Title: Statistical Mechanics (PHYS 602) - Lecture 7

Date: Oct 06, 2009 10:30 AM

URL: http://pirsa.org/09100128

Abstract:

Renormalization: $a \dashrightarrow 3a = a'$ $W_K\{\sigma\} \dashrightarrow W_{K'}\{\mu\}$ $Z' = Z$ $K' = R(K)$

Scale Invariance at the critical point: $\dashrightarrow$ $K_c = R(K_c)$

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

if $t=0$ then $t'=0$

ordered region ($t>0$) goes into ordered region ($t'>0$)

disordered region goes into disordered region

if t is small, $t' = bt$. $b = (a'/a)^x$ defines x. b can be found through a numerical calculation.

coherence length: $\xi = \xi_0\, a\, t^{-\nu}$ 2d Ising has $\nu=1$; 3d has $\nu \approx 0.64$....

$\xi = \xi'$ $\xi_0\, a\, t^{-\nu} = \xi_0\, a'\, (t')^{-\nu}$

so $\nu = 1/x$

number of lattice sites: $N = \Omega/a^d$ $N' = \Omega/a'^d$

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

Free energy: F = non-singular terms $+ N f_c(t) = F'$ = non-singular terms $+ N' f_c(t')$

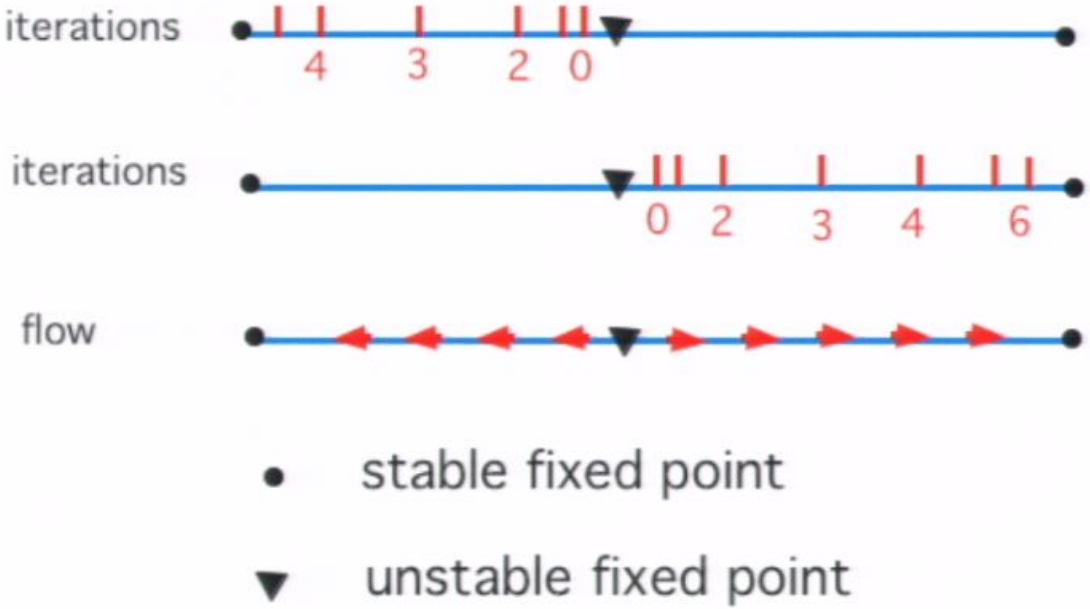
$f_c(t) = f_c^0\, t^{dx}$

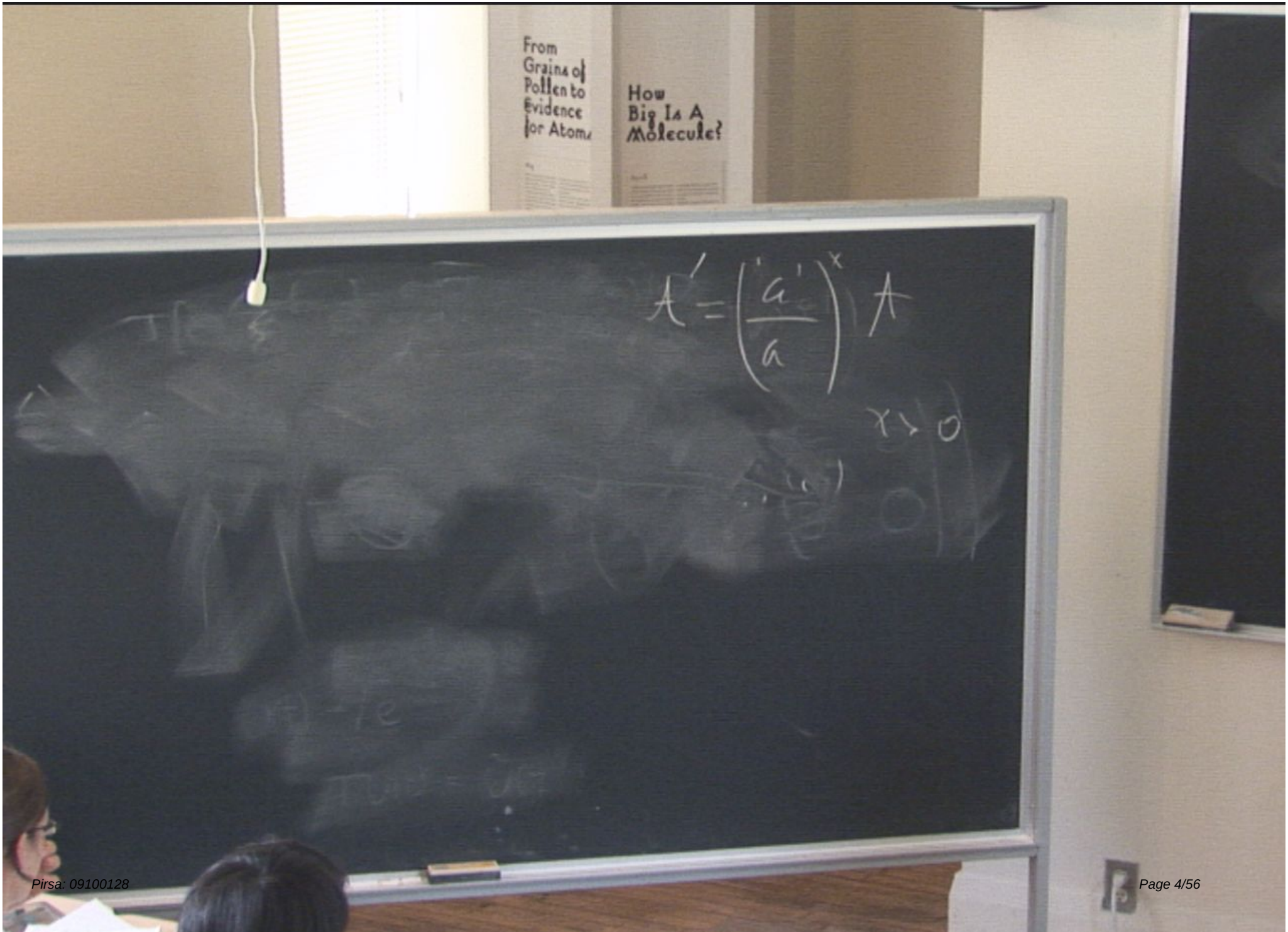
Specific heat: $C = d^2F/dt^2 \sim t^{dx-2}$ form of singularity determined by x

One can do many more roughly analogous calculations and compare with experiment and numerical simulation. Everything works!

However notice that this is not a complete theory. It is a *phenomenological* theory. We have no way to find x from theory

renormalizations of couplings

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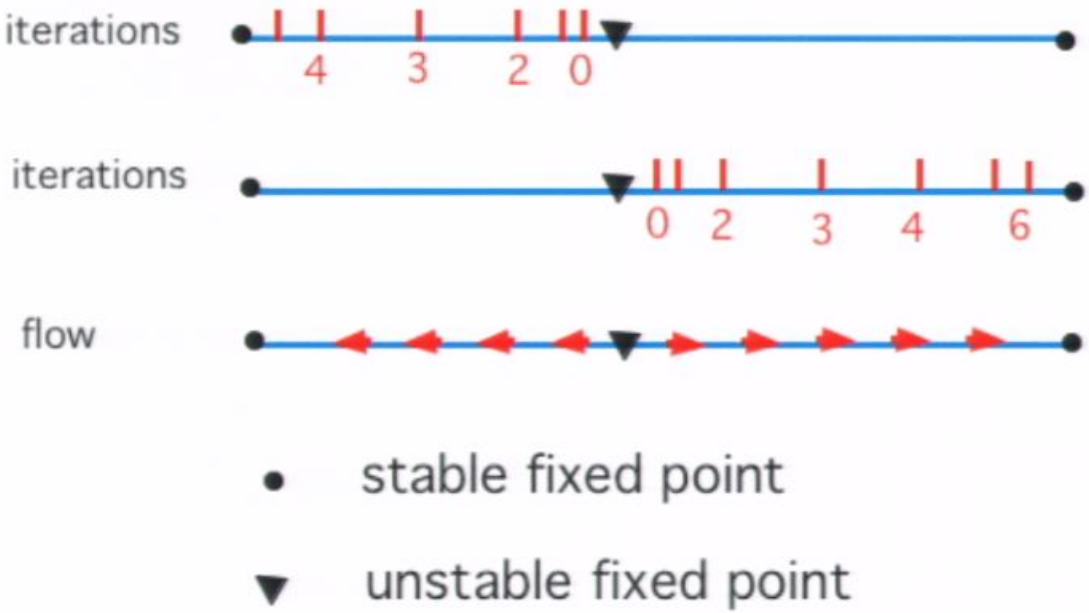


Homework:

Add a term in $\Sigma_j (h\ \sigma_j)$ to the weighting function, W, for the one dimensional Ising Hamiltonian. Find the value of the average spin in the presence of a small magnetic field h. Define the magnetic susceptibility as the derivative of the magnetization with respect to h at fixed K. Show that this susceptibility diverges as K goes to infinity. Shows that it is proportional to a sum of fluctuations in the magnetization.

The three-state Potts model is just like the Ising model except that its "spin" variable σ_j can take on three values $= -1, 0, 1$. It has $w(\sigma_j, \sigma_{j+1}) = K$ if the two variables are the same and zero otherwise. Find the partition function and coherence length of the one dimensional model. How does the renormalization work for ?

What is the critical temperature of the three-state Potts model on the square lattice in two dimensions?

Solution to Diffusion Equation Cannot be Carried Backward in Time

The wave equation is $(\partial_t^2 - \partial_x^2)F = 0$

Its general solution is $F(x,t)=G(x-ct)+H(x+ct)$

This is a global solution. It enables you to look forward or back infinitely far in the future or the past without losing accuracy. Find solution from $F(x,0) = \partial_x F(x,0) = 1$ for $0<x<1$ and $F(x,0) = \partial_x F(x,0) = 0$ otherwise. Use $c=2$

A global solution to the diffusion equation is $\rho(x,t)= \int dk \ \exp[ikx-\lambda k^2 t] \ g(k)$

with $g(k)= \int dx \ \exp[-ikx] \ \rho(x,0)/(2\pi)$ as initial data.

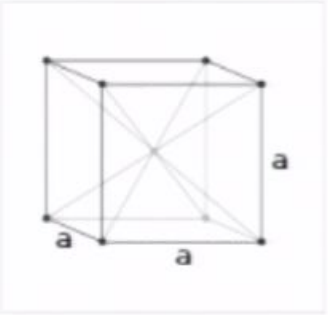
Small rapidly varying errors at t=0 will produce small errors for positive t and huge errors for negative t. You cannot extrapolate backward in time. Information gets lost as time goes forward.

Solve for $\rho(x,0)=1$ for $0<x<1$ and $\rho(x,0) = 0$ otherwise. Use $\lambda=2$. Plot solution for t=0,2,4. What happens for t= −2?

Boltzmann noted that equations of classical mechanics make sense if t is replaced by −t. (In fact, it just replaces momenta, *p*, by -*p*.) But diffusion equation has a solution which does not make sense. Where did we go from sense to nonsense?

Higher Dimensions

Reason for putting many different calculations on a lattice is that the lattice provides a simplicity and control not available in a continuum system. There is no ambiguity about how things very close to one another behave, because things cannot get very close. They are either at the same point or different points



Body-centered cubic

So now I would like to talk about a random walk in a d-dimensional system by considerin a system on a simple lattice constructed as in the picture. The lattice sites are given by $\mathbf{x} = a(n_1, n_2, n_3, ...)/2$. The n's are integers. There are two possible kinds of assignments for the n's: Either they are all even e.g. $\mathbf{x} = a(0,2,-4, ...)/2$ or they are all odd, for example $\mathbf{x} = a(1,3,-1, ...)/2$. If all hopping occurs from one site to a nearest neighbor site, the hops are through one of 2^d vectors of the form $\xi_\alpha = a(m_1, m_2, m_3, ...)/2$, where each of the m's have magnitude one, but different signs for example a(1,-1,-1, ...). We use a lattice constant, a, which is twice as big as the one shown in the picture.

We then choose to describe the system by saying that in each step, the coordinate hops through one of the nearest neighbor vectors, ξ_α , which one being choosen at random. This particular choice makes the entire coordinate, $\mathbf{x}$, have components which behave entirely independently of one another, and exactly the same as the one-dimensional coordinate we have treated up to now.

Part 4: Diffusion and Hops

From Discrete to Continuous
- Hopping on a Lattice
- Notation: Even and Odd
- From one step to many
- An example

Continuous
- Langevin equation
- An integration
- Gaussian Properties
- Generating Function
- A probability

Discrete
- A generating Function
- A probability
- calculation
- we get an answer!
- fourier transform formulation
- binomial theorem

Higher Dimension
- continued
- probability density
- One dimension
- Current

Diffusion equation
- Higher Dimension
- You cannot go back

Hopping: From Discrete to Continuous

We are going to be spending some time talking about the physics of a particle moving in a solid. Often this motion occurs as a set of discrete hops. The particle gets stuck someplace, sits for a while, acquires some energy from around it, hops free, gets caught in some trap, and then sits for a while. I'm going to describe two mathematical idealizations of this motion: discrete hopping on a lattice and continuous random motion.

One point is to see the difference between the two different topologies represented by a continuous and a discrete system. One often approximates one by the other and lots of modern physics and math is devoted to figuring out what is gained and lost by going up and back.

There is a fine tradition to this. Boltzmann, one of the inventors of statistical mechanics, liked to do discrete calculations. So he often represented things which are quite continuous, like the energy of a classical particle by discrete approximations,

