Title: Statistical Mechanics (PHYS 602) - Lecture 11

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Abstract:

PERIMETER PI INSTITUTE FOR THEORETICAL PHYSICS

Start here

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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.

But sometimes MFT works quite well, mostly when there are many particles within a force range as in BCS superconductors and in electrodynamics of materials.

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

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

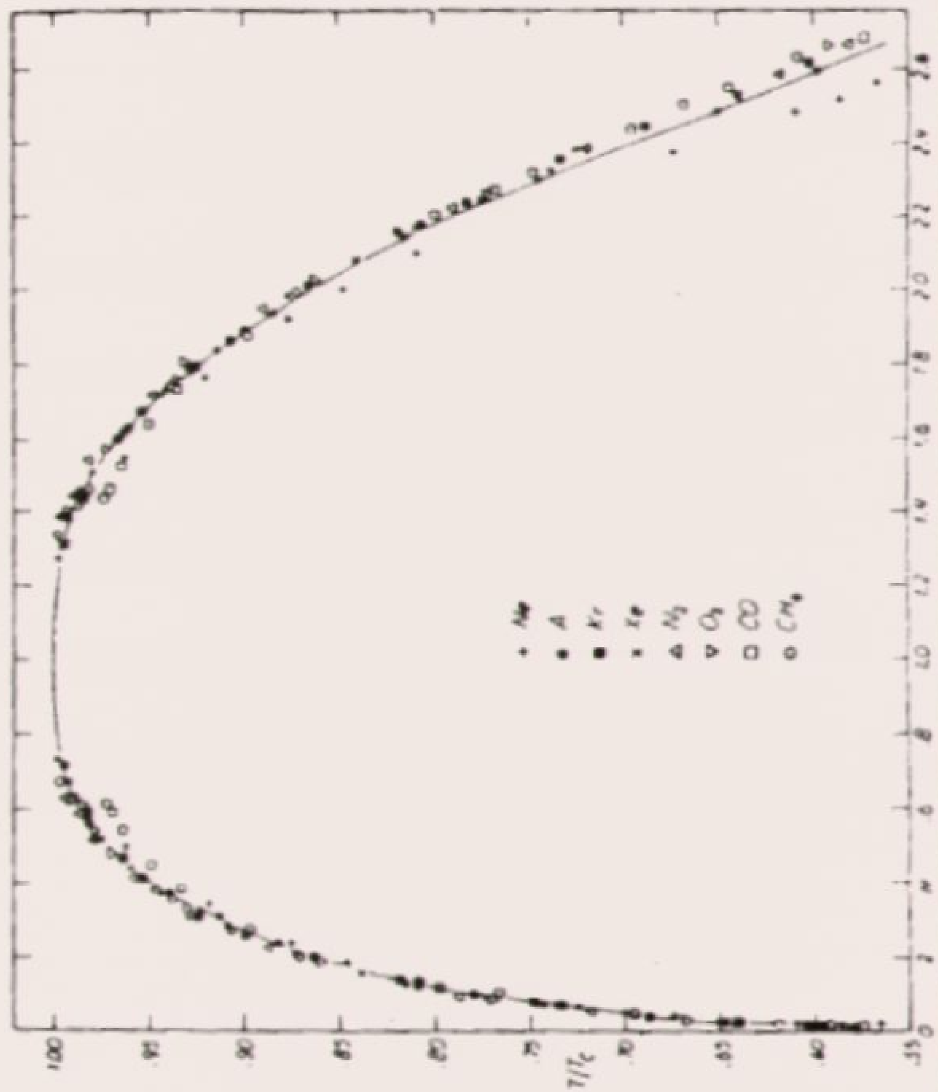
How could these divergences occur? Mean field theory does roughly predicts them, but its detailed predictions are incorrect.

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.

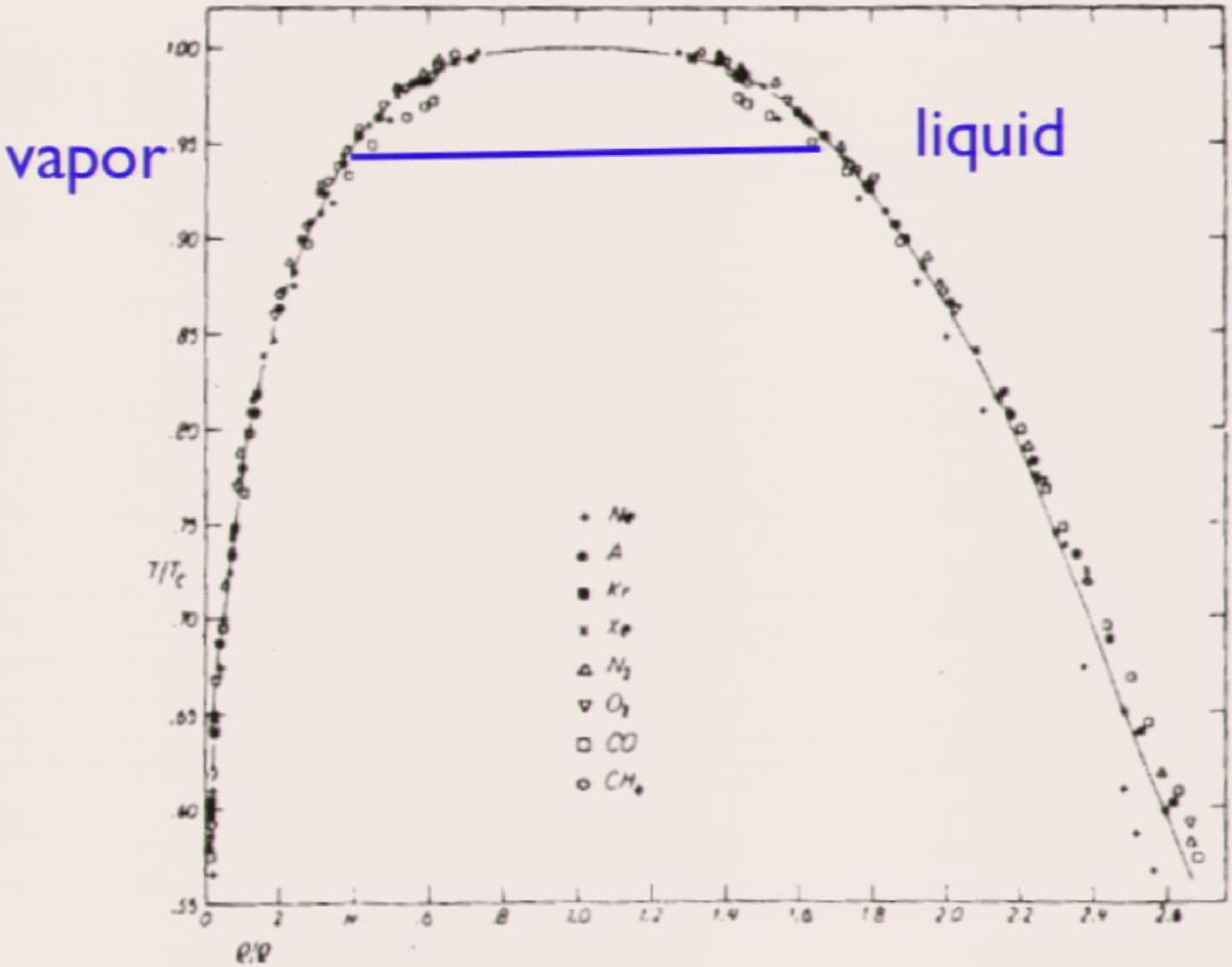


Figure 1.6 Reduced densities of coexisting liquid and gas phases for a number of simple molecular fluids (Guggenheim 1945). The experimental points support a law of corresponding states, but the universal curve is cubic rather than quadratic as required by van der Waals' theory.

Specific descriptors of critical region of fluids:

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

Experimental data, fluids

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

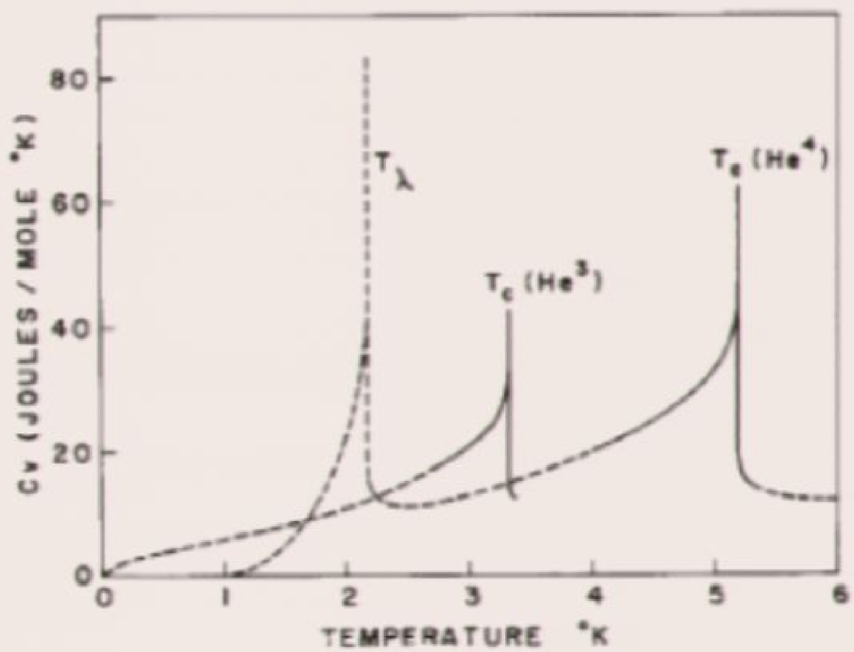
It predicts transitions in one-dimensional systems with finite-range interactions at non-zero temperatures. (In fact, these transitions never occur.)

