Title: Statistical Mechanics (PHYS 602) - Lecture 1

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Abstract:

# Fundamentals of Statistical Physics

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text:

Statistical Physics,

Statics, Dynamics, Renormalization

Leo Kadanoff

I also referred often to *Wikipedia* and found it accurate and helpful.

## Part I: Once over lightly

Concepts which specifically belong to statistical physics
Interesting Physical Science Advances have a Major Statistical Component
Probabilities: One die
Quantum Stat Mech
Classical Stat Mech
Averages from Derivatives
Thermodynamics
From Quantum to Classical: The Ising model
Degenerate Distributions
Thermodynamic Phases
Phase Transitions
Random Walk
Brownian Dynamics
Big Words

# Where do we come from?

Undergraduate Institution:

Major:

Theory, Experiment, Simulation

Research:

## Concepts which specifically belong to statistical physics:

Not in few particle quantum mechanics or in Classical Mechanics

- Temperature

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Not in few particle quantum mechanics or in Classical Mechanics

- Temperature

temperature pressure, entropy, (B,D,H,E), phase, phase transition, liquid, solid, gas, plasma, probability density matrix, correlation, entanglement, chaos. order, butterfly effect, reaction rate, chemical potential,

# Concepts which specifically belong to statistical physics:

Not in few particle quantum mechanics or in Classical Mechanics

- Temperature

# Interesting Physical Science Advances have a Major Statistical Component

Bekenstein-Hawking: entropy of black holes

Fluctuation spectrum of 3 degree kelvin background radiation

Bell's theorem: statistics of quantum measurements

source of complexity in the universe

probabilities of hearing from civilizations elsewhere in universe

Why do markets crash?

Time Reversal Invariance: Nature of Irreversability

Probabilities of major earth-asteroid collision

Probabilistic interpretation of quantum mechanics and of wave functions.

Is our universe likely?

# Part 2. Start with Probabilities: Dice

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

probability of choosing a side with number $\alpha = \rho_\alpha$ $\rho_\alpha = N_\alpha/N$ i.1

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

$r_\alpha$ = relative probability of $\Sigma_\alpha\ r_\alpha$ $\rho = r_\alpha/z$

fair dice --> all probabilities ll values of $\alpha$

average number on a throw $\alpha = 3.5$

general rule: To calculate th
function $f(\alpha)$ that gives the p $(\alpha)\rho_\alpha$ i.3
will come out will be $\alpha$, you

Do we understand what th . loaded die? An
average from a loaded die? the other values,
and these others were all 'hat would we have
for the average throw on t

# Part 2. Start with Probabilities: Dice

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

probability of choosing a side with number $\alpha = \rho_\alpha$ $\qquad \rho_\alpha = N_\alpha / N \qquad$ i.1

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

$r_\alpha$ = relative probability of event $\alpha$. e.g. for fair dice $r_\alpha$ = const $\qquad z = \sum_\alpha r_\alpha \qquad \rho = r_\alpha / z$

fair dice --> all probabilities are equal --> $\qquad \rho_\alpha = 1/6 \qquad$ for all values of $\alpha$

average number on a throw =

$$< \alpha >= \sum_\alpha \rho_\alpha \alpha = 3.5$$

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

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

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# Part 3: Lattices

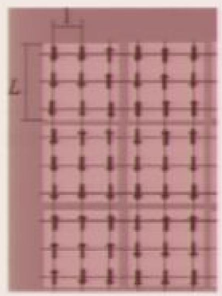
## Renormalization for d-2 Ising model

A. Pokrovskii & A. Patashinskii, Ben Widom, myself, Kenneth Wilson.

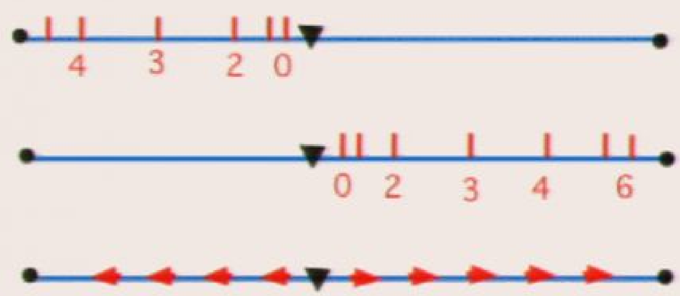
$Z = \mathrm{Trace}_{\{\sigma\}} \exp(W_K\{\sigma\})$

nagine that each box in the picture has in it a
ariable called $\mu_R$, where the **R**'s are a set of new
ttice sites with nearest neighbor separation $3a$. Each
ew variable is tied to an old ones via a
enormalization matrix $G\{\mu, \sigma\} = \prod_R g(\mu_R, \{\sigma\})$
here g couples the $\mu_R$ to the

$\sigma$'s in the corresponding box. We take each $\mu_R$ to
e ±1 and define g so that,
$\sum_\mu g(\mu, \{s\}) = 1$. For example, $\mu$ might be
efined to be an Ising variable with the
ame sign as the sum of $\sigma$'s in its box



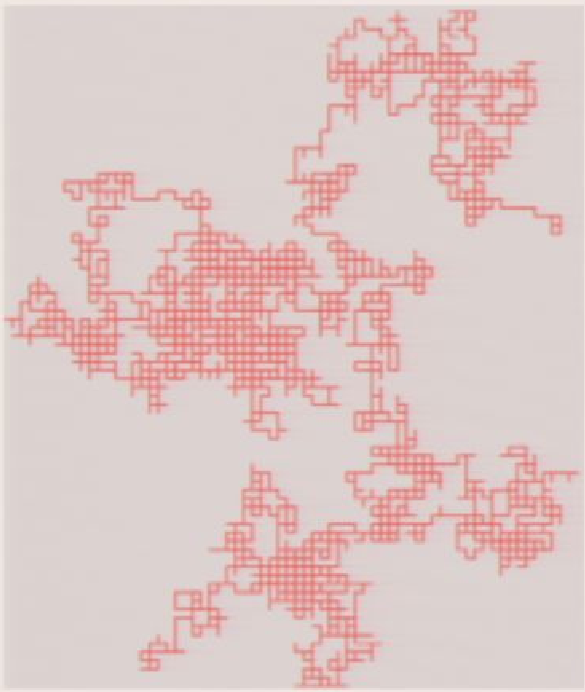

fewer degrees of fr
produces "block renor




• stable fixed point

▼ unstable fixed point

# Part 4: Random Walks & Diffusion



http://particlezoo.files.wordpress.com/2008/09/randomwalk.png

# Part 5 : Statistics of Motion

Albert Einstein (1905) explained this dancing by many, many collisions with molecules in fluid

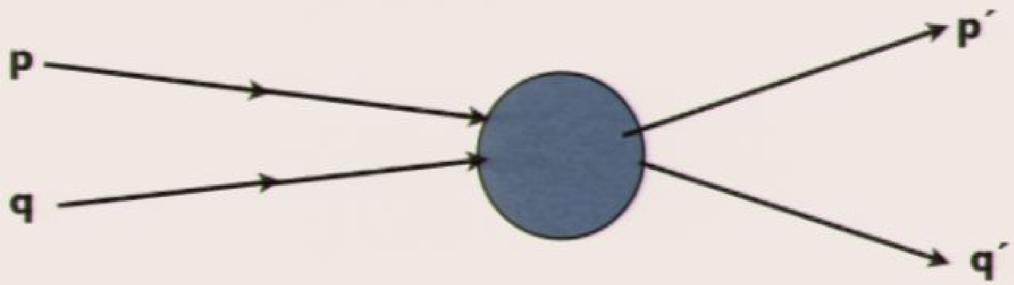
$$dp/dt = ...... + \eta(t) - p/\tau$$

$p=(p_x, p_y, p_z)$ $\qquad$ $\eta = (\eta_x, \eta_y, \eta_z)$

$\eta(t)$ is a Gaussian random variable resulting from random kicks produced by collisions. Since the kicks have random directions $\langle\eta(t)\rangle=0$. Different collisions are assumed to be statistically independent

$$\langle\eta_j(t)\, \eta_k(s)\rangle = \Gamma\,\delta(t-s)\,\delta_{j,k}$$

$$\partial_t f(\mathbf{p},\mathbf{r},t) + (\mathbf{p}/m)\cdot\nabla_{\mathbf{r}} f(\mathbf{p},\mathbf{r},t) - \nabla_{\mathbf{r}} U(\mathbf{r},t)\cdot\nabla_{\mathbf{p}} f(\mathbf{p},\mathbf{r},t) = \text{ effects of collisions}$$



# Part 6: Bose & Fermi: (probably not this time)

particle statistics, i.e. the symmetry properties of the particles' wave functions, have a major role in determining the behavior of many interesting physical systems. This is especially true when the system is degenerate, i.e. there is a sufficiently high density of identical particles so that there could be a substantial overlap of the wave functions involved. Important degenerate systems include:

for fermions:

- the electrons in atoms
- 

for non-conserved bosons

- 

for conserved bosons:

- 

# Part 7: Phase Transitions and Mean Fields

phases of matter:

•

which symmetries of nature have been lost in the snowflake?

