Title: Statistical Mechanics (PHYS 602) - Lecture 9

Date: Oct 15, 2010 10:30 AM

URL: http://pirsa.org/10100028

Abstract:

PERIMETER INSTITUTE FOR THEORETICAL PHYSICS

Mean Field Theory: more is the same

one spin

Ising model, spin, simplified atom $\quad \sigma = \pm 1$

one spin in a magnetic field $\quad H = -\sigma\mu B = -kT\sigma h$

statistical average: $\quad <\sigma>= \tanh(h)$

many spins

spin in a magnetic field, dimension d $\quad -H/kT = K\sum_{nn}\sigma_r\sigma_s + h\sum_r \sigma_r$

focus on one spin, at ***r***: that spin feels $\quad h + K \sum_{\mathbf{s}\text{ nn to }\mathbf{r}} \sigma_{\mathbf{s}}$

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in MFT more is the same

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ocus on one spin $\quad -H_{eff}/(kT) = \sigma_r[h_r + K\sum_s <\sigma_s>]$

tatistical average: $\quad h_{eff} = [h + Kz <\sigma>]$ z=number of nn

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

or, if there is space variation, $h_{eff} = h_{\mathbf{r}} + K \sum_{\mathbf{s}\ nn\ to\ \mathbf{r}} <\sigma_{\mathbf{s}}>$

We shall focus on these equations for a time. This is an approximation called MFT. It has many qualitatively useful aspects.

Look near criticality

The simplest interesting thing happens for small $<\sigma>$, with no field. Expand in $<\sigma>$ and h and find

$$h_{eff} = [h + Kz < \sigma >]$$
$$< \sigma > = \tanh(h_{eff})$$

lowest order: $h_{eff}=Kz<\sigma>$

$<\sigma >=h_{eff}$

which has the solution Kz=1.

Pick $K=K_c=1/z$ as a critical value of K.

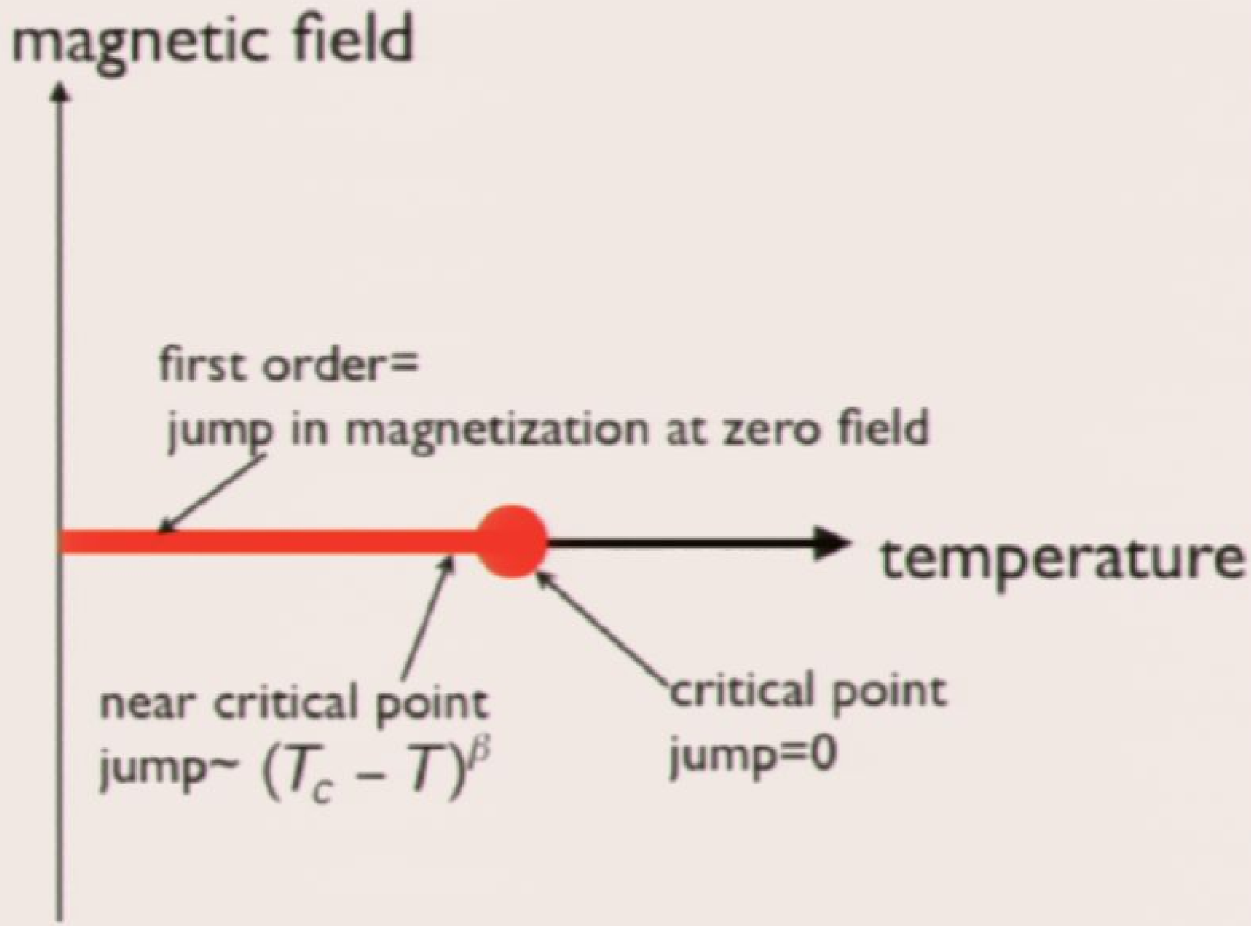
Write Kz=1-t, t is temperature deviation from criticality, now write next order expansion as $<\sigma> = (1-t) <\sigma> +h - <\sigma>^3/3$ or

$t <\sigma> = h - <\sigma>^3/3$

this is now the result of mean field theory near the critical point. Notice that MFT gives a simple cubic equation for order parameter near critical point.

Magnetic Phase Diagram

Conceptually, the simplest phase transitions occur in ferromagnetic materials in which neighboring spins tend to align in the same direction making a magnetic field in that direction. Below a critical temperature, Tc, this alignment can occur even in the absence of an applied magnetic field.



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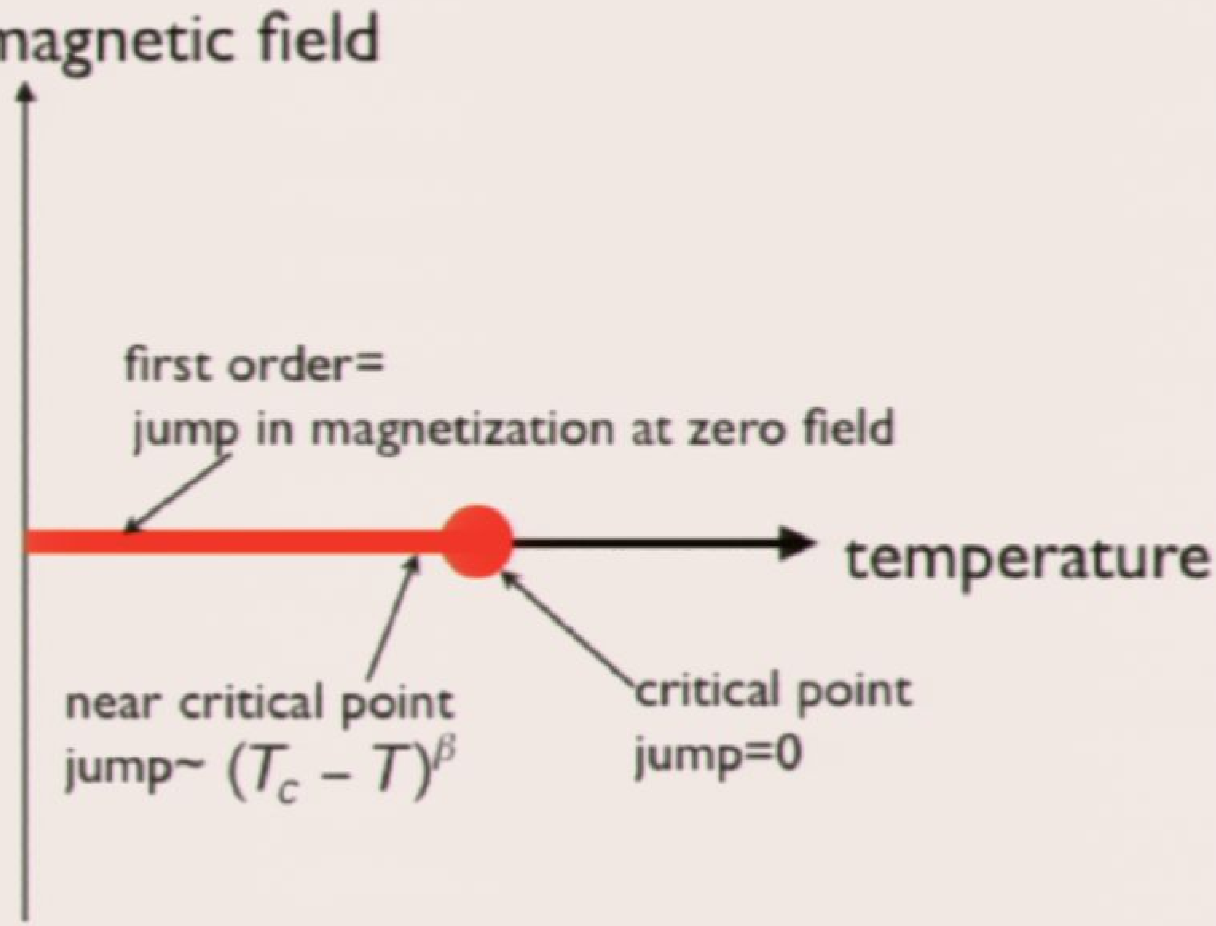

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easiest problem: Ising ferromagnet spin, $\sigma_{\mathbf{r}}$ at each site of lattice, each spin takes on values plus or minus one.

problem defined by

$$-H/(kT) = K \sum_{nn} \sigma_r \sigma_s + h \sum_r \sigma_r$$

free energy defined by

$$-F/(kT) = \ln \sum_{\{\sigma_r = \pm 1\}} \exp\left[-H\{\sigma_r\}/(kT)\right]$$

<σ> depends on K and h. Even when h=0, if K>0 spins line up and <σ> chooses to be non-zero.

Focus on Ising model to see nature of MFT's.

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$$\tanh x \simeq x - \frac{x^3}{3}$$

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Calculate results

$t <\sigma> = h - <\sigma>^3/3$

$h=0$ $t>0$ implies $<\sigma>=0$ no magnetization for $T>T_c$ and zero field

$h=0$ $t<0$ implies $<\sigma>=0$ or $<\sigma>=\pm(-3t)^\beta$ with $\beta=½$

spontaneous magnetization for $T<T_c$ and zero field

0 solution has higher free energy and is ruled out

(thermodynamics demands minimum free energy)

also at $t=0$ we find $<\sigma>= h^{1/\delta}$ $\delta=3$

susceptibility $=\partial<\sigma>/\partial h =1/|t|$ for $h=0$ $t>0$ note divergence

same qualitative results hold near all critical points,

qualitatively correct, near most $d=3$ critical points

quantitatively wrong (e.g. β approximately ⅓)

The divergence in the susceptibility is an important result. It shows the extreme sensitivity of the critical point region to parametric changes, These divergences in the thermodynamics will be one key to understanding critical point behavior.

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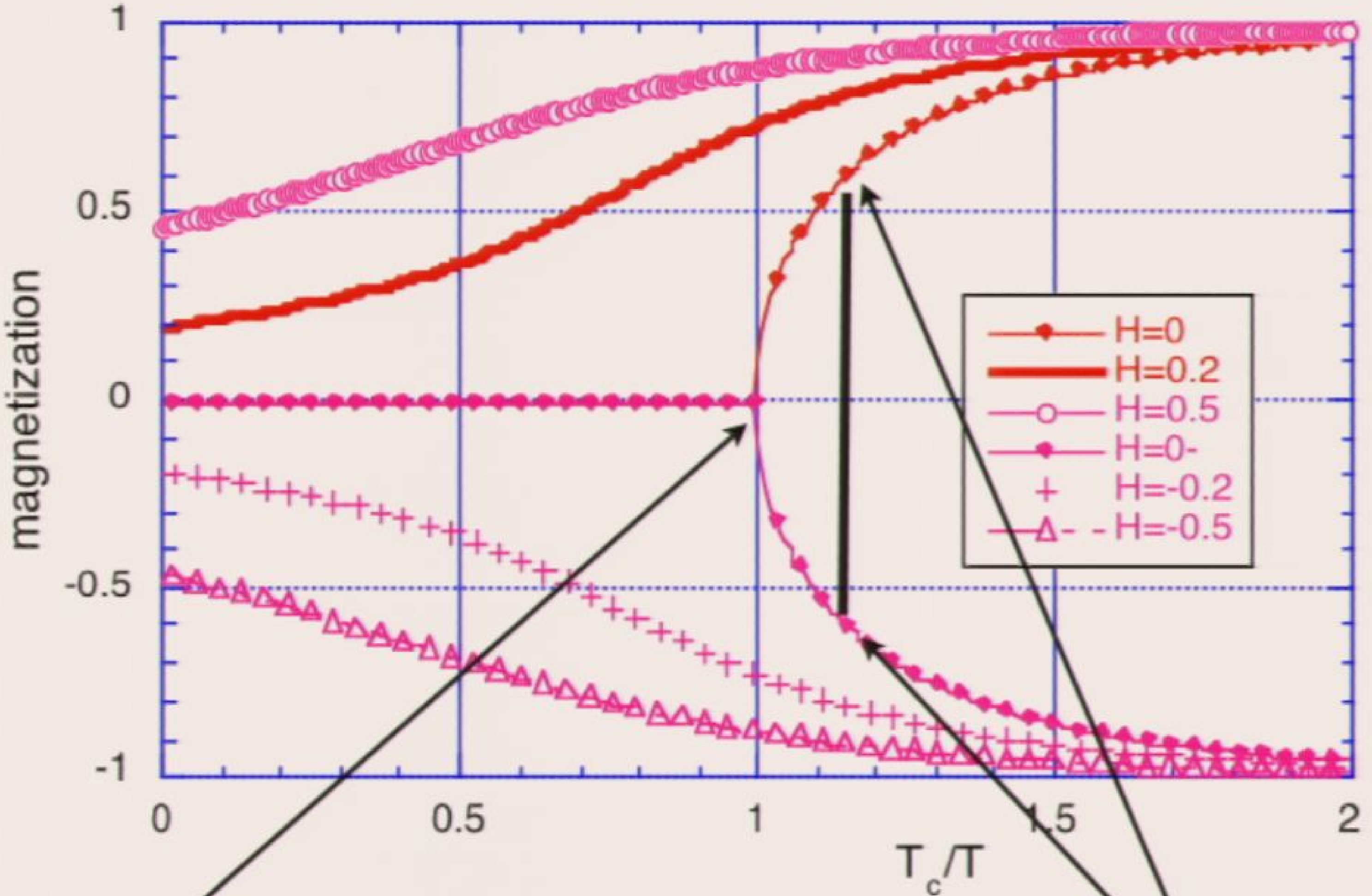

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First order phase transition

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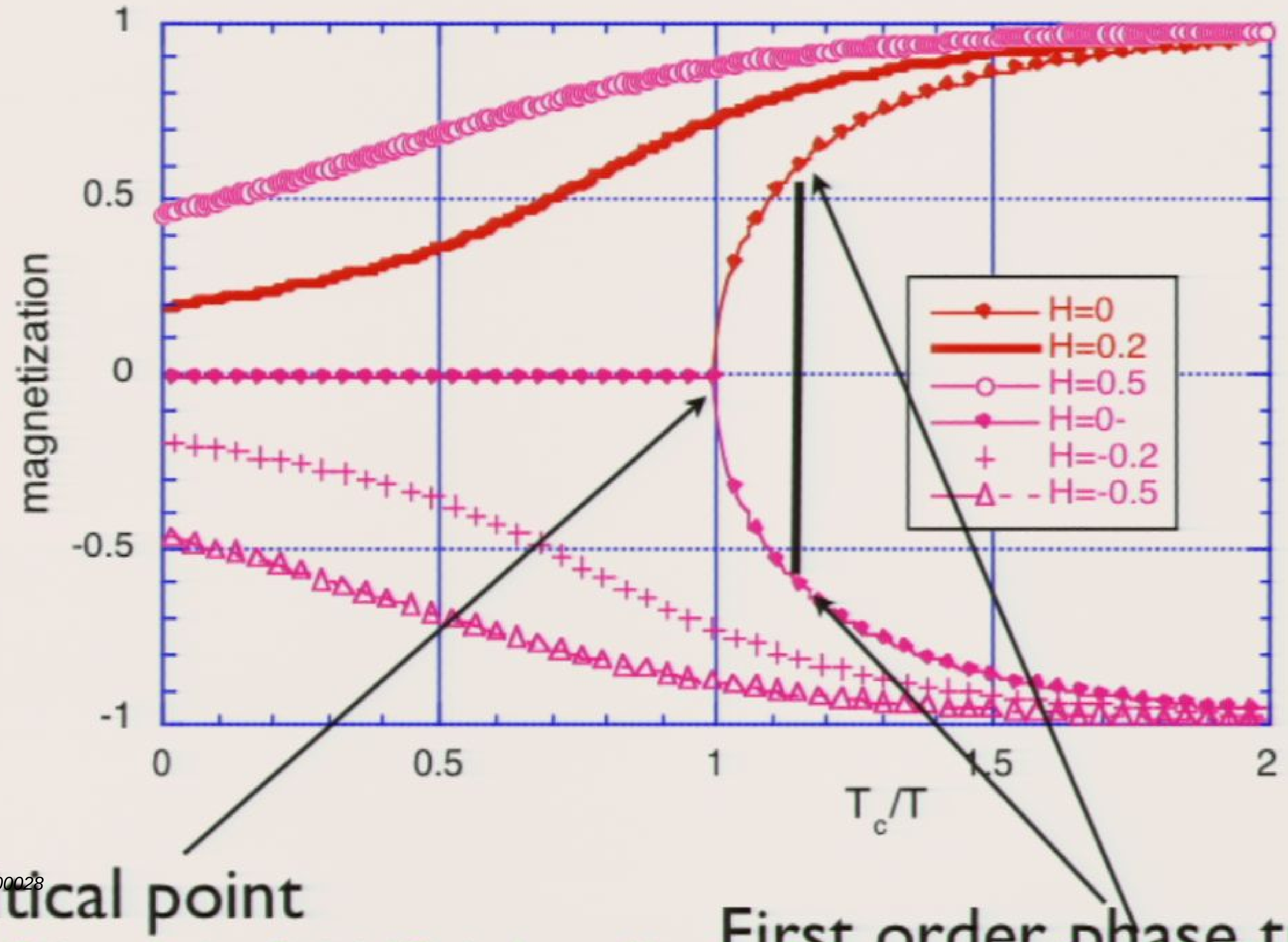