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

Theoretical work

Onsager solution (1943) for 2D Ising model gives infinity in specific heat and order parameter index β=1/8 (Yang)-- contradicts Landau theory which has β=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 β=1/8 in two dimensions and β=1/3 in three and not the Landau\van der Waals value, β=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.

L. Onsager, Phys. Rev. **65** 117 (1944)

C.N, Yang, Phys. Rev. **85** 808 (1952)

C. Domb, *The Critical Point*, Taylor and Francis, 1993

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.

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

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.

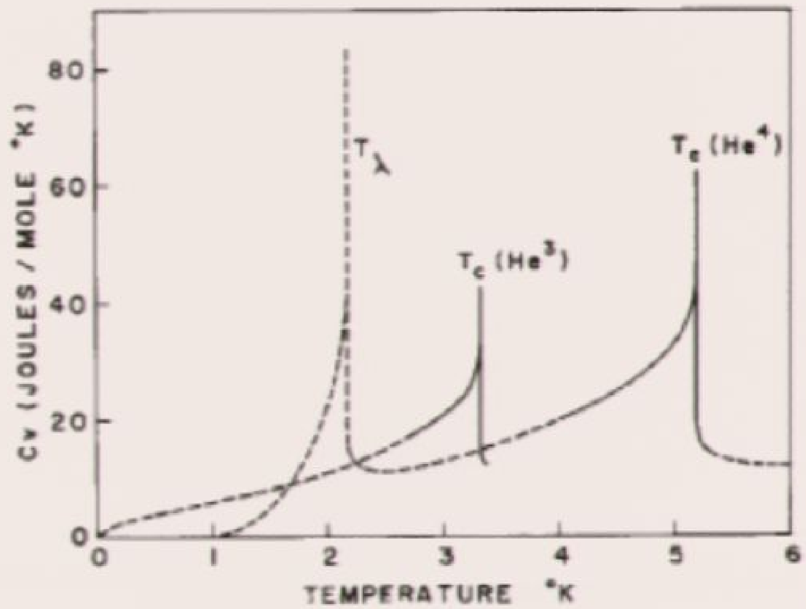
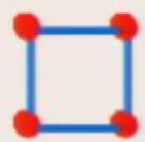


FIGURE 1. C_v of He^3 and He^4 at their respective critical den[sities] is plotted as a function of temperature. The solid curves are the present work.

Moldover and Little (1966)

Mean field theory is never right in giving 1st order transitions in systems like

or even this:



r for describing any two or three dimensional system near its critical point.

ean field theory says that order is produced by the time-average alignment of neighboring oms producing more alignment and thereby producing closed chains of interaction.

know this is wrong. Broken symmetry alignment must extend over entire system. Linkage egions should not be broken if one link goes "wrong". Fluctuations will always make this open. When fluctuations are important mean field theory is wrong.

What's wrong with MFT

- The interaction between phase transitions and spatial topology is ignored.
- Important fluctuations in the critical region are ignored. Specifically, in jump in order parameter proportional to $(-t)^{\beta}$ as $t=T-T_c$ goes to critical point, MFT gives $\beta = 1/2$, experiments give a smaller number.
- In using it, people were looking for the wrong "universality" or "law of corresponding states". Einstein(1902), Uhlenbeck(1952), and others look for quantitative similarities among equations of state across the entire phase diagram. That is a chimera.
- Everyone focuses on average forces or "potentials of mean force" . Fluctuations are ignored. Fluctuations often dominate, as in one dimension.

chimera |kīˈmi(ə)rə; kə-| (also chimaera)

noun

1 (Chimera) (in Greek mythology) a fire-breathing female monster with a lion's head, a goat's body, and a serpent's tail.

• any mythical animal with parts taken from various animals.

2 a thing that is hoped or wished for but in fact is illusory or impossible to achieve : the economic sovereignty you claim to defend is a chimera.

3 Biology an organism containing a mixture of genetically different tissues, formed by processes such as fusion of early embryos, grafting, or mutation : the sheeplike goat chimera.

• a DNA molecule with sequences derived from two or more different organisms, formed by laboratory manipulation.

4 (usu. chimaera) a cartilaginous marine fish with a long tail, an erect spine before the first dorsal fin, and typically a forward projection from the snout. • Subclass Hoplocephali: three families, in particular Chimaeridae. See also

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How can we do better?

• J. van der Waals (1870) and a contemporary, J.E. Verschaffelt, knew mean field theory was, experimentally, wrong near critical point, but nobody paid attention.

• David Ruelle(~1969): calculates phase transition properties with systems approaching infinite size, and prescribed order on the boundaries.

• Guggenheim (1945) compiles jump behavior of fluids, but looks at entire phase diagram, rather than critical region. Focused upon wrong place.

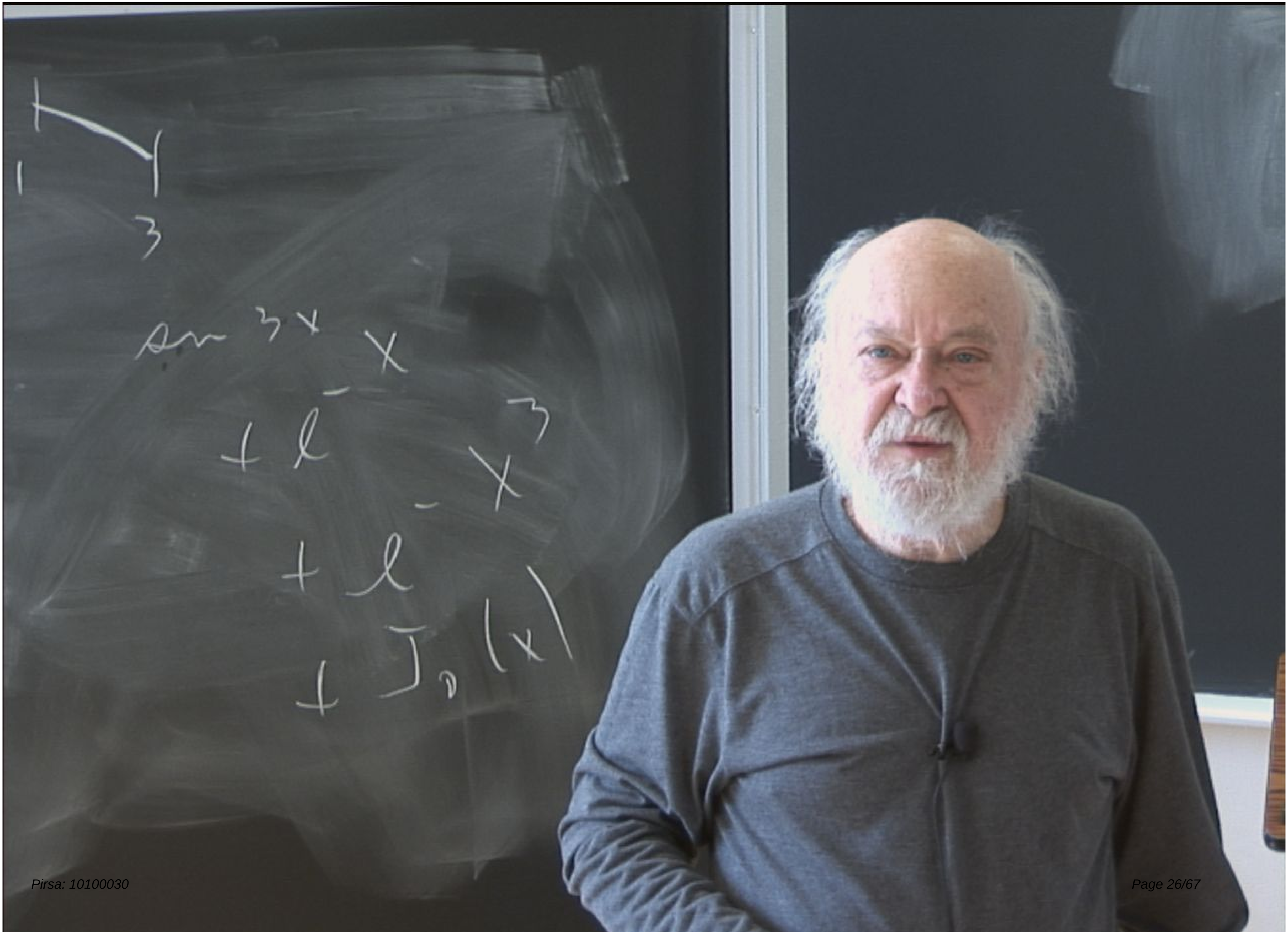
• Landau (~1960) knows that fluctuations matter a lot for turbulence calculation, but does not know how to extend this idea to behavior near critical point.