•

•

are they really lost?

http://azahar.files.wordpress.com/2008/12/snowflake_.jpg

# Part 8: After Mean Fields: Big Words

Universality:

In appropriate limits, very different systems can have essentially identical properties

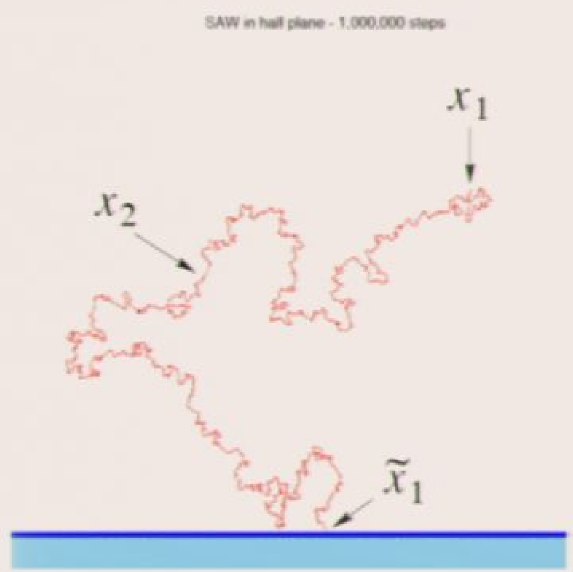
Scale Invariance

Systems look the same at different spatial scales

Renormalization

Take advantage of scale invariance and universality to produce a theory of phase transitions.

A scale invariant walk:



# Conformal Symmetry in Statistical Physics

Correlations, Maps, and symmetries on the Riemann sphere

$z \dashrightarrow z+a$

$z \dashrightarrow \lambda z$

$z \dashrightarrow 1/z$

# A start:

Ising system has as its basic variable a spin, $\sigma_z$ which takes on the values ±1.

We shall use the abbreviation, $\sigma$ for this spin.

The behavior of a physical system is described by its Hamiltonian. If we put this spin in a magnetic field in the z-direction it has a Hamiltonian $H = -\mu B_z \sigma$ .

Statistical Mechanics is defined by a probability. Here the probability is

$\rho(\sigma) = (1/z)\ \exp[-H/(k_B T)] = (1/z)\ \exp[\mu B_z \sigma/(k_B T)]$

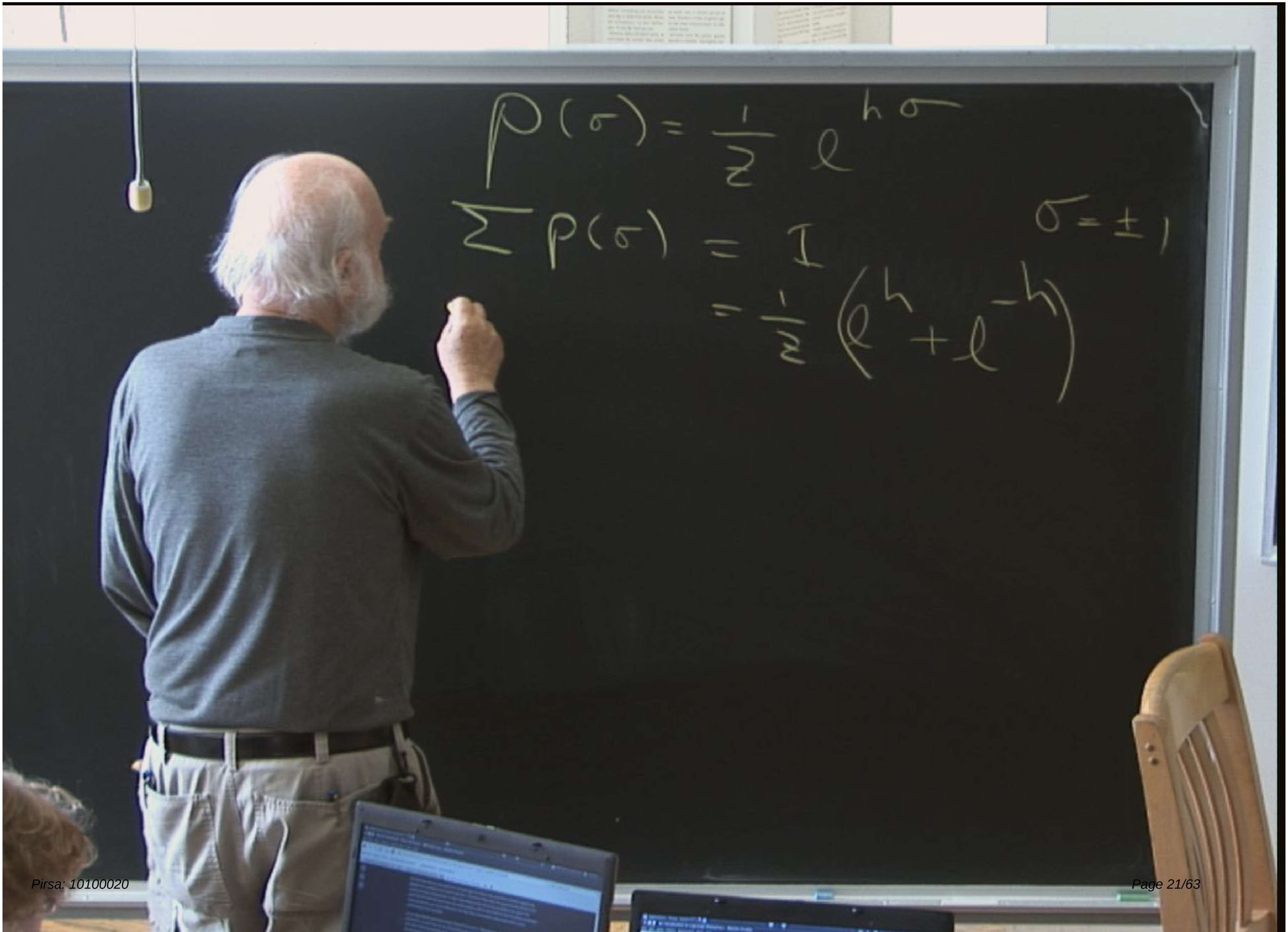
We describe this by using the abbreviation, $h$, for the parameters in the probability

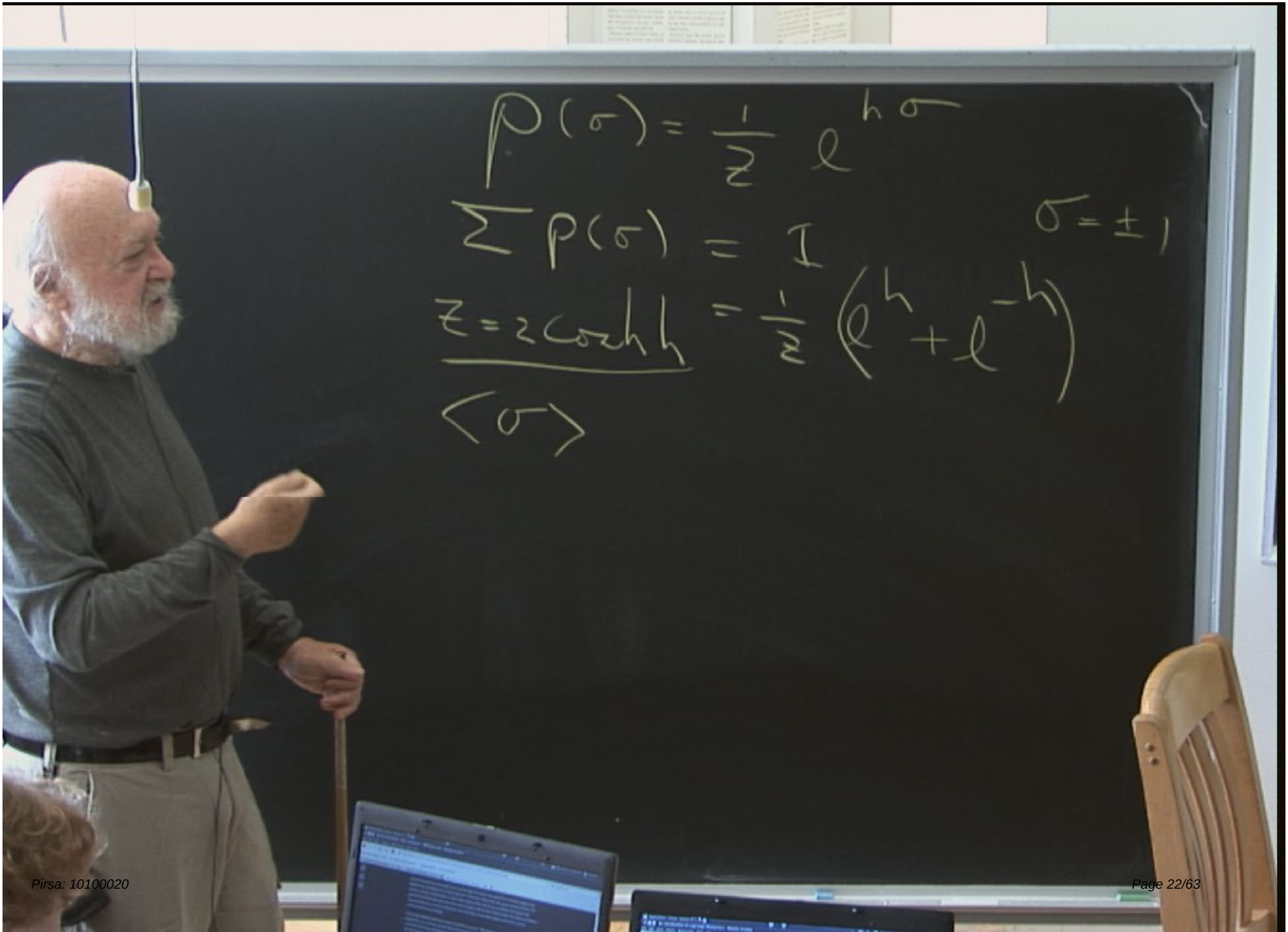
$\rho(\sigma) = (1/z)\ \exp(h\ \sigma) \qquad h = \mu B_z /(k_B T)$

normalization: total probability $=1= \rho(1) + \rho(-1) = (1/z)\ \exp(h) + (1/z)\ \exp(-h)$
therefore $z = \exp(h) + \exp(-h) = 2 \cosh h$

average $X = \langle X \rangle = \sum_\alpha \rho(\alpha)\ X_\alpha$

therefore $\langle \sigma \rangle = \rho(1)1 + \rho(-1)(-1) = 1/(2 \cosh h)\ \{\exp(h) - \exp(-h)\}$
$= (2 \sinh h) /(2 \cosh h) = \tanh h$


