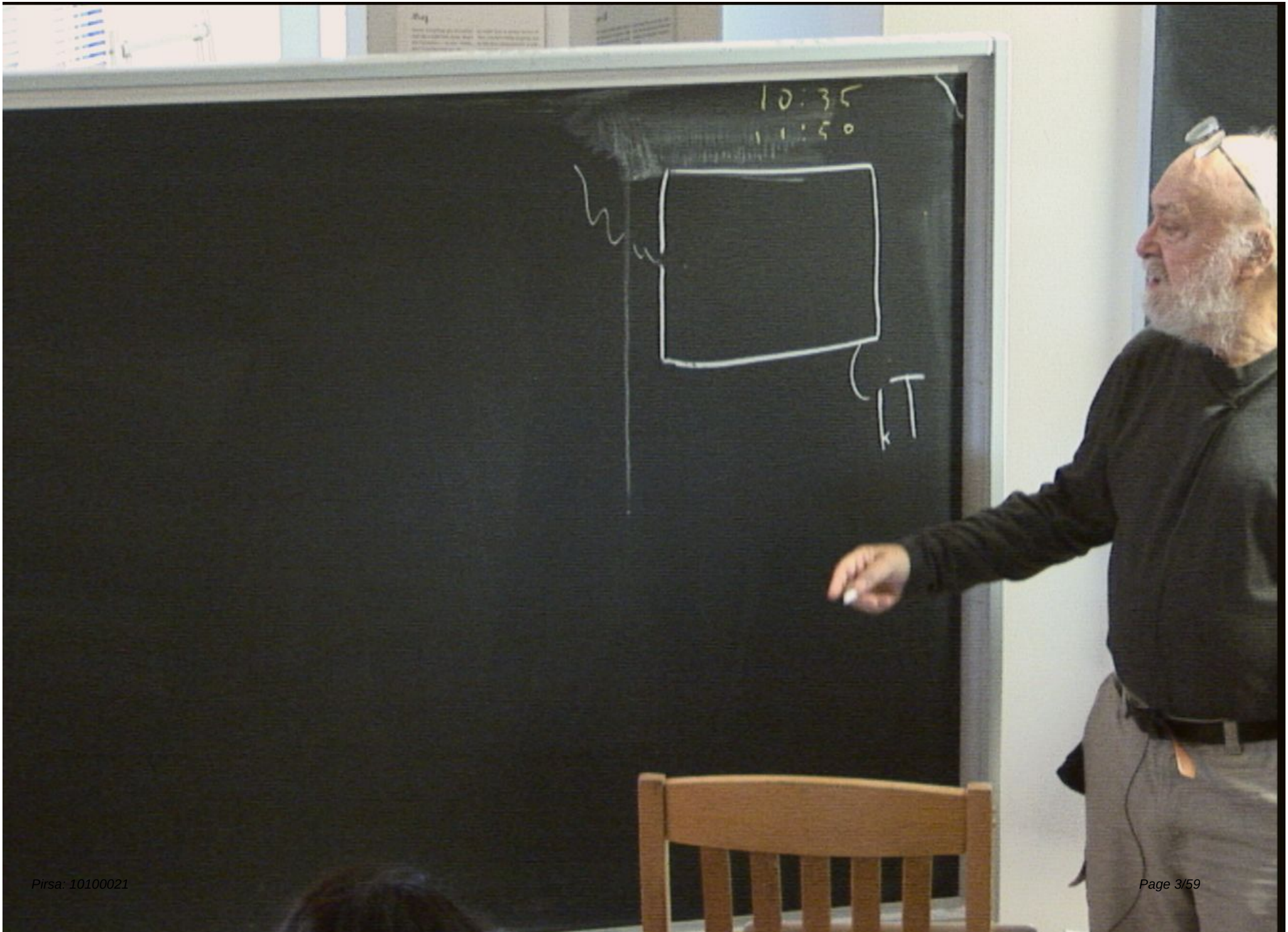
Title: Statistical Mechanics (PHYS 602) - Lecture 2

Date: Oct 05, 2010 10:30 AM

URL: http://pirsa.org/10100021

Abstract:


PERIMETER
INSTITUTE FOR THEORETICAL PHYSICS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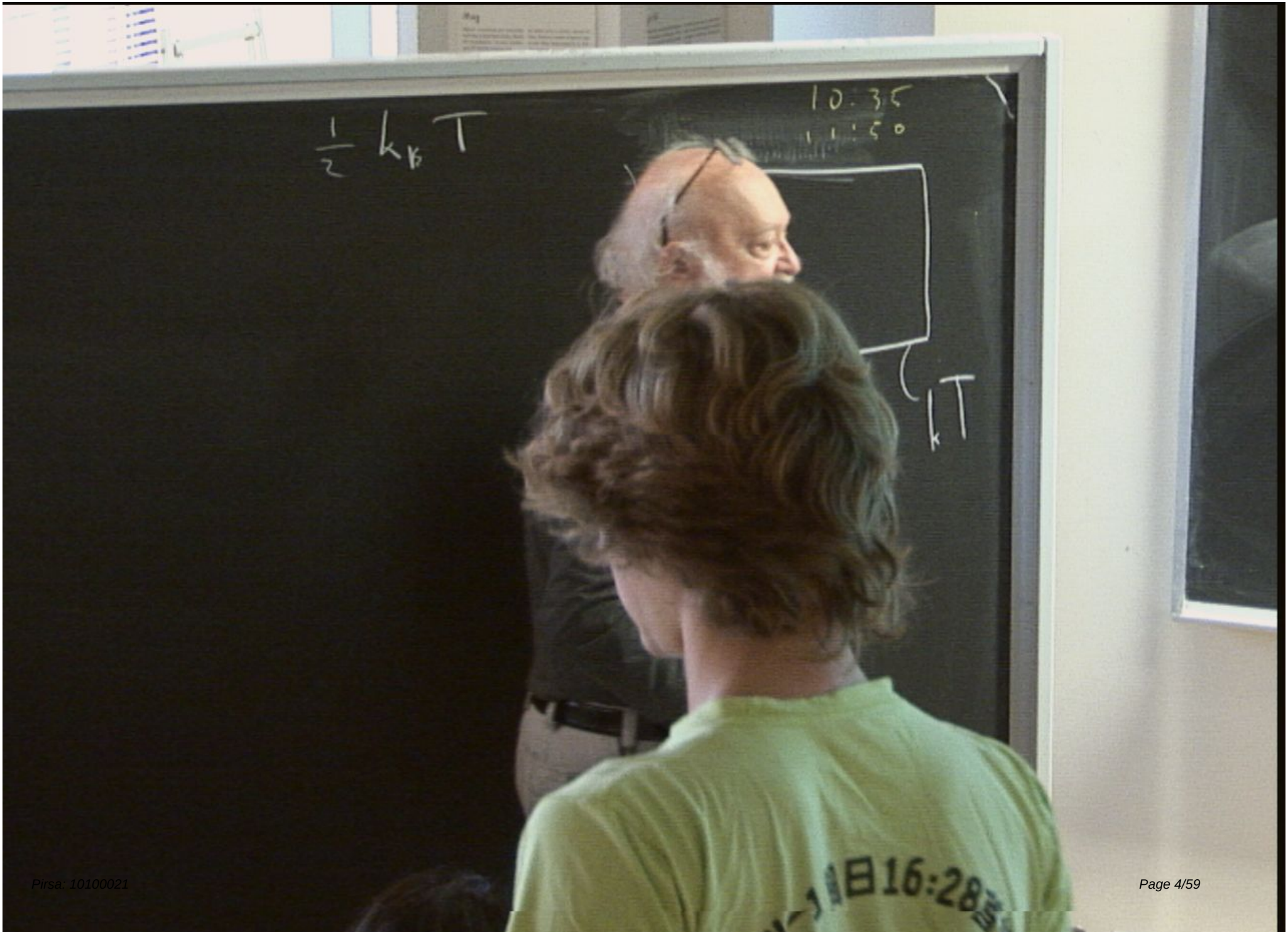
kT


$\frac{1}{2} k_B T$
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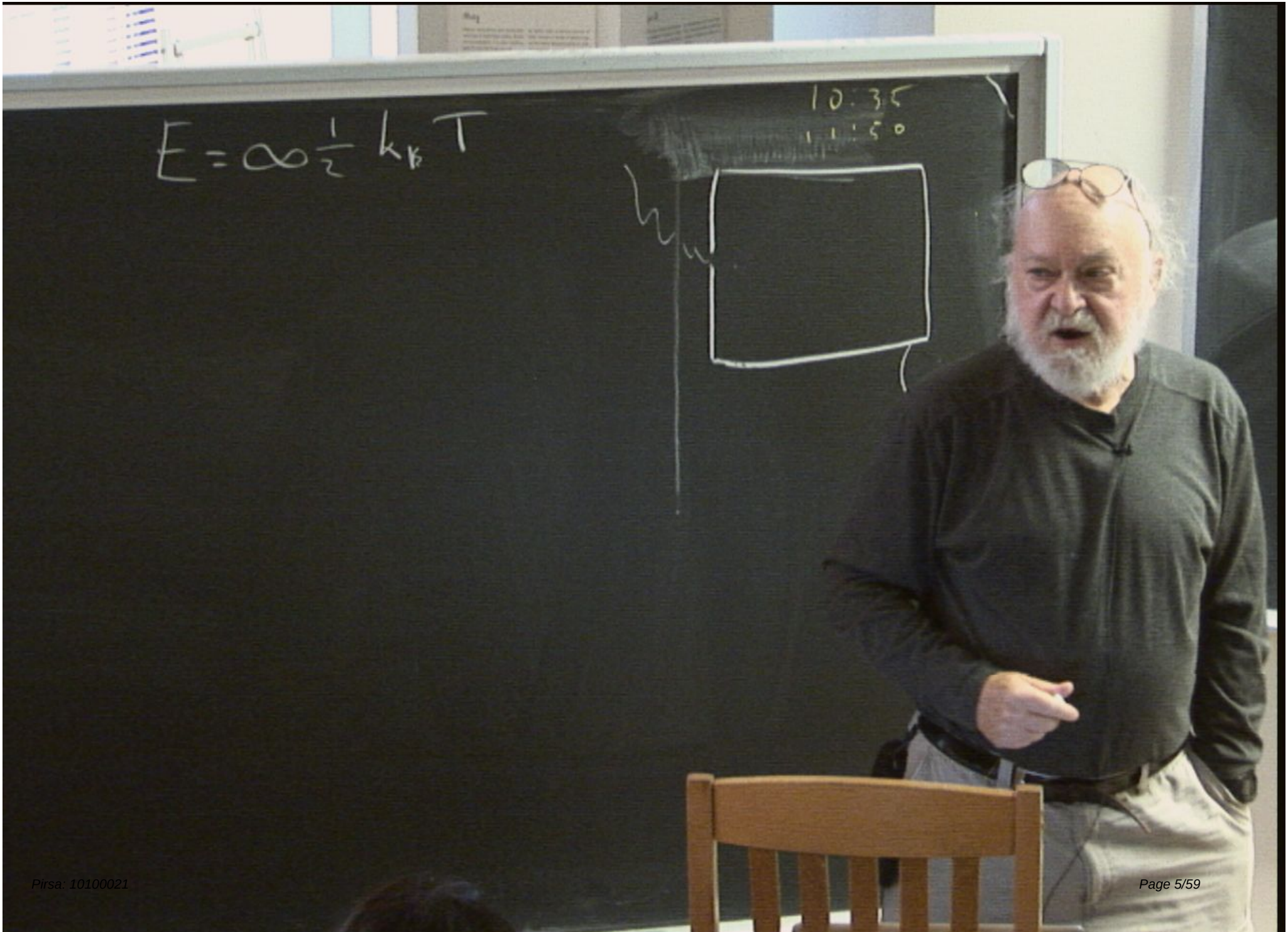
kT


$E = \infty \frac{1}{2} k_B T$
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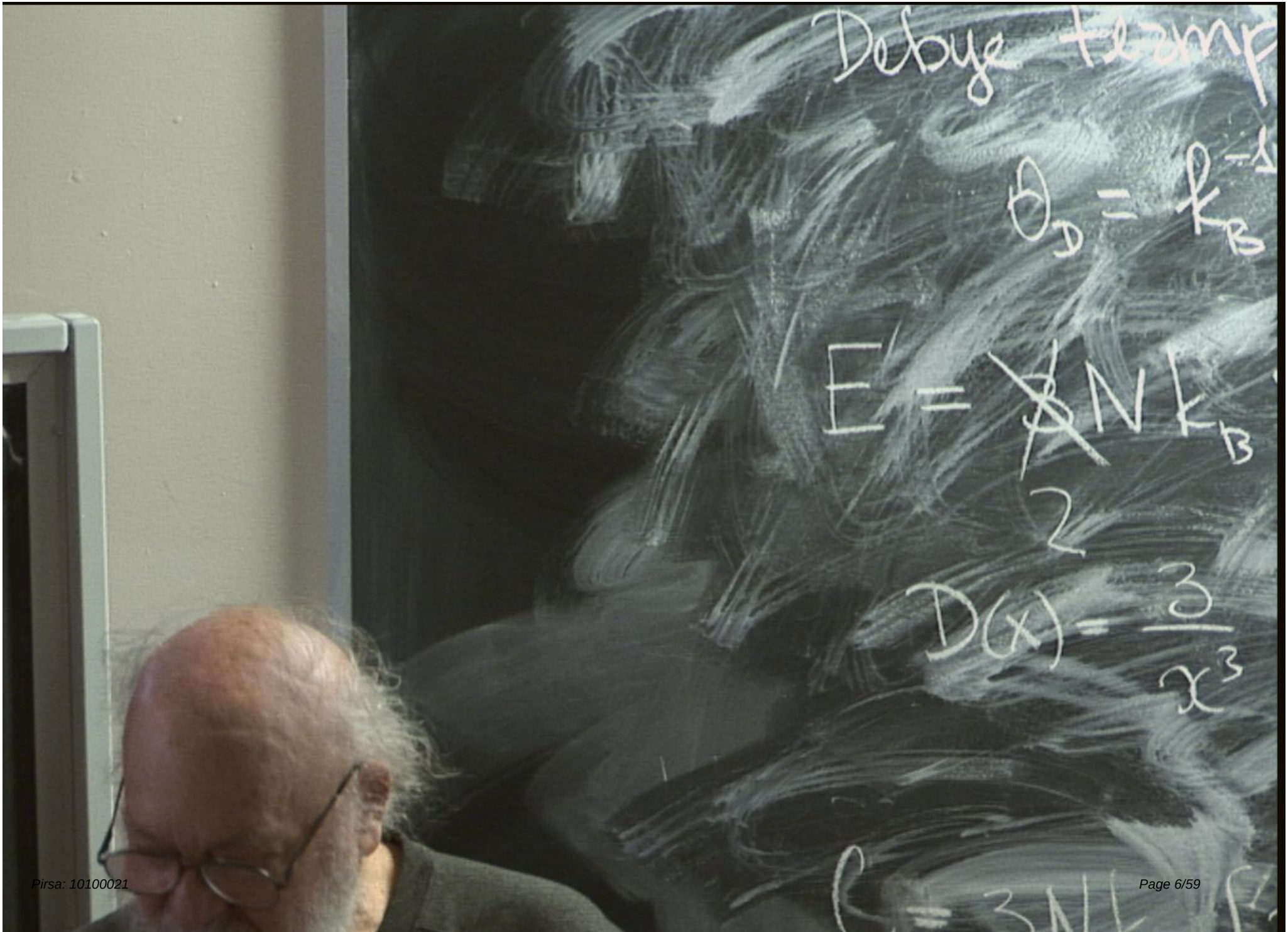
Debye temp
$\Theta_D = k_B$
$E = \frac{3}{2} N k_B$
$D(x) = \frac{3}{x^3}$

Start Here

I believe that my notes are correct in the definition of variance

$=\langle(X - \langle X\rangle)^2\rangle$

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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

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

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, $M_{i,j} = \delta_{i,j} m_i$ then it follows at once that $Z = \Pi_i (2\pi/m_i)^{1/2}$ since the determinant of M is the product of its eigenvalues. If M is not diagonal we form linear combinations of the ϕ's that are eigenstates of the matrix, M. If we use those linear combinations as integration variables, then our formula for the integration immediately follows once again.