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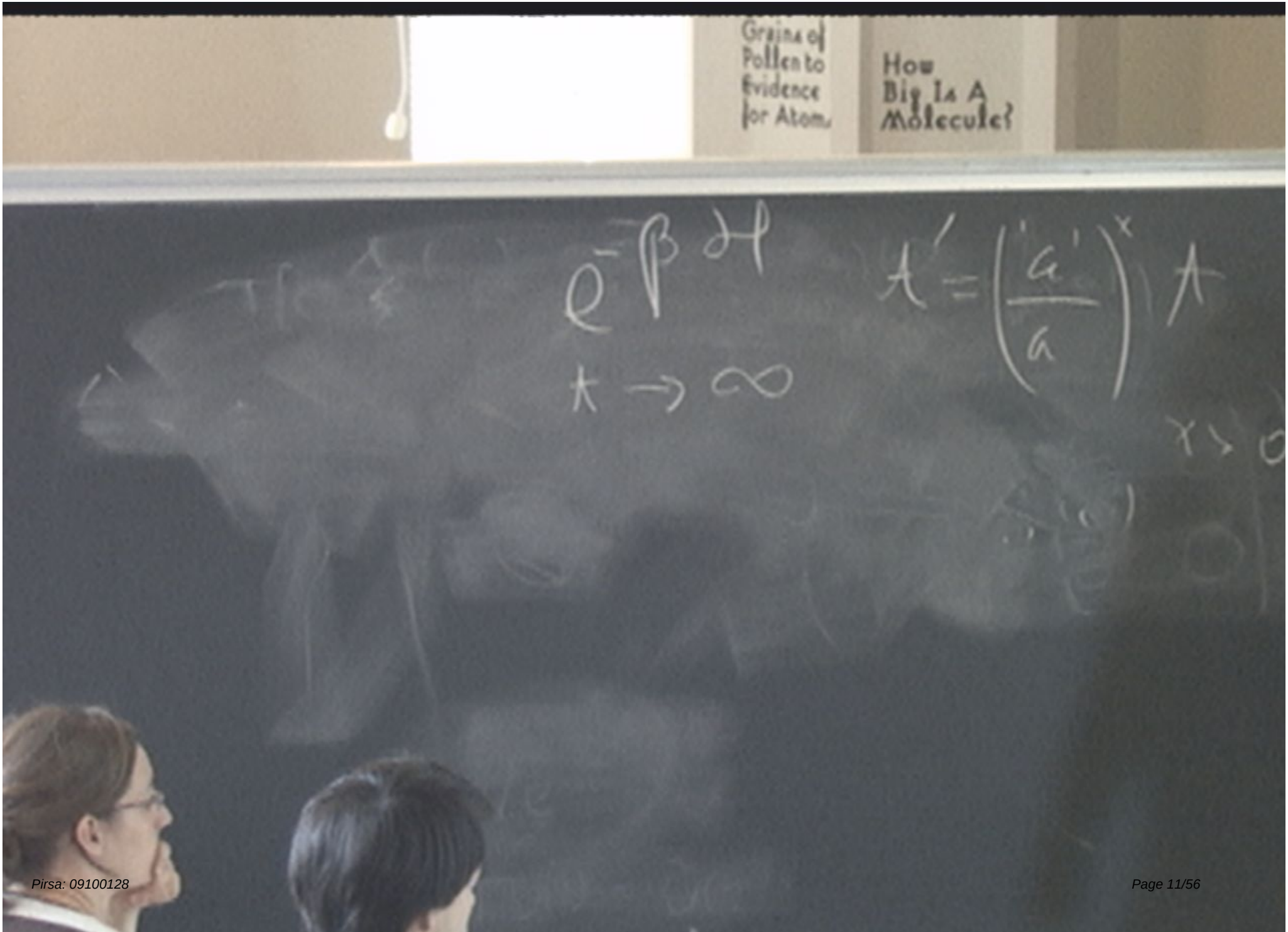
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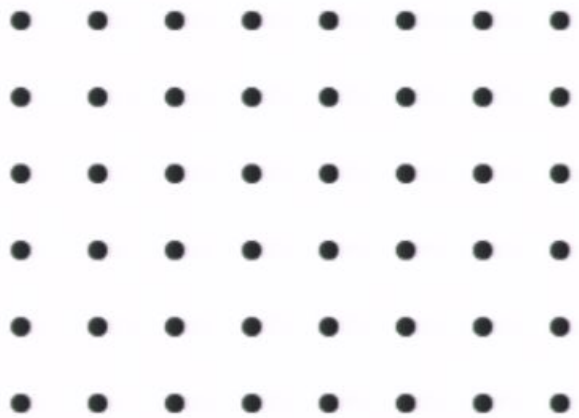
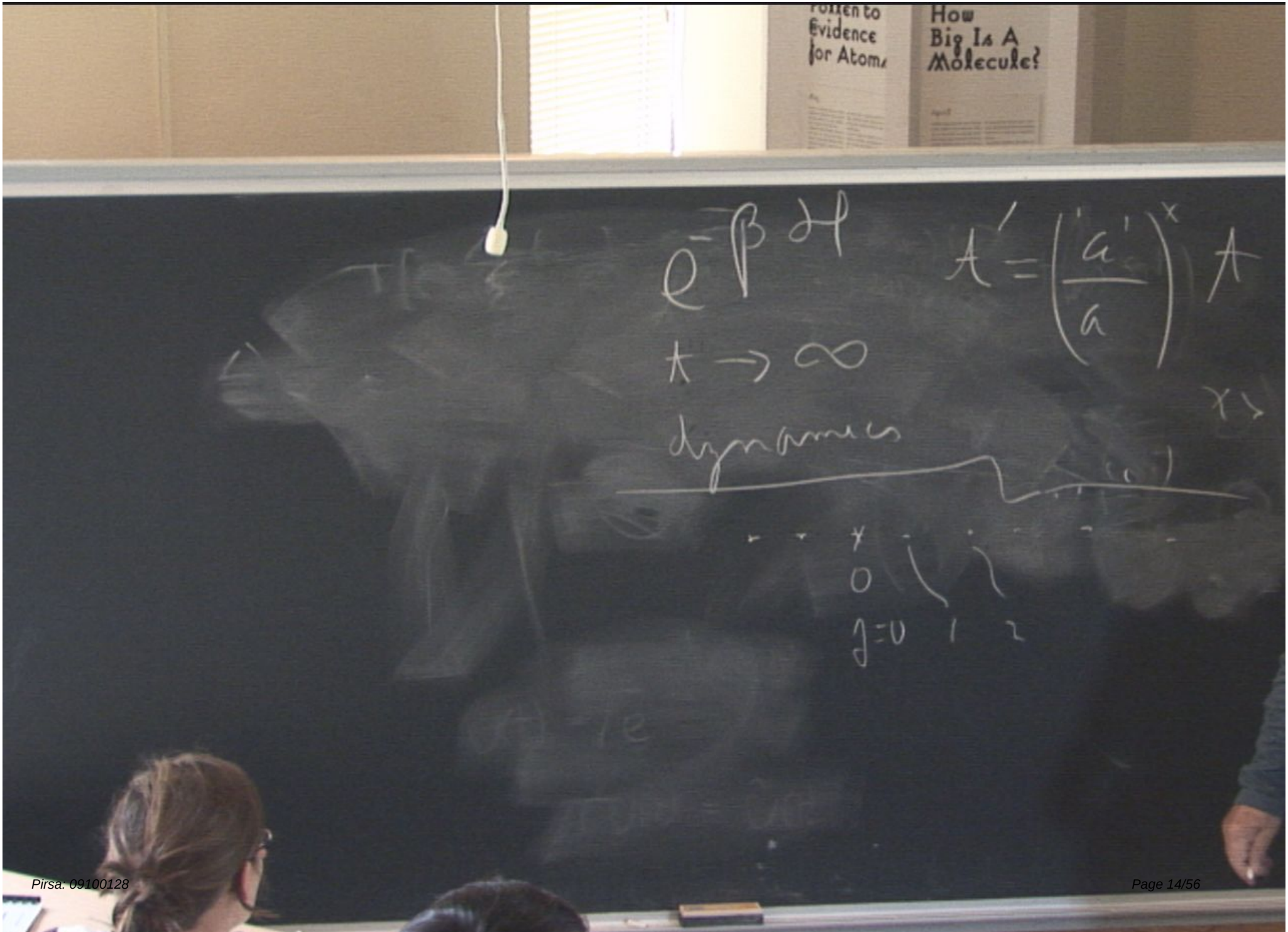
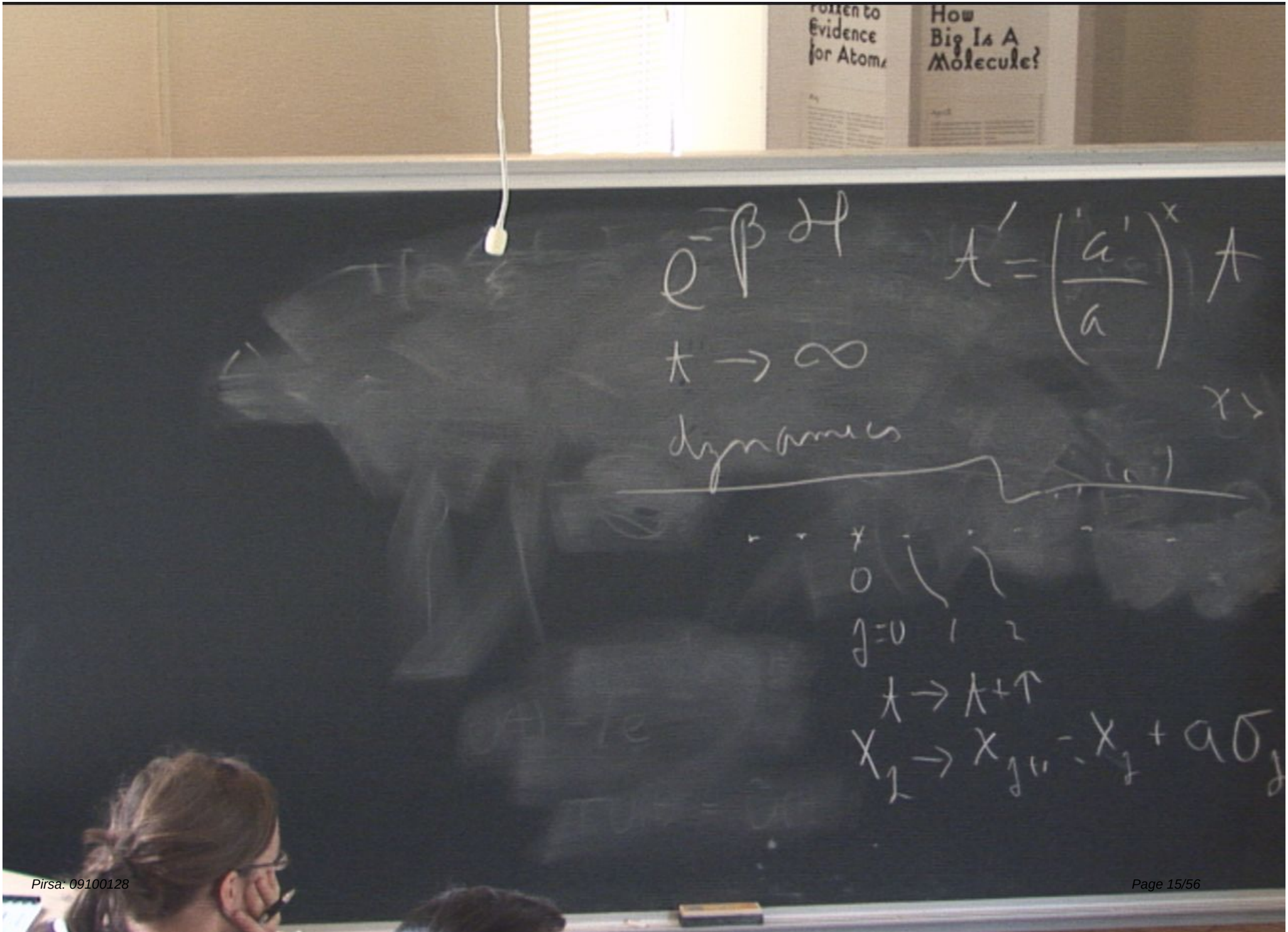
Hopping On a Lattice

A lattice is a group of sites arranged in a regular pattern. One way of doing this can be labeled by giving the position $r=(n_1,n_2,....)a$ where the n's are integers. If we include all possible values of these integers, the particular lattice generated is called is called the simple hypercubic lattice. We show a picture of this lattice in two dimensions.



This section is devoted to developing the concept of a random walk. We could do this in any number of dimensions. However, we shall approach it is the simplest possible way by first working it all out in one dimension and then stating results for higher dimensions A random walk is a stepping through space in which the successive steps occur at times $t=M\,\tau$. At any given time, the position is X(t), which lies on one of the a lattice sites, $x=an$, where n is an integer. In one step of motion one progress from $X(t)$ to $X(t+\tau) = X(t)+ a\sigma_j$, where σ_j is picked at random from among the two possible nearest neighbor hops along the lattice, σ_j $=1$ or $\sigma_j = -1$. Thus, $<\sigma_j>=0$, but of course the average its square is non-zero and is given by $<\sigma_j^2>=1$. We assume that we start at zero, so that our times $t = j\,\tau$. It is not accidental that we express the random walk in the same language as the Ising model. We do this to emphasize that geometric problems can often be expressed in algebraic form and vice versa.


How
Big Is A
Molecule?
$e^{-\beta \mathcal{H}}$
$A' = \left(\frac{a'}{a}\right)^x A$
$t \to \infty$
dynamics
x
0
j=0 1 2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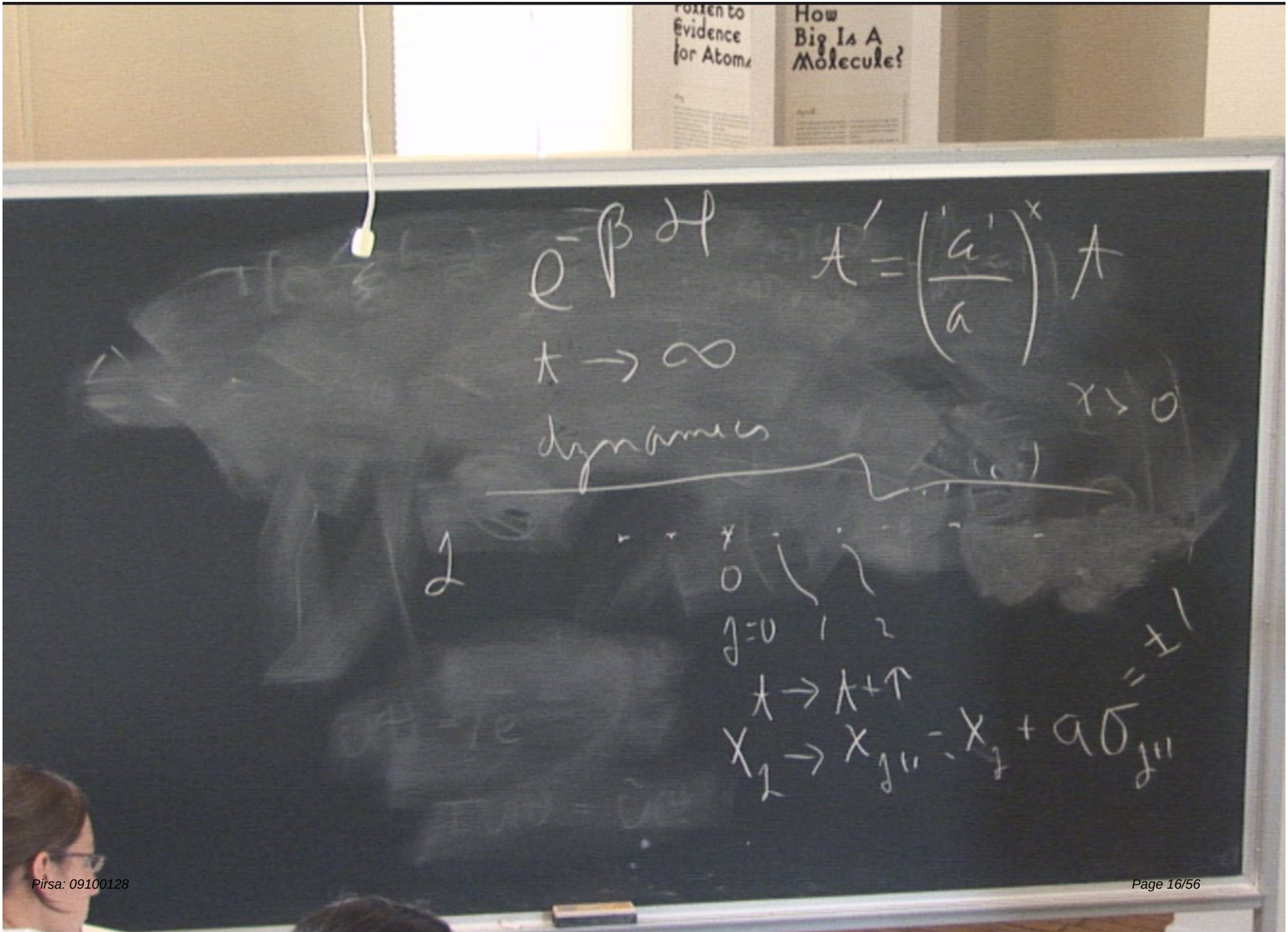
$j=0 \quad 1 \quad 2$
$t \to t+\tau$
$X_j \to X_{j+1} - X_j + a\sigma_j$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dynamics
$x > 0$
$j = 0 \quad 1 \quad 2$
$t \to t + \tau$
$X_1 \to X_{j+1} = X_j + a\sigma_{j+1}$
$= \pm 1$

From one step to many steps

We start from the two statements that $<\sigma_j>=0$ and that $<\sigma_j \sigma_k>=\delta_{j,k}$

On the average, on each step the walker goes left as much as right. and thus as a result th average displacement of the entire walk is zero

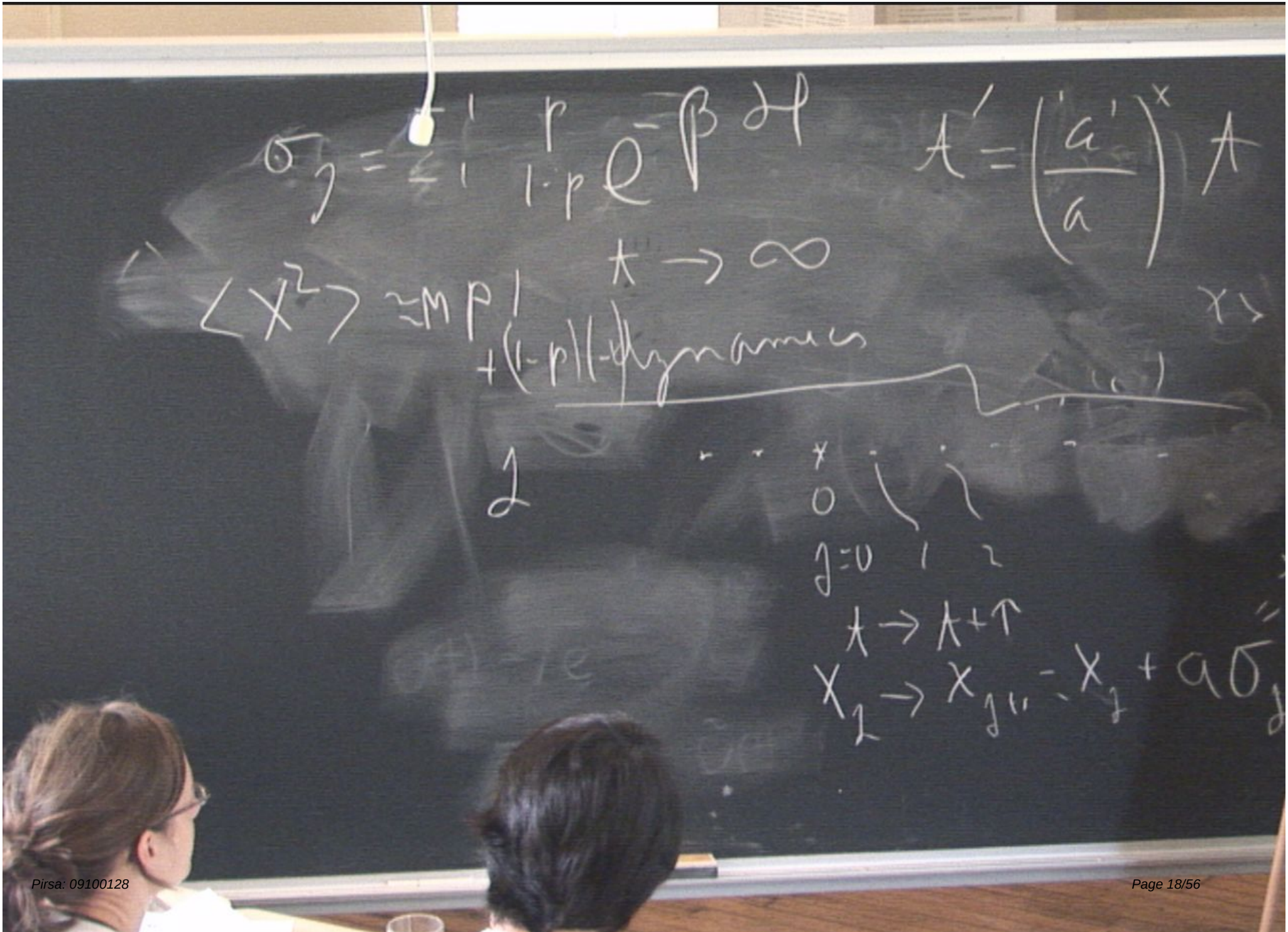
$$< X(t) >= a\sum_{j=1}^{M} < \sigma_j >= 0 \qquad \text{iv.1}$$

However, of course the mean squared displacement is not zero, since

$$< X(t)^2 >= a^2 \sum_{j,k=1}^{M} < \sigma_j \sigma_k >= a^2 \sum_{j,k=1}^{M} \delta_{j,k} = a^2 M \qquad \text{iv.2}$$

Our statement is the same that in a zero field uncoupled Ising system, the maximum magnetization is proportional to the number of spins, but the typical magnetization is only proportional to the square root of that number. Typical fluctuations are much, much smaller than maximum deviations.

