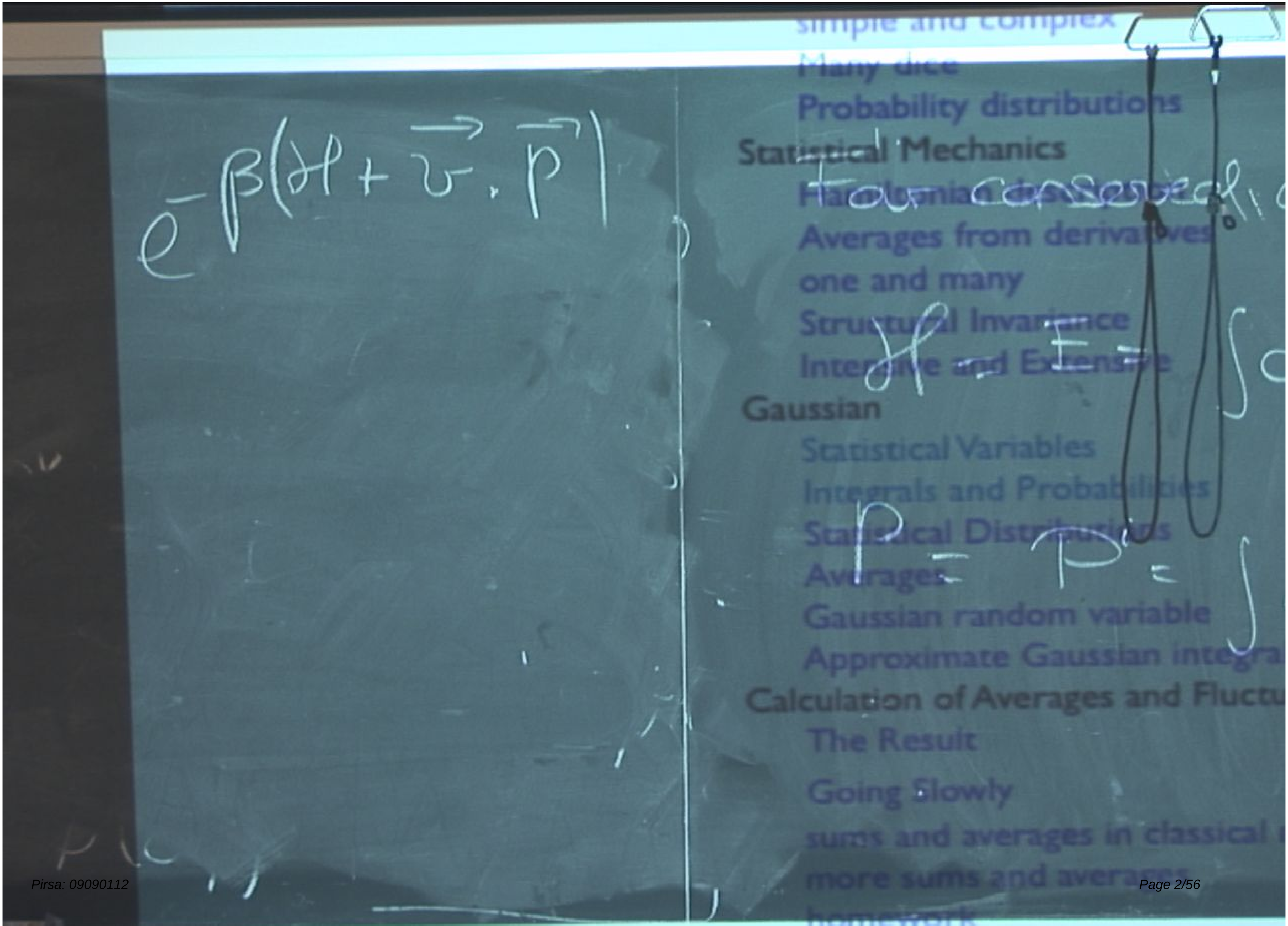
Title: Statistical Mechanics (PHYS 602) - Lecture 2

Date: Sep 29, 2009 10:30 AM

URL: http://pirsa.org/09090112

Abstract:


Probability distributions
Statistical Mechanics
Averages from derivatives
one and many
Structural Invariance
Intensive and Extensive
Gaussian
Statistical Variables
Integrals and Probabilities
Statistical Distributions
Averages
Gaussian random variable
Approximate Gaussian integra
Calculation of Averages and Fluctu
The Result
Going Slowly
sums and averages in classical
more sums and averages
homework
Four conserved
$e^{-\beta(\mathcal{H}+\vec{v}\cdot\vec{p})}$

Part 2: Basics of Statistical Physics

Probabilities

- Simple probabilities
- averages
- Composite probabilities
- Independent events
- simple and complex
- Many dice
- Probability distributions

Statistical Mechanics

- Hamiltonian description
- Averages from derivatives
- one and many
- Structural Invariance
- Intensive and Extensive

Gaussian

- Statistical Variables
- Integrals and Probabilities
- Statistical Distributions
- Averages
- Gaussian random variable
- Approximate Gaussian integrals

Calculation of Averages and Fluctuations

- The Result
- Going Slowly
- sums and averages in classical mechanics
- more sums and averages
- homework

Simple probabilities (reprise)

mutually exclusive events described by $\alpha=1,2,3,\ldots\ldots$

number of times α turns up$=N_\alpha$; total number of events N $N = \sum_\alpha N_\alpha$

probability of getting a side with number α is ρ_α $\rho_\alpha=N_\alpha/N$ ii.1

total probability =1 --> $\sum_\alpha \rho_\alpha = 1$ ii.2

relative probability: relative chance that α will turn up $=r_\alpha$, e.g. fair dice have r_α =constant

from r to ρ $z = \sum_\alpha r_\alpha$ normalize (=fix up size) : $\rho_\alpha = r_\alpha/z$

cubic dice 6 sides: fair dice --> all probabilities are equal -->
$r_\alpha=1$ --> $z=6$ --> $\rho_\alpha=1/6$ for all values of α

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Averages (reprise)

$\rho_\alpha = 1/6$

average number on a throw= $<\alpha>=(\sum_\alpha \alpha N_\alpha)/N$

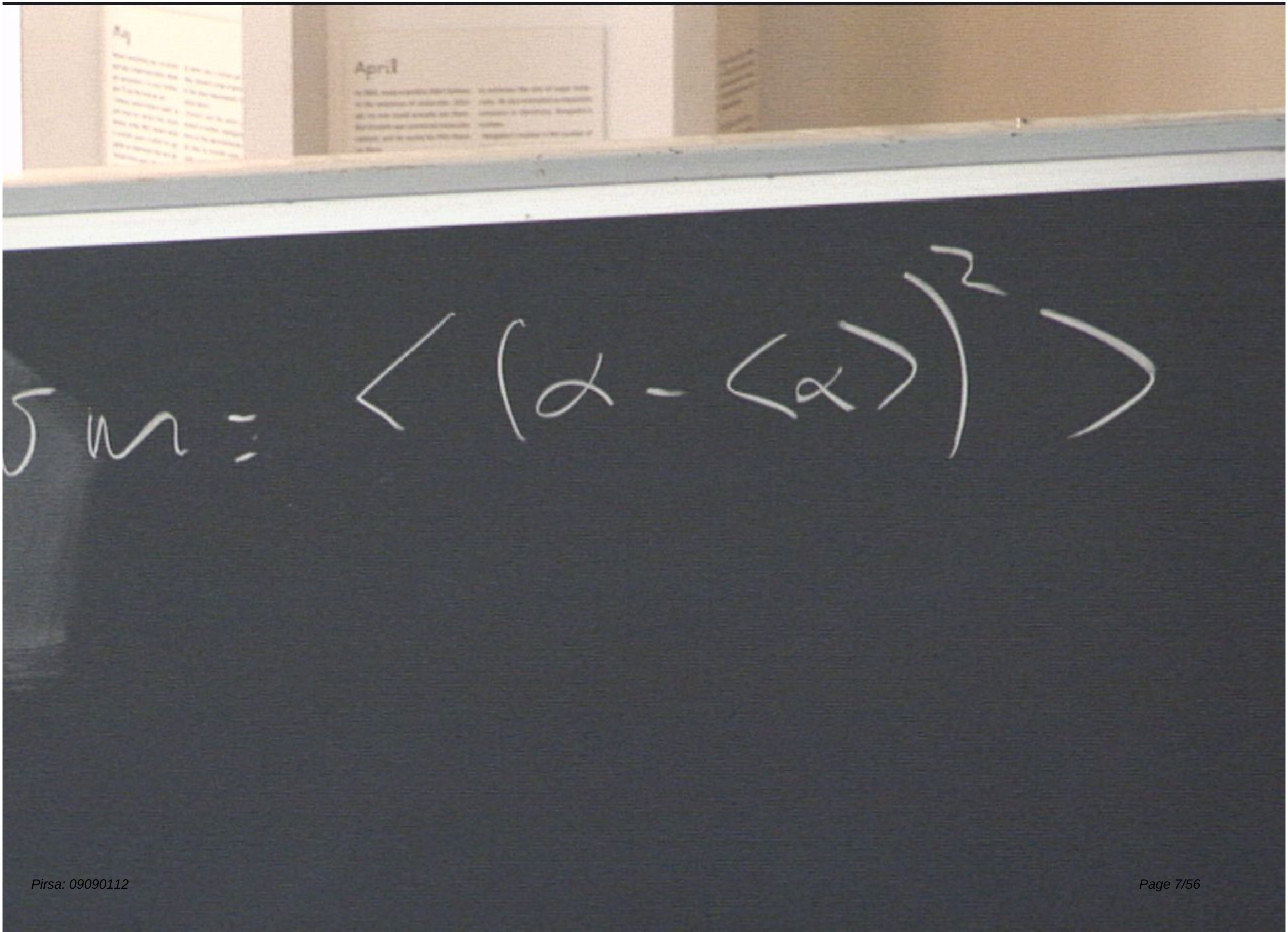
average number on a throw = $< \alpha >= \sum_\alpha \rho_\alpha \alpha = 3.5$

