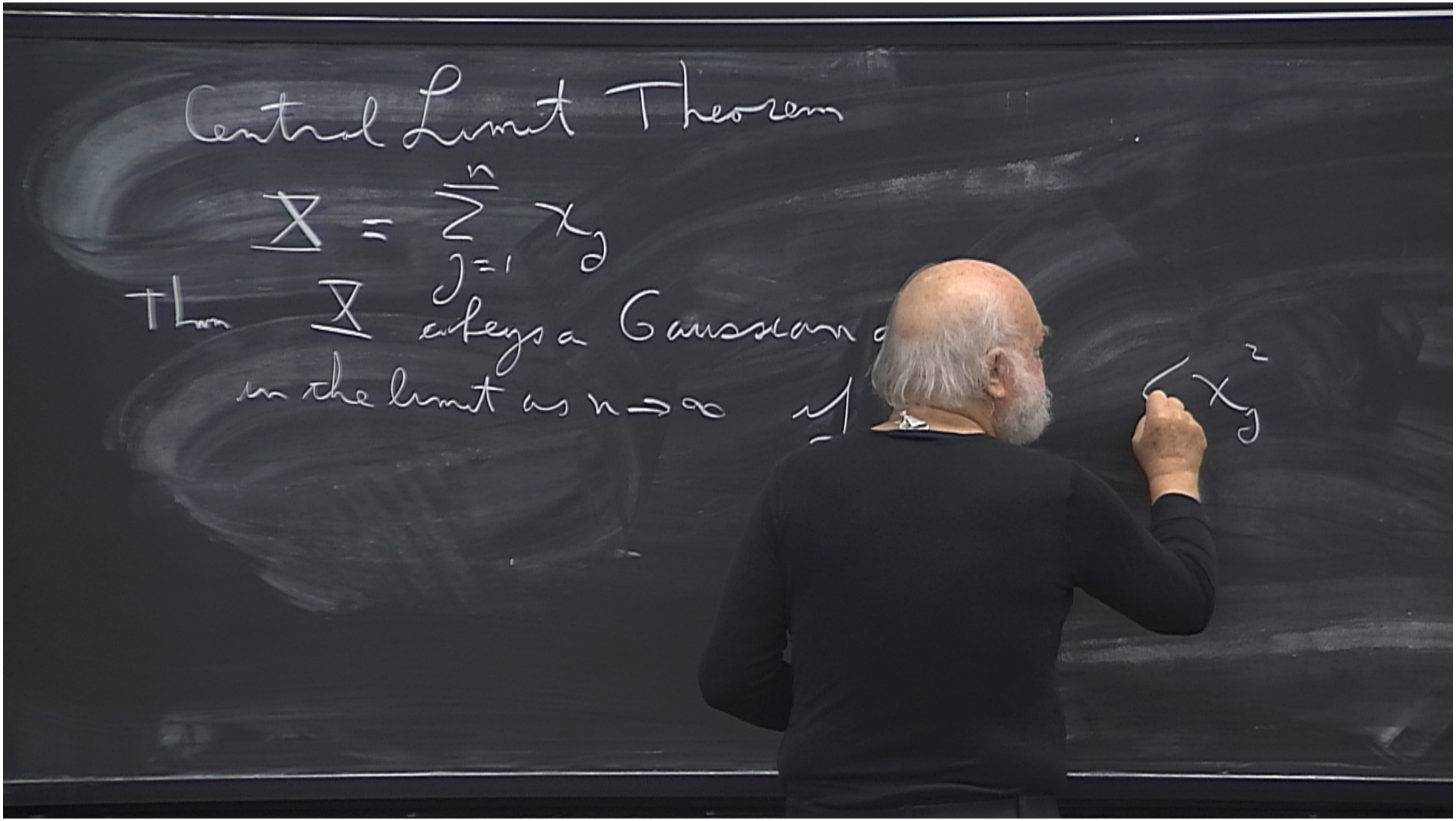
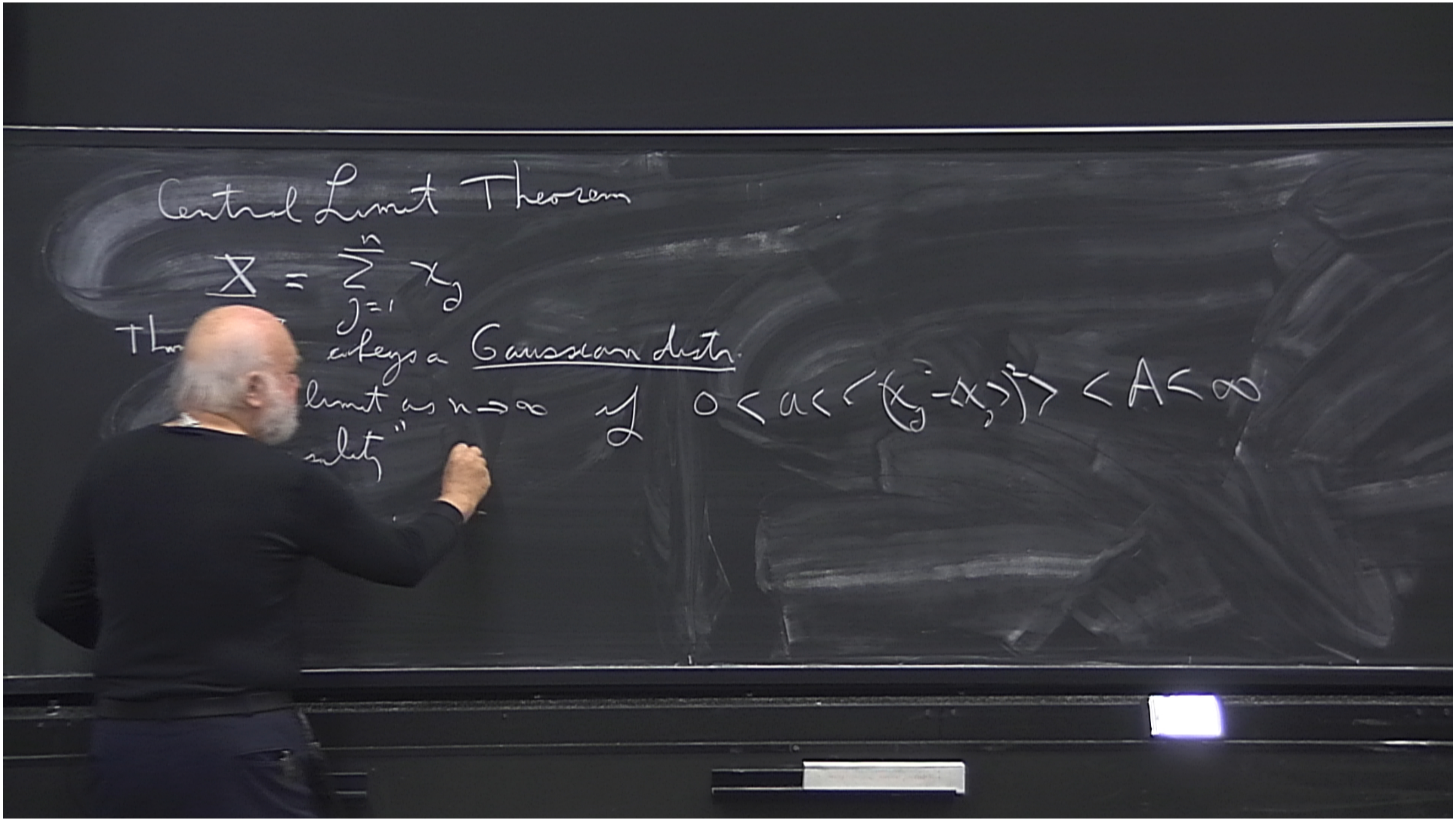
Title: Statistical Mechanics - Lecture 7

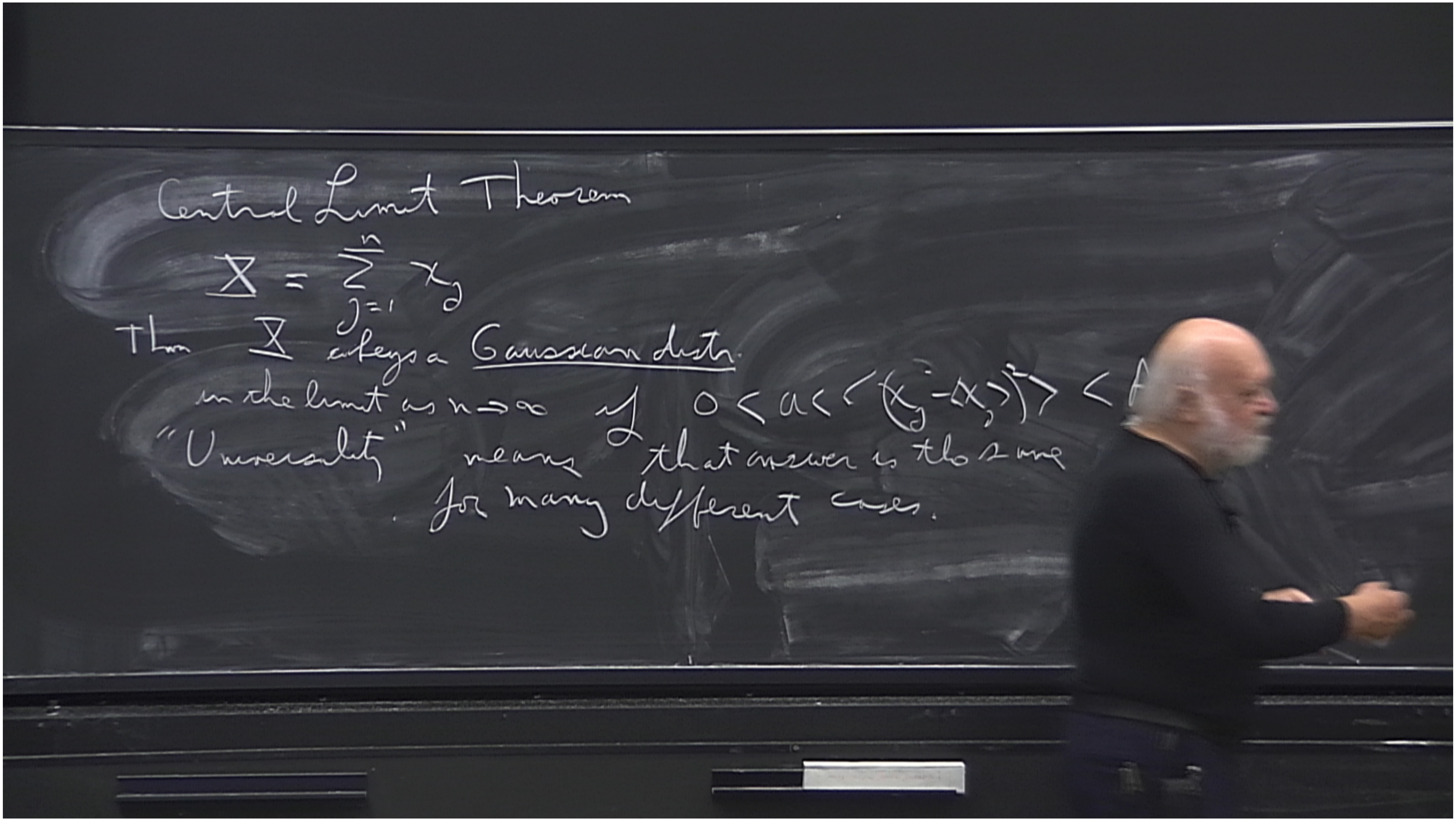
Date: Oct 12, 2011 10:30 AM

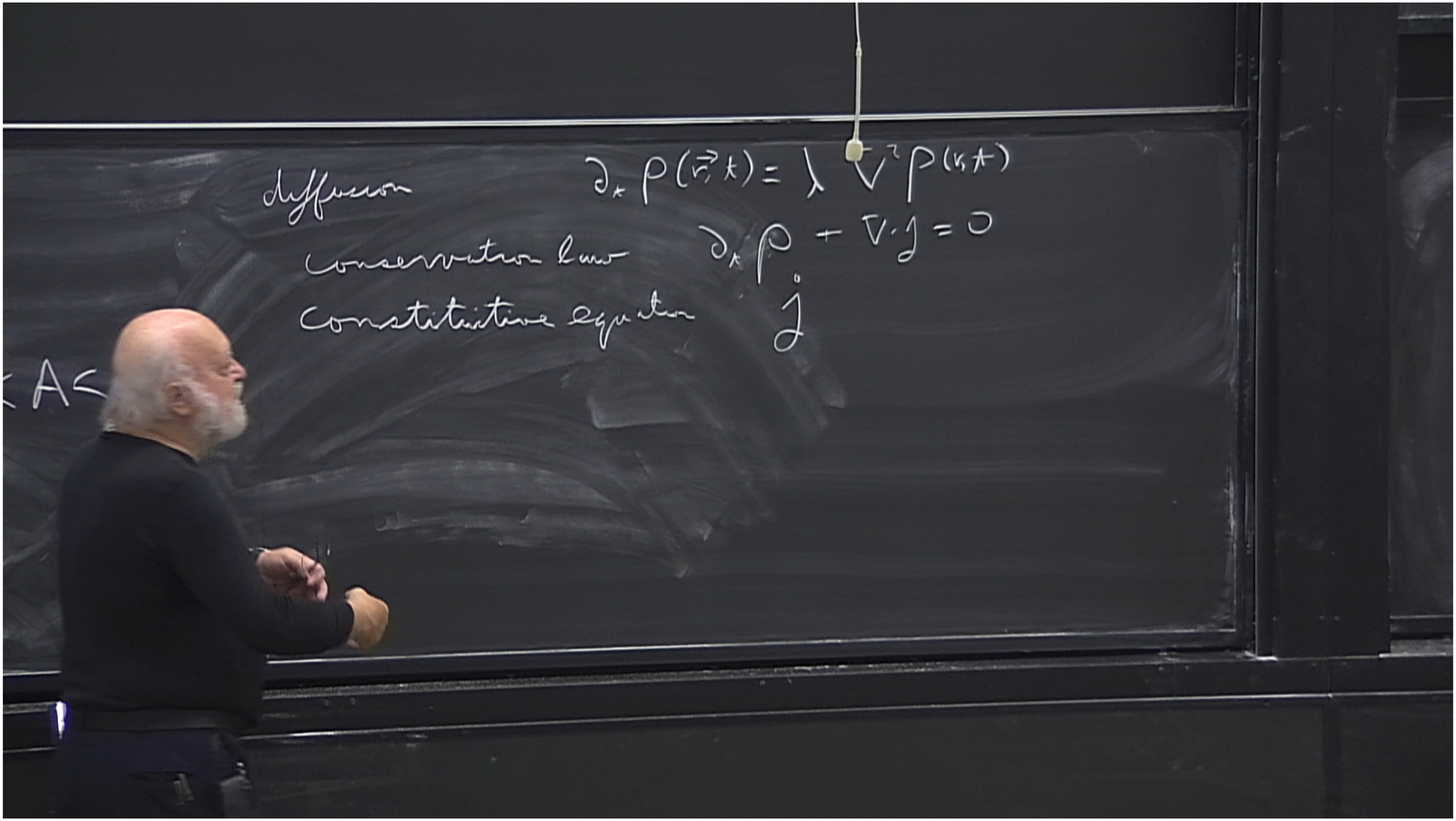
URL: http://pirsa.org/11100034

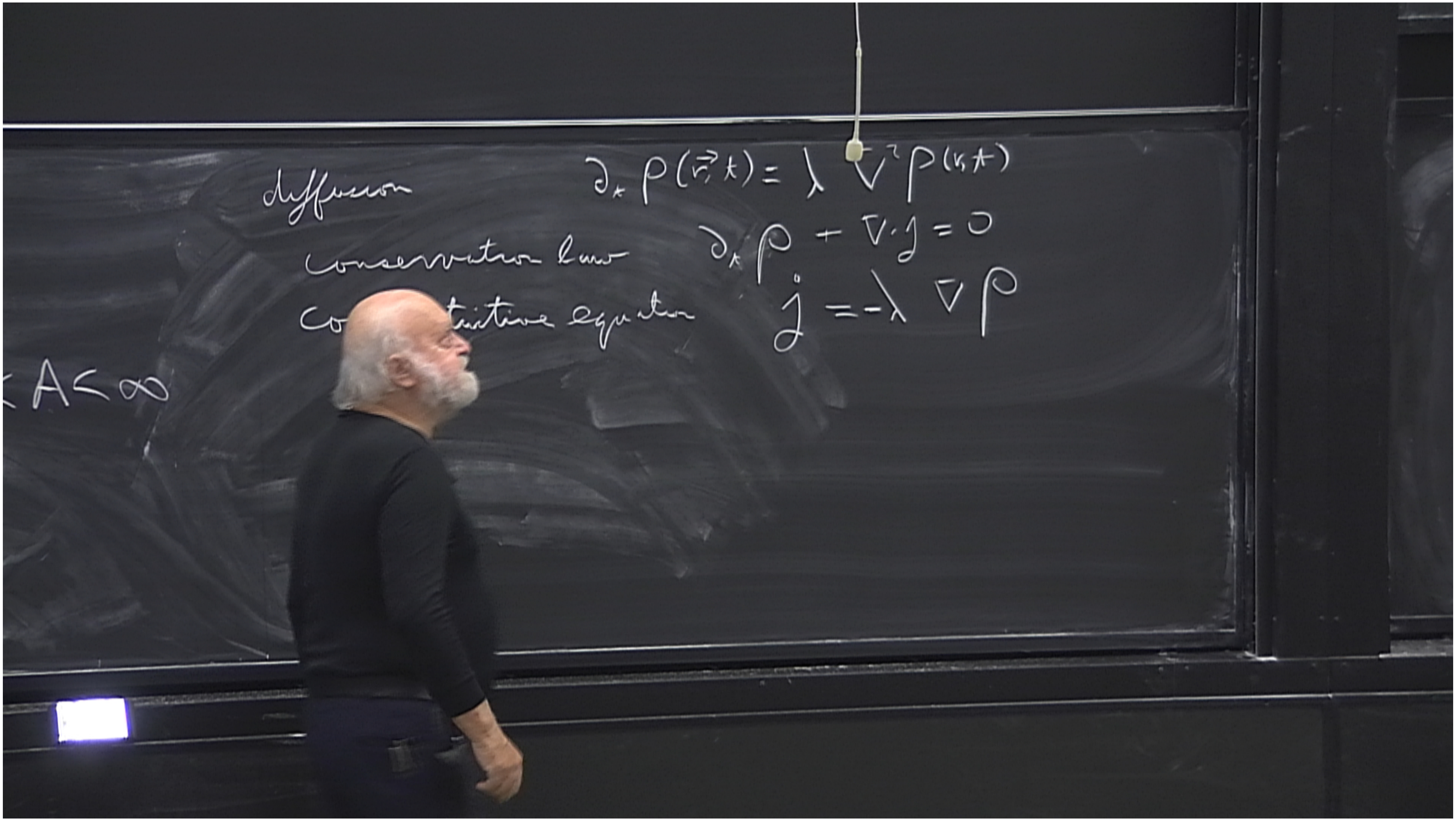
Abstract:


Central Limit Theorem
$X = \sum_{j=1}^{n} x_j$
Then X obeys a Gaussian
in the limit as $n \to \infty$


Central Limit Theorem
X = Σ_{j=1}^n x_j
obeys a Gaussian distr.
limit as n → ∞ if 0 < a < ⟨(x_j − ⟨x_j⟩)²⟩ < A < ∞


Central Limit Theorem
$X = \sum_{j=1}^{n} x_j$
Then X obeys a Gaussian distn.
in the limit as $n \to \infty$ if $0 < a < \langle (x_j - \langle x_j \rangle)^2 \rangle < A$
"Universality" means that answer is the same
for many different cases.