We can see this fact by noting that the root mean square average of X^2 is $a\sqrt{M}$, which is the typical end-to-end distance of this random walk. This distance is is much smaller than the maximum distance which would be covered were all the steps to go in the same direction. In that case we would have had a distance aM.
Thus, a random walk does not, in net, cover much ground.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$+(1-p)(1-q)$ dynamics
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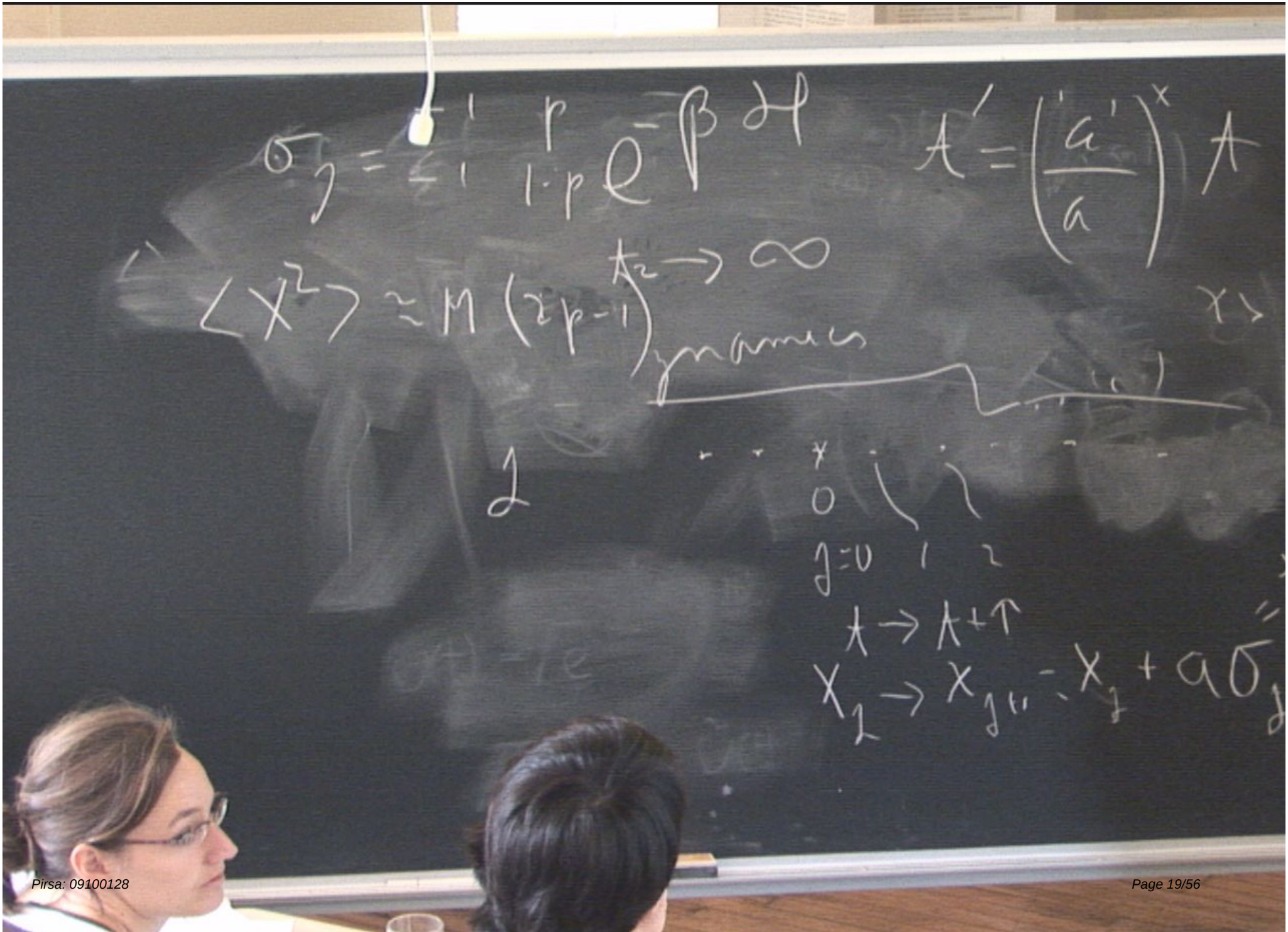
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$r \cdot p e^{-\beta \mathcal{H}}$
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Δ
$\langle X^2 \rangle \simeq M (2p-1)$
$\lambda_2 \to \infty$
$x >$
x
0
$j = 0 \quad 1 \quad 2$
$\lambda \to \lambda + \uparrow$
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Gaussian Properties of Continuous Random Walk

In the continuous case, $X(t)$ is composed of a sum, or rather integral, of many pieces which are uncorrelated with one another. According to the central limit theorem, such a sum or integral is a Gaussian random variable. Hence, we know everything there is to know about it. Its average is zero and its variance is a^2t/τ . Consequently, it has a probability distribution

$$< \rho(X(t) = x) >= \left(\frac{\tau}{2\pi a^2 t}\right)^{1/2} e^{-x^2\tau/(2a^2t)} \qquad \text{iv.9}$$

Now we have said everything there is to say about the continuous random walk. As an extra we can exhibit the generating function for this walk:

$$< \exp[iqX(t)] >= e^{-q^2a^2t/(2\tau)}$$

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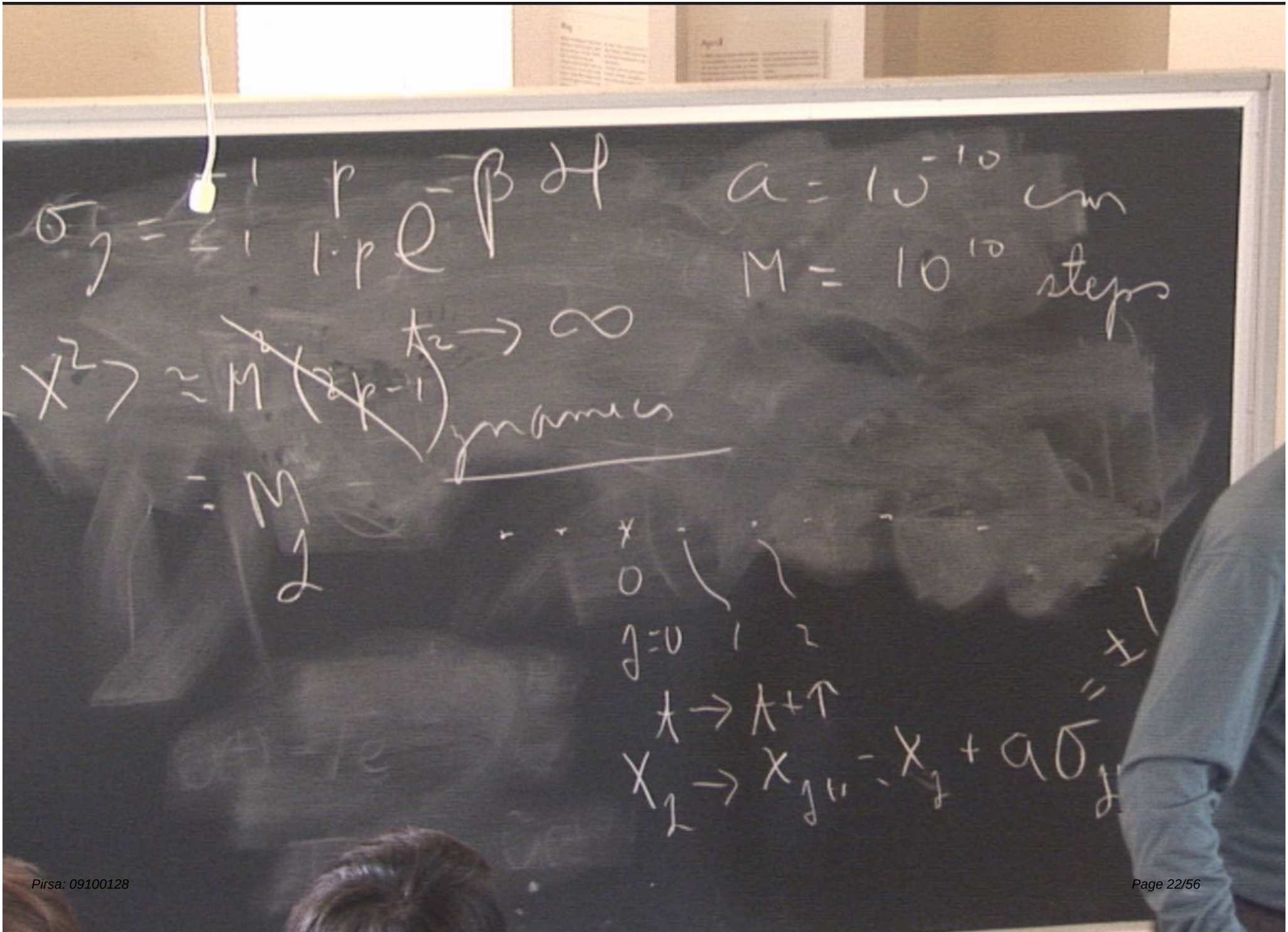
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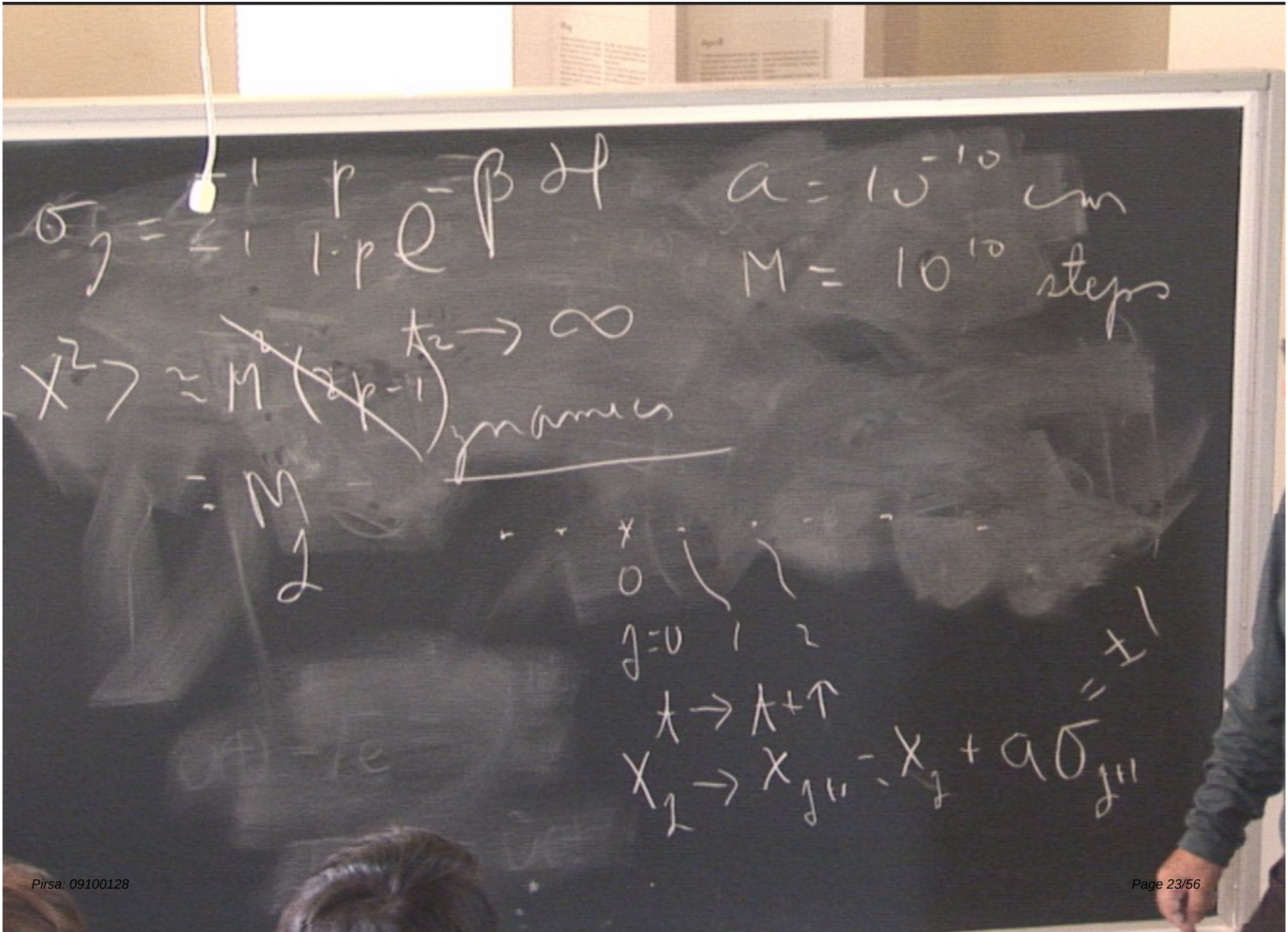
dynamics
$j = 0 \quad 1 \quad 2$
$t \to t + \tau$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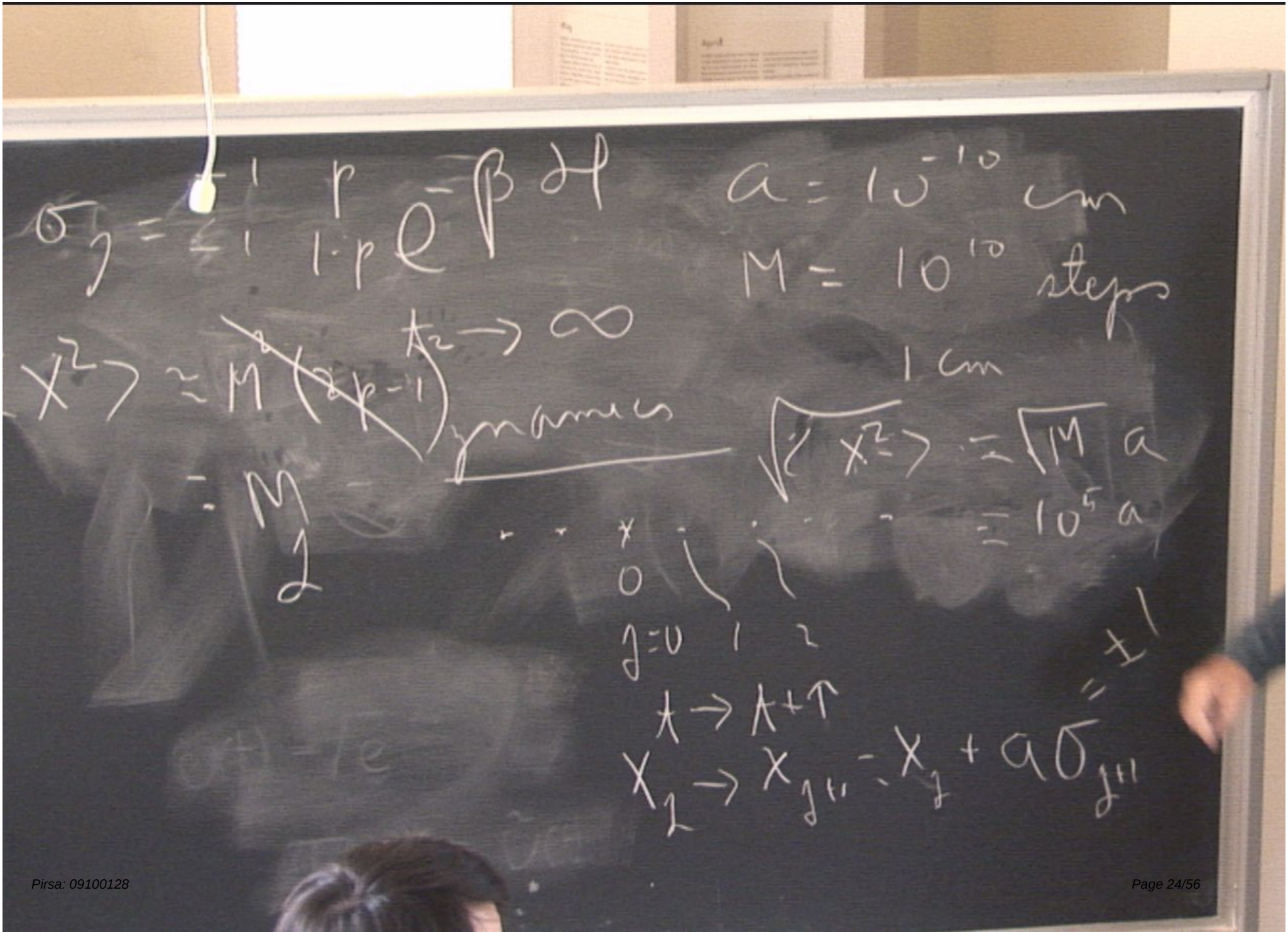
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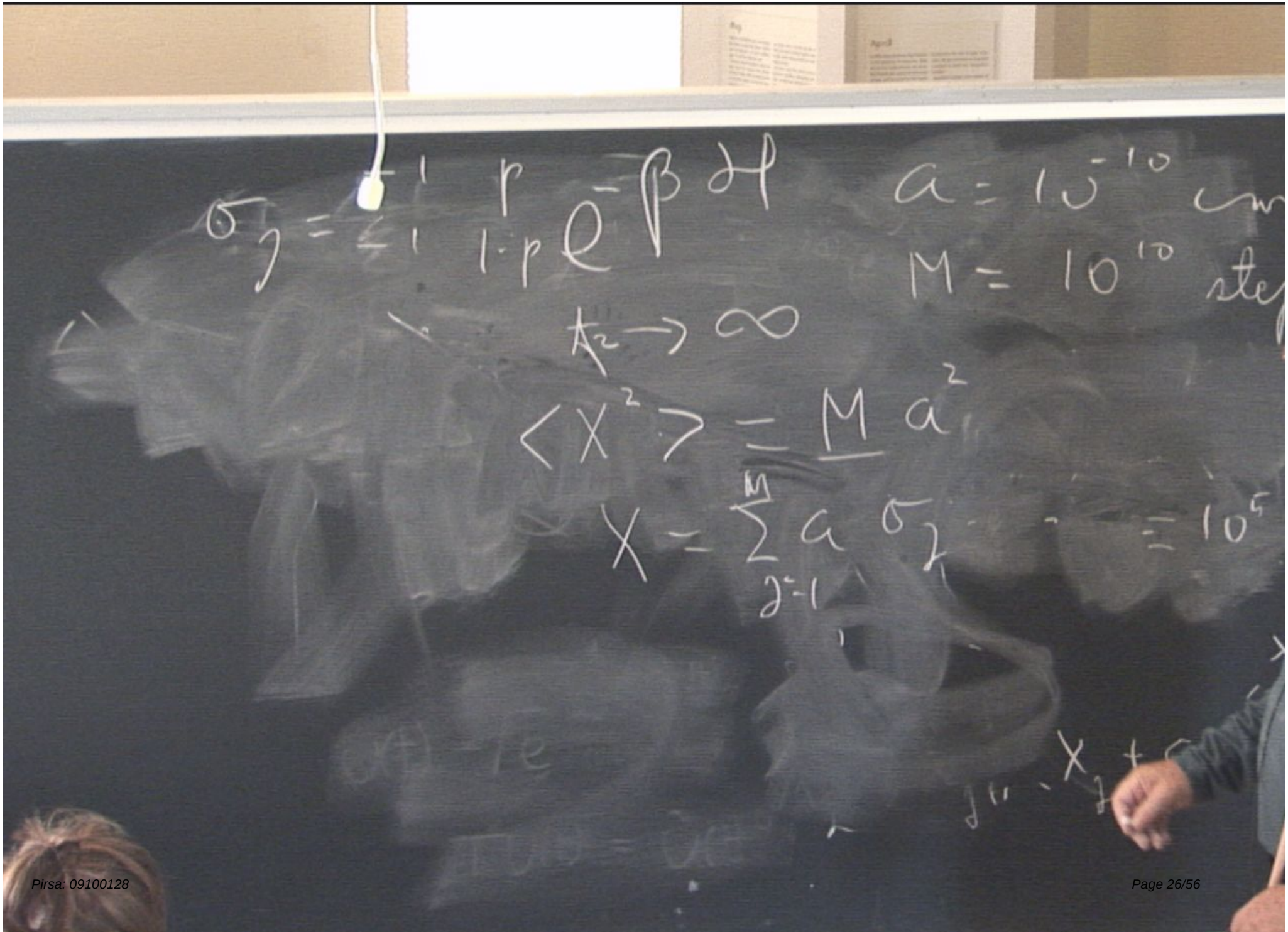
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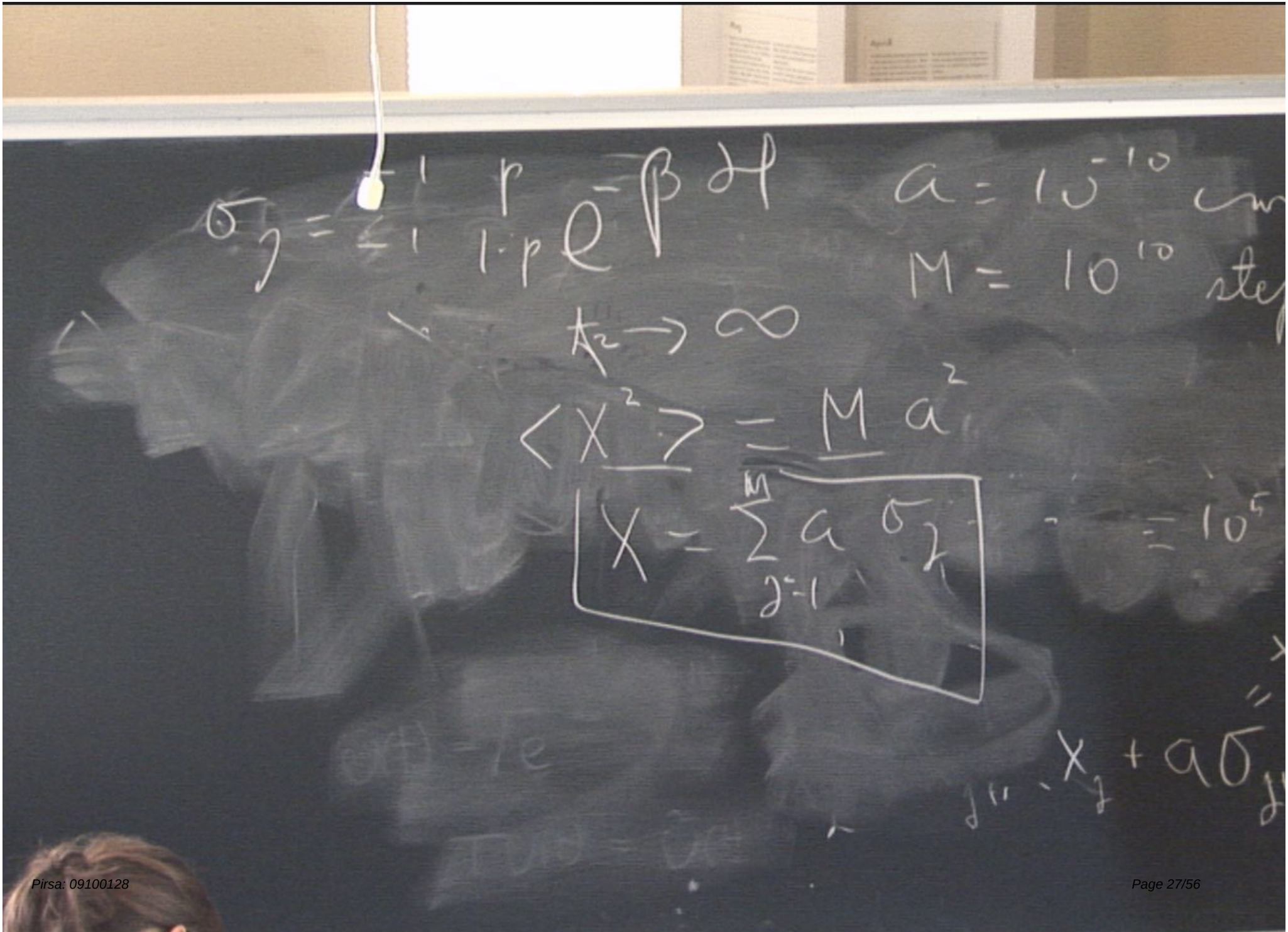
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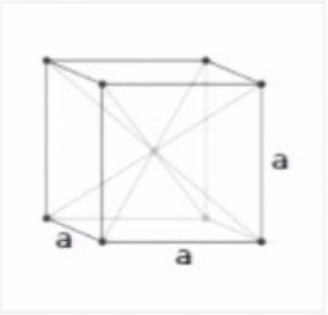