$<\alpha^2>=?$ $<(\alpha-<\alpha^2>)^2> = ?$ This last quantity is called the variance of α

general rule: To calculate the average of any function $f(\alpha)$ that gives the probability that what will come out will be α, you use the formula

$$< f(\alpha) >= \sum_\alpha f(\alpha)\rho_\alpha \qquad \text{ii.3}$$

Do we understand what this formula means?? How would we describe a loaded die? An average from a loaded die? If I told you that $\alpha=2$ was twice as likely as all the other values, and these others were all equally likely, what would be the relative probability? What would we have for the average throw on the die?


April
$\delta m = \langle (\alpha - \langle \alpha \rangle)^2 \rangle$

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Composite Probabilities

α and β are two different kinds of events

α might describe the temperature on January 1, ρ_α computed as N_α / N

β might describe the precipitation on December 31, with probabilities ρ'_β

Both kinds of events are complete $\sum_\alpha \rho_\alpha = 1$ $\sum_\beta \rho'_\beta = 1$

The prime indicates that the two probabilities are quite different from one another.

Let $\rho_{\alpha,\beta}$ be the probability that both will happen. The technical term for this is a joint probability. The joint probability satisfies $\sum_{\alpha,\beta} \rho_{\alpha,\beta} = 1$

$\rho(\alpha|\beta)$ is the probability that event α occurs if that we know that event β has or will occur. This quantity is called a conditional probability. It obeys $\rho(\alpha|\beta) = \rho_{\alpha,\beta} / \rho'_\beta$

Something must happen, implies that $\sum_\alpha \rho(\alpha \mid \beta) = 1$

Independent Events

Physically two events are independent if the outcome of one does not affect the outcome of the other. It is a mutual relation, if α is independent of β then β is independent of α.

This can then be stated in terms of conditional probabilities. If $\rho(\alpha|\beta)$ is independent* of β then we say α and β are statistically independent. After a little algebraic manipulation, it follows that the joint probability $\rho_{\alpha,\beta}$ obeys

$$\rho_{\alpha,\beta} = \rho_\alpha \ \rho'_\beta$$

equivalently, two events are statistically independent, if the number of times both show up is expressed in terms of the number of times each one individually shows up as

$$N_{\alpha,\beta} = N_\alpha N'_\beta / N$$

This can be generalized to the statement that a series of *m* different events are statistically independent if the joint probabilities of the outcomes of all these events is simply the product of all the *m* individual probabilities.

The word uncorrelated is also used to describe statistically independent quantities.

* note multiple uses of the word "independent"!

Simple and Complex

definition: simple outcome: can happen only one way: like 2 coming up when a die in thrown

definition: complex outcome: can happen several ways: like 7 coming up when two dice are thrown.

One should calculate probability of complex outcome as a sum of probabilities of simple outcomes.

If the simple outcomes are equally likely, probability of complex outcome is the number of different simple outcomes times the probability of a single simple outcome. There is lots of counting in statistical mechanics. The number of ways that something can happen is often denoted by the symbol W. Entropy is given by

Entropy $S=k \ln W$, where $k=k_B$ is Boltzmann's constant. This equation is on Boltzmann's tombstone. He committed suicide.

what is minimum value of S ?

can you think of a way of getting sub-minimum values of S ?

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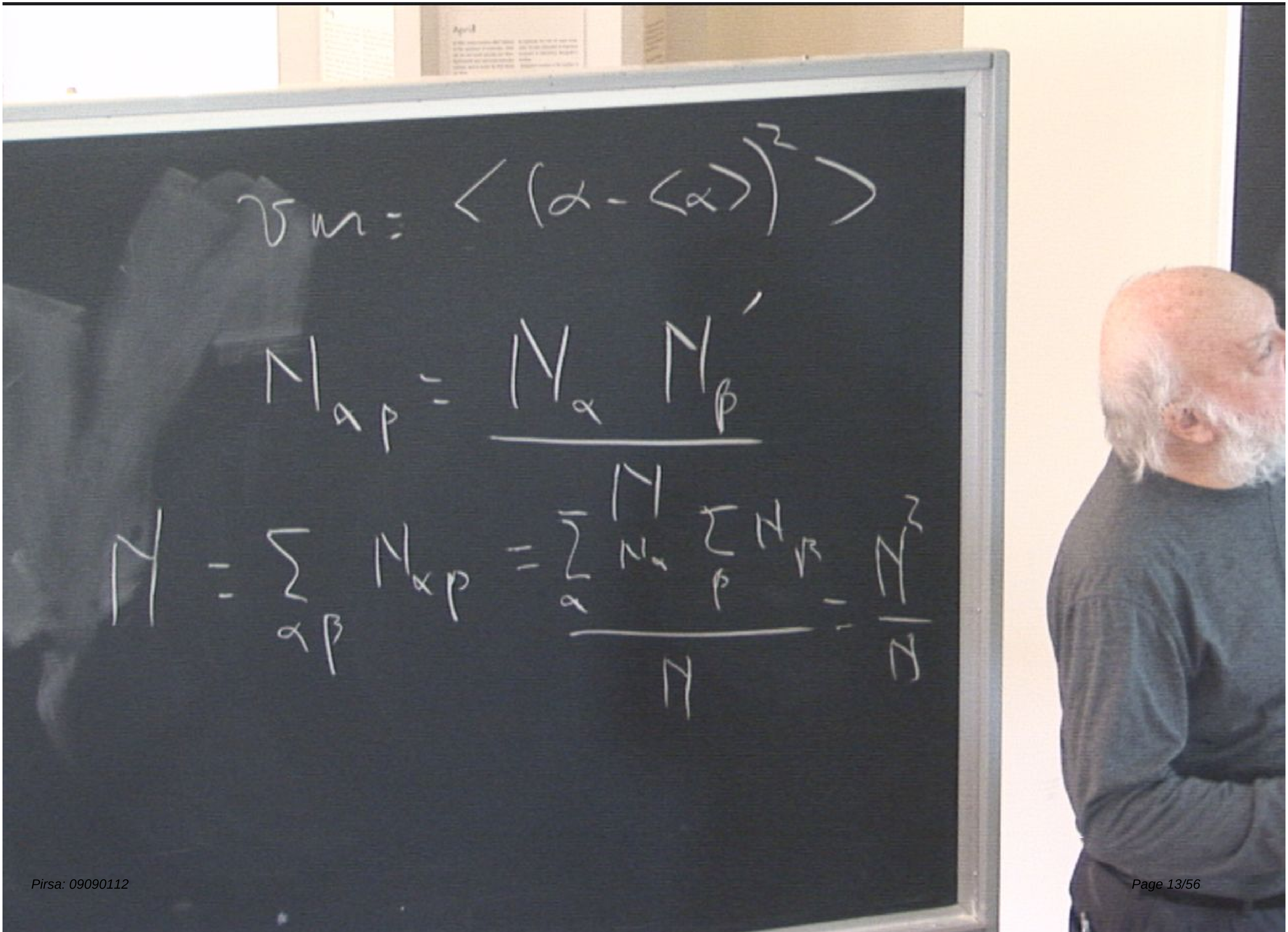
$var = \langle (\alpha - \langle \alpha \rangle)^2 \rangle$
$N_{\alpha\beta} = \frac{N_\alpha N_\beta'}{N}$
$N = \sum_{\alpha\beta} N_{\alpha\beta} = \frac{\sum_\alpha N_\alpha \sum_\beta N_\beta}{N} = \frac{N^2}{N}$

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Many Dice

Given two fair dice
what is the average sum and product of what turns up

Given two dice independent of one another: one fair and the other one unfair. How does one describe the probabilities of the outcome of throwing both dice together?

what is the chance, rolling two fair dice, that we shall roll an eleven, a seven?

Now we roll one hundred dice all at the same time. What is the average of the sum of the dice-values. How can one define a root mean square fluctuation in this value? How big is it?

Probability Distributions

So far we have talked about discrete outcomes. A die may take on one of six possible values. But measured things are often continuous. For example, in one dimension, the probability that a quantum particle will be found between x and x+dx is given in terms of the wave function, $|\psi(x)|^2 dx$. In this context, the squared wave function appears as a probability density. In general, we shall use the notation $\rho(x)$ for a probability density, saying that $\rho(x)\ dx$ is the probability for finding a particle between x and x+dx. The general properties of such probability densities are simple. They are positive. Since the total probability of some x must be equal to one they satisfy the normalization condition

$$\int_{-\infty}^{+\infty} \rho(x)\ dx = 1$$

For example, in classical statistical mechanics, the probability density for finding a particle with x-component of momentum equal to p is

$$(\frac{2\pi\beta}{m})^{1/2}\ \exp[-\beta\ p^2/(2m)]$$

This is called a Gaussian probability distribution, i.e. one that is based on $\exp(-x^2)$. Such distributions are very important in theoretical physics.