$p(\sigma) = \frac{1}{Z} e^{h\sigma}$
$\sum p(\sigma) = 1$
$= \frac{1}{Z}(e^{h} + e^{-h})$
$\sigma = \pm 1$


$\rho(\sigma) = \frac{1}{Z} e^{h\sigma}$
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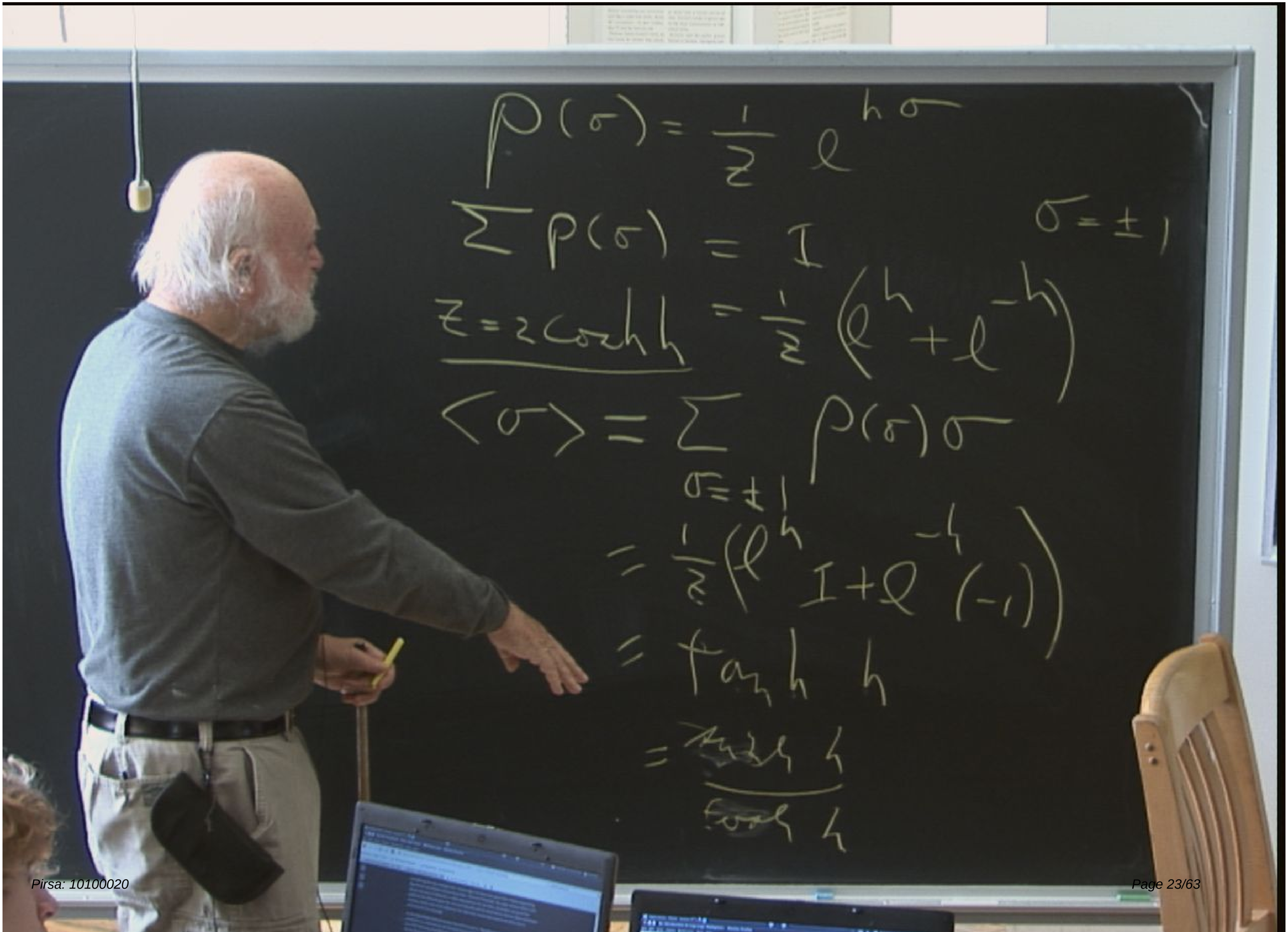
$Z = 2\cosh h = \frac{1}{2}\left(e^{h} + e^{-h}\right)$
$\langle \sigma \rangle$



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$\langle\sigma\rangle = \sum_{\sigma=\pm 1} \rho(\sigma)\sigma$
$= \frac{1}{Z}\left(e^{h} 1 + e^{-h}(-1)\right)$
$= \tanh h$
$= \frac{\sinh h}{\cosh h}$

$$\rho(\sigma) = \frac{1}{Z} e^{h\sigma}$$

$$\sum \rho(\sigma) = 1 \qquad \sigma = \pm 1$$

$$\underline{Z = 2\cosh h} = \frac{1}{Z}\left(e^{h} + e^{-h}\right)$$

$$\langle \sigma \rangle = \sum_{\sigma = \pm 1} \rho(\sigma)\,\sigma$$

$$= \frac{1}{Z}\left(e^{h}\, 1 + e^{-h}(-1)\right)$$

$$= \tanh h$$

$$= \frac{\sinh h}{\cosh h}$$

# Averages from Derivatives

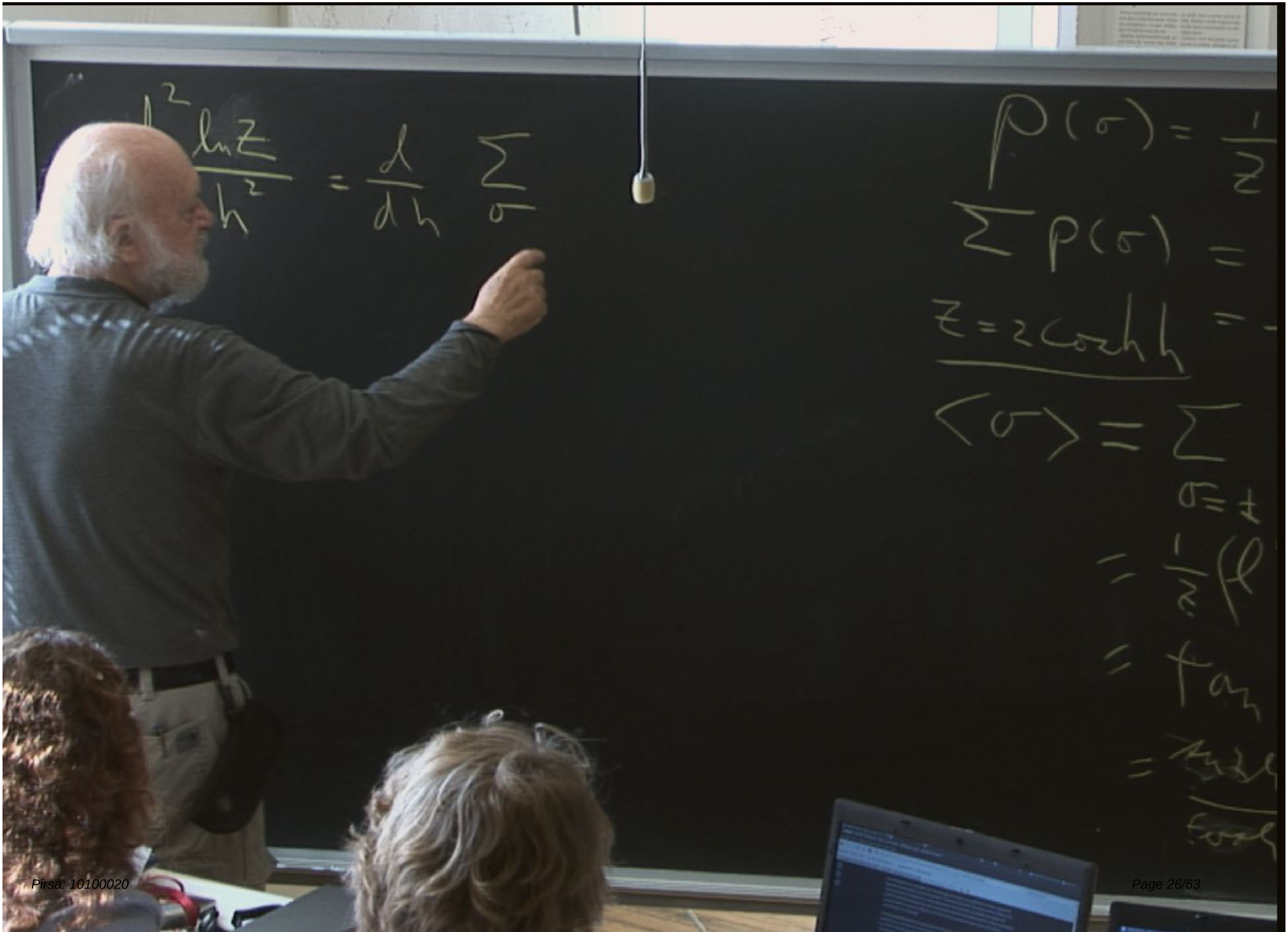
$$z = \sum_{\sigma} \exp(h\sigma) = 2\cosh h$$