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!

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.

Calculation of Averages and Fluctuations: Reprise

The usual way: in general

Let's start from a Hamiltonian on a Lattice

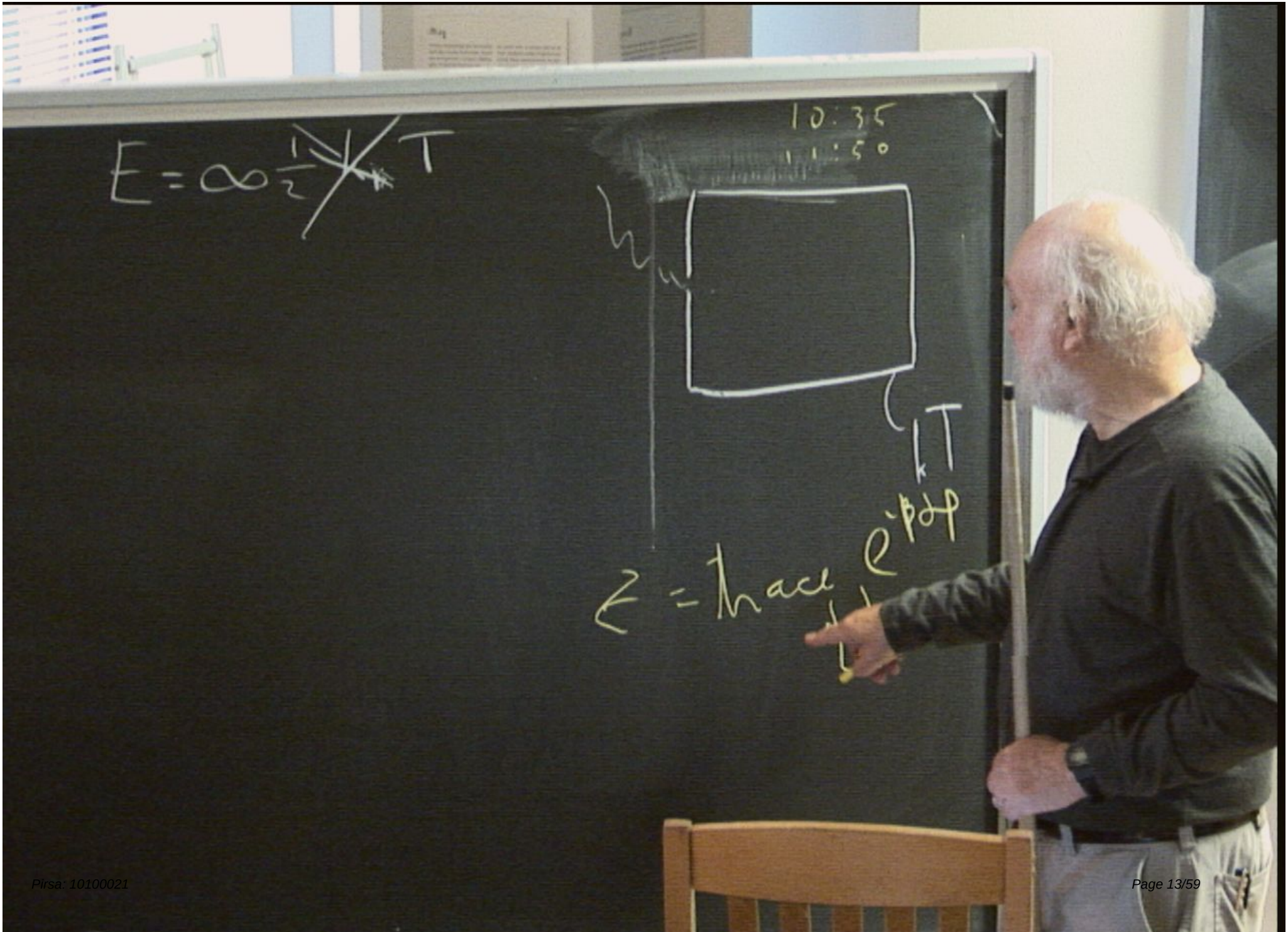
$$W\{\sigma\}=-\beta H\{\sigma\} = \sum_r h_r\sigma_r + \sum_{<r,s>} K\sigma_r\sigma_s$$

This Hamiltonian defines what is called the Ising model. The first sum is a sum over all lattice sites, ***r***. The second sum is a sum over nearest neighbors. The field, h_r, which depends upon ***r***, multiplies a spin variable which is different, of course, different on each site. The notation $\{\sigma\}$ says that these things depend upon many spin variables. You can assume that the spin variables take on the value +1 or -1 if you want, but the argument below on this slide is very general and the result does not depend upon what σ might be. Start from Z =Tr exp $W\{\sigma\}$ where Tr means a summation over all possible values of all the spin variables. It is a repeat of the argument that we have given before to say that

$$<\sigma_r>= \partial \ln Z/ \partial h_r$$

The partial derivative means that we hold all other h's constant. The second derivative is given by

$$<\sigma_r \sigma_s> - <\sigma_r><\sigma_s>= <[\sigma_r - <\sigma_r>][\sigma_s-<\sigma_s>]> = \partial^2 \ln Z/ \partial h_s \partial h_r = \partial <\sigma_s>/ \partial h_r$$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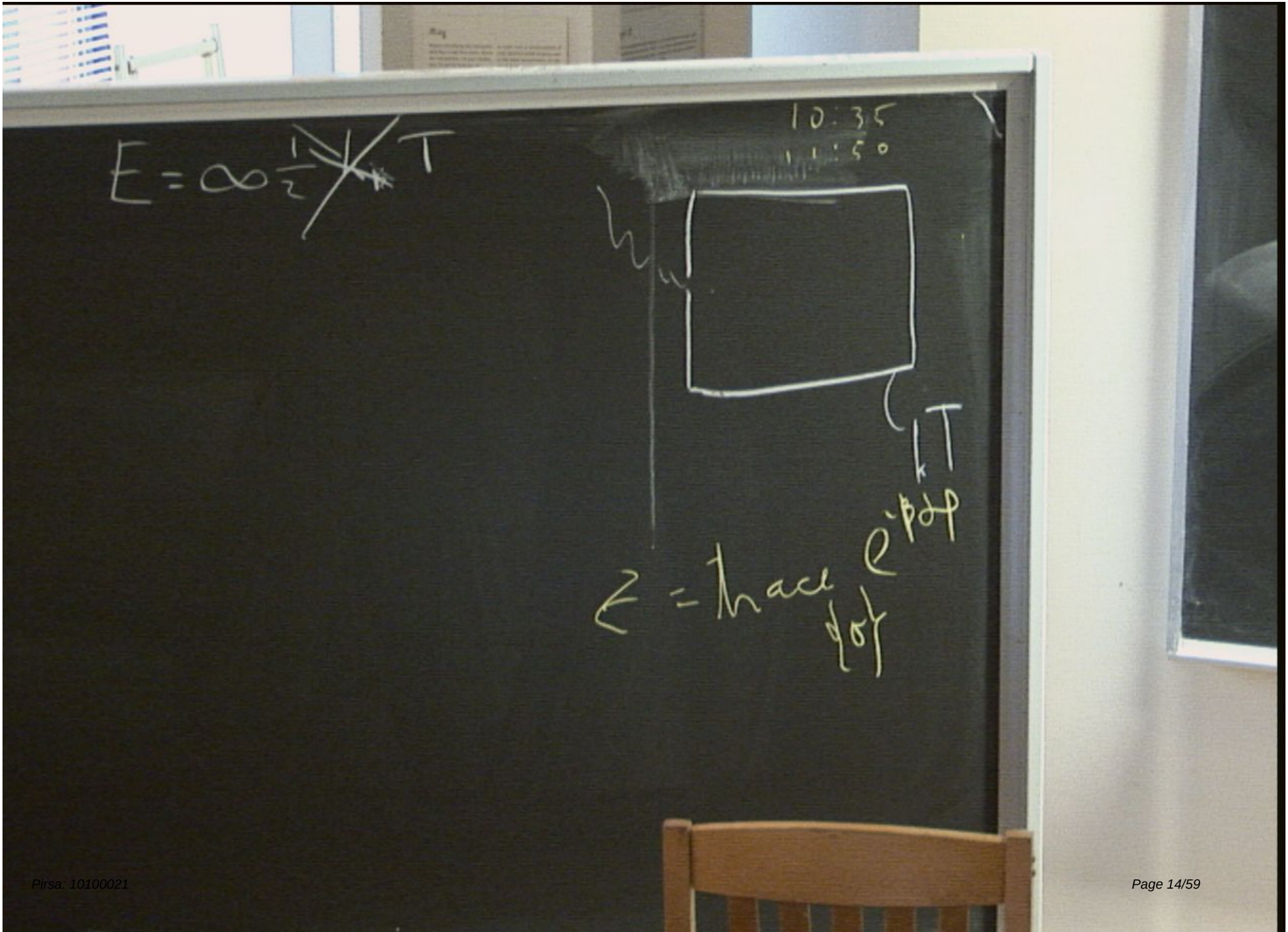
10:35
11:50
kT
Z = Trace e^{-βH}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Sums and Averages in Classical Mechanics

The probability distribution for a single 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. The partition function, is

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

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

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

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

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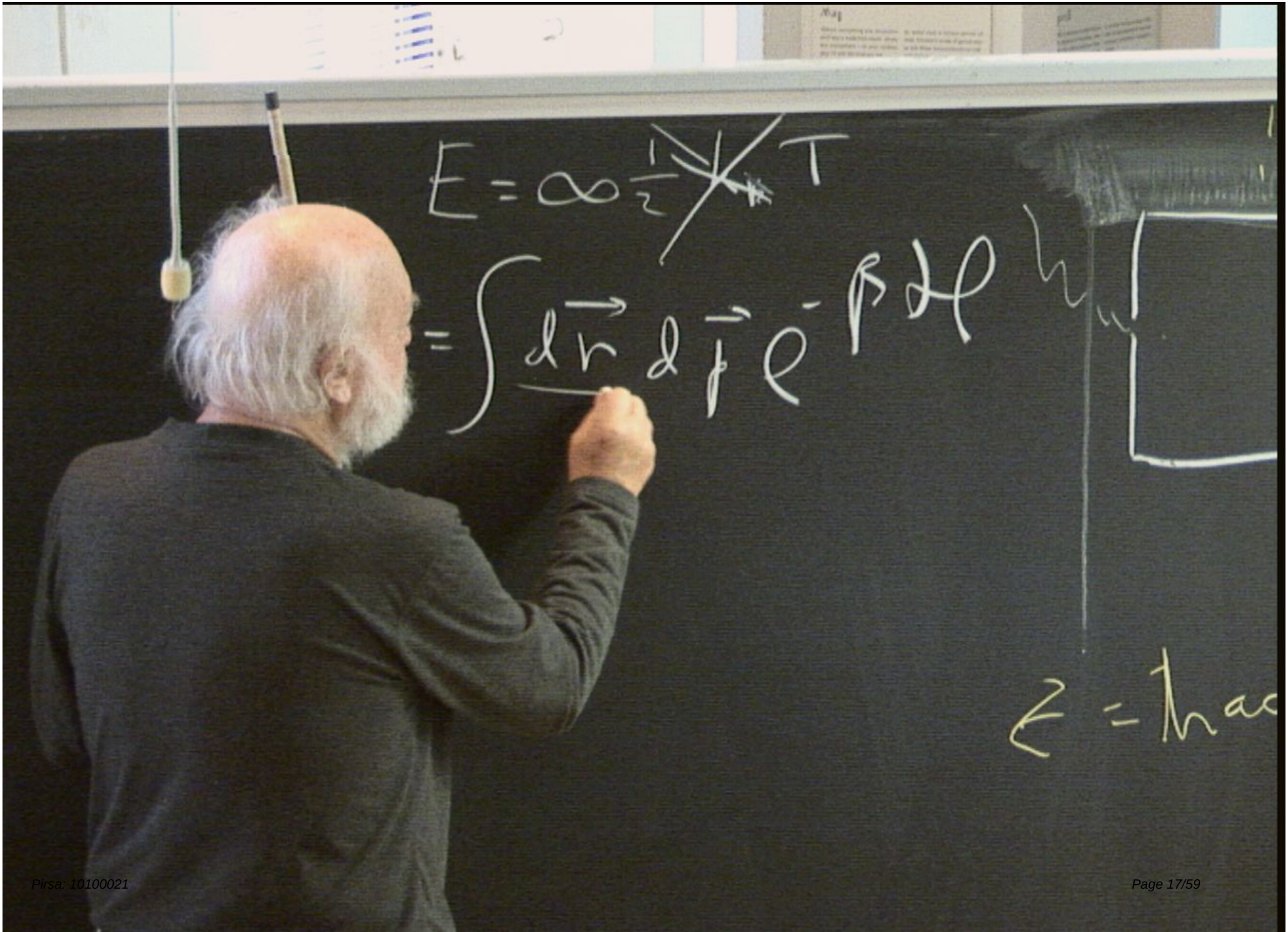
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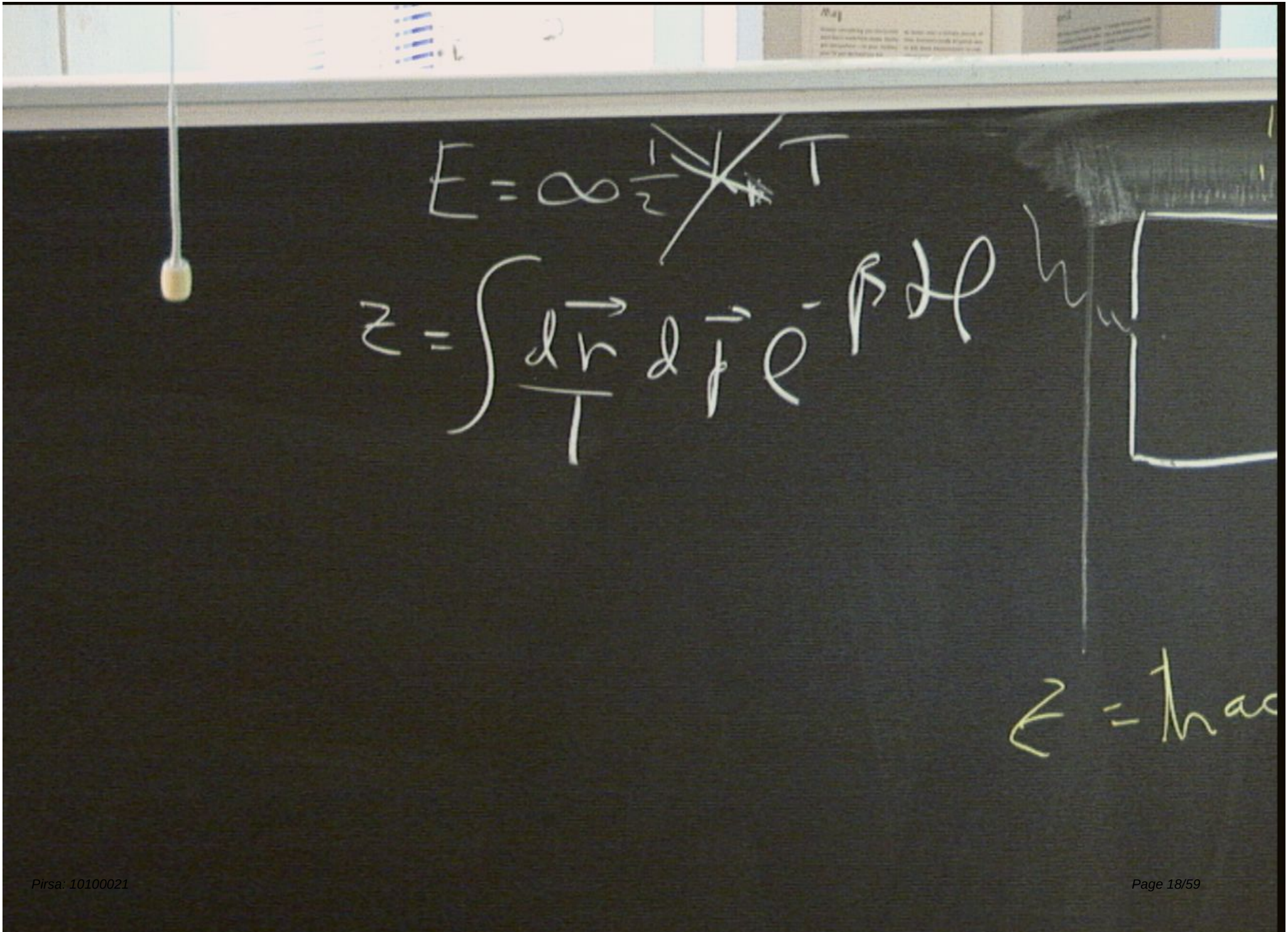
$E = \infty \frac{1}{2} \not{k} T$
$Z = \int \frac{d\vec{r}}{T} d\vec{p} e^{-\beta \mathcal{H}}$
$\mathcal{L} = \hbar \omega$