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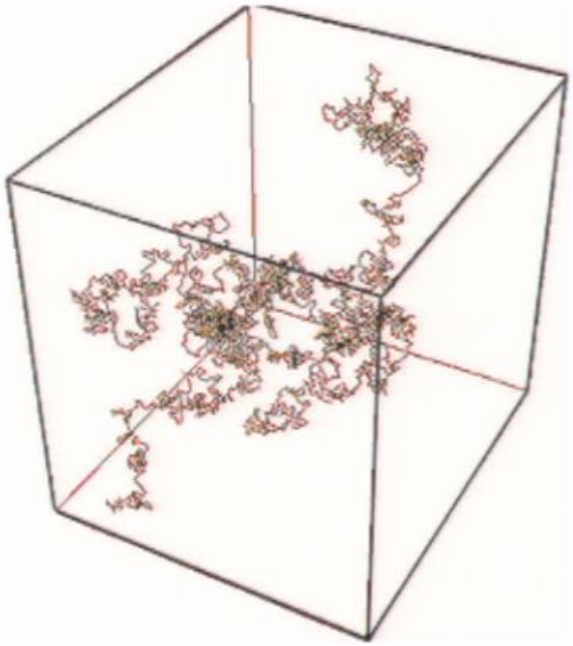
RANDOM WALKS

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



dspace.mit.edu/.../CourseHome/index.htm

Higher Dimensions.....continued

We denote the probability density of this d-dimensional case by a superscript d and the one for the previous one-dimensional case of by a superscript 1. As an additional difference, the d-dimensional object will be a function of space and time rather than n and M. After a while, we shall focus entirely upon the higher dimensional case and therefore drop the superscripts. We have

$$\rho^d_{a\mathbf{n},M\tau} = \prod_{\alpha=1}^{d} \rho^1_{n_\alpha,M}$$

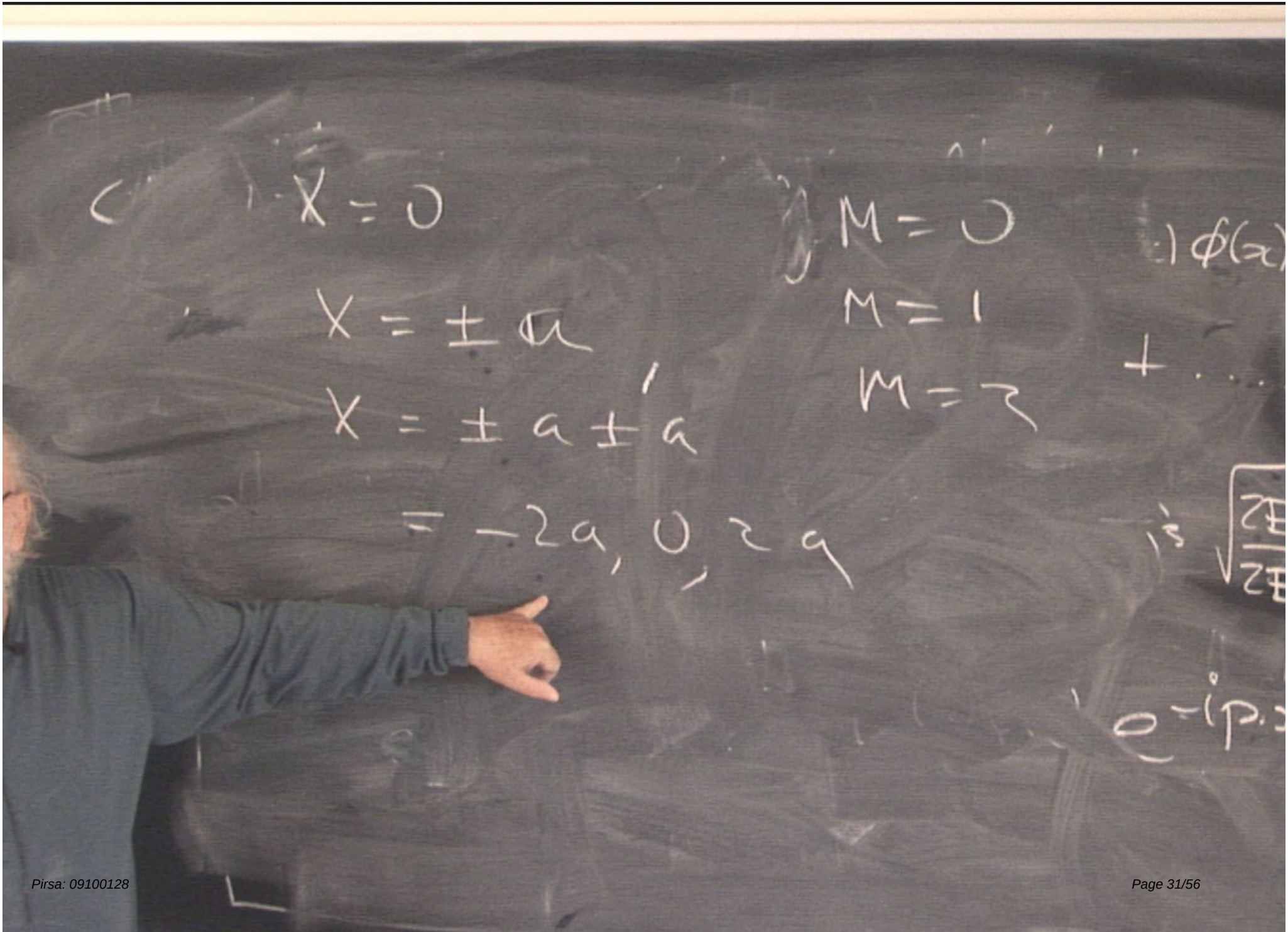
However, we can jump directly to the answer for the continuum case, If the probability distribution for the discrete case is simply the product of the one-dimensional distributions so must be the continuum distribution. The one-dimensional equation answer in eq iv.9 was

$$< \rho(X(t) = x) >= \left(\frac{\tau}{2\pi a^2 t}\right)^{1/2} e^{-x^2\tau/(2a^2t)} \qquad \text{iv.9}$$

so that the answer in d dimensions must be

$$< \rho(\mathbf{R}(t) = \mathbf{r}) >= \left(\frac{\tau}{2\pi a^2 t}\right)^{d/2} e^{-r^2\tau/(2a^2t)}$$

