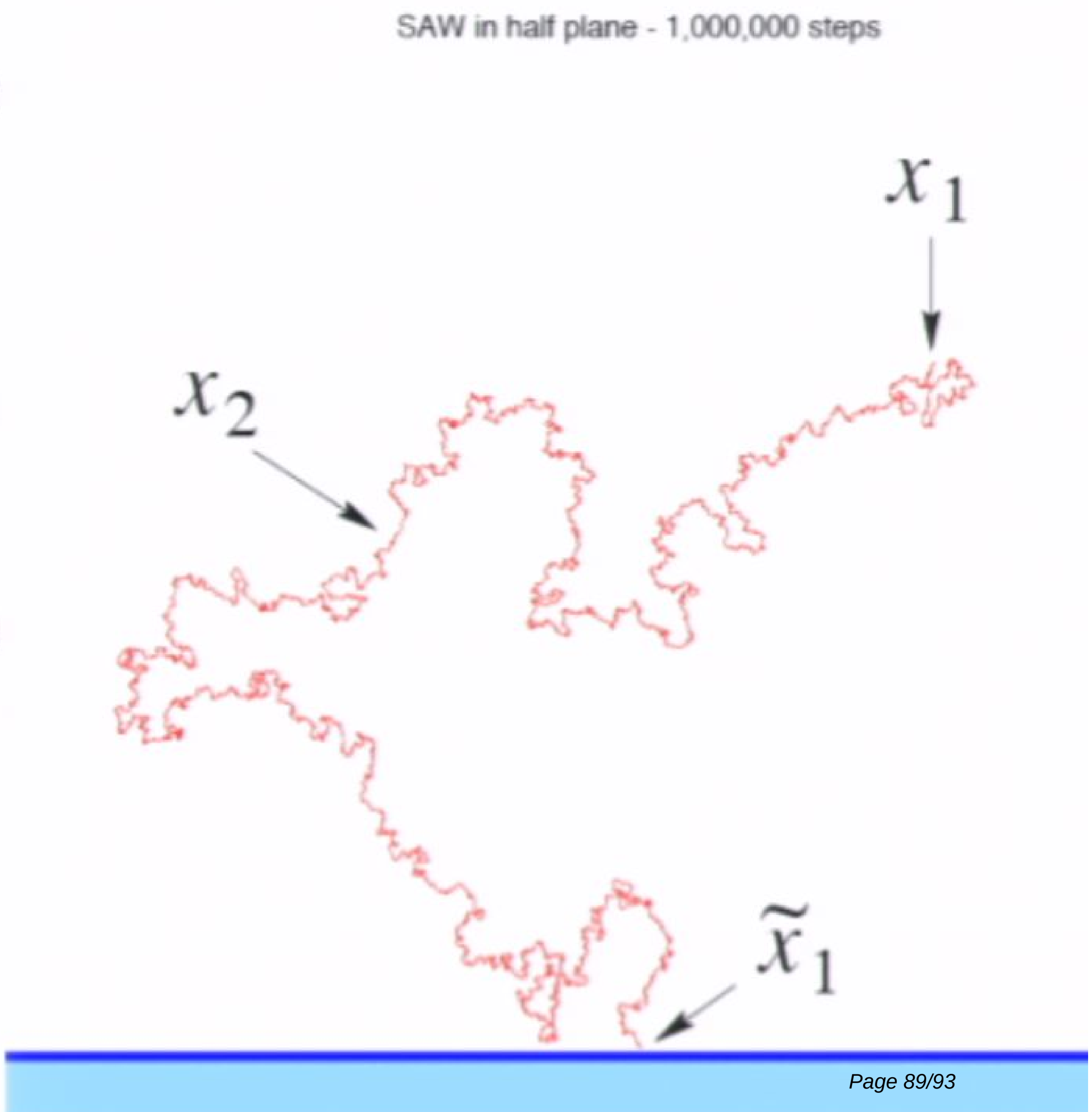

SLE-II

)efine a critical cluster as the shape
·f cluster of spins pointed in the
ame direction in an Ising model, or
·f a connected set of occupied sites
ı a percolation problem.