One and Many

Imagine a material with many atoms, each with its own spin. The system has a Hamiltonian which is a sum of the Hamiltonia of the different atoms

$$H = \sum_{\alpha=1}^{N} h\sigma_{\alpha}$$

and a probability distribution

$$\rho = \exp(-\beta H) / Z = (1/Z)\prod_{\alpha=1}^{N} \exp(h\sigma_{\alpha})$$

which is a product of pieces which belong to the different atoms. The different pieces are then *statistically independent* of one another. Note that the partition function is

$$Z = \prod_{\alpha=1}^{N} \sum_{\sigma^{\alpha}=\pm 1} \exp(h\sigma^{\alpha}) = (2\cosh h)^{N} = z^{N} \qquad \text{ii.4}$$

so that the entire probability is a product of N pieces connected with the N atoms

$$\rho\{\sigma\} = \prod_{\alpha} [\exp(h\sigma_{\alpha}) / z]$$

The appearance of a product structure depends only upon having a Hamiltonian which is a sum of terms referring to individual parts of the system

Hamiltonian is sum <---> stat mech probability is product <---> statistical independence

$$\rho_{\alpha\beta}, \quad \mathcal{V}m = \langle$$

$$= \rho_\alpha \, \rho_\beta$$

$$N_{\alpha\beta} =$$

$$N = \sum_{\alpha\beta} N_{\alpha\beta} =$$

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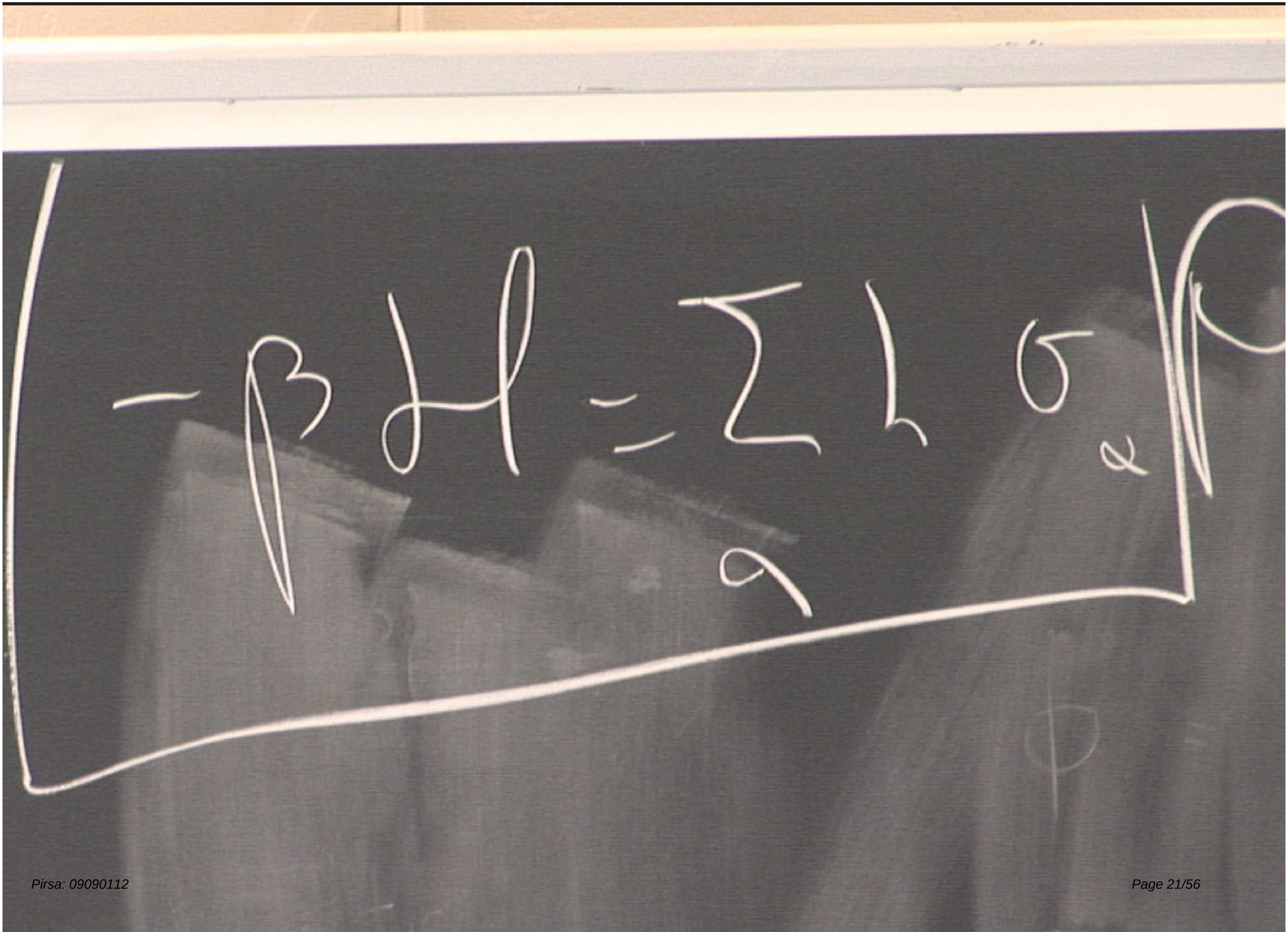
$-\beta\mathcal{H} = \sum_q h \, \sigma_\alpha$

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Structural invariance

Note how the very same structure which applies to one atom $\exp(-\beta H)/Z$ carries over equally to many atoms.

This structural invariance is characteristic of the mathematical basis of physical theories. Newton's gravitational theory seemed natural because the same law which applied to one apple equally applies to an entire planet composed of apples.

This same thing works for electromagnetism.

A wave function is the same sort of thing for one electron or many.

The structure of space and time has a similar invariance property. Remember that a journey of a thousand miles starts with but a single step. The similarity between a single step and a longer distance is a kind of structural invariance. This invariance of space is called a scale invariance. It is quite important in all theories of space and time.

Gaussian Statistical Variables

A Gaussian random variable, X, is one which has a probability distribution which is the exponential of a quadratic in X.

$$\rho(x) = [\beta/(2\pi)]^{1/2} \exp[-\beta(x-\langle X\rangle)^2/2]$$

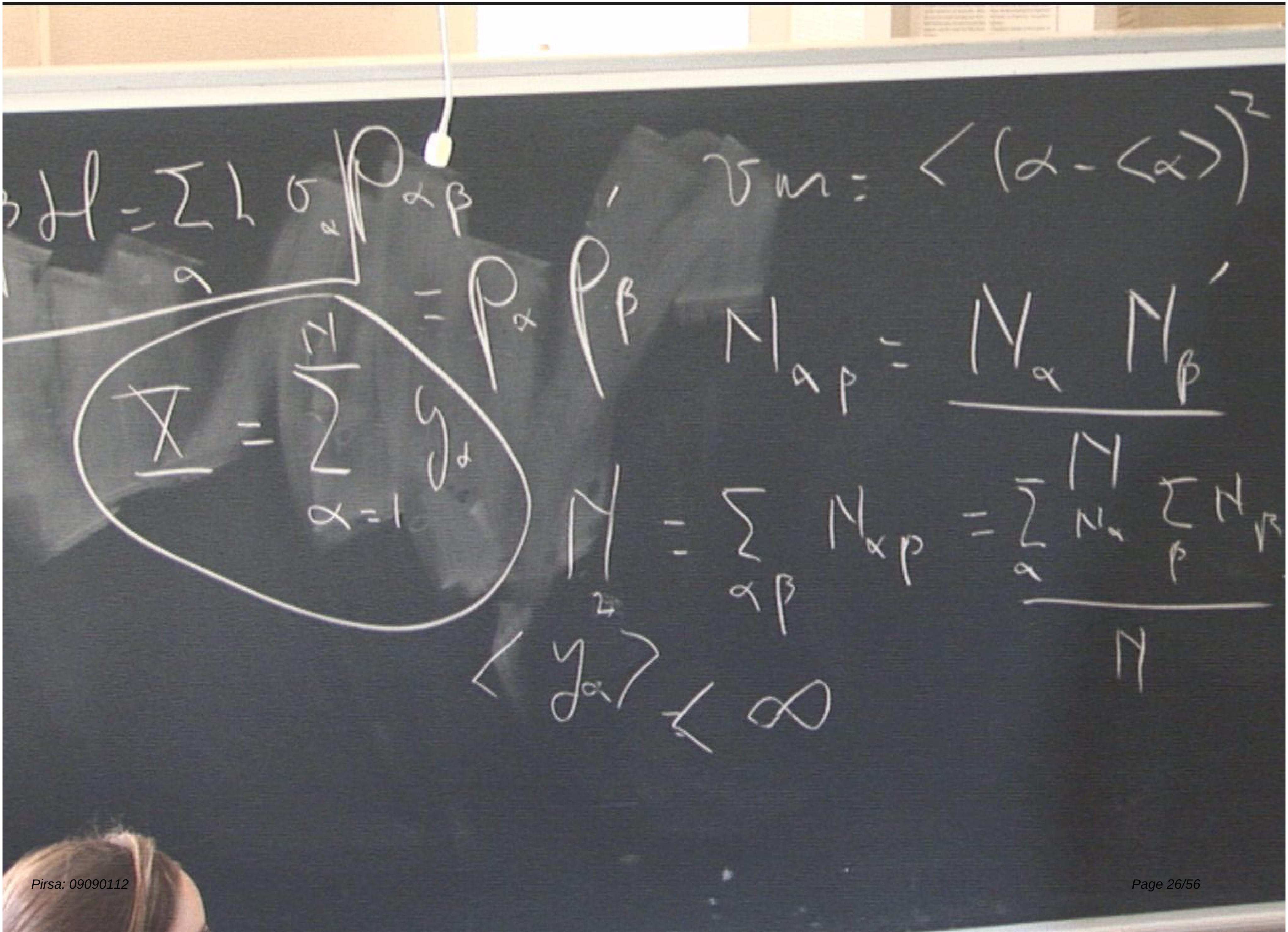
$1/\beta$ is the variance of this distribution.