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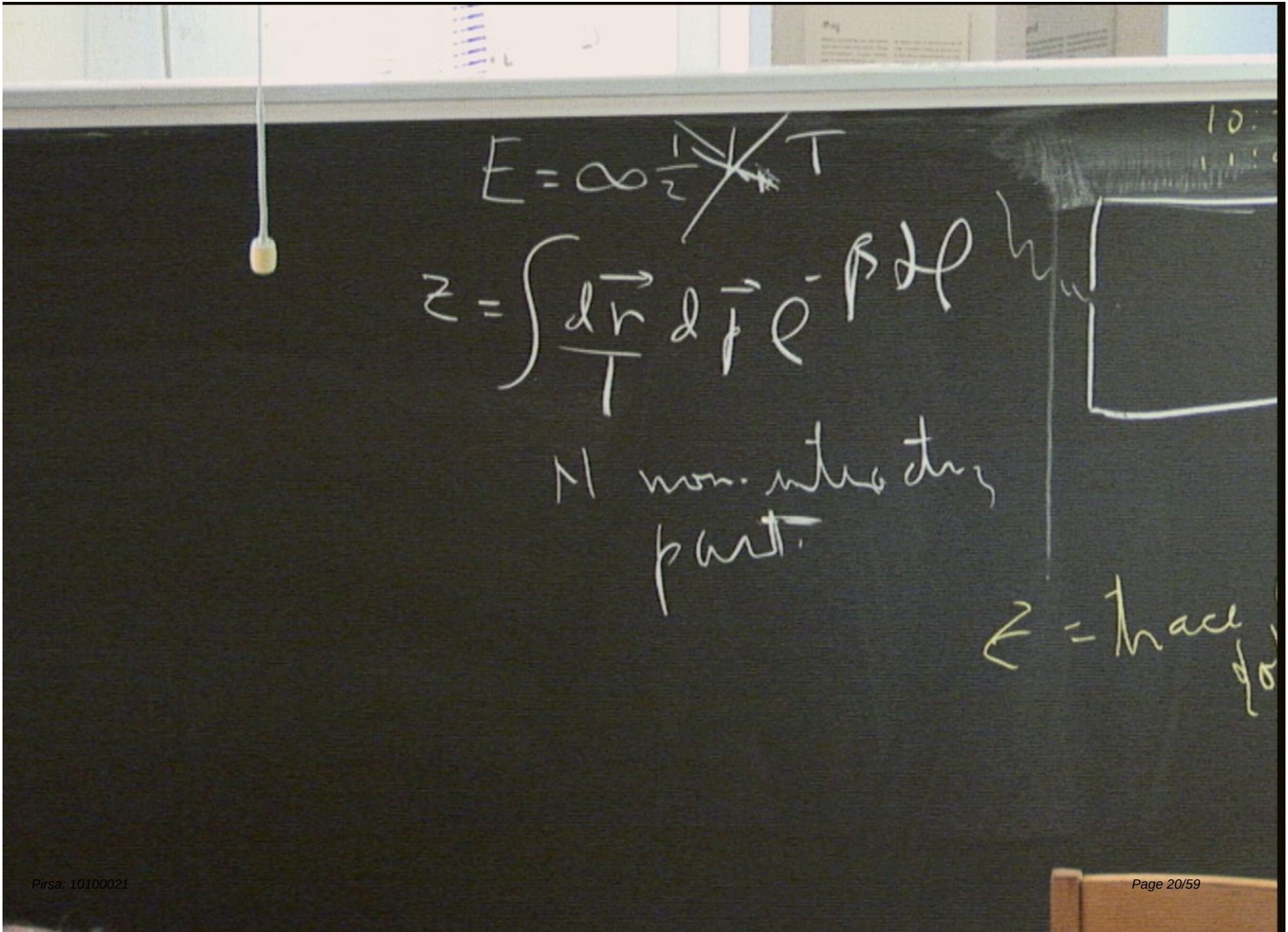
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N non-interacting
particles
$Z = \text{Trace}$

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More sums and averages

The normalization condition for the probability is $\int d\mathbf{p}\, d\mathbf{r}\, \rho(\mathbf{p},\mathbf{r}) = \langle 1 \rangle = 1$

The normalization for the distribution function is $\int d\mathbf{p}\, d\mathbf{r}\, f(\mathbf{p},\mathbf{r}) = N$

The pressure, P, is defined as the total momentum transfer to a wall per unit of area and unit of time. Call these dA and dt. Since a low density gas is the same all over, the number hitting is the number within the distance $p_x/m\, dt$ of the area, for $p_x > 0$, and hence the number within the volume $p_x/m\, dt\ dA$ which is $\int d\mathbf{p}\, f(\mathbf{p},\mathbf{r})\, p_x/m\, dt\ dA$ with the integral covering all $\mathbf{p}$'s with the condition that $p_x > 0$. If a particle hits the wall and bounces back it transfers momentum $2p_x$.

do we need specular reflection condition??

Therefore the total momentum transferred is $\int d\mathbf{p}\, f(\mathbf{p},\mathbf{r})\, p_x/m\, dt\ dA\ 2p_x$ once again with the condition that $p_x > 0$. An integral over all momenta would give a result twice as large. In the end we get that the pressure is

$$P = \int d\mathbf{p}\, f(\mathbf{p},\mathbf{r})\, p_x^2/m$$

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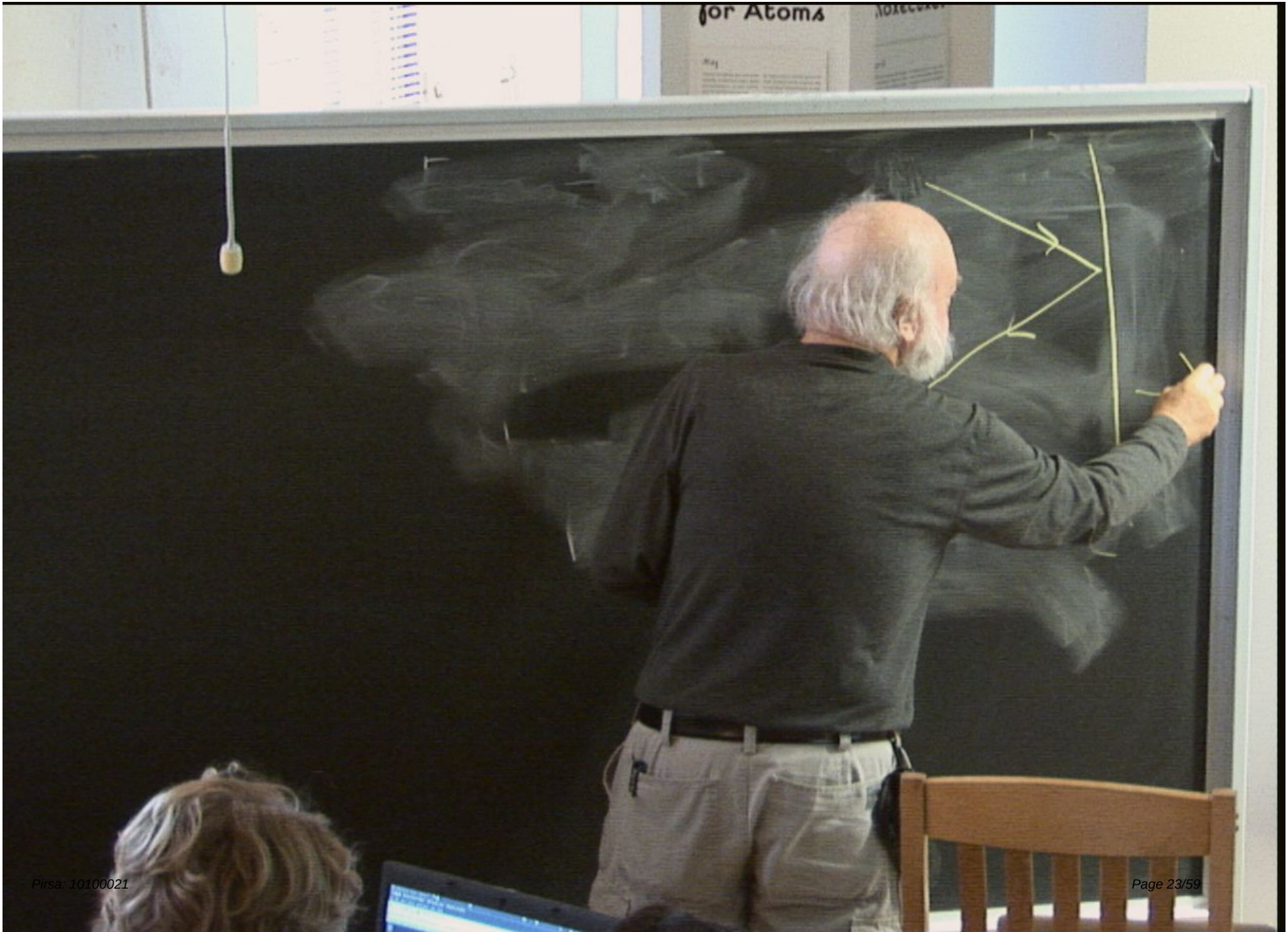
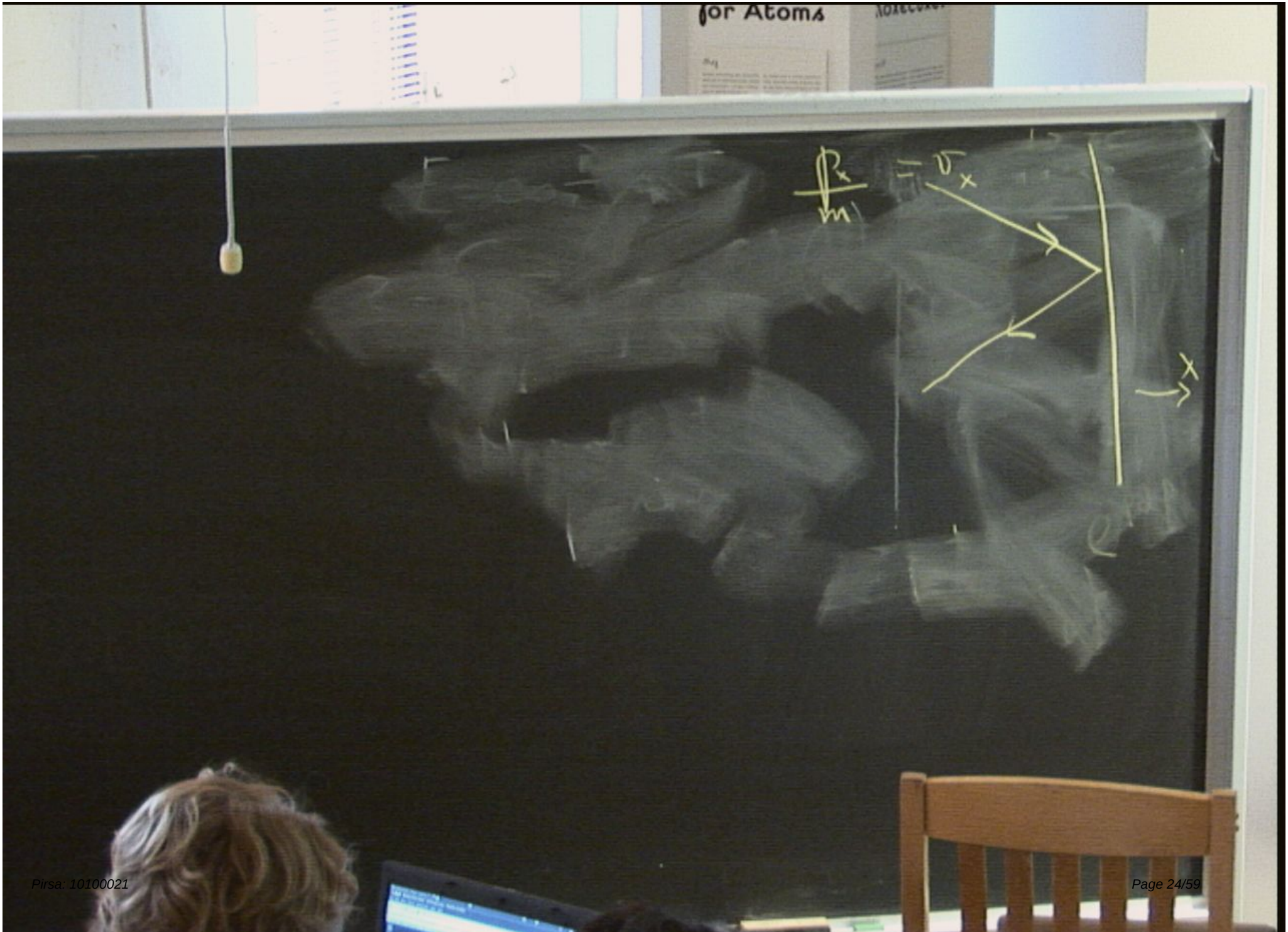
The partition function is the sum over all variables of $\exp(-\beta H)$. For large N, it can be interpreted as $W \exp(-\beta \langle H \rangle)$, where W is the number of configuration which enter. Boltzmann got W in terms of the entropy as $\ln W = S/k$. We put together previous results and find