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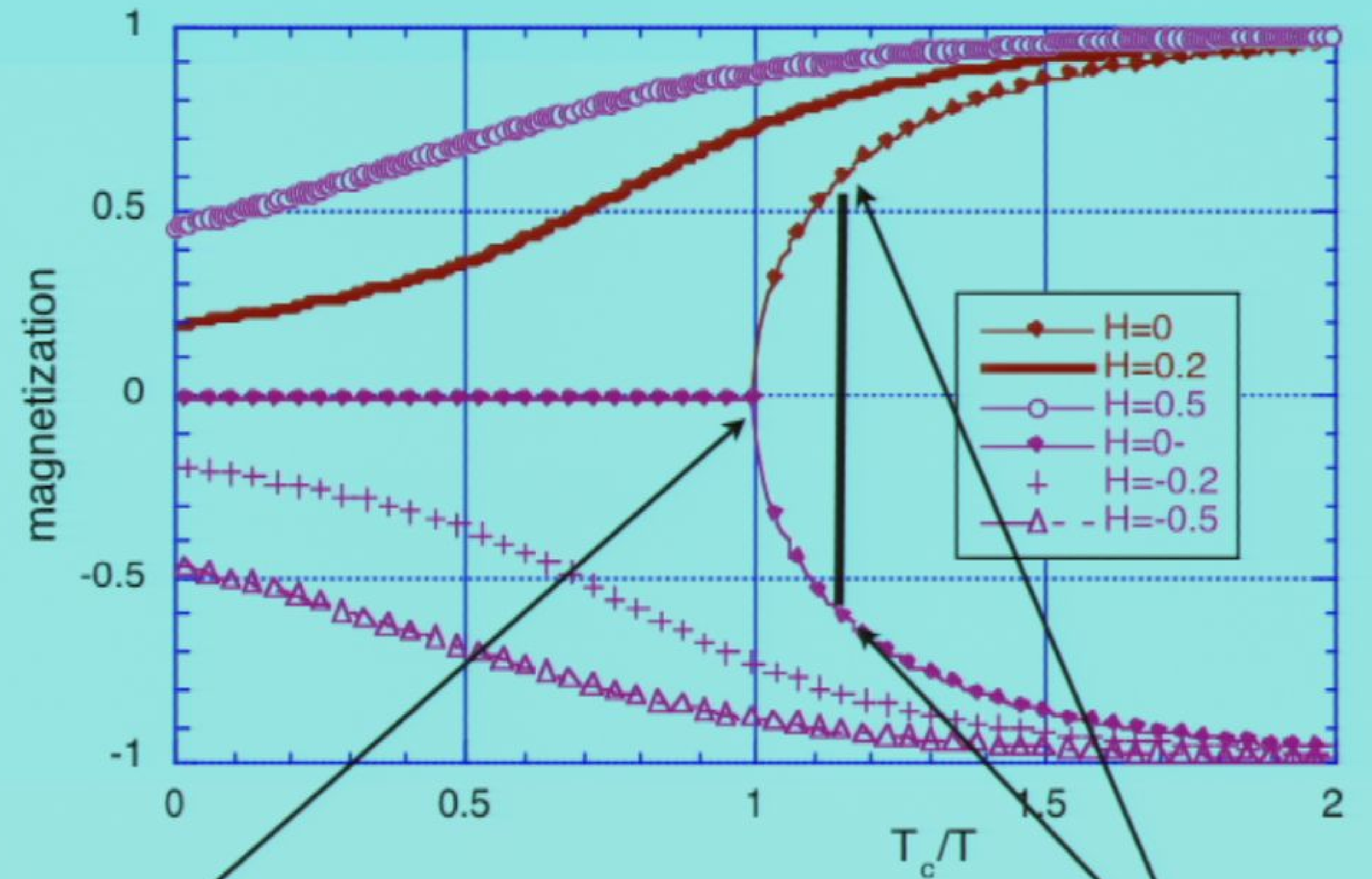

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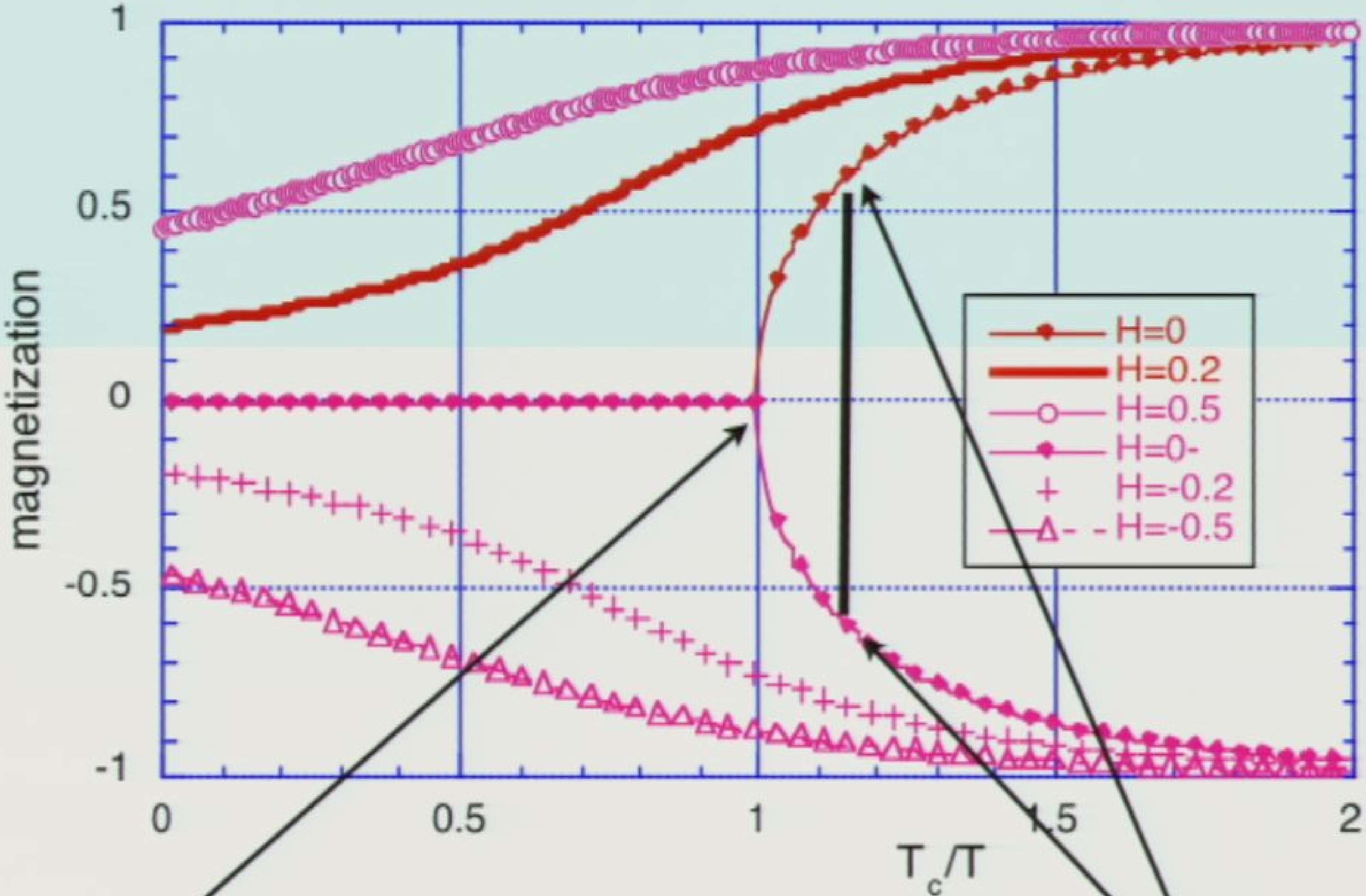

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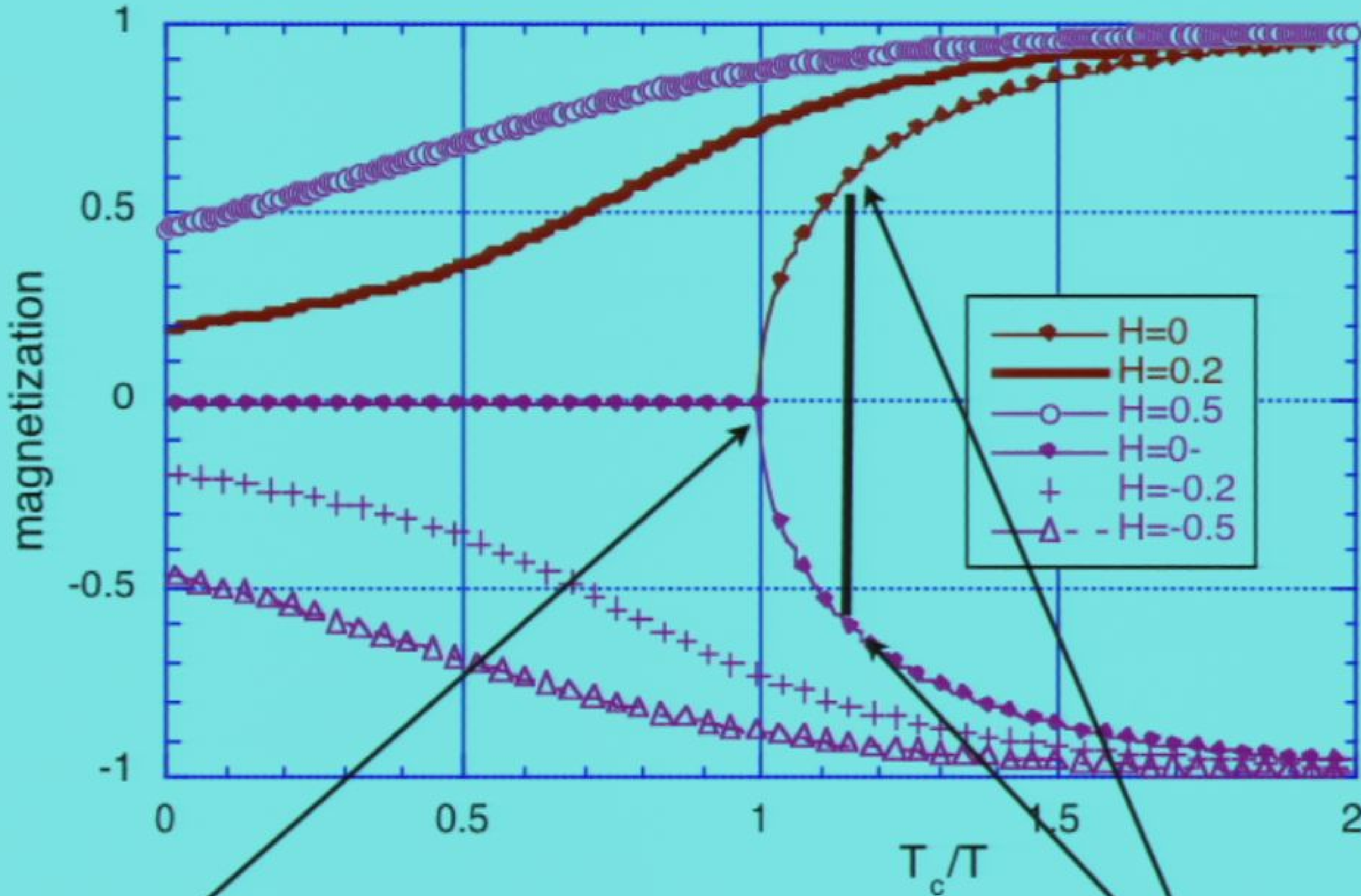

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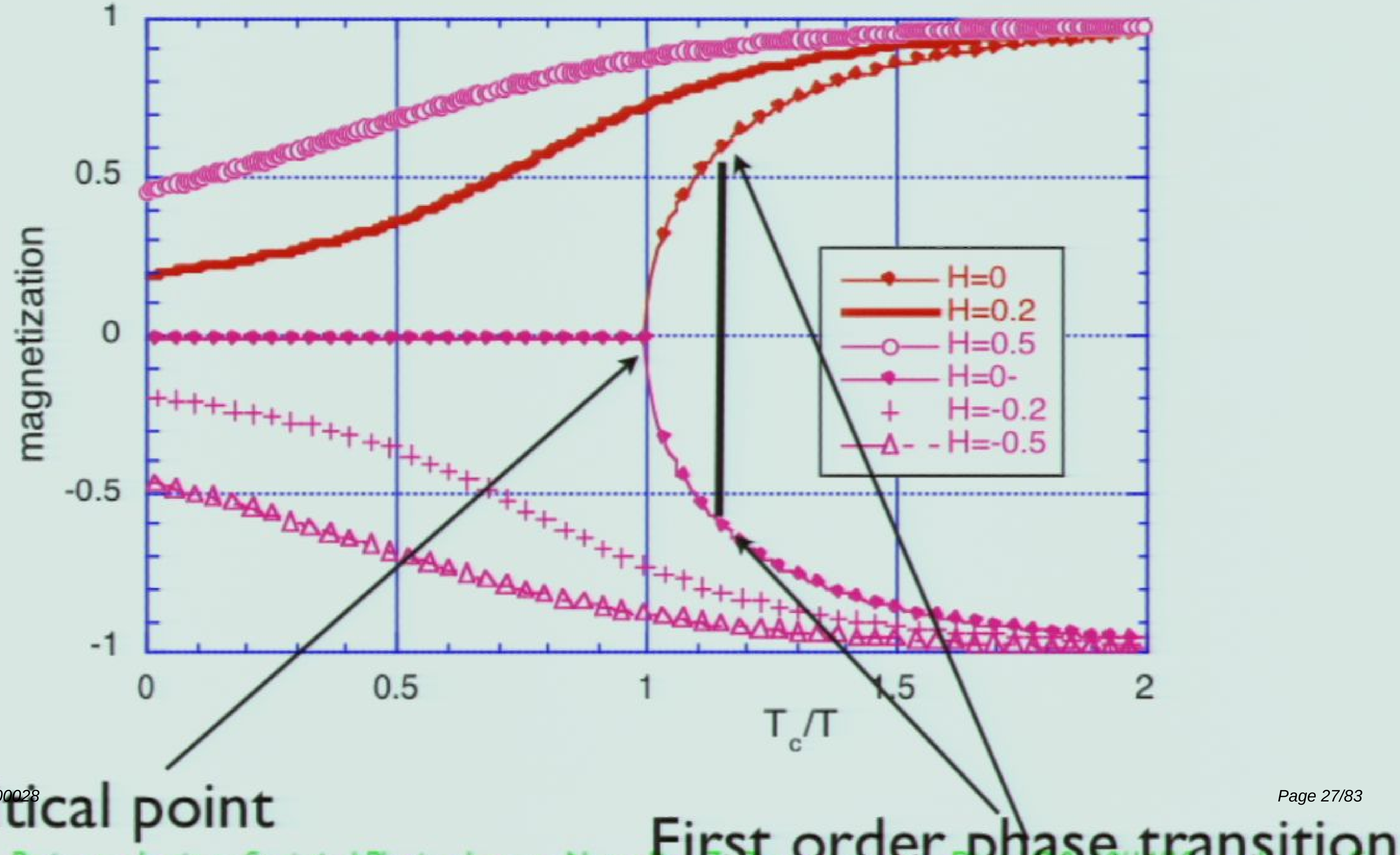