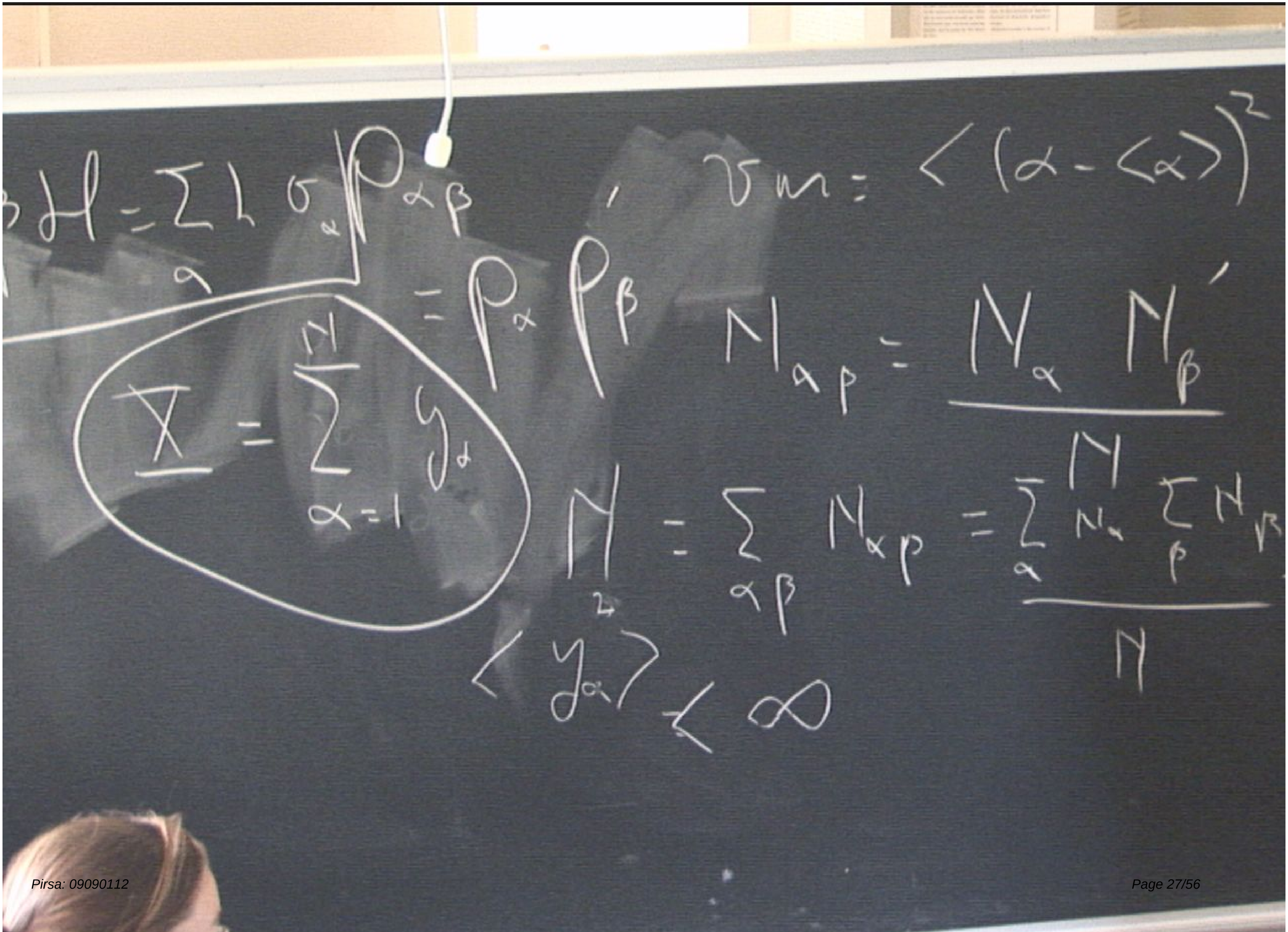
The sum of two statistically independent Gaussian variables is also Gaussian. How does the variance add up?

A Gaussian variable is an extreme example of a structurally stable quantity.

Central Limit Theorem: A sum of a large number of individually quite small random variables need not be small, but that sum is, to a good approximation, a Gaussian variable, given only that the variance of the individual variables is bounded.

Carl Friedrich Gauss (1777 – 1855)


ρ_αβ = ρ_α ρ'_β
N_αβ = N_α N'_β / N
X = Σ_{α=1}^{N} y_α
N = Σ_{αβ} N_αβ
⟨y_α⟩ < ∞



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Gaussian integrals and Gaussian probability distributions

Gaussian integrals are of the form

$$I = \int dx \, \exp(-ax^2/2 + bx + c)$$

with *a*, *b*, and *c* being real numbers, complex numbers, or matrices.
They are very, very useful in all branches of theoretical physics.

We define the probability that the random variable *X* will take on the value between *x* and *x*+*dx* as $\rho(X=x)dx$ or more simply as $\rho(x)dx$

There is a canonical form for Gaussian probability distributions, namely

$$\rho(X=x) = \left(\frac{\beta}{2\pi}\right)^{1/2} \exp[-\beta(x - \langle X \rangle)^2/2]$$

produced by "completeing the square". Here $1/\beta$ is the variance and $\langle X \rangle$ is the average of the random variable, X.

For Gaussian probability distributions, there is a very important result:

$$\langle \exp(iqX) \rangle = \exp(iq\langle X \rangle)\exp[-q^2/(2\beta)] \qquad \text{ii.5}$$

prove this

Notice how the β that appears in the numerator of the probability distribution reappears in the

Gaussian Distributions

According to Ludwig Boltzmann (1844 – 1906) and James Clerk Maxwell (1831-1879) the probability distribution for a particle in a weakly interacting gas as is given by

$$\rho(p,r) = (1/z)\exp(-\beta H)$$
$$H = [p_x^2 + p_y^2 + p_z^2]/2m + U(r)$$

Here, the potential holds the particles in a box of volume Ω, so that U is zero inside a box of this volume and infinite outside of it. As usual, we go after thermodynamic properties by calculating the partition function,

$$z = \Omega[\int dp \exp(-\beta p^2/(2m))]^3 = \Omega(2\pi m/\beta)^{3/2} \qquad \text{ii.6}$$

In the usual way, we find that the average energy is $3/(2\beta) = (3/2)kT$. The classical result is the average energy contains a term 1/2 kT for each quadratic degree of freedom. Thus a harmonic oscillator has $\langle H \rangle = kT$.

lint for theorists: Calculations of Z (or of its quantum equivalent, the vacuum energy) are nportant. Once you can get this quantity , you are prepared to find out most other things bout the system.