$W \exp(-3N/2) = z^N = \Omega^N (2\pi\, m\, kT)^{3N/2}$ so that $S/k = N [\ln \Omega + 3 (\ln (2\pi\, e\, m\, kT))/2]$


for Atoms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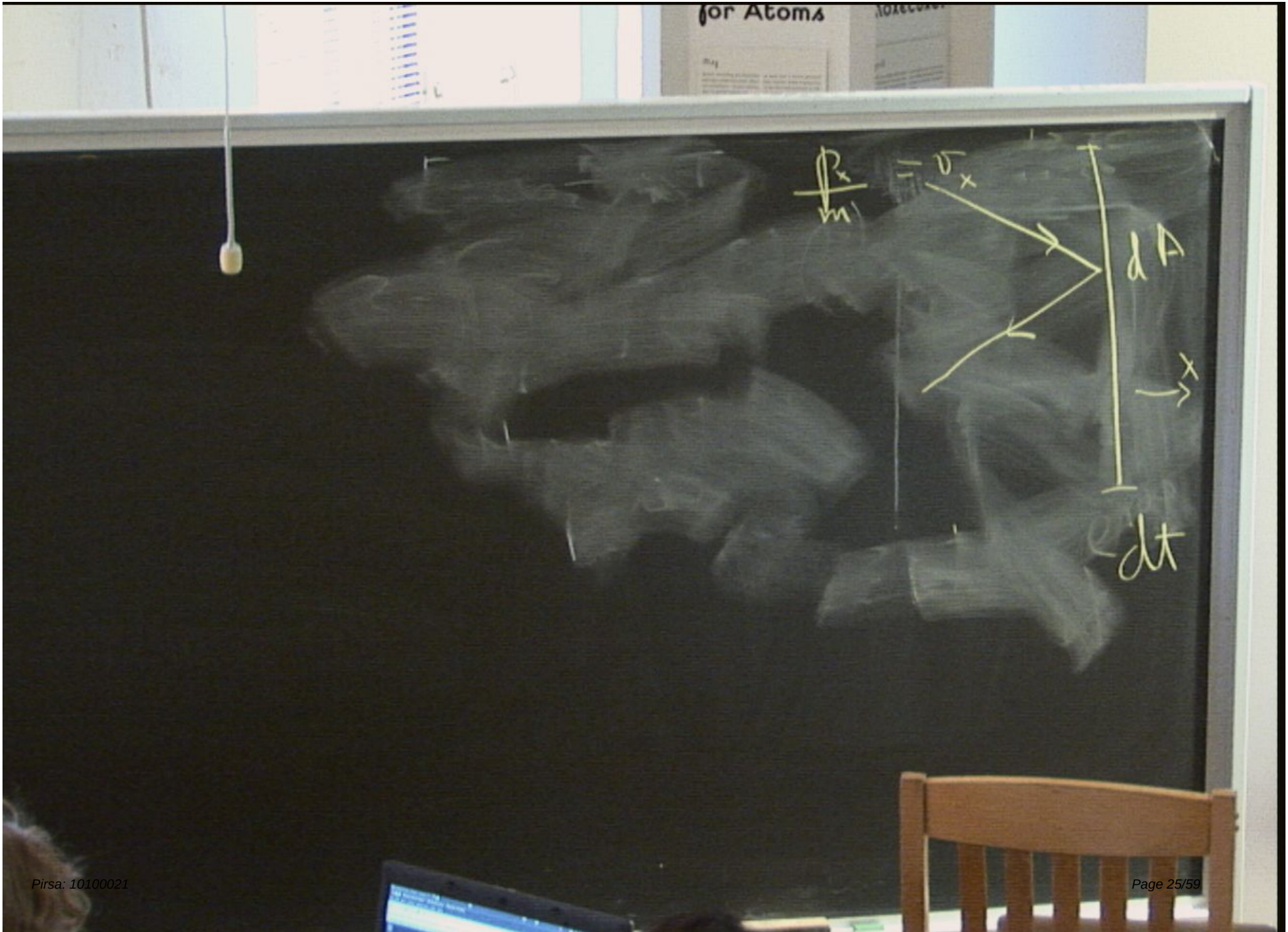
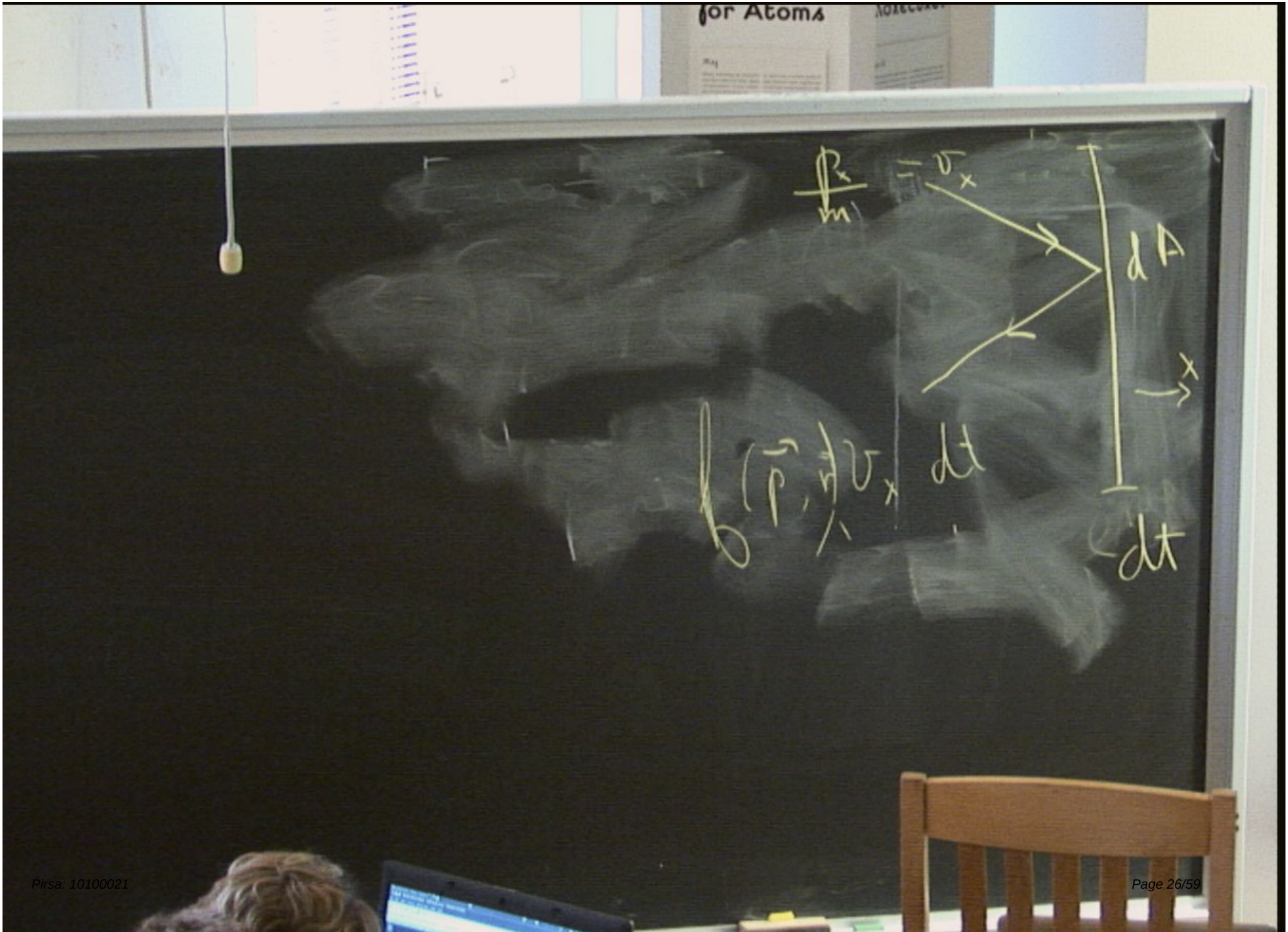

for Atoms
$\frac{p_x}{m} = v_x$
dA
x
dt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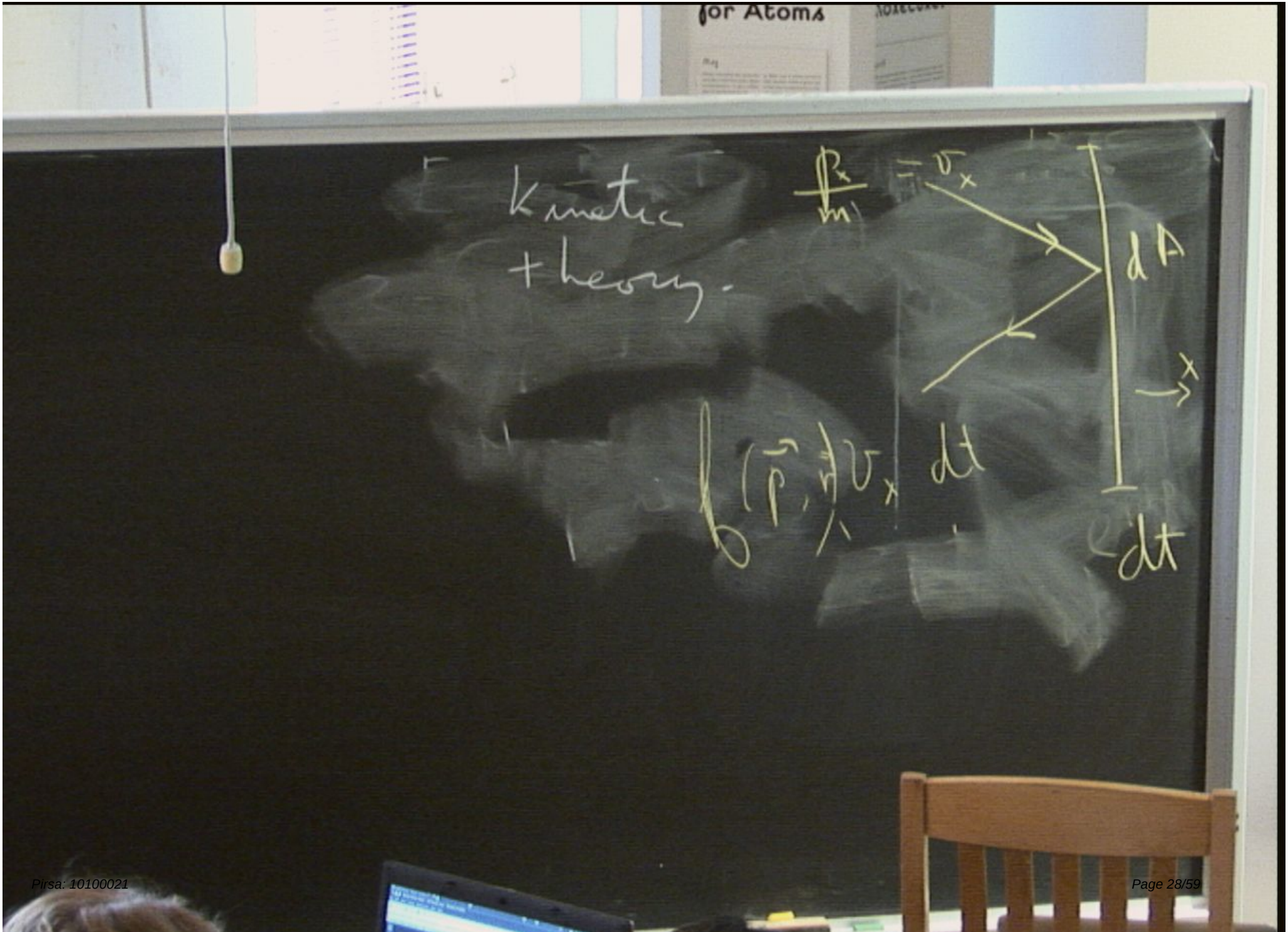
for Atoms
Kinetic
+ theory.
$\frac{P_x}{m} = v_x$
dA
x
$\int f(\vec{r},\vec{v}) v_x \, dt$
dt

From Classical Stat Mech to Quantum to RG

All of quantum mechanics on one slide

To do quantum mechanics, one starts with a complete set of states $|q)$ and $(p|$ which have the ortho-normality property $(q|q') = \delta_{q,q'}$ and a completeness relation

$$\sum_q |q)(q| = 1 \qquad (4.1)$$

and a trace operation

$$\text{trace } \mathcal{P} = \sum_q (q|\mathcal{P}|q) \qquad (4.2)$$

Heisenberg representation $P(t)=e^{-iHt}\, P\, e^{iHt}$. Let $T(t) = e^{-iHt}$

Partition Function $Z(\beta)$ = trace $T(-i\beta)=\sum_\alpha \exp(-\beta\varepsilon_\alpha)$

Average $\langle Q\rangle = [\text{trace } T(-i\beta)\, Q]/\, Z(\beta)$

Two Times $\langle Q(s)\, P(t)\rangle = [\text{trace } T(-i\beta)\, Q(s)\, P(t)\,]/\, Z(\beta)$