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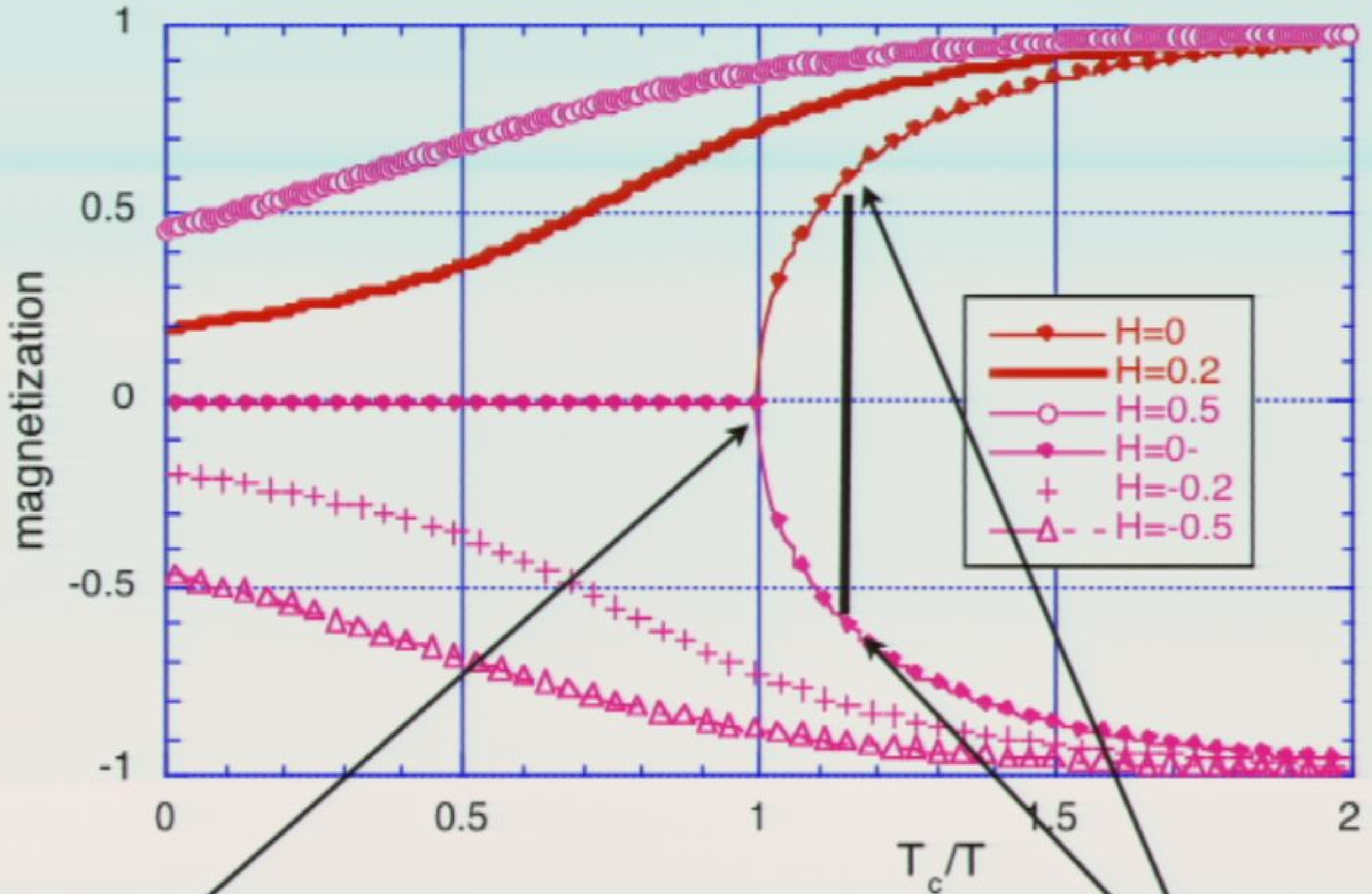

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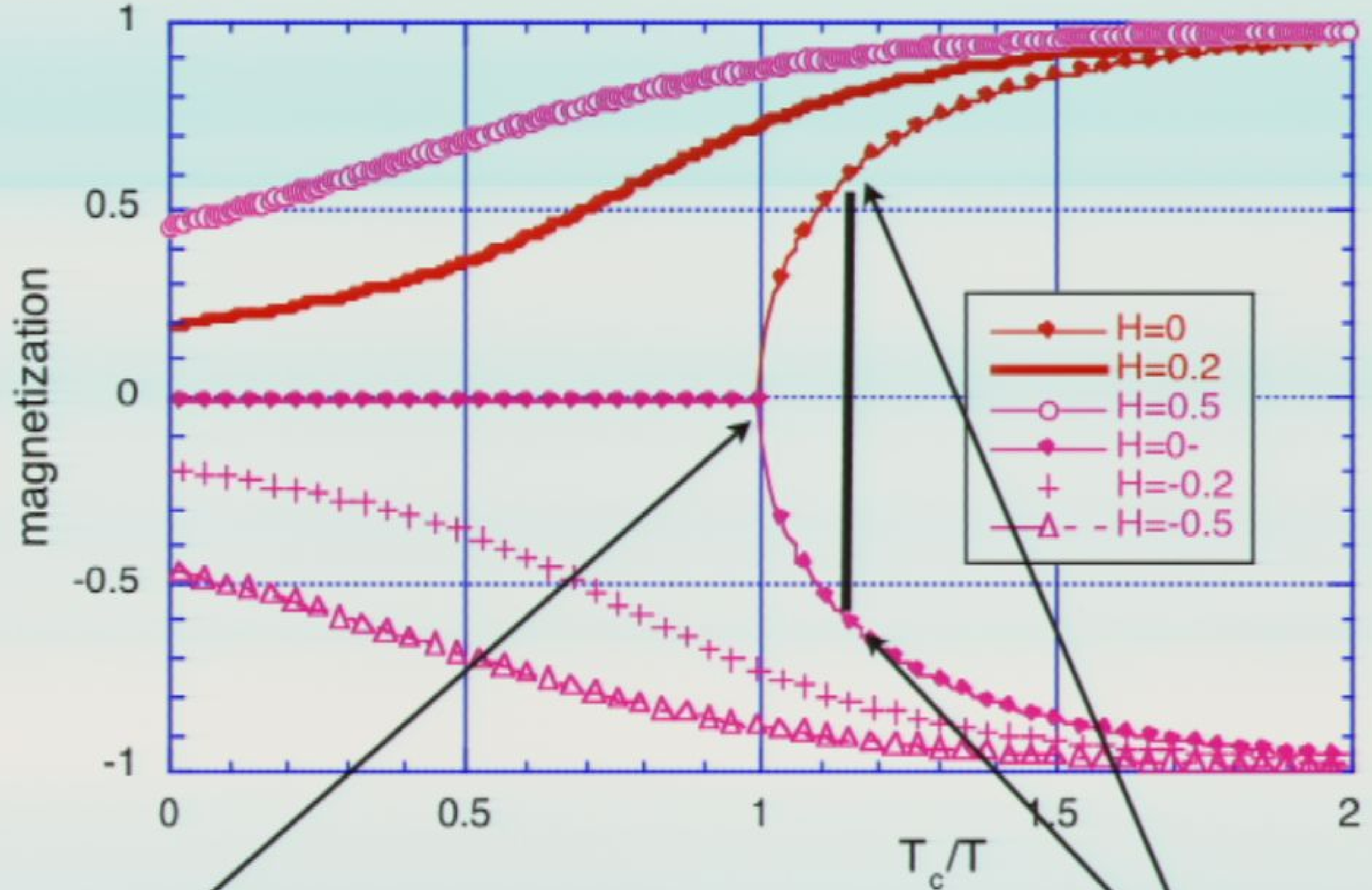

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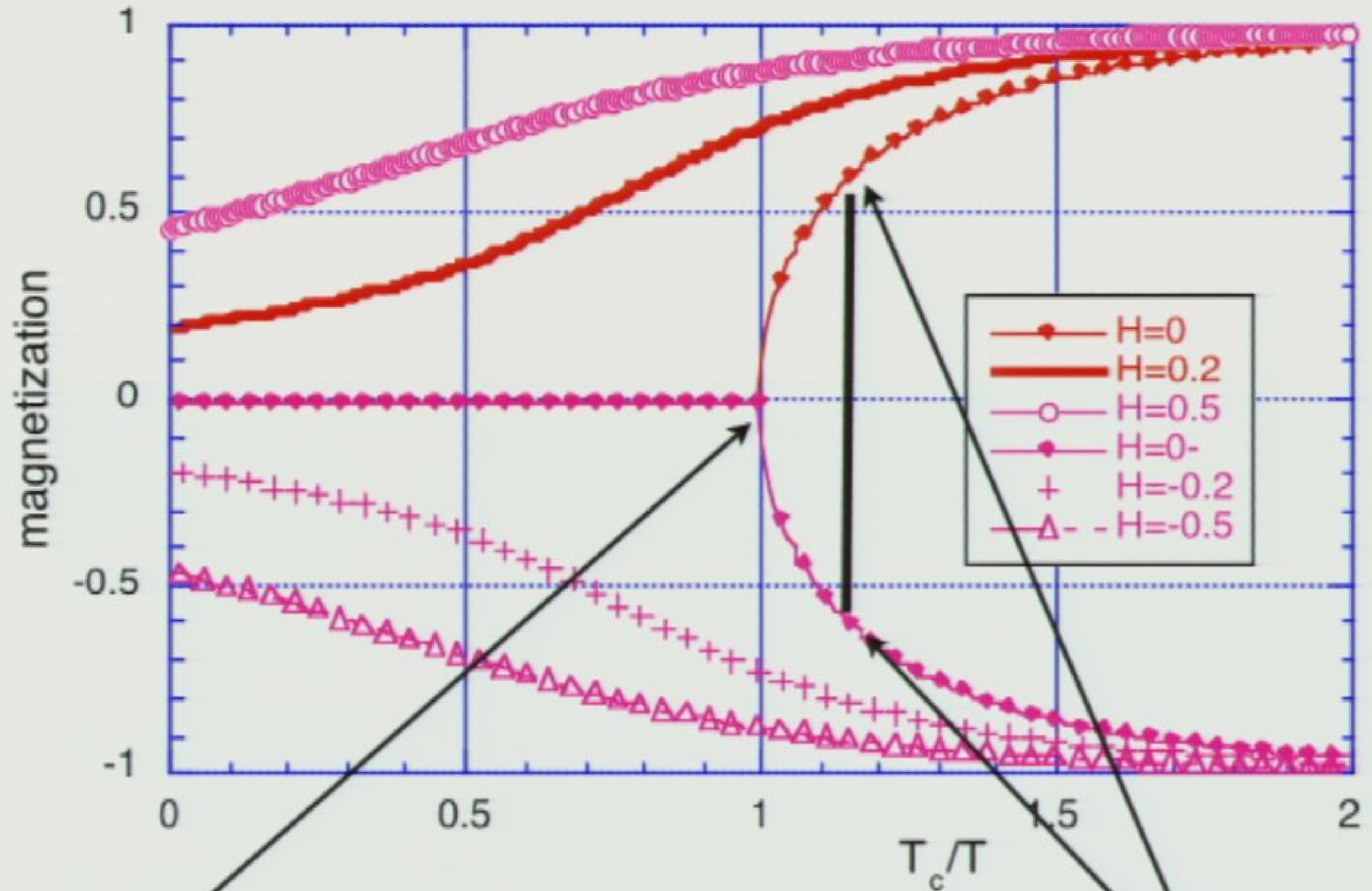

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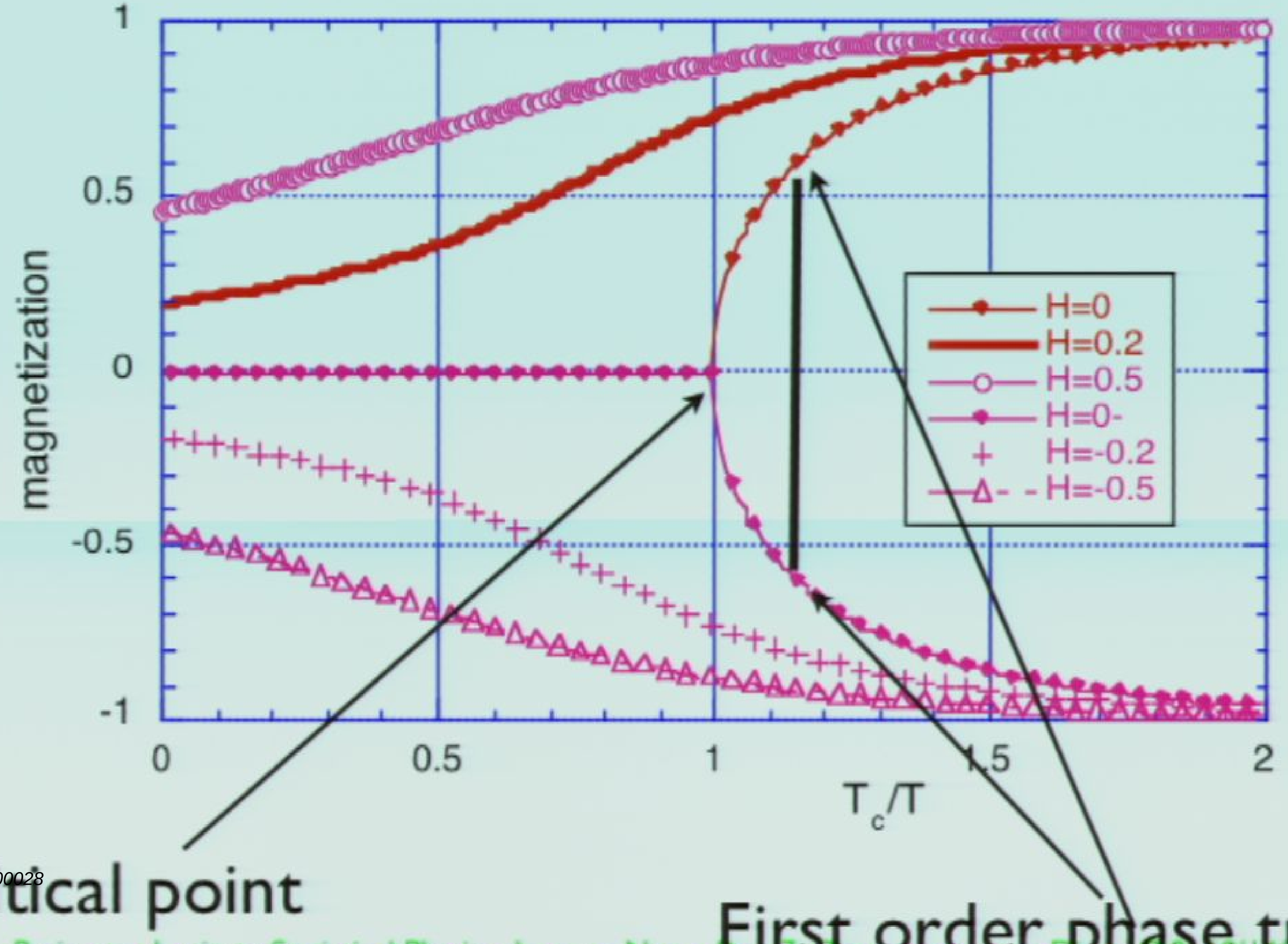

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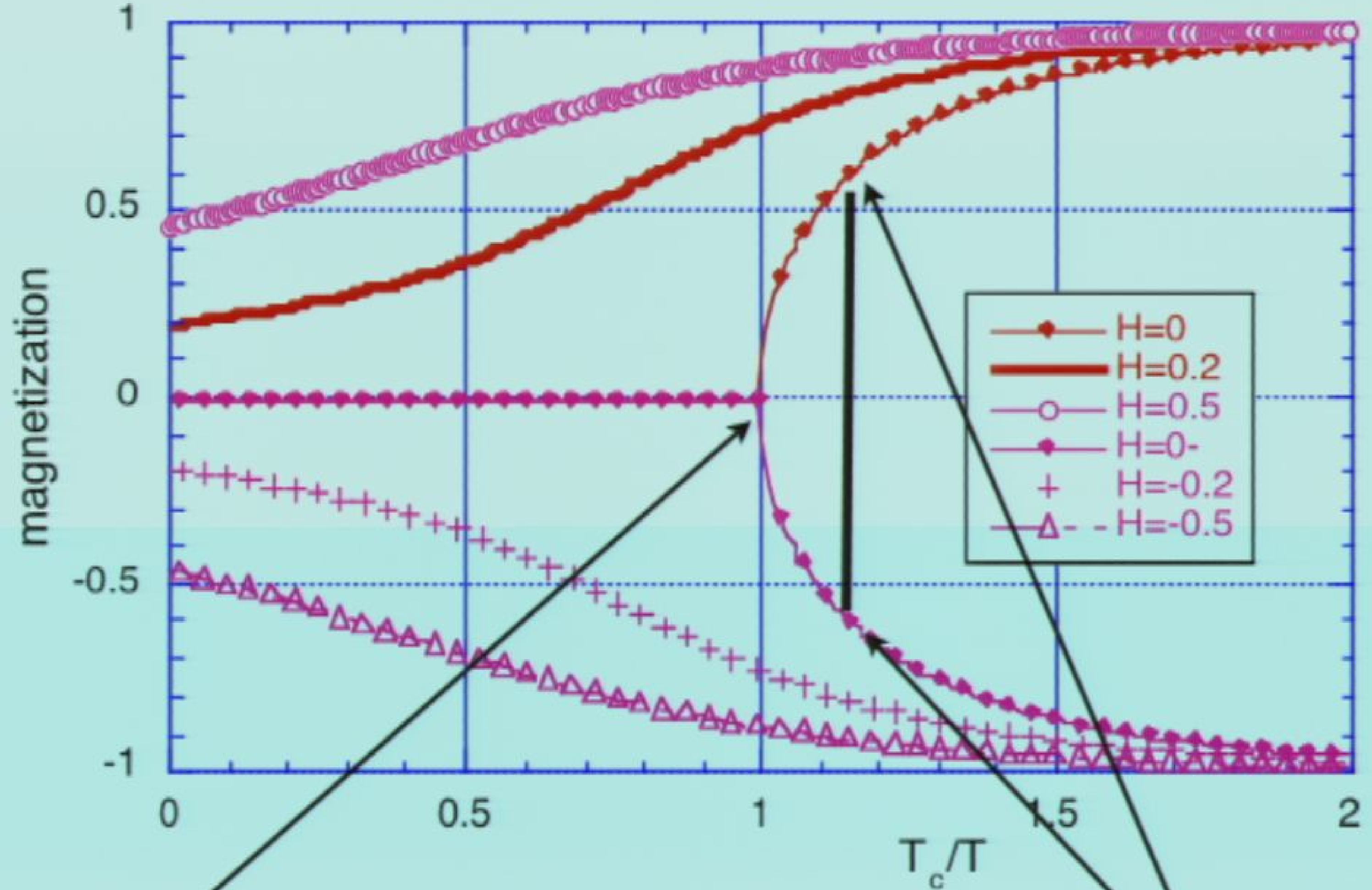