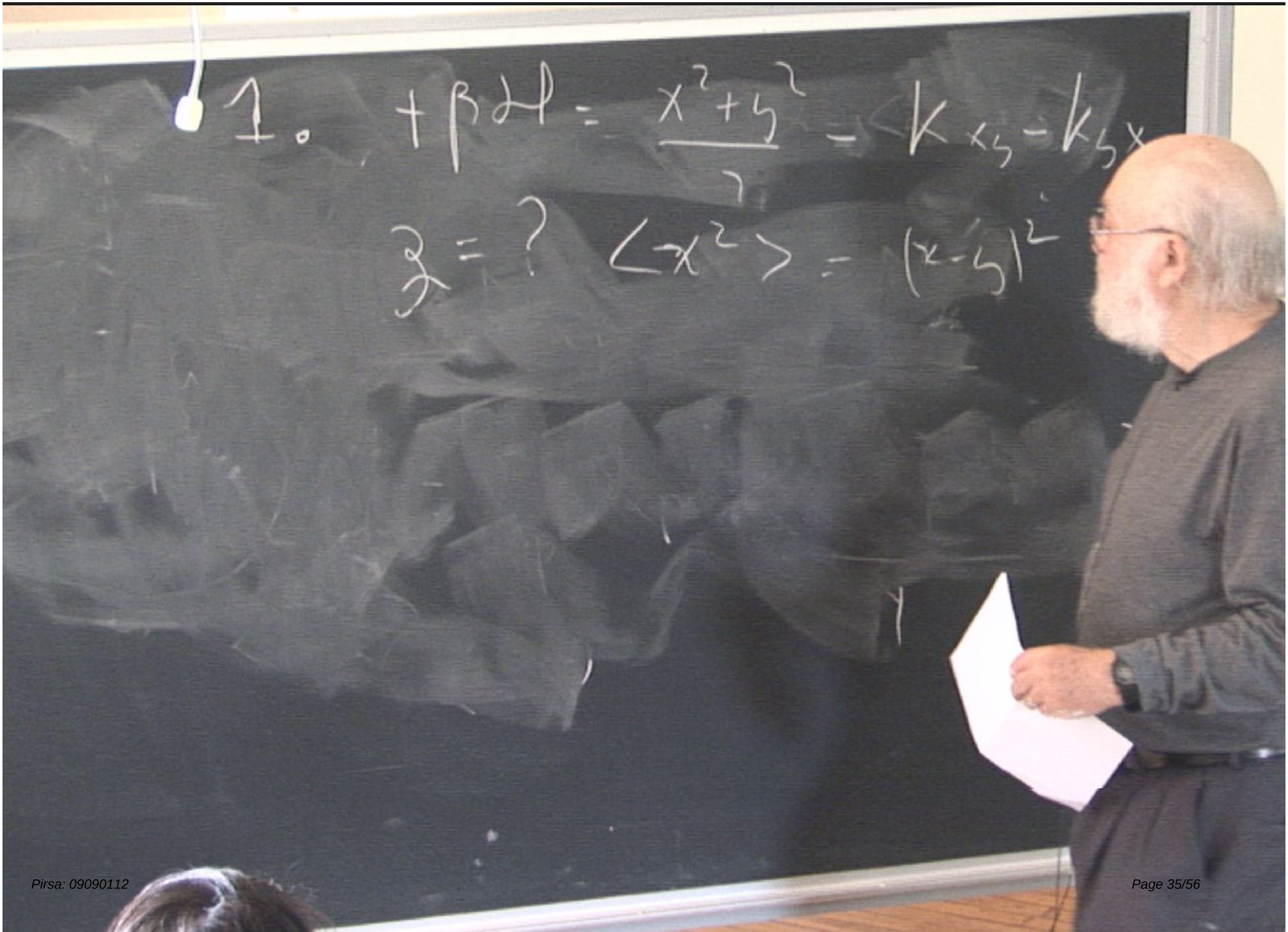
$$+\beta \partial H = \frac{x^2+y^2}{2} = K_{xy} - K_{yx}$$

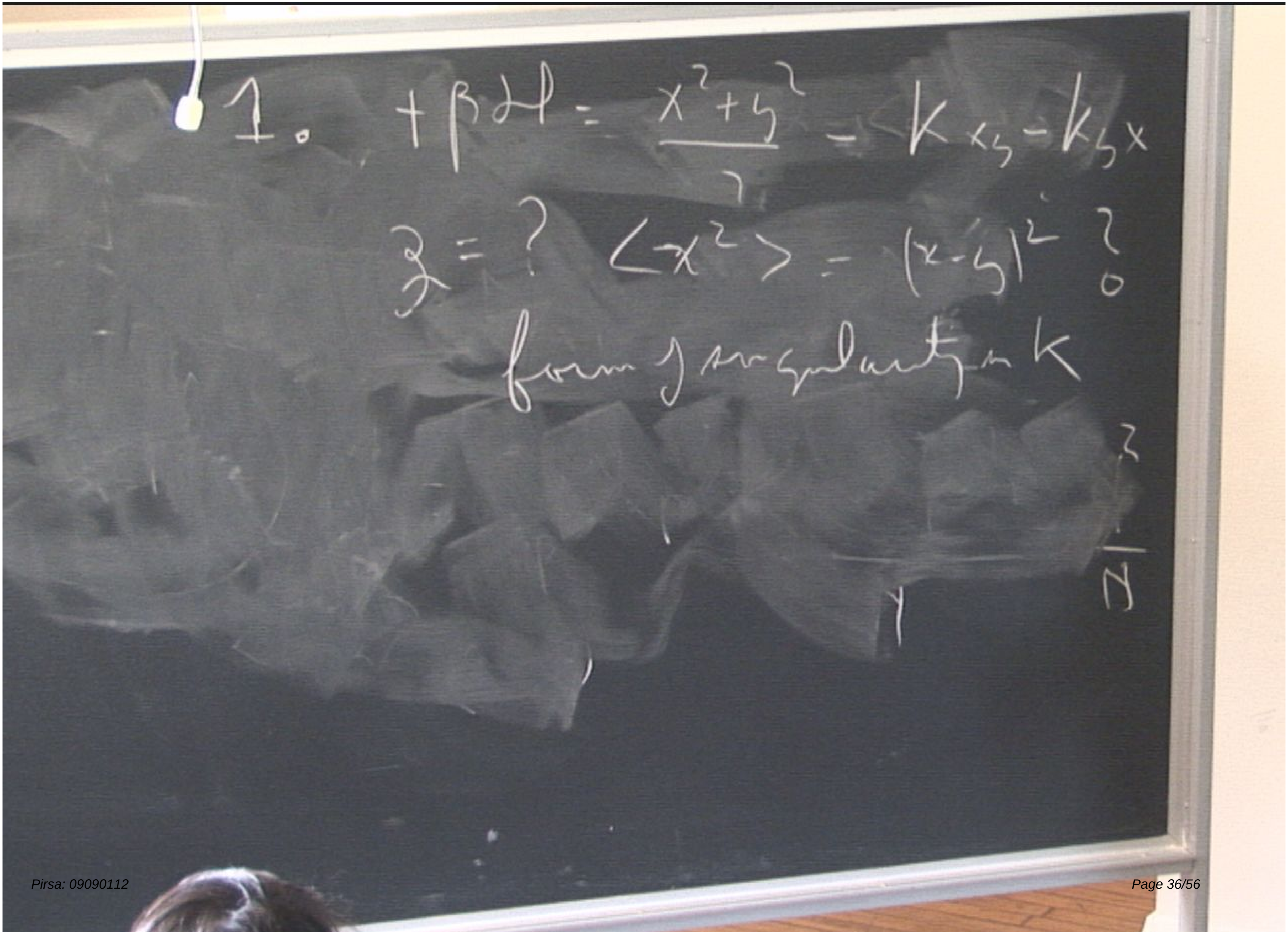
$$z = ? \quad \langle x^2 \rangle = (x-y)^2 \; ? \; 0$$

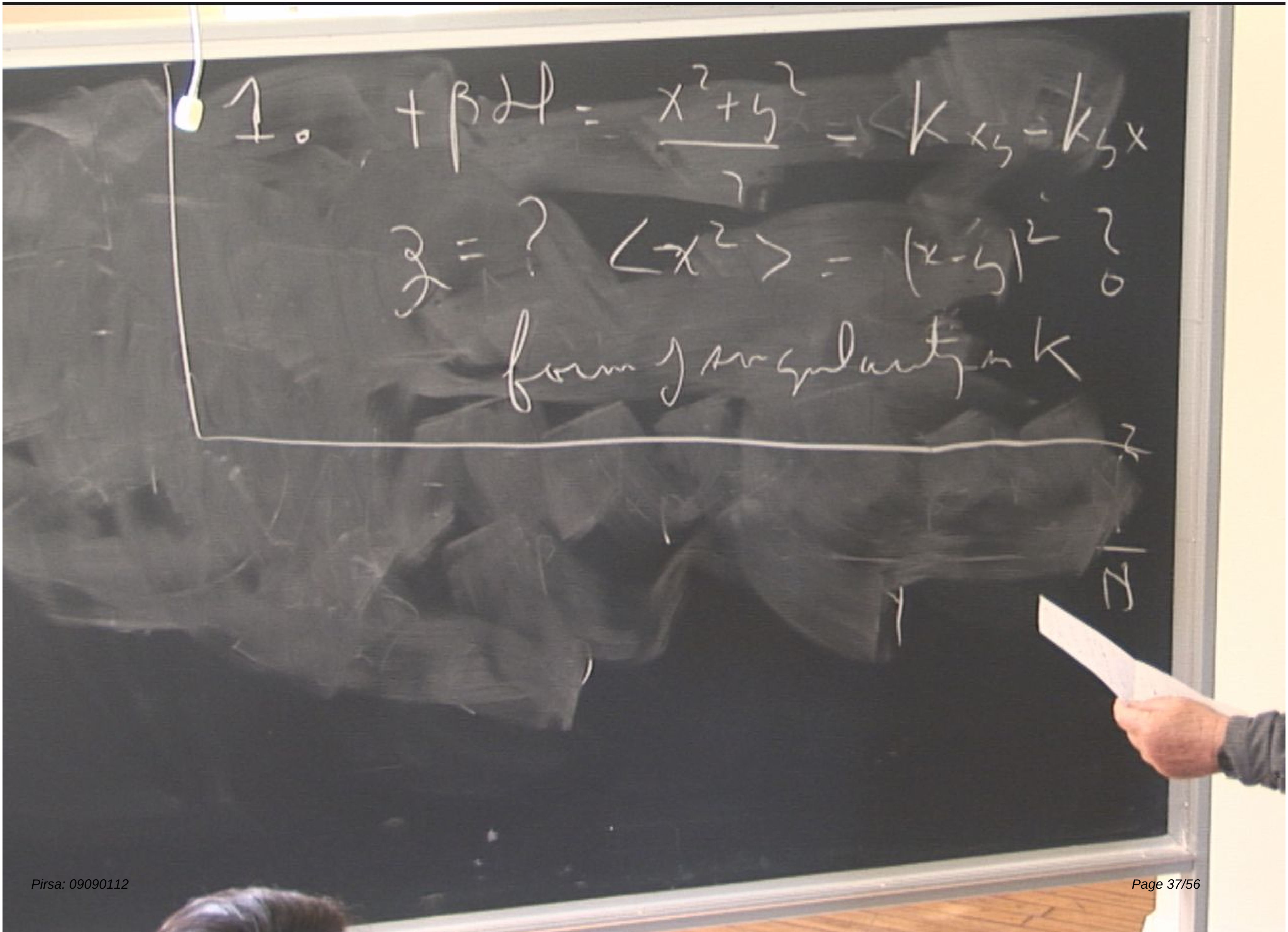
$$\sqrt{N} \sum_{\alpha=1}^{N} y_\alpha$$