For grand canonical ensemble use $T(t)= exp[-i(H-\mu N)t]$

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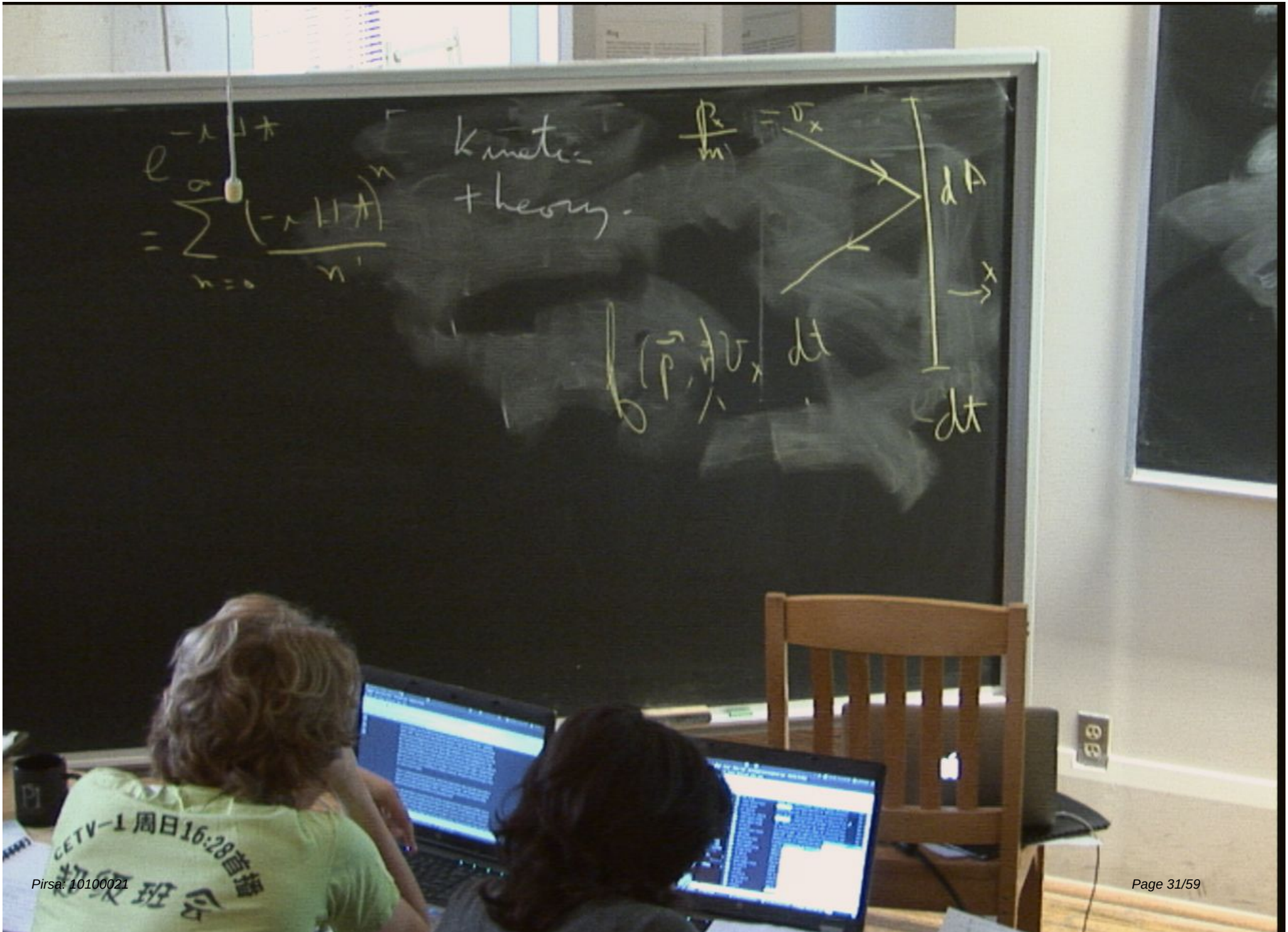
Kinetic
+ theory.
dA
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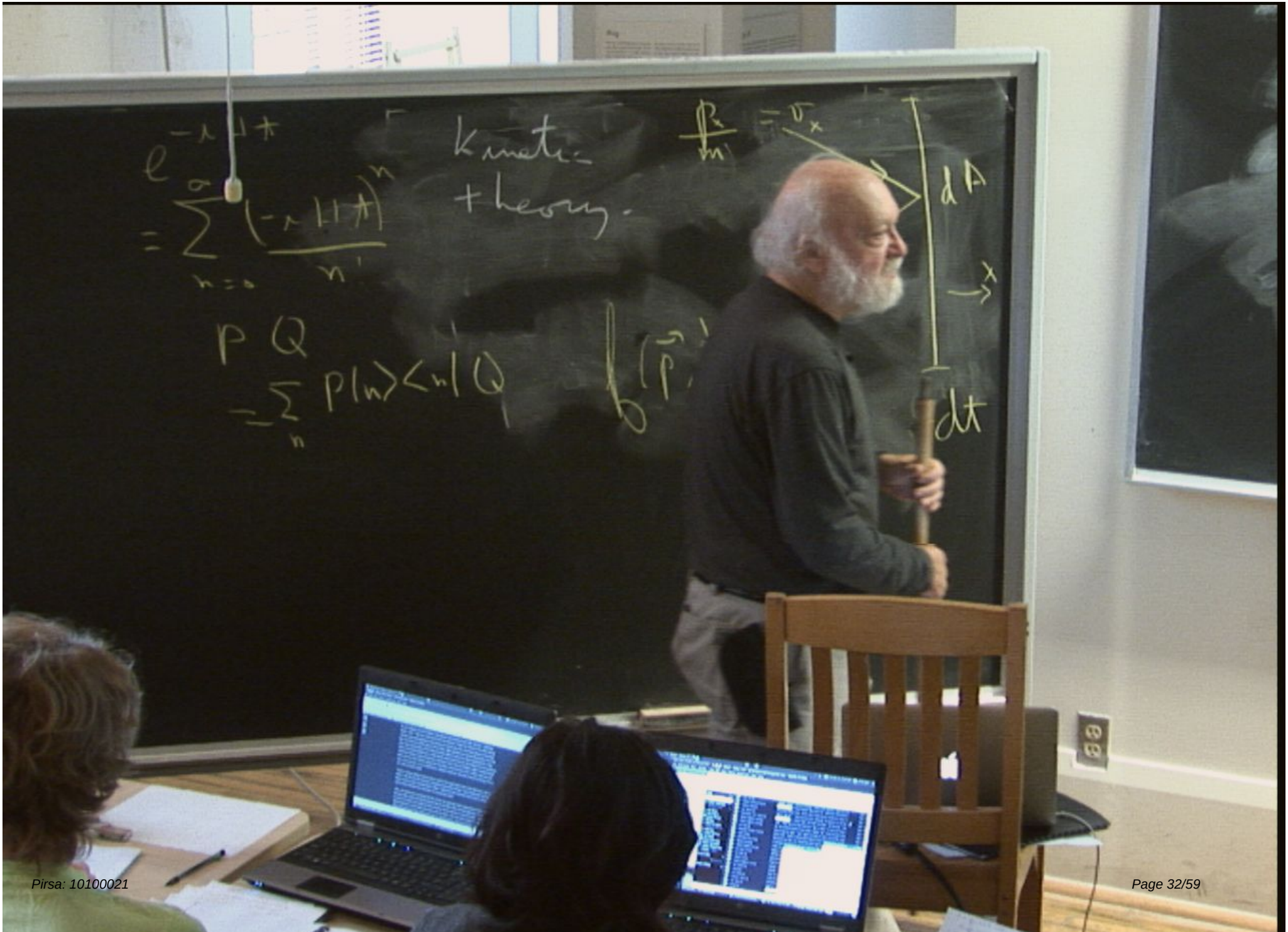
CETV-1 周日16:28首播
物理班会


kinetic
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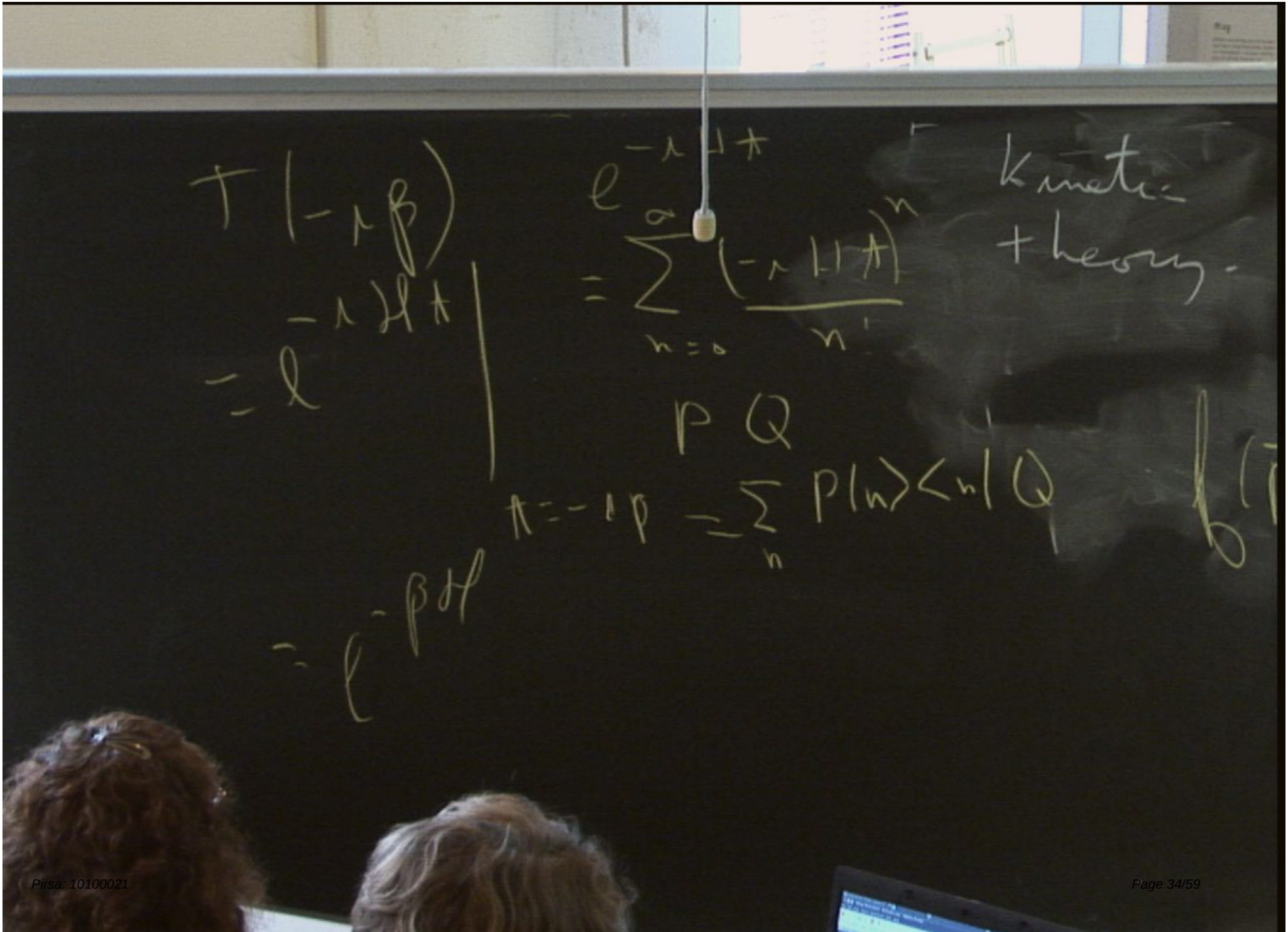

kinetic
+ theory.
pQ
$\sum_n p|n\rangle\langle n|Q$

From Classical Stat Mech to Quantum to RG

All of quantum mechanics on one slide

To do quantum mechanics, one starts with a complete set of states $|q)$ and $(p|$ which have the ortho-normality property $(q|q') = \delta_{q,q'}$ and a completeness relation

$$\sum_q |q)(q| = 1 \qquad (4.1)$$

and a trace operation

$$\text{trace } \mathcal{P} = \sum_q (q|\mathcal{P}|q) \qquad (4.2)$$

Heisenberg representation $P(t)=e^{-iHt}\, P\, e^{iHt}$. Let $T(t) = e^{-iHt}$

Partition Function $Z(\beta) =$ trace $T(-i\beta)=\sum_\alpha \exp(-\beta\varepsilon_\alpha)$

Average $\langle Q\rangle = [\text{trace } T(-i\beta)\, Q]/\, Z(\beta)$

Two Times $\langle Q(s)\, P(t)\rangle = [\text{trace } T(-i\beta)\, Q(s)\, P(t)\,]/\, Z(\beta)$

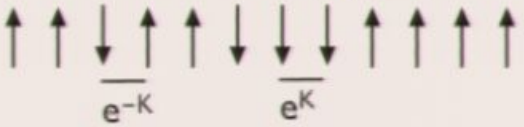
For grand canonical ensemble use $T(t)= exp[-i(H-\mu N)t]$

The Ising Linear Chain

We calculate the partition function in the simplest case of this kind. Take an Ising model with spins σ_j at sites $j = 1, 2, \ldots, N$. Take the magnetic field to be zero and arrange the couplings so that immediately neighboring sites (j and $(j+1)$ have a coupling K. The statistical weight for two neighboring sites having spin-values σ and σ' is then defined to be

$$e^{w(\sigma,\sigma')} = e^{K\sigma\sigma'} = (\sigma|\mathcal{T}|\sigma') \qquad (4.17)$$

linear chain



This kind of two by two system is generally analyzed in terms of the Pauli matrices which are the four basic matrices that we can use to span this two by two space. They are

$$\mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad (4.18)$$

In going up and back between the notation of equations (4.17) and (4.18) we have to think a little. In (4.17), we interpret σ and σ' as eigenvalues of the matrix τ_3. Any two by two matrix, M, can be written in terms of the eigenstates corresponding to these eigenvalues:

$$M = \begin{pmatrix} (-1|M|-1) & (-1|M|1) \\ (1|M|-1) & (1|M|1) \end{pmatrix}.$$

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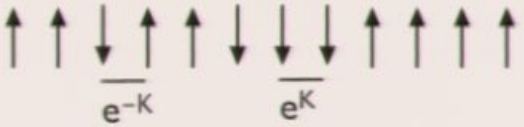

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The transfer Matrix

A useful form for these Pauli matrices is

$$(\sigma|\mathbf{1}|\sigma') = \delta_{\sigma,\sigma'} \qquad (\sigma|\tau_1|\sigma') = \delta_{\sigma,-\sigma'} \qquad (4.19b)$$
$$(\sigma|\tau_2|\sigma') = i\sigma\delta_{\sigma,-\sigma'} \qquad (\sigma|\tau_3|\sigma') = \sigma\delta_{\sigma,\sigma'}$$

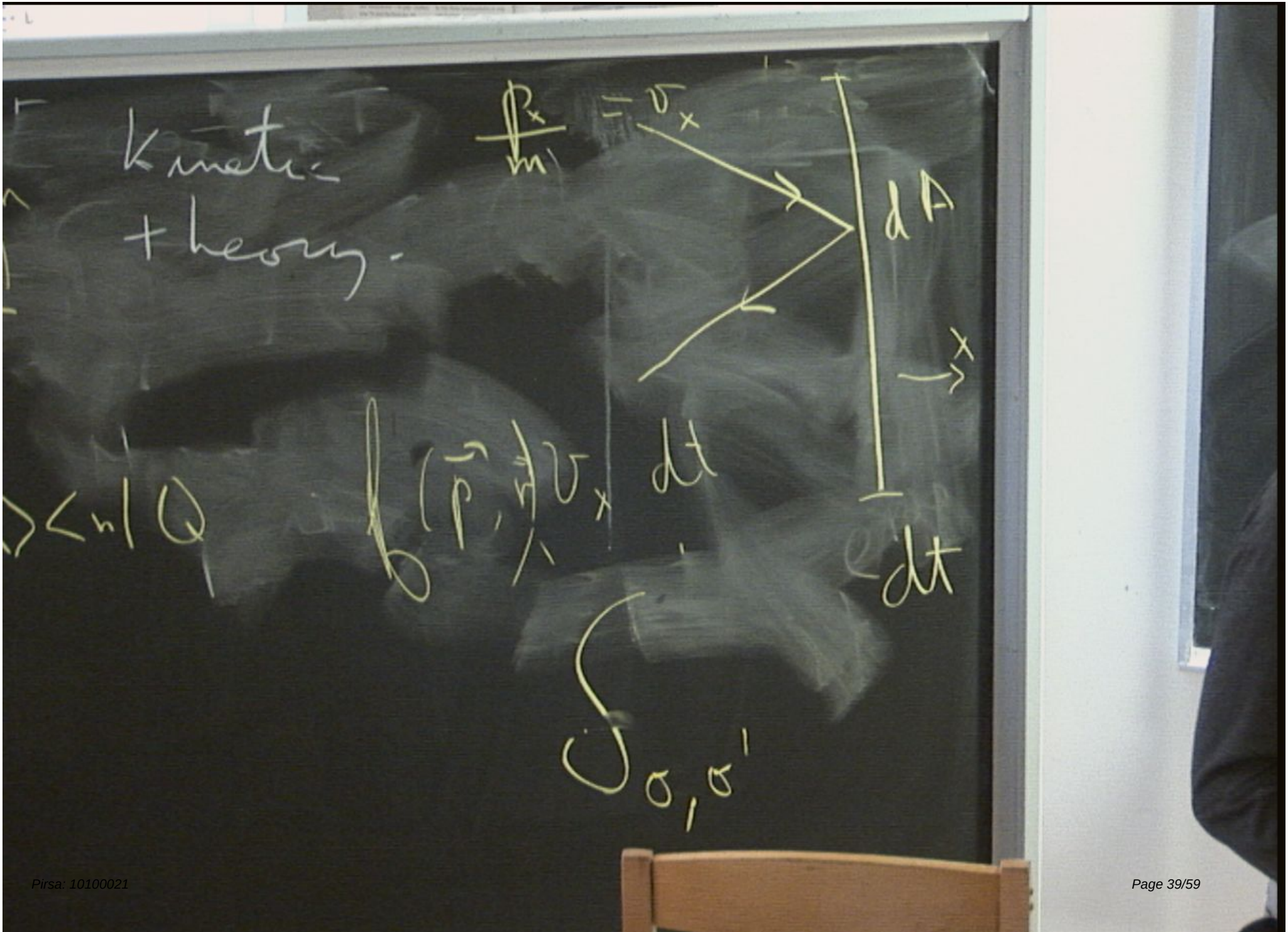
these matrices have a very direct physical meaning.
The matrix τ_3 is diagonal in the σ-representation and represents the spin. Conversely, τ_1 has only off-diagonal elements. It is an operator whose effect is to change the σ-value.