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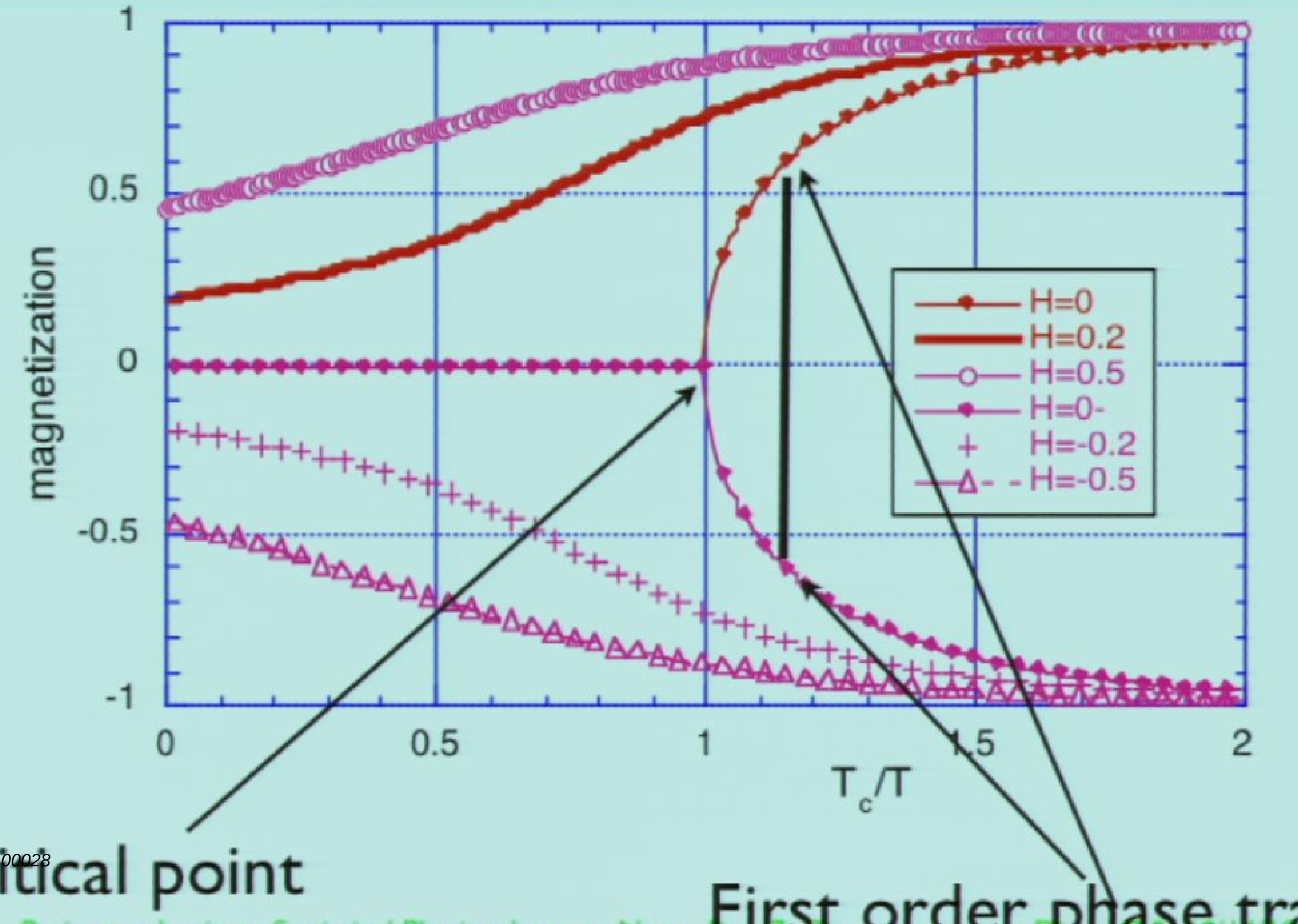

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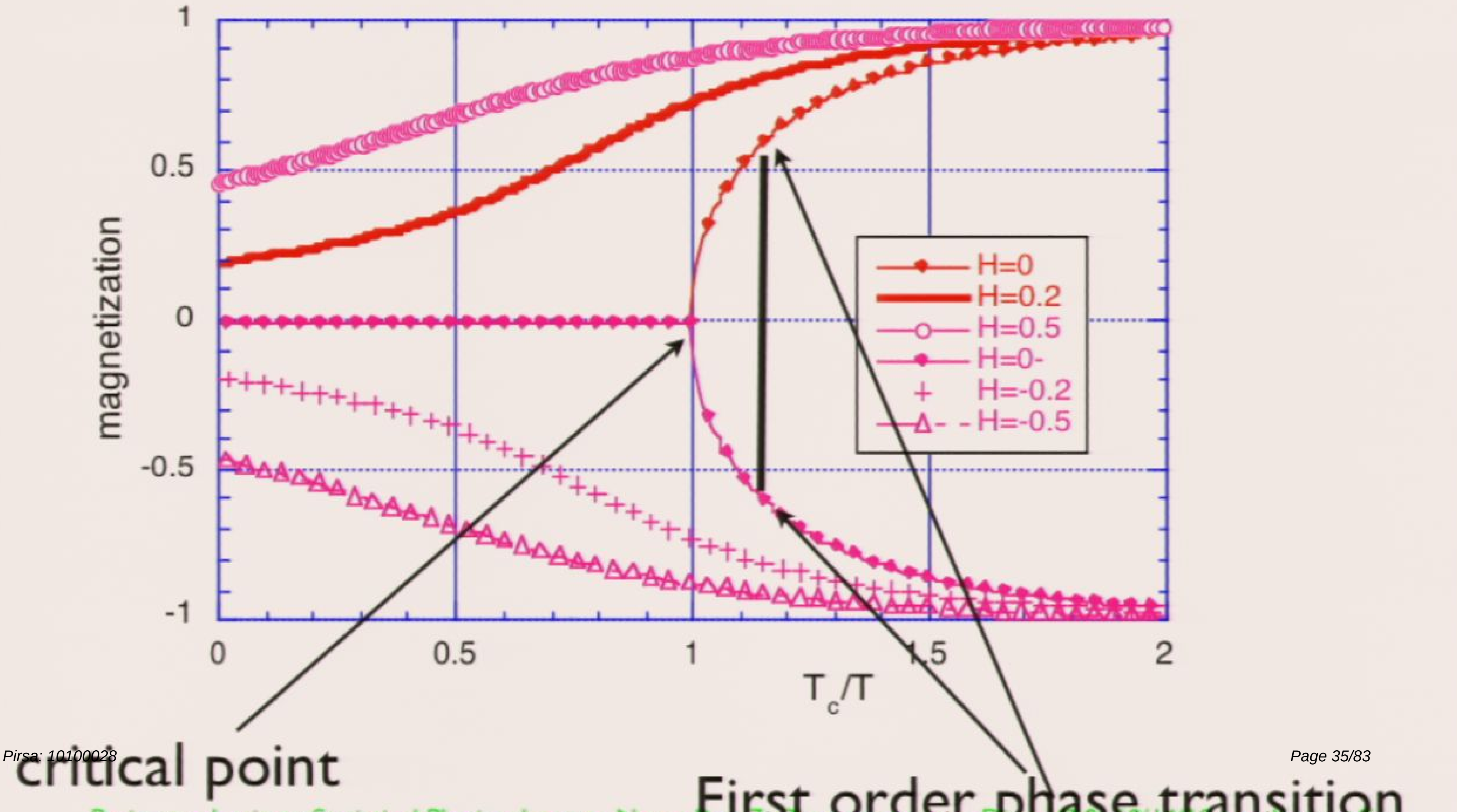

More MFT: Try to understand divergence of $\chi = \partial\langle\sigma\rangle/\partial h$ by finding form for correlation function

$d\langle\sigma_{\mathbf{r}}\rangle/d\, h_{\mathbf{u}}$ is correlation function $g(\mathbf{r-u}) = \langle[\sigma_{\mathbf{r}} - \langle\sigma_{\mathbf{r}}\rangle]\,[\sigma_{\mathbf{u}} - \langle\sigma_{\mathbf{u}}\rangle]$

since for t>0 and small h

$\langle\sigma_r\rangle = h_{eff} = h_{\mathbf{r}} + K \sum_{\mathbf{s}\ nn\ to\ \mathbf{r}} \langle\sigma_{\mathbf{s}}\rangle$ with $K=(1-t)/z$

$0=\delta_{\mathbf{r,u}} - t\, g(\mathbf{r-u}) + \sum_{\mathbf{r}} {}_{\mathbf{s}\ nn\ to\ \mathbf{r}} [g(\mathbf{s-u}) - g(\mathbf{r-u})]/z$

define Fourier transform: $G(q)=\sum \exp[-i\mathbf{q}.(\boldsymbol{r-u})]\, g(\boldsymbol{r-u})$ so that

$0=1 + \Big[-t + 2\sum_{i=1,2\ldots d} [\cos(aq_i) - 1]/z\Big]\, G(\mathbf{q})$

One can then see the long-wavelength form of G by expanding in q to find $G(q) = 1/[t+a^2q^2/z]$.

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and the long-wavelength form $G(q) = 1/[t+a^2q^2/z]$.

One can then invert the Fourier transform and perform the integral to find that , for d=3

$$g(\mathbf{r-s})= \int dq/(2\pi)^d \exp[i\mathbf{q}.(\mathbf{r-u})]\, G(\mathbf{q})$$
$$=\exp[-|\,\mathbf{r-s}\,|/\xi]/[2\pi\,|\,\mathbf{r-s}\,|$$

The correlation length, ξ, is given by $\xi=a/(zt)^{1/2}$

Note that at fixed separation, the correlation function does not diverge as criticality is approached. It is the range of correlations which grows and causes the divergence. This is an important result.

One More Conclusion from MFT

Go after E=<H> when h=0, no variation in space

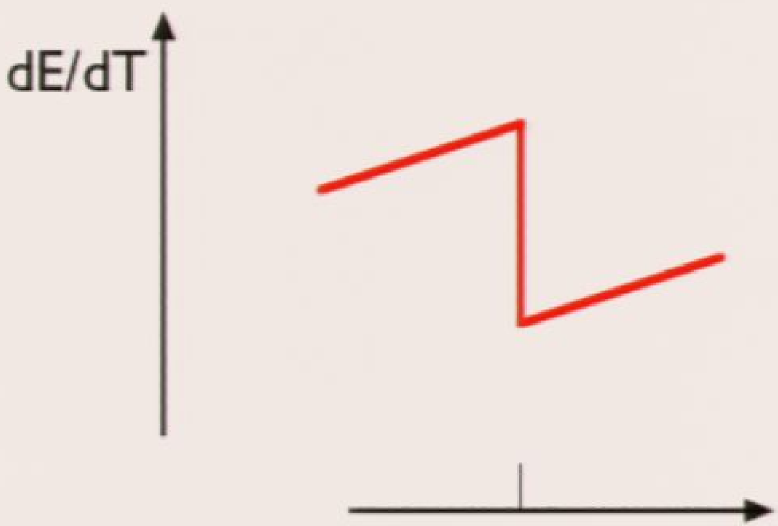
$$-H / kT = K \sum_{nn} \sigma_r \sigma_s + h \sum_r \sigma_r$$

Ve assume neighboring spins are uncorrelated

-$\langle H \rangle/(kT) = Kz \langle\sigma\rangle \langle\sigma\rangle$ + other effects

ear T_c $\langle\sigma\rangle^2 = 0$ above T_c $\langle\sigma\rangle^2 = -3t$ below

Hence specific heat, d <H>/dT has a jump at T_c. It looks like



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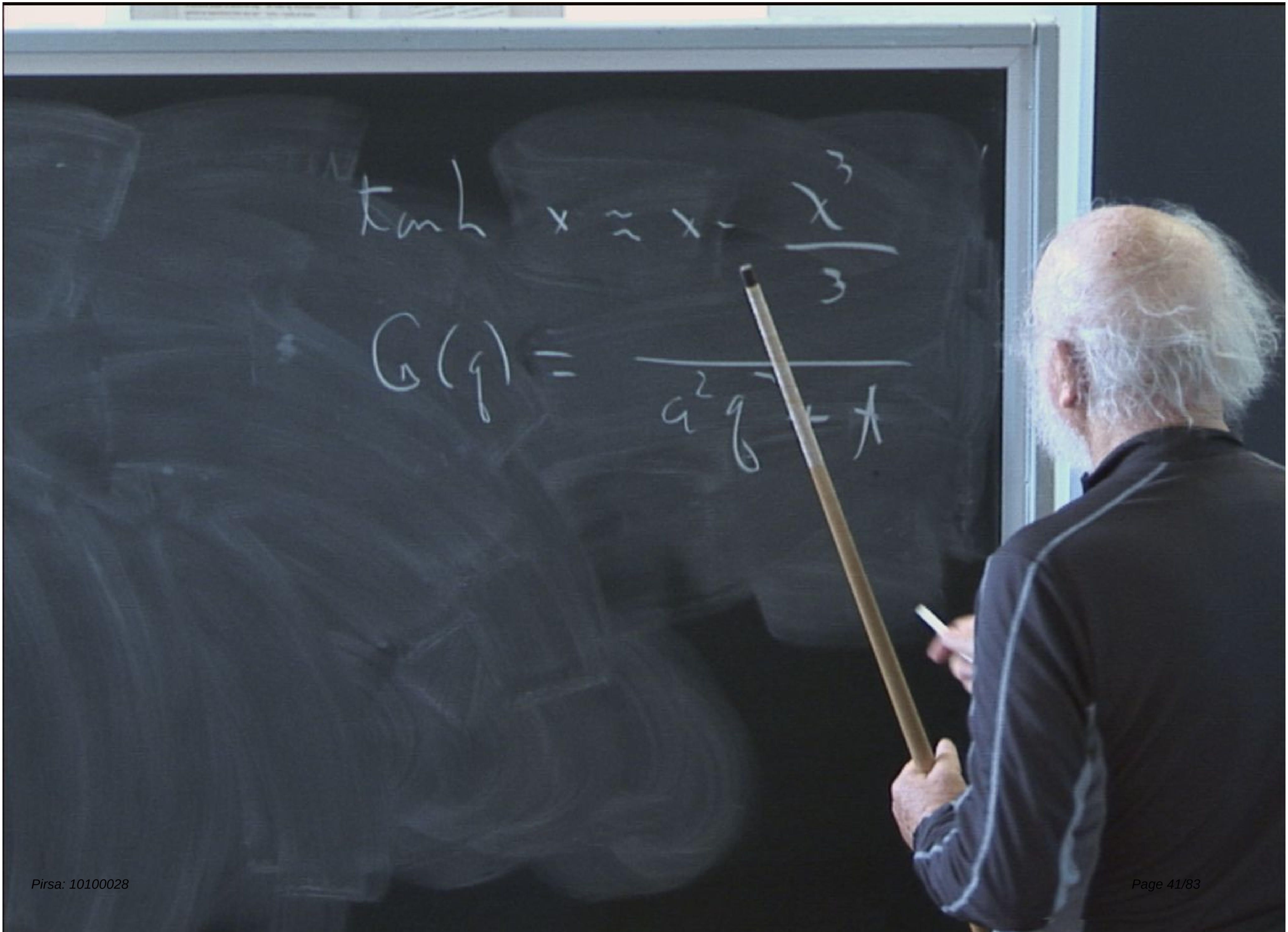
$\tanh x \approx x - \frac{x^3}{3}$
$G(q) = \frac{\quad}{a^2 q^2 + \lambda}$