Here the bold faced quantities are vectors, viz $\mathbf{r^2} = x^2 + y^2 + ...$

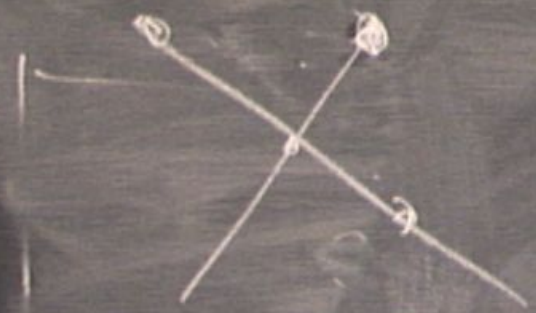

X = 0
M = 0
X = ± a
M = 1
X = ± a ± a
M = 2
= −2a, 0, 2a

$X = 0$

$X = \pm a$

$X = \pm a \pm a$

$= -2a, 0, 2a$



$M = 0$

$M = 1$

$M = 2$

$|\phi(x)|$

$+ \ldots$

$\sqrt{\frac{2E_p}{2E_k}}$

$e^{-ip \cdot x}$

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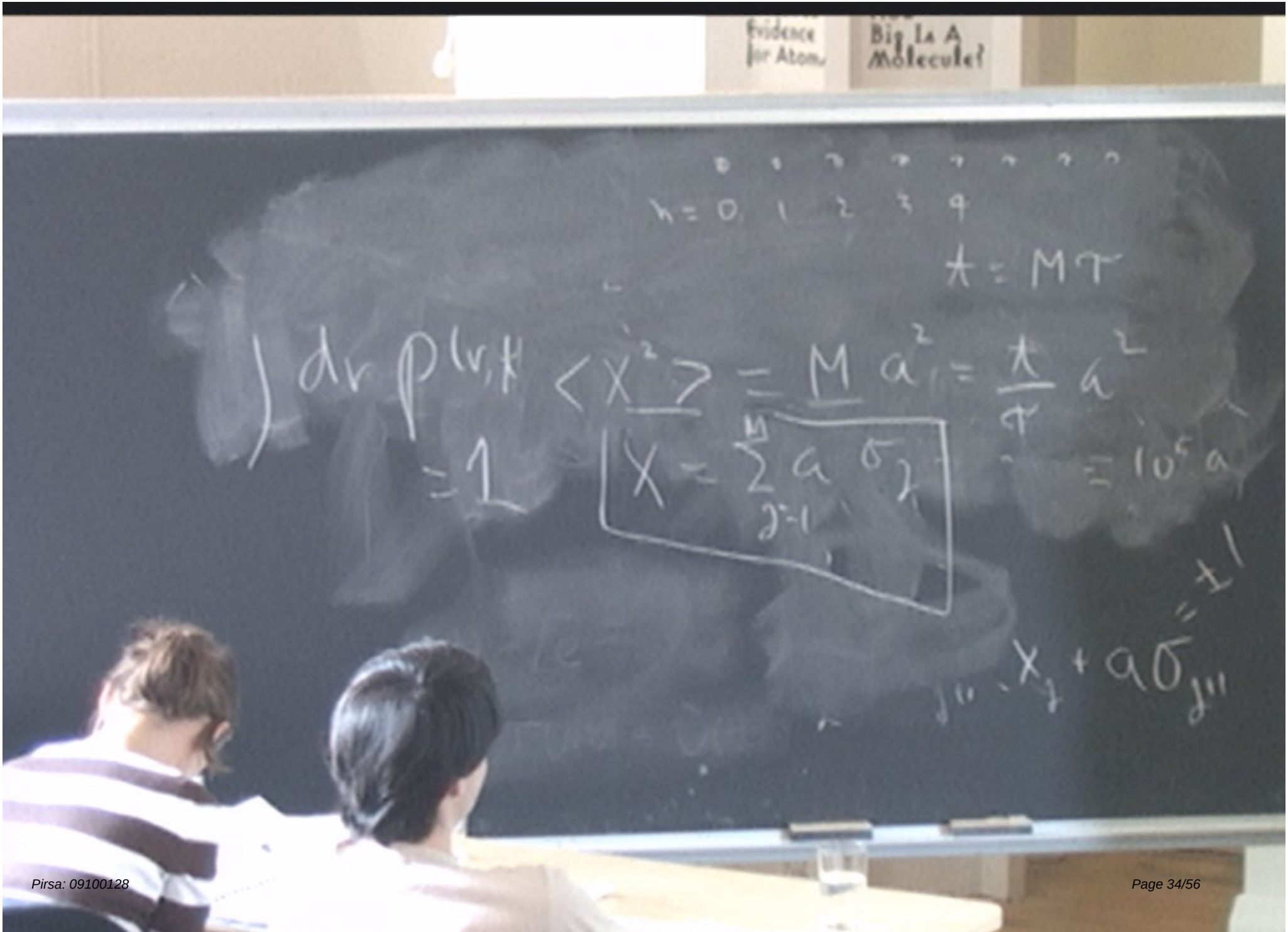
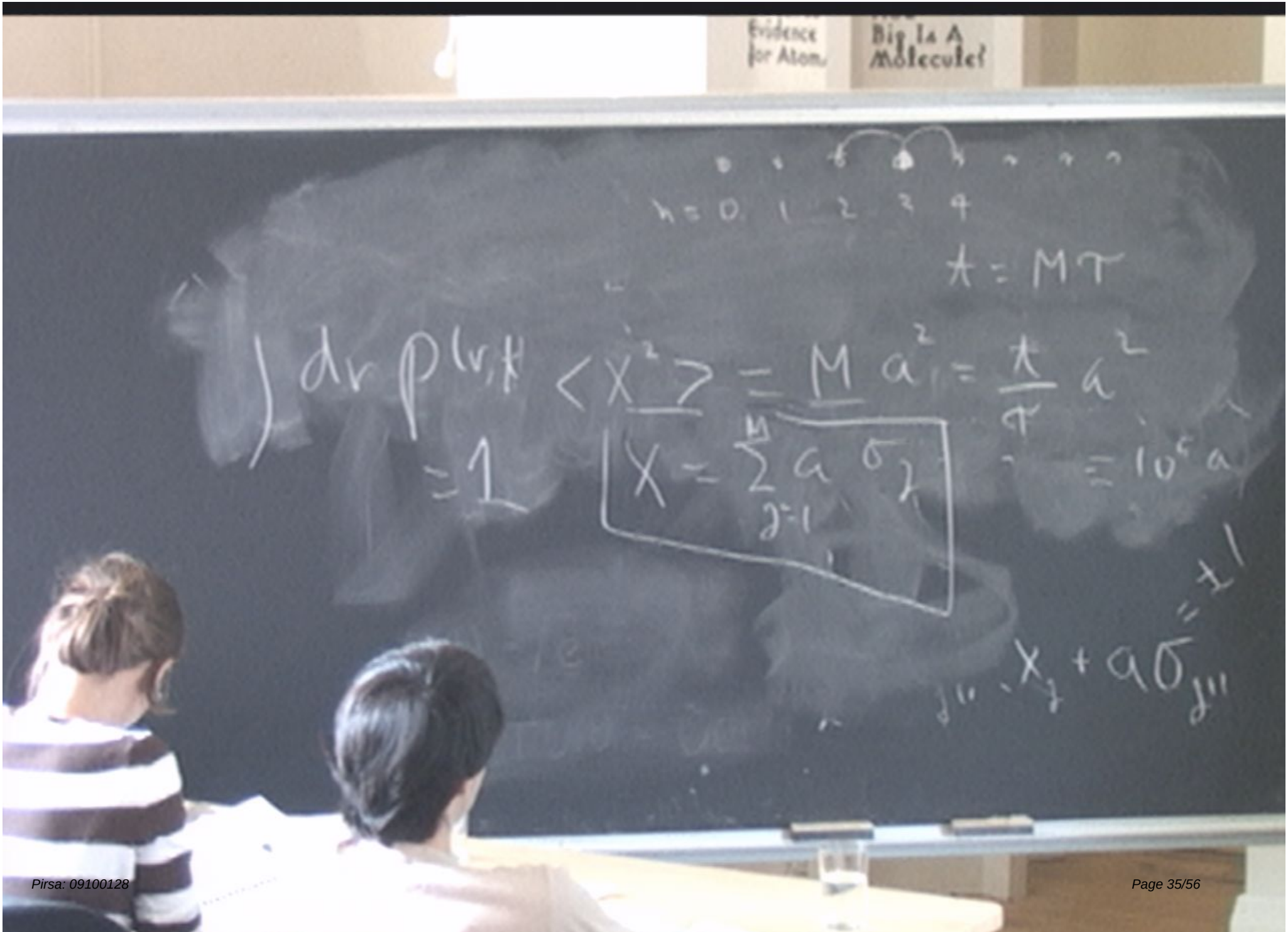
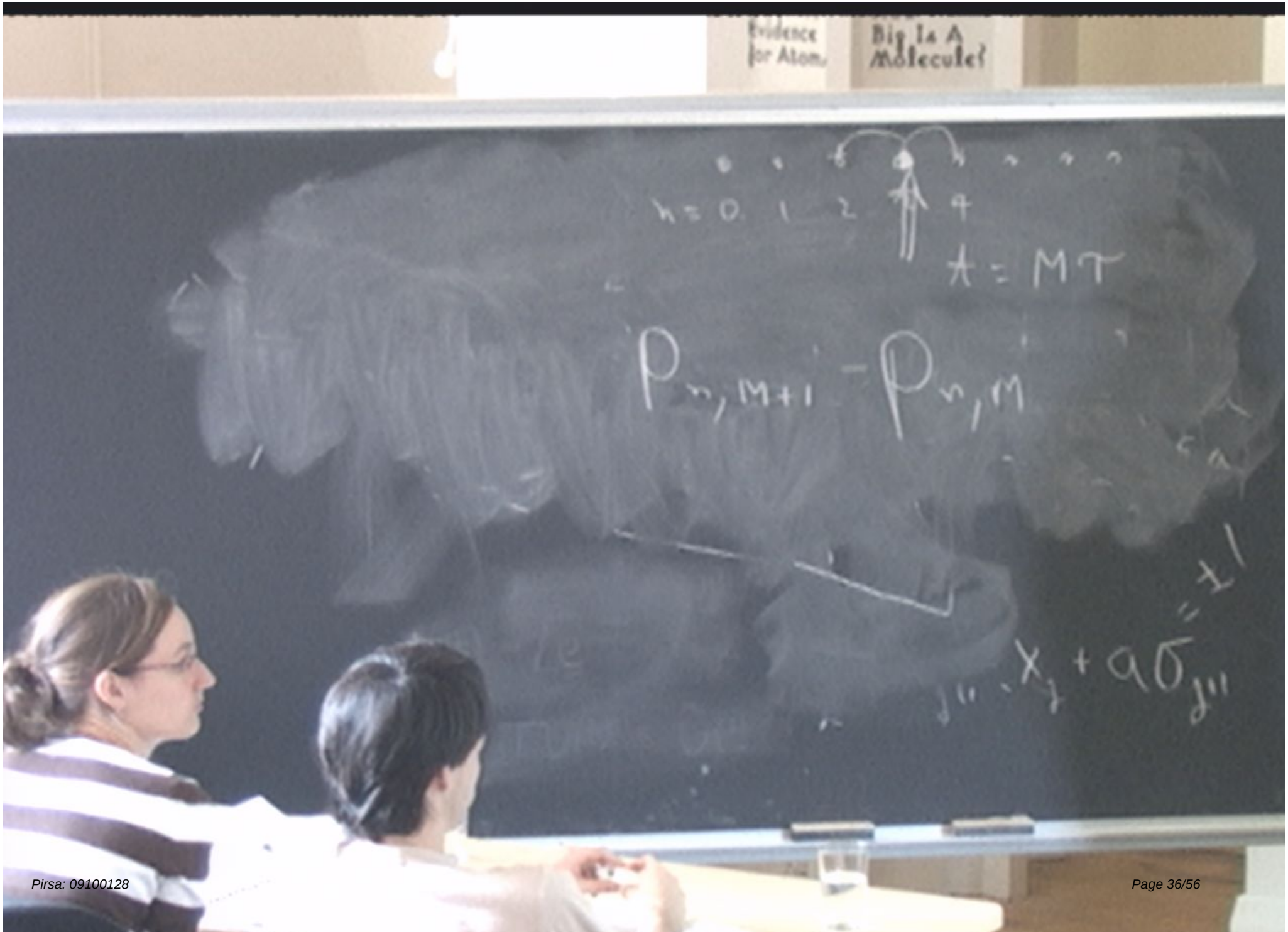
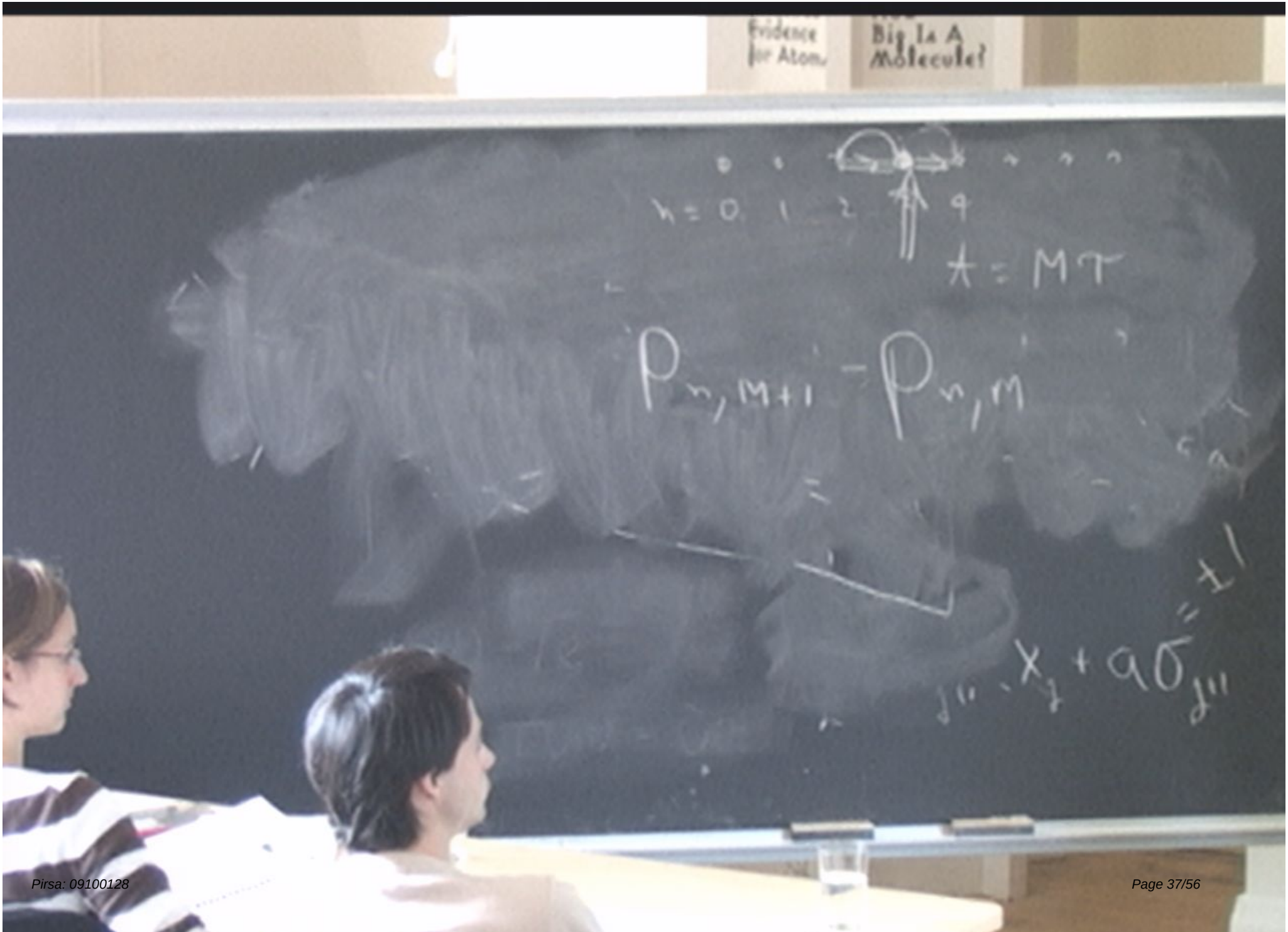
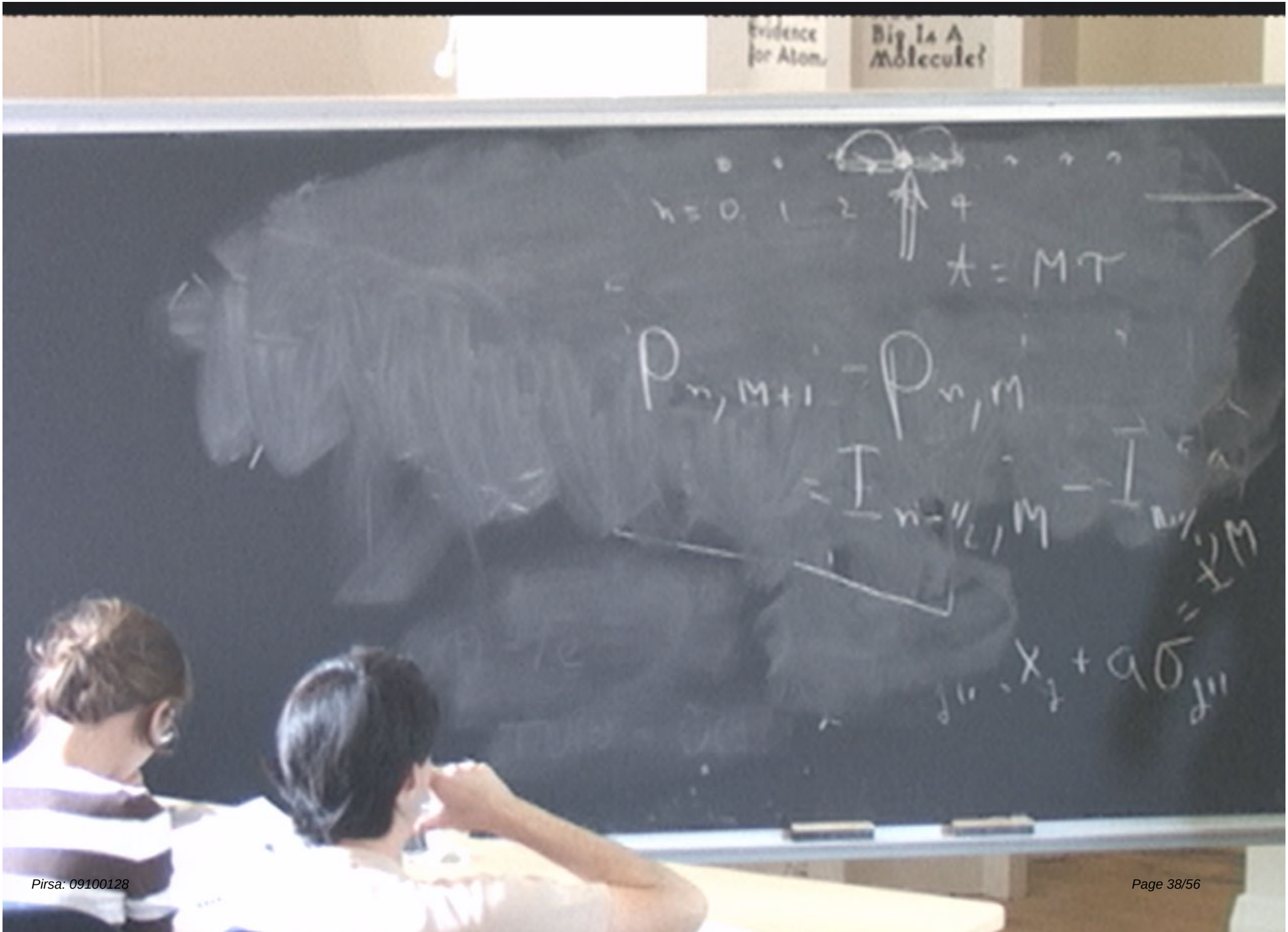