$$e^{K\sigma\sigma'} = (\sigma|T|\sigma') = \frac{1+\sigma\sigma'}{2}e^{K} + \frac{1-\sigma\sigma'}{2}e^{-K} \qquad (4.20)$$

$$= \cosh K + \sigma\sigma' \sinh K$$

$$= \langle\sigma| \; e^{K}\mathbf{1} + e^{-K}\boldsymbol{\tau}_1 \; |\sigma'\rangle$$

Here the matrices in **bold** are the ones defined in eq. 4.19b. We can also write this same quantity one more way as an exponential in $\boldsymbol{\tau}_1$


kinetic
+ theory.
dA
dt
dt

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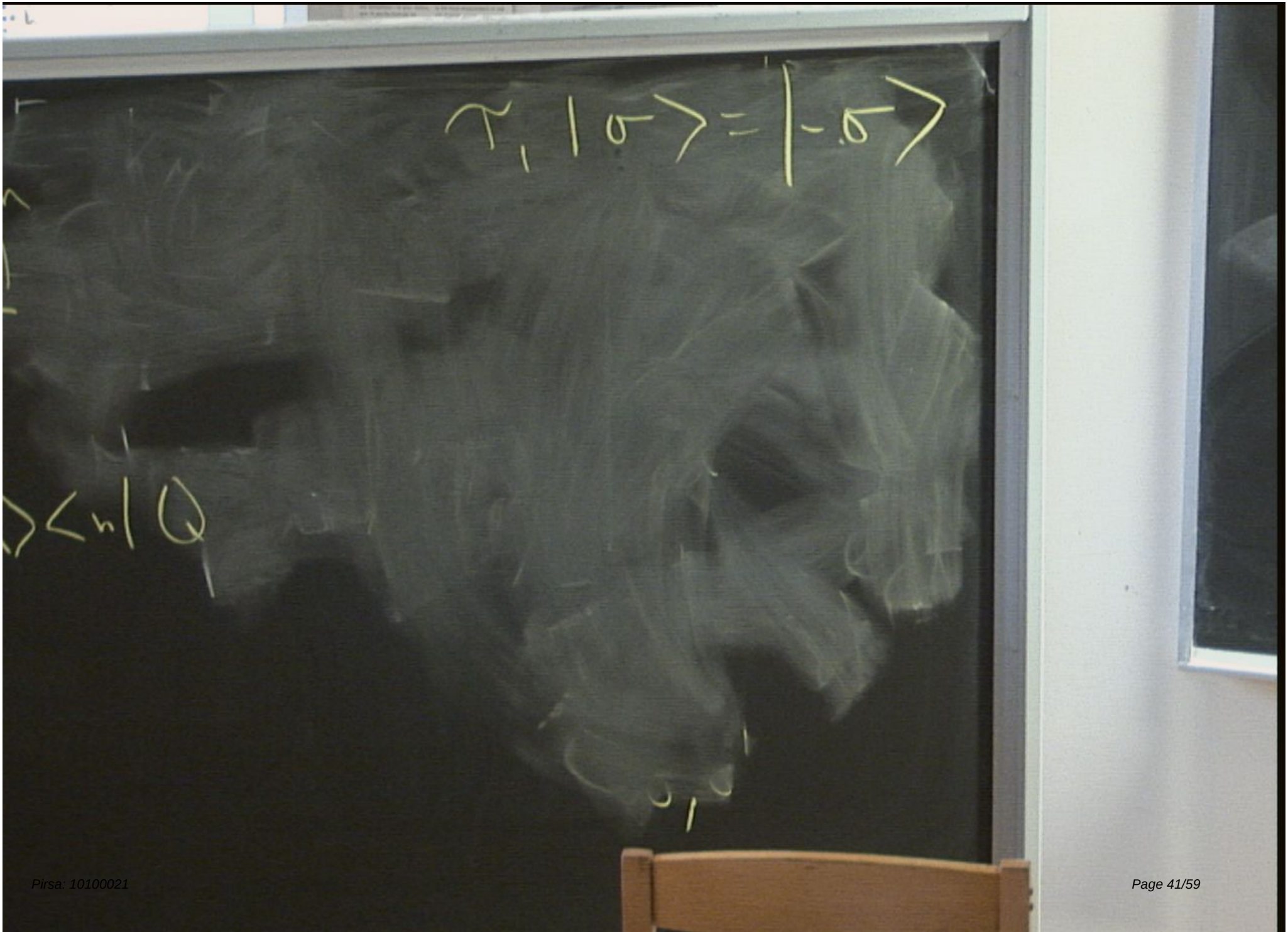
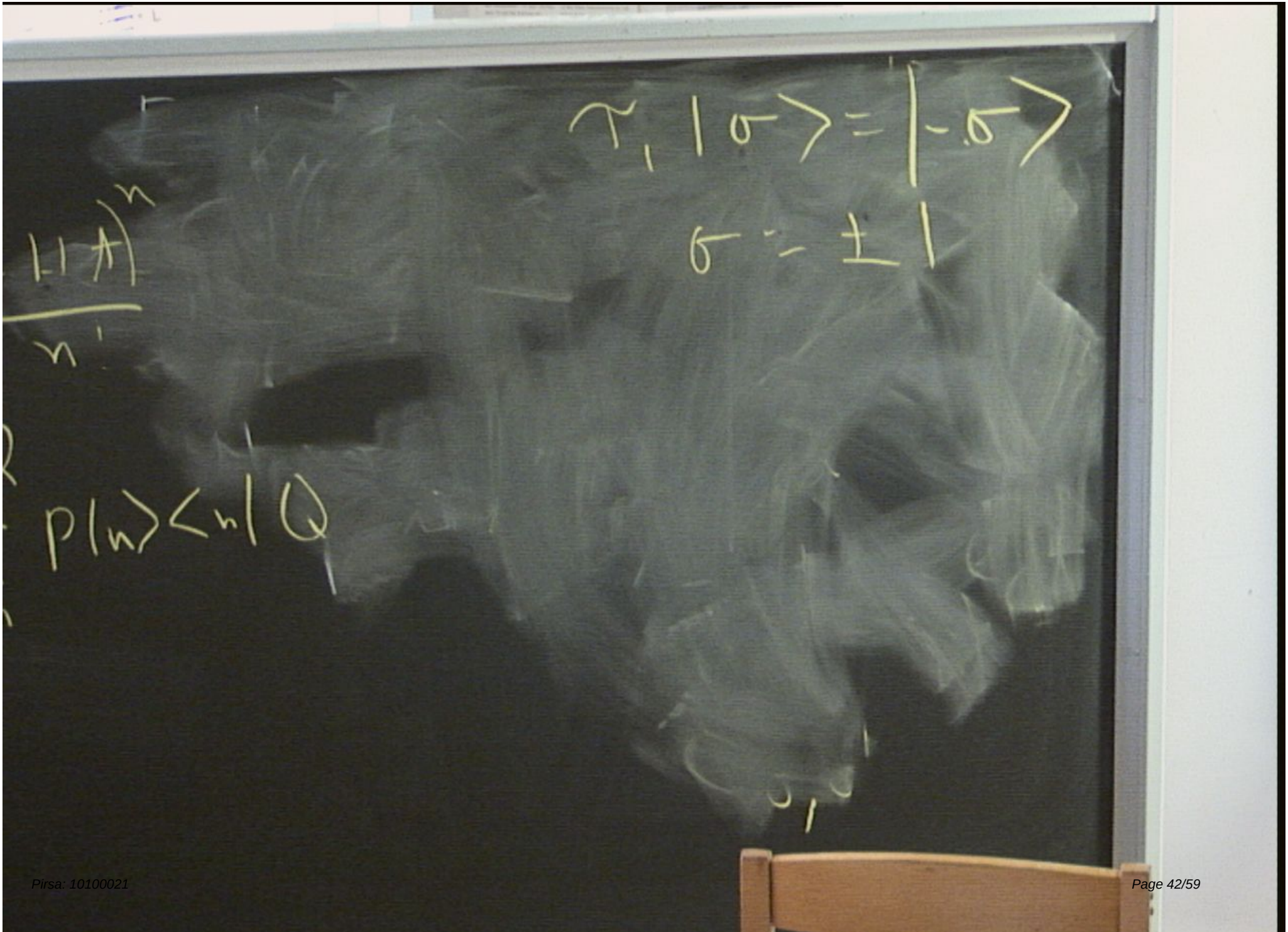

$\tau_1 |\sigma\rangle = |-\sigma\rangle$
$\rangle\langle n| Q$


$\tau_1 |\sigma\rangle = |-\sigma\rangle$
$\sigma = \pm 1$
$\frac{(1+A)^n}{n!}$
$P|n\rangle\langle n|Q$

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The matrix element of the transfer matrix, *T*, is equal to e^K when σ = σ' and equal to e^{-K} otherwise. In symbols,

$$e^{K\sigma\,\sigma'} = (\sigma|T|\sigma') = \frac{1+\sigma\sigma'}{2}e^{K} + \frac{1-\sigma\sigma'}{2}e^{-K} \qquad (4.20)$$

$$= \cosh K + \sigma\,\sigma' \sinh K$$

$$= e^{K}\,\mathbf{1} + e^{-K}\,\boldsymbol{\tau}_1$$

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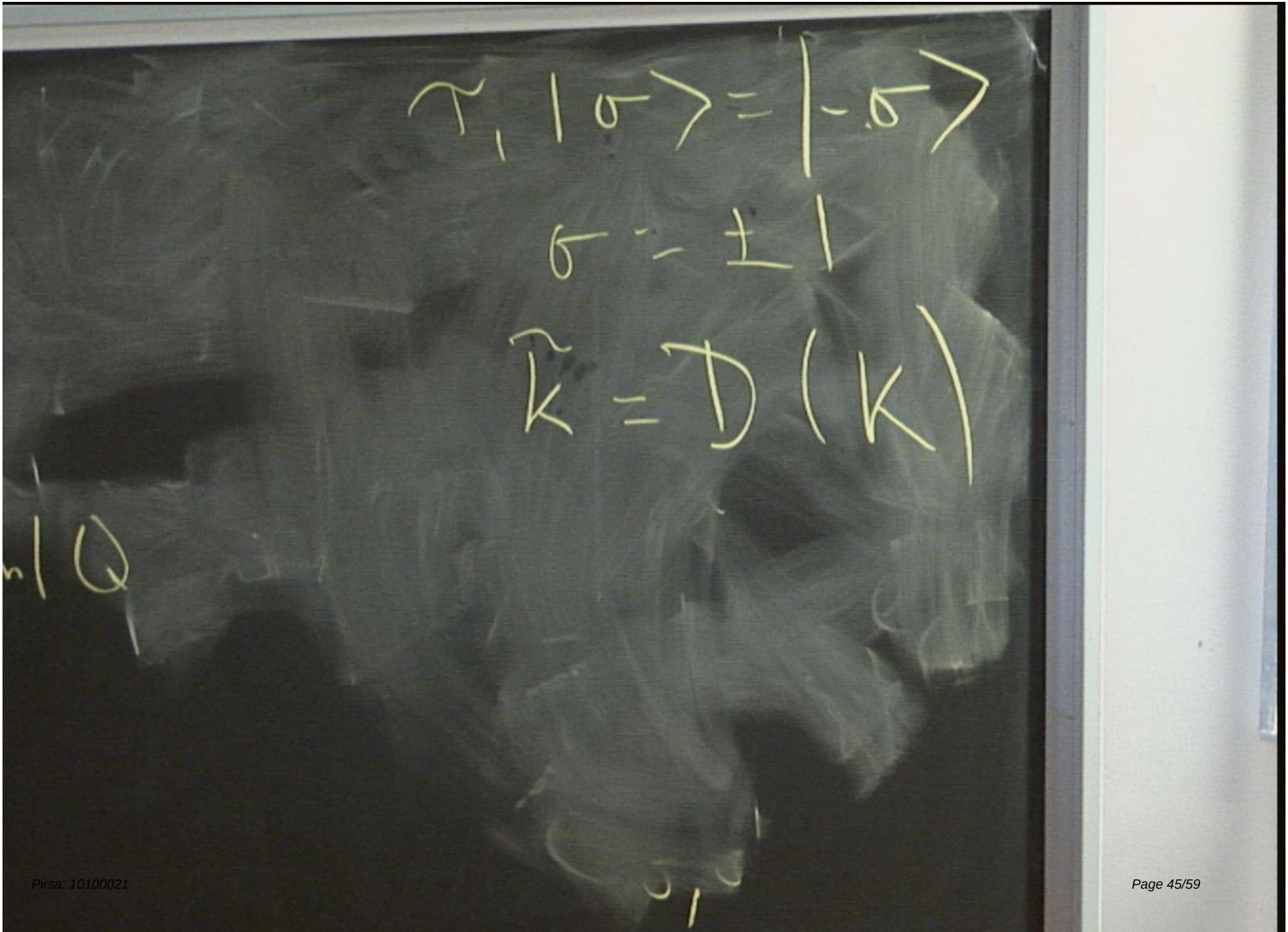
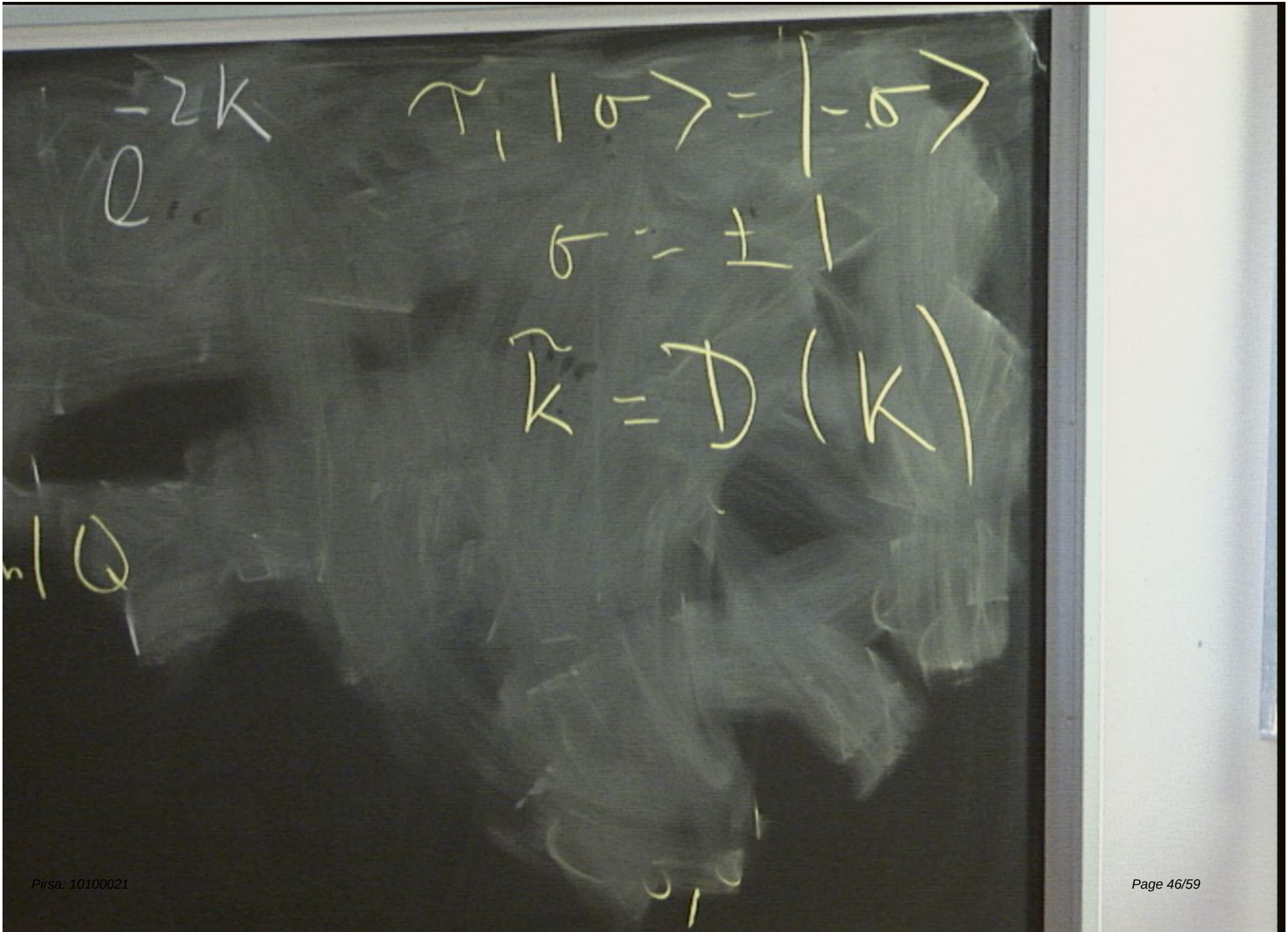
$$e^{K\sigma\sigma'} = <\sigma|e^{\tilde{K}_0+\tilde{K}\tau_1}|\sigma'> = e^{\tilde{K}_0} <\sigma|\cosh(\tilde{K}) + \sinh(\tilde{K})\tau_1|\sigma'>$$