• T.D. Lee and C.N. Yang (1952) Show that there are singularities in F produced by zeros in partition function in complex h-plane.

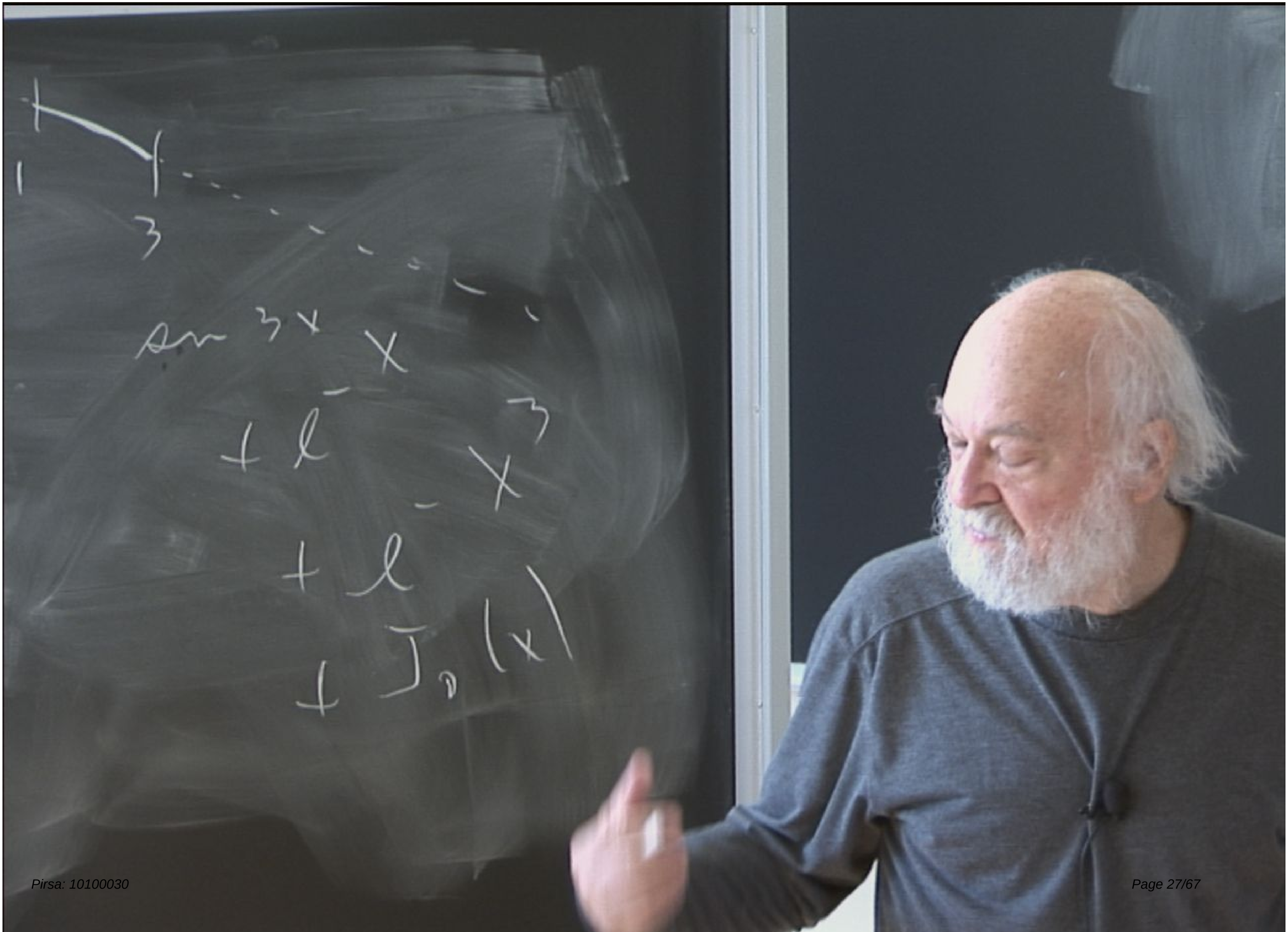
• Lars Onsager (~1943)produces exact solution of two dimensional Ising model. Solution does not look anything like MFT behavior. This focuses attention on critical point. At last people noticed singularities.

What is needed?

A theory which took into account fluctuations and also extended singularity theorem.   It's coming in the next lecture.



+ l
+ l
+ J(x)



Or $e^{-\frac{1}{x^2}}$ $\qquad \frac{\sin 3x}{x}$

$+\ e^{-x}$

$e^{-1/x^2}\,\frac{2}{x^3}$ $\qquad +\ e^{-x^3}$

$+\ J_0(x)$

1

3

$\partial_x\; e^{-\frac{1}{h^2}}$

$\sin 3x \quad x^{-}$

$+\, e^{-x^3}$

$e^{-1/x^2} \quad \frac{2}{x^3} \quad + e^{-x}$

$+\, J_0(x)$

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

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The physics is in fluctuations

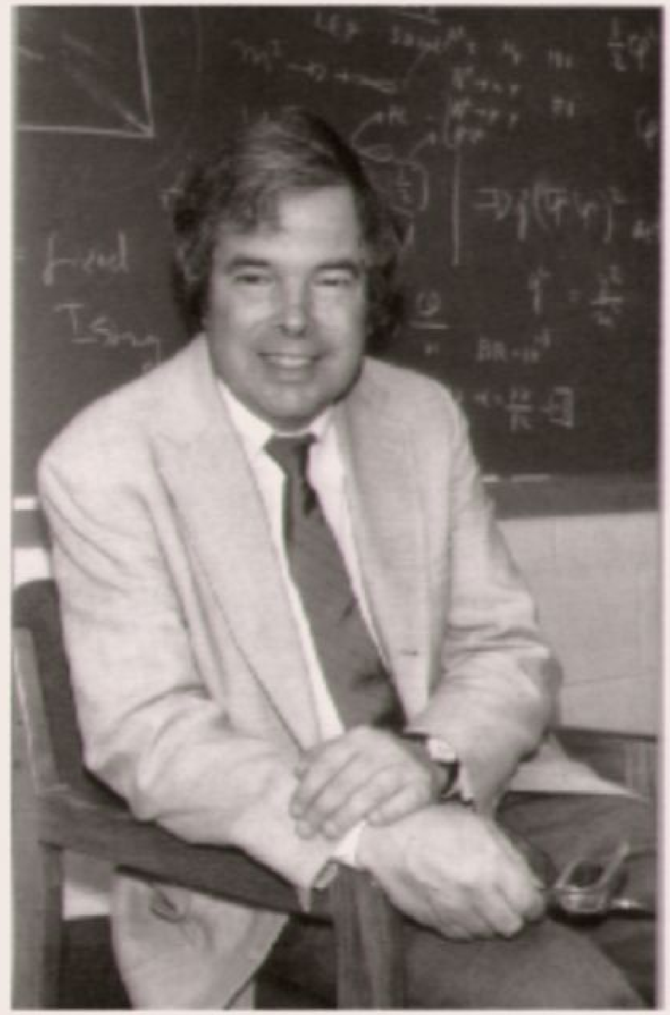
which extend over an indefinite range at critical point. t and h limit range of fluctuations to finite value, called the correlation length, ξ. How can we convert this fact into a theory?

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



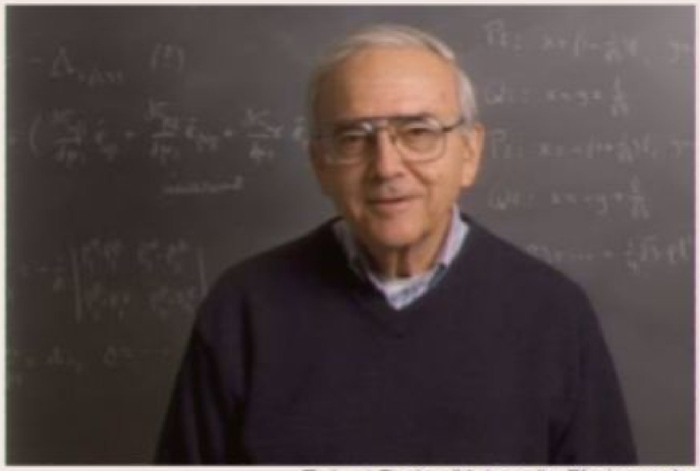
Kenneth G. Wilson

Toward the revolution

The phenomenology

en Widom noticed the most significant caling properties of critical phenomena, ut did not detail where they might have ome from.

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

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

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

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
$< \sigma(r_1)\ \sigma(r_2) \ldots\ldots \sigma(r_m) > \sim 1/r^{mx}$
1964, 1966: This is a good idea but produces a partially wrong answer $x \neq 3/2$. (It is actually close to 1/2.)