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$$G(q) = \frac{1}{a^2 q^2 + t}$$

$$\left.\frac{\partial \sigma_r}{\partial h_u}\right|_{h=0} = g(r,u)\Big|_{h=0;\, t>0}$$

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$$\tanh x \approx x - \frac{x^3}{3}$$

$$G(q) = \frac{1}{a^2 q^2 + t}$$

$$\left.\frac{\partial \sigma_r}{\partial h \cdot u}\right|_{h=0} = g(r \cdot a)\Big|_{h=0,\, t>0}$$

$$-r/\xi$$

$$g(r) = \frac{a}{r}$$

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Generalized Mean Field Schemes I

Landau generalized the many different MFT's that existed by assuming an expansion of the free energy in an order parameter, here symbolized by M = magnetization

$$F=\int dr[a-hM+tM^2+cM^4+(\nabla M)^2]$$

note: no cubic term. This free energy applies to symmetry of Ising model

expansion assumes a small order parameter (works near critical point) and small fluctuations (works far away?!)

h is magnetic field

t is proportional to $(T-T_c)$

minimize F in M: result General Solution $M(h, (T-T_c))$

singularity as t,h both go through zero!

singularity as h goes through zero for $T < T_c$

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

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

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

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

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

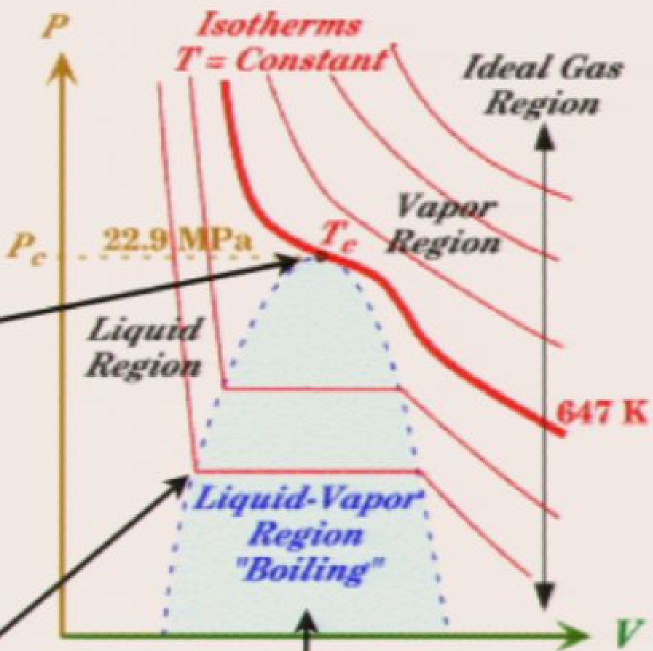
Further he says singular term in free energy given by excitations of size of coherence length with kT per excitation. They fill all space, giving

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

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

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

inite size of real systems cuts off
ıfinities, for example, in the
erivative of density with respect to
ressure, at some very large value.



ıite size of real systems produces
ıall regions of rounding here rather
an sharp corners

statistical mechanics mostly fails
in boiling region.

his same approach is still in extensive use.

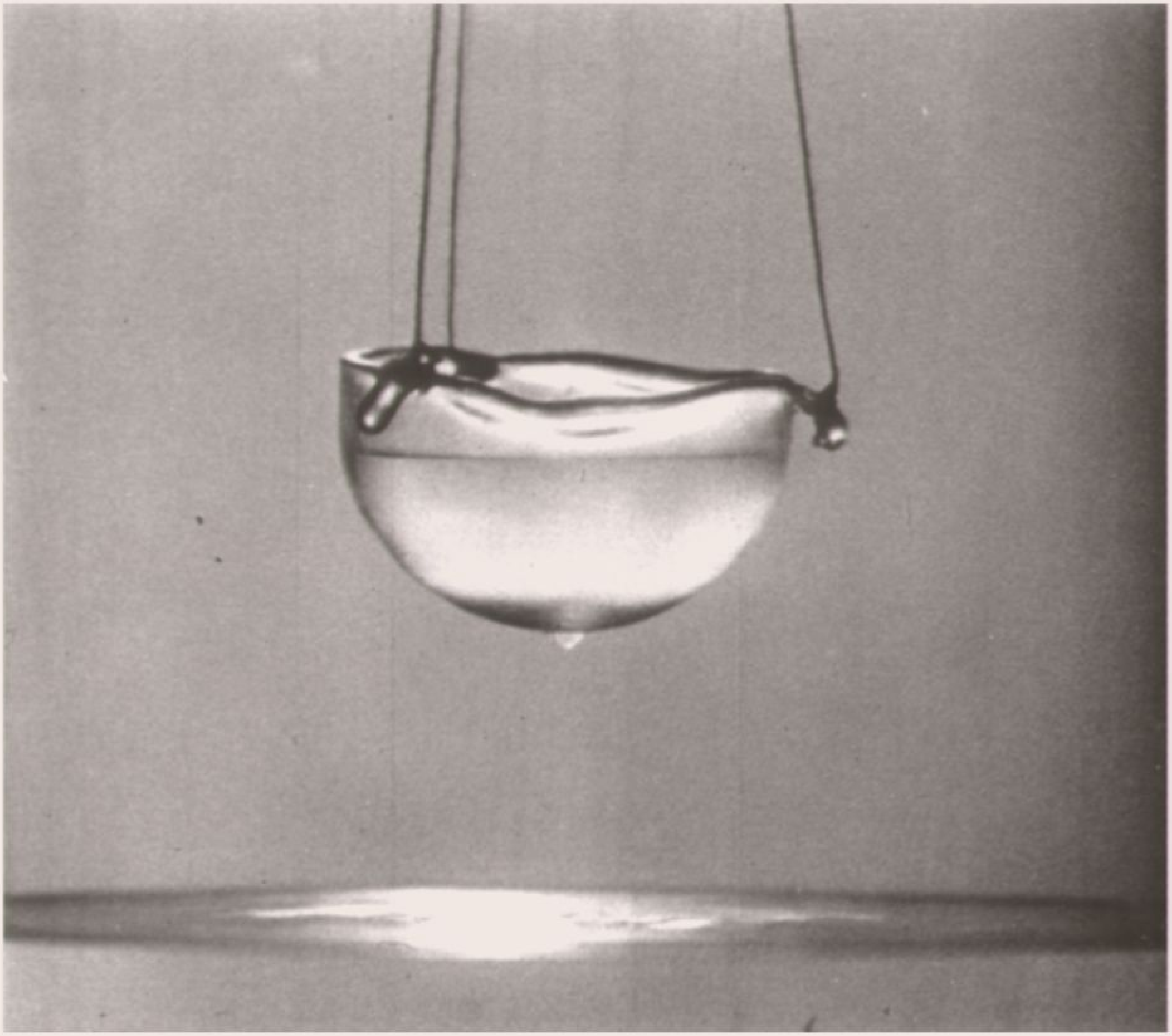
$$= \mathcal{F}_n + \int d\mathbf{r} \left\{ \frac{1}{2m} |\nabla\Psi(\mathbf{r})|^2 + \alpha(T)|\Psi(\mathbf{r})|^2 + U(\mathbf{r})|\Psi(\mathbf{r})|^2 + \frac{b}{2}|\Psi(\mathbf{r})|^4 \right\}$$

Superfluid density near the critical temperature in the presence of random planar defects

D. Dalidovich, A.J. Berlinsky and C. Kallin

Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada L8S 4M1

(Dated: November 14, 2008)



Wikipedia

"Hydrodynamics" and transport in different phase of matter

Different phases of matter are qualitatively different. The only exception mentioned here is the liquid/vapor system in which both phases are qualitatively similar.

Each kind of phase has its own kind of long-wave-length or transport process. For example, a liquid has no rigidity so it cannot transfer a torque over a long distance, but a solid can. At low frequencies momentum transfer in liquids involve one kind of sound wave and two components of diffusion limited by viscosity. The latter is described by the Navier Stokes equations, extensively used in fluid research.

$\partial_t \mathbf{v}(r,t) = \eta \nabla^2 \mathbf{v}(r,t) + \nabla p(r,t) \qquad \nabla \cdot \mathbf{v}(r,t) = 0$

In contrast, solids have three modes of sound propagation: one longitudinal and two transverse.

Liquid

Superfluidity

Superfluidity is a phase of matter in which viscosity of a fluid vanishes, while heat capacity becomes infinite. These unusual effects are observed when liquids, typically of helium-4 or helium-3, overcome friction in surface interaction at a stage (known as the "lambda point", which is temperature and pressure, for helium-4) at which the liquid's viscosity becomes zero. Also known as a major facet in the study of quantum hydrodynamics, it was discovered by Pyotr Kapitsa, John F. Allen, and Don Misener in 1937 and has been described through phenomenological and microscopic theories. In the 1950s Hall and Vinen performed experiments establishing the existence of quantized vortex lines. In the 1960s, Rayfield and Reif established the existence of quantized vortex rings. Packard has observed the intersection of vortex lines with the free surface of the fluid, and Avenel and Varoquaux have studied the Josephson effect in superfluid ^{4}He.

Wikipedia

Evaluate correlation function

we had $G(q)=\sum_{\boldsymbol{r}} \exp[-i\mathbf{q}.(\boldsymbol{r}-\boldsymbol{u})]\, g(\boldsymbol{r}-\boldsymbol{u})$

and the long-wavelength form $G(q) = 1/[t+a^2q^2/z]$.

One can then invert the Fourier transform and perform the integral to find that , for d=3

$$g(\mathbf{r}-\mathbf{s})=\int dq/(2\pi)^d \exp[i\mathbf{q}.(\mathbf{r}-\mathbf{u})]\, G(\mathbf{q})$$
$$=\exp[-|\,\mathbf{r}-\mathbf{s}\,|/\xi]/[2\pi\,|\,\mathbf{r}-\mathbf{s}\,|$$

The correlation length, ξ, is given by $\xi=a/(zt)^{1/2}$

Note that at fixed separation, the correlation function does not diverge as criticality is approached. It is the range of correlations which grows and causes the divergence. This is an important result.

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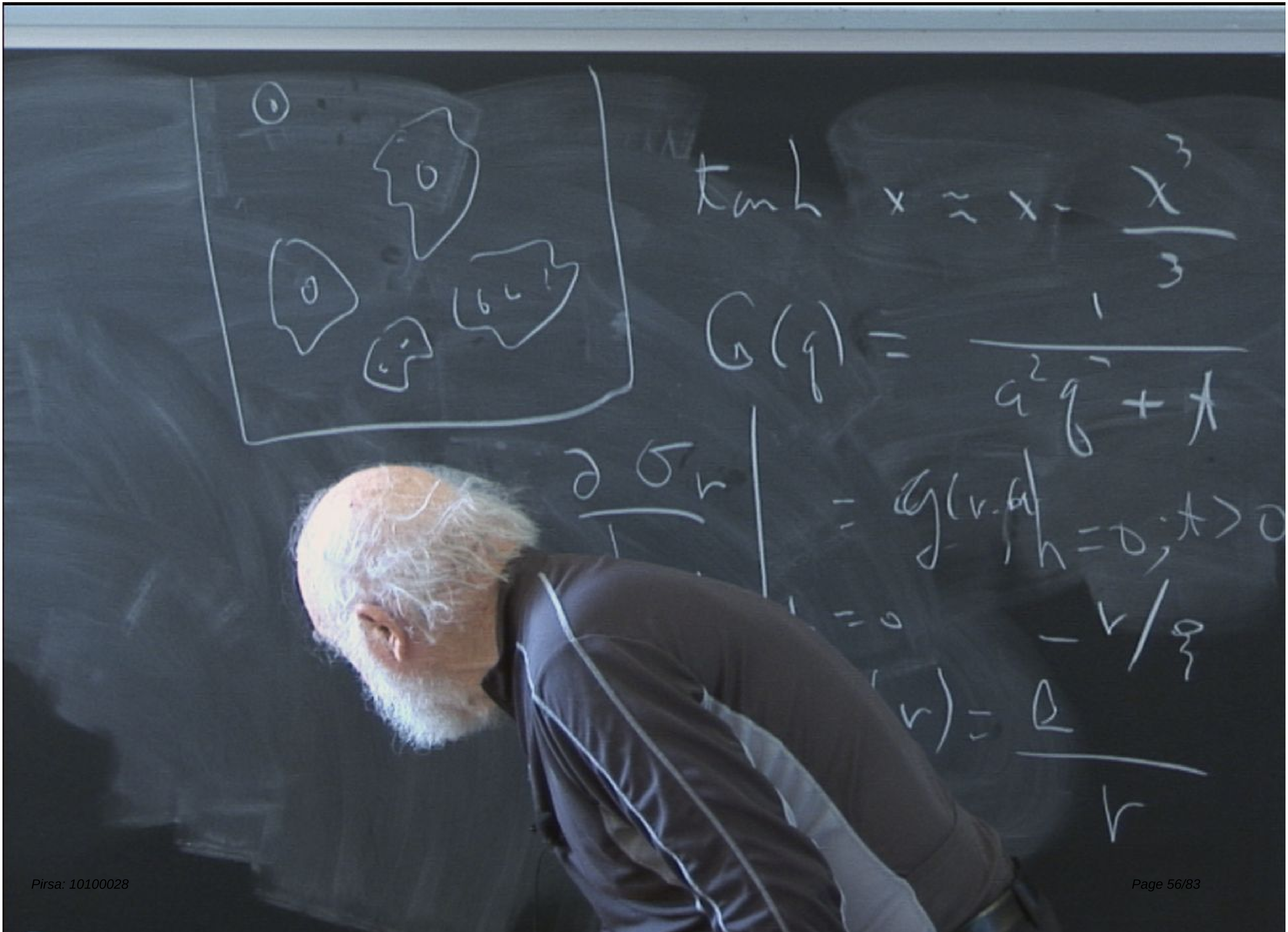
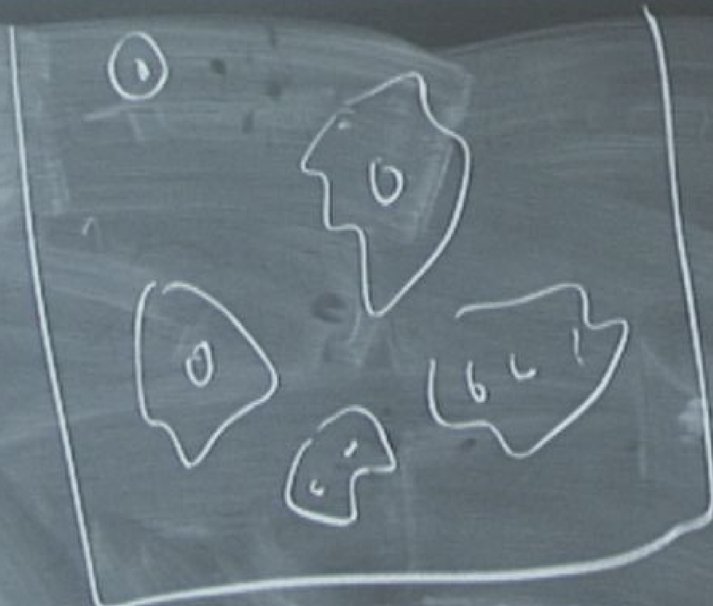