The quantity $\tilde{K}$ depends upon *K*. For a simpler writing, I* call this function of K by another name and write it as D(*K*). The reason for using the symbol D will be apparent in a moment. Using the ration of the term in I and the term in $\boldsymbol{\tau}_1$, I find

$\tanh D(K) = e^{-2K}$ so that $K = -\ln[\tanh(D(K))]/2$

* stacking symbols as in K^~ is very hard in keynote


$\tau_1 |\sigma\rangle = |-\sigma\rangle$
$\sigma = \pm 1$
$\tilde{K} = \mathcal{D}(K)$


$-2k$
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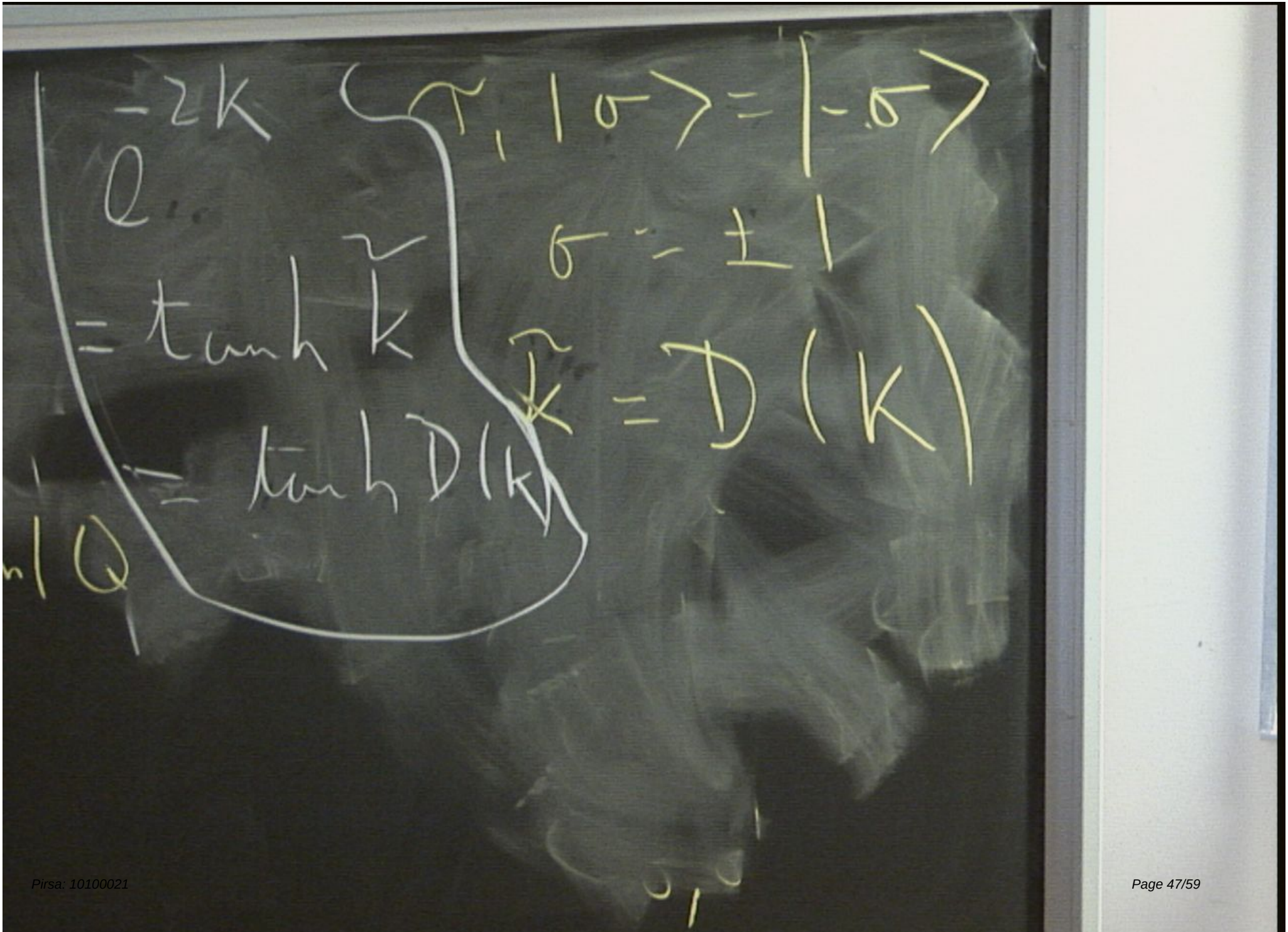
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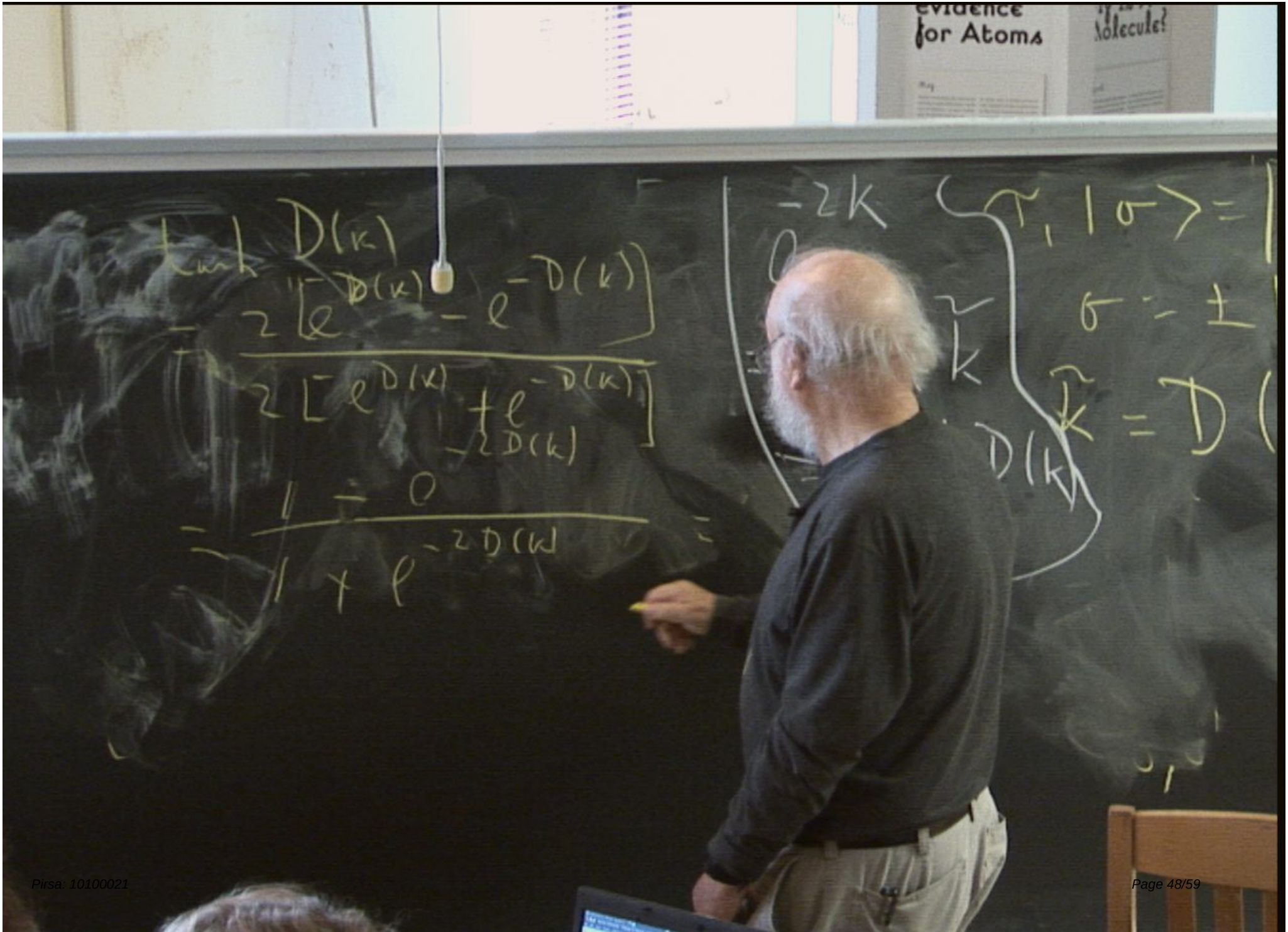
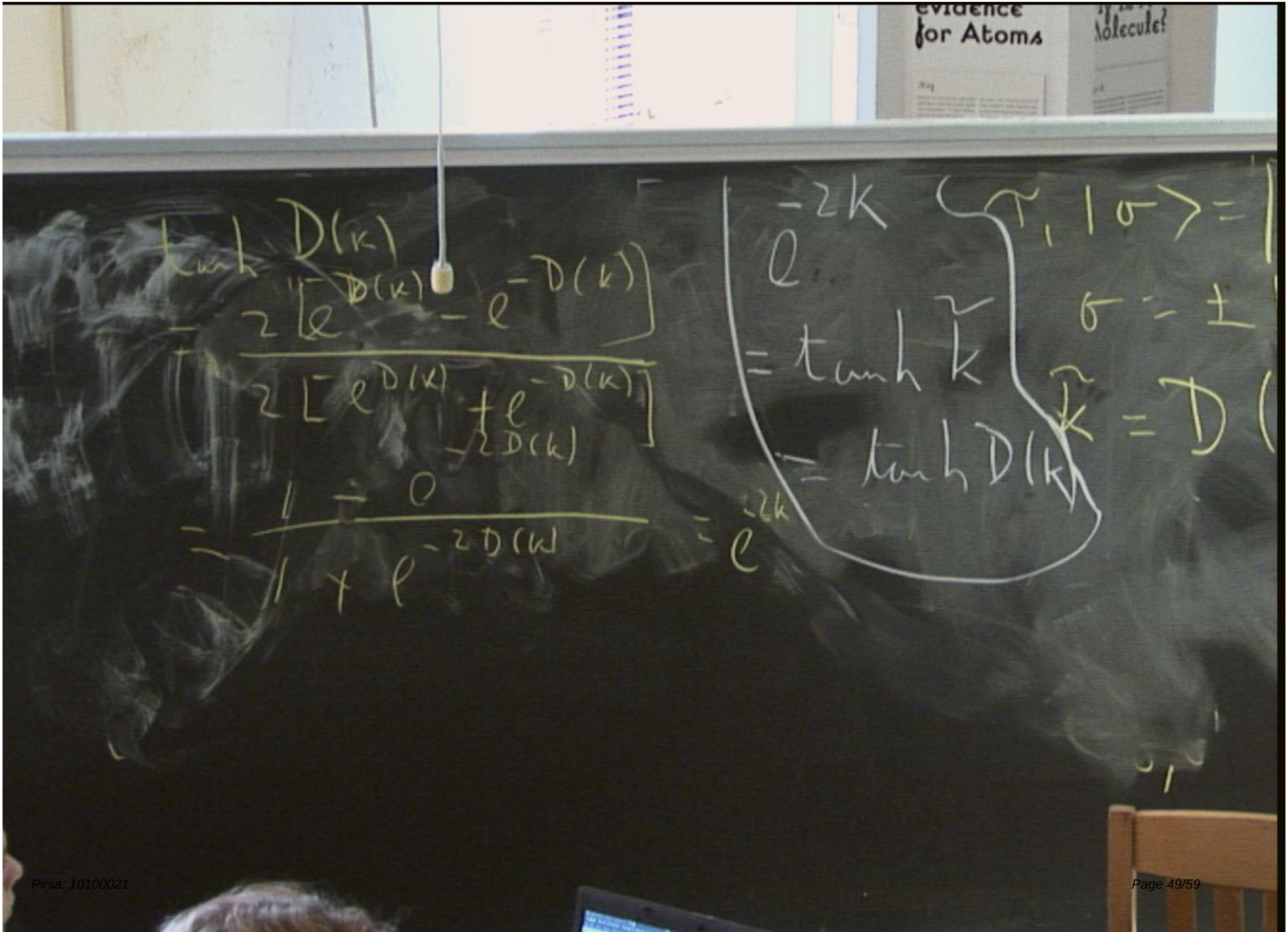

for Atoms
Molecule?