$$N = \sum_{\alpha\beta} N_{\alpha\beta} = \frac{\sum_\alpha N_\alpha \sum_\beta N_\beta}{N} = \frac{N^2}{N}$$

$$\langle y_\alpha^2 \rangle < \infty$$




1. + βH = (x² + y²)/2 − K xy − K yx
Z = ? ⟨x²⟩ = (x−y)² ?
form of singularity in K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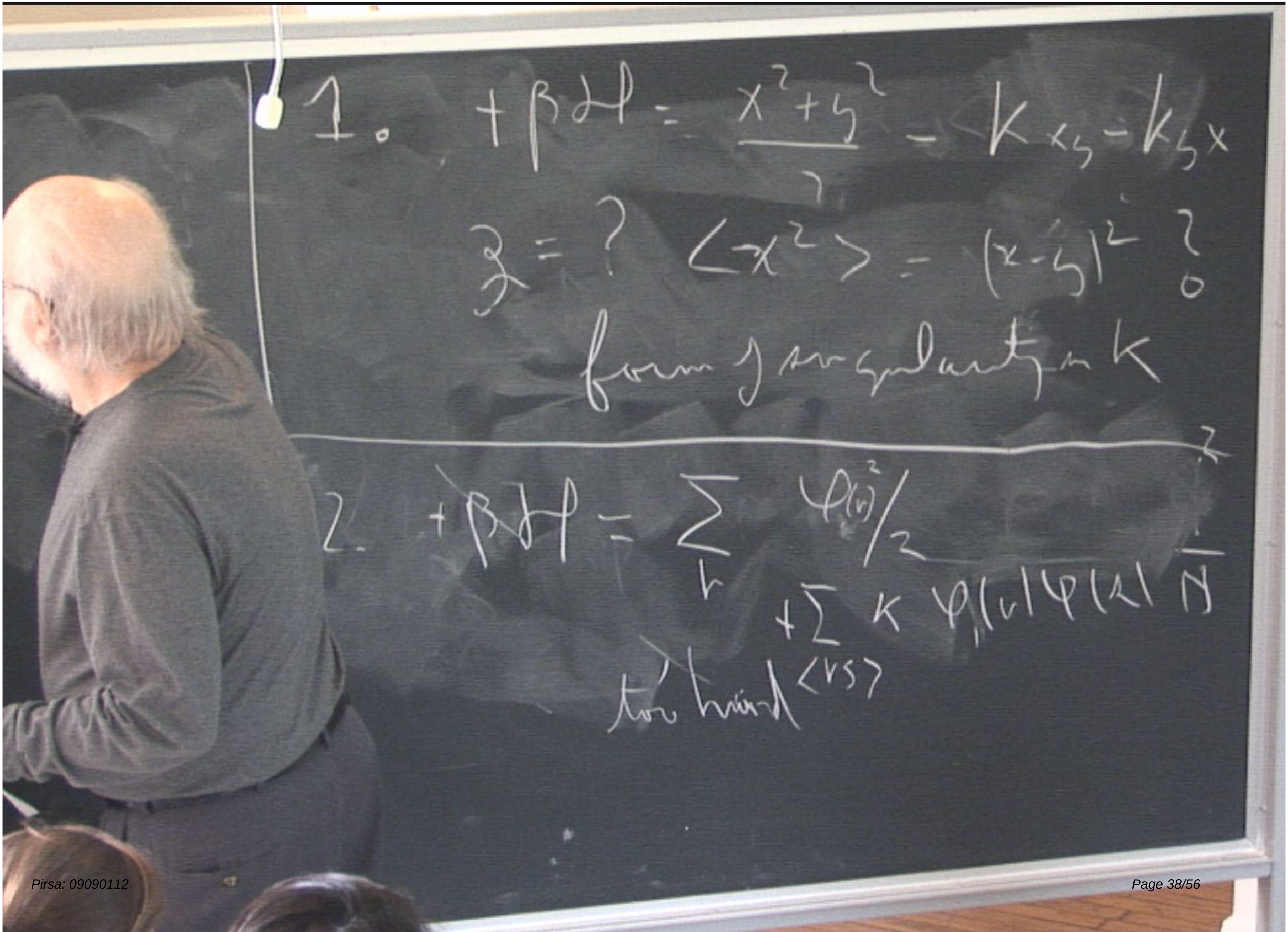
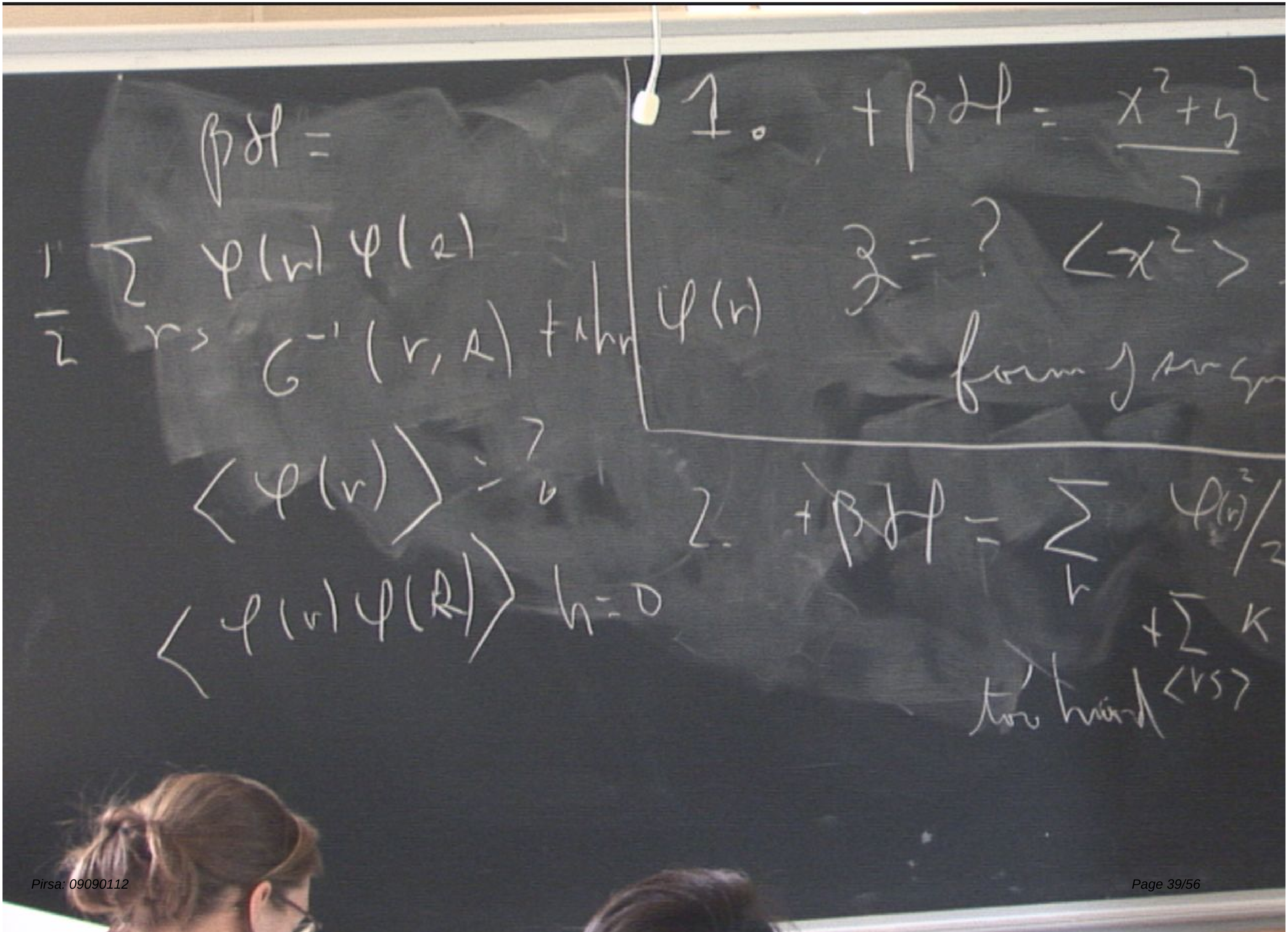

1. +βH = (x²+y²)/2 − Kxy − Kyx
z = ? ⟨x²⟩ = (x−y)² ?
form of singularity in K
2. +βH = Σ φ(r)²/2
+Σ K φ(r)φ(r')
1/N
too hard ⟨rs⟩


βH =
1/2 Σ_rs φ(r) φ(s) G^-1 (r, s) + Σ h_r φ(r)
⟨φ(r)⟩ = ?
⟨φ(r) φ(R)⟩ h=0
1. +βH = (x^2 + y^2)/2
Z = ? ⟨x^2⟩
2. +βH = Σ_r φ(r)^2/2
+ Σ_⟨rs⟩ K

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$$z = \Omega[\int dp \exp(-\beta p^2/(2m))]^3 = \Omega(2\pi m/\beta)^{3/2} \qquad \text{ii.6}$$

In the usual way, we find that the average energy is $3/(2\beta) = (3/2)kT$. The classical result is the average energy contains a term 1/2 kT for each quadratic degree of freedom. Thus a harmonic oscillator has $\langle H\rangle = kT$.