tanh x ≈ x − x^3/3
G(q) = 1/(a^2 q^2 + A)
h = 0
−r/ξ
Q/r



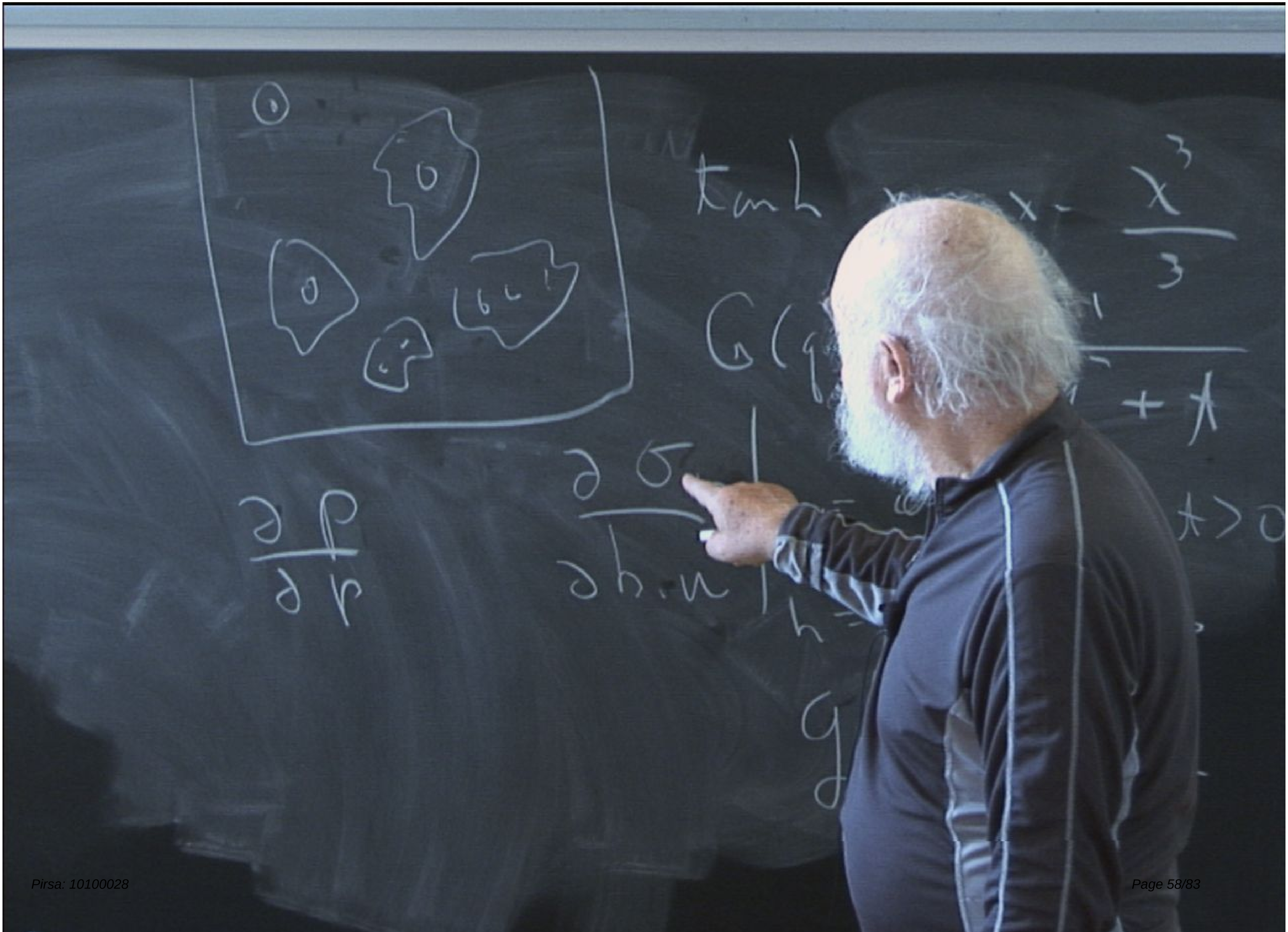
$$\tanh x \approx x - \frac{x^3}{3}$$

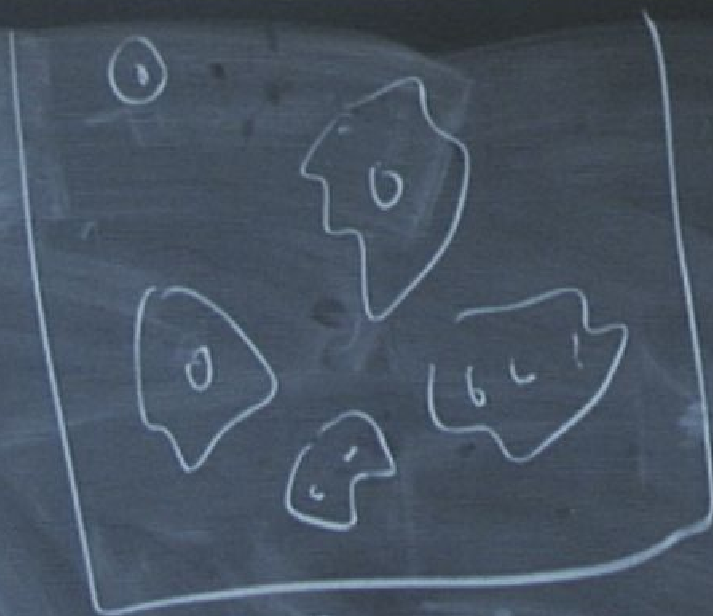
$$G(q) = \frac{1}{a^2 q^2 + t}$$

$$\left.\frac{\partial \sigma_r}{\partial h_0}\right|_{h=0} = g(r,0) \quad ;\ h=0,\ t>0$$

$$-r/\xi$$

$$g(r) = \frac{Q}{r}$$


tanh



$$\tanh x \approx x - \frac{x^3}{3}$$

$$G(q) = \frac{1}{a^2 q^2 + \lambda}$$

$$\boxed{\frac{\partial \rho}{\partial p}} \to \infty \qquad \frac{\partial \sigma_r}{\partial h.u}\Bigg|_{h=0} = g(r,a)\Big|_{h=0,\ \lambda>0} \quad e^{-r/\xi}$$

$$g(r) = \frac{Q}{r}$$

Evaluate correlation function

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$$\tanh x \approx x - \frac{x^3}{3}$$

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One More Conclusion from MFT

Go after E=<H> when h=0, no variation in space

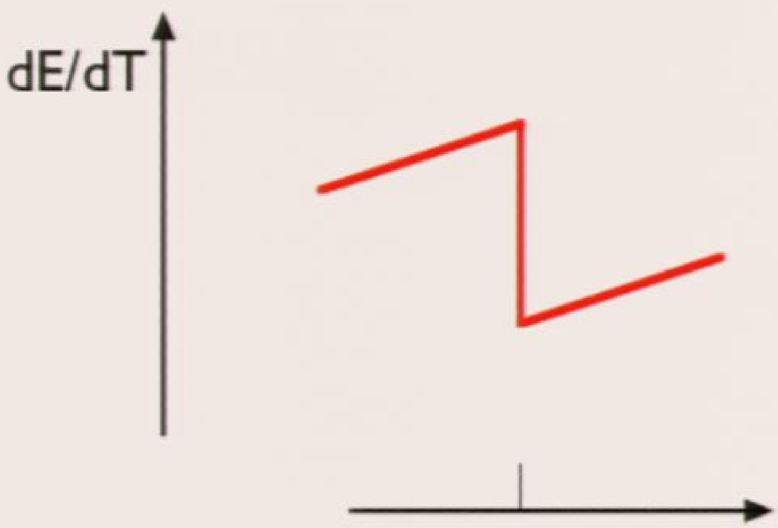
$$-H / kT = K\sum_{nn} \sigma_r \sigma_s + h\sum_{r} \sigma_r$$

Ve assume neighboring spins are uncorrelated

$-\langle H\rangle/(kT) = Kz\langle\sigma\rangle\ \langle\sigma\rangle$ + other effects

ear T_c $\langle\sigma\rangle^2 = 0$ above T_c $\langle\sigma\rangle^2 = -3t$ below

Hence specific heat, d <H>/dT has a jump at T_c. It looks like



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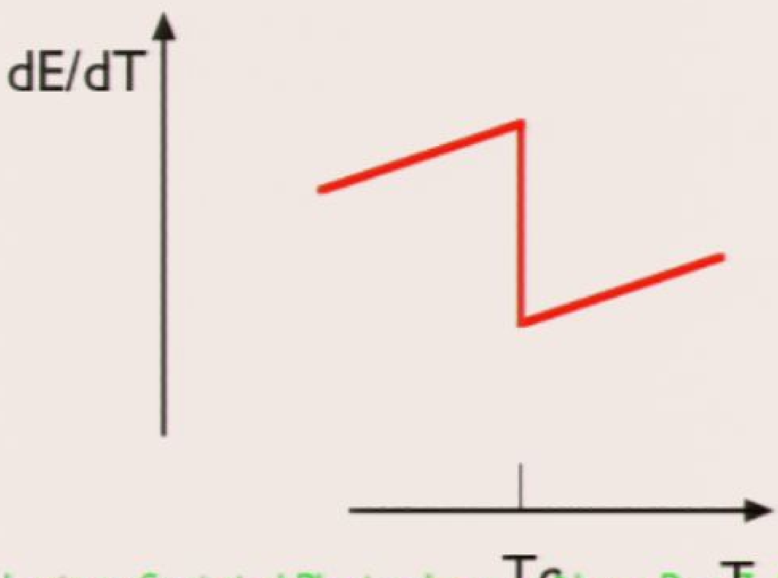

More applications

I have just described in an abbreviated form mean field theory, particularly as it is applied near critical points. Putting aside the specialization for behavior near critical points, a tremendous amount of this kind of work has been done. For each one of a huge variety of phase transitions, scientists have discovered their order parameters, and constructed theories describing the discontinuities in these parameters that we characterize as "phase transitions".

This work has been very important and enlightening. It has led us to a working understanding of some of the different phases of matter and the uses to which they might be put. It is not precisely accurate but it gives a good working understanding of the many different kinds of phase transitions.

The high point of this work was the 1957 Bardeen, Cooper, Schrieffer theory of superconductivity, which provided a very accurate description if the superconductors then under study.

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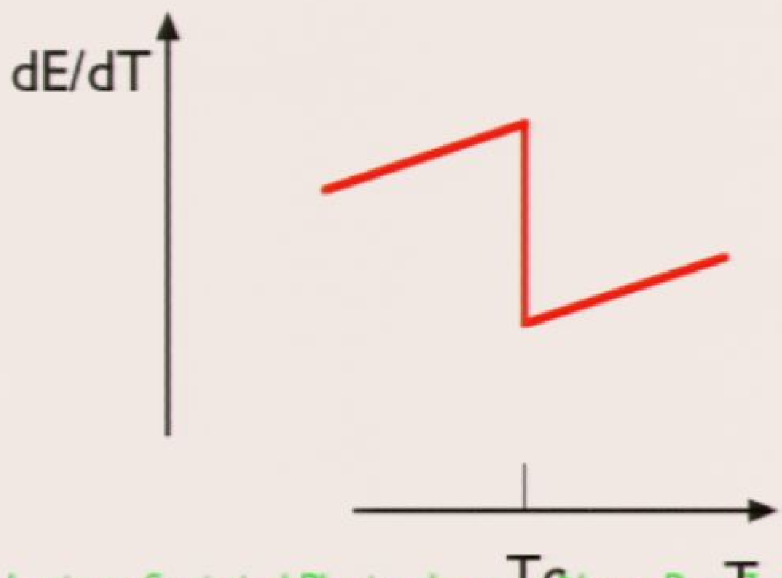

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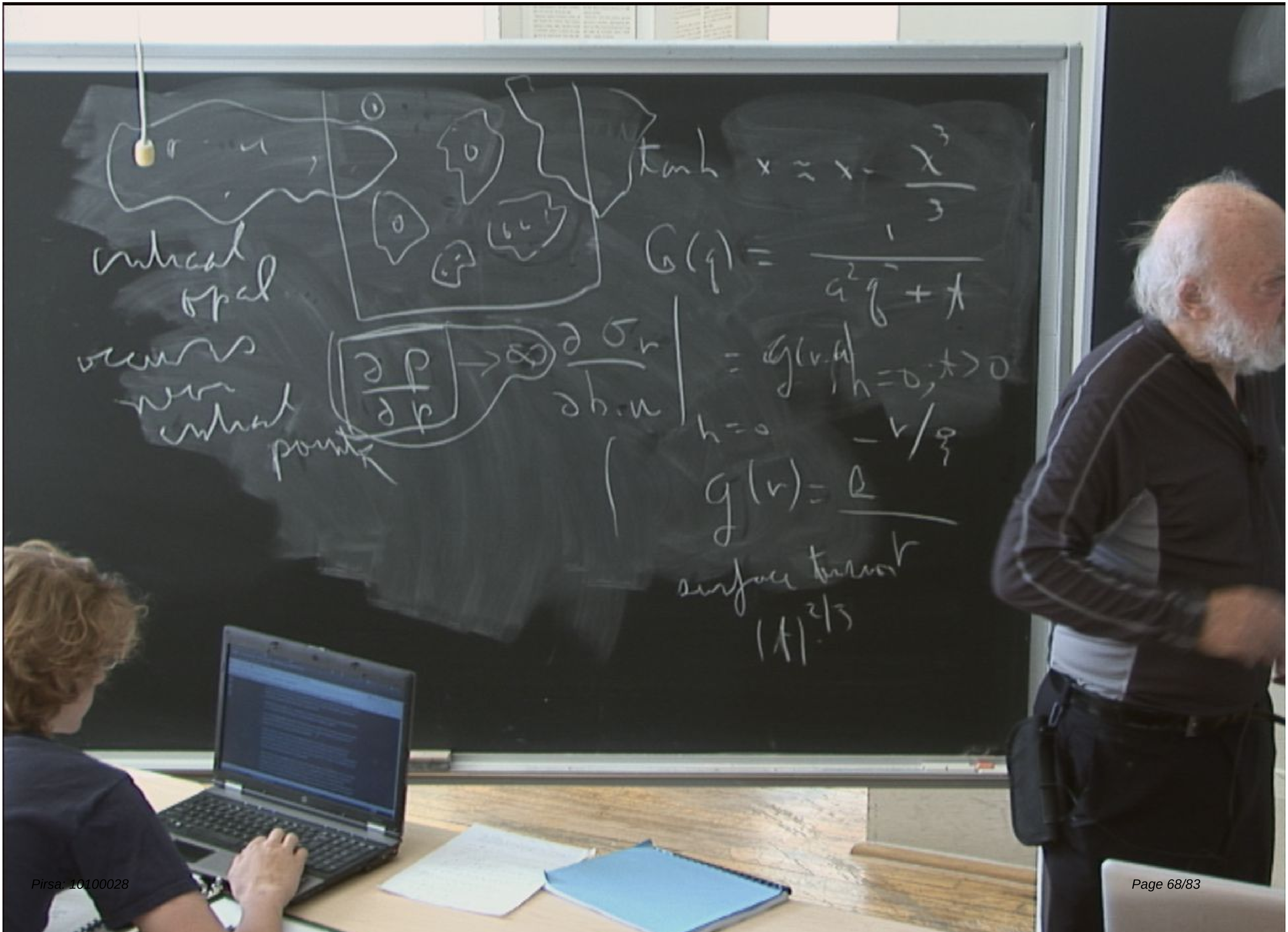
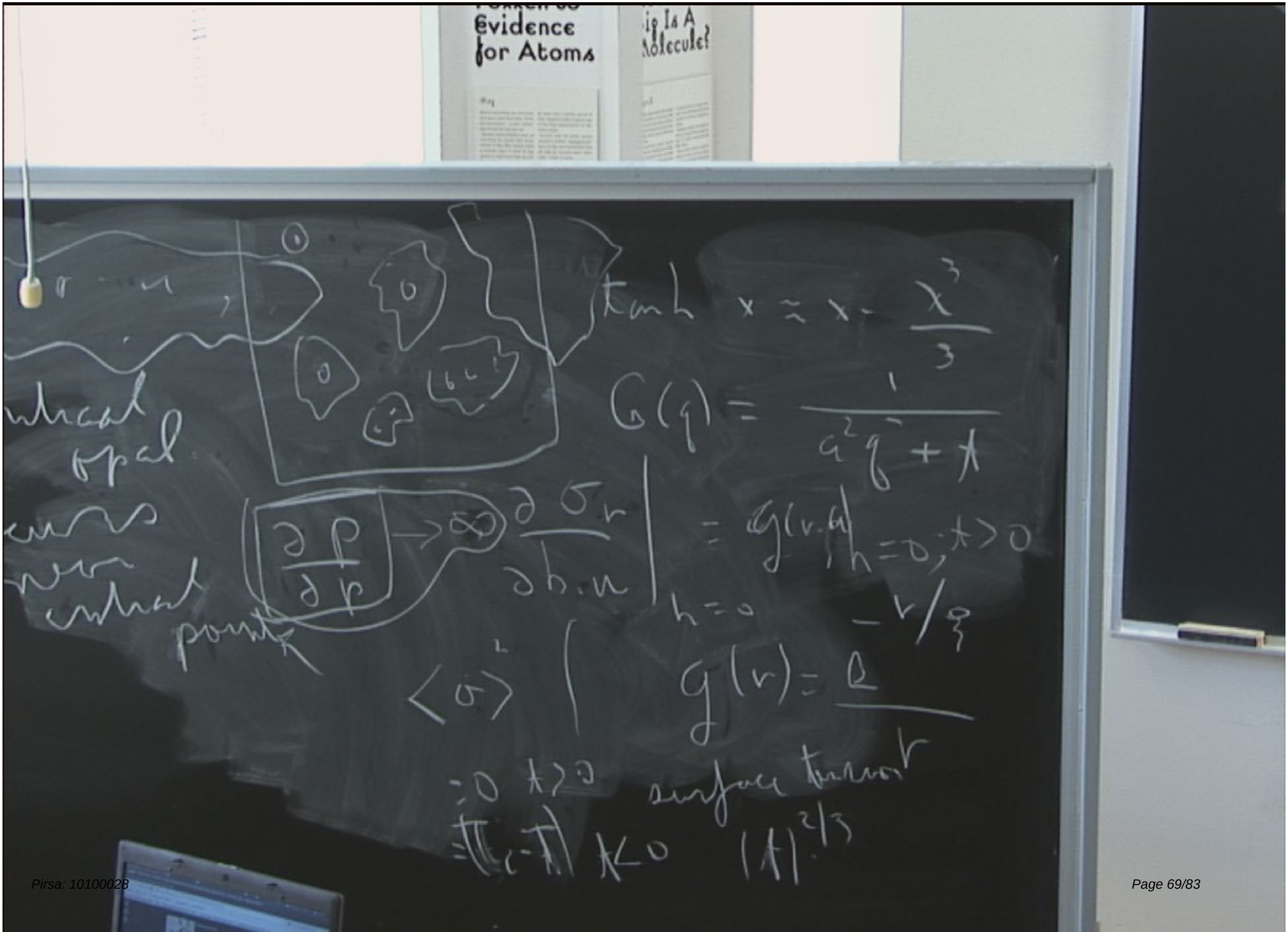
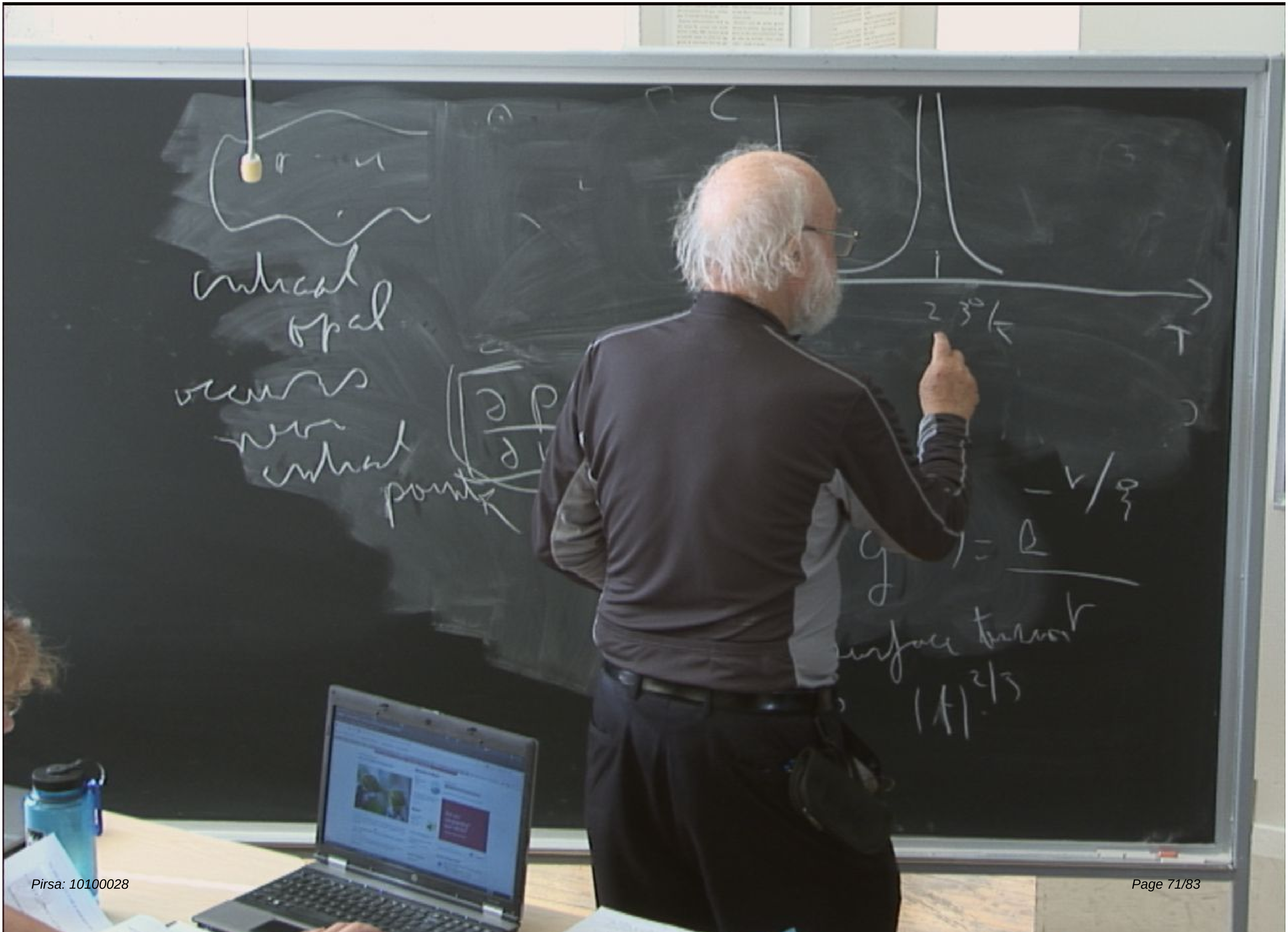