$$d(\ln z) / dh = \sum_{\sigma} \sigma \exp(h\sigma) / z = <\sigma> = \tanh h$$

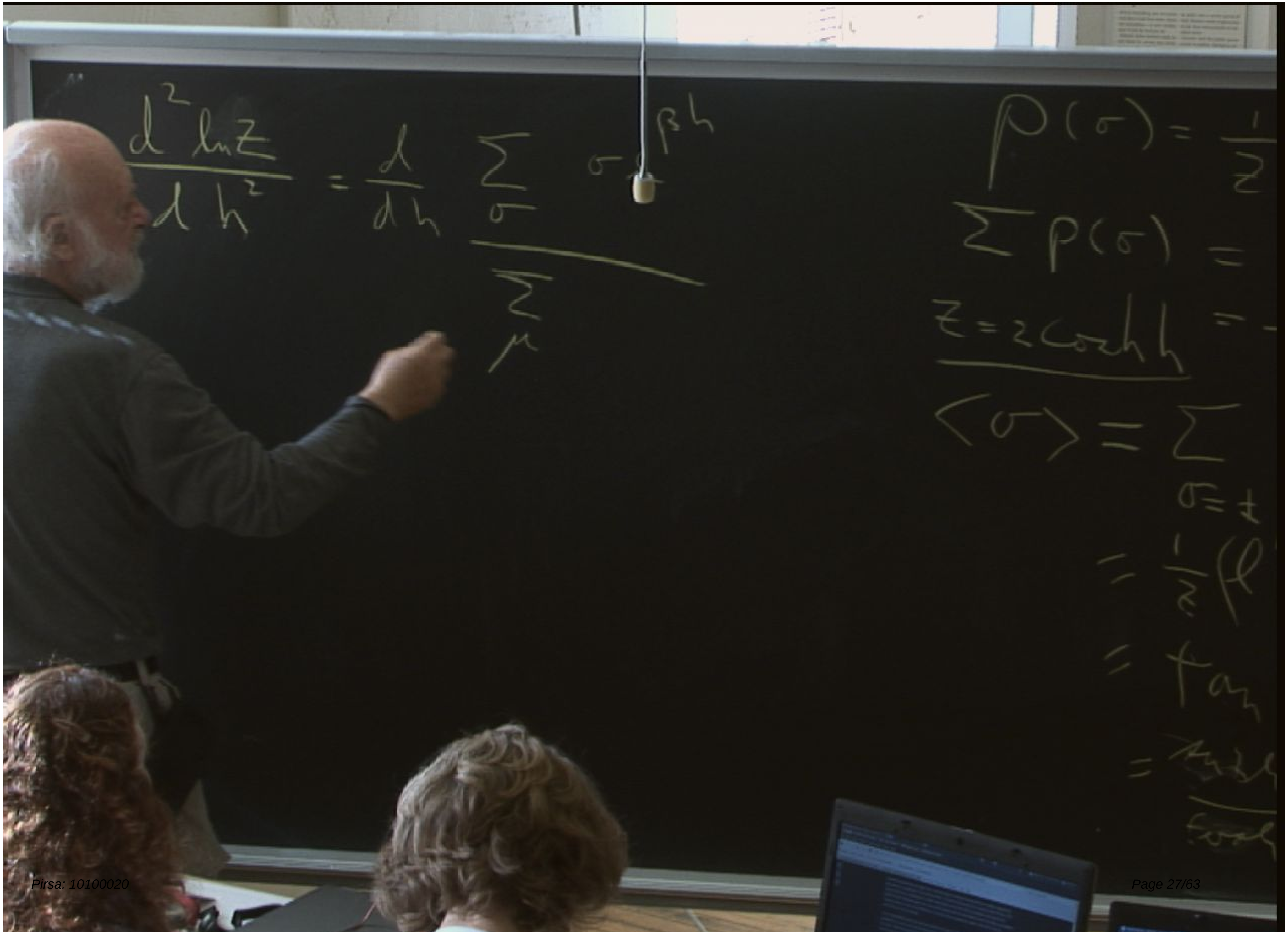
$$d^2(\ln z) / (dh)^2 = \sum_{\sigma} (\sigma - <\sigma>)^2 \exp(h\sigma) / z = <(\sigma - <\sigma>)^2>$$