Hint for theorists: Calculations of Z (or of its quantum equivalent, the vacuum energy) are important. Once you can get this quantity , you are prepared to find out most other things about the system.

Gaussian Averages

The usual way

Let one particle be confined to a box of volume Ω. Let U(r) be zero inside the box and + infinity outside. Then, in three dimensions

$$Z=\int d^3p\, d^3r\, \exp(-\beta[p^2/(2m)+U(r)])=\Omega(2\pi m/\beta)^{3/2}$$

Let $\varepsilon = [p^2/(2m)+U(r)]$

$$\partial \ln Z/ \partial\beta=-(1/Z)\int d^3p\, d^3r\, \varepsilon \exp(-\beta\varepsilon)= -<\varepsilon>$$

$$<\varepsilon>=3/(2\beta)=(3/2)kT$$

(The usual way)^2

$$\partial^2 \ln Z /\partial\beta^2= -\partial<\varepsilon>/\partial\beta= \quad ???$$

Let N particles be confined to a box of volume Ω. What is the RMS fluctuation in the pressure?

Gaussian Distributions

According to Ludwig Boltzmann (1844 – 1906) and James Clerk Maxwell (1831-1879) the probability distribution for a particle in a weakly interacting gas as is given by

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Insert Gaussian Homework

do two variables

do N variables

hint: these are "complete the square" exercises

hint: do formal linear algebra on N variables

Rapidly Varying Gaussian random variable

Later on we shall make use of a time-dependent gaussian random variable, $\eta(t)$. In its usual use, $\eta(t)$ is a very rapidly varying quantity, with a time-integral which behaves like a Gaussian random variable. Specifically, it is defined to have two properties:

$$<\eta(t)>=0$$

$X(t) = \int_s^t du\, \eta(u)$ is a Gaussian random variable with variance $\Gamma\,|s-t|$.

Here Γ defines the strength of the oscillating random variable.

Approximate Gaussian Integrals

It is often necessary to calculate integrals like

$$I = \int_a^b dx\, e^{Mf(x)}$$

in the limit as M goes to infinity. Then the exponential varies over a wide range and the integral appears very difficult. But, in the end it's easy. The main contribution will come at the maximum value of f in the interval [a,b]. Assume there is a unique maximum and the second derivative exists there. For definiteness say that the maximum occurs at $x=0$, with $a<0<b$. Then we can expand the exponent and evaluate the integral as

$$I \approx e^{Mf(0)} \int_a^b dx\, e^{Mf''(0)x^2/2+....} \approx e^{Mf(0)} \int_{-\infty}^{\infty} dx\, e^{Mf''(0)x^2/2+....} = e^{Mf(0)} \left(\frac{2\pi}{-Mf''(0)} \right)^{1/2}$$

Notice that because we have assumed that zero is a maximum, the second derivative is negative. Because M is large and positive, we do not have to include any further higher order terms in x. For the same reason we can extend the limits of integration to infinity. With that, it's done!

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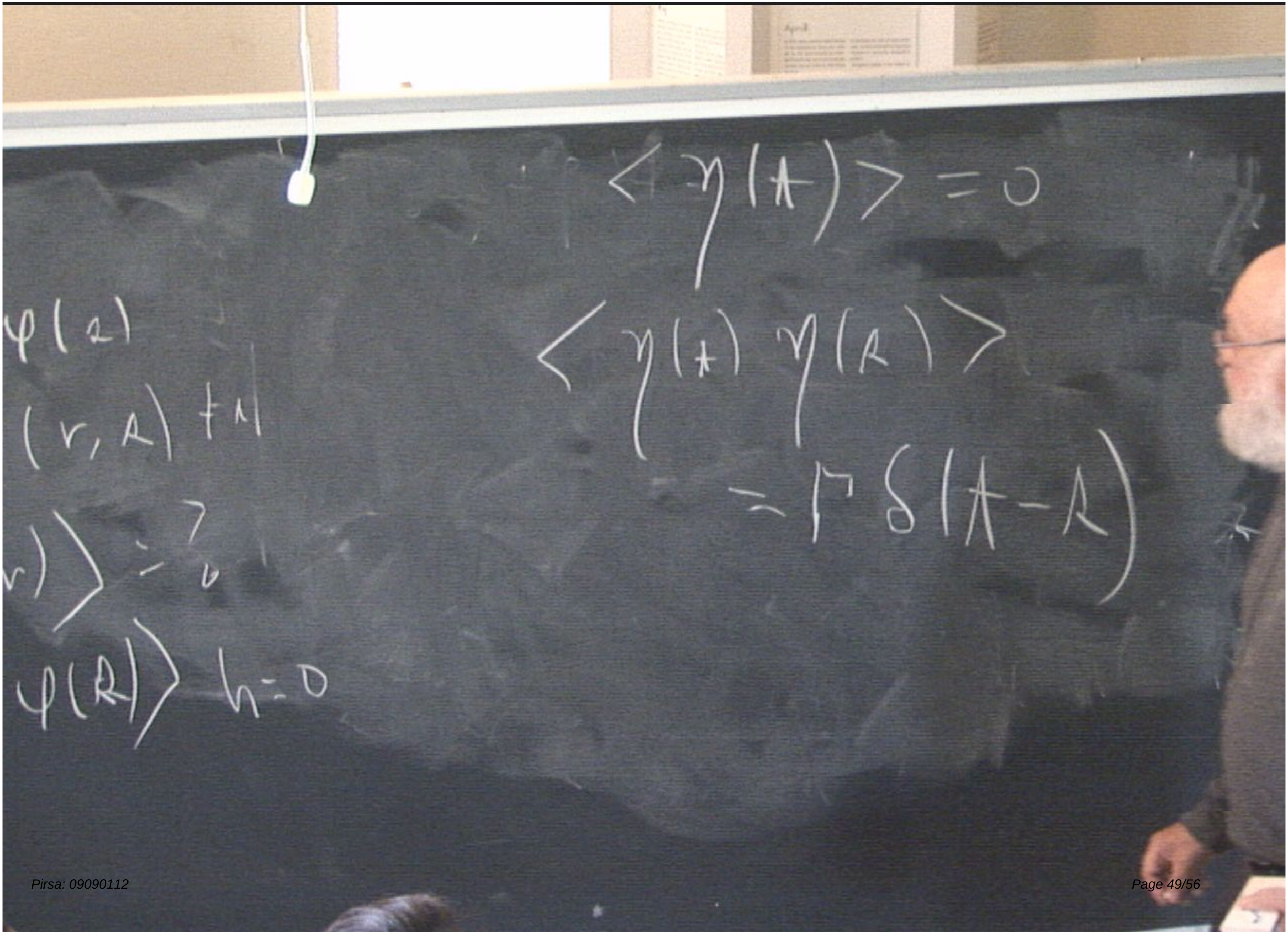

⟨η(x)⟩ = 0
⟨η(x) η(R)⟩
= Γ δ(x − R)