critical opal
occurs near critical point
tanh x ≈ x - x^3/3
G(q) = 1/(a^2 q^2 + t)
h=0, t>0
h=0
surface tension
|t|^2/3


Evidence
for Atoms

Superfluidity

Superfluidity is a phase of matter in which viscosity of a fluid vanishes, while heat capacity becomes infinite. These unusual effects are observed when liquids, typically of helium-4 or helium-3, overcome friction in surface interaction at a stage (known as the "lambda point", which is temperature and pressure, for helium-4) at which the liquid's viscosity becomes zero. Also known as a major facet in the study of quantum hydrodynamics, it was discovered by Pyotr Kapitsa, John F. Allen, and Don Misener in 1937 and has been described through phenomenological and microscopic theories. In the 1950s Hall and Vinen performed experiments establishing the existence of quantized vortex lines. In the 1960s, Rayfield and Reif established the existence of quantized vortex rings. Packard has observed the intersection of vortex lines with the free surface of the fluid, and Avenel and Varoquaux have studied the Josephson effect in superfluid ^{4}He.

Wikipedia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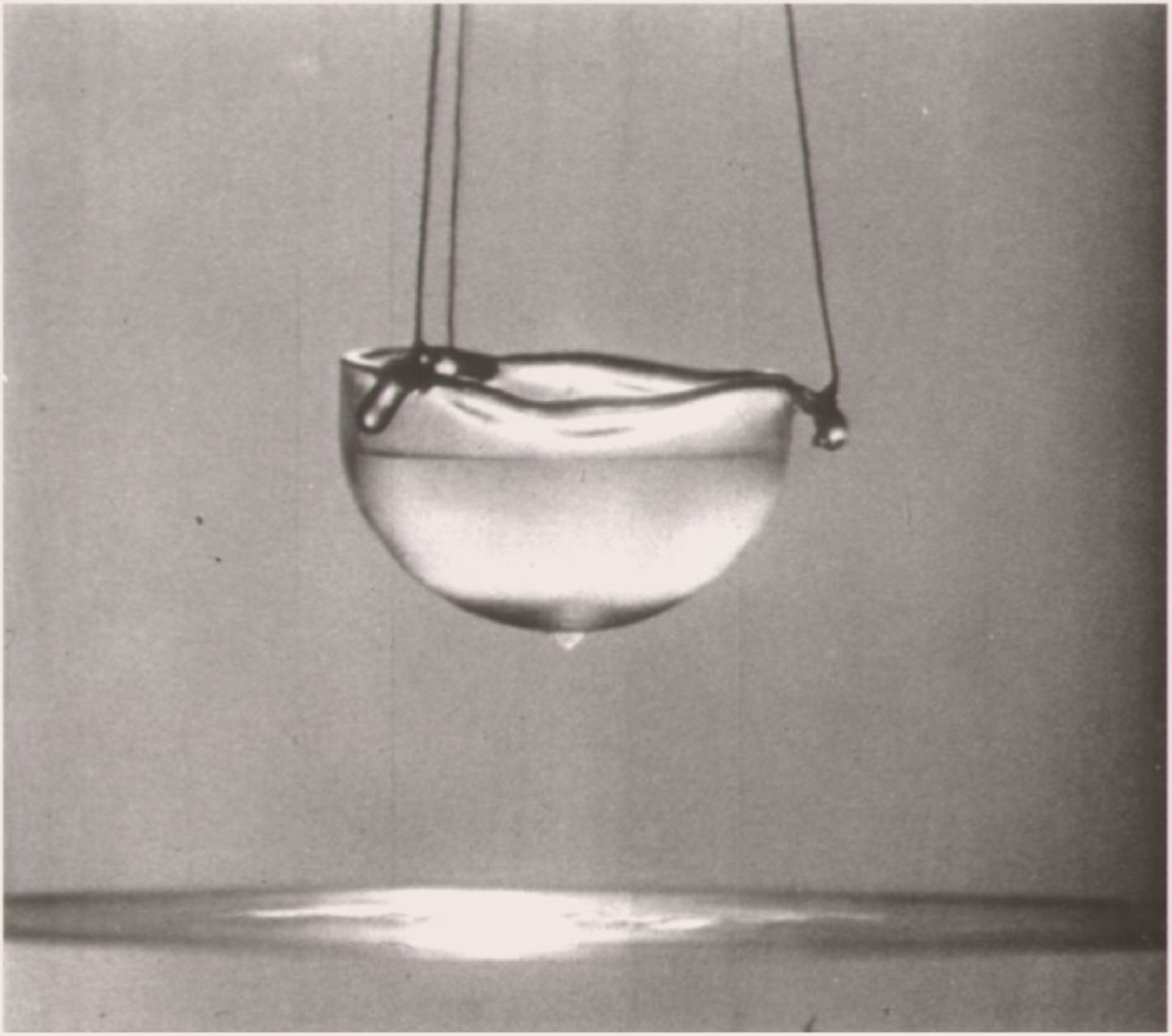

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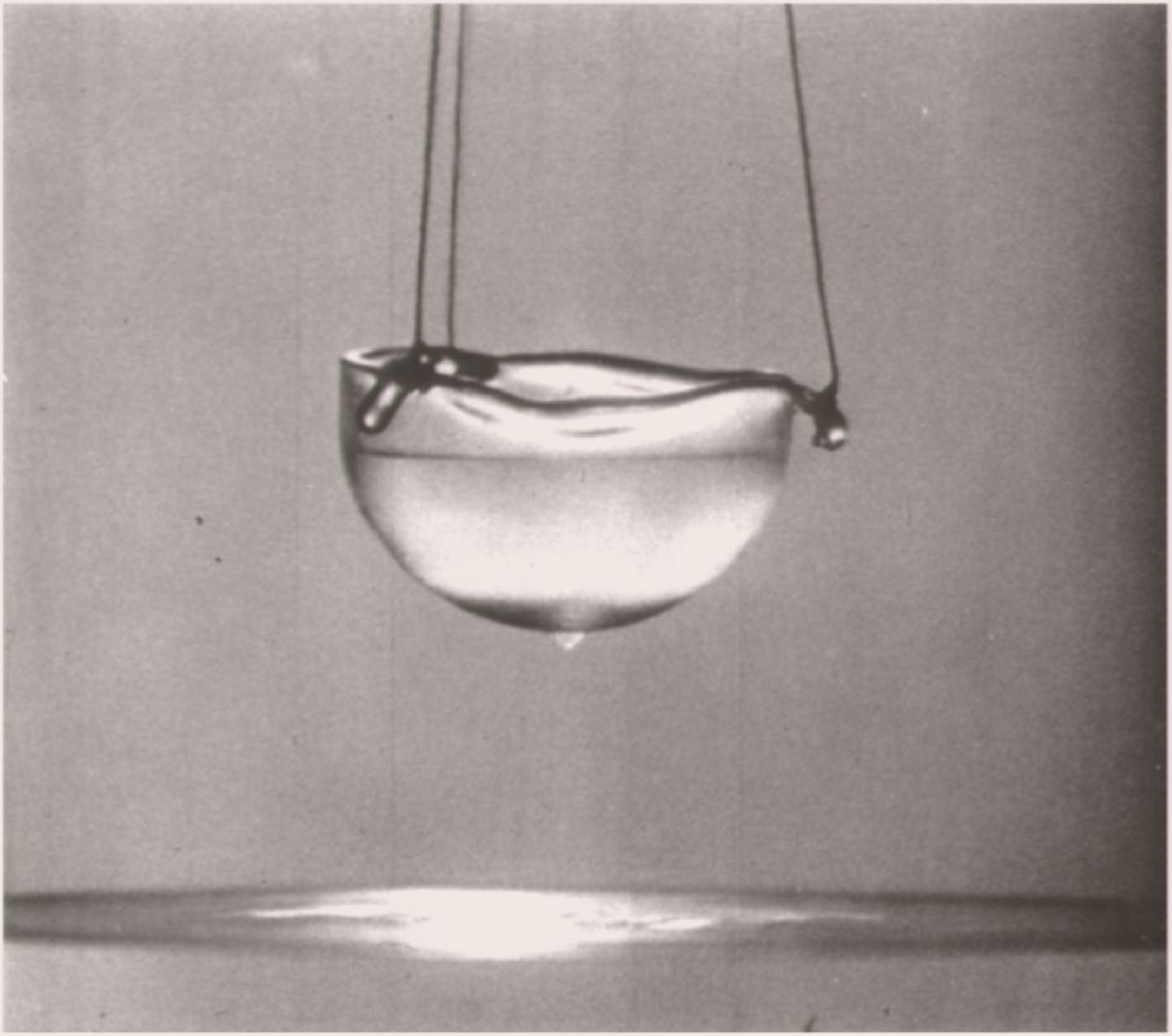