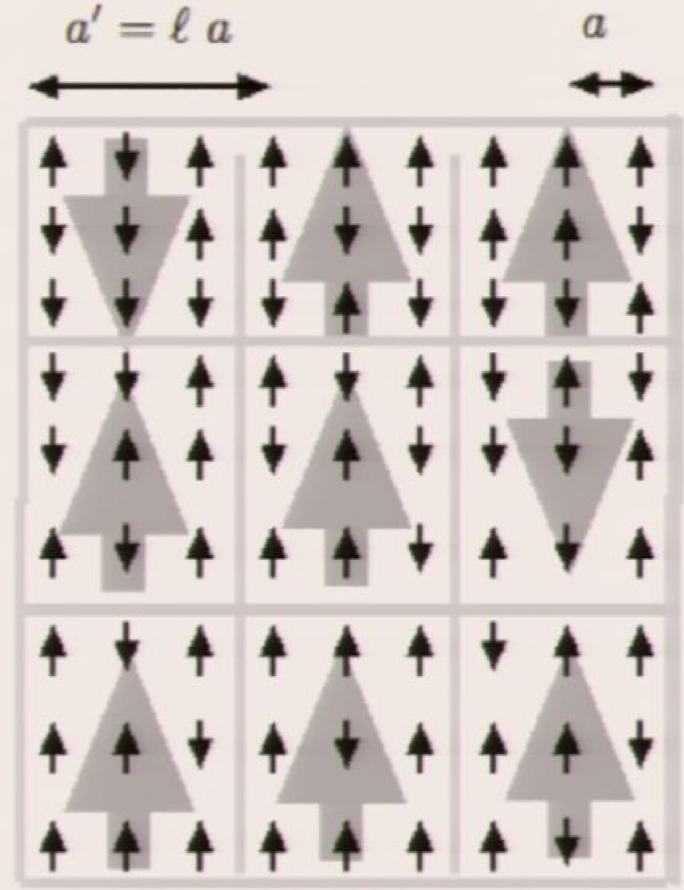
Before Widom, Michael E. Fisher introduces scaling ideas, and the two basic indices in his 1965 paper in the University of Kentucky conference on phase transitions. He bases his approach upon an insightful view of droplets of the different phases driving the thermodynamics. However, he misses the relation between correlation length and thermodynamics.

Kadanoff (1966) .....

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.



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

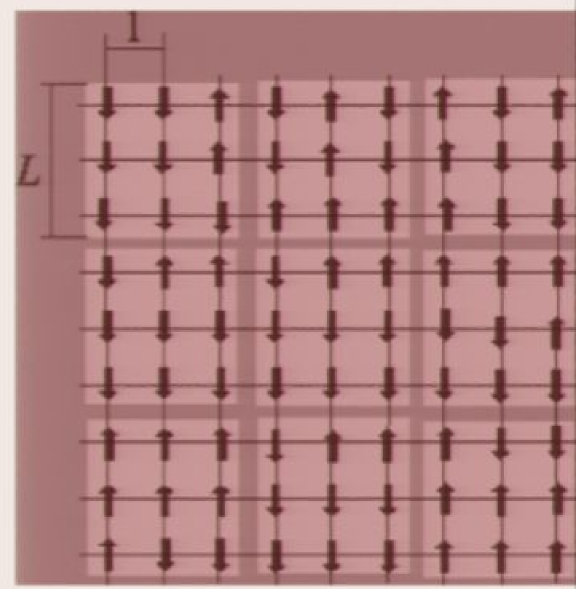
$$h' = h\ \ell^{y_h}$$

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

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, $\Sigma_\mu\, g(\mu,\{s\}) = 1$.

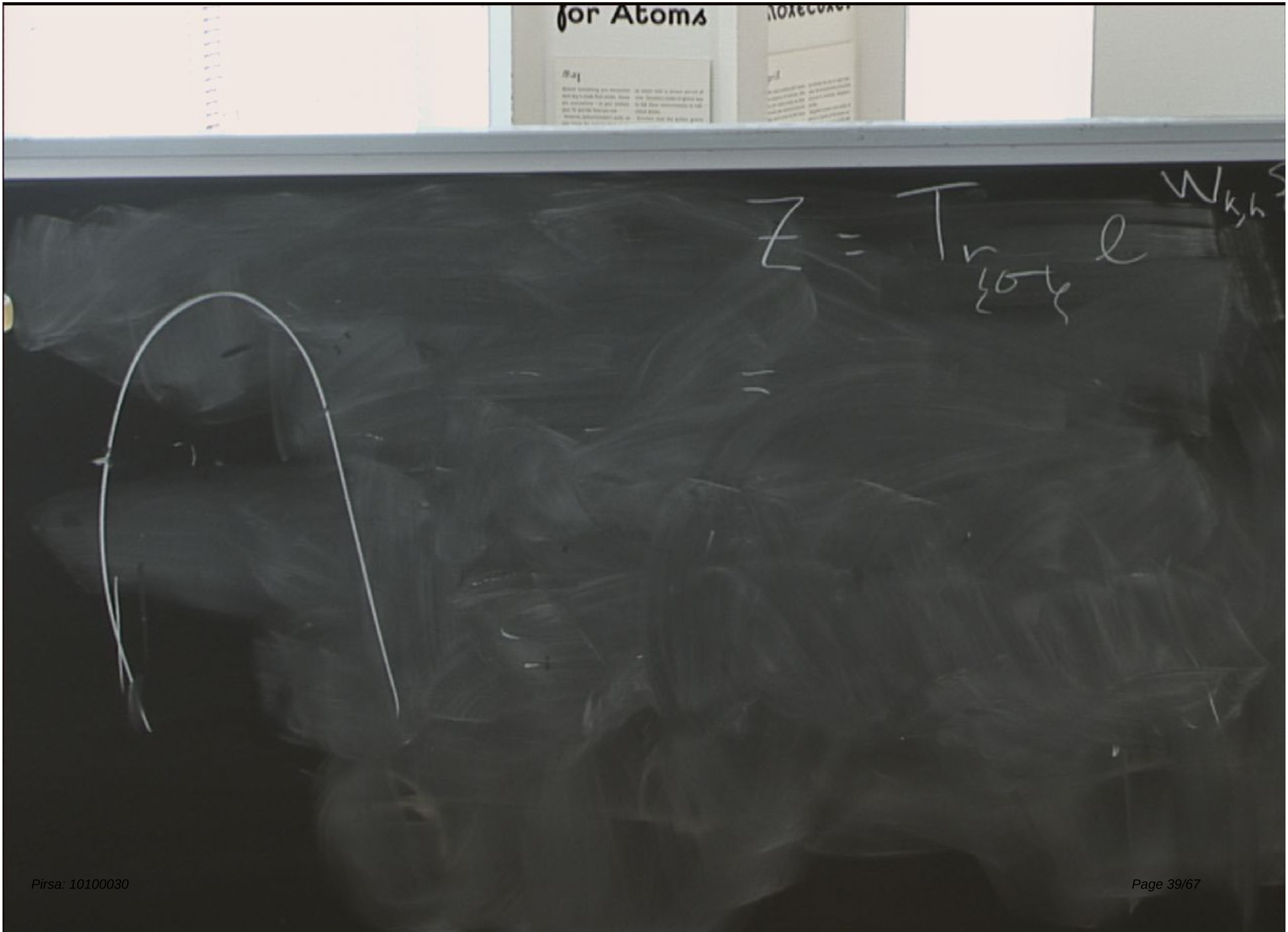


fewer degrees of freedom produces "block renormalization"

Now we are ready. Define $\exp(W'\{\mu\}) = \text{Trace}_{\{\sigma\}}\, G\{\mu, \sigma\} \exp(W_K\{\sigma\})$

Notice that $Z = \text{Trace}_{\{\mu\}} \exp(W'\{\mu\})$

If we could ask our fairy god-mother what we wished for now, it would be that we came back to the same problem as we had at the beginning: $W'\{\mu\} = W_{K'}\{\mu\}$ where the subscript represents the three relevant


for Atoms
$Z = \mathrm{Tr}_{\{\sigma\}}\, e^{W_{k,h}}$

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$$= \mathrm{Tr}_{\{\mu\}}$$

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$$= \mathrm{Tr}_{\{\mu\}}\, \mathrm{Tr}_{\{\sigma\}}\, G(\{\mu,\sigma\})\, e^{W}$$

$$\mathrm{Tr}_{\{\mu\}}\, G(\{\mu\},\{\sigma\}) = 1$$

$$Z = \mathrm{Tr}_{\xi\sigma\zeta}\, e^{W_{k,h}}$$

$$= \mathrm{Tr}_{\{\mu\},\zeta}\ \mathrm{Tr}_{\xi\sigma\zeta}\, G\{\mu,\sigma\}\, e^{W_k}$$