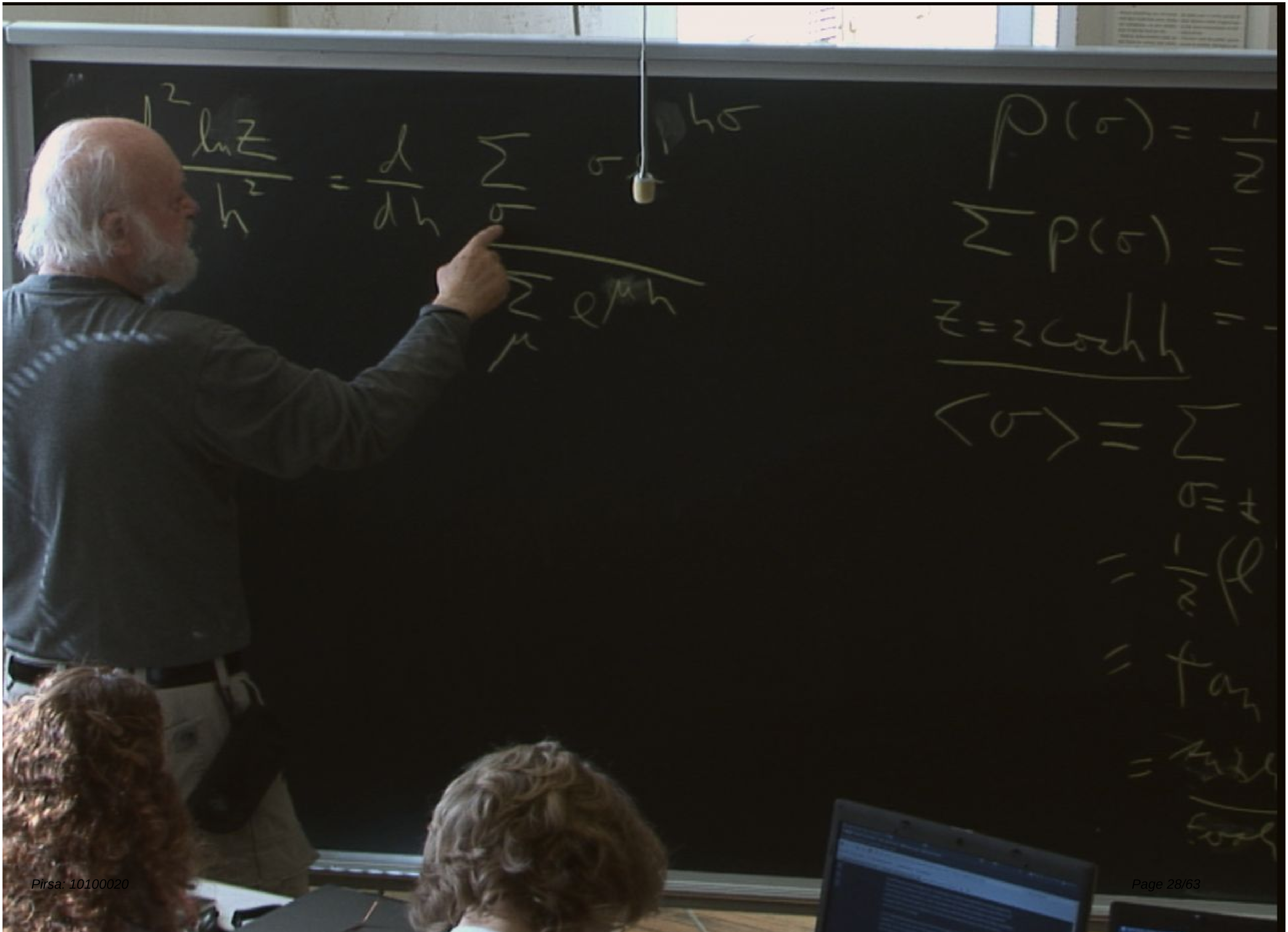
$$= 1 - <\sigma>^2 = 1 - (\tanh h)^2$$

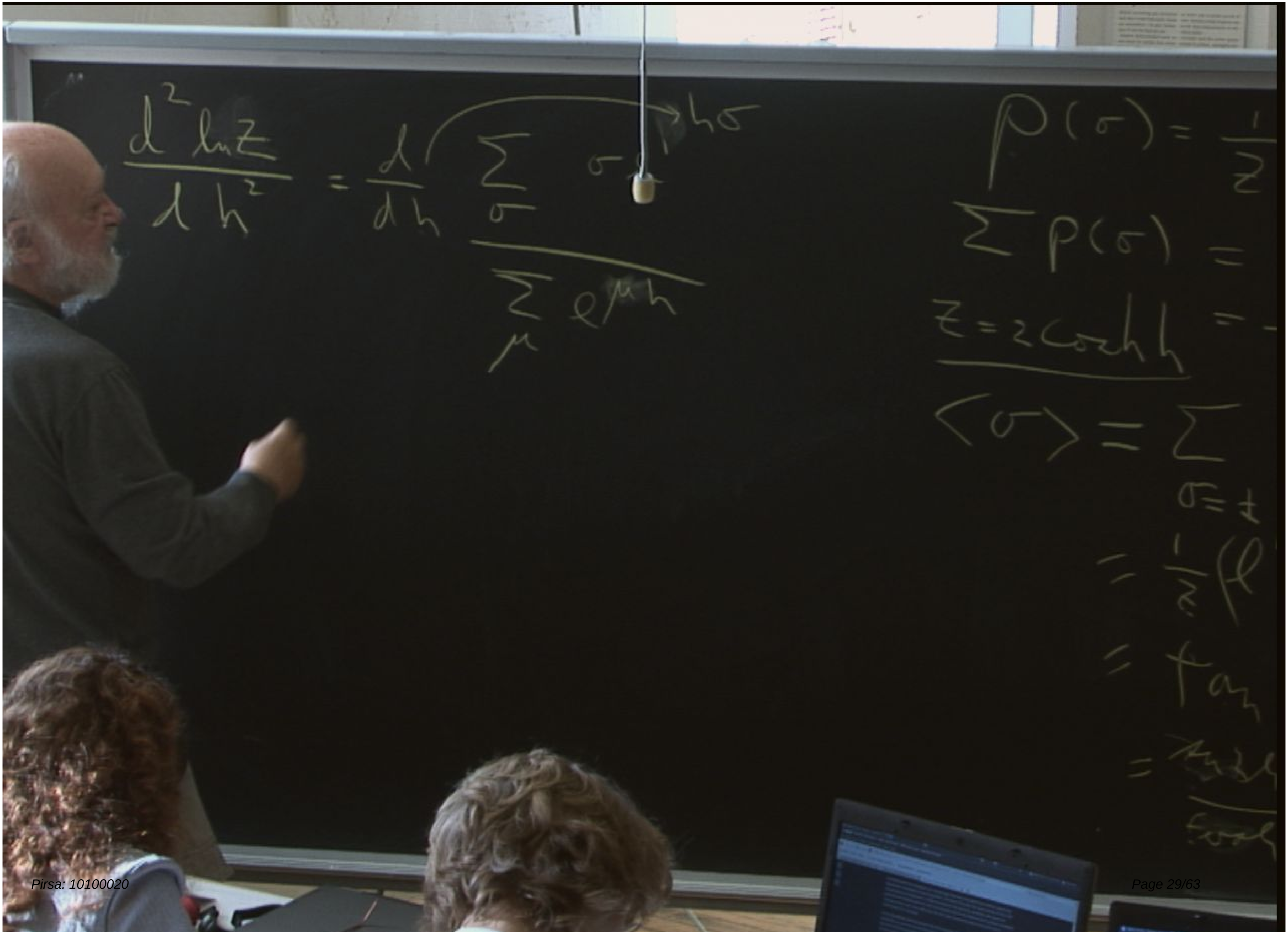
All derivatives of the log of the partition function are thermodynamic functions of some kinds. As I shall say below, we expect simple behavior from the log of Z but not Z itself. The derivatives described above are respectively called the magnetization, $M=<\sigma>$ and the magnetic susceptibility, $\chi$, = dM/dH. The analogous first derivative with respect to $\beta$ is minus the energy. The next derivative with respect to $\beta$ is proportional to the specific heat, or heat capacity, another traditional thermodynamic quantity. The derivative of partition function with respect to volume is the pressure.



$\frac{d}{dh} \sum_\sigma$
$\rho(\sigma) = \frac{1}{Z}$
$\sum p(\sigma) =$
$Z = 2\cosh h$
$\langle\sigma\rangle = \sum$
$\sigma = \pm$


$\frac{d^2 \ln Z}{d h^2} = \frac{d}{dh} \sum_\sigma \sigma e^{\beta h}$
$\sum_\mu$
$\rho(\sigma) = \frac{1}{Z}$
$\sum p(\sigma) =$
$Z = 2\cosh h$
$\langle \sigma \rangle = \sum$
$\sigma = \pm$


Z = 2cosh h
⟨σ⟩ = Σ
σ = ±



d²lnZ/dh² = d/dh Σσ σ e^{hσ} / Σμ e^{μh}
ρ(σ) = 1/Z
Σ p(σ) =
Z = 2cosh h
⟨σ⟩ = Σ
σ=±
= 1/Z
= tan

$$\frac{d^2 \ln Z}{dh^2} = \frac{d}{dh} \frac{\sum_\sigma \sigma \, e^{h\sigma}}{\sum_\mu e^{\mu h}}$$

$$\rho(\sigma) = \frac{1}{Z}$$

$$\sum p(\sigma) =$$

$$\underline{Z = 2\cosh h} =$$

$$\langle \sigma \rangle = \sum$$

$\sigma = \pm$

$$= \frac{1}{Z}(e$$

$$= \tan$$

$$= \frac{\sinh}{\cosh}$$

# Averages from Derivatives

$$z = \sum_{\sigma} \exp(h\sigma) = 2\cosh h$$

$$d(\ln z) / dh = \sum_{\sigma} \sigma \exp(h\sigma) / z = <\sigma> = \tanh h$$

$$d^2(\ln z) / (dh)^2 = \sum_{\sigma} (\sigma - <\sigma>)^2 \exp(h\sigma) / z = <(\sigma - <\sigma>)^2>$$

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# End Survey: Start More Intensive/Extensive Discussions

Do you know what intensive and extensive mean in statistical physics?

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# Homework

Work out the value of the pressure for a classical relativistic gas with H=|**p**|c. Do this both by using kinetic theory, as just above, and also by differentiating the partition function.

The Hamiltonian for N particles in a fluid is $H= \sum_\alpha \mathbf{p}_\alpha^2/(2m) + \sum_{\alpha<\beta} V(r_\alpha - r_\beta)$. If the interaction, V, is weak we can assume that the particles move independently of one another. What is the value of the pressure? How does this result relate to van der Waals' approximate equation of state for a fluid?

The length of a random walk of $N$ steps is of the form of a sum of $N$ iid variables $\sigma_j$ each of which takes on the values 0 and ±1 with equal probability. What is the probability that a walker who takes 1000 steps will end up at a point at least 30 steps away from her starting point? (A relative accuracy of two decimal digits will suffice.)

## 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

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# Simple probabilities (reprise)

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

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

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

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

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

from r to $\rho$ $z = \sum_\alpha r_\alpha$ 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 $\alpha$

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# Composite Probabilities

$\alpha$ and $\beta$ are two different kinds of events

$\alpha$ might describe the temperature on January 1, $\rho_\alpha$ computed as $N_\alpha / N$

$\beta$ might describe the precipitation on December 31, with probabilities $\rho'_\beta$

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 $\alpha$ occurs if that we know that event $\beta$ 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 $\alpha$ is independent of $\beta$ then $\beta$ is independent of $\alpha$.

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

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

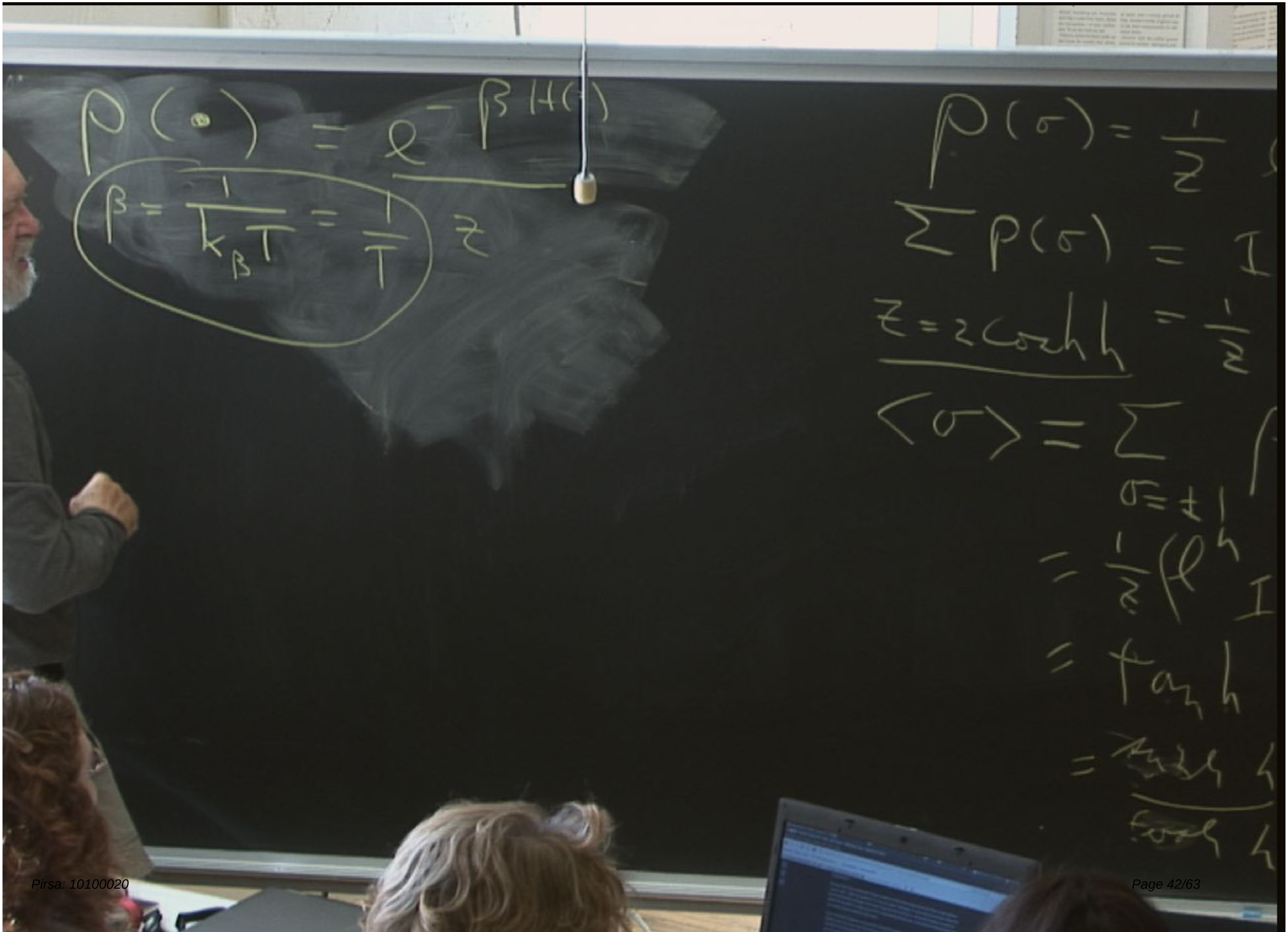
equivalently, two events are statistically independent, if the number of times both show up is expressed in terms of the number of times each one individually shows up as

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

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"!