diffusion $\partial_t \rho(\vec{r},t) = \lambda \nabla^2 \rho(r,t)$
conservation law $\partial_t \rho + \nabla \cdot j = 0$
constitutive equation j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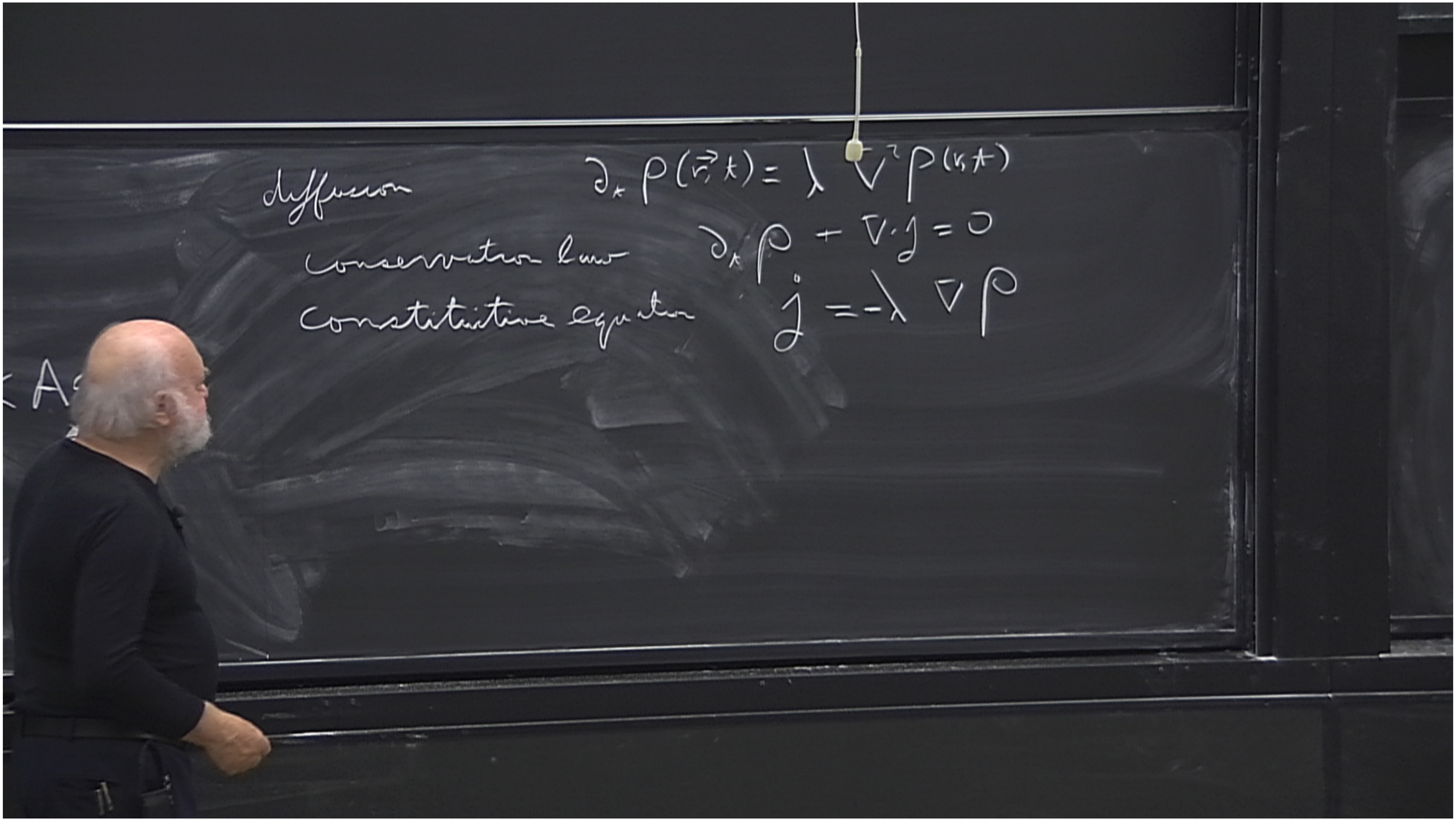
conservation law
∂t ρ + ∇·j = 0
j = −λ ∇ρ
equation
A < ∞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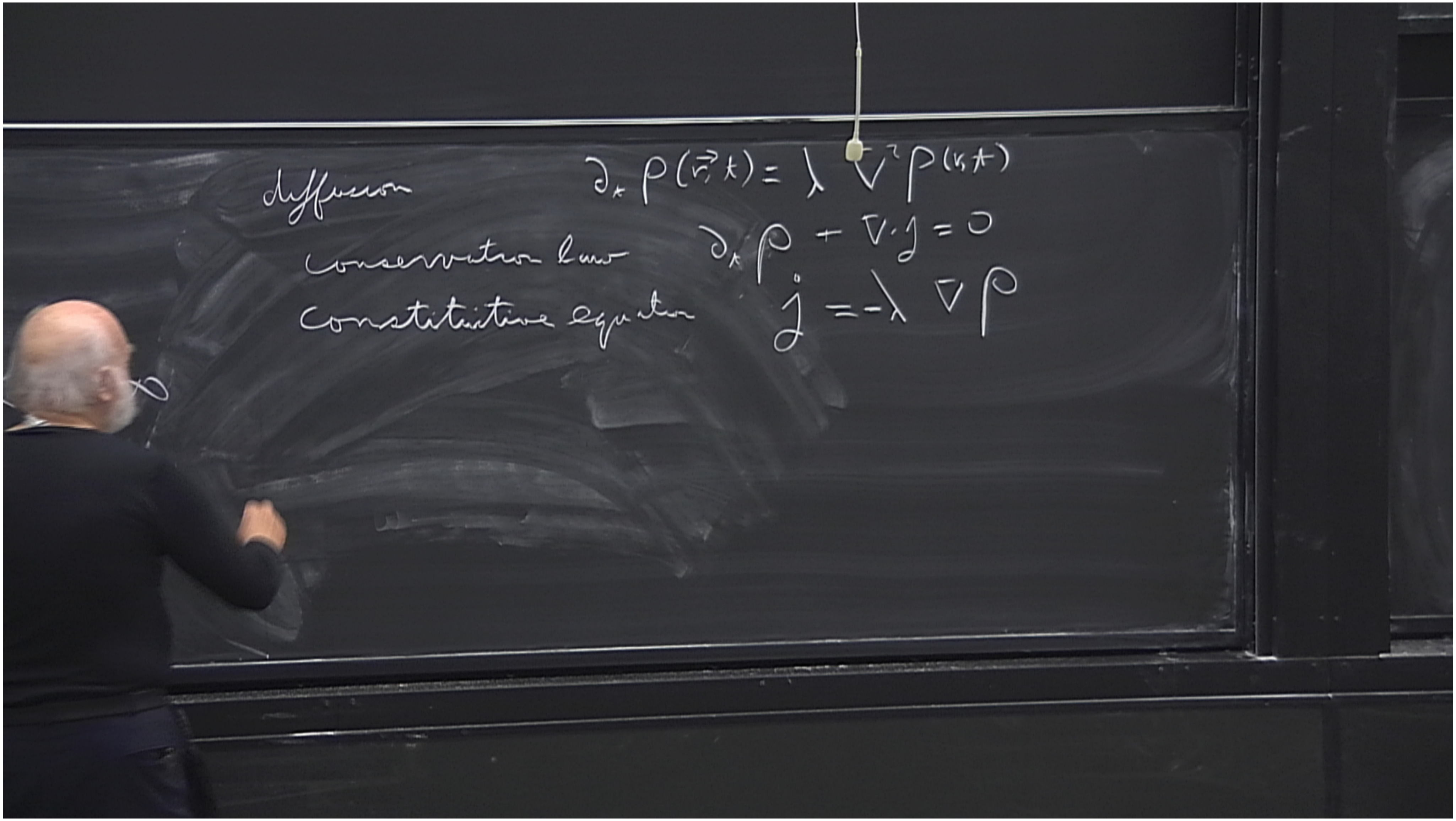
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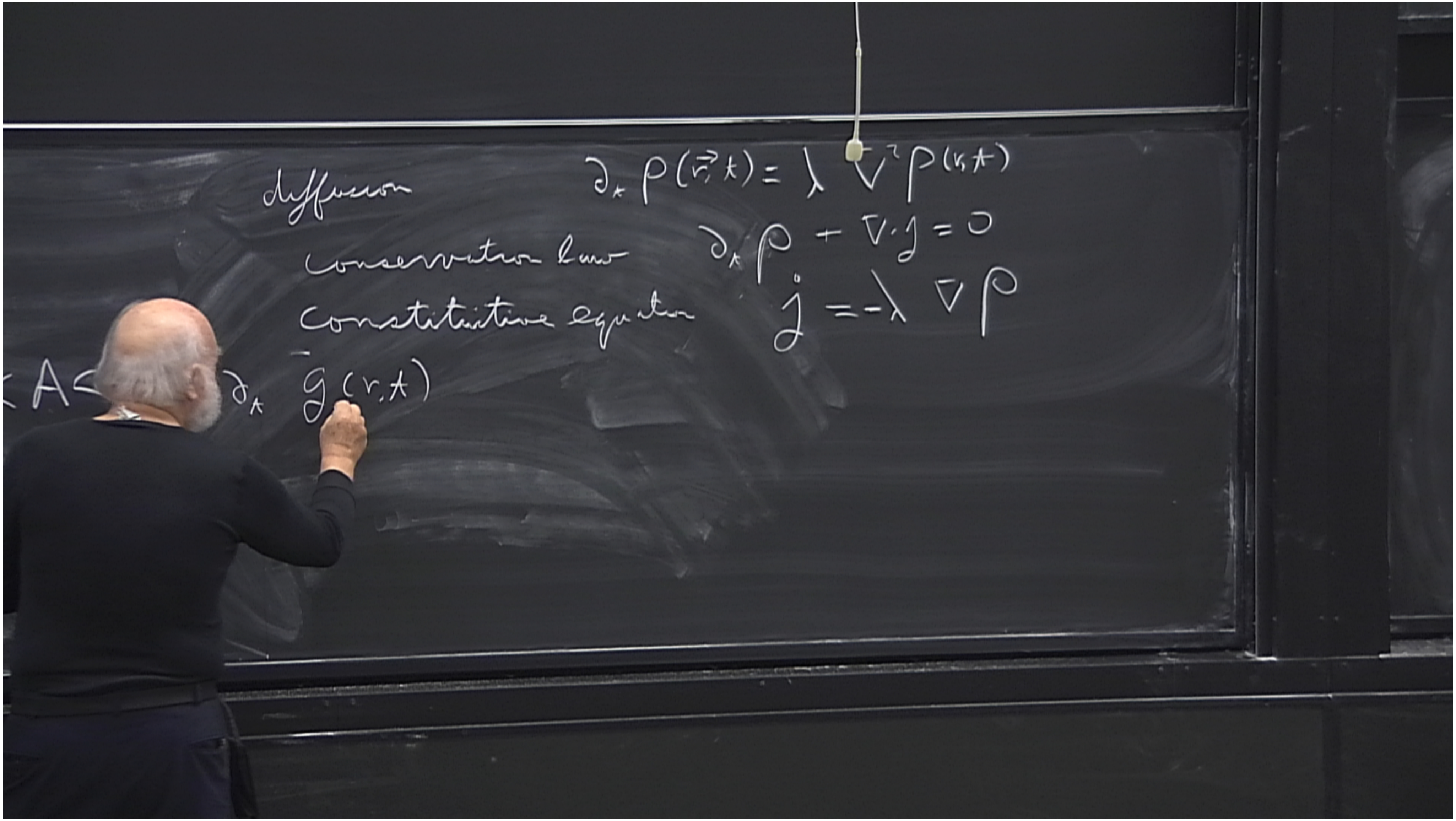
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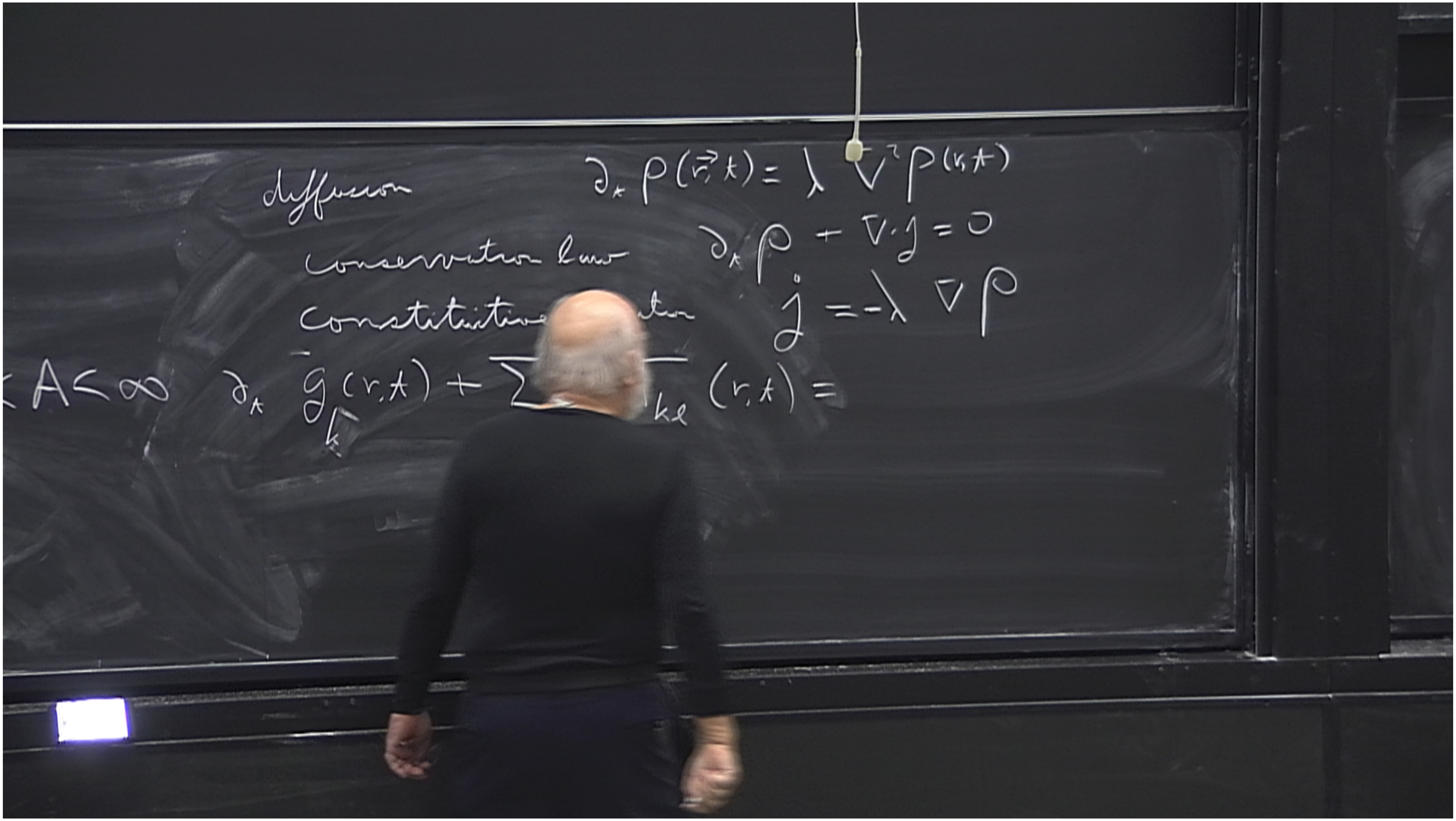
$j = -\lambda \nabla \rho$
$\partial_t \bar{g}(r,t)$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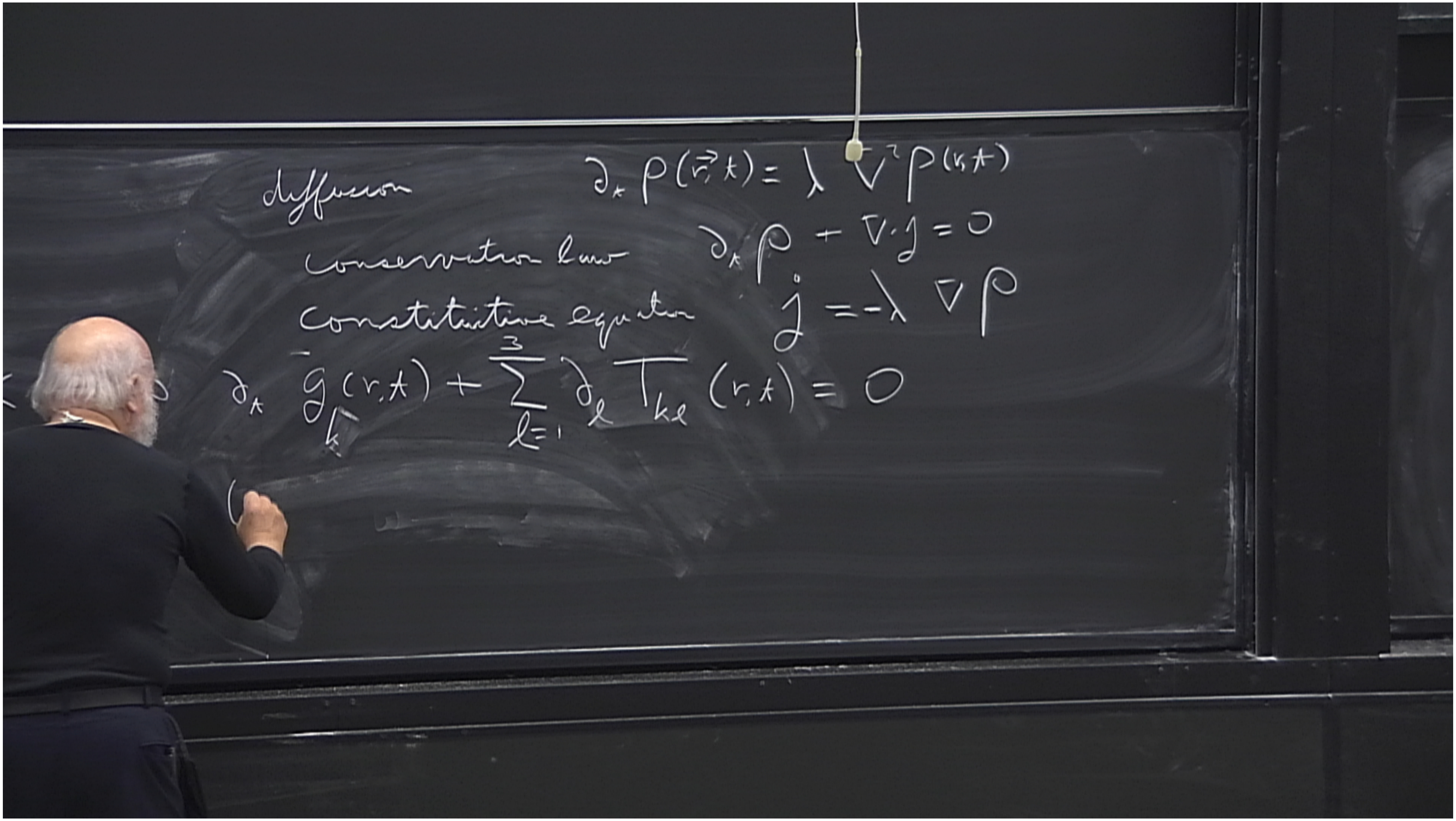
conservation law
∂t ρ + ∇·j = 0
j = -λ ∇ρ
A < ∞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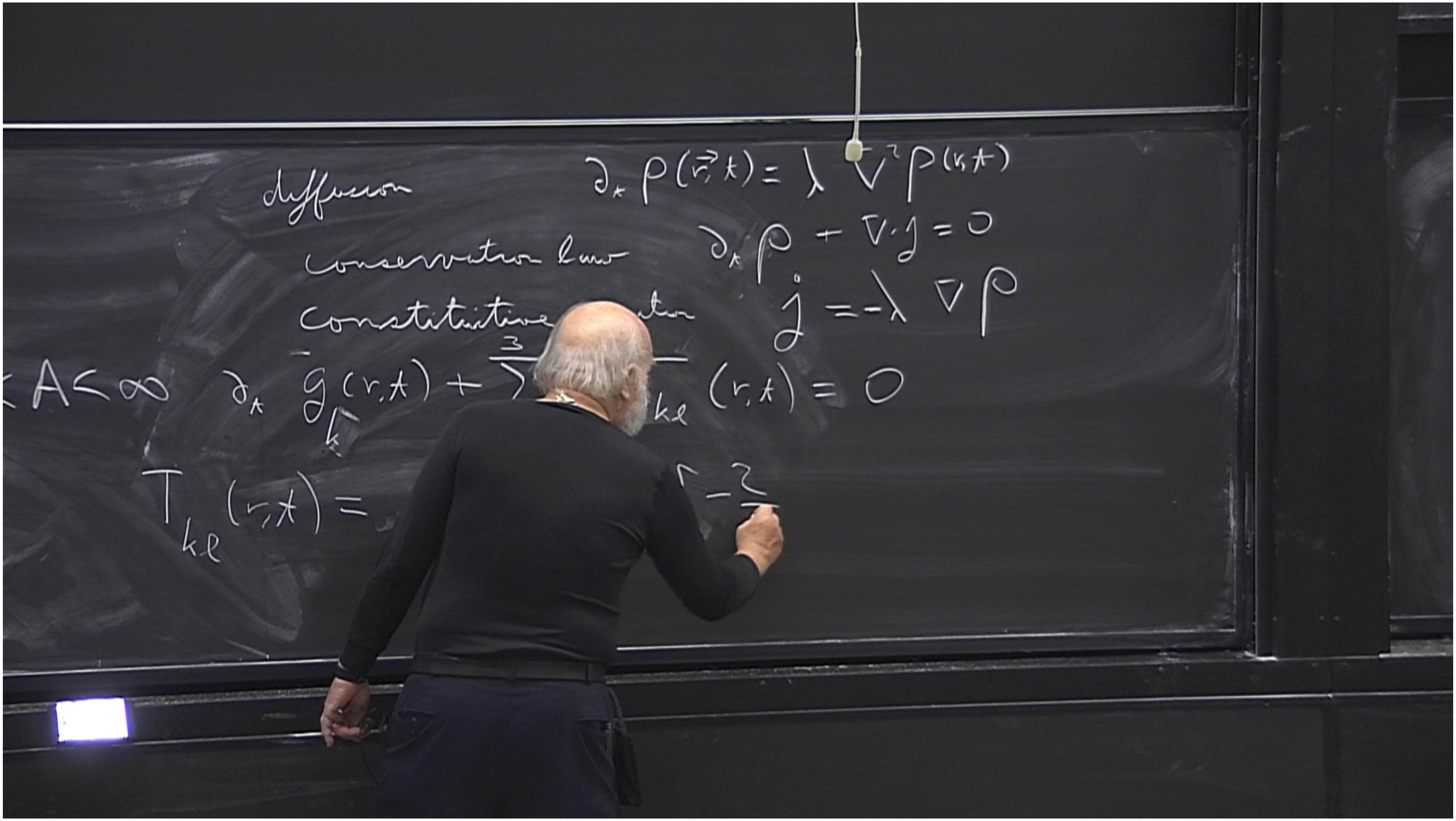
$\partial_t g_k(r,t) + \sum_{l=1}^{3} \partial_l T_{kl}(r,t) = 0$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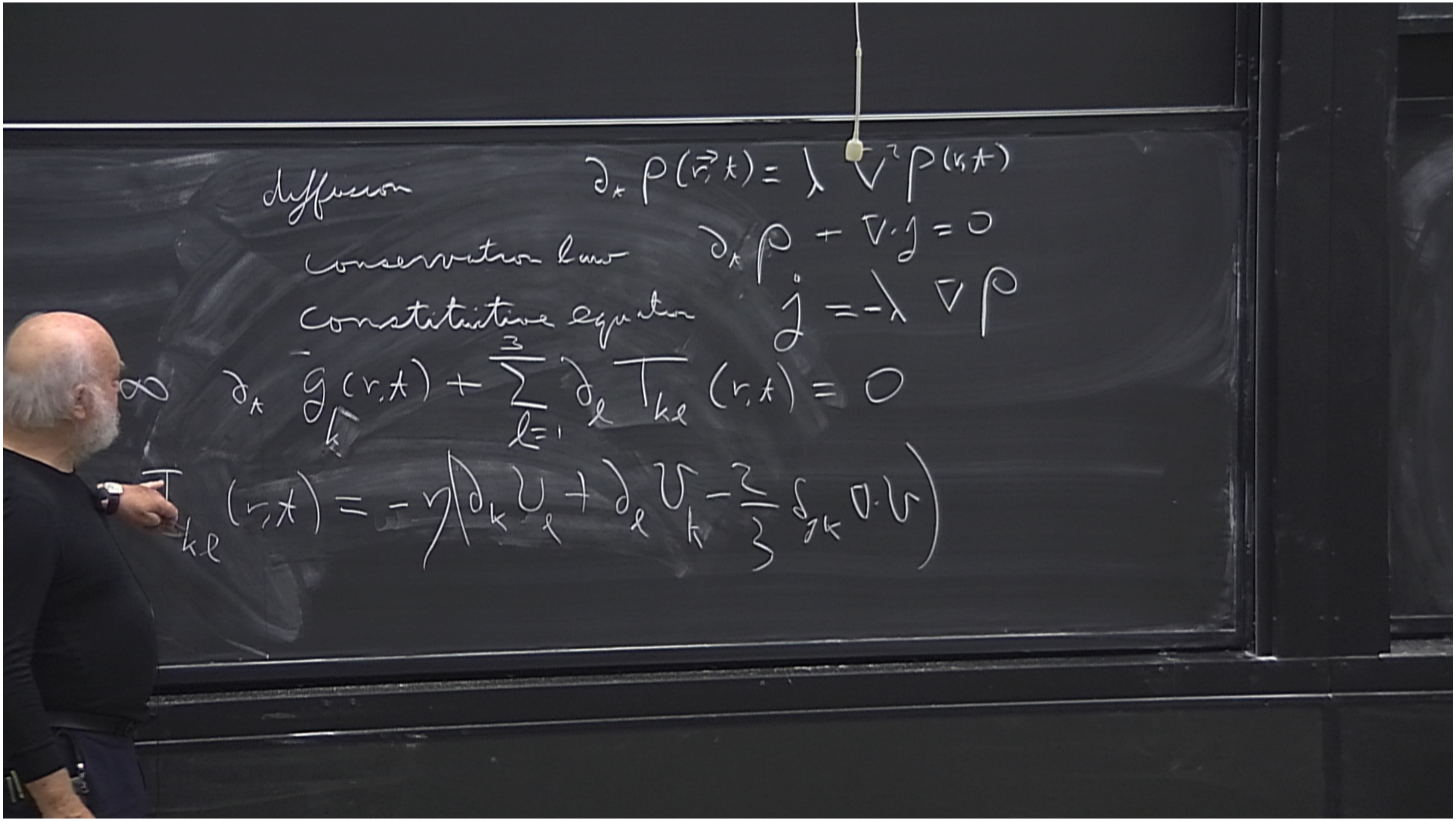
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conservation law $\partial_t \rho + \nabla \cdot j = 0$
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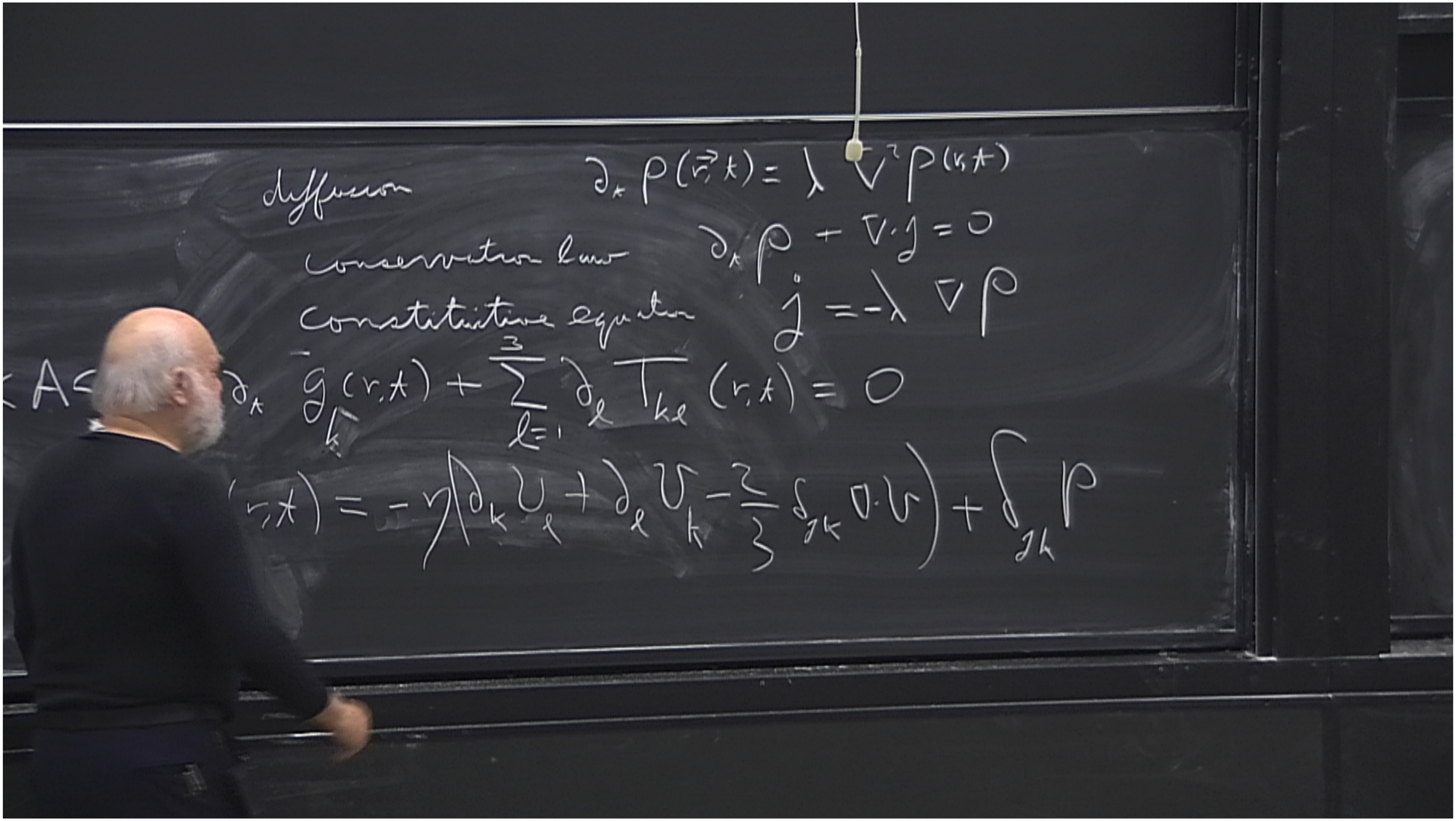
$\partial_t g_k(r,t) + \sum_{l=1}^{3} \partial_l T_{kl}(r,t) = 0$
$T_{kl}(r,t) = -\eta(\partial_k v_l + \partial_l v_k - \frac{2}{3}\delta_{lk} \nabla \cdot v)$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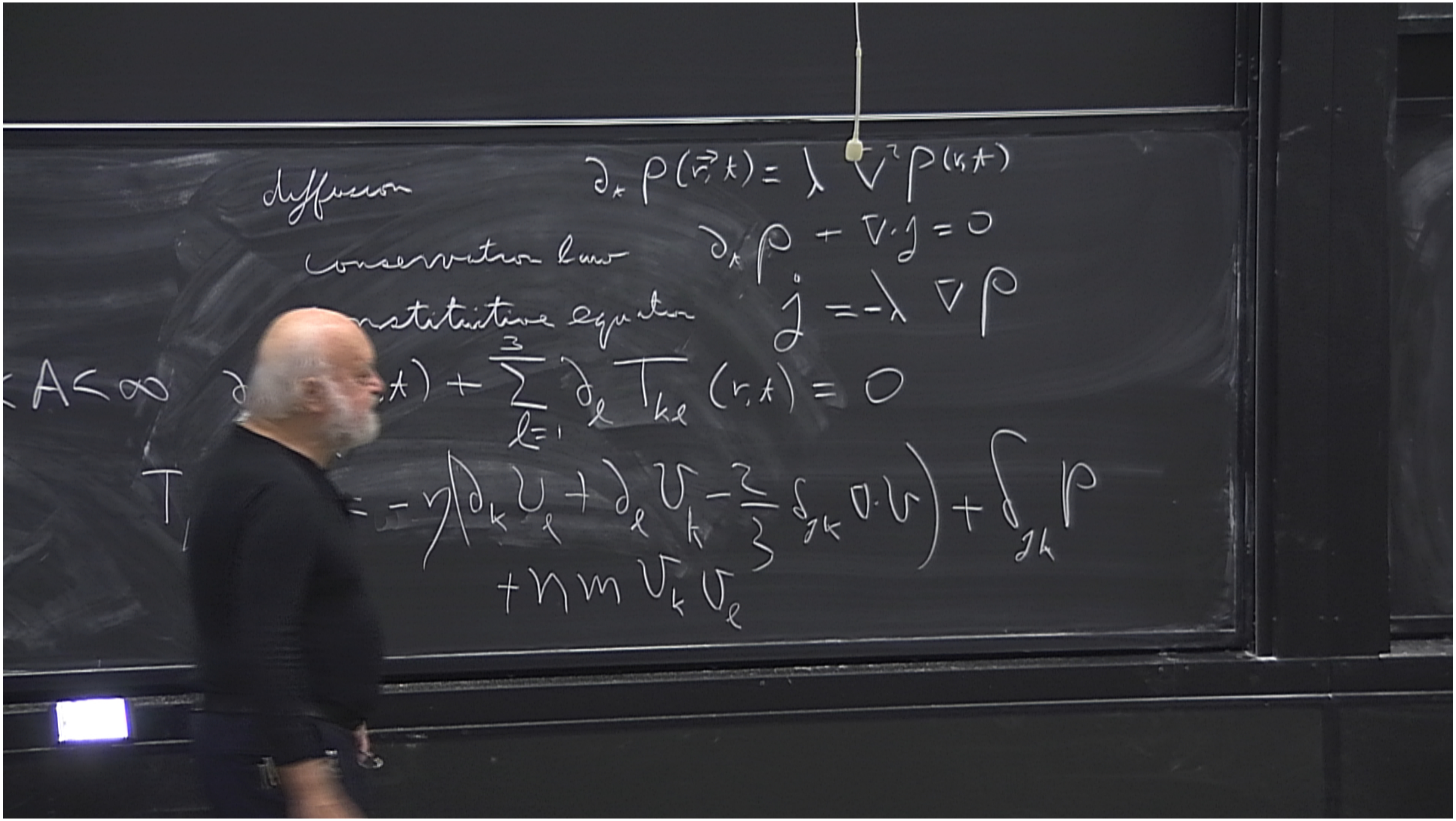
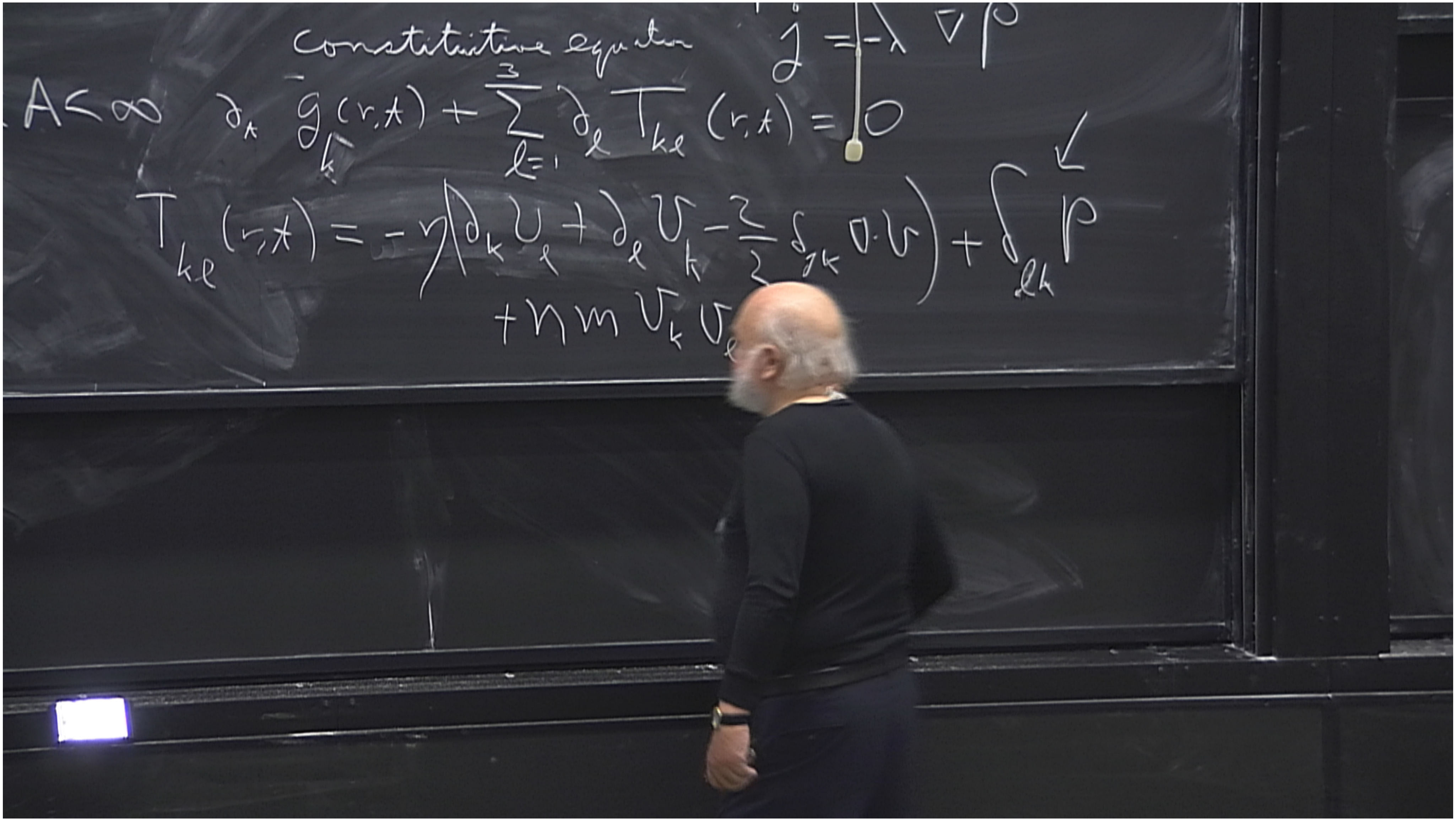
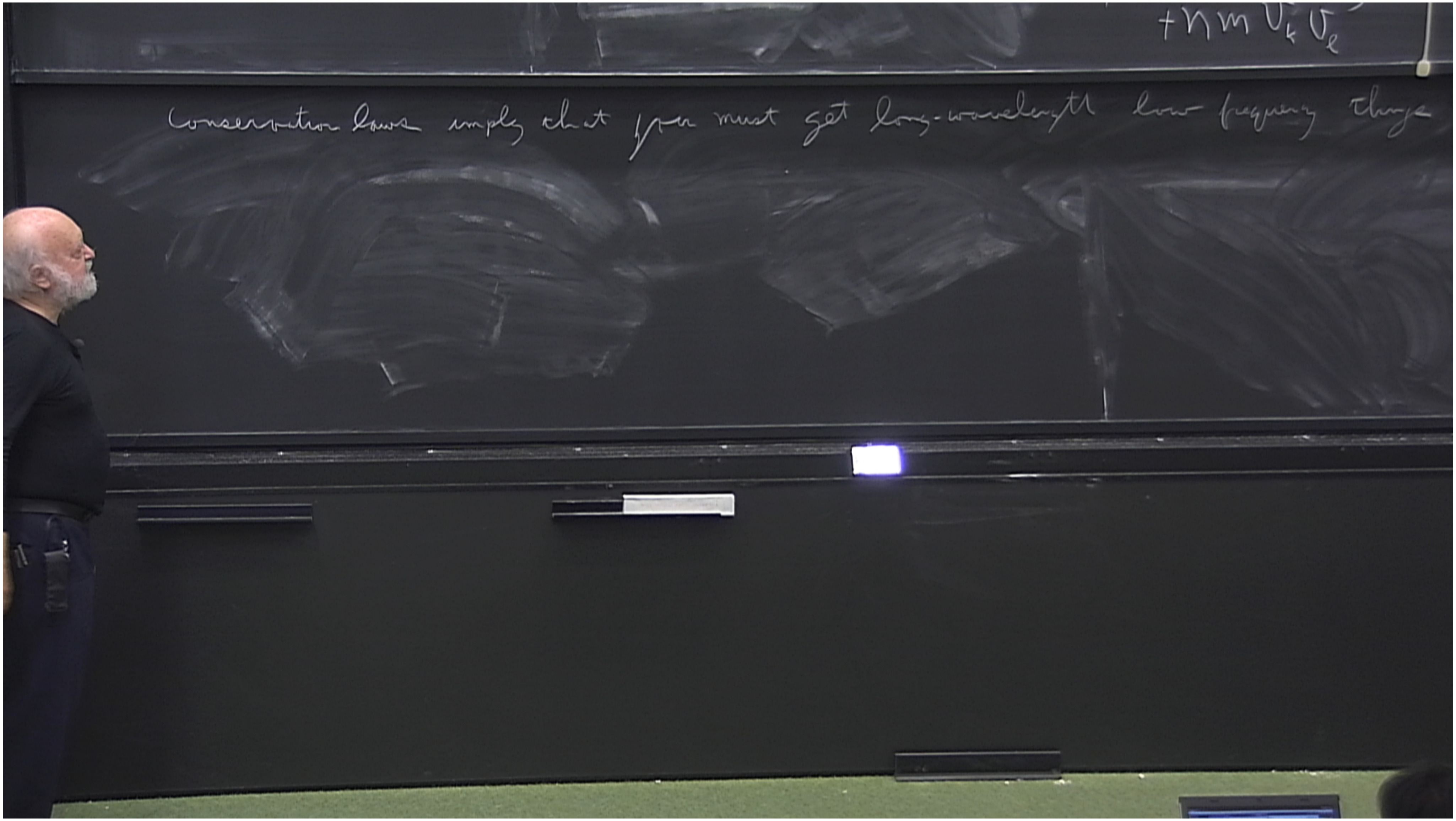
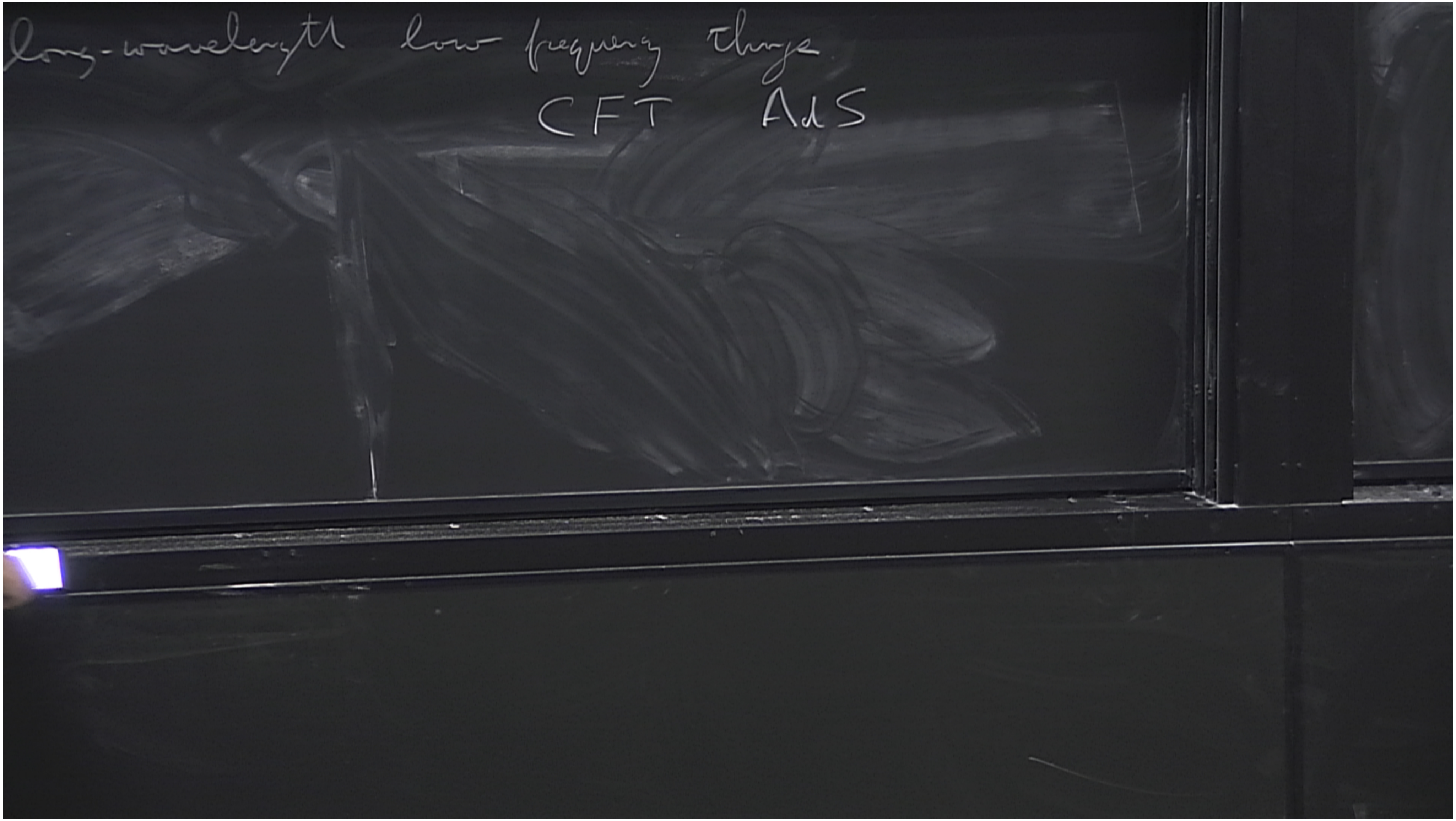
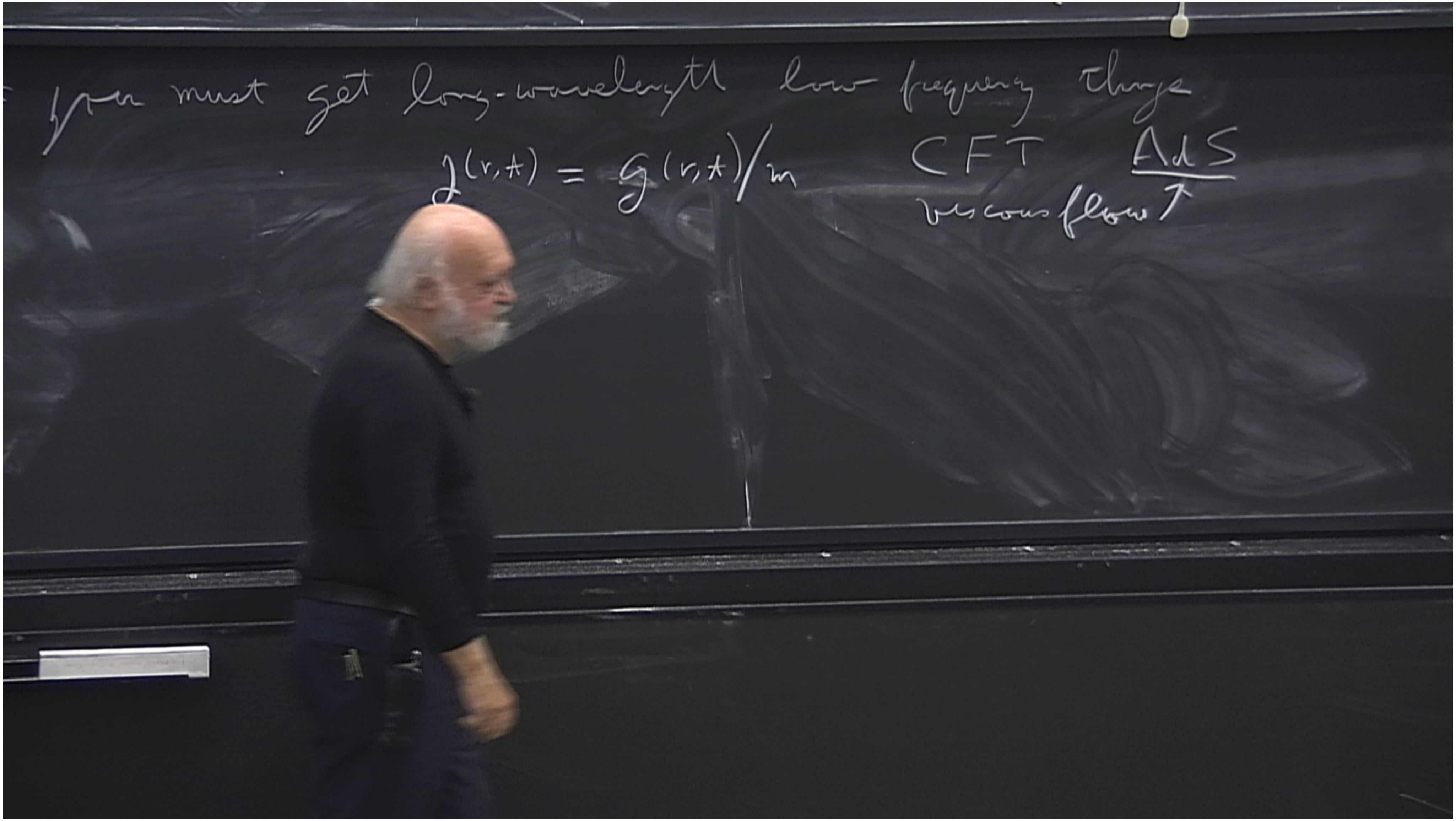
conservation law ∂t ρ + ∇·j = 0
constitutive equation j = -λ ∇ρ
∂t g_k(r,t) + Σ_{l=1}^{3} ∂_l T_kl(r,t) = 0
(r,t) = -η(∂_k v_l + ∂_l v_k - 2/3 δ_lk ∇·v) + δ_lk p