$$\mathrm{Tr}_{\{\mu\}}\, G(\{\mu\},\{\sigma\}) = 1$$

$$e^{W'\{\mu\}}$$

$\# \ g(\mu, \sigma's)$

blocks

μ has orign

$= \ \mu \quad \sum_{\text{block}} \sigma's$

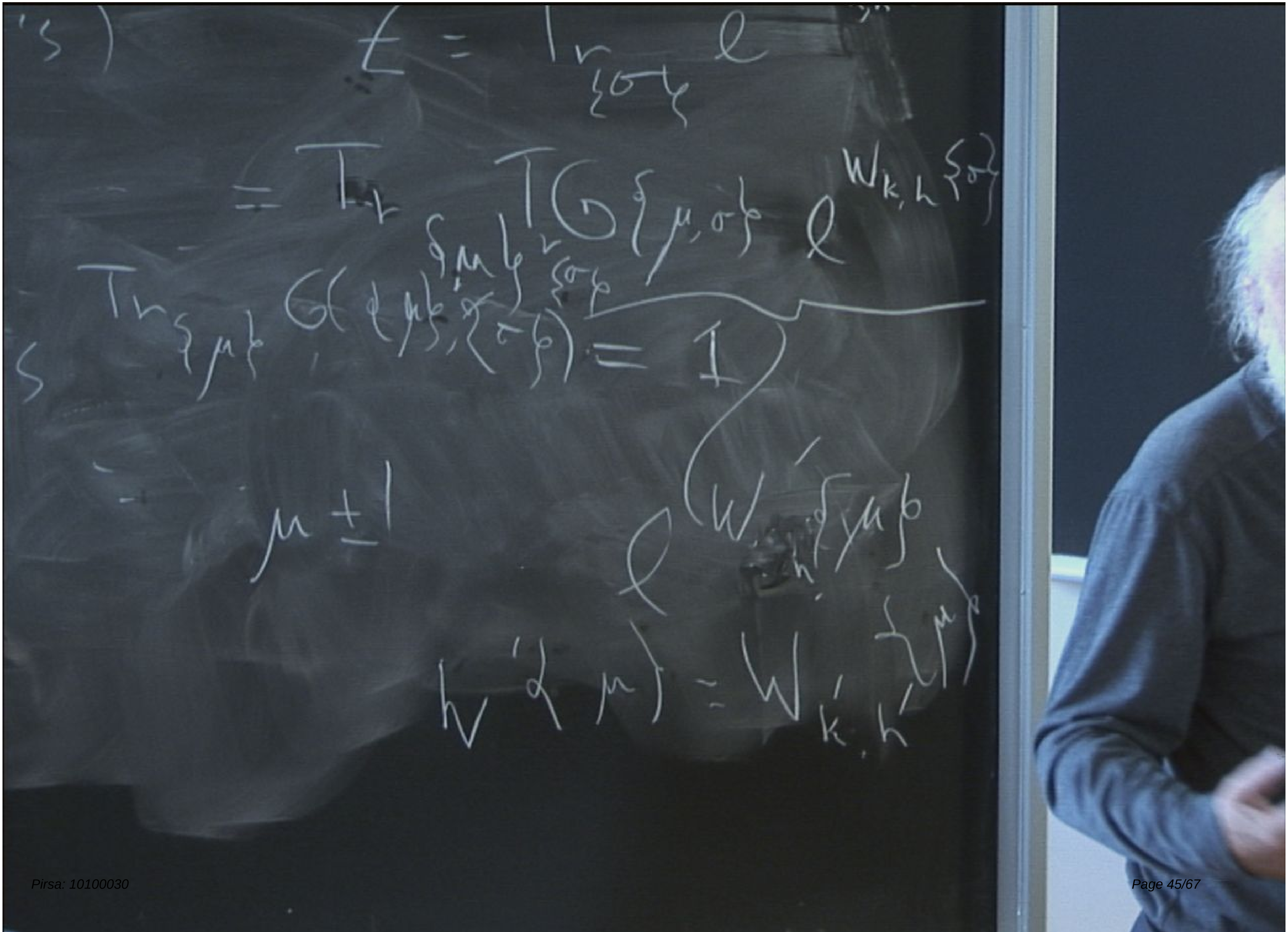
$Z = \mathrm{Tr}_{\{\sigma\}} e$

$= \mathrm{Tr}_{\{\mu\}} \ \mathrm{Tr}_{\{\sigma\}} G\{\mu, \sigma\}$

$\mathrm{Tr}_{\{\mu\}} G(\{\mu\}, \{\sigma\}) = 1$

$\mu \pm 1$

e^{W}



Z = Tr e
= Tr Tr G({μ,σ}) e
Tr G({μ},{σ}) = 1
μ ± 1

Renormalization for Ising model in any dimension; reprise

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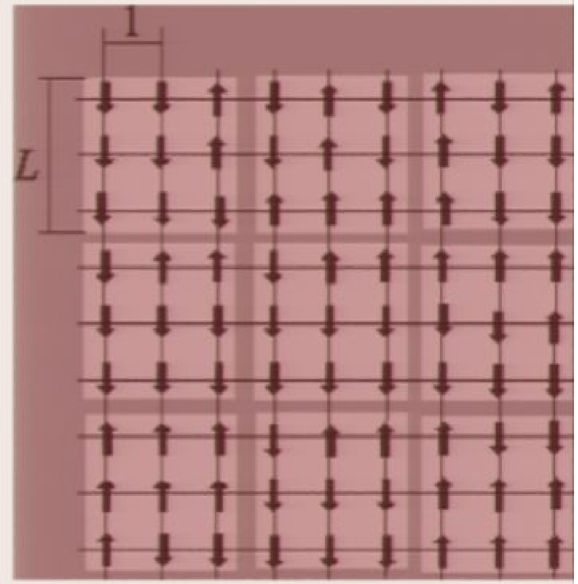

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Renormalization

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

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

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

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

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

b's can be found through a numerical calculation.

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: $N=\Omega/a^d$ $\quad N'=\Omega/a'^d$

$N'/N = a^d / a'^d = (a'/a)^{-d}$

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

$f_c(t) = f_c^0\, t^{dx}$

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

Fields: Relevant, Irrelevant, marginal, ...

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

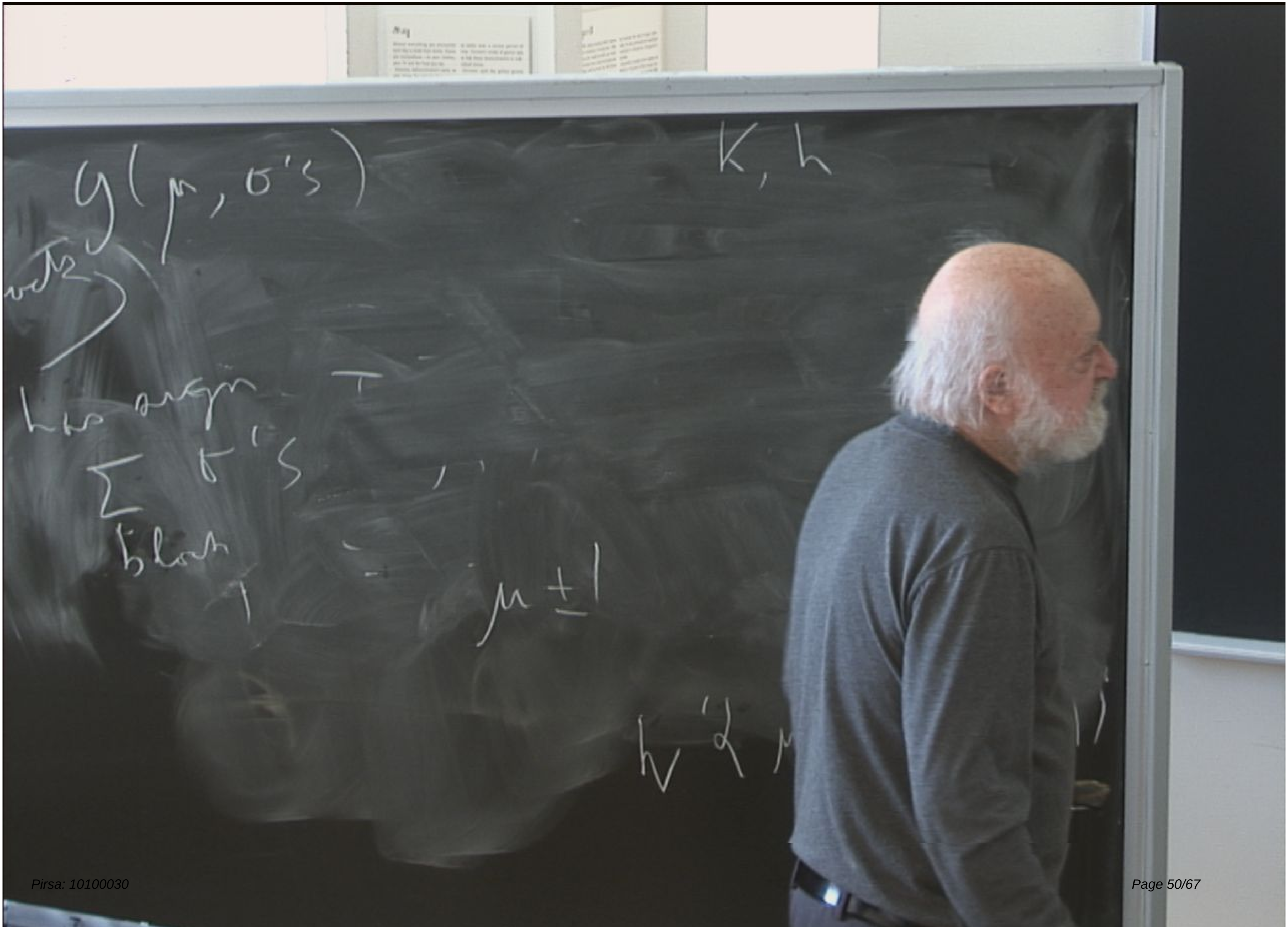
there are a few relevant fields: like t,h, K_0, which grow at larger length scales, completely dominate large-scale behavior