ρ(σ) = e^{-βH(σ)} / Z
β = 1/(k_β T) = 1/T
ρ(σ) = 1/Z
Σ ρ(σ) = 1
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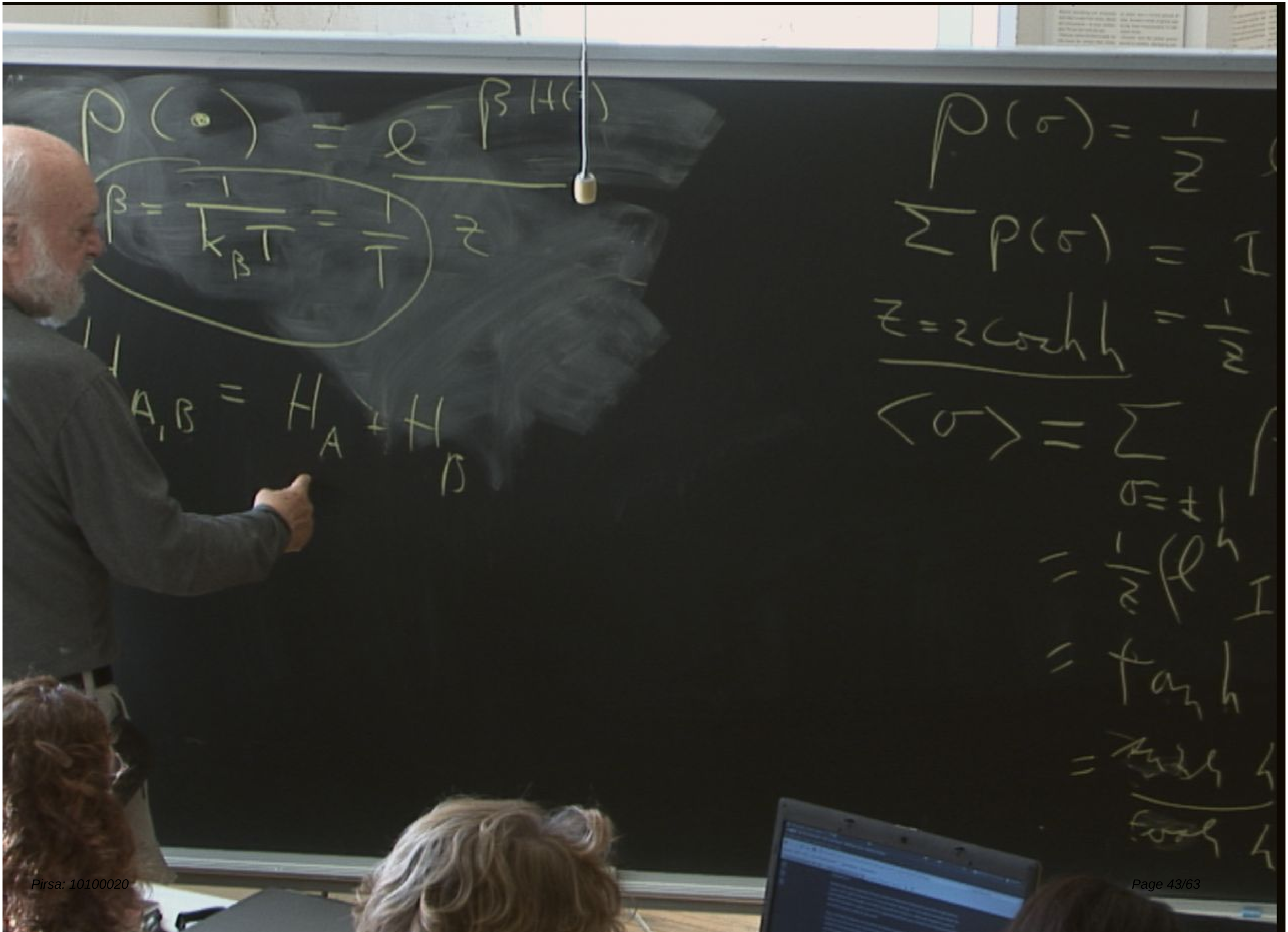
ρ(σ) = 1/Z
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H_{A,B} = H_A + H_B
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⟨σ⟩ = Σ
σ = ±1
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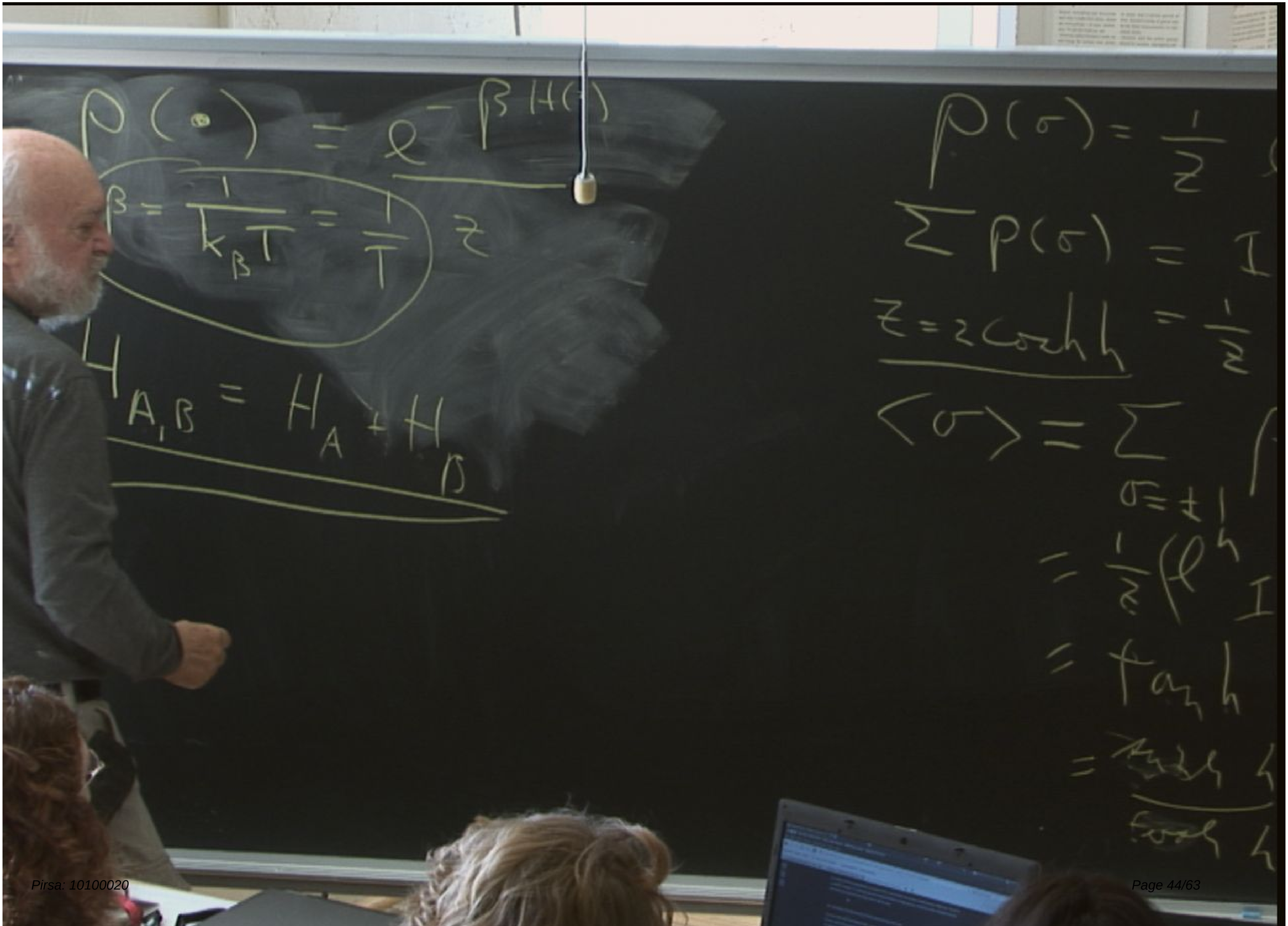
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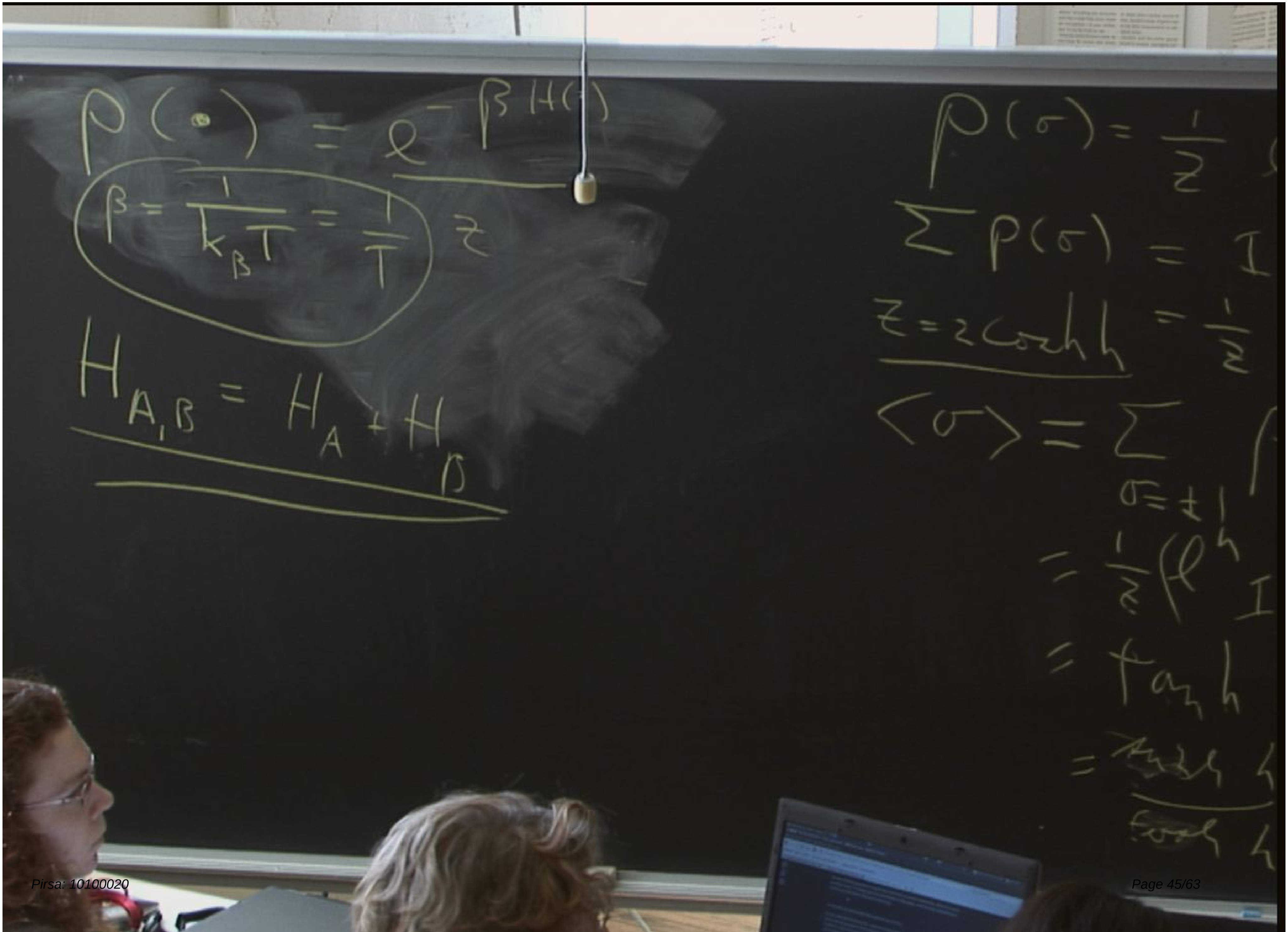
$\beta = \frac{1}{k_\beta T} = \frac{1}{T}$
$H_{A,B} = H_A + H_B$
$\rho(\sigma) = \frac{1}{Z}$
$\Sigma\, \rho(\sigma) = 1$
$Z = 2\cosh h$
$\langle\sigma\rangle = \sum_{\sigma=\pm 1}$
$= \tanh h$