Evidence for Atom
Big Is A Molecule?
$t = M\tau$
$\int dr\, \rho(r,t) = 1$
$\langle x^2 \rangle = M a^2 = \frac{t}{\tau} a^2$
$X = \sum_{j=1}^{M} a\, \sigma_j$
$= 10^5 a$
$= \pm 1$
$\sigma_{j+1} = X_j + a\sigma_{j+1}$


Evidence for Atom
Big Is A Molecule?
h = 0 1 2 3 4
t = MT
$\int dr\, \rho(r,t) = 1$
$\langle \dot{X}^2 \rangle = \frac{M a^2}{\tau} = \frac{t}{\tau} a^2$
$X = \sum_{j=1}^{M} a\, \sigma_j$
$= 10^6 a$
± 1
$X_j + a\sigma_{j+1}$


Evidence for Atom
Big Is A Molecule?
h = 0 1 2 4
A = MT
$P_{n,M+1} - P_{n,M}$
$X_j + q\sigma_{jn}$
$= \pm 1$


Evidence for Atom
Big Is A Molecule?
n = 0 1 2 q
A = MT
$P_{n,M+1} - P_{n,M}$
$X_1 + q\sigma$


Evidence for Atom
Big Is A Molecule?
n = 0 1 2 q
A = MT
P n, M+1 - P n, M
= I n-1/2, M - I
± M
X + qσ

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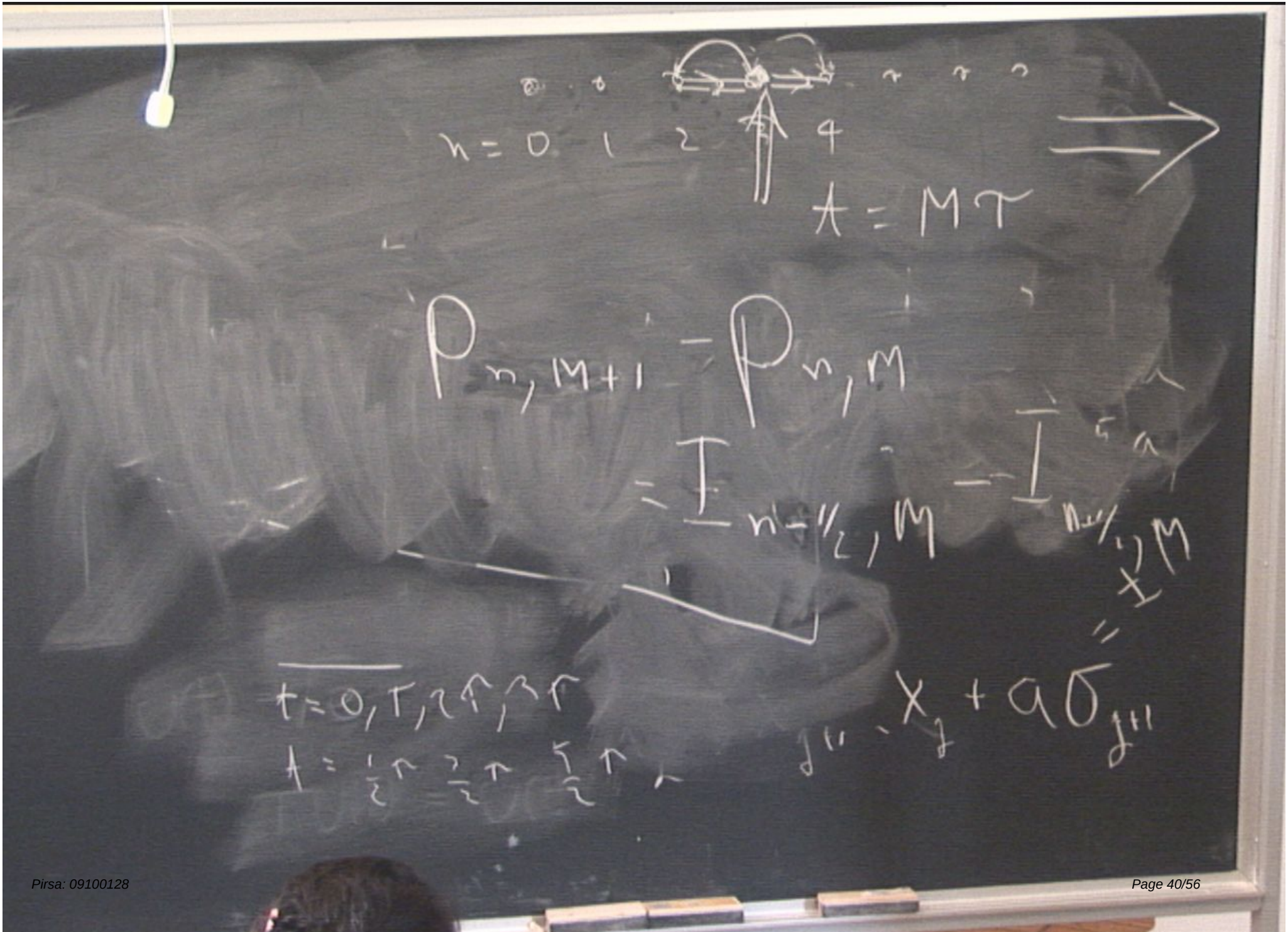
n = 0 1 2 q
t = Mτ
P n, M+1 = P n, M
t = 0, τ, 2τ, 3τ
t = 1/2 τ 3/2 τ 5/2 τ

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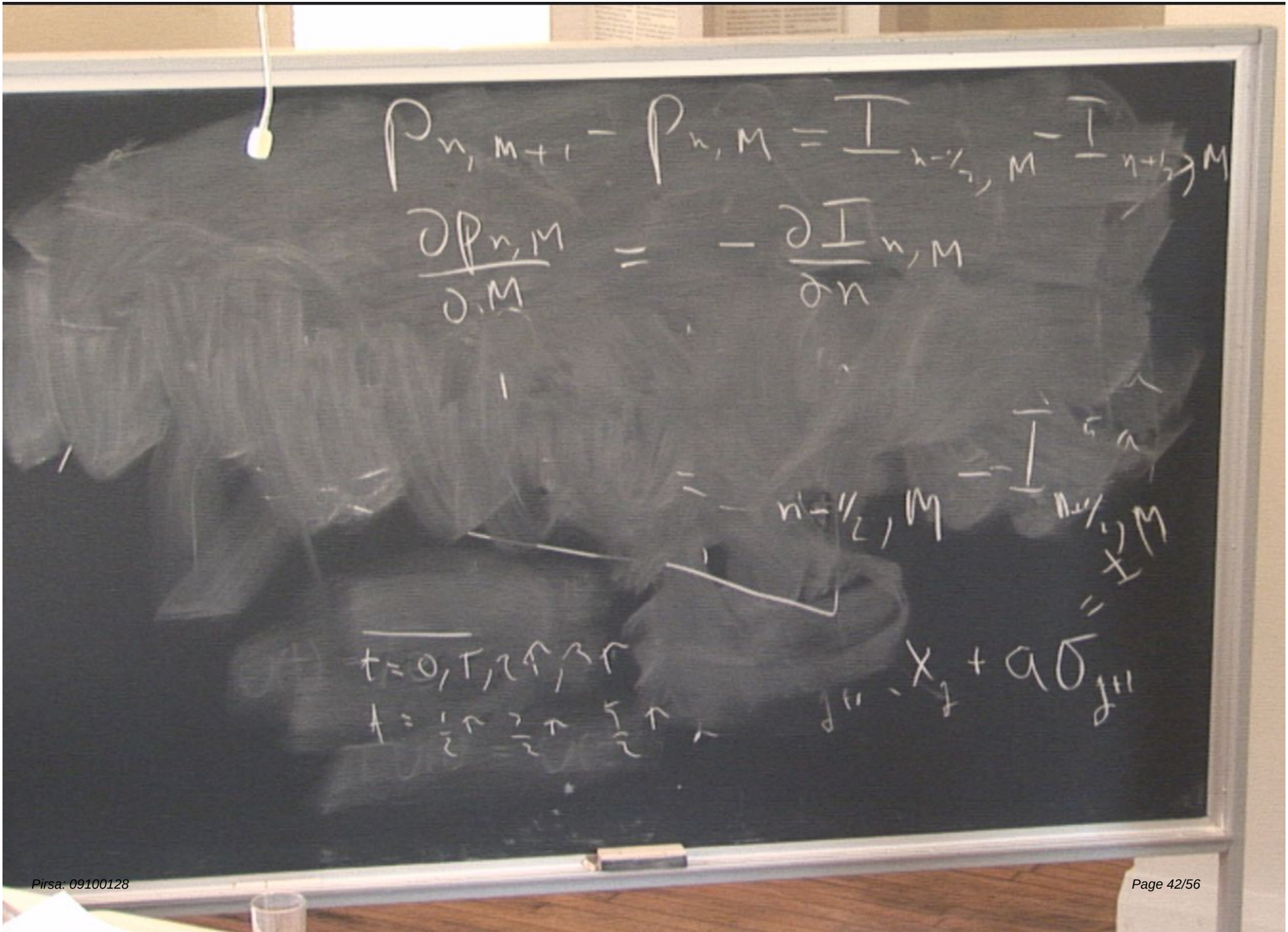
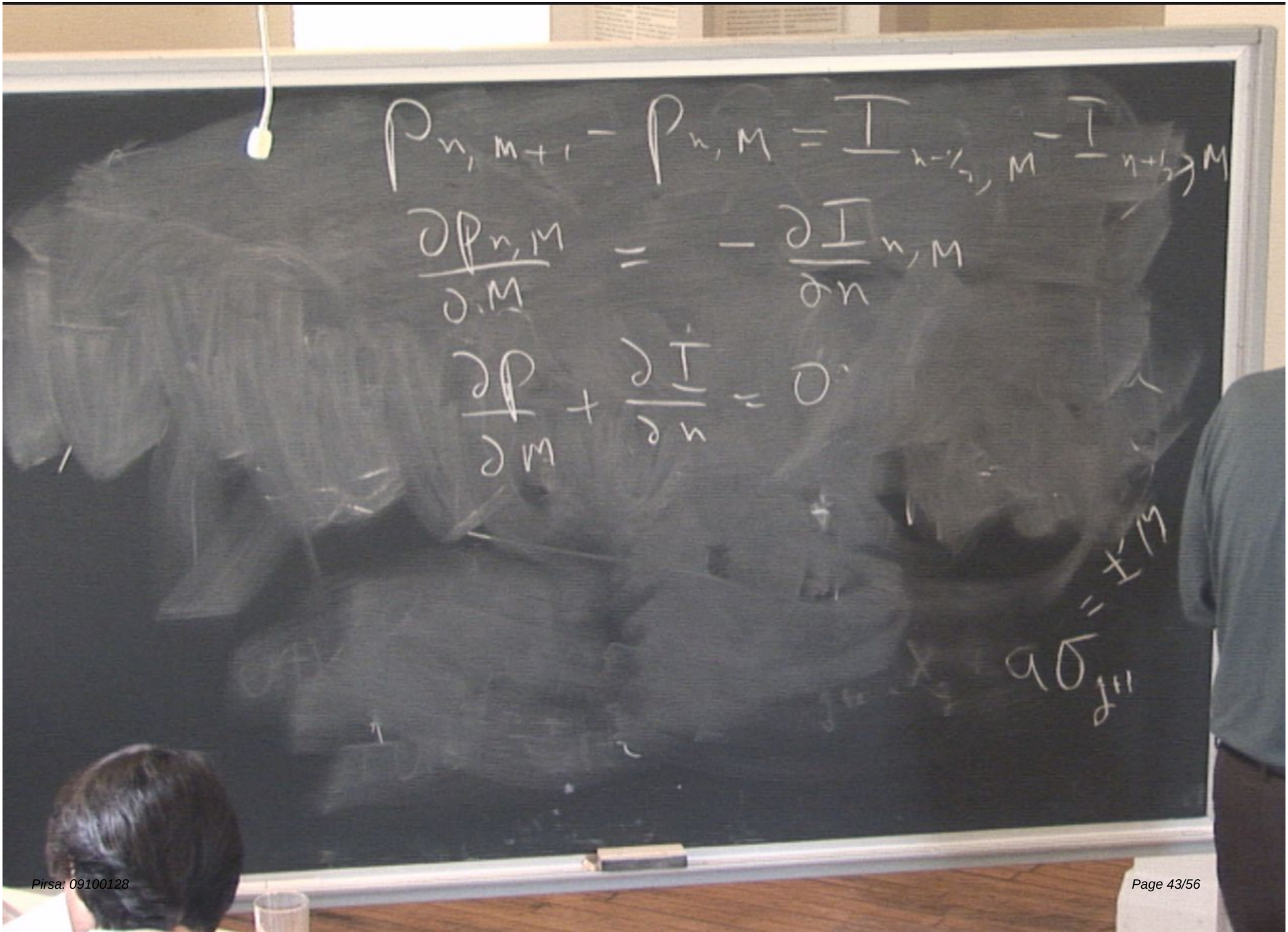
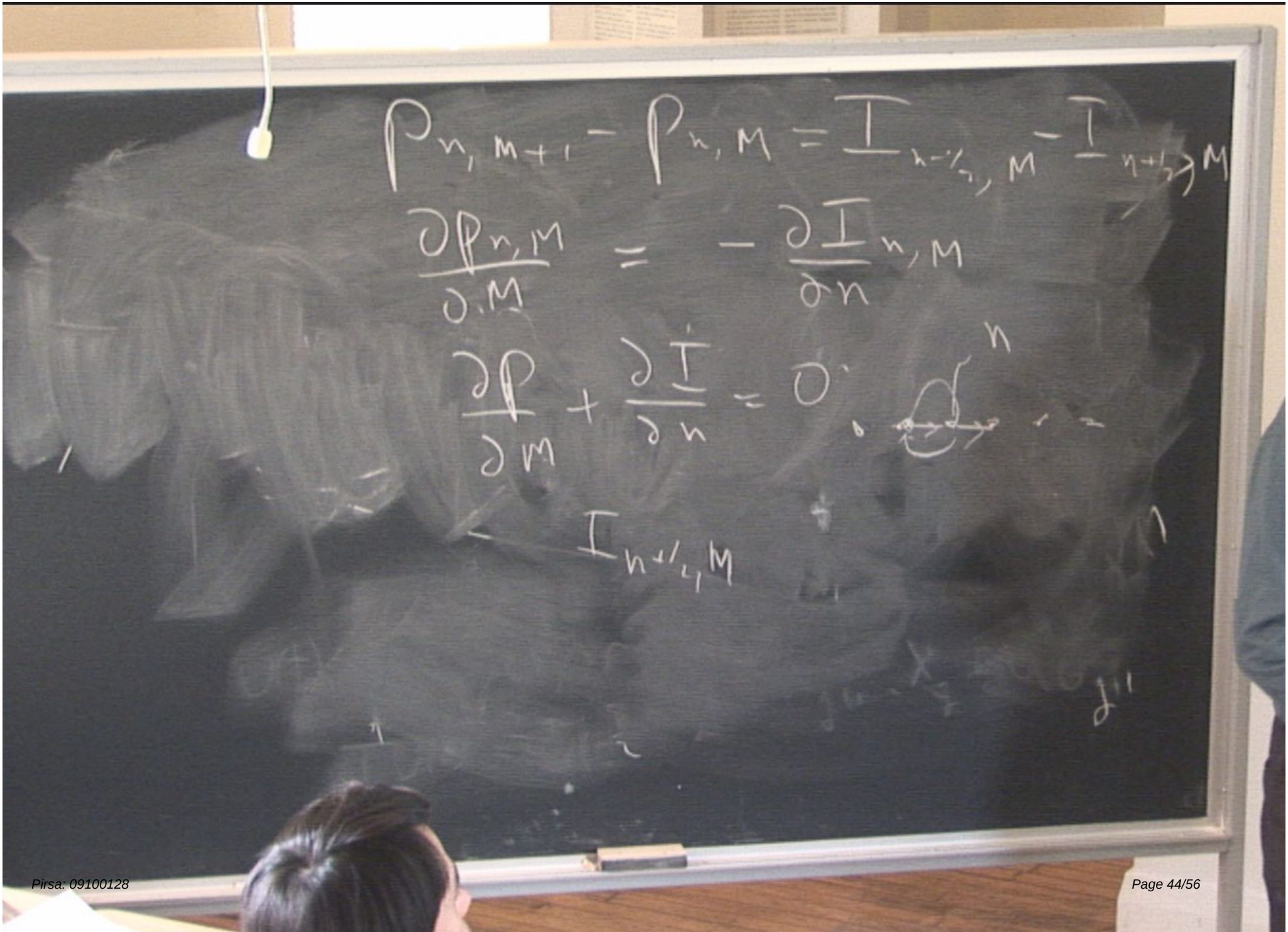