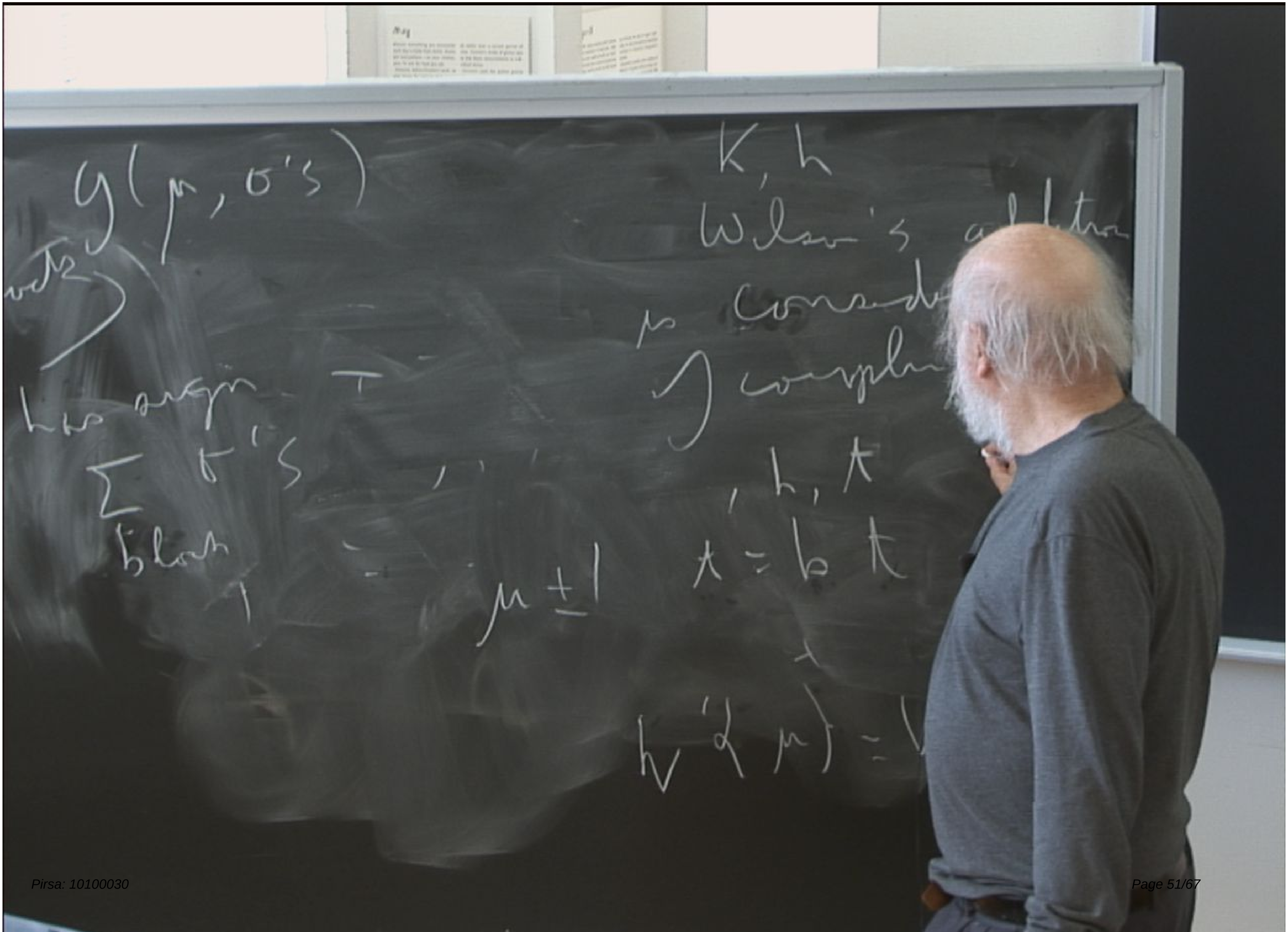
there are many irrelevant fields: they have $|b|<1$, don't play a role at large scales

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).


g(μ, σ's)
K, h
Σ σ's
μ ± 1



$g(\mu, \sigma\text{'s})$

with

has origin

Σ σ's

block

$\mu \pm 1$

K, h

Wilson's addition

consider lots of couplings

$, h, \tau$

$\tau = b\,\tau$

$|b| > 1$

$h'(\mu) = W'_{k,h}$

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).

A Worthwhile Phenomenology

Weaknesses of phenomenology:

i. One cannot calculate everything: value of x's unknown

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.

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 $a' = \ell a$

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.

ℓ has to cancel out of everything

e.g. coherence length, ξ, is $a\, t^{-1/yt}$ and is equally $a'\, (t')^{-1/yt}$

$$a' = \ell a$$

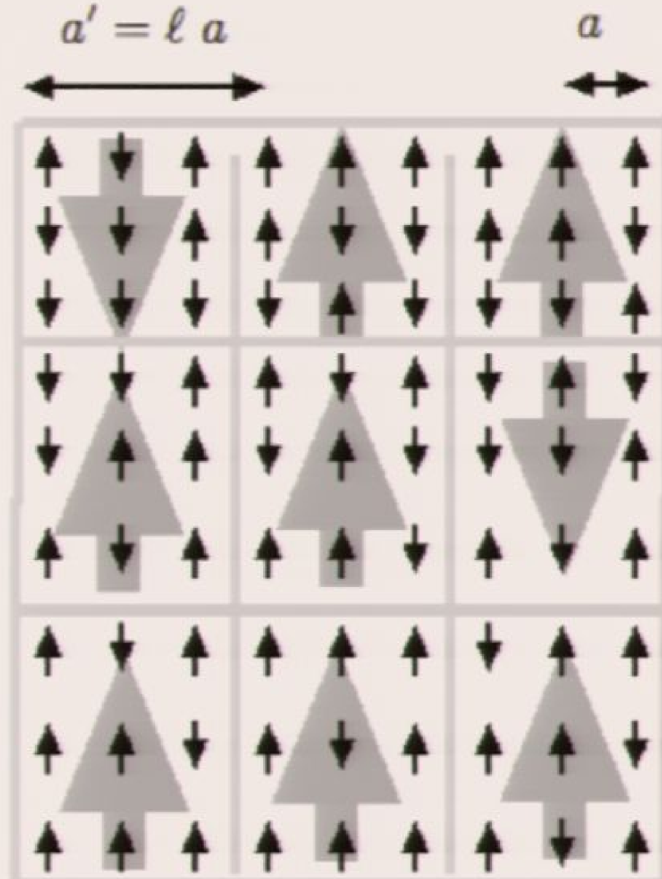
$$t' = t\ \ell^{y_t}$$

The ℓ 's cancel out. Good!

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"

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.