'roblem: Define the ensemble of
luster shapes for any critical
ituation. Before Schramm's work
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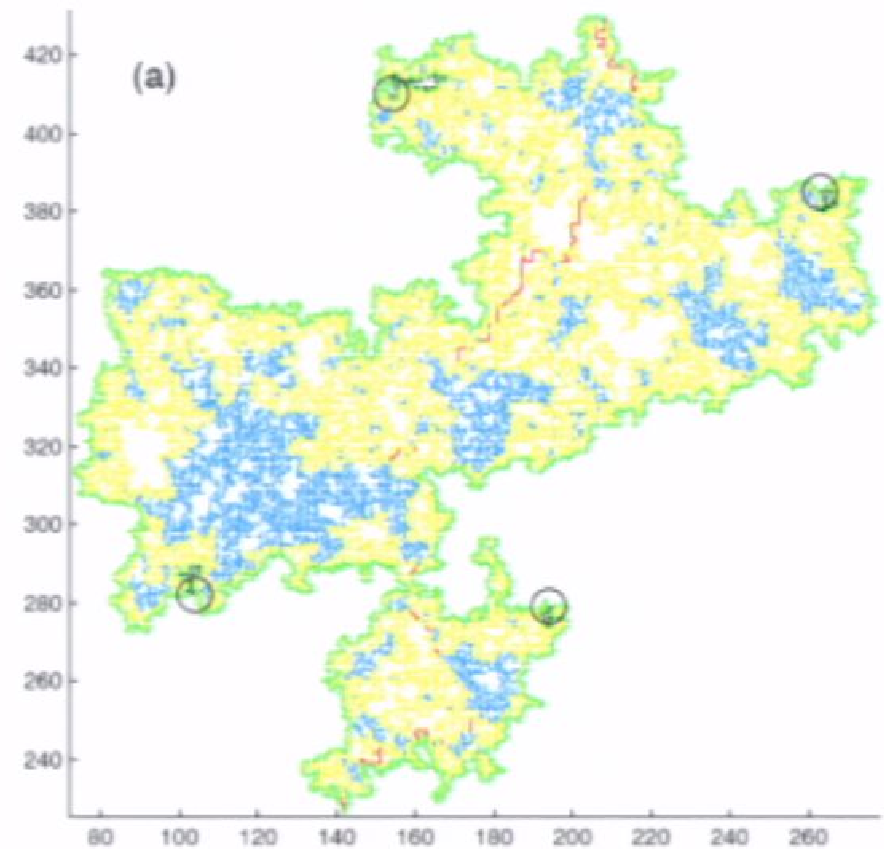
ıroblems.



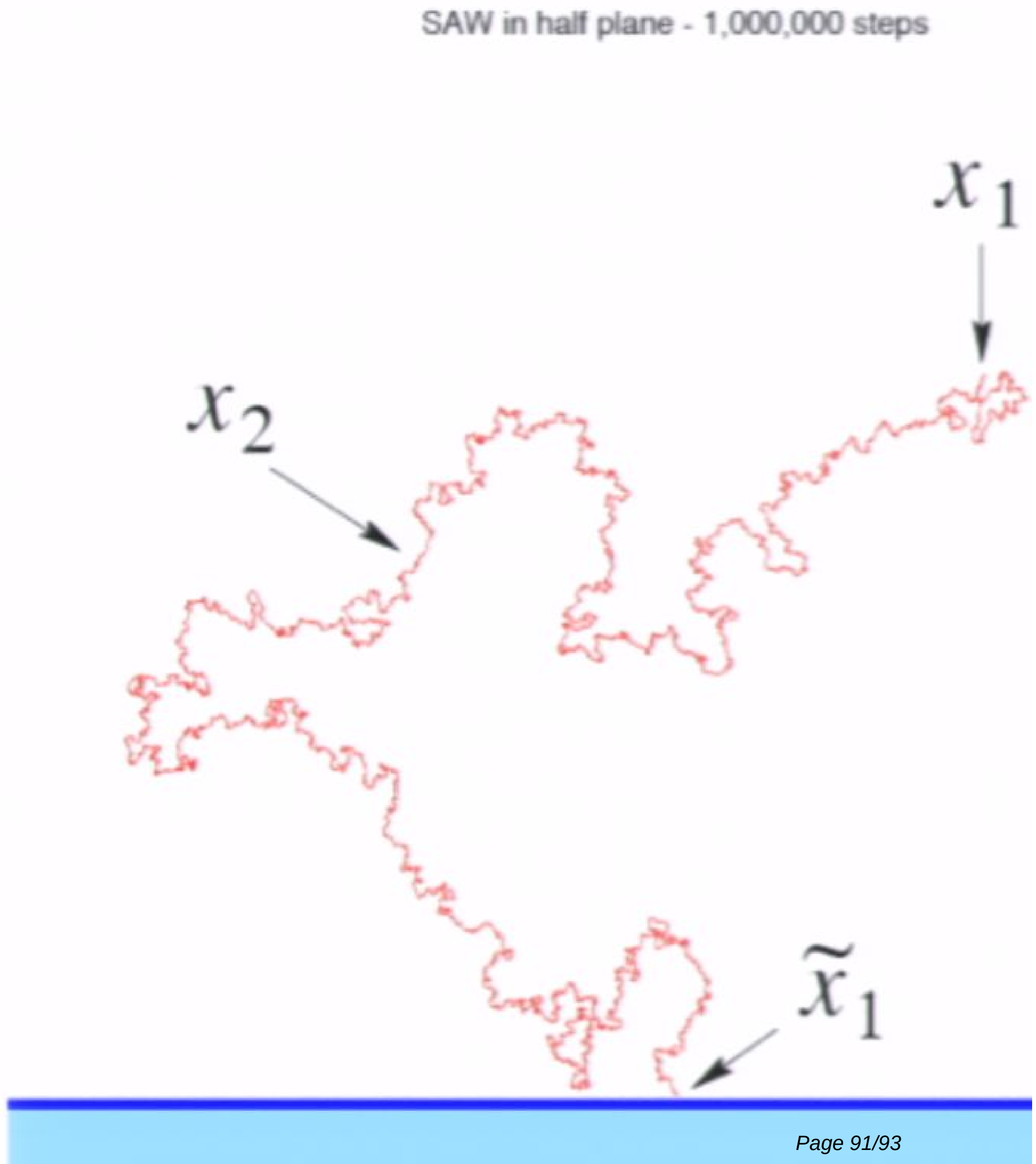
(J. Asikainen et al., 2003)