$\rho_{n,m+1} - \rho_{n,m} = I_{n-1/2,m} - I_{n+1/2,m}$
$\frac{\partial \rho_{n,m}}{\partial m} = -\frac{\partial I_{n,m}}{\partial n}$


$\rho_{n,m+1} - \rho_{n,m} = \bar{I}_{n-\frac{1}{2},m} - \bar{I}_{n+\frac{1}{2},m}$
$\frac{\partial \rho_{n,m}}{\partial m} = -\frac{\partial \bar{I}}{\partial n}_{n,m}$
$\frac{\partial \rho}{\partial m} + \frac{\partial \bar{I}}{\partial n} = 0$
$q\sigma = \pm m$


$\rho_{n,m+1} - \rho_{n,m} = I_{n-1/2,m} - I_{n+1/2,m}$
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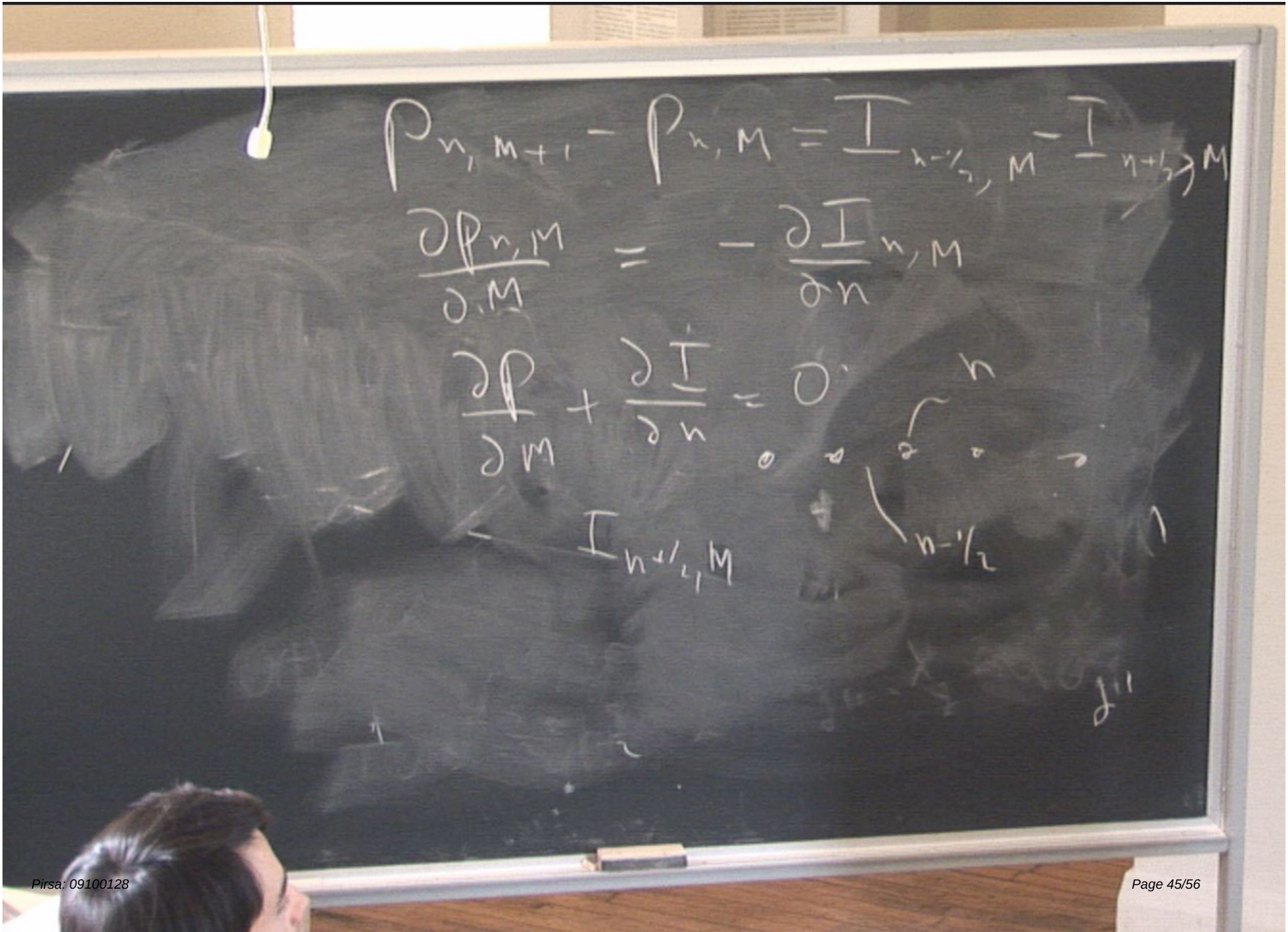
$I_{n+1/2,m}$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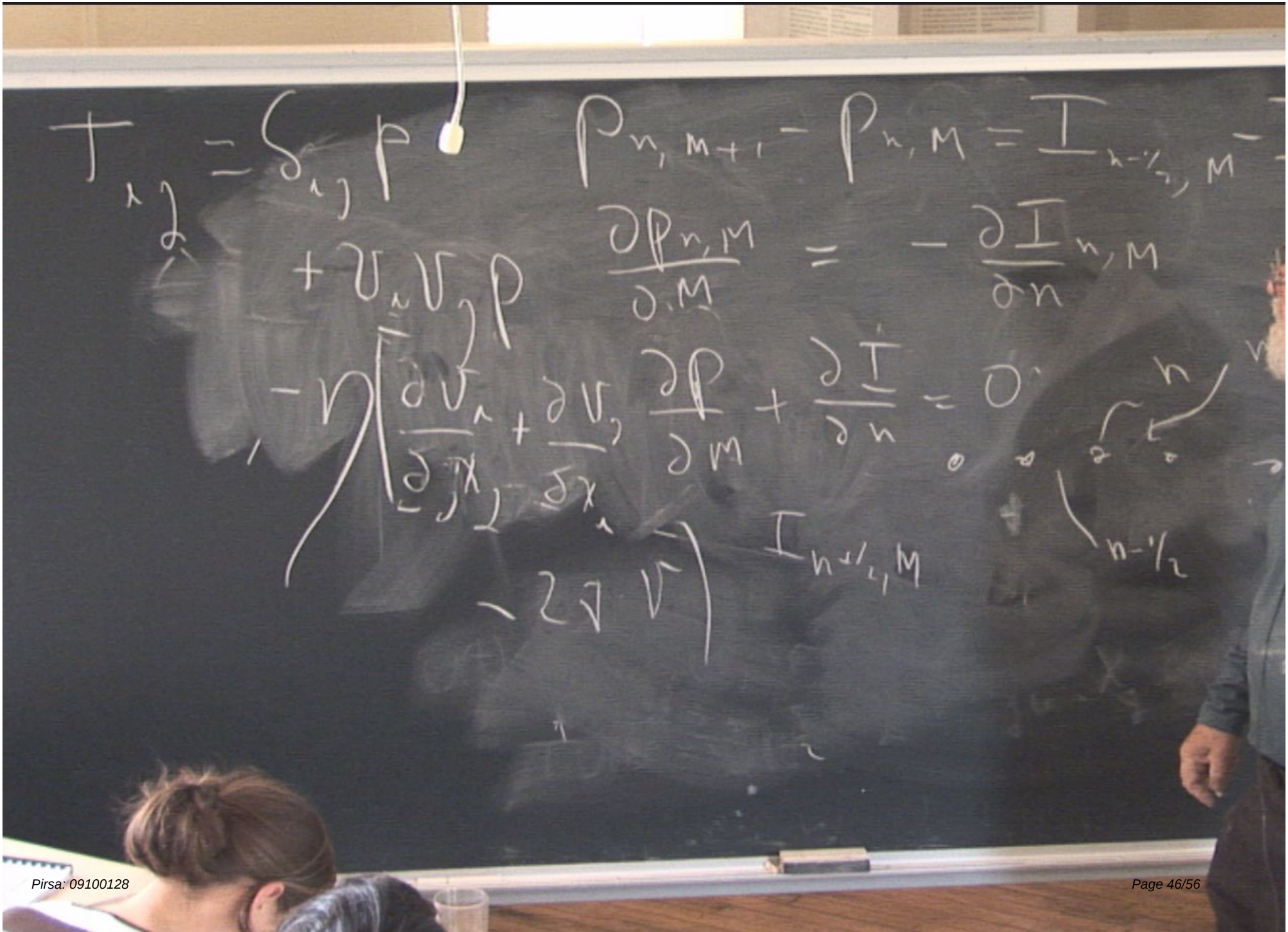
$\frac{\partial \rho}{\partial M} + \frac{\partial I}{\partial n} = 0$
$I_{n+1/2,M}$
$n-1/2$



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The Current

We do not have a full statement of the of what is happening until we can specify the current. An approximate definition of a current in a conservation law is called a constitutive equation. We now write this down.

Our hopping model says that a $I_{n+1/2,M}$ is given a contribution +1 when the site at n is occupied at time M, and σ_n is equal to +1. On the other hand it is given a contribution -1 when the site at n +1 is occupied at time M, and σ_{n+1} is equal to -1. Since there is a probability 1/2 for each of the σ−events the value of *I* is

$$I_{n+1/2,m} = (\rho_{n,m} - \rho_{n+1,m}) / 2$$ constitutive equation

Once again, we write the difference in terms of a derivative, getting

$$I_{n,m} = -(\partial \rho_{n,m} / \partial n) / 2$$ constitutive equation

This can then be combined with the conservation law to give the diffusion equation

$$\partial \rho_{n,M} / \partial M = \partial^2 \rho_{n,M} / \partial\, n^2 / 2$$

which can be written in dimensional form as

$$\frac{\partial \rho}{\partial t} = \lambda \frac{\partial^2 \rho}{\partial\, x^2}$$ diffusion equation

with the diffusion coefficient being given by $\lambda = a^2/(2\,\tau)$

Diffusion Equation

This equation is one of several equations describing the slow transport of physical quantities from one part of the system to another. When there is slow variation is space, the conservation law guarantees that the rate of change in time will also be slow. In fact this is part of a general principle which permits only slow changes as a result of a conservation law. This general principle is much used in the context of quantum field theory and condensed matter physics. The idea is connected with the construction of the kind of particle known as a Nambu-Goldstone boson, named for two contemporary physicists, my Chicago colleague Yoichiro Nambu and the MIT theorist Jeffrey Goldstone.

Solution to Diffusion Equation Cannot be Carried Backward in Time

The wave equation is $(\partial_t^2 - \partial_X^2)F = 0$

Its general solution is $F(x,t)=G(x-ct)+H(x+ct)$

This is a global solution. It enables you to look forward or back infinitely far in the future or the past without losing accuracy. Find solution from $F(x,0) = \partial_X F(x,0) = 1$ for $0<x<1$ and $F(x,0) = \partial_X F(x,0) = 0$ otherwise. Use $c=2$

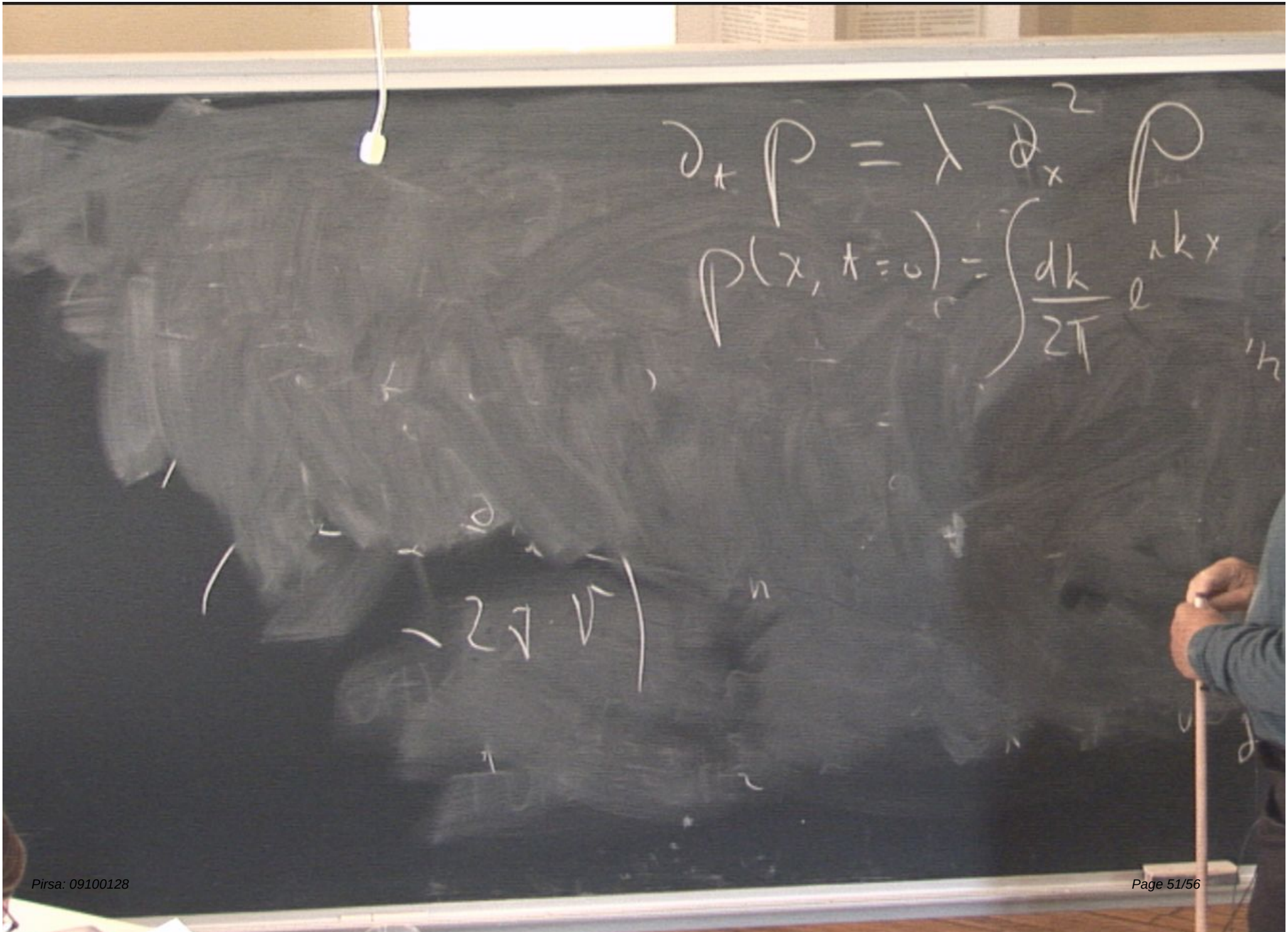
A global solution to the diffusion equation is $\rho(x,t)= \int dk \ \exp[ikx-\lambda k^2 t] \ g(k)$

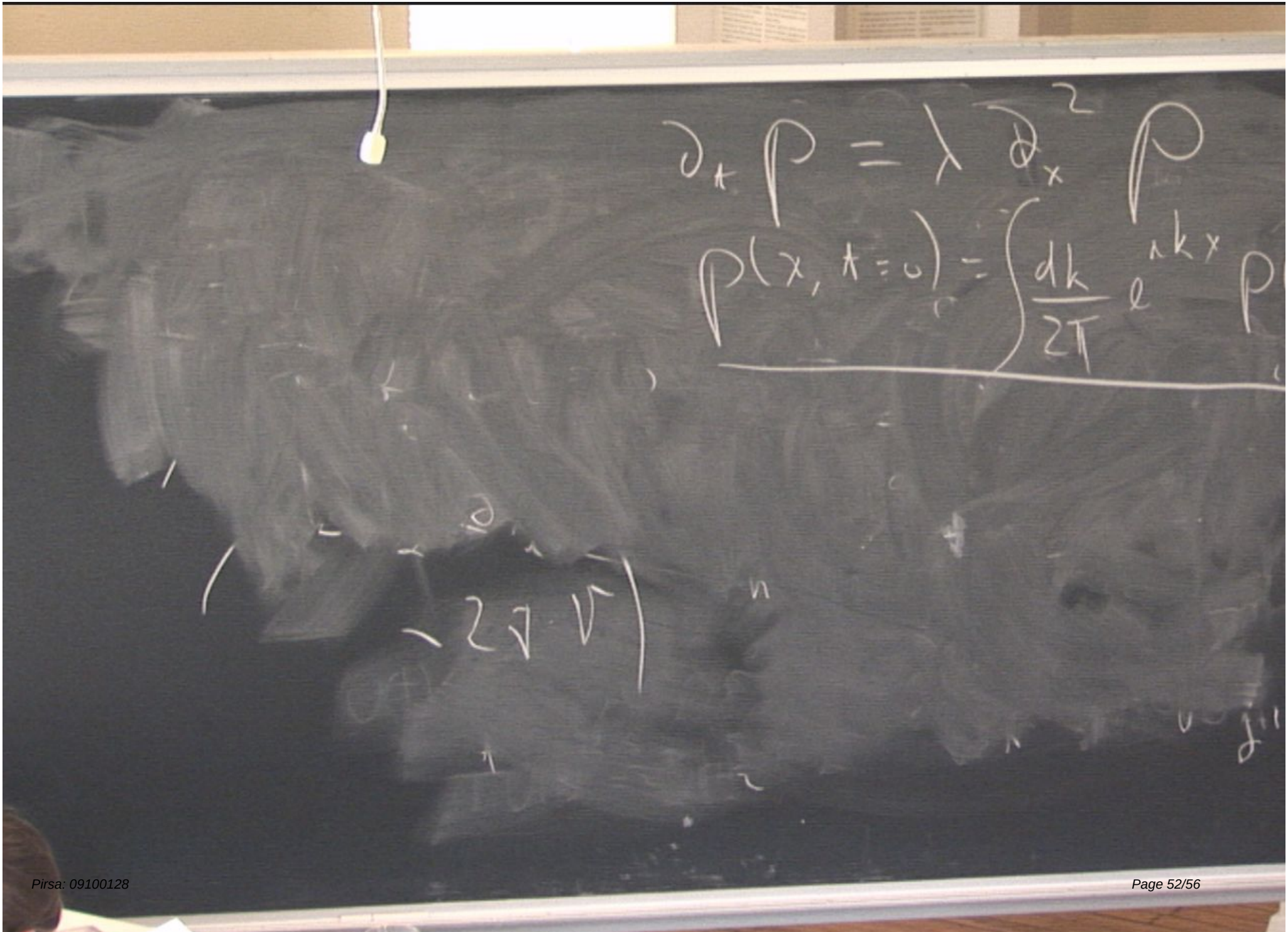
with $g(k)= \int dx \ \exp[-ikx] \ \rho(x,0)/(2\pi)$ as initial data.