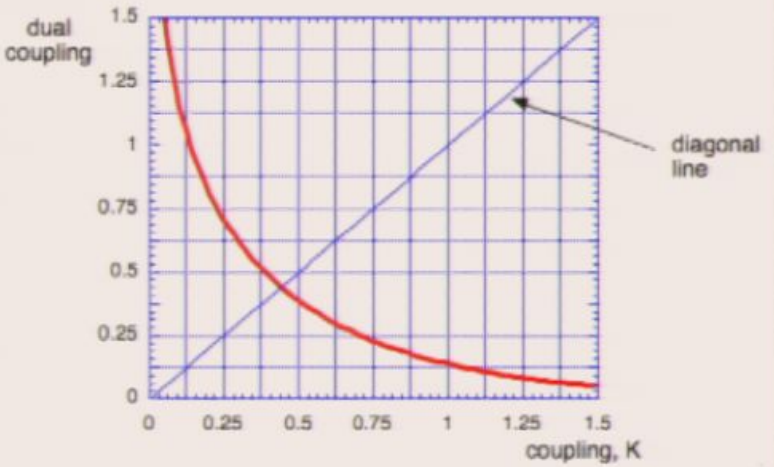

evidence
for Atoms
Molecule?
tanh D(k)
= 2[e^{D(k)} − e^{−D(k)}] / 2[e^{D(k)} + e^{−D(k)}]
= (1 − e^{−2D(k)}) / (1 + e^{−2D(k)})
e^{−2k̃} ⟨τ, | σ⟩ =
= tanh k̃
= tanh D(k)
σ = ±
k̃ = D(

Dual Coupling

This same expression can be written as
$1 = e^{-2K} + e^{-2D(K)} + e^{-2K}\, e^{-2D(K)}$
so whatever the relation is between D(K) and K there is exactly the same relation between K and D(K). This is why D(K) is called the dual of K.
Consequently K=D(D(K)).

Therefore two applications of the dual operation takes you back to precisely the same function.

This function has the property that when *K* is strong its dual is weak and *vice versa*. This property has proven to be very important in both statistical physics and particle physics. Often we know both a basic model and its dual. Often models are hard to solve in strong coupling but easy to solve when the coupling is weak. But the dual models have weak coupling when the basic model has strong coupling. So then we get an indirect solution of the basic model.



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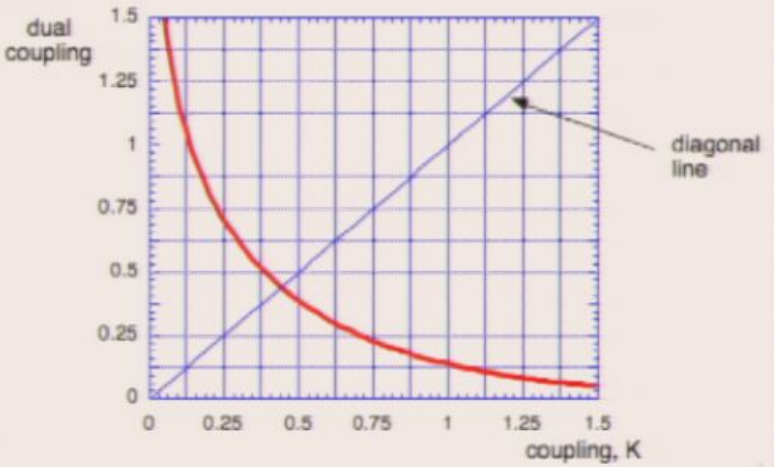

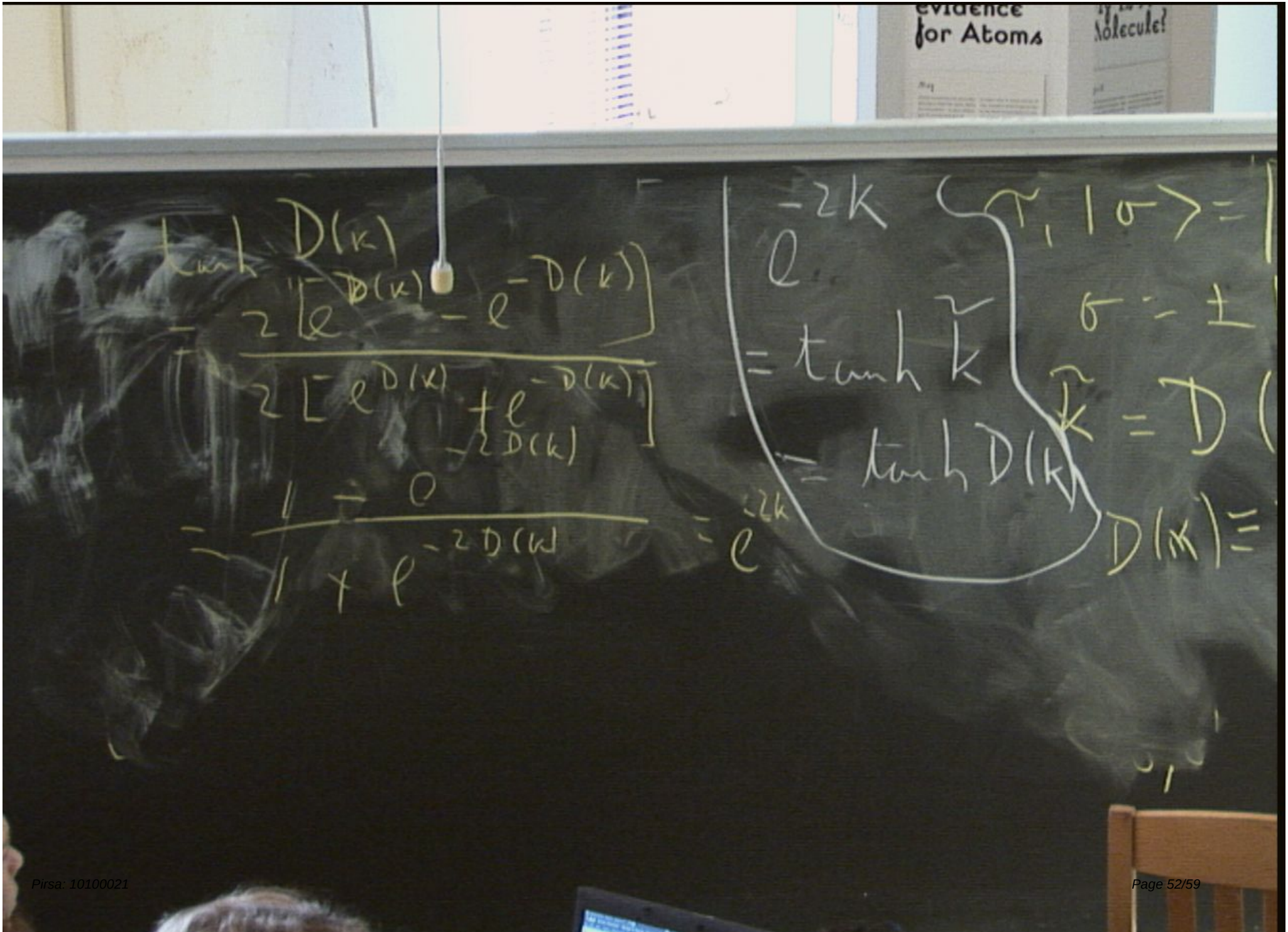
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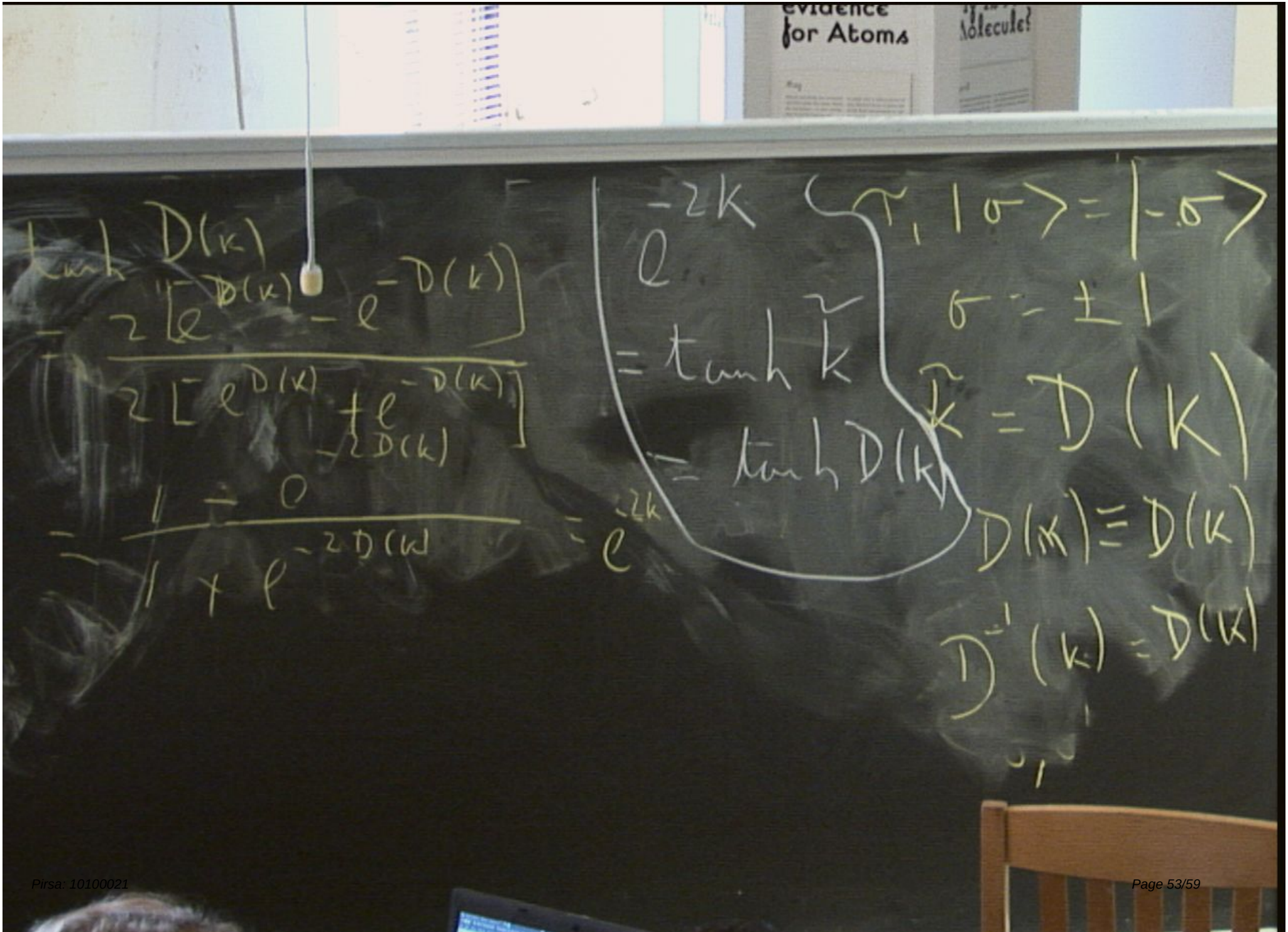
for Atoms
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$= e^{-2k}$
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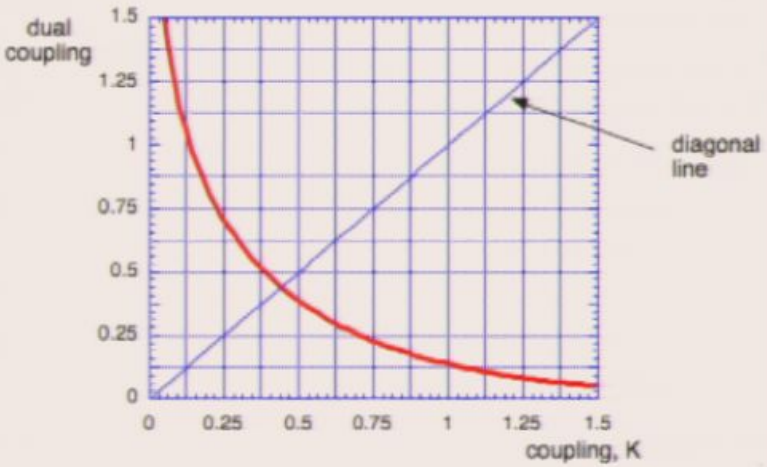

Solution of the one-dimensional Ising model

From equation 4.20, we find that the partition function of the one-dimensional Ising model is

$$Z = \text{ trace } (e^K \mathbf{1} + e^{-K} \tau_1)^N$$

But the trace is a sum over eigenvalues and the eigenvalues of τ_1 are plus or minus one. Thus, the answer is:

$$Z = (2 \cosh K)^N + (2 \sinh K)^N \qquad (4.25)$$

If N is very large, the first term is much larger than the second and thus in this limit of large system size:

$$-\beta F = \ln Z = N \ln(2 \cosh K) \qquad (4.26)$$

What quantum mechanics problem have we solved?

More about quantum from the Long Chain

We should be able to say more about quantum problems based upon the analysis of the long chain. For example let us imagine that we wish to calculate the average of some quantum operator, $X(q)$, which happens to be diagonal in the q-representation. The text book goes through a long song and dance to prove a rather obvious result. You have seen that the trace in equation 4.10 pushes us into a sum over energy states, and if N is very large that sum reduces to a projection onto the ground state of the system. Specifically,

$$Z = \mathrm{trace}_{q_1}\mathrm{trace}_{q_2}\ldots\mathrm{trace}_{q_n}\prod_{j=1}^{N}\exp(w(q_j,q_{j+1})) \qquad (4.10)$$

becomes $Z=\mathrm{trace}\ \exp(-NH)\approx \exp(-N\varepsilon_0)$

So if we insert an X, for any any operator X, in that sum the result should give what happens to that X in the ground state, specifically

$$(1/Z)\ \mathrm{Trace}_{\{q\}}\ \exp[W\{q\}]\ X = \langle 0|\ X(q)\ |0\rangle$$

In this way, we can use statistical mechanics to calculate the average of any operator in the ground state. If we do not take N to infinity, we can do the corresponding calculation to calculate the average of any operator at a inverse temperature ($\beta-$ value) equal to $N\ \tau$.

By playing with the times in an appropriate fashion, we can even calculate time-dependent correlation functions in the ground state or in a finite-temperature state.

Statistical Correlations in a Long Chain

We should be able lots about the statistical mechanics of a the long chain with Ising style interactions. For example, let us calculate the average of the jth spin on a long chain or the correlations among the spins in the chain. Start from

$$Z = \mathrm{Tr}\ \exp[\ \sum_{j=1}^{N} K\sigma_{j+1}\sigma_j]$$

$$< \sigma_k >= (1/Z)\mathrm{Tr}\,\sigma_k\ \exp[\ \sum_{j=1}^{N} K\sigma_{j+1}\sigma_j]$$

$$< \sigma_k\sigma_{k+r} >= (1/Z)\mathrm{Tr}\,\sigma_k\sigma_{k+r}\ \exp[\ \sum_{j=1}^{N} K\sigma_{j+1}\sigma_j]$$

Here Tr means "sum over all the N spin-values". We use periodic boundary conditions. In this equation all the σ's are numbers, and they commute with each other.

We can make the calculation easier by replacing all the couplings by their expressions in terms of Pauli spins matrices giving these three calculations as, first,

$$Z=\mathrm{trace}_\tau \prod_{j=1}^{N} \exp\,(\tilde{K}_0 + \tilde{K}\tau_1) = \mathrm{trace}_\tau \exp[N\,(\tilde{K}_0 + \tilde{K}\tau_1)]$$

$$= (2\cosh K)^N + (2\sinh K)^N \qquad \approx \quad (2\cosh K)^N$$

The ≈ is an approximate equality which holds for large *N*. Note that in this limit the term with eigenvalue of $\tau_1 = 1$ dominates because the dual coupling is positive.

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