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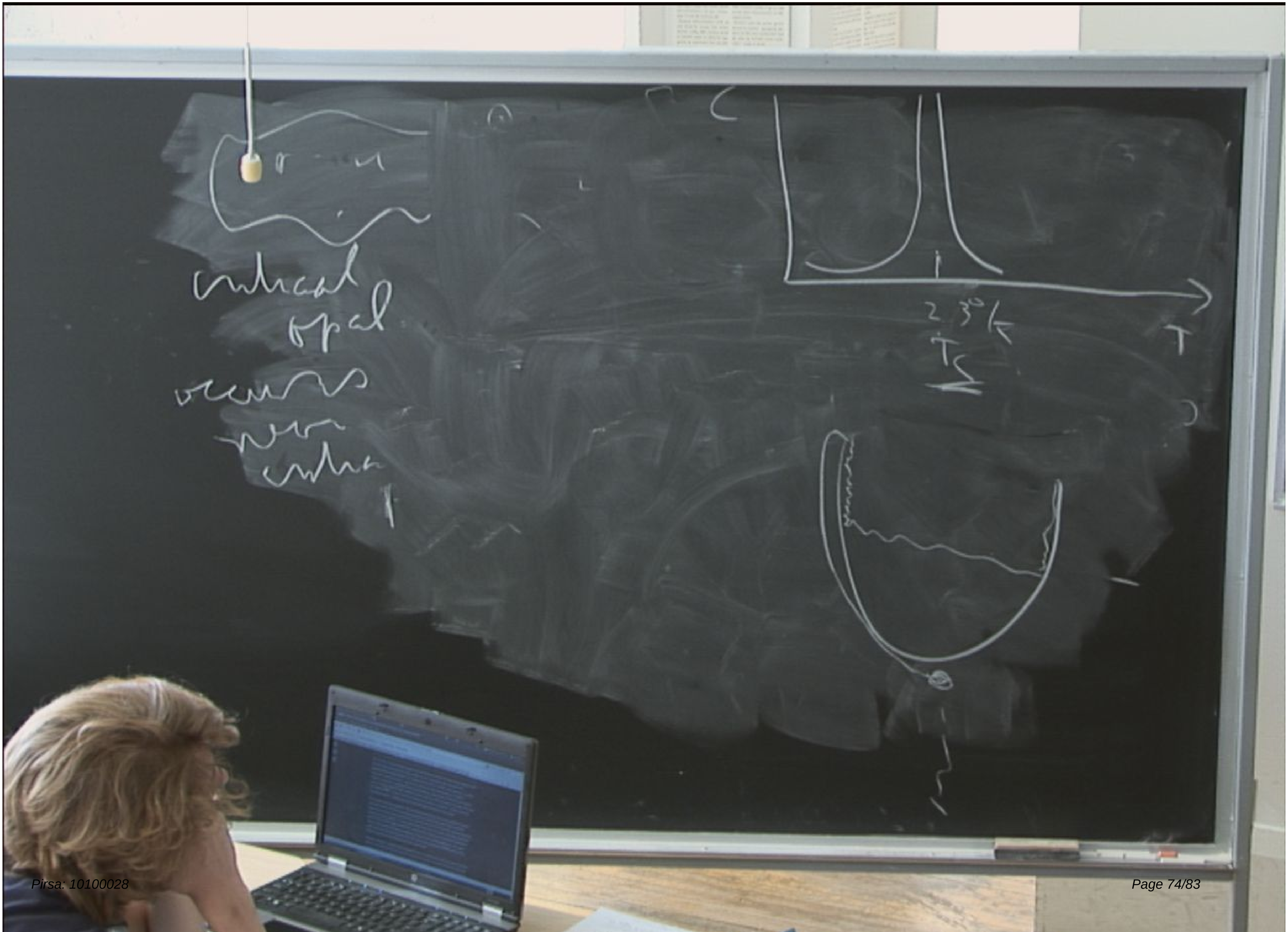
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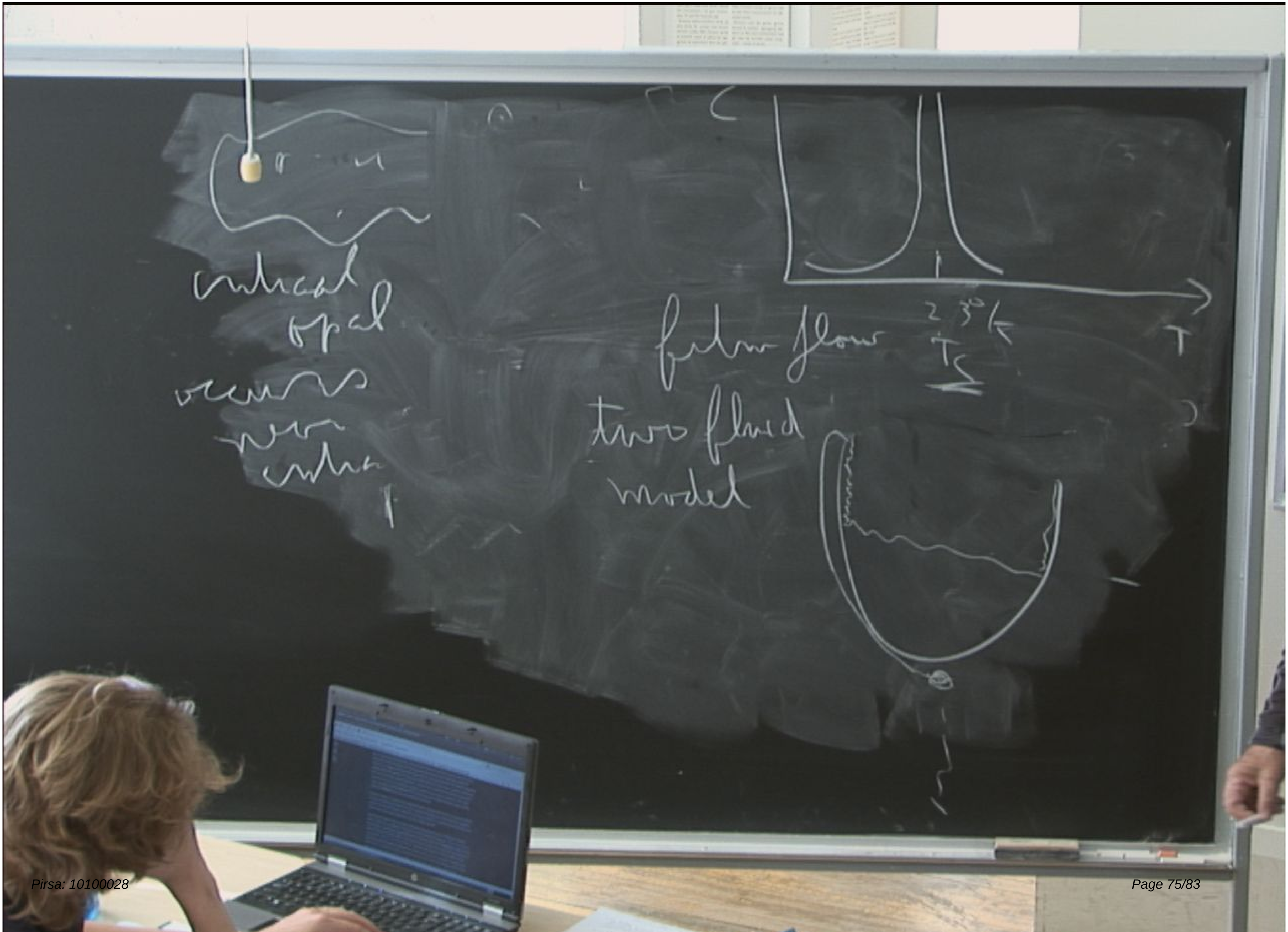
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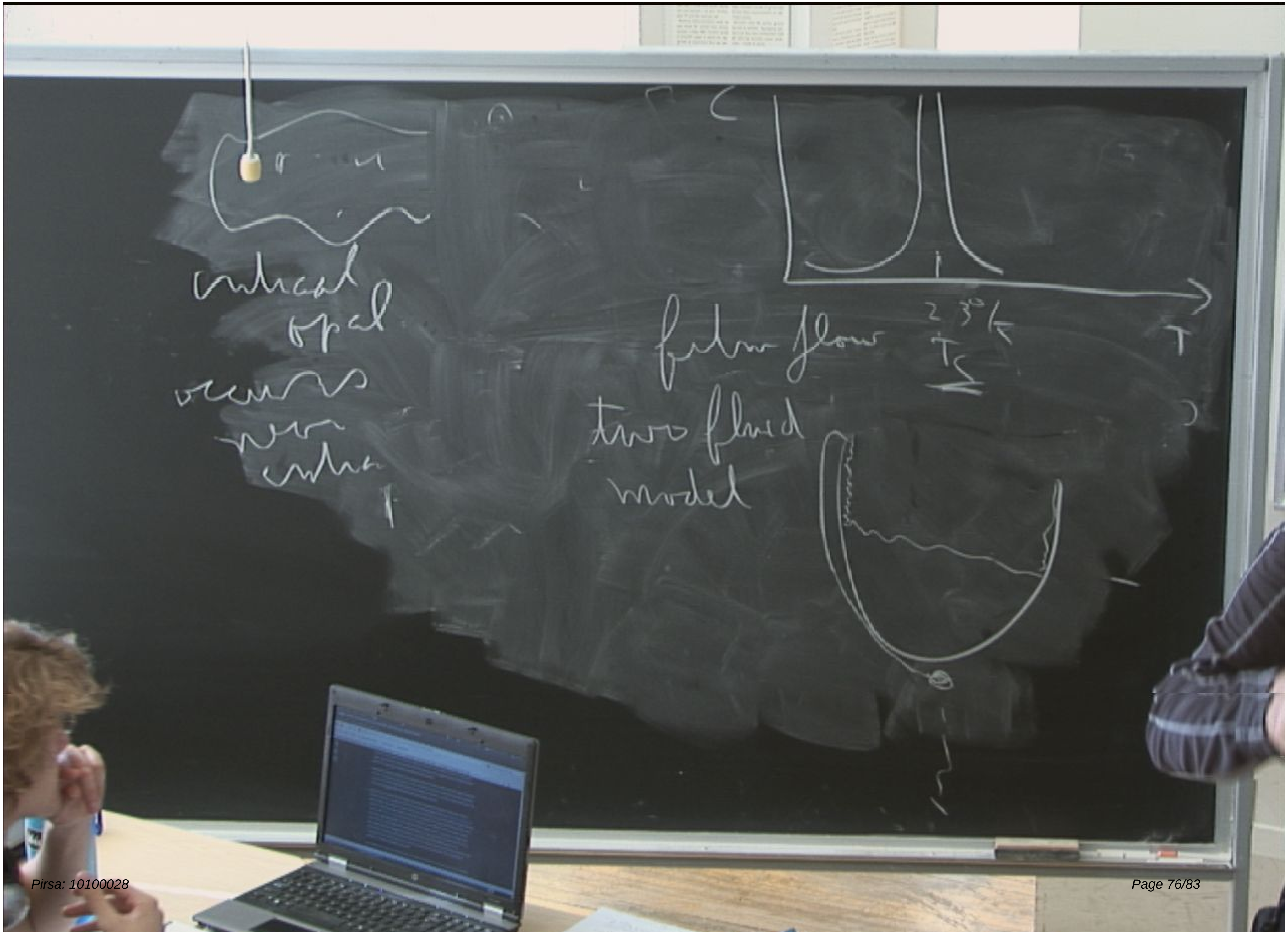
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Order Parameter, generalized

One very important moment occurred in 1937, when Landau pointed out the basic unity among all the different MFT's.

• Landau suggested that phase transitions were manifestations of a broken symmetry, and used the order parameter to measure the extent of breaking of the symmetry.

• in ferromagnet, parameter = magnetization
• in fluid, order parameter = density
• in Ising model, order parameter = $<\sigma>$

L.D. Landau

Generalized Mean Field Schemes I

Landau generalized the many different MFT's that existed by assuming an expansion of the free energy in an order parameter, here symbolized by M = magnetization

note: no cubic term. This free energy applies to symmetry o Ising mode

$$F=\int dr[a-hM+tM^2+cM^4+(\nabla M)^2]$$

expansion assumes a small order parameter (works near critical point) and small fluctuations (works far away?!)

h is magnetic field

t is proportional to $(T-T_c)$

minimize F in M: result General Solution $M(h, (T-T_c))$

singularity as t,h both go through zero!

singularity as h goes through zero for $T< T_c$

Superconductors

An analogous situations holds in the normal low-temperature superconductors of the sort described by BCS. These have the usual solid transport processes, produced by the superconducting quasi-particles and in addition an equation for the condensate, called the Landau-Ginzburg equation. The latter is a form of Landau's equation for a critical system, with a complex wave function representing the behavior of the order parameter. Their equations take the form

$$\alpha\psi + \beta|\psi|^2\psi + \frac{1}{2m}\left(-i\hbar\nabla - 2e\mathbf{A}\right)^2\psi = 0$$

$$\mathbf{j} = \frac{2e}{m}\mathrm{Re}\left\{\psi^*\left(-i\hbar\nabla - 2e\mathbf{A}\right)\psi\right\}$$

where j is the electrical current produced by the superflow. Note the 2e. That's because the wave function describes Cooper pairs. One can include a time derivative in the first equation to describe slow temporal changes.

Brian Josephson

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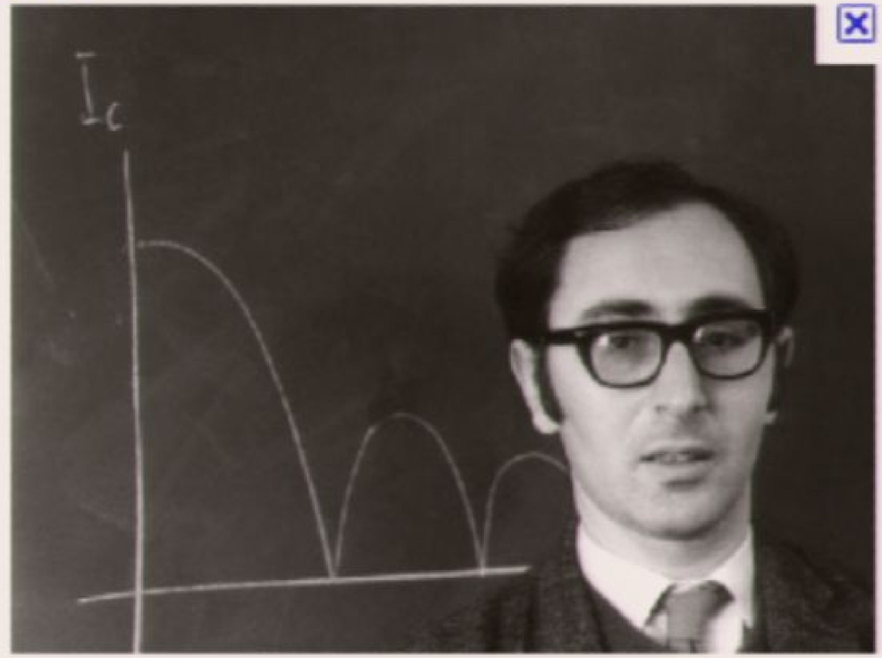

Josephson, B.D., 1964: "Coupled Superconductors", *Review of Modern Physics*, **36** [1P1].
Josephson, B.D., 1965: "Supercurrents through Barriers", *Advances in Physics*, **14** [56].
Josephson, B.D., 1992: "Telepathy Works", *New Scientist*, **135** [1833], 50-50.
Josephson, B.D., 1992: "Defining Consciousness", *Nature*, **358** [6388], 618-618.

anecdote tells of Werner Heisenberg and Dirac sailing on a cruise ship to a conference in Japan in August 29. "Both still in their twenties, and unmarried, they made an odd couple. Heisenberg was a ladies' man who nstantly flirted and danced, while Dirac—'an Edwardian geek', as [biographer] Graham Farmelo puts it—fered agonies if forced into any kind of socialising or small talk. 'Why do you dance?' Dirac asked his npanion. 'When there are nice girls, it is a pleasure,' Heisenberg replied. Dirac pondered this notion, then rted out: 'But, Heisenberg, how do you know beforehand that the girls are nice?'"[

Superfluidity

Superfluidity is a phase of matter in which viscosity of a fluid vanishes, while heat capacity becomes infinite. These unusual effects are observed when liquids, typically of helium-4 or helium-3, overcome friction in surface interaction at a stage (known as the "lambda point", which is temperature and pressure, for helium-4) at which the liquid's viscosity becomes zero. Also known as a major facet in the study of quantum hydrodynamics, it was discovered by Pyotr Kapitsa, John F. Allen, and Don Misener in 1937 and has been described through phenomenological and microscopic theories. In the 1950s Hall and Vinen performed experiments establishing the existence of quantized vortex lines. In the 1960s, Rayfield and Reif established the existence of quantized vortex rings. Packard has observed the intersection of vortex lines with the free surface of the fluid, and Avenel and Varoquaux have studied the Josephson effect in superfluid ^4He.

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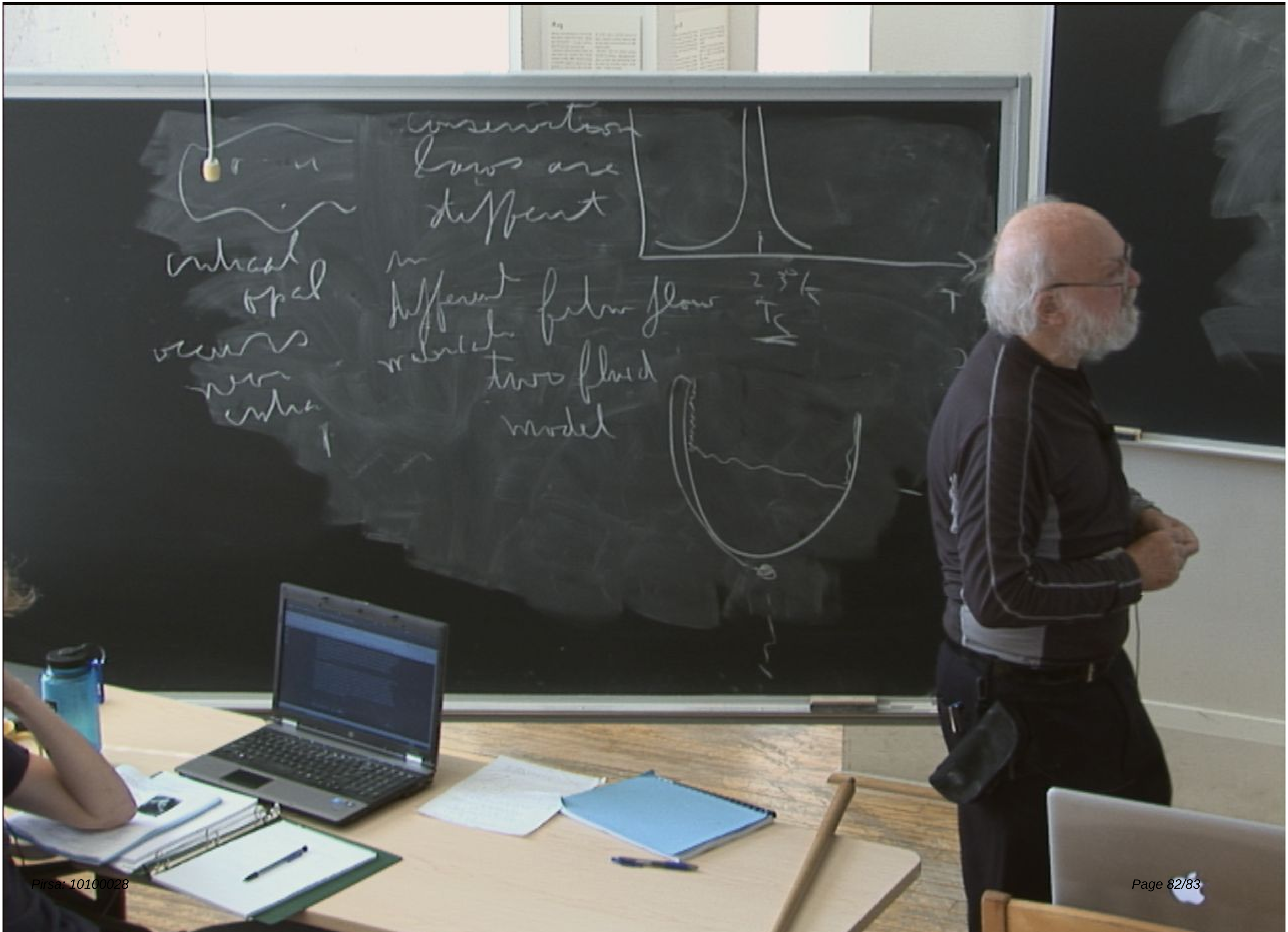
laws are
different
two fluid
model

transport in different phases ...continued

Superfluids have special "super" flow processes which cannot occur in an ordinary liquid. In the simplest time-independent limit the slow changes are described by a non-linear Schrodinger equation of the form

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r}^2} + V(\mathbf{r}) + \frac{4\pi\hbar^2 a_s}{m}|\psi(\mathbf{r})|^2\right)\psi(\mathbf{r}) = \mu\psi(\mathbf{r}),$$

The right hand side comes from a term in i $(h/2\pi)\partial_t\psi$, in a situation in which the energy is given by the chemical potential μ.

This is called the Gross-Pitaevski equation, and applies at very low temperatures. At higher temperatures, the flow equations are described as two-fluid equations, because the flow can be roughly understood as a simultaneous flow of normal fluid and superfluid. Some very special effects are produced. For example film flow.