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

$$\boxed{\vec{K}' = \vec{R}(\vec{K})}$$

K, h

Wilson's additi

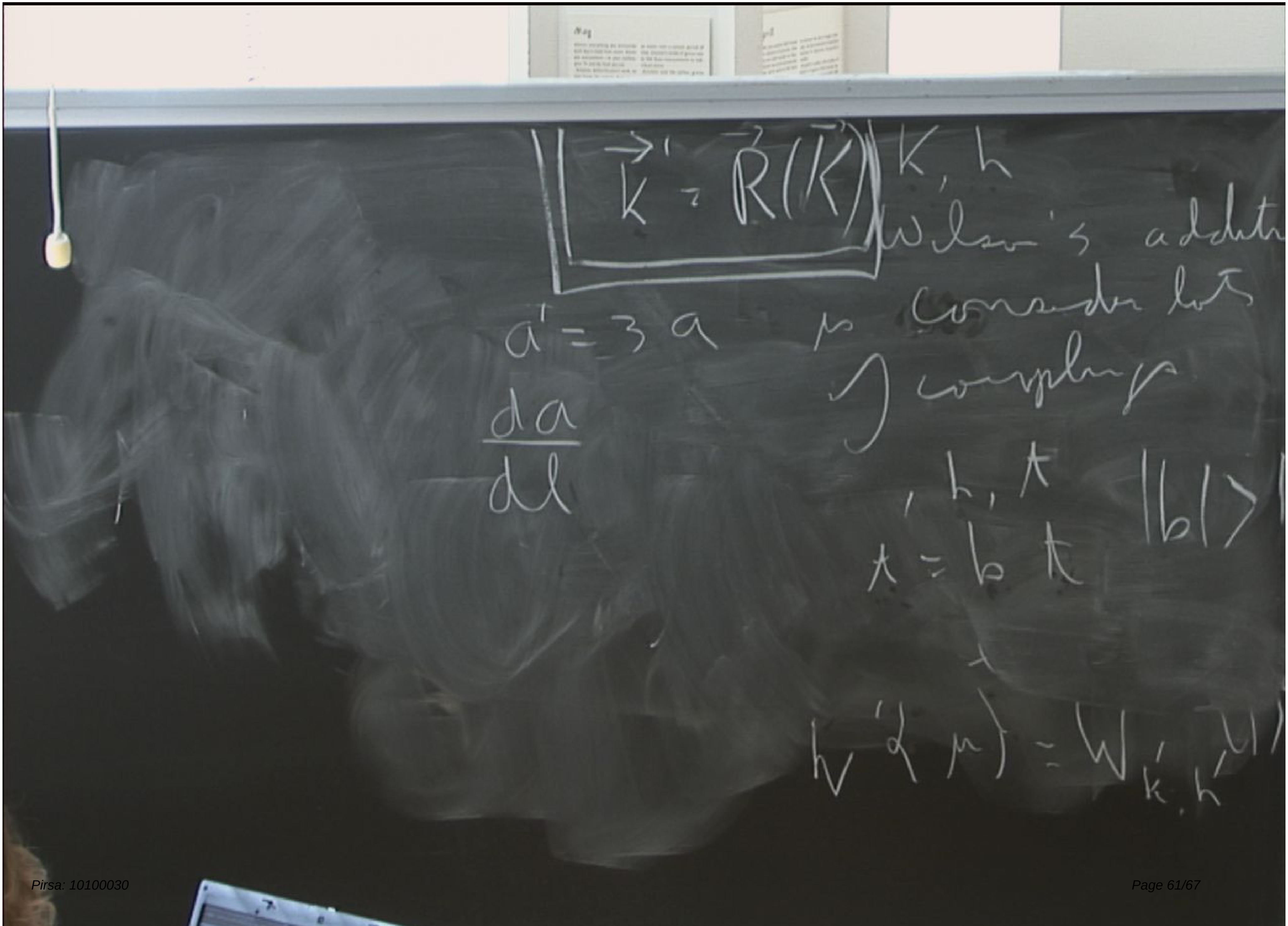
consider lots

of couplings

h, t

$t = b\, t$

$h'(\mu) =$


$\vec{k}' = \vec{R}(\vec{k})$
k, h
Wilson's
consider lots of couplings
$a' = 3a$
$\frac{da}{dl}$
h, t
$t' = b\,t$
$|b| >$
$h'(\mu) = W_{k,h}$

$$\boxed{\vec{k}' = \vec{R}(\vec{K})}$$

K, h

Wilson's additi[ve]

consider lots

of couplings

$a' = 3a$

$\frac{da}{dl}$

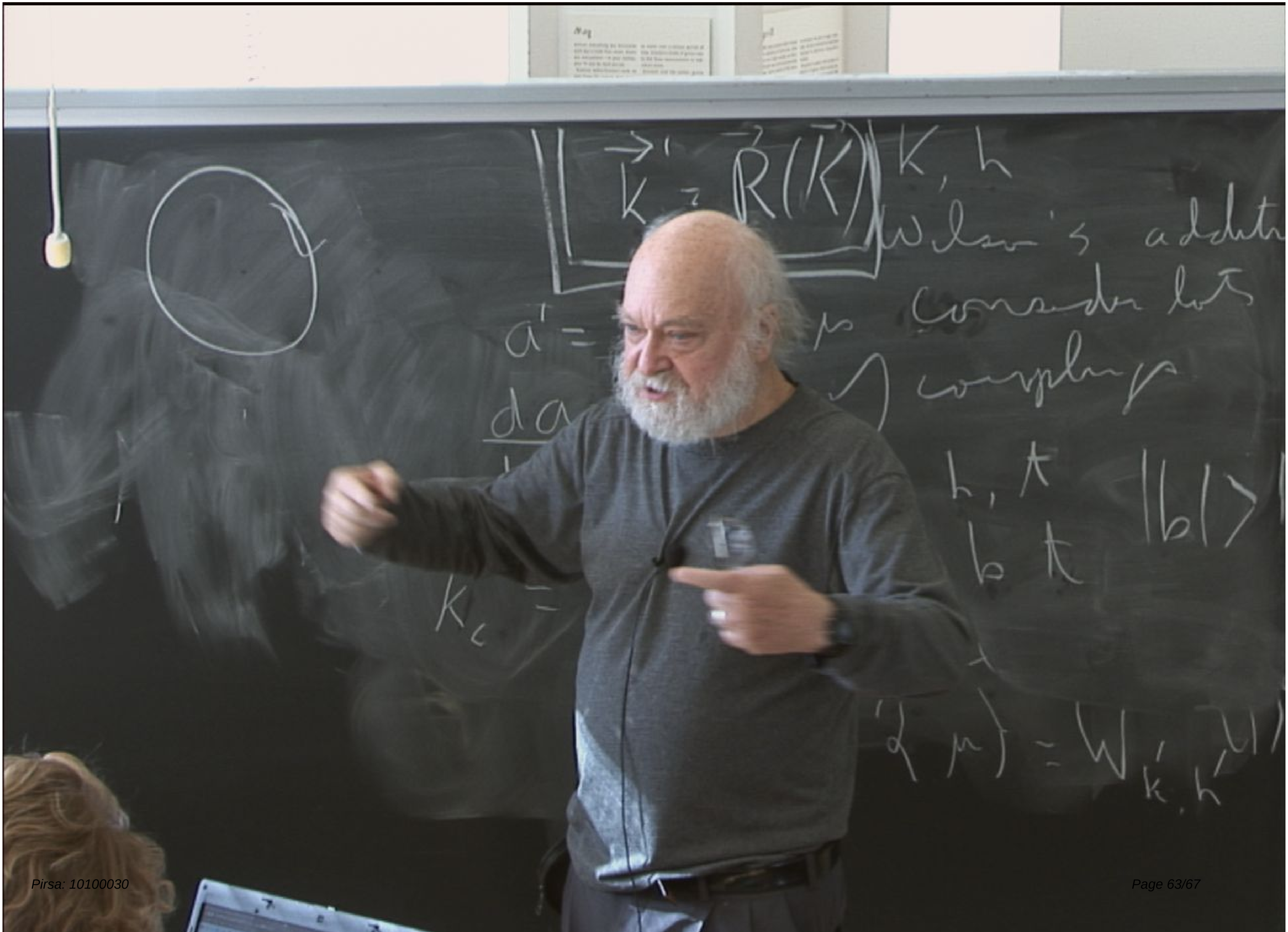
$\vec{k}_i = \vec{R}(\vec{k}_i)$

h, t

$t = b\,t$

$|b|>$

$W'(\mu) = W_{k,h}'(l)$


Wilson's
consider lots
couplings

e three kinds fixed points:

g coupling: K,h go to infinity   describes e.g. liqu

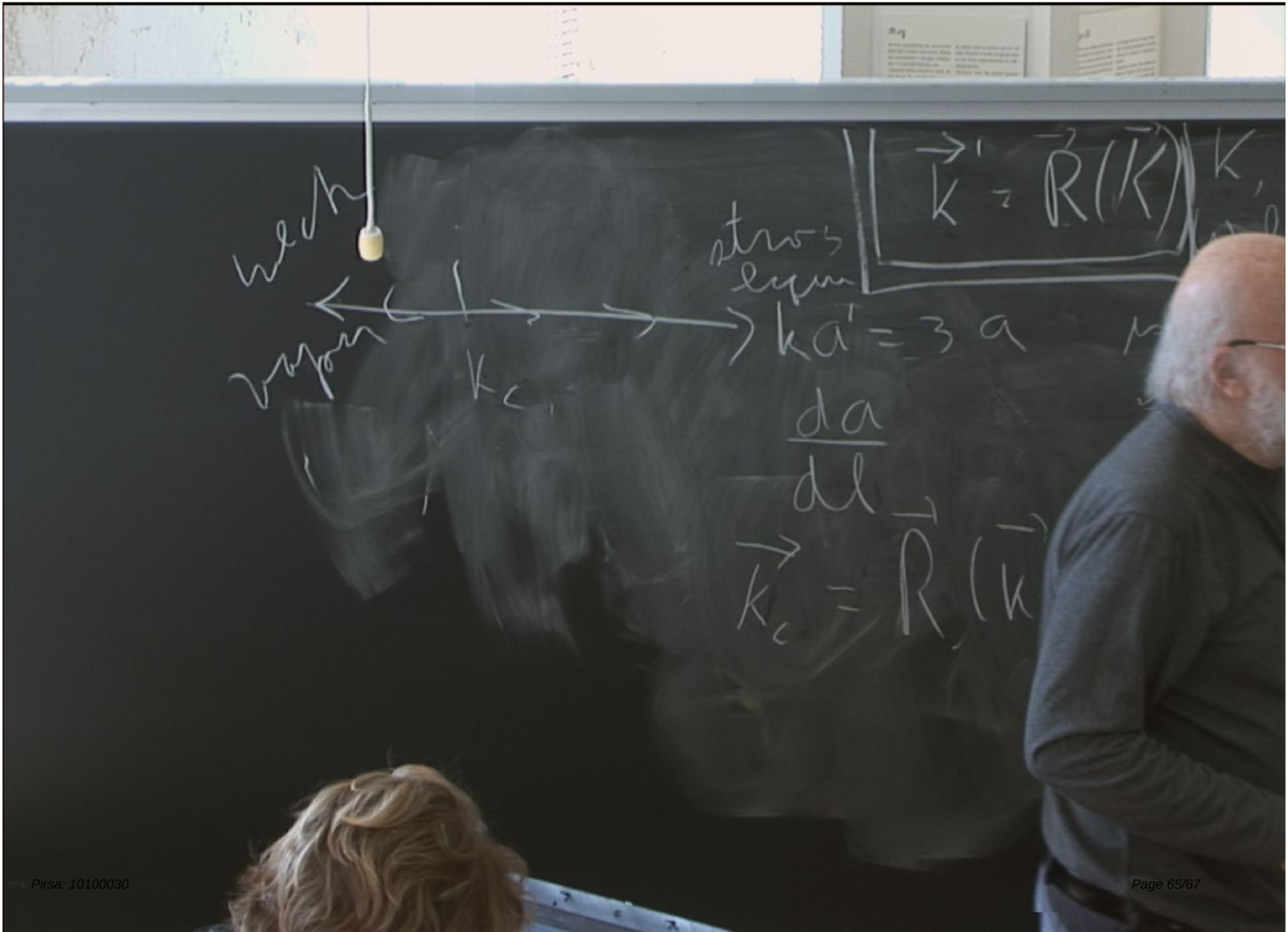
k coupling: K, h go to zero   describes e.g. vap