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* 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 ?

# 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

$$Z = \prod_{\alpha=1}^{N} \sum_{\sigma^\alpha=\pm1} \exp(h\sigma^\alpha) = (2\cosh h)^N = z^N \qquad \text{ii.4}$$

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

## 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. The same law which gives the force for a single electron also gives the force pattern produced outside a spherically symmetric object containing many charged particles.

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.

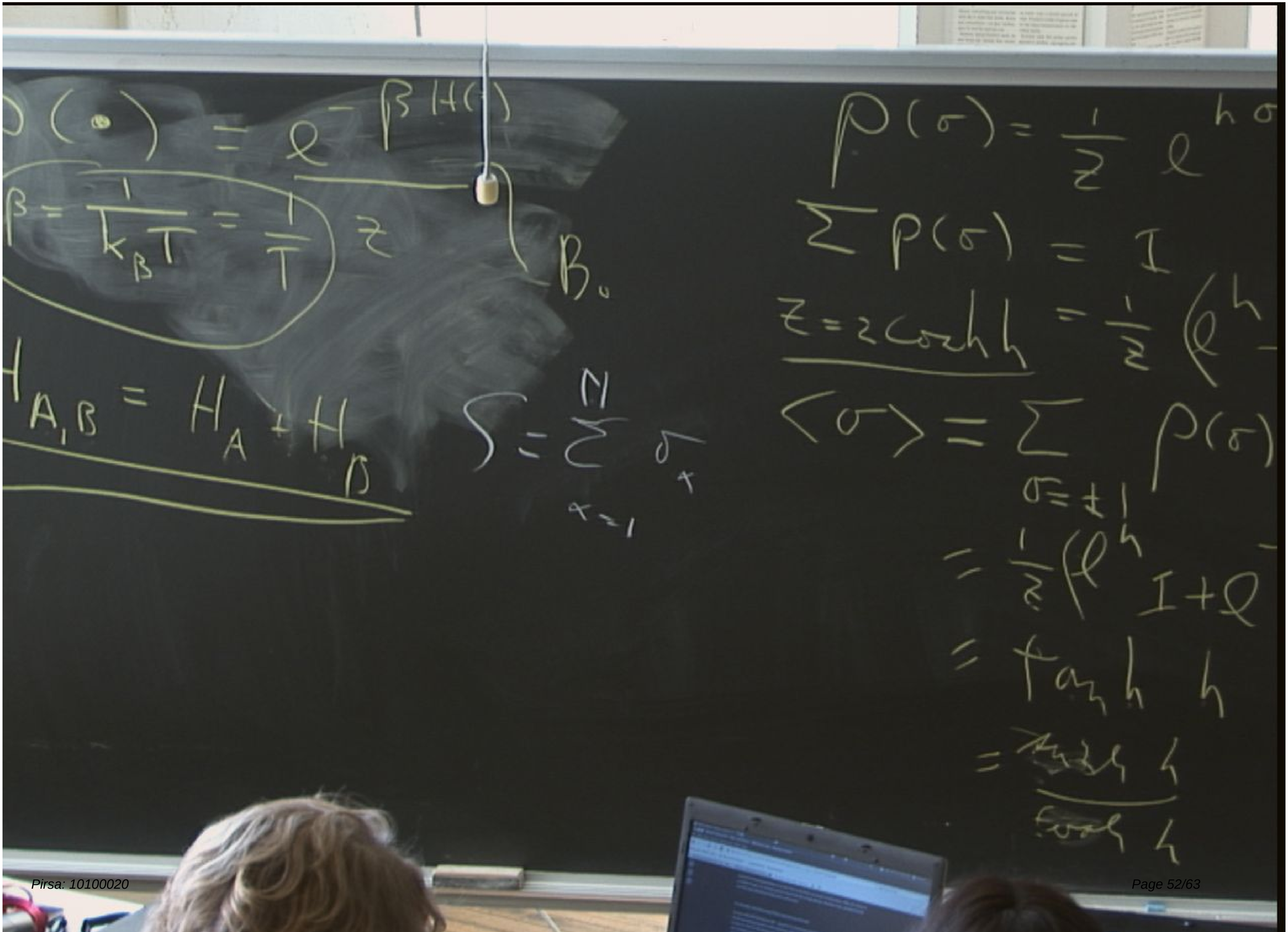
The sum of two statistically independent Gaussian variables is also Gaussian. How does the variance add up?

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 each of the individual variables is bounded.

Carl Friedrich Gauss (1777 – 1855)

A Gaussian distribution has a lot of structurally invariant properties.