Small rapidly varying errors at t=0 will produce small errors for positive t and huge errors for negative t. You cannot extrapolate backward in time. Information gets lost as time goes forward.

Solve for $\rho(x,0)=1$ for $0<x<1$ and $\rho(x,0) = 0$ otherwise. Use $\lambda=2$. Plot solution for t=0,2,4. What happens for t= −2?

Boltzmann noted that equations of classical mechanics make sense if t is replaced by −t. (In fact, it just replaces momenta, *p*, by *-p.)* But diffusion equation has a solution which does not make sense. Where did we go from sense to nonsense?


$\partial_t \rho = \lambda \partial_x^2 \rho$
$\rho(x, t=0) = \int \frac{dk}{2\pi} e^{ikx}$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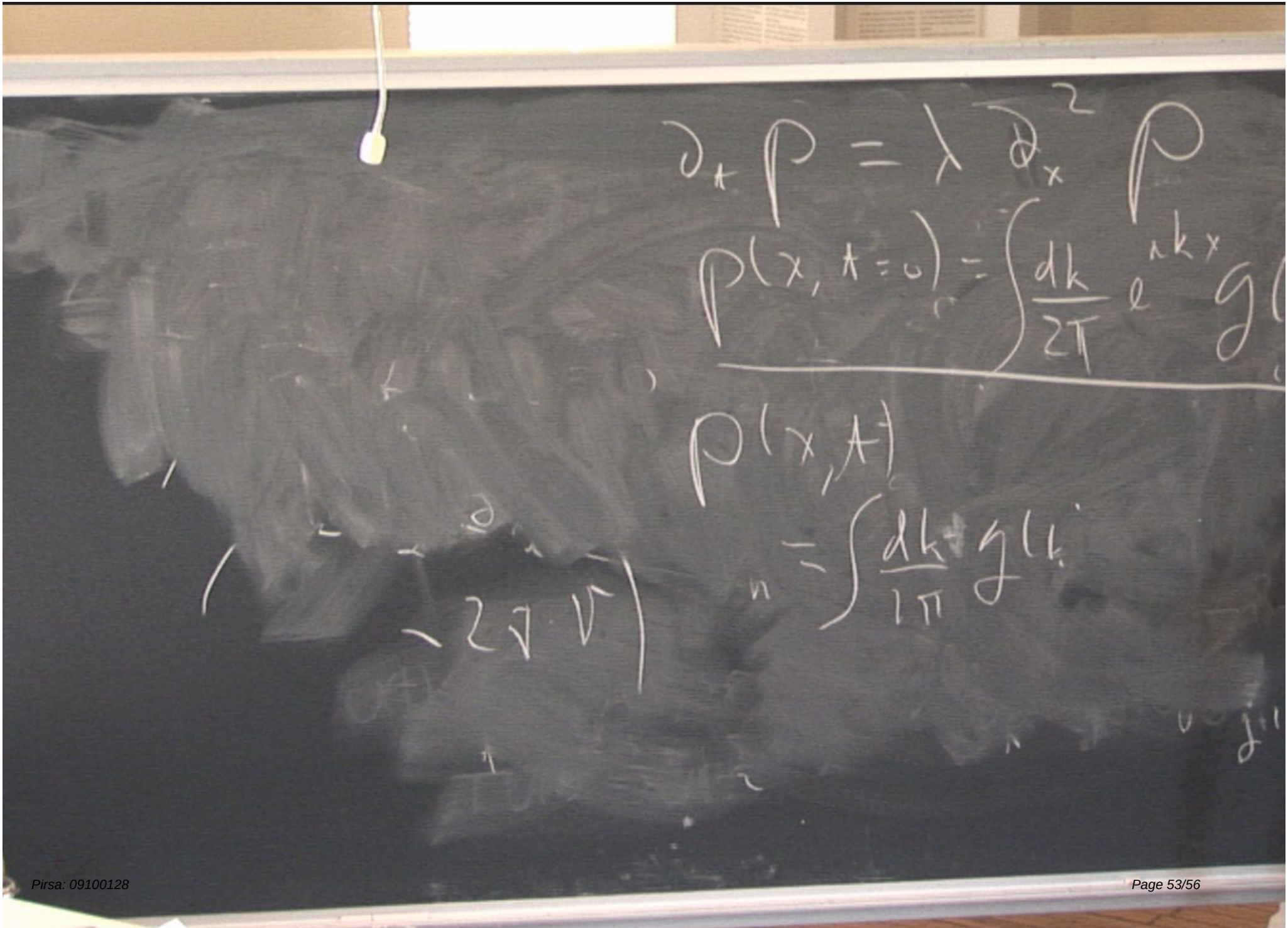
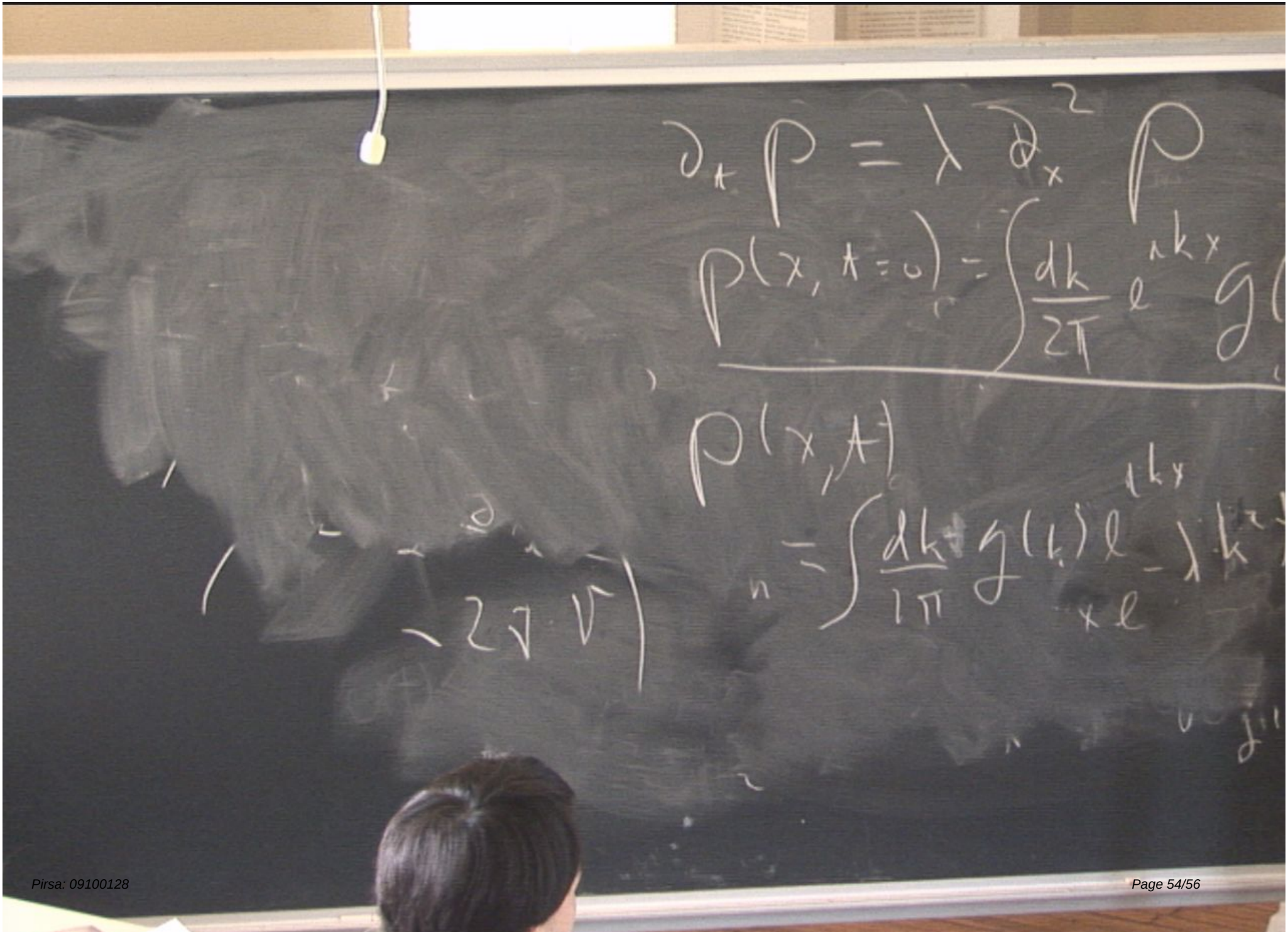

$\partial_t \rho = \lambda \partial_x^2 \rho$
$\rho(x, t=0) = \int \frac{dk}{2\pi} e^{ikx} g($
$\rho(x,t)$
$= \int \frac{dk}{2\pi} g($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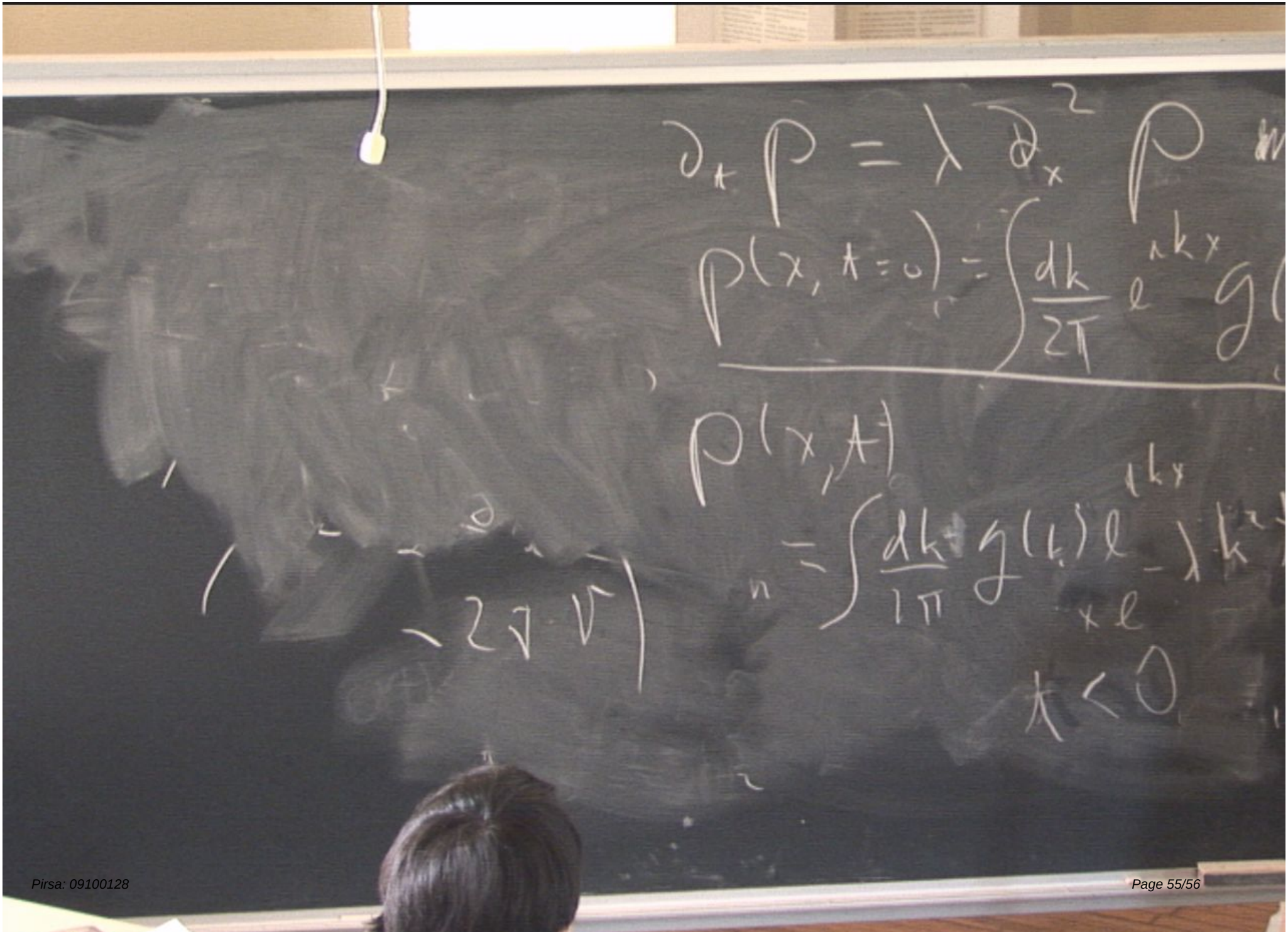
$= \int \frac{dk}{2\pi} g(k) e^{ikx} e^{-\lambda k^2}$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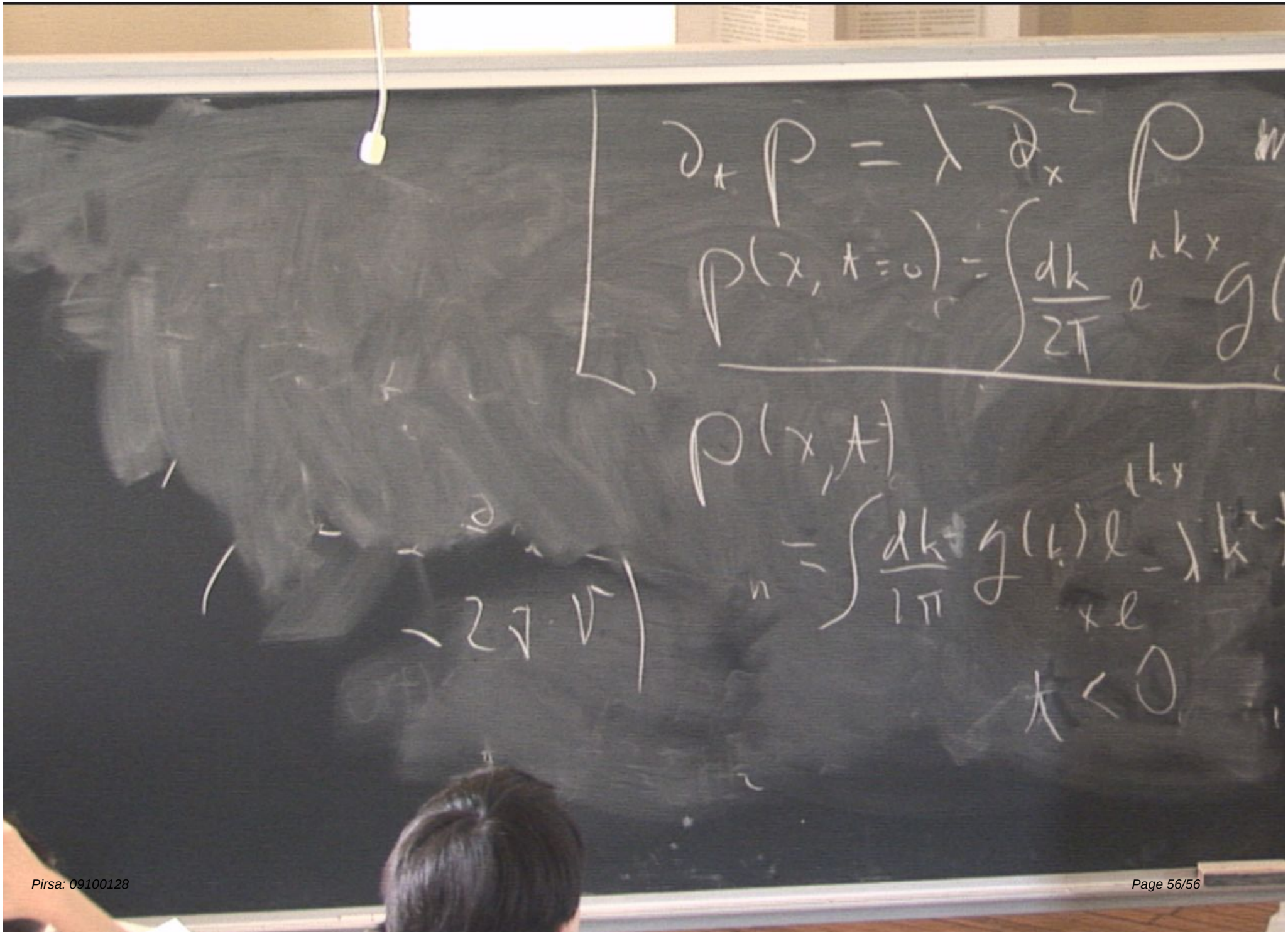
$t < 0$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