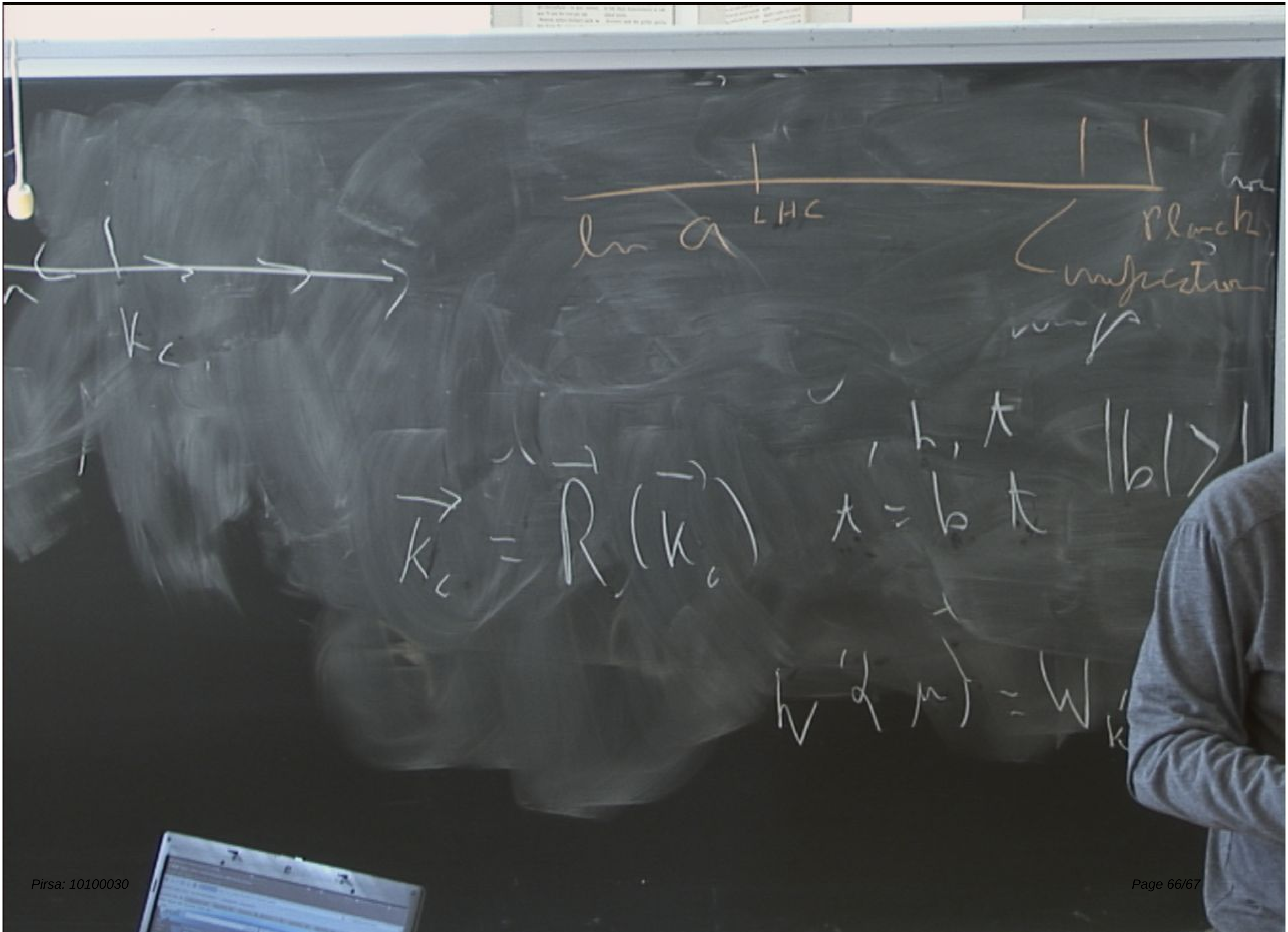
cal: K set to K_c h set to zero, critical point

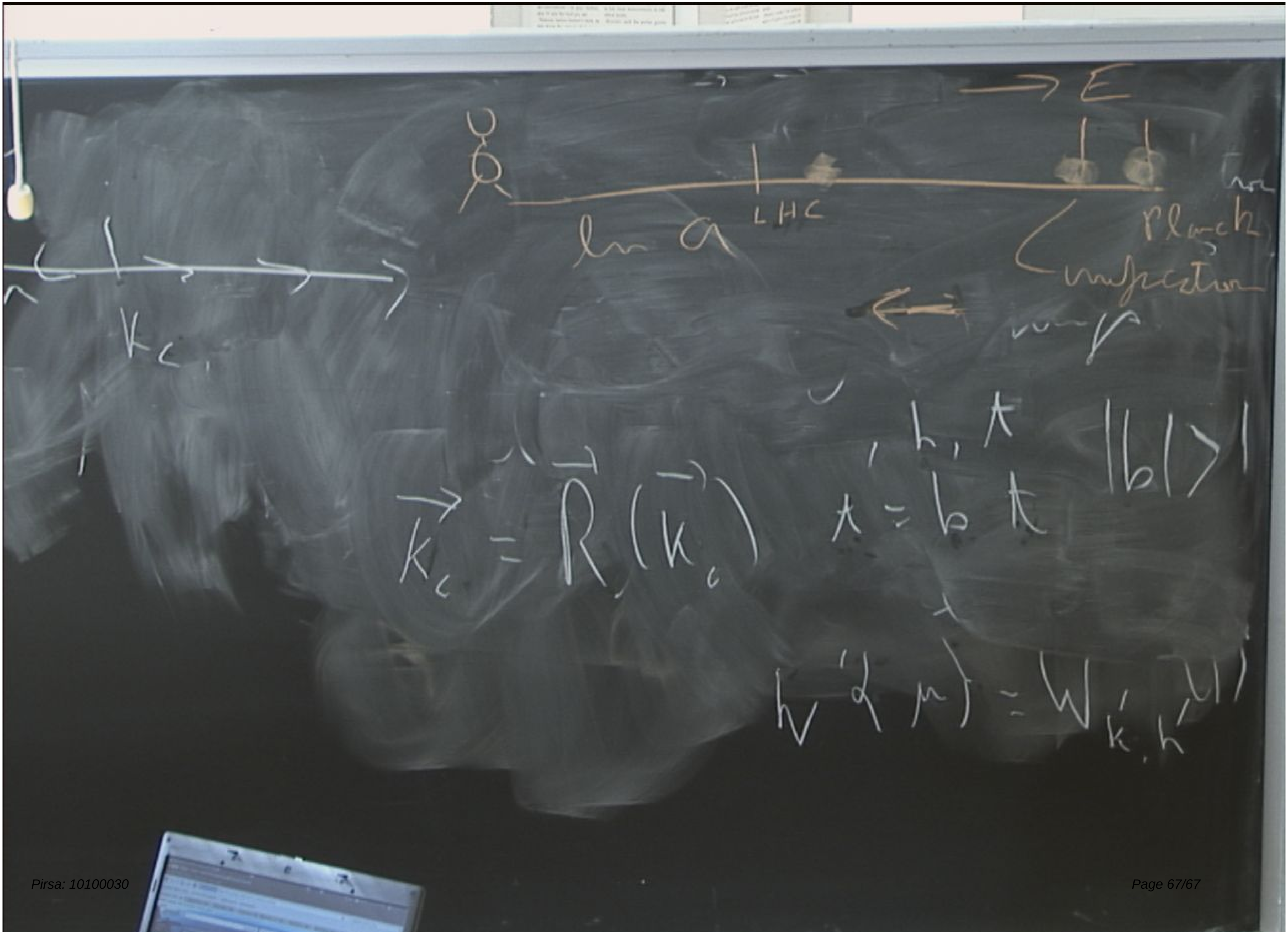
erent in destinations encode different behavior.

t symmetries and spatial dimensions produce differe

ints.


k' = R(K)
ka' = 3 a
da
dl
k_c = R(k


ln a
LHC
Planck
unification


E
ln a
LHC
Planck
unification
$\vec{k}_c = \bar{R}(\vec{k}_c)$
$x = b\,x$
$|b| > 1$