ρ(•) = e^{-βH(σ)}
β = 1/(k_β T) = 1/T
Z
B_0
H_{A,B} = H_A + H_B
S = Σ_{α=1}^{N} σ_α
ρ(σ) = 1/Z e^{hσ}
Σ p(σ) = 1
Z = 2 cosh h = 1/Z (e^h
⟨σ⟩ = Σ_{σ=±1} ρ(σ)
= 1/Z (e^h 1 + e
= tanh h
= sinh h / cosh h

# 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

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

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

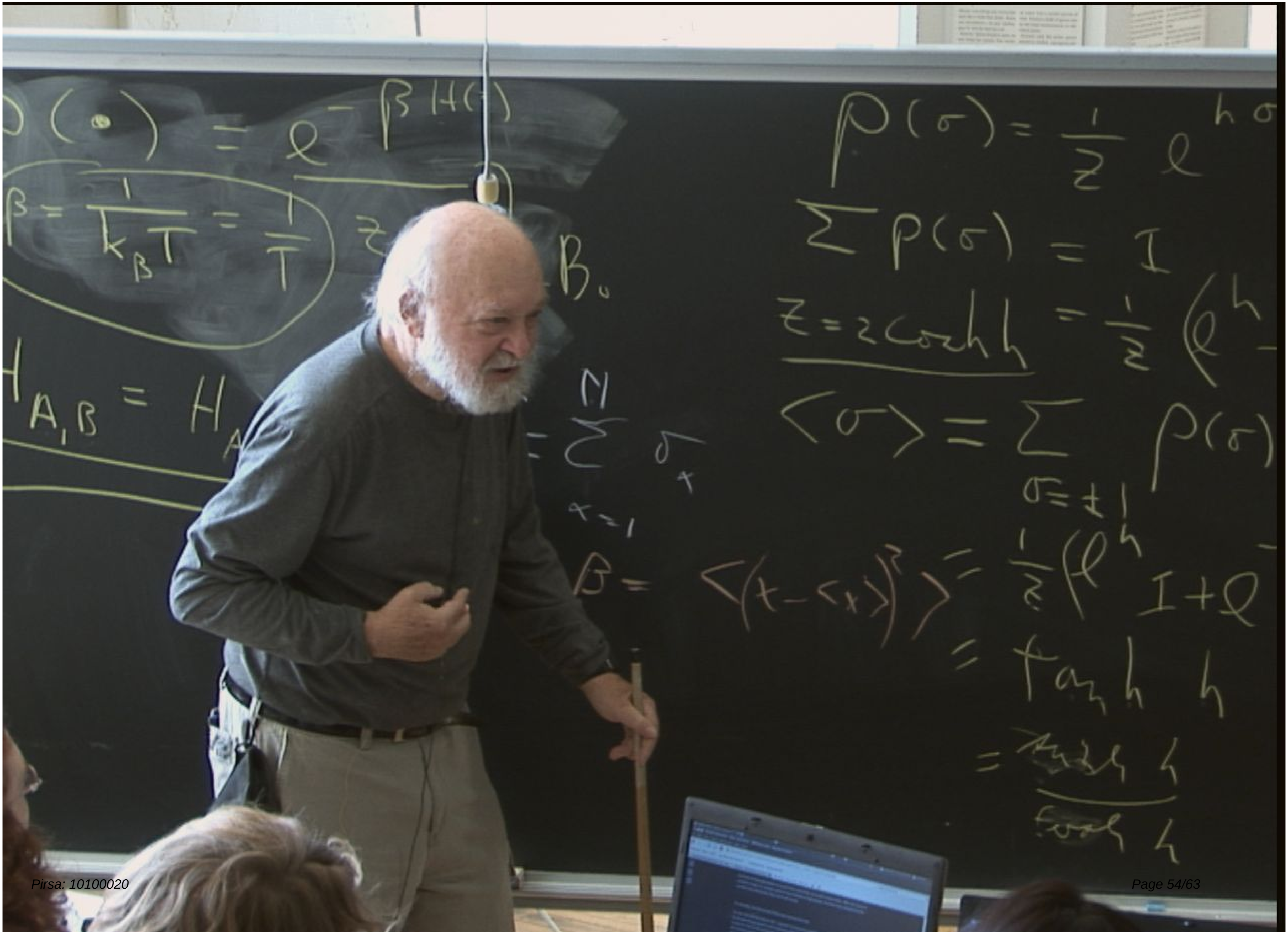
$$\rho(x) \sim \exp[-ax^2/2+bx+c] = \exp[-a(x-b/a)^2/2+b^2/(2a)+c]$$

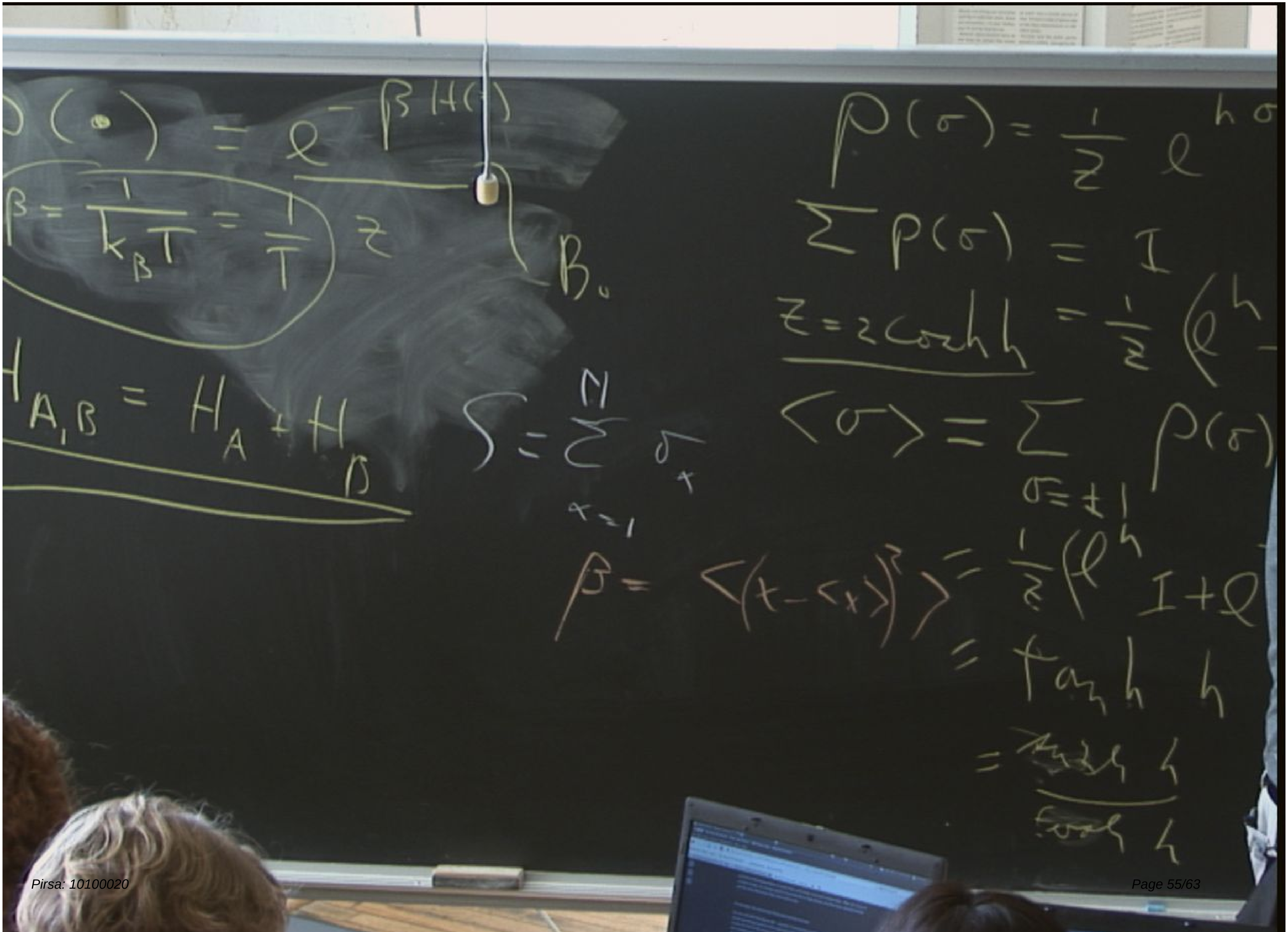
so pick $c=-b^2/(2a)+[\ln(\beta/2\pi)]/2$ we now have the canonical form

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

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

Notice how the $\beta$ that appears in the numerator of the probability distribution reappears in the denominator of the average.


Σ p(σ) = 1
Z = 2 cosh h
= tanh h



$\rho(\sigma) = \frac{1}{Z} e^{h\sigma}$
$\sum p(\sigma) = 1$
$Z = 2\cosh h$
$\langle\sigma\rangle = \sum_{\sigma=\pm1} \rho(\sigma)$
$= \tanh h$
$\beta = \frac{1}{k_B T} = \frac{1}{T}$
$H_{A,B} = H_A + H_B$
$S = \sum_{x=1}^{N} \sigma_x$
$\beta = \langle(x - \langle x\rangle)^2\rangle$

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## 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 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, $z = \int dp\,dr \exp[-\beta H]$

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

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 $kT/2$ for each quadratic degree of freedom. Thus a harmonic oscillator has $<H>=kT$.

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. Specifically $\ln Z = -F/T$ $\quad d(F/T) = -(p/T)\,d\Omega + <E>d\beta$ so knowing Z you can calculate average energy and pressure.

# Gaussian Averages

## The usual way

Let one particle be confined to a box of volume $\Omega$. 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)$^2$

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

# Many variables are as easy as one

Let M be an N by N symmetric real matrix with N positive real eigenvalues, $m_1, m_2, \ldots, m_\mu, \ldots m_N$ are the eigenvalues of this matrix. We can then easily calculate an integral involving many Gaussian variables by taking linear combinations of variables to diagonalize the matrix, M, giving

$$Z = \int d\phi_1 ... d\phi_N \exp[-\frac{1}{2} \sum_{i,j} \phi_i M_{i,j} \phi_j] = \left[(2\pi)^N / \det M\right]^{1/2}$$

The last equality follows from the fact that the determinant of M is the product of its eigenvalues. More specifically, if $M_{i,j}$ is a diagonal matrix,

# 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 $\Gamma$ 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

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

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!

We shall have an integral just like this later on.

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 a very large positive number.

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

$$\partial \ln Z / \partial\beta = -(1/Z)\int d^3p \; d^3r \; \varepsilon \exp(-\beta\varepsilon) = -\langle\varepsilon\rangle$$

$$\langle\varepsilon\rangle = 3/(2\beta) = (3/2)kT$$

## (The usual way)$^2$

$$\partial^2 \ln Z / \partial\beta^2 = -\partial\langle\varepsilon\rangle/\partial\beta = \;???$$

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