$\varphi(x)$

$(r, s) + n$

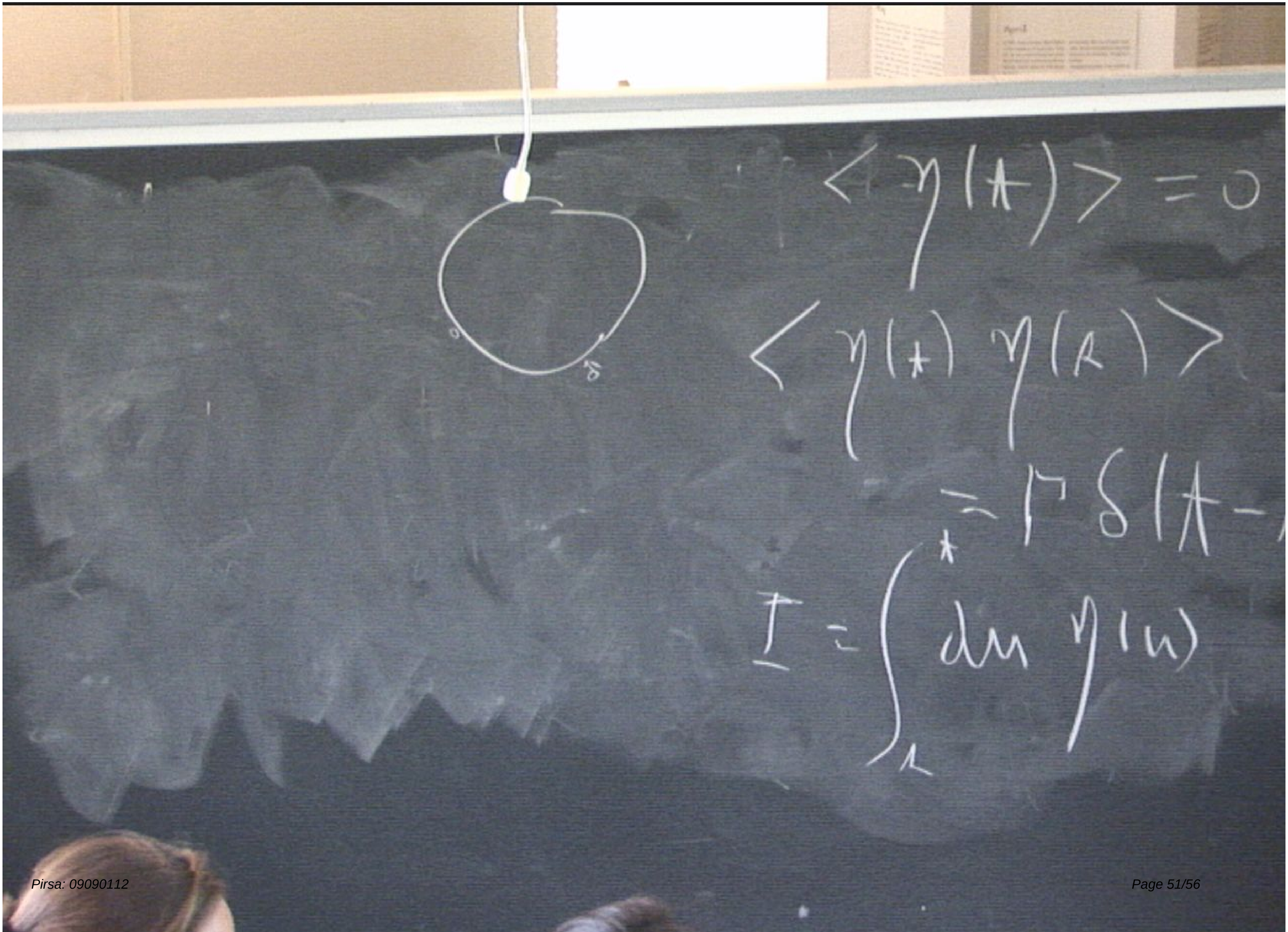
$r)\rangle = 0$

$\varphi(R)\rangle \; h = 0$

$$\langle \eta(t) \rangle = 0$$

$$\langle \eta(t)\,\eta(s) \rangle = \Gamma\,\delta(t-s)$$

$$I = \int_s^t du\, \eta(u)$$


⟨η(A)⟩ = 0
⟨η(A) η(B)⟩
= Γ δ(A −
I = ∫ du η(u)
A
B

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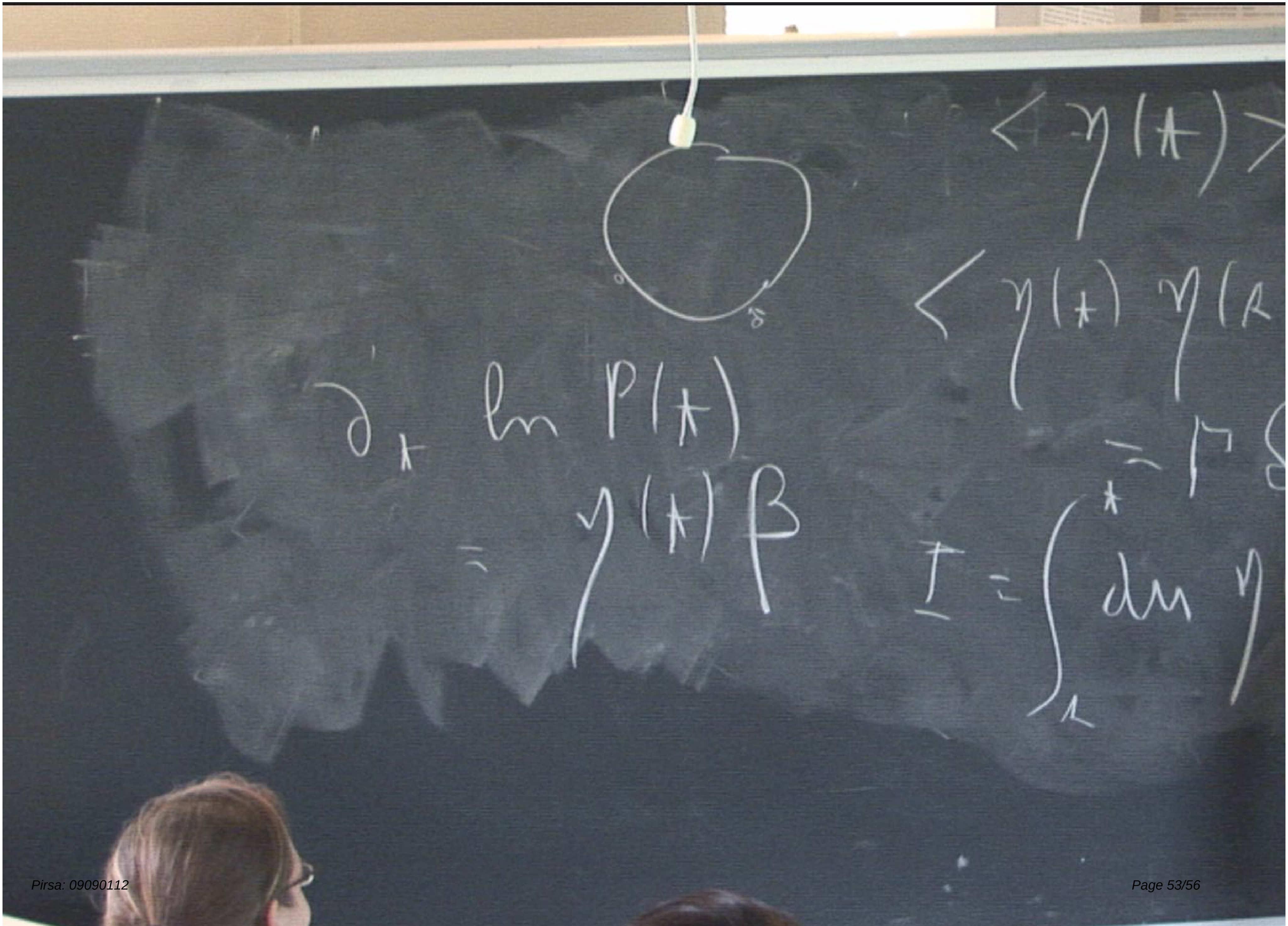
∂t ln P(t)
= η(t) β
<η(t)>
<η(t) η(t
I = ∫ du η

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Let's do it now. Calculate $I = \int dx\ [\cos x]^M \exp(ikx)$ with the integral going from 0 to $\pi/2$ and M being very

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Sums and Averages in Classical Mechanics

'he probability distribution for a single particle in a weakly interacting gas as is given by

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$$z = \Omega[\int dp\, \exp(-\beta p^2/(2m))]^3 = \Omega(2\pi m/\beta)^{3/2}$$

The average of any function of **p** and **r** is given by

$\langle g(\mathbf{p},\mathbf{r})\rangle = \int d\mathbf{p}\, d\mathbf{r}\, \rho(\mathbf{p},\mathbf{r})\, g(\mathbf{p},\mathbf{r})$

Since there are N particles in the system $N\, d\mathbf{p}\, d\mathbf{r}\, \rho(\mathbf{p},\mathbf{r})$ is the number of particles which have position and momentum within $d\mathbf{p}\, d\mathbf{r}$ about the phase space point $\mathbf{p},\mathbf{r}$. The quantity $N\rho(\mathbf{p},\mathbf{r})=f(\mathbf{p},\mathbf{r})$ is called the distribution function. The total amount of the quantity represented by $g(\mathbf{p},\mathbf{r})$ is given in terms of the distribution function as

total amount of $g = \int d\mathbf{p}\, d\mathbf{r}\, f(\mathbf{p},\mathbf{r})\, g(\mathbf{p},\mathbf{r})$

Example: We calculated the average energy $\langle \mathbf{p}^2/(2m) \rangle = 3\, kT/2 = \int d\mathbf{p}\, d\mathbf{r}\, \rho(\mathbf{p},\mathbf{r})\, \mathbf{p}^2/(2m)$

The total energy in the system is $\int d\mathbf{p}\, d\mathbf{r}\, f(\mathbf{p},\mathbf{r})\, \mathbf{p}^2/(2m) = 3N\, kT/2$.