diffusion
∂_t ρ(r⃗,t) = λ ∇² ρ(r,t)
conservation law
∂_t ρ + ∇·j = 0
j = −λ ∇ρ
+ n m v_k v_l


Constitutive equation

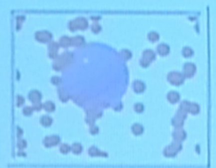

+ηm v_k v_ℓ
Conservation laws imply that you must get long-wavelength low frequency things


long-wavelength low frequency things
CFT AdS


you must get long-wavelength low frequency things
CFT
AdS
viscous flow

Brownian motion:

Robert Brown (1773-1858) saw particles of pollen "dance around" in fluid under microscope. This motion was caused by many tiny particles hitting the grains of pollen.



The many moving tiny particles are of course **molecules of the liquid.** They were too small to see under a microscope when Brownian motion was discovered, but it was obvious they were there. You can see the molecules of liquid hitting the bigger particle in the animation on the left. (The size of the molecules has been dramatically *increased* in order to make them visible).

http://www.worsleyschool.net/science/files/brownian/motion.html

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

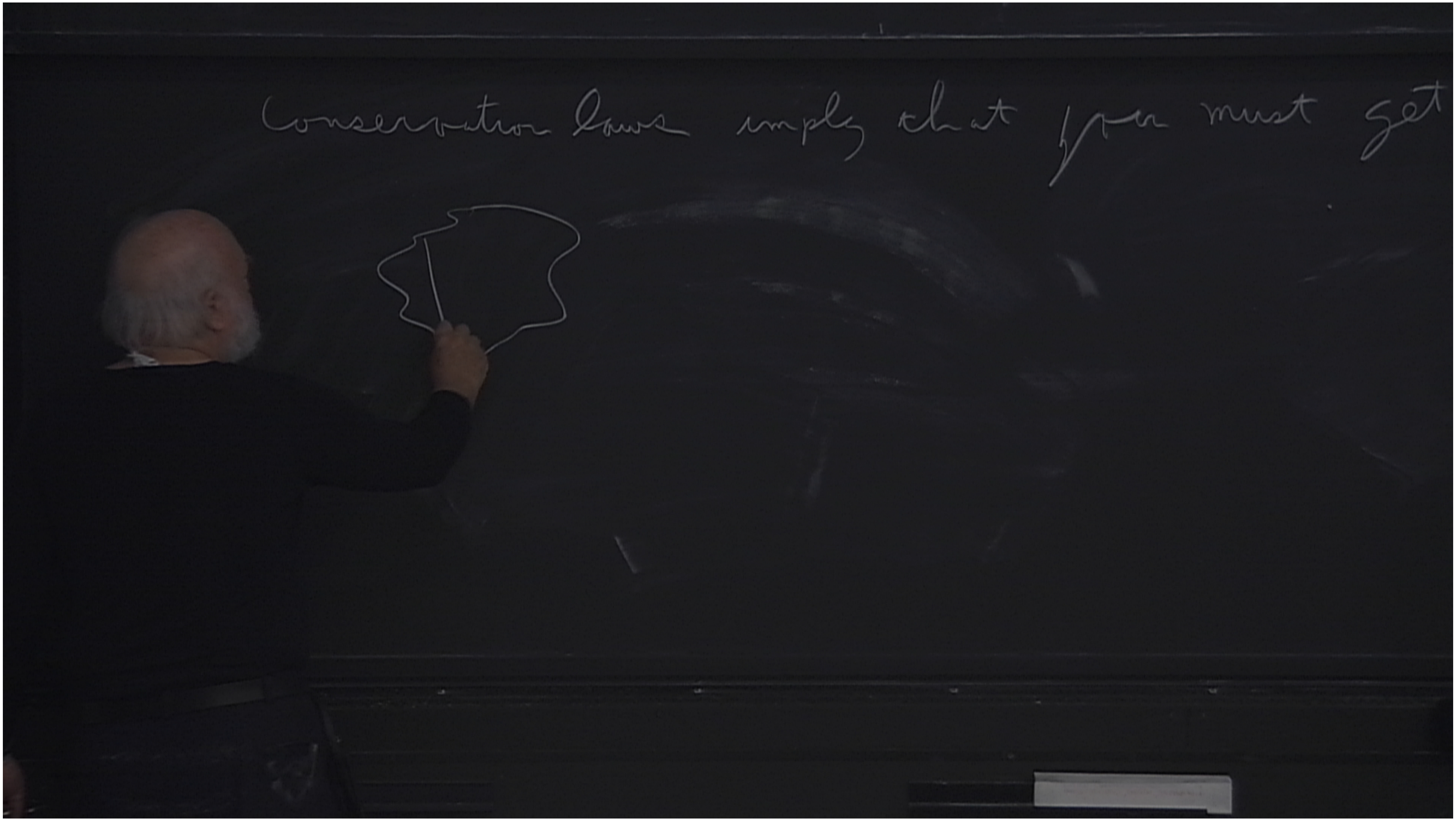
$$dp/dt = \ldots\ldots + \eta(t) - p/\tau$$

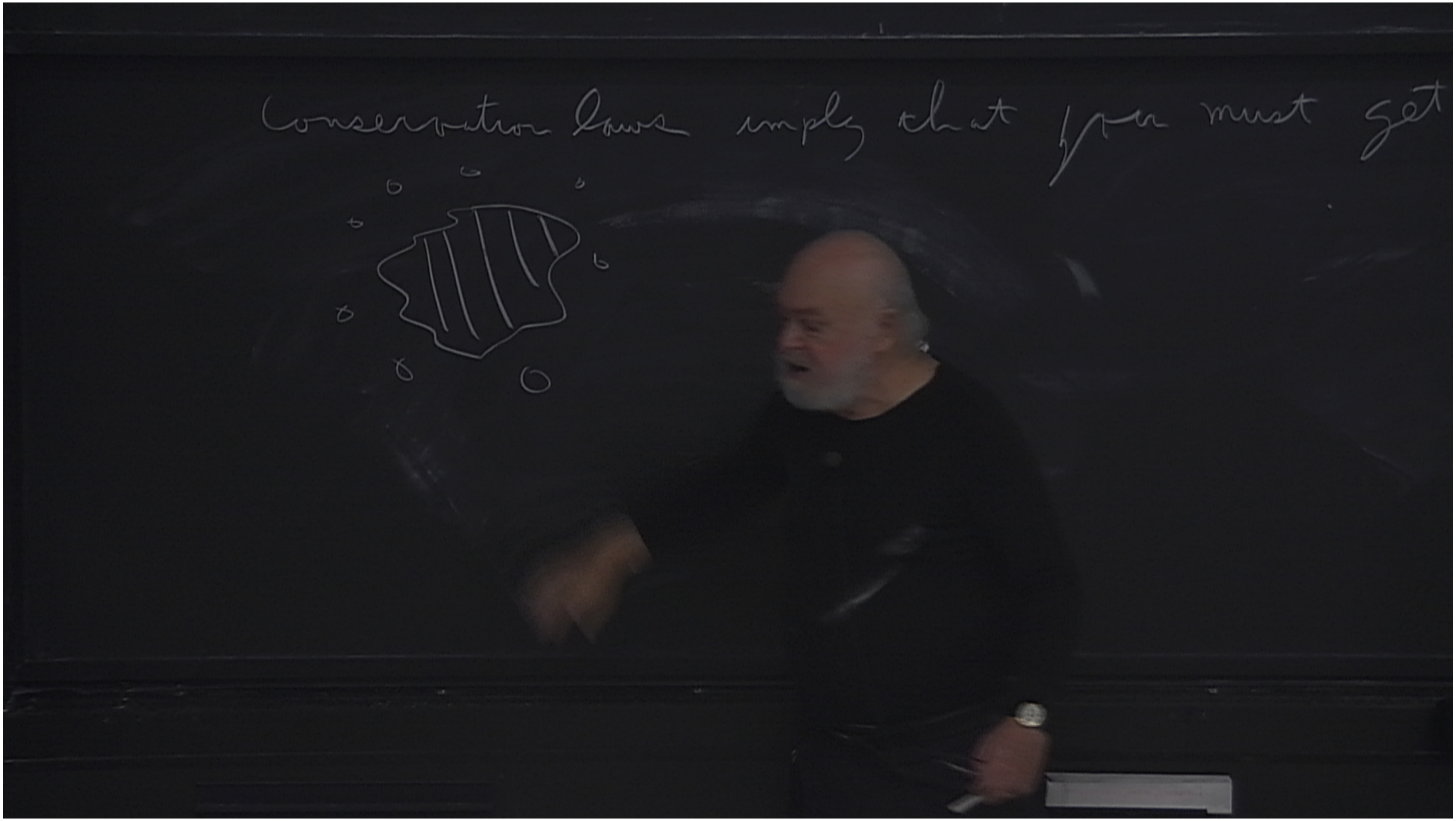
$p=(p_x, p_y, p_z)$ $\qquad \eta = (\eta_x, \eta_y, \eta_z)$ $\qquad$ v.1

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

$<\eta_j(t)\ \eta_k(s)> = \Gamma \delta(t-s)\delta_{j,k}$ $\qquad$ v.2

The relaxation time, τ, describes friction slowing down as the particles moves through the medium. In contrast Γ describes the extra momentum picked up via the collisions. Both represent the same physical effect, little particles hitting our big one. However, they operate in a somewhat different fashion. The individual kicks point in every which direction and only in the long run produce any concerted change in momentum. On the other hand the term in τ is a friction tending to continually push our particle toward smaller speeds relative to the medium.


Conservation laws imply that you must get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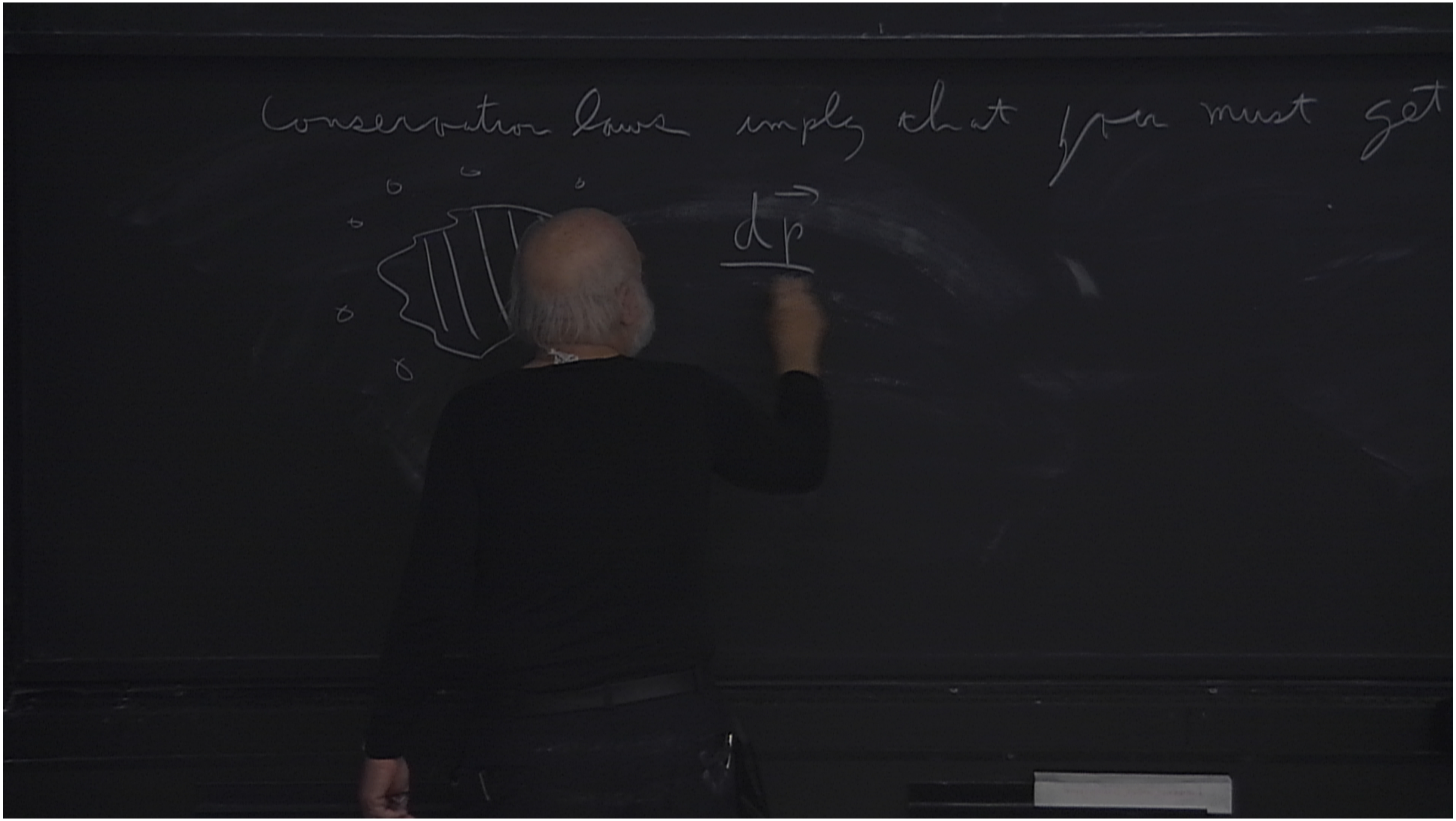
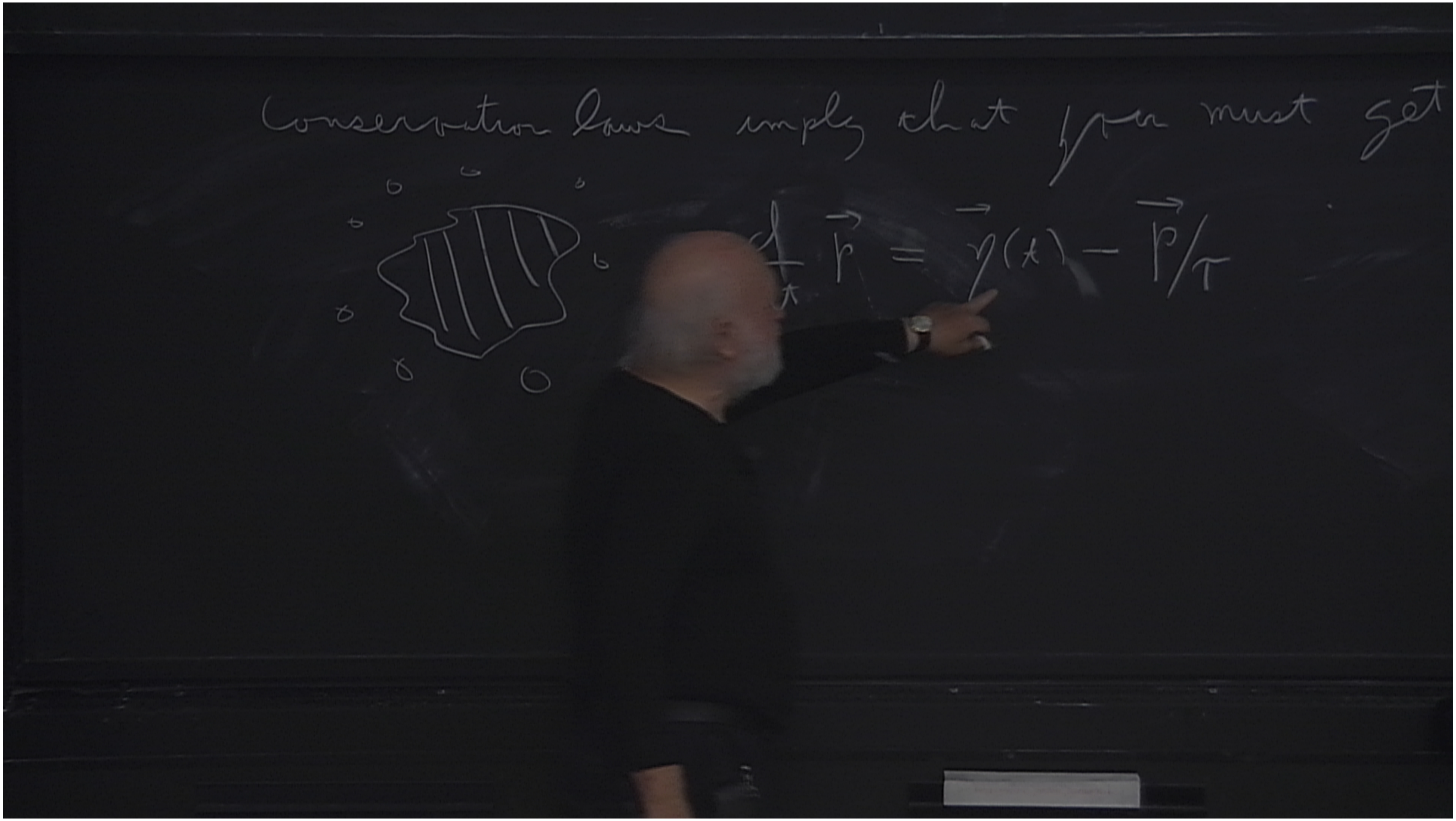
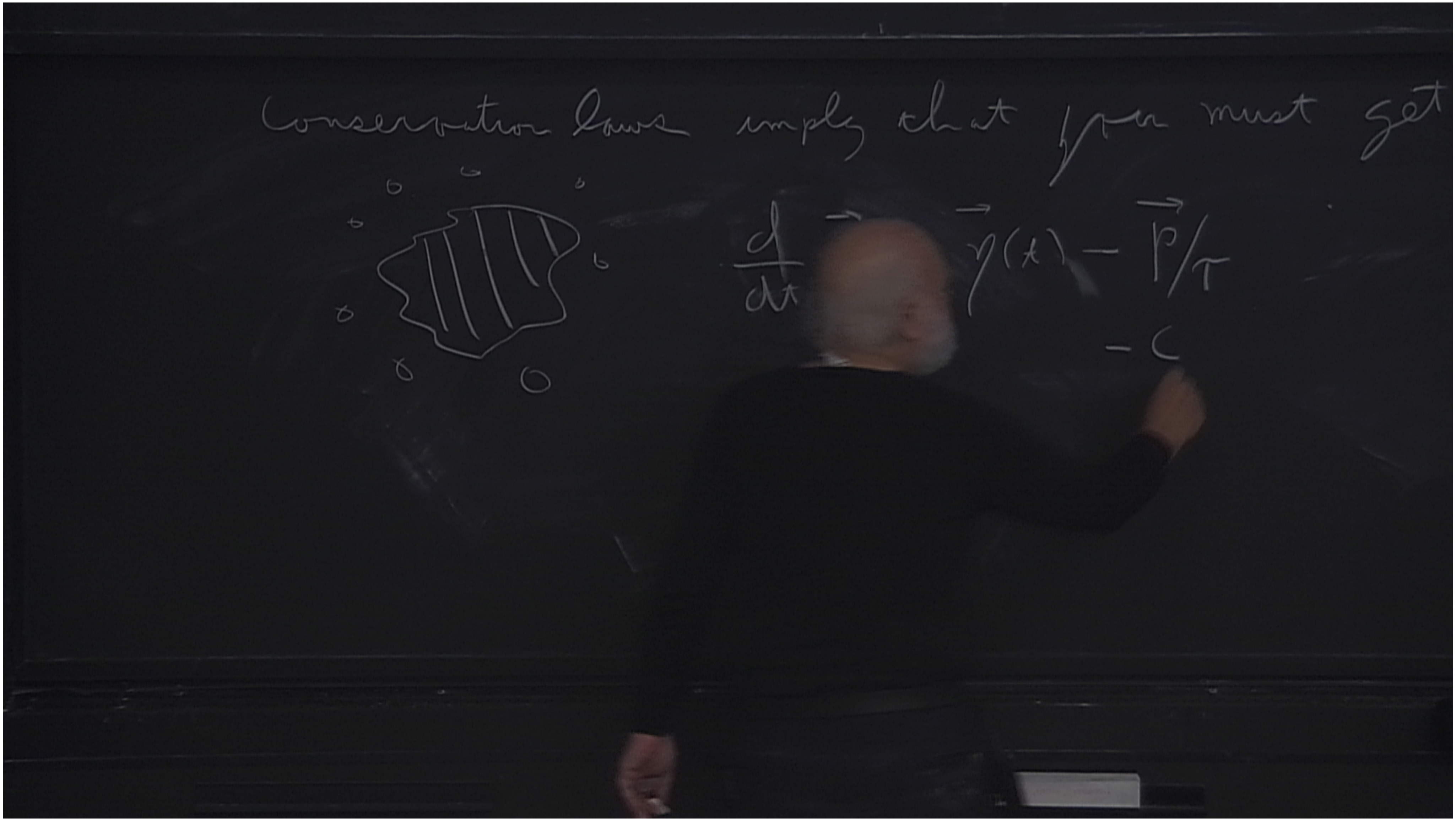

Conservation laws imply that you must get
dp⃗


Conservation laws imply that
must get
$\frac{d}{dt}\vec{p} = \vec{\eta}(t) - \vec{p}/\tau$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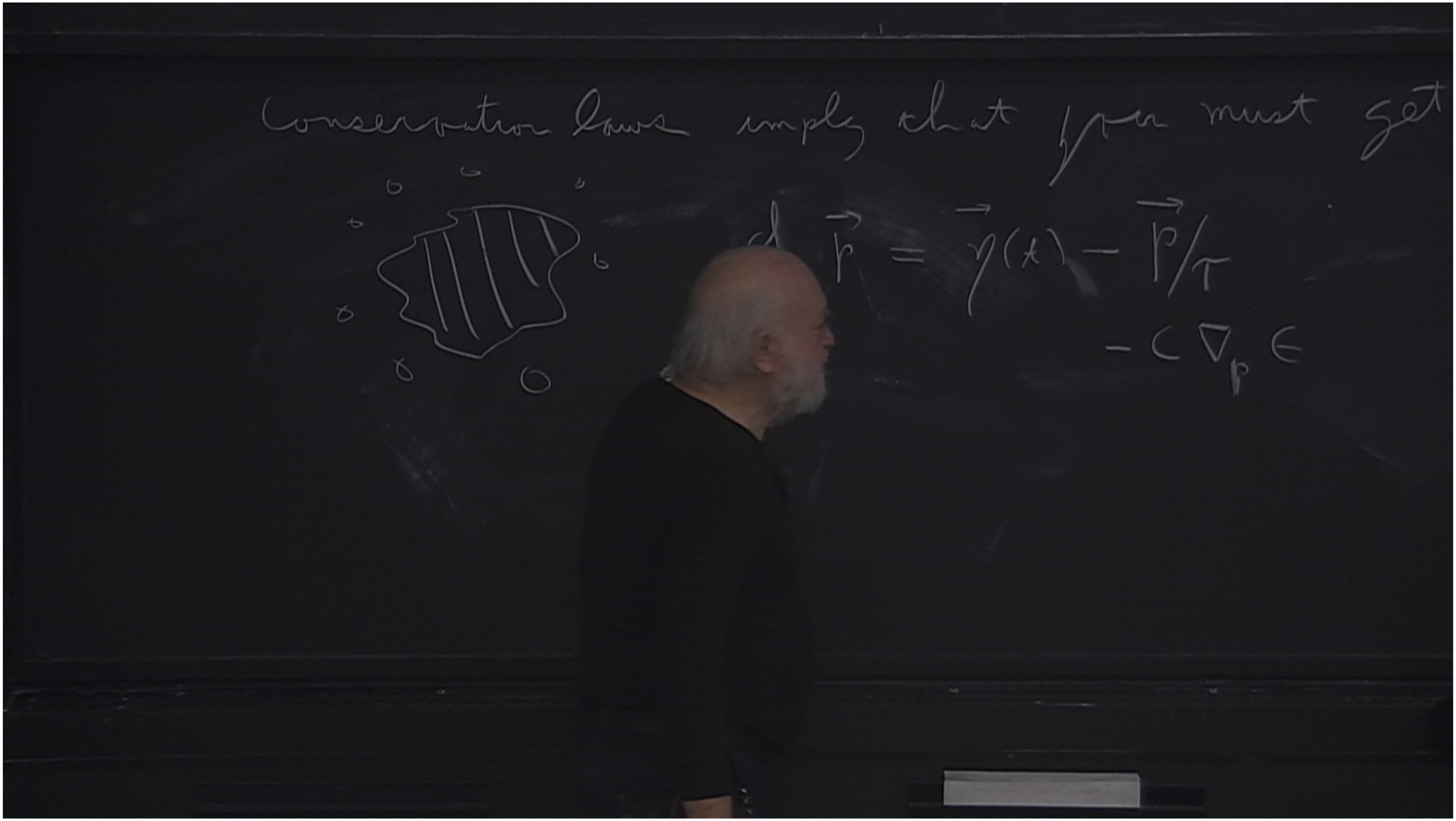
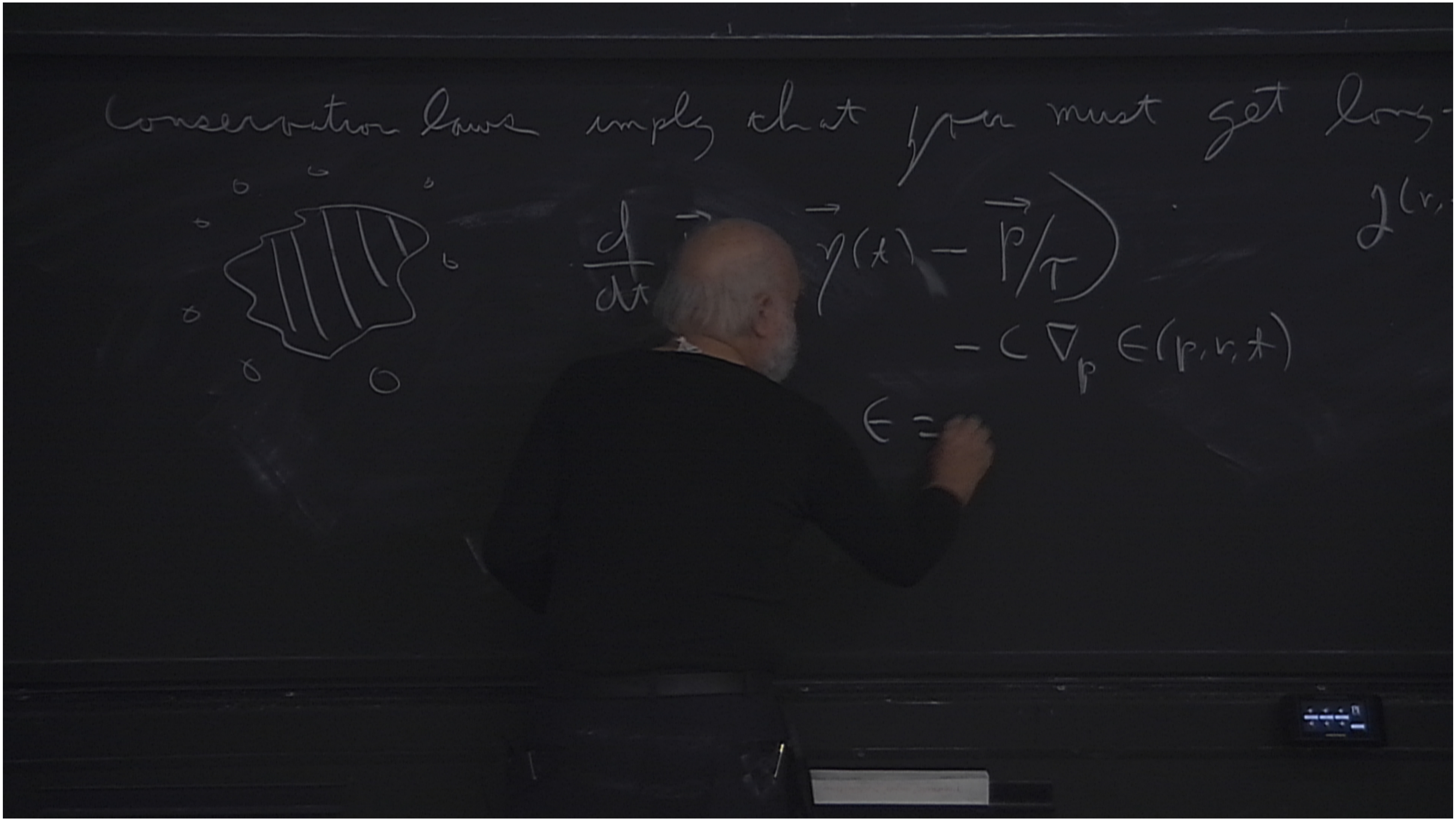
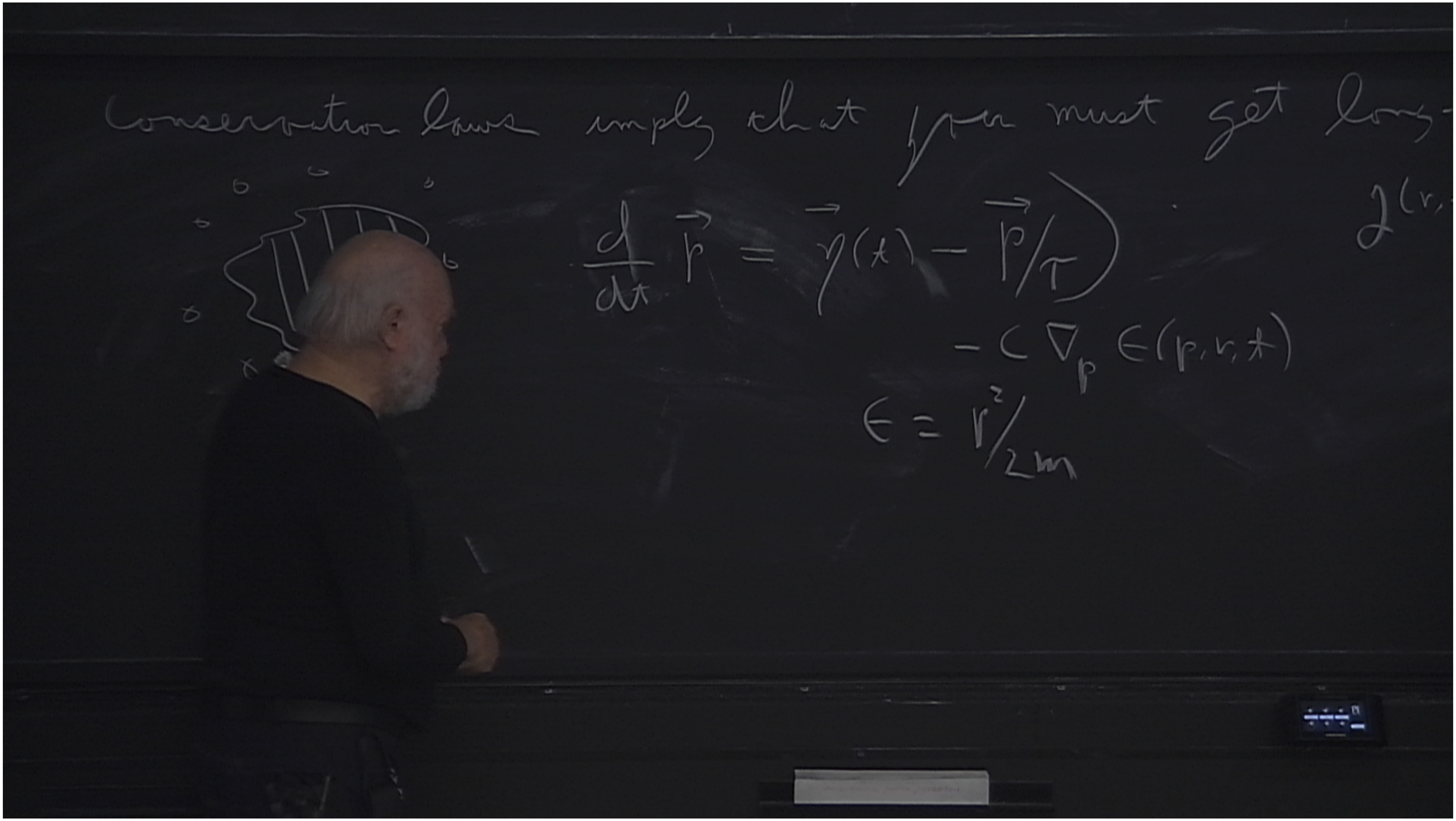
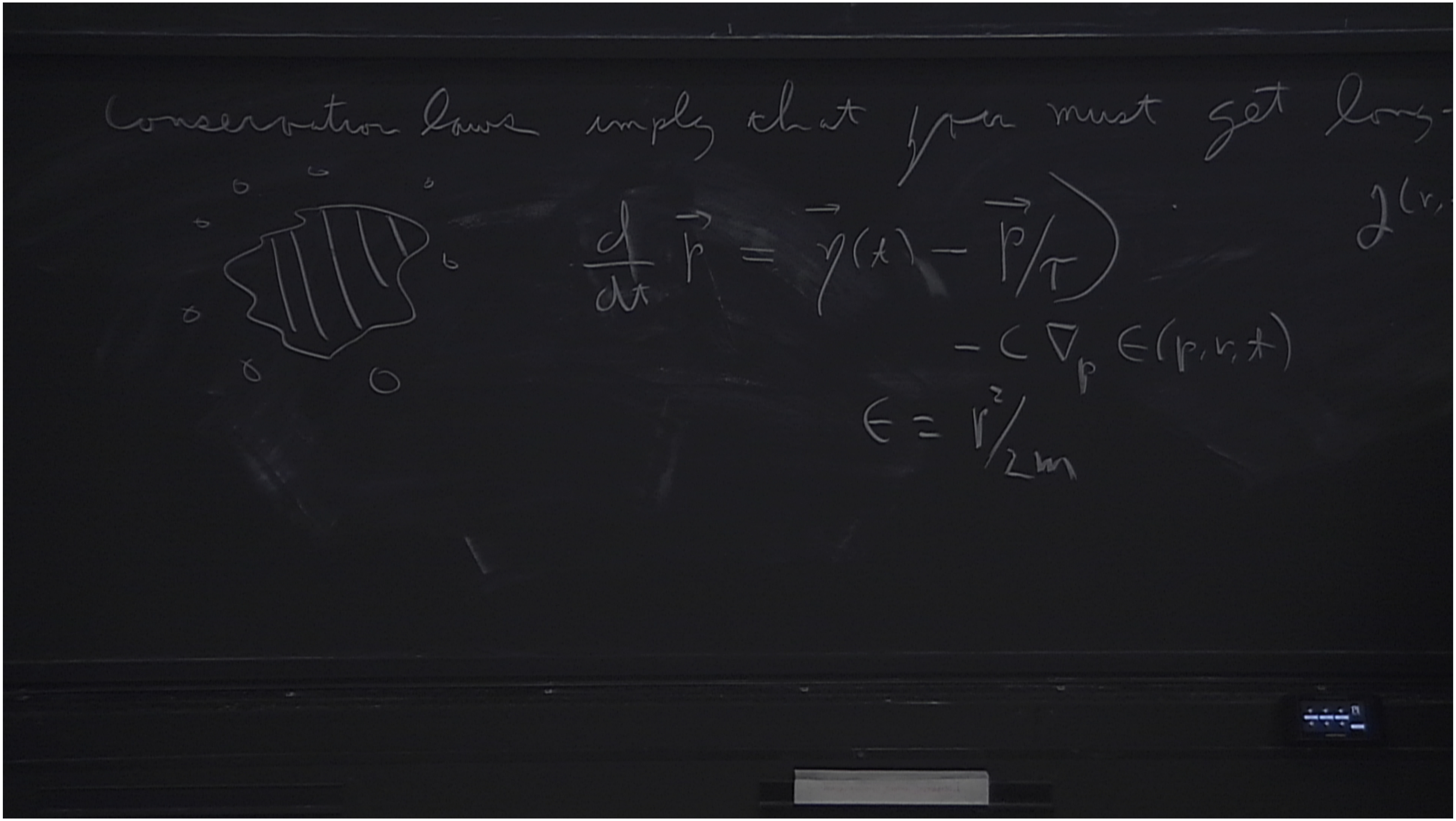

Conservation laws imply that you must get
d p = η(t) − p/τ
− C ∇p ∈


Conservation laws imply that you must get long-


Conservation laws imply that you must get long-
d/dt p = η(t) − p/τ
− c ∇p ∈(p,r,t)
∈ = p²/2m



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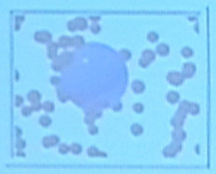

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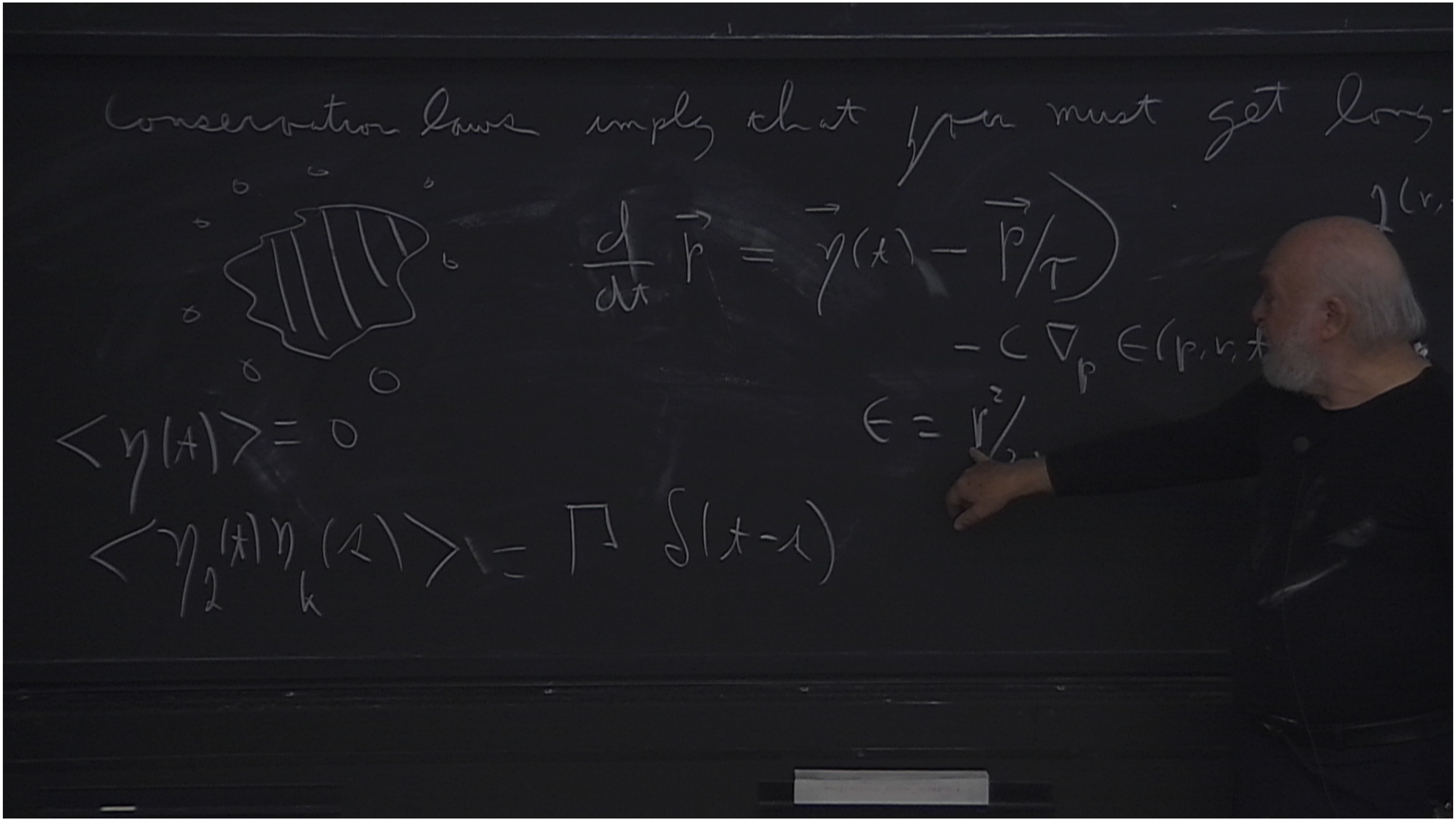
1


Conservation laws imply that you must get long-
d/dt p = η(t) − p/τ
− C ∇p ε(p, r, t
ε = p²/2
<η(t)> = 0
<η_i(t) η_k(s)> = Γ δ(t−s)

Calculate momentum from $dp/dt = \ldots\ldots + \eta(t) - p/\tau$

We have previously calculated the solution to this kind of **Langevin** equation for position. Now we do it for momentum.

Solution to equation v.1: $$P(t) = \int_{-\infty}^{t} dt' \; \eta(t') \exp(-\frac{t-t'}{\tau}) \qquad \text{v.3}$$

Because *P(t)* is a sum of many random variables, according to the central limit theorem, it must be a Gaussian random variable. Therefore it has a Gaussian probability distribution. In equilibrium, *P(t)* should have the variance, M kT, with M being the mass of the Brownian particle. In equilibrium it will have the Maxwell-Boltzmann probability distribution

$$\rho(\mathbf{p}) = (\frac{\beta}{2\pi M})^{3/2} \exp[-\beta p^2/(2M)]$$

Notice that if this works out for us, it will be our first "proof" that the ideas of Gibbs, Boltzmann, and Maxwell about the canonical distribution was correct. So we would have a proof that this "law" works, at least in this situation. Previously, we used this result without having any evidence that it was correct.

In physic[illegible] often use laws long before there is any substantial proof that they are co[illegible] little bits of evidence, intuition, and guesswork and gradually conv[illegible] hat idea X "must be" right. If X is attractive, we hold on to that [illegible] overwhelming evidence to the contrary.

2

Calculate Average

$$< p_j(t) p_k(s) >= \int_{-\infty}^{t} du \int_{-\infty}^{t} dv < \eta_j(u)\eta_k(v) > \ \exp[-(t-u+s-v)/\tau]$$

$$< p_j(t) p_k(s) >= \int_{-\infty}^{t} du \int_{-\infty}^{s} dv \Gamma \delta_{j,k} \delta(u-v) \exp[-(t-u)/\tau - (s-v)/\tau] \qquad \text{v.4}$$

.... if $t > s$ the integral over v always gets a contribution from the delta-function integral in u so that this expression then becomes

$$< p_j(t) p_k(s) >= \int_{-\infty}^{s} dv \, \Gamma \delta_{j,k} \exp[-(t+s-2v)/\tau]$$

$$= \frac{\delta_{j,k}}{2} \Gamma \tau \exp[-|t-s|/\tau] \qquad \text{v.5}$$

so we see that $p_j^2/(2M)$, where M is the mass of the Brownian particle, is on one hand given by

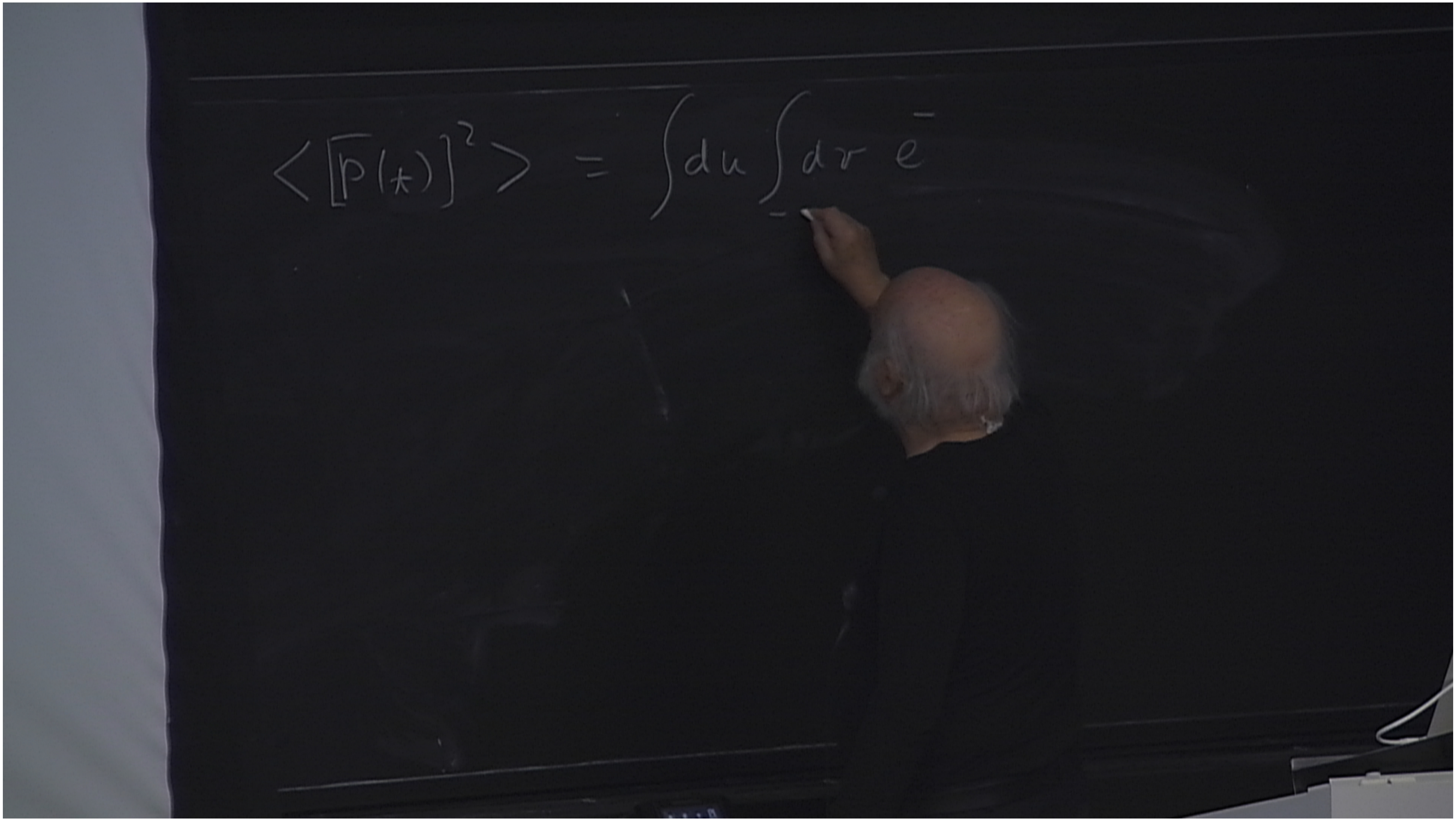
$$< \frac{p_j^2}{2M} >= \Gamma \tau / (4M)$$

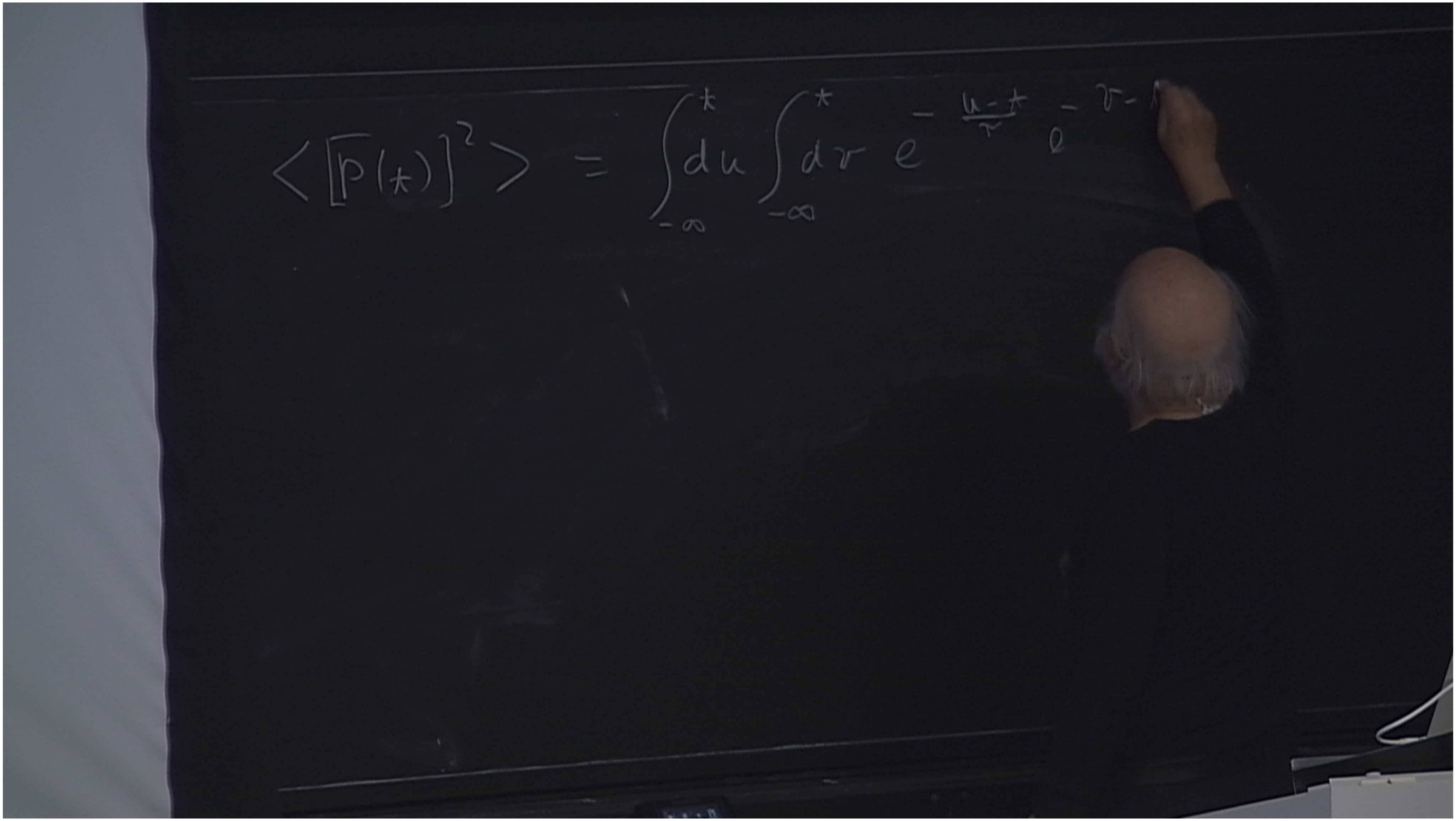
On the other hand, we know that in classical physics this quantity is kT/2. Thus we obtain the relation between the two parameters in the Einstein model.

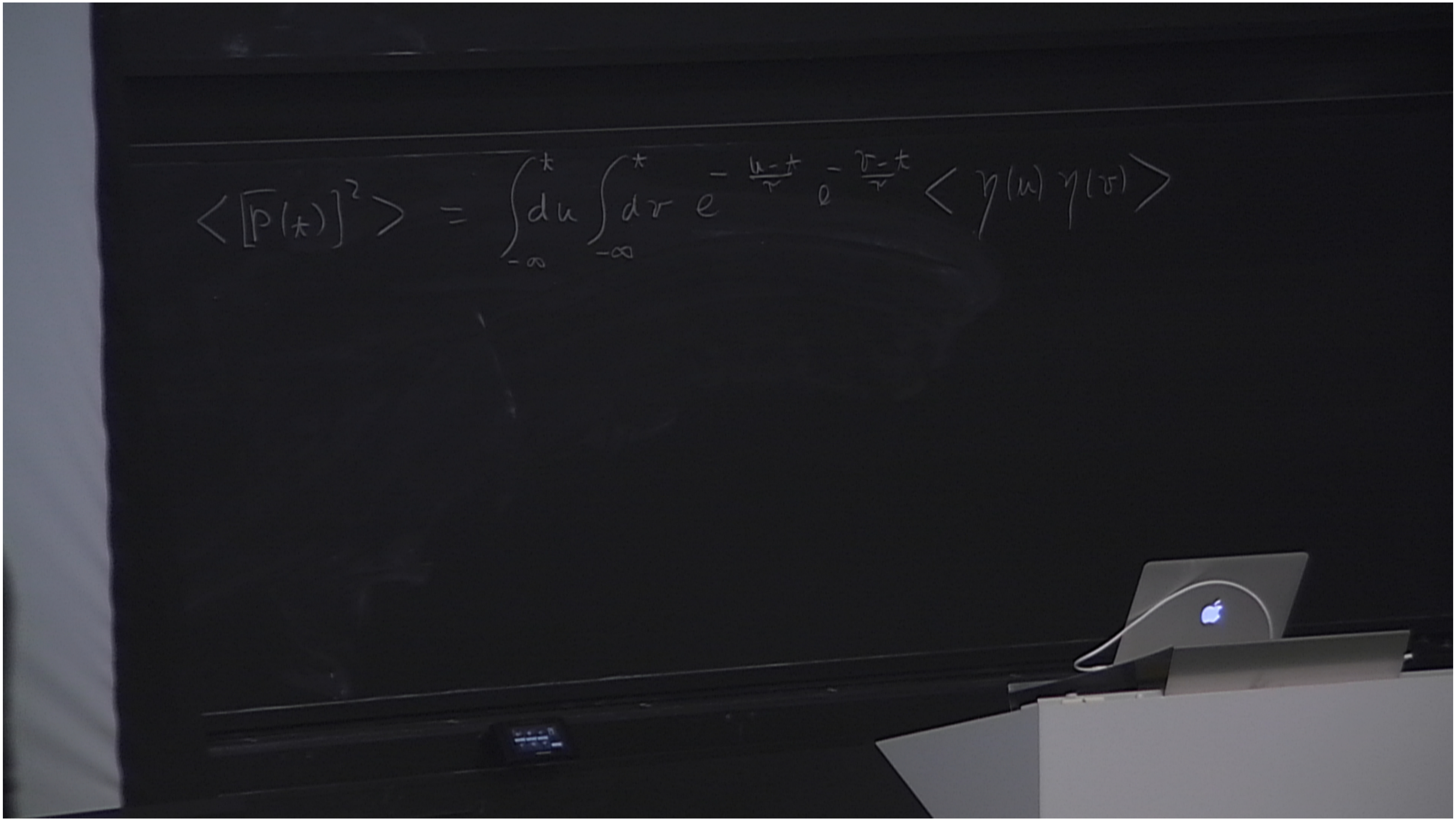
$$\Gamma \tau = 2MkT$$

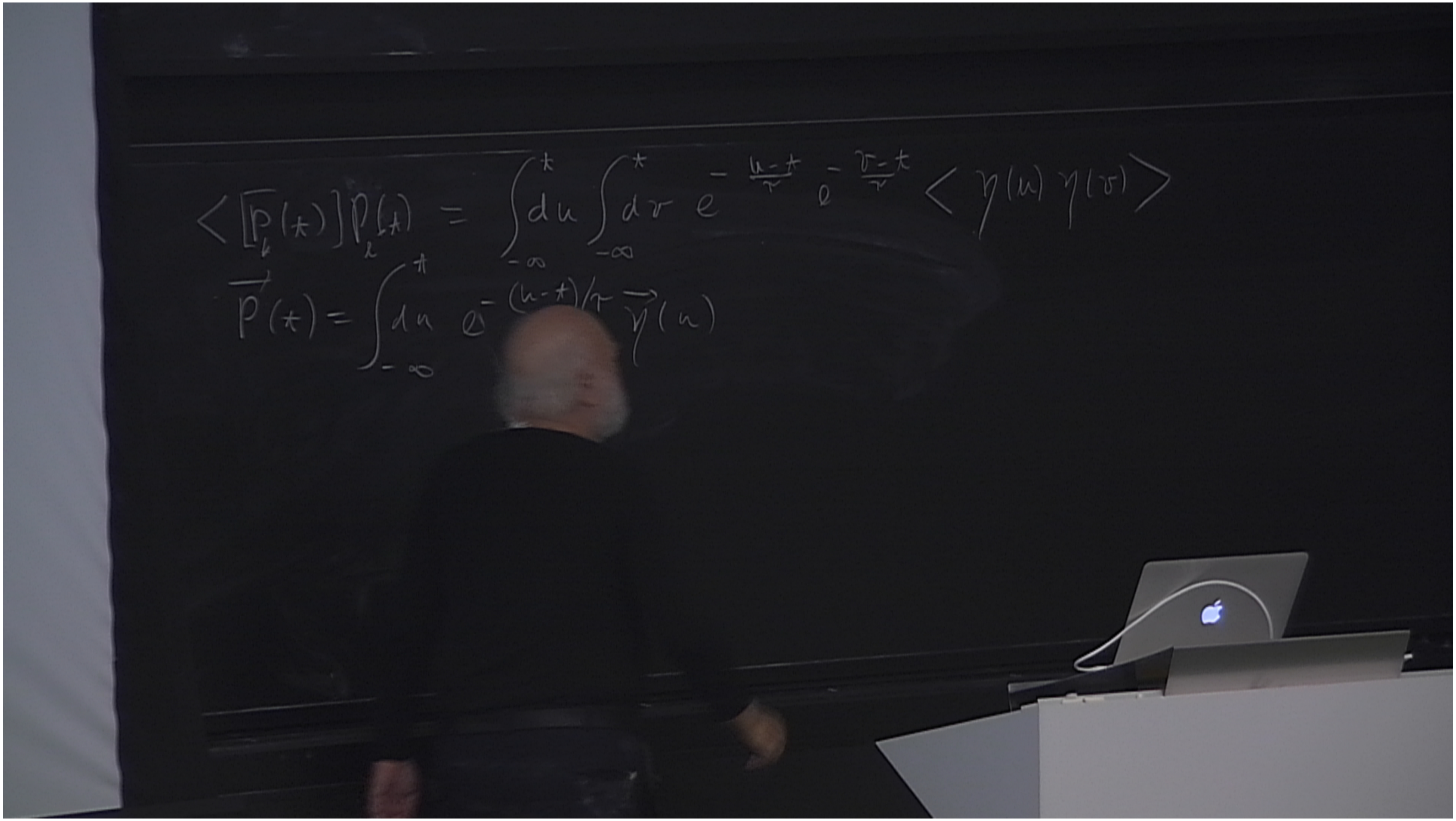
v.6

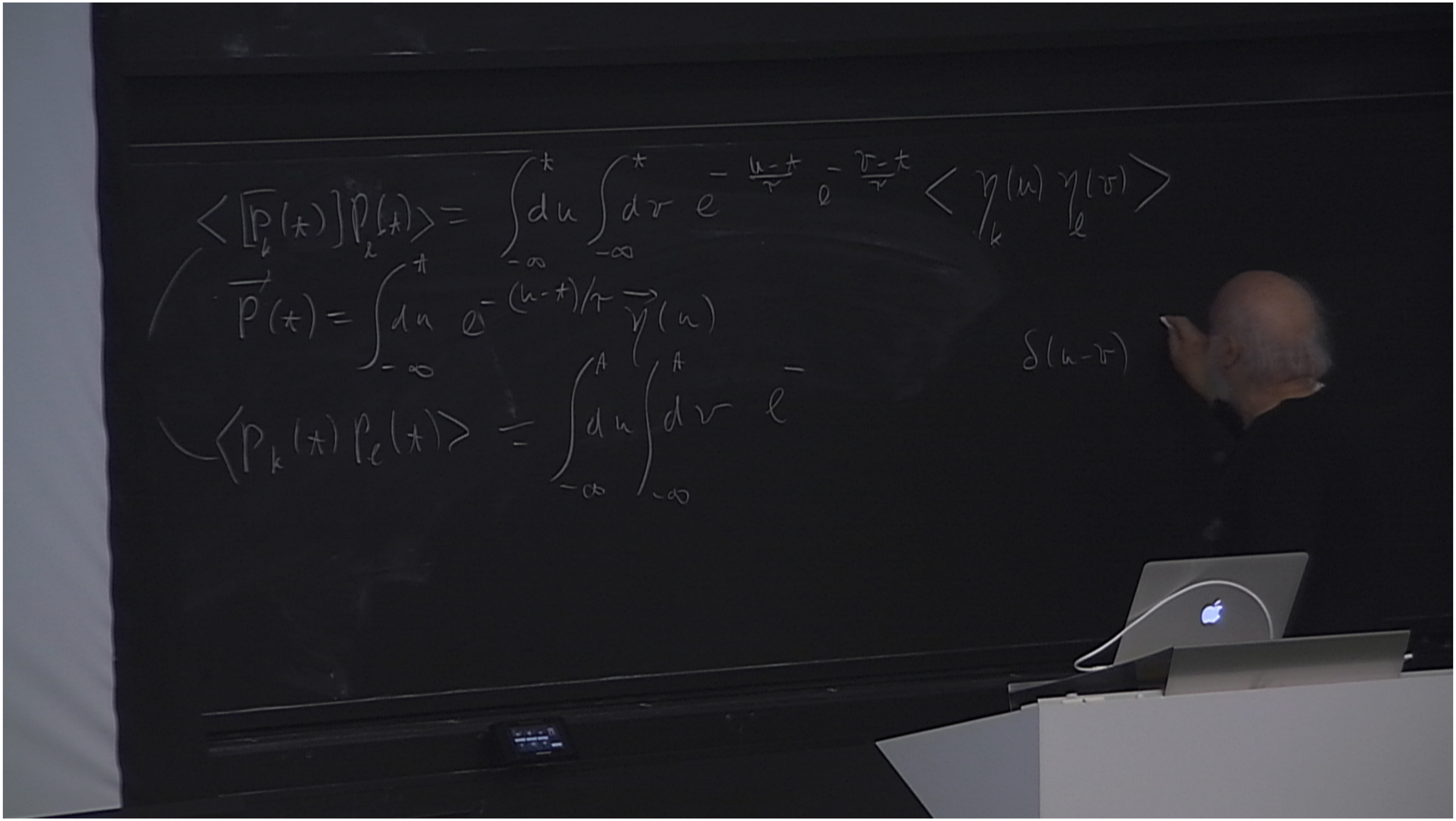
3

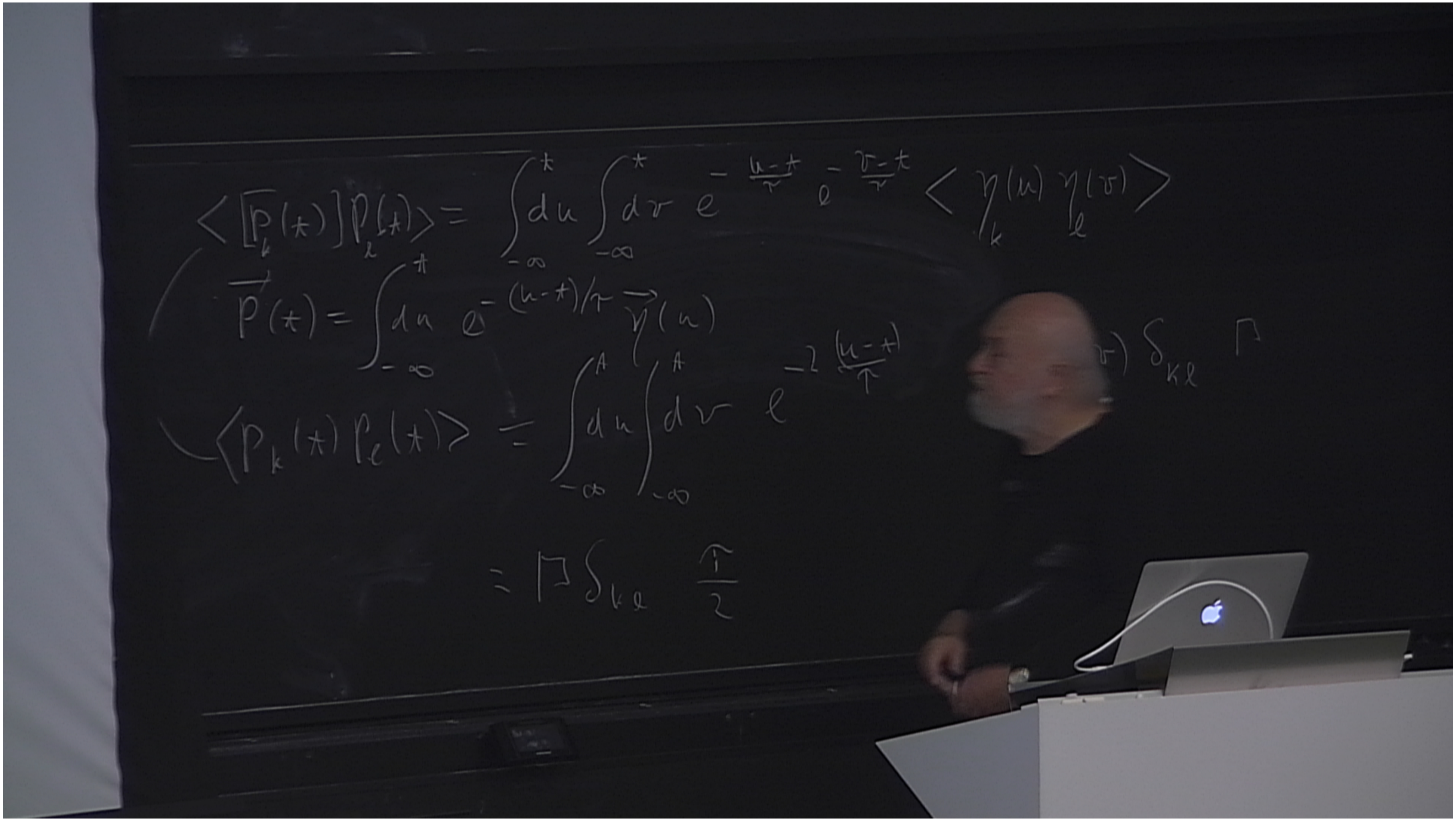

$\langle [p(t)]^2 \rangle = \int du \int dv\, e^{-}$

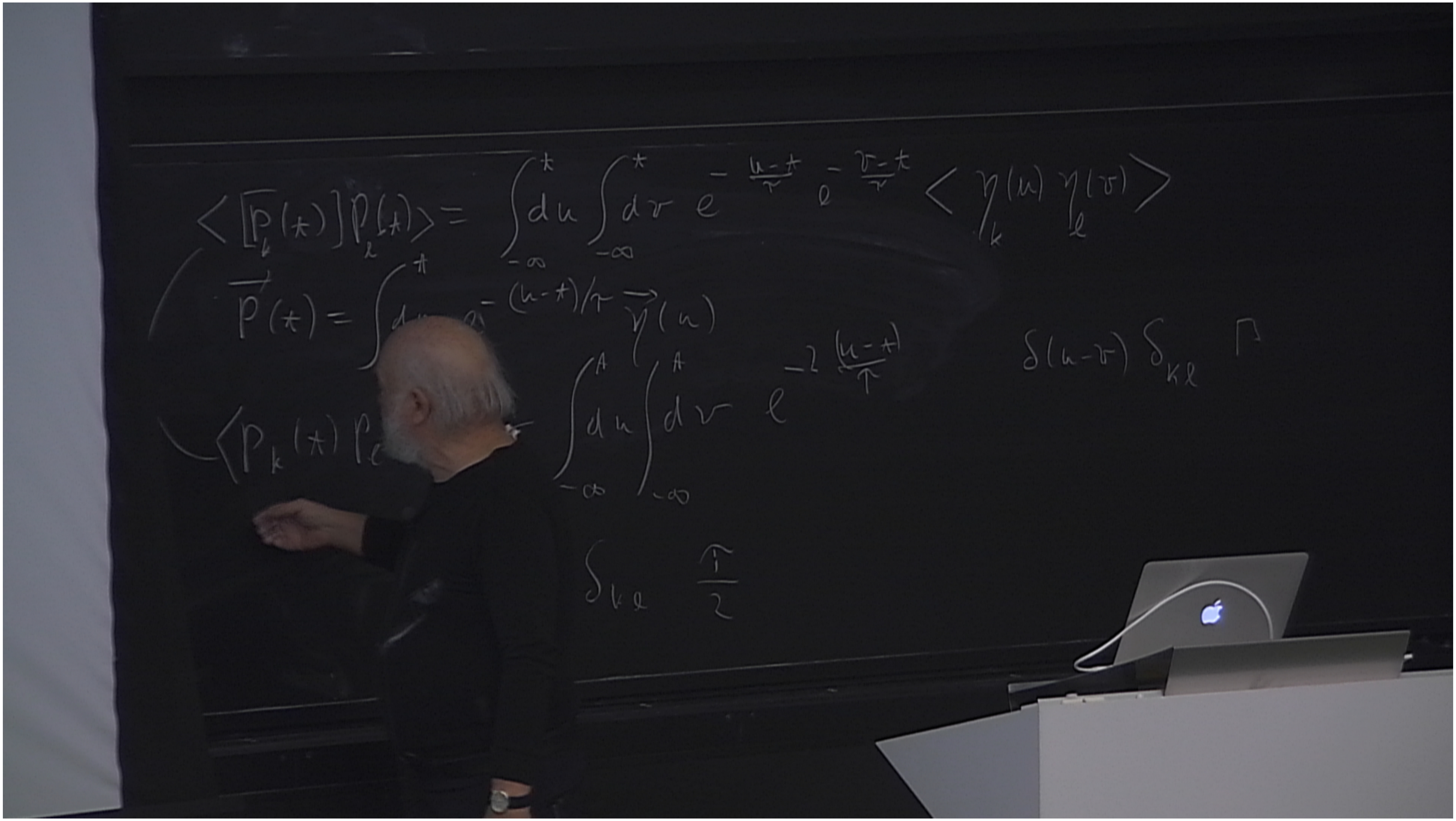

$\langle [p(t)]^2 \rangle = \int_{-\infty}^{t} du \int_{-\infty}^{t} dv \, e^{-\frac{u-t}{\tau}} e^{-\frac{v-}{}}$

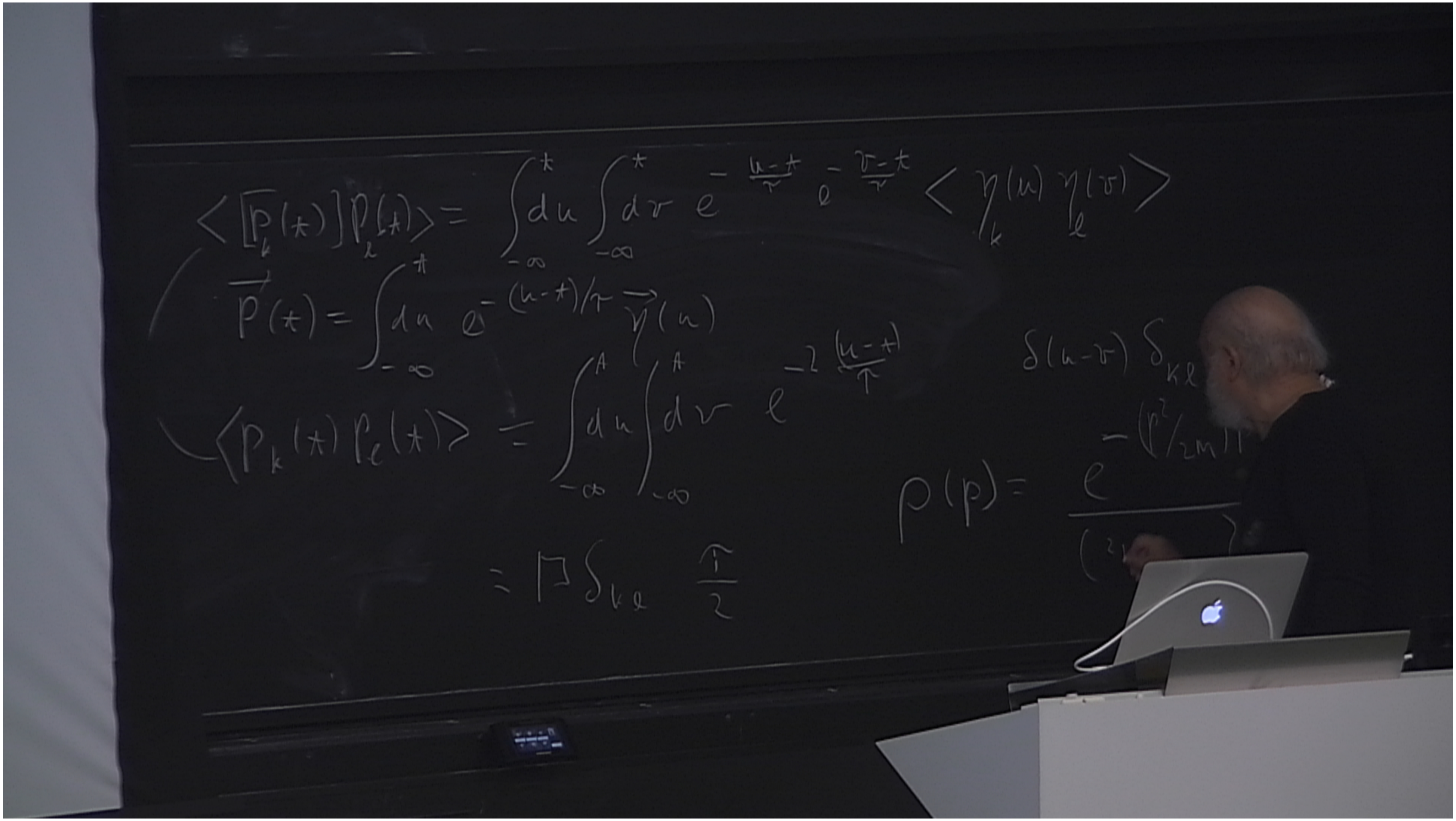

$\langle [p(t)]^2 \rangle = \int_{-\infty}^{t} du \int_{-\infty}^{t} dv \, e^{-\frac{u-t}{\tau}} e^{-\frac{v-t}{\tau}} \langle \eta(u)\, \eta(v) \rangle$

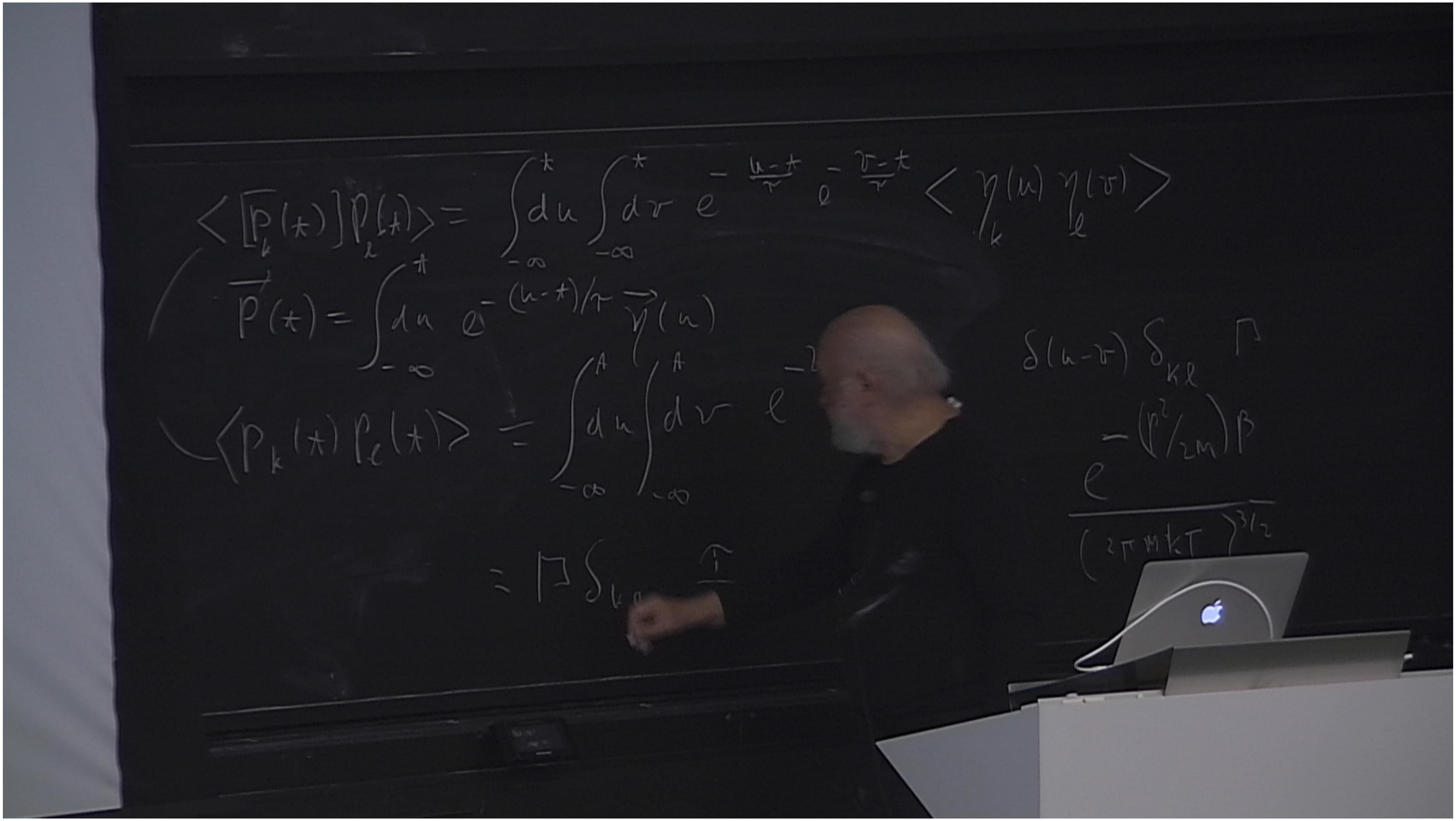

$\langle [p_k(t)] p_l(t) \rangle = \int_{-\infty}^{t} du \int_{-\infty}^{t} dv \, e^{-\frac{u-t}{\tau}} e^{-\frac{v-t}{\tau}} \langle \eta(u) \eta(v) \rangle$
$\vec{p}(t) = \int_{-\infty}^{t} du \, e^{-(u-t)/\tau} \vec{\eta}(u)$


⟨[p_k(t)] p_l(t)⟩ = ∫_{-∞}^{t} du ∫_{-∞}^{t} dv e^{-(u-t)/τ} e^{-(v-t)/τ} ⟨η_k(u) η_l(v)⟩
p(t) = ∫_{-∞}^{t} du e^{-(u-t)/τ} η(u)
⟨p_k(t) p_l(t)⟩ = ∫_{-∞}^{t} du ∫_{-∞}^{t} dv e^{-}
δ(u-v)

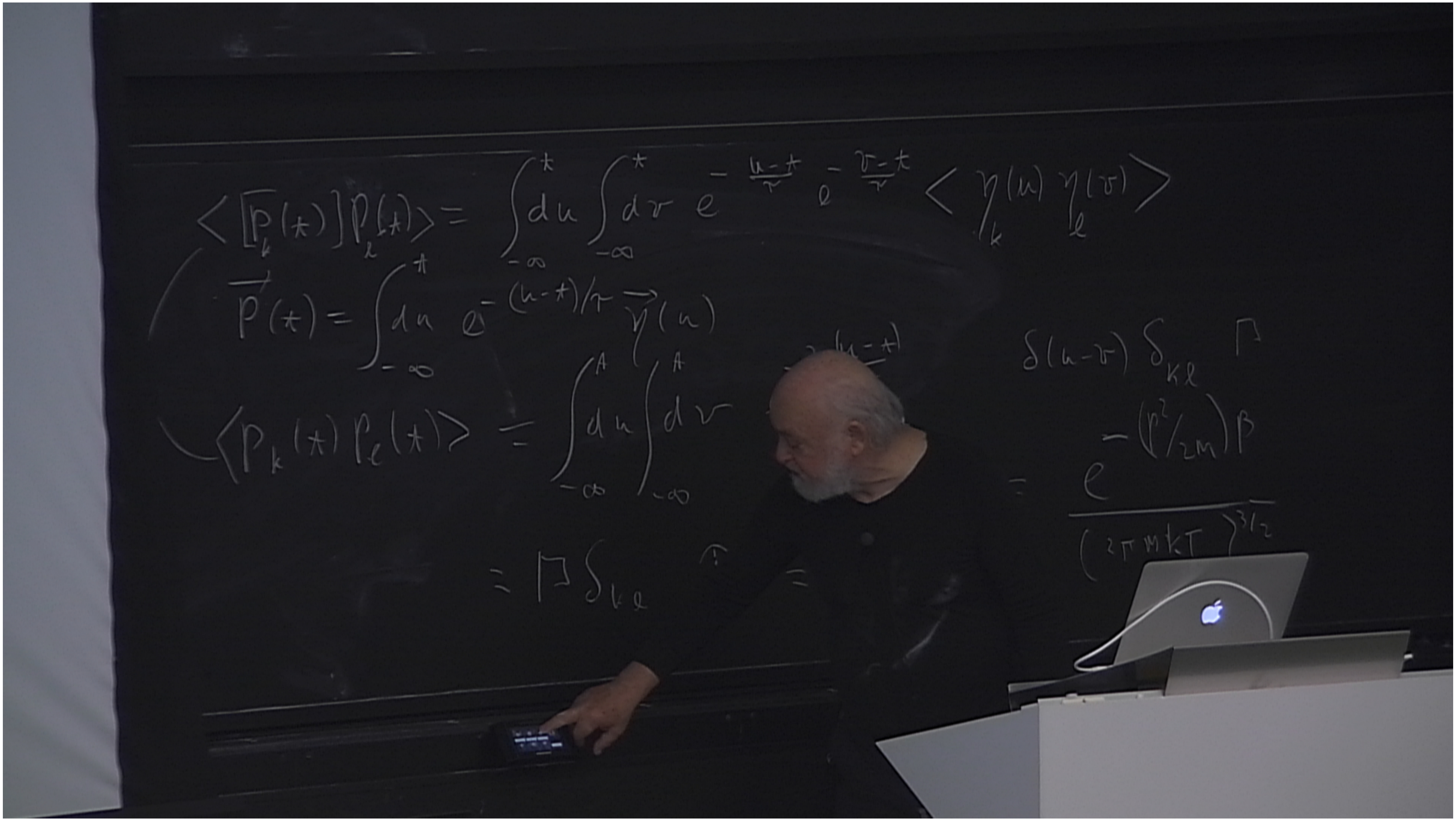



⟨[p_k(t)] p_l(t)⟩ = ∫_{-∞}^{t} du ∫_{-∞}^{t} dv e^{-(u-t)/τ} e^{-(v-t)/τ} ⟨η_k(u) η_l(v)⟩
p(t) = ∫ du e^{-(u-t)/τ} η(u)
δ(u-v) δ_{kl} Γ
⟨p_k(t) p_l ... = ∫_{-∞}^{t} du ∫_{-∞}^{t} dv e^{-2(u-t)/τ}
δ_{kl} τ/2


$\langle [p_k(t)] p_l(t) \rangle = \int_{-\infty}^{t} du \int_{-\infty}^{t} dv \, e^{-\frac{u-t}{\tau}} e^{-\frac{v-t}{\tau}} \langle \eta_k(u) \eta_l(v) \rangle$
$\vec{p}(t) = \int_{-\infty}^{t} du \, e^{-(u-t)/\tau} \vec{\eta}(u)$
$\langle p_k(t) p_l(t) \rangle = \int_{-\infty}^{t} du \int_{-\infty}^{t} dv \, e^{-2\frac{(u-t)}{\tau}}$
$= \Gamma \delta_{kl} \frac{\tau}{2}$
$\delta(u-v) \delta_{kl}$
$\rho(p) = e^{-(p^2/2m)}$



$\langle [p_k(t)] p_\ell(t) \rangle = \int_{-\infty}^{t} du \int_{-\infty}^{t} dv \, e^{-\frac{u-t}{\tau}} e^{-\frac{v-t}{\tau}} \langle \eta_k(u) \eta_\ell(v) \rangle$
$\vec{p}(t) = \int_{-\infty}^{t} du \, e^{-(u-t)/\tau} \vec{\eta}(u)$
$\langle p_k(t) p_\ell(t) \rangle = \int_{-\infty}^{t} du \int_{-\infty}^{t} dv \, e^{-2}$
$= \Gamma \delta_{k\ell}$
$\delta(u-v) \delta_{k\ell} \; \Gamma$
$\frac{e^{-(p^2/2m)\beta}}{(2\pi m k T)^{3/2}}$



<[p_k(t)] p_l(t)> = ∫_{-∞}^{t} du ∫_{-∞}^{t} dv e^{-(u-t)/τ} e^{-(v-t)/τ} < η_k(u) η_l(v) >
p(t) = ∫_{-∞}^{t} du e^{-(u-t)/τ} η(u)
<p_k(t) p_l(t)> = ∫_{-∞}^{t} du ∫_{-∞}^{t} dv
= Γ δ_{kl}
δ(u-v) δ_{kl} Γ
= e^{-(p²/2m)β} / (2πmkT)^{3/2}

Calculate momentum from $d\mathbf{p}/dt = ... + \eta(t) - \mathbf{p}/\tau$

We have previously calculated the solution to this kind of **Langevin** equation for position. Now we do it for momentum.

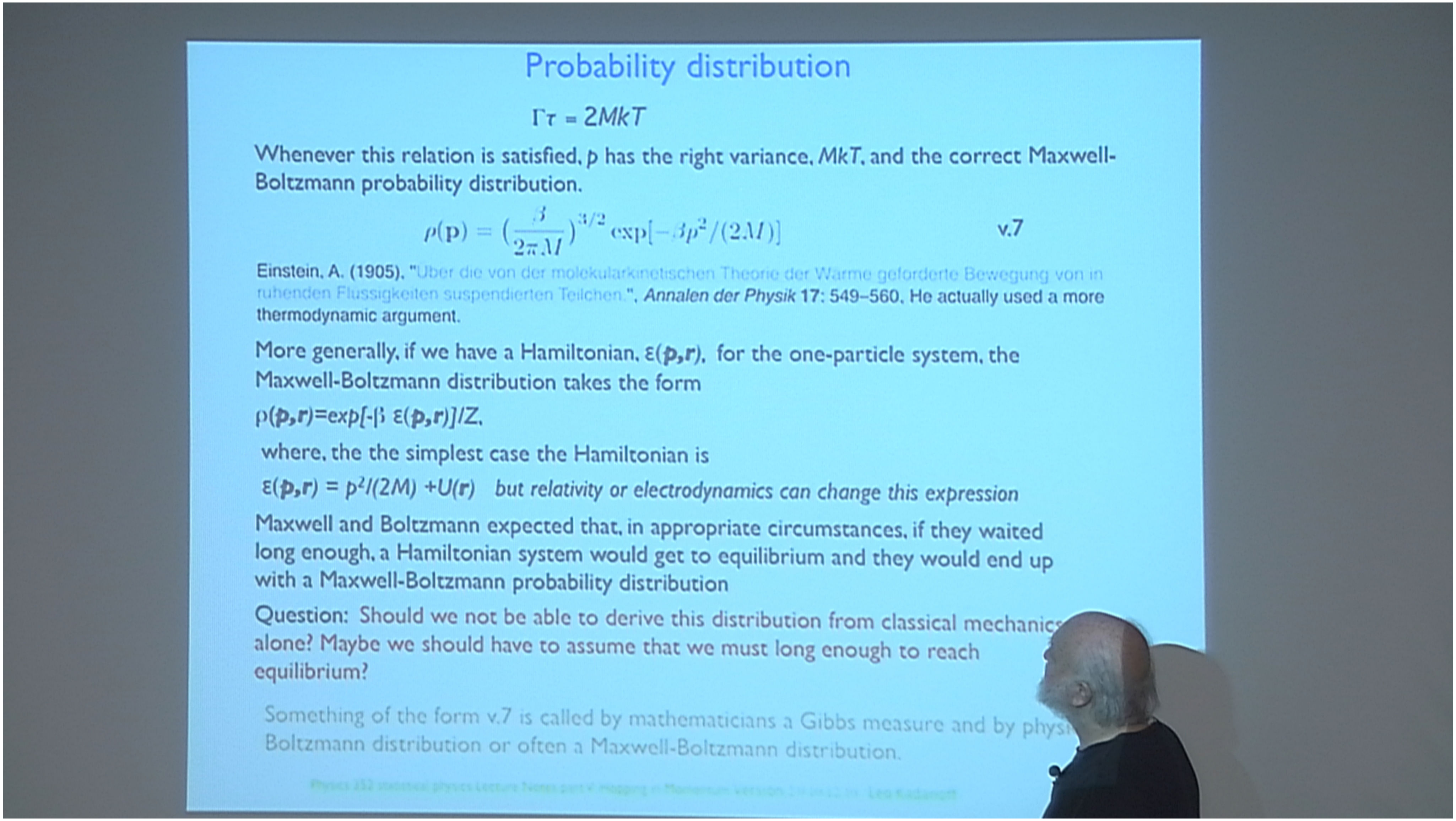
Solution to equation v.1:
$$P(t) = \int_{-\infty}^{t} dt' \ \eta(t') \exp(-\frac{t-t'}{\tau}) \qquad \text{v.3}$$

Because *P(t)* is a sum of many random variables, according to the central limit theorem, it must be a Gaussian random variable. Therefore it has a Gaussian probability distribution. In equilibrium, *P(t)* should have the variance, M kT, with M being the mass of the Brownian particle. In equilibrium it will have the Maxwell-Boltzmann probability distribution

$$\rho(\mathbf{p}) = (\frac{\beta}{2\pi M})^{3/2} \exp[-\beta p^2/(2M)]$$

Notice that if this works out for us, it will be our first "proof" that the ideas of Gibbs, Boltzmann, and Maxwell about the canonical distribution was correct. So we would have a proof that this "law" works, at least in this situation. Previously, we used this result without having any evidence that it was correct.

In physics, we often use laws long before there is any substantial proof that they are correct. We use little bits of evidence, intuition, and guesswork and gradually convince ourselves that idea X "must be" right. If X is attractive, we hold on to that view until there is overwhelming evidence to the contrary.


Probability distribution
$\Gamma\tau = 2MkT$
Whenever this relation is satisfied, p has the right variance, MkT, and the correct Maxwell-Boltzmann probability distribution.
$\rho(\mathbf{p}) = (\frac{\beta}{2\pi M})^{3/2} \exp[-\beta p^2/(2M)]$ v.7
Einstein, A. (1905). "Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flussigkeiten suspendierten Teilchen.", *Annalen der Physik* 17: 549–560. He actually used a more thermodynamic argument.
More generally, if we have a Hamiltonian, $\varepsilon(\boldsymbol{p},\boldsymbol{r})$, for the one-particle system, the Maxwell-Boltzmann distribution takes the form
$\rho(\boldsymbol{p},\boldsymbol{r}) = \exp[-\beta\, \varepsilon(\boldsymbol{p},\boldsymbol{r})]/Z$.
where, the the simplest case the Hamiltonian is
$\varepsilon(\boldsymbol{p},\boldsymbol{r}) = p^2/(2M) + U(\boldsymbol{r})$ *but relativity or electrodynamics can change this expression*
Maxwell and Boltzmann expected that, in appropriate circumstances, if they waited long enough, a Hamiltonian system would get to equilibrium and they would end up with a Maxwell-Boltzmann probability distribution
Question: Should we not be able to derive this distribution from classical mechanic
alone? Maybe we should have to assume that we must long enough to reach equilibrium?
Something of the form v.7 is called by mathematicians a Gibbs measure and by physi
Boltzmann distribution or often a Maxwell-Boltzmann distribution.

Statistical and Hamiltonian Dynamics

We have that the equilibrium $\rho = \exp(-\beta H)/Z$. How can this arise from time dependence of system? One very important possible time-dependence is given by Hamiltonian mechanics

$$\frac{dq_\alpha}{dt} = \frac{\partial \mathcal{H}}{\partial p_\alpha}$$

$$\frac{dp_\alpha}{dt} = -\frac{\partial \mathcal{H}}{\partial q_\alpha}$$

The simplest case is a particle moving in a potential field with a Hamiltonian

$$\mathcal{H} = \mathbf{p}^2/(2M) + U(\mathbf{r})$$

and consequently equations of motion

$$\frac{d\mathbf{p}}{dt} = -\nabla U$$

$$\frac{d\mathbf{r}}{dt} = \mathbf{p}/M$$

The statistical mechanics of such situa[illegible] by a probability density function $\rho(\mathbf{p},\mathbf{r},t)$ such that the probability of [illegible]icle in a volume element **dp dr** about **p,r** at time t is $\rho(\mathbf{p},\mathbf{r},t)$ **dp dr** [illegible]estion is, what is the time-dependence of this probability density? [illegible] how do we get equilibrium statistical mechanics as a consequence o[illegible]

Time Dependence of Dynamical systems:
A much more general problem

Instead of carrying around the variables $\boldsymbol{p}$ and $\boldsymbol{q}$, let me do something with much simpler formulas. I'm going to imagine solving the dynamical systems problem in which there is a differential equation

$$dX_k/dt=V_k(\boldsymbol{X}(t),t)$$

to get a solution $\boldsymbol{X}(t)$. Note that $\boldsymbol{X}(t)$ is the solution vector while $X_k(t)$ is one component of that vector. On the other hand $\boldsymbol{x}$ is simply a vector of numbers haveing the same number of components as $\boldsymbol{X}(t)$. I will made extensive use of a probability function $\rho(\boldsymbol{x},t)\, d\boldsymbol{x}$ which is the probability that the solution will be in the interval $d\boldsymbol{x}= \prod_k dx_k$ about $\boldsymbol{x}$.

This $\rho(\boldsymbol{x},t)$ is a probability distribution because, when we start out, the initial data is not just one value of x but a probability distribution, given by $\rho(x,0)$. So the situation at a later time must be described by a probability distribution then as well. So what is the time dependence of the probability distribution? One way to approach this problem is to ask what does the distribution mean. Specifically, if we have some function $g(\boldsymbol{X})$ of the particle coordinates at time t, that function has an average at time t given by

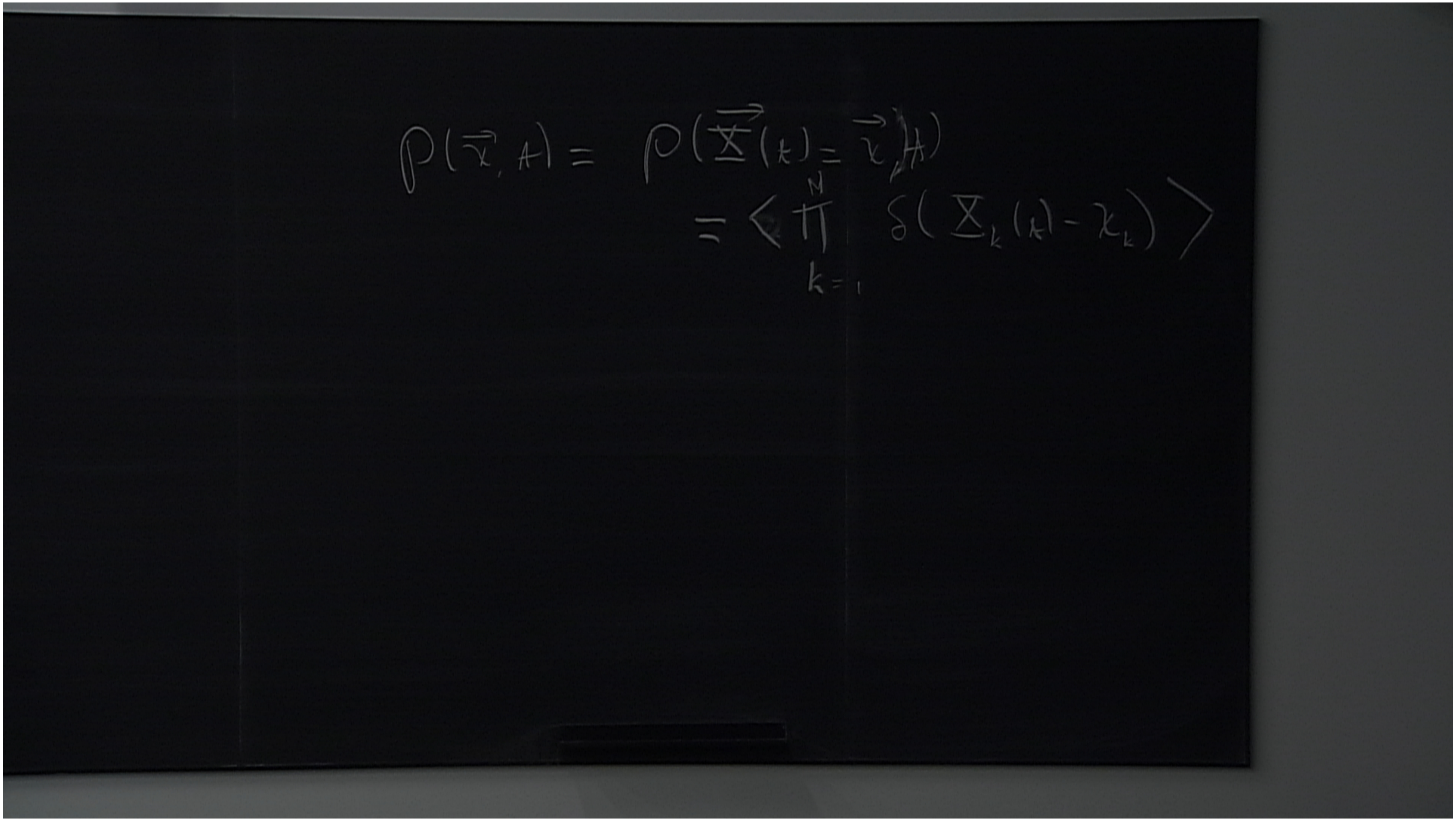
$\int dx\, g(\boldsymbol{x})\, \rho(\boldsymbol{x},t)$. A formula that agrees with this definition is to take

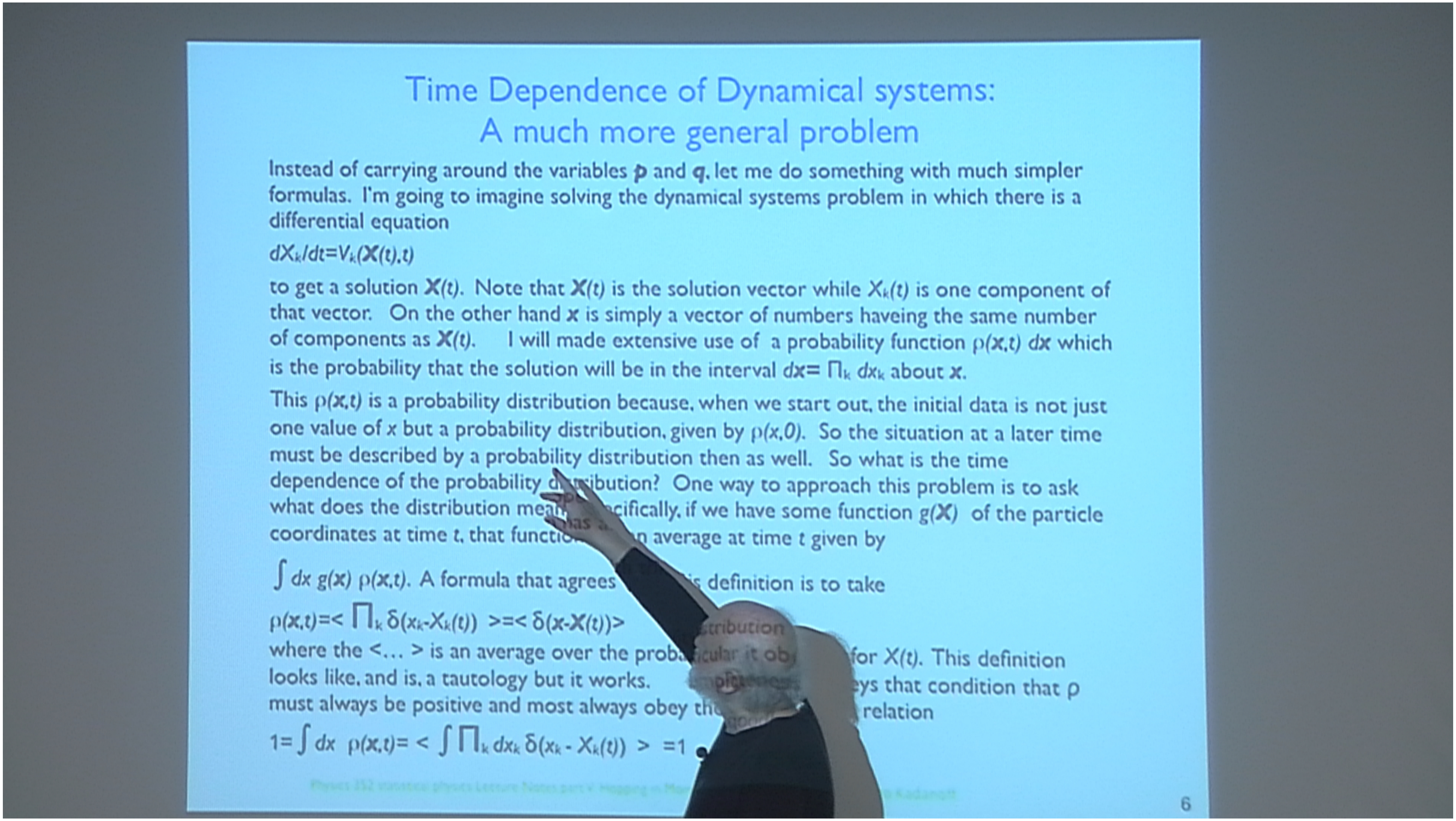
$$\rho(\boldsymbol{x},t)=< \prod_k \delta(x_k-X_k(t)) >=< \delta(\boldsymbol{x}-\boldsymbol{X}(t))>$$

where the <... > is an average over the probability distribution for $X(t)$. This definition looks like, and is, a tautology but it works. In particular it obeys that condition that ρ must always be positive and most always obey the completeness relation

$$1=\int dx\ \rho(\boldsymbol{x},t)= < \int \prod_k dx_k\, \delta(x_k - X_k(t)) > =1$$

good!


$\rho(\vec{x}, t) = \rho(\vec{X}(t) = \vec{x}, t)$
$= \left\langle \prod_{k=1}^{N} \delta(X_k(t) - x_k) \right\rangle$


Time Dependence of Dynamical systems:
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Instead of carrying around the variables p and q, let me do something with much simpler formulas. I'm going to imagine solving the dynamical systems problem in which there is a differential equation
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to get a solution X(t). Note that X(t) is the solution vector while X_k(t) is one component of that vector. On the other hand x is simply a vector of numbers haveing the same number of components as X(t). I will made extensive use of a probability function ρ(x,t) dx which is the probability that the solution will be in the interval dx= Π_k dx_k about x.
This ρ(x,t) is a probability distribution because, when we start out, the initial data is not just one value of x but a probability distribution, given by ρ(x,0). So the situation at a later time must be described by a probability distribution then as well. So what is the time dependence of the probability
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ys that condition that ρ must always be positive and most always obey th
relation
1= ∫ dx ρ(x,t)= < ∫ Π_k dx_k δ(x_k - X_k(t)) > =1
6

Time Dependence of $\rho(\mathbf{x},t)$

To calculate the time-dependence, differentiate $\rho(\mathbf{x},t)$ with respect to time, holding the coordinate vector, $\mathbf{x}$, fixed. Since $\rho(\mathbf{x},t) = < \prod_k \delta(x_k - X_k(t)) >$, we can use the usual rules for differentiation to find

$$\partial_t \rho(\mathbf{x},t) = < \sum_j [\partial_t \delta(x_j - X_j(t))\,] \prod_{k \neq j} \delta(x_k - X_k(t)) >$$

$$= - < \sum_j \partial_t X_j(t)\, \partial_{x_j} \prod_k \delta(x_k - X_k(t)) >$$

The time derivative of $X_j(t)$ is $V_j(\mathbf{X}(t),t)$. Thus we obtain

$$- < \sum_j \partial_{x_j} V(X_j(t),t) \prod_k \delta(x_k - X_k(t)) >$$

with the derivative on the left, I can replace the X in V by x

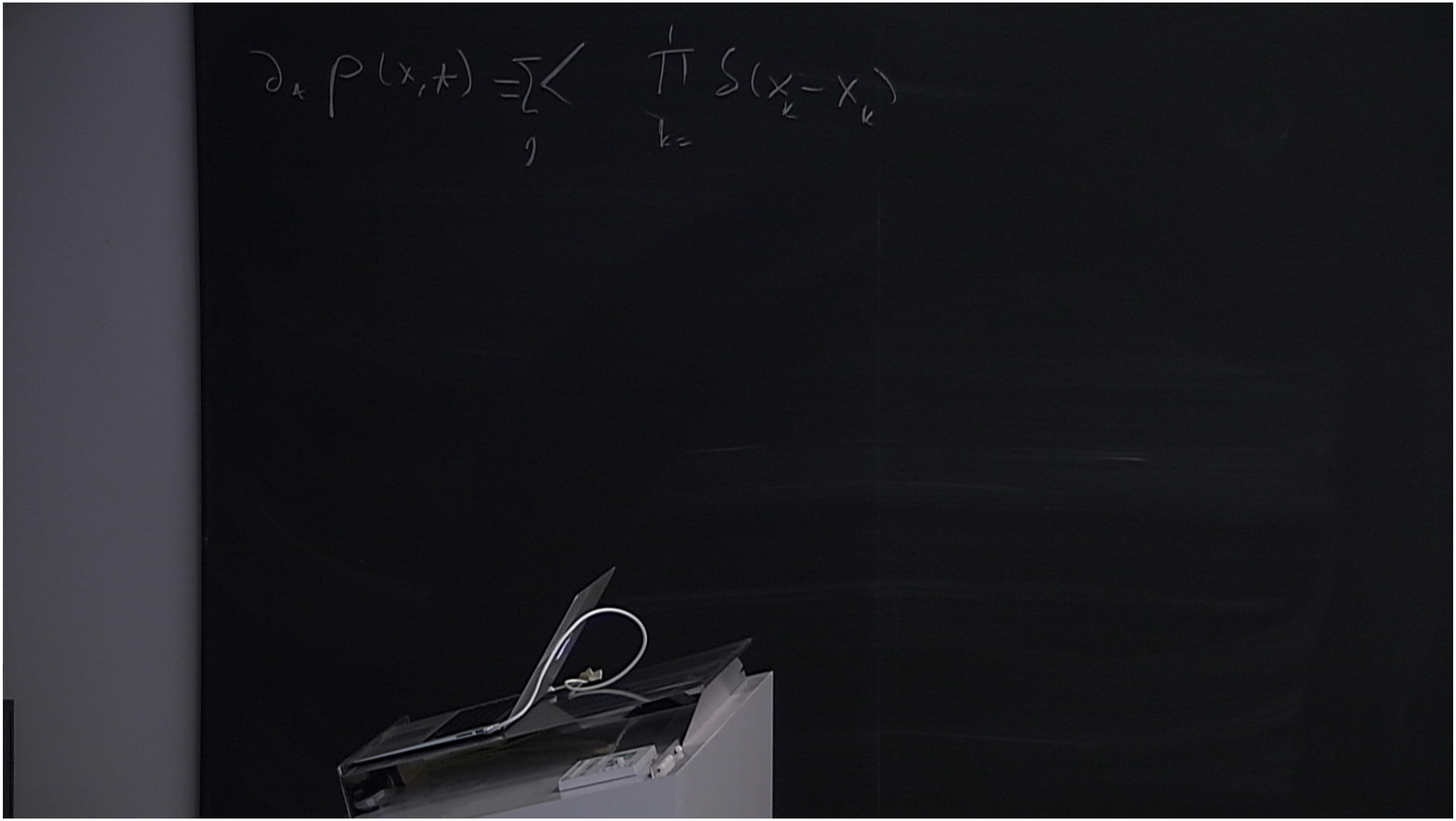
$$\partial_t \rho(\mathbf{x},t) + \sum_j \partial_{x_j} V_j(\mathbf{x},t) < \prod_k \delta(x_k - X_k(t)) > = 0$$ or more compactly

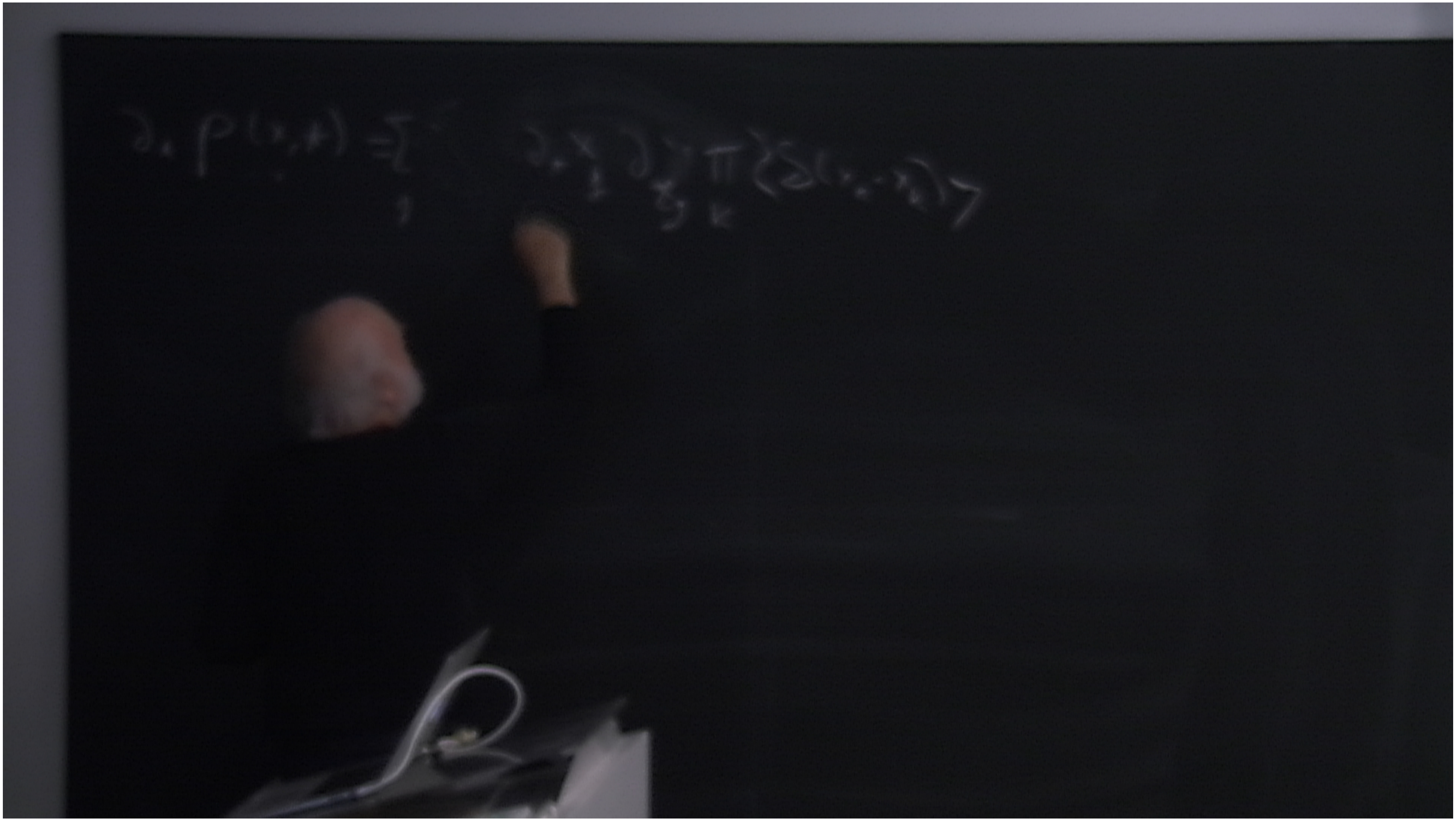
$$\partial_t \rho(\mathbf{x},t) + \sum_j \partial_{x_j} [\, V_j(\mathbf{x},t)\, \rho(\mathbf{x},t)] = 0$$ or more compactly yet

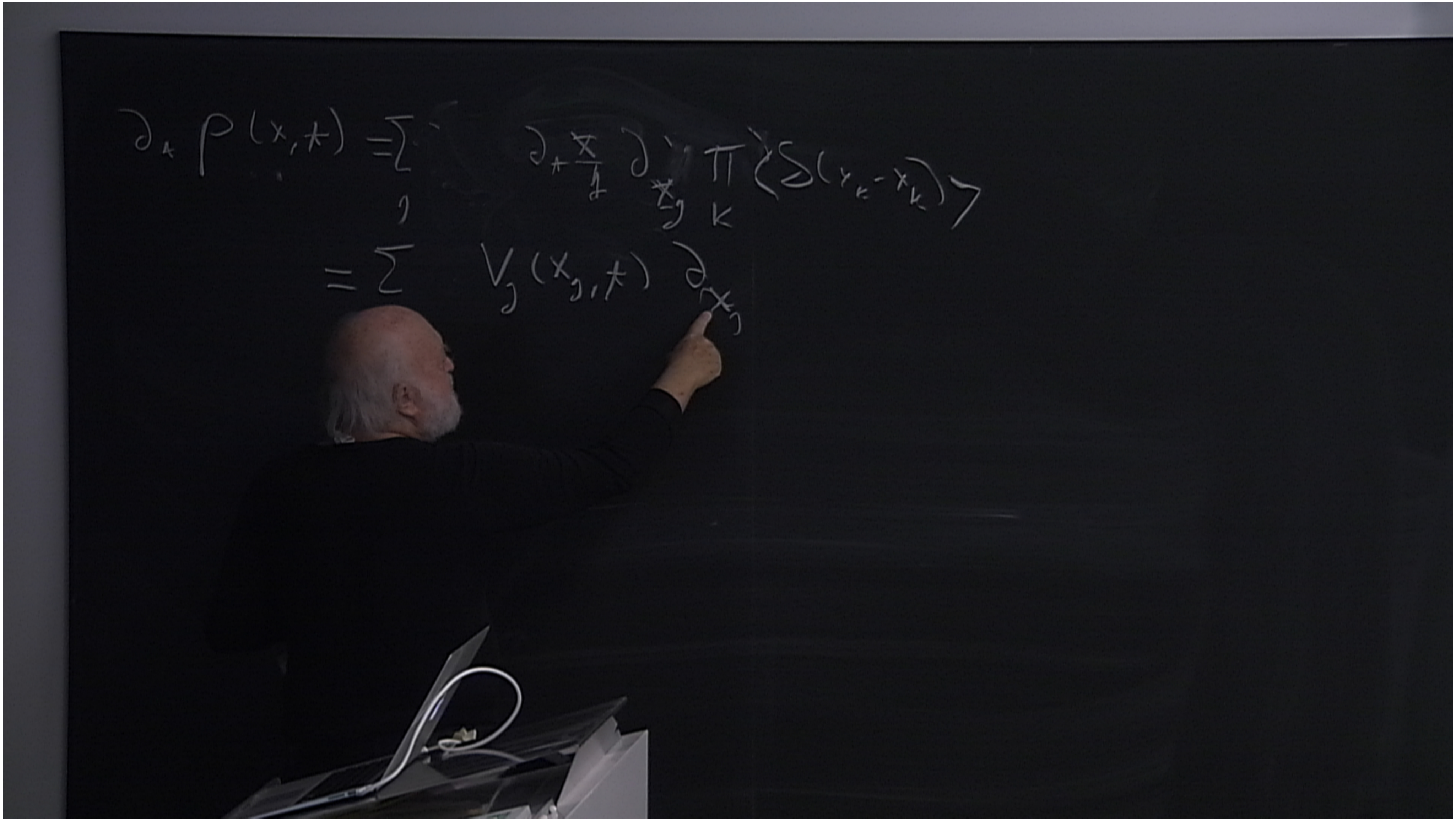
$$\partial_t \rho + \nabla \cdot [\, \mathbf{V} \rho] = 0$$

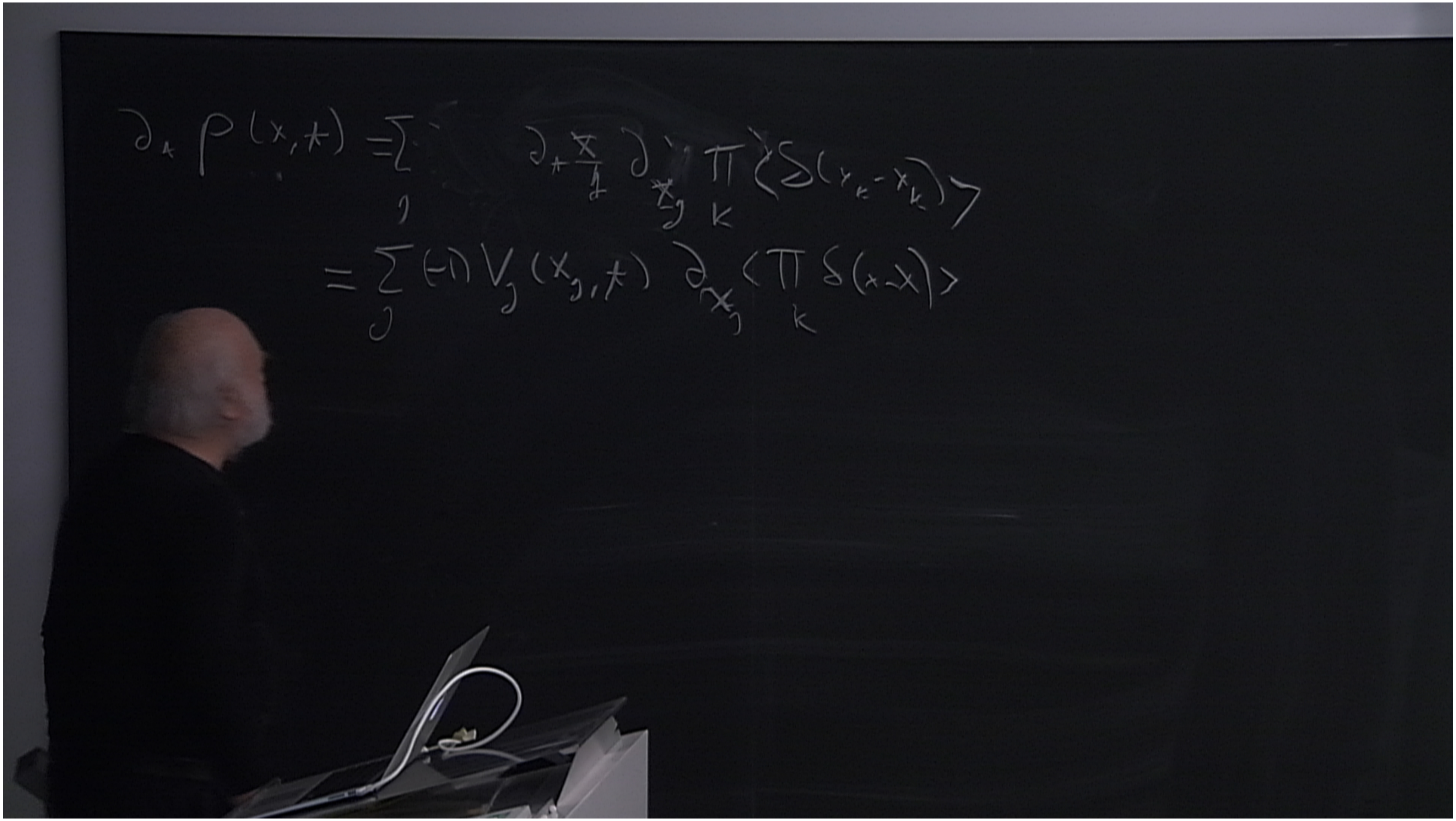
This result is of the form of a local conservation law with the jth. component of the probability current being the velocity, V_j, times the probability, ρ.

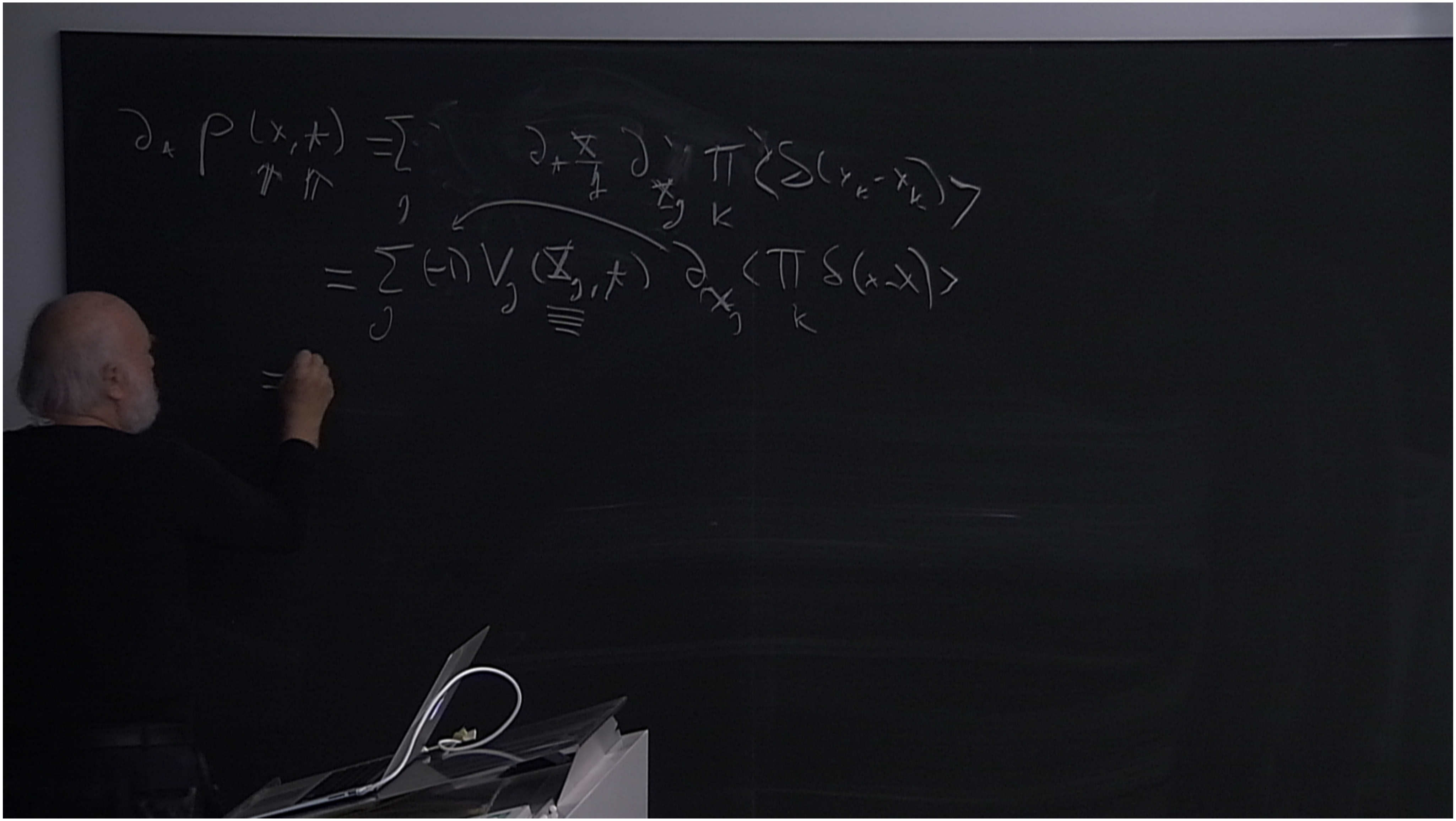
Notice how the spatial gradient appears on the far left in the local conservati[on] law. This placement guarantees that the probability density will have a time-independent integral. Why?

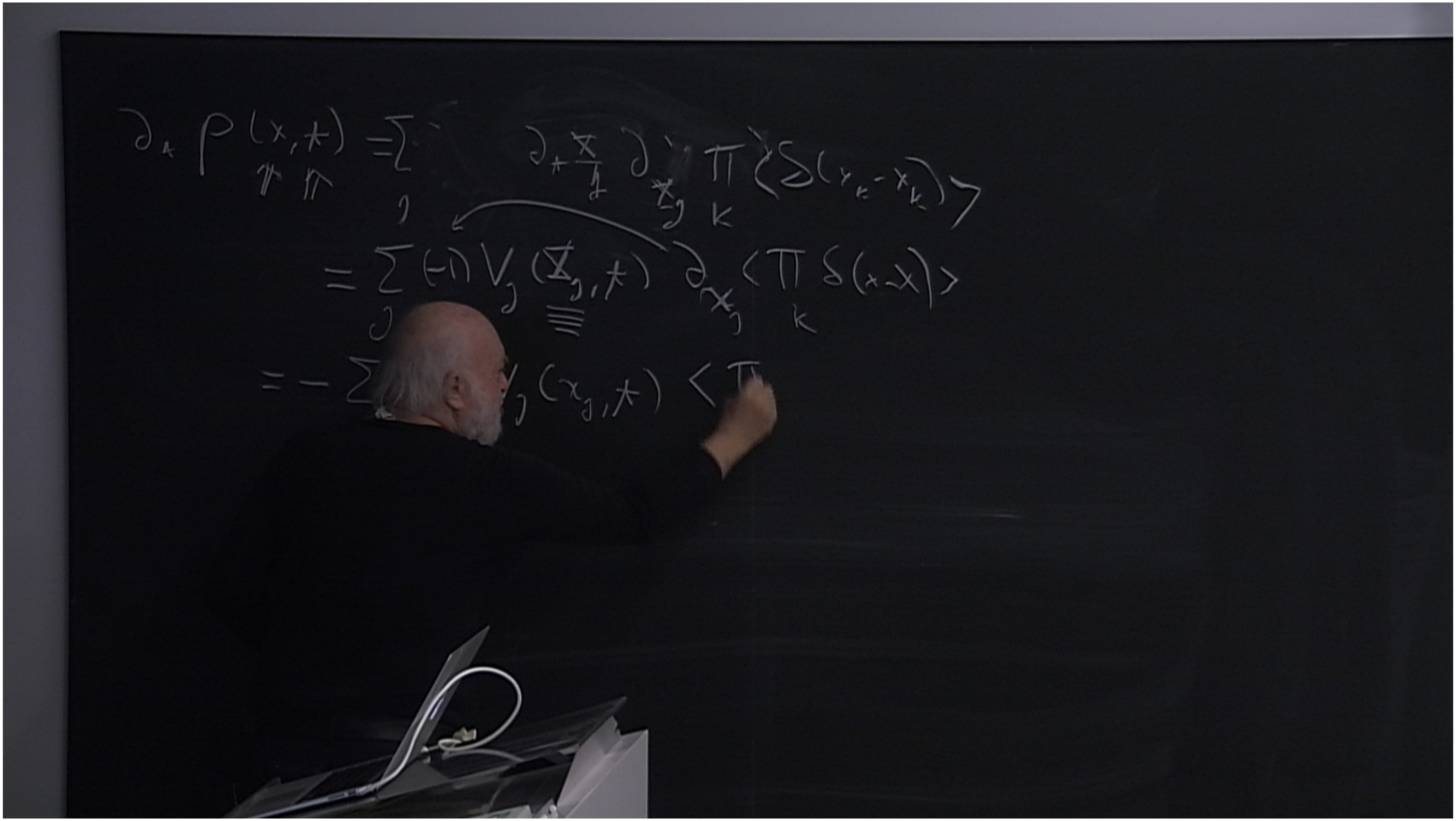

$\partial_t \rho(x,t) = \sum_j \langle \prod_{k=} \delta(x_k - x_k)$

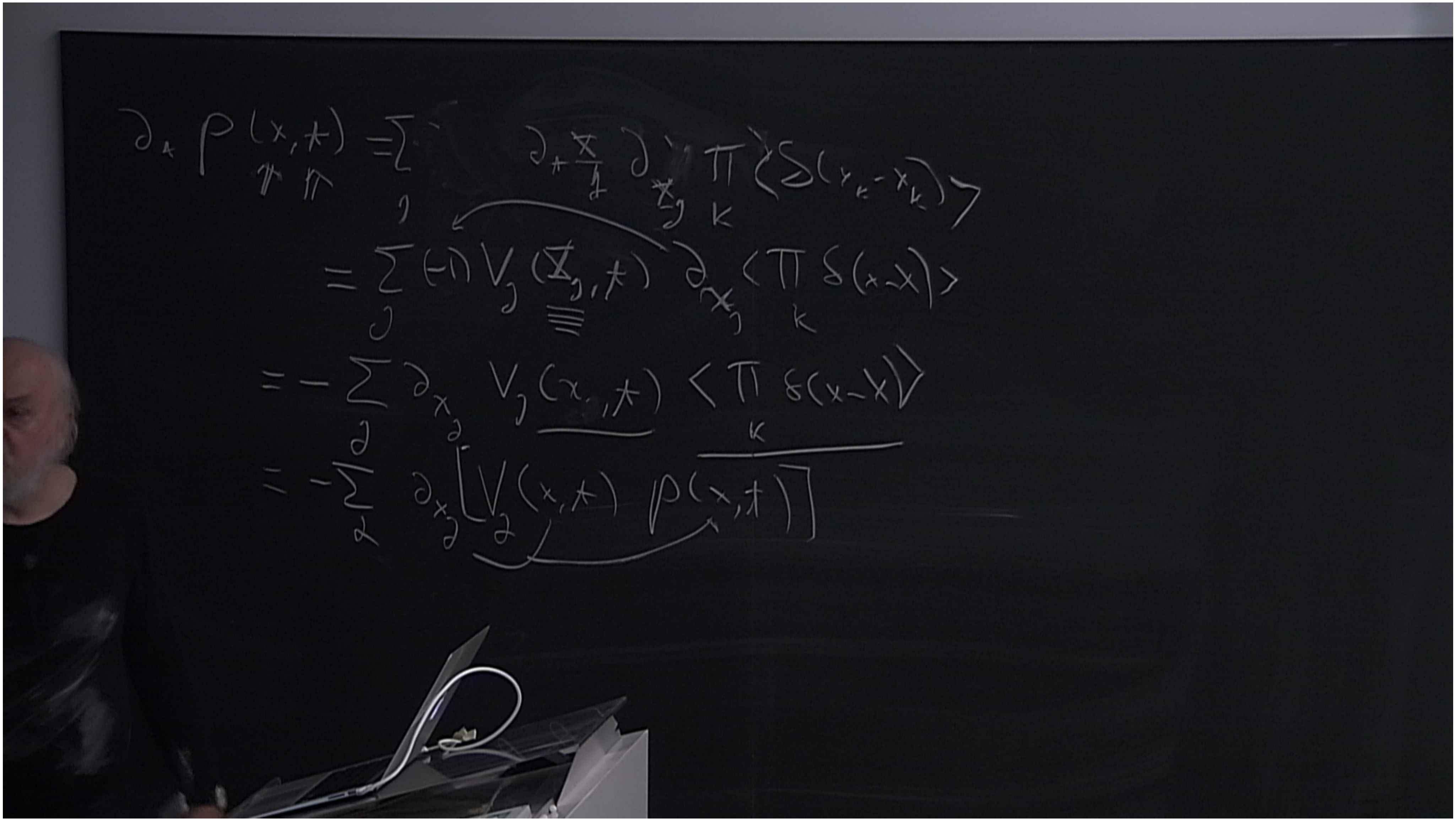



$\partial_t \rho(x,t) = \sum_j \partial_t x_j \, \partial_{x_j} \prod_k \langle \delta(x_k - x_k) \rangle$
$= \sum_j V_j(x_j,t) \, \partial_{x_j}$

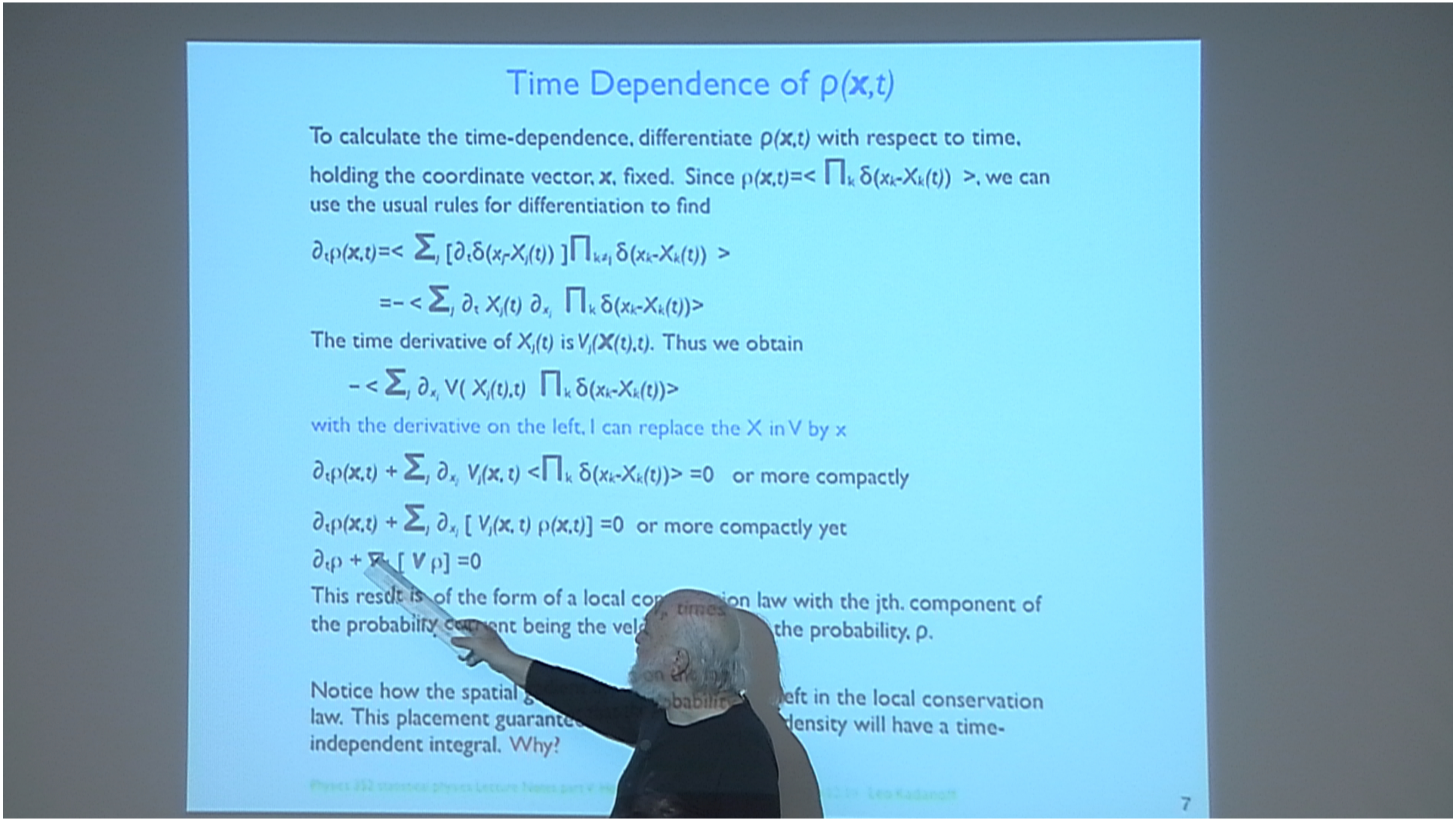

$\partial_t \rho(x,t) = \sum_j \partial_t X_j \, \partial_{X_j} \prod_k \langle \delta(x_k - X_k) \rangle$
$= \sum_j (-1) V_j(X_j, t) \, \partial_{X_j} \langle \prod_k \delta(x - X) \rangle$


∂_t ρ(x, t) = Σ_j ∂_t X_j ∂_{X_j} Π_k ⟨δ(x_k − X_k)⟩
= Σ_j (−1) V_j(X_j, t) ∂_{X_j} ⟨Π_k δ(x − X)⟩
=





$\partial_t \rho(x,t) = \sum_j \partial_t X_j \, \partial_{X_j} \prod_k \langle \delta(x_k - X_k) \rangle$
$= \sum_j (-1) V_j(X_j, t) \, \partial_{X_j} \langle \prod_k \delta(x - X) \rangle$
$= -\sum_j \partial_{x_j} V_j(x, t) \langle \prod_k \delta(x - X) \rangle$
$= -\sum_j \partial_{x_j} [V_j(x,t) \, \rho(x,t)]$


Time Dependence of $\rho(\mathbf{x},t)$
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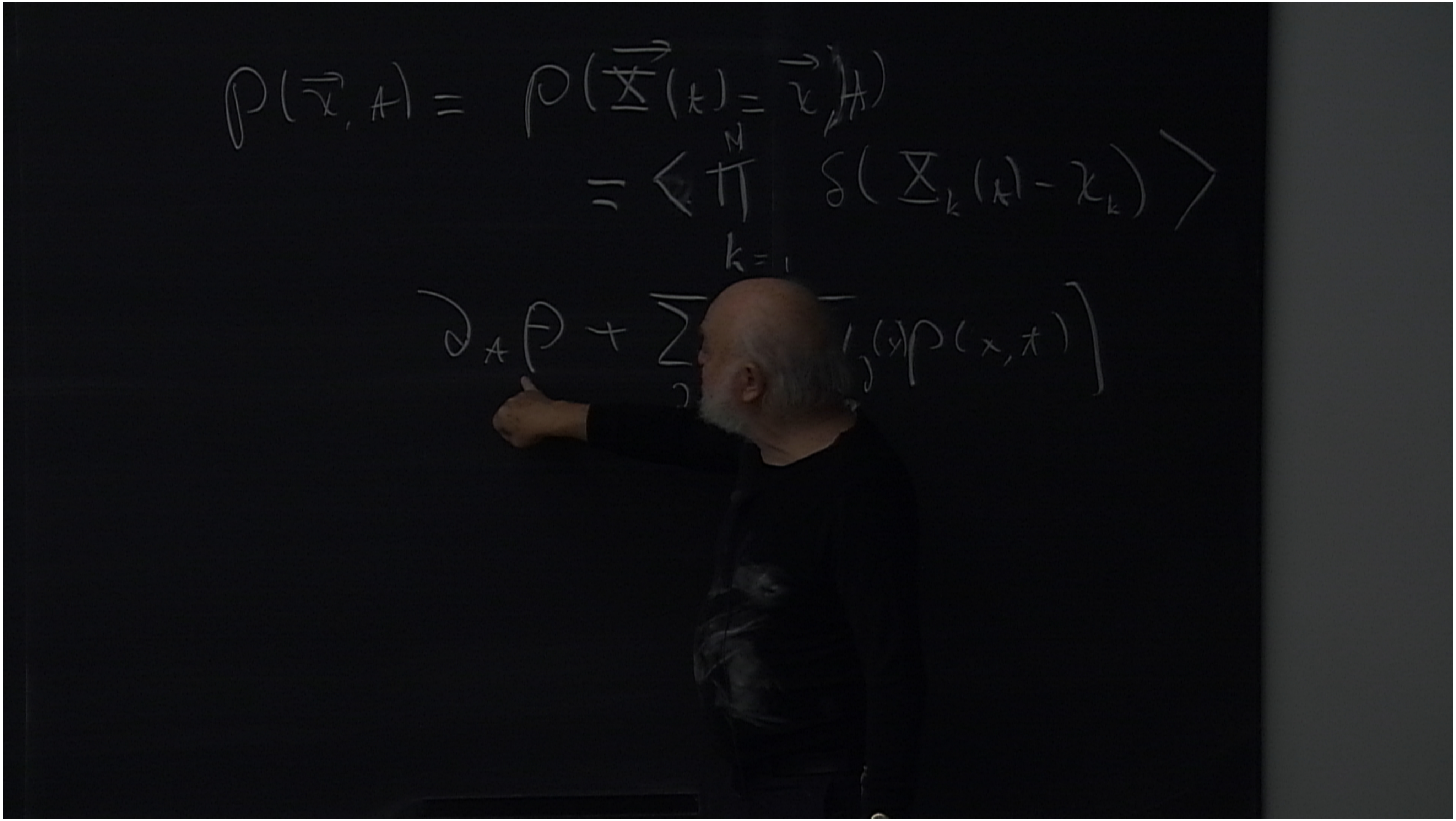
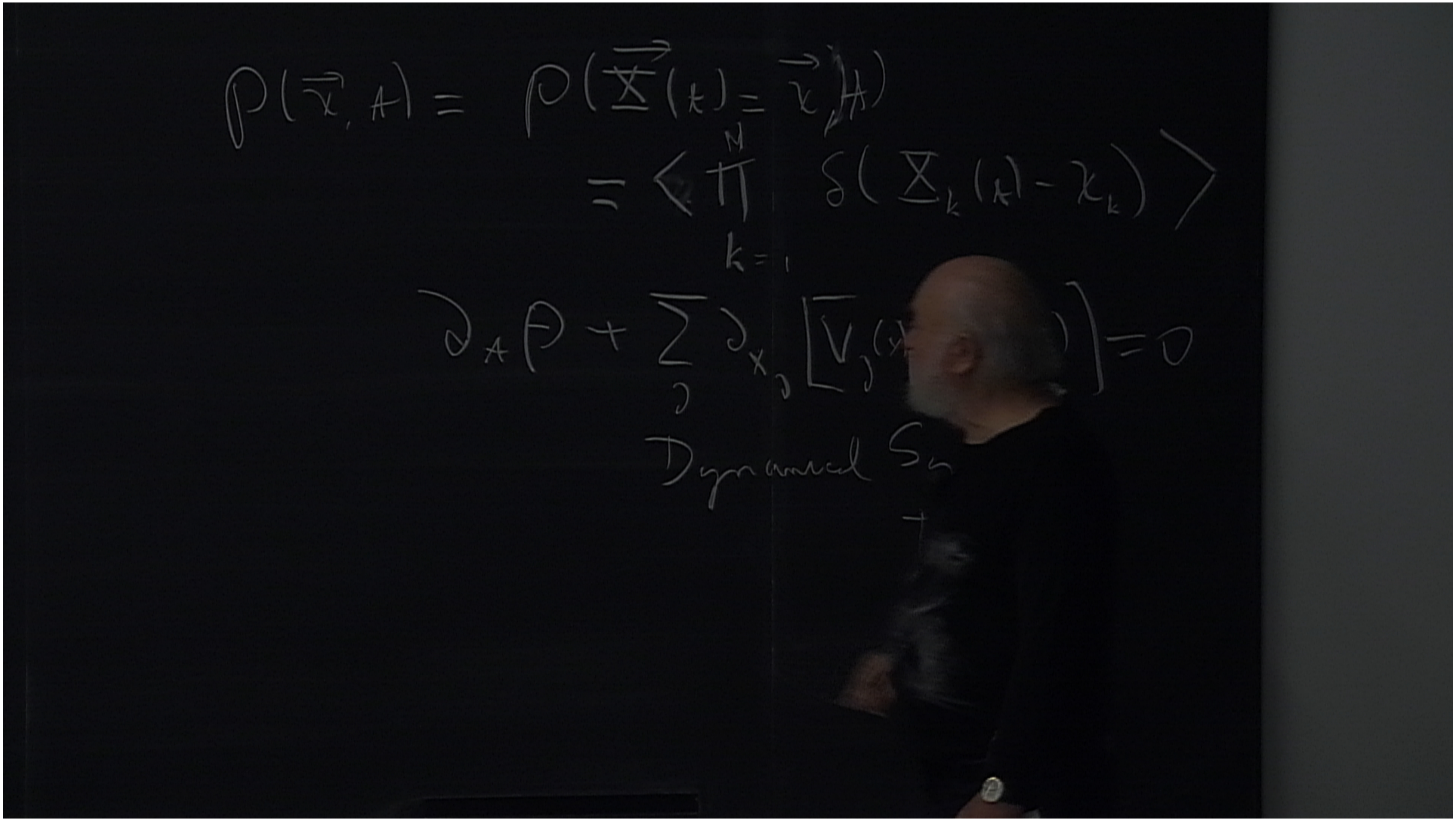
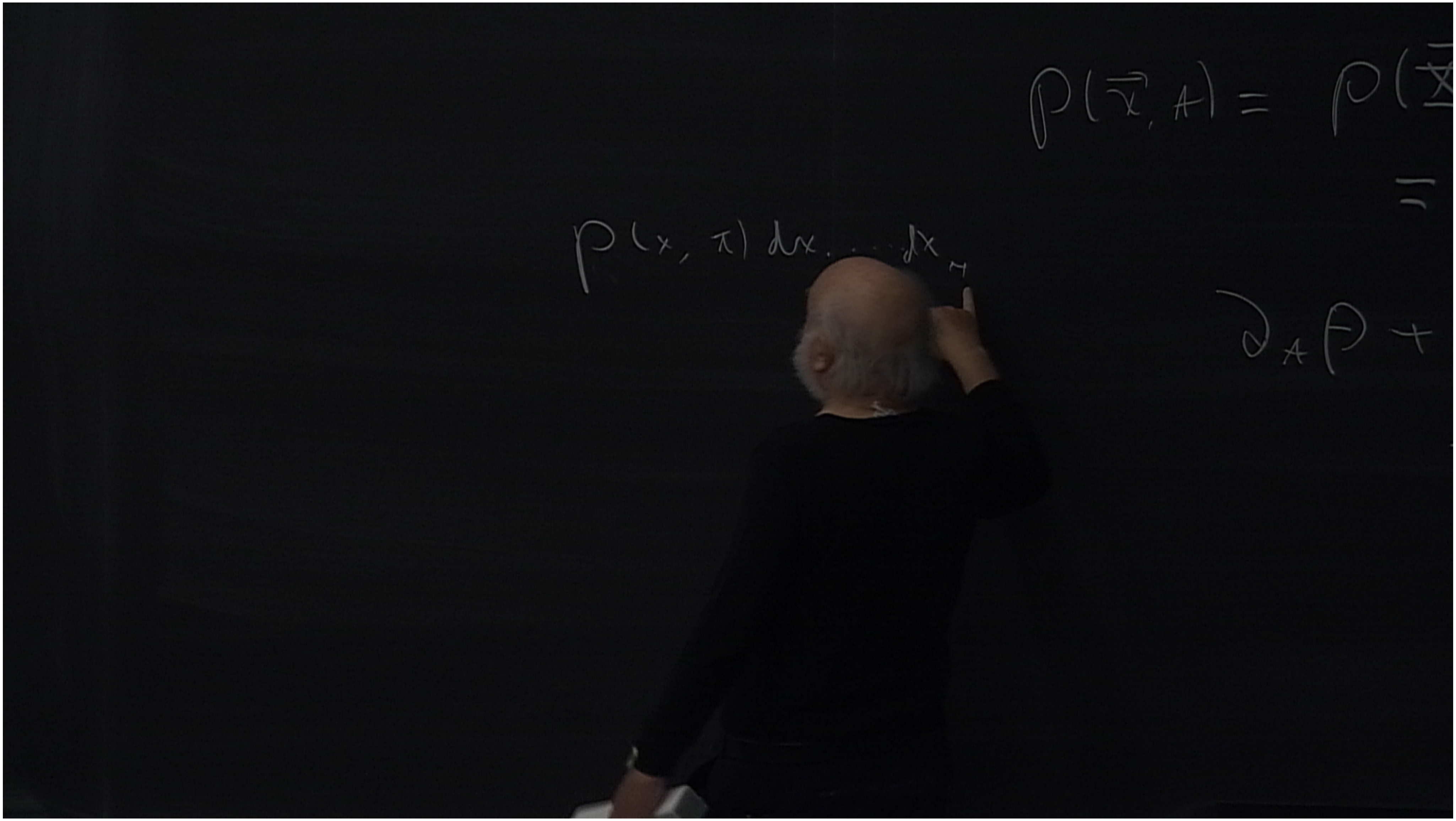
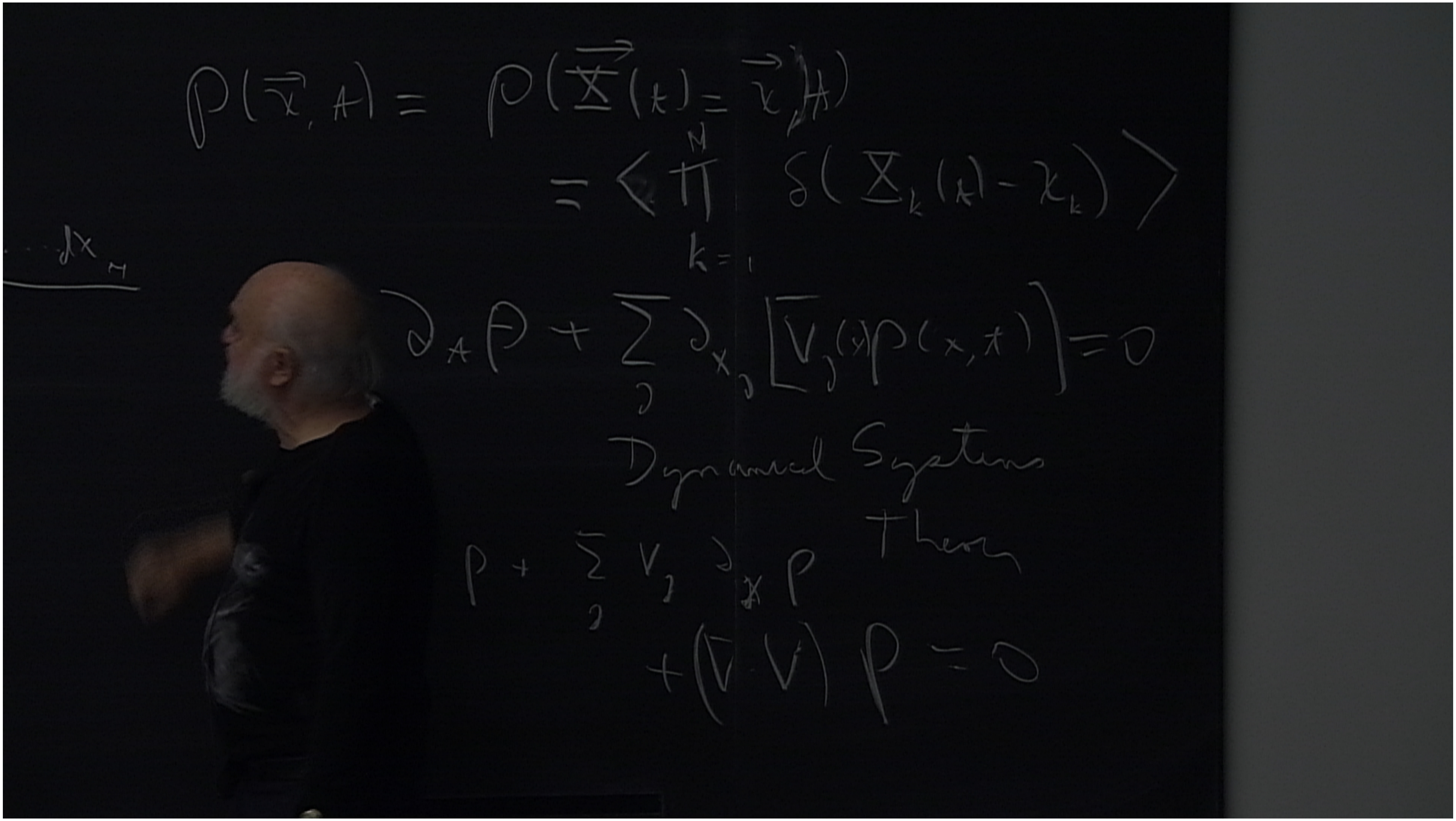
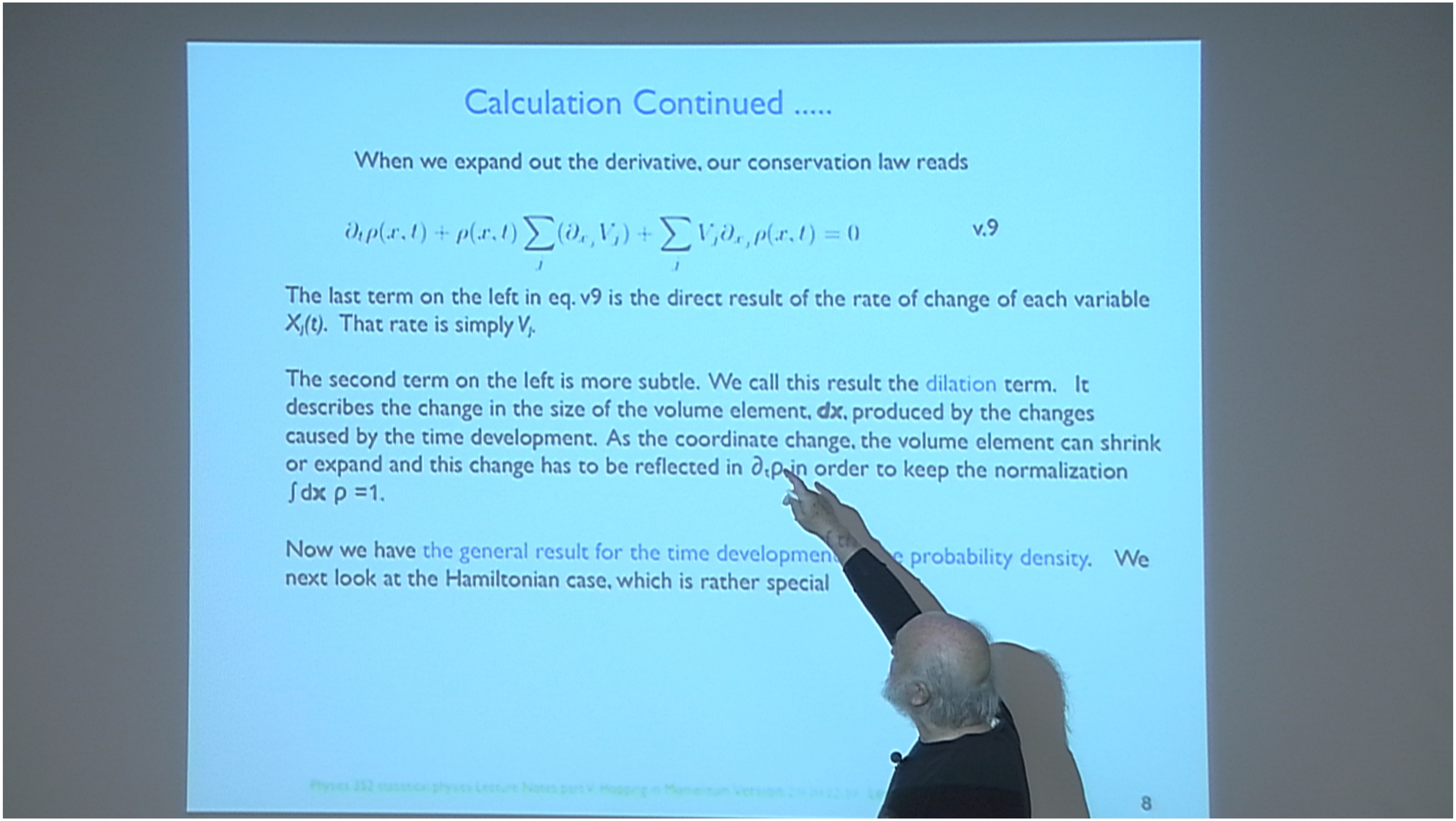
holding the coordinate vector, $\mathbf{x}$, fixed. Since $\rho(\mathbf{x},t)=\langle \prod_k \delta(x_k-X_k(t)) \rangle$, we can
use the usual rules for differentiation to find
$\partial_t\rho(\mathbf{x},t)=\langle \sum_j [\partial_t\delta(x_j-X_j(t))] \prod_{k\neq j} \delta(x_k-X_k(t)) \rangle$
$=-\langle \sum_j \partial_t X_j(t)\, \partial_{x_j} \prod_k \delta(x_k-X_k(t))\rangle$
The time derivative of $X_j(t)$ is $V_j(\mathbf{X}(t),t)$. Thus we obtain
$-\langle \sum_j \partial_{x_j} V(X_j(t),t) \prod_k \delta(x_k-X_k(t))\rangle$
with the derivative on the left, I can replace the X in V by x
$\partial_t\rho(\mathbf{x},t) + \sum_j \partial_{x_j} V_j(\mathbf{x}, t) \langle\prod_k \delta(x_k-X_k(t))\rangle =0$ or more compactly
$\partial_t\rho(\mathbf{x},t) + \sum_j \partial_{x_j} [V_j(\mathbf{x}, t)\, \rho(\mathbf{x},t)] =0$ or more compactly yet
$\partial_t\rho + \nabla \cdot [V \rho] =0$
This result is of the form of a local con ion law with the jth. component of
the probability current being the vel the probability, ρ.
Notice how the spatial eft in the local conservation
law. This placement guarante density will have a time-
independent integral. Why?
7


ρ(x, t) = ρ(X(t) = x, t)
= < ∏ δ(X_k(t) − x_k) >
k=1




ρ(x̄, t) = ρ(x̄
ρ(x, τ) dx ... dx
∂_t ρ +


Dynamical Systems
Theory


Calculation Continued .....
When we expand out the derivative, our conservation law reads
$\partial_t \rho(x,t) + \rho(x,t) \sum_j (\partial_{x_j} V_j) + \sum_j V_j \partial_{x_j} \rho(x,t) = 0$
v.9
The last term on the left in eq. v9 is the direct result of the rate of change of each variable $X_j(t)$. That rate is simply V_j.
The second term on the left is more subtle. We call this result the dilation term. It describes the change in the size of the volume element, **dx**, produced by the changes caused by the time development. As the coordinate change, the volume element can shrink or expand and this change has to be reflected in $\partial_t \rho$ in order to keep the normalization $\int d\mathbf{x}\, \rho = 1$.
Now we have the general result for the time developmen
probability density. We next look at the Hamiltonian case, which is rather special
8

Calculation concluded .....

$$\partial_t \rho(x,t) + \rho(x,t)\sum_j (\partial_{x_j} V_j) + \sum_j V_j \partial_{x_j}\rho(x,t) = 0$$

The Hamiltonian case is special. There are two kinds of coordinates $x_j = q_\alpha$ with $V_j = \partial_{p_\alpha} H$ and $x_j = p_\alpha$ with $V_j = -\partial_{q_\alpha} H$. In that case, the dilation term is

$(\partial_{q_\alpha} \partial_{p_\alpha} H - \partial_{p_\alpha} \partial_{q_\alpha} H)\rho$ which, of course, vanishes

This result, called Liouville's theorem, says that the size