percolation cluster after Duplantier

Problem: Define the ensemble of cluster shapes for any critical situation.

Answer: Look for the ensemble of shapes formed from the singularities in the solution to the differential equation

where is a random walk on a line with correlations

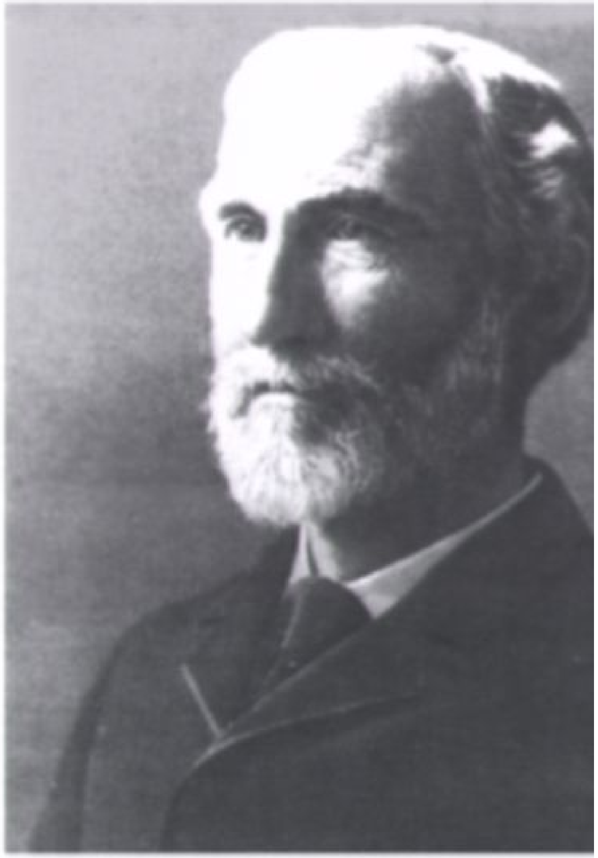


Summary

Critical behavior occurs at but one point of the phase diagram of a typical system. It is anomalous in that it is usually dominated by fluctuations rather than average values. These two facts provide a partial explanation of why it took until the 1960s before it became a major scientific concern. Nonetheless most of the ideas used in the eventual theoretical synthesis were generated in this early period.

Around 1970, these concepts were combined with experimental and numerical results to produce a complete and beautiful theory of critical point behavior.

In the subsequent period the "revolutionary synthesis" radiated outward to (further) inform particle physics, mathematical statistics, various dynamical theories...



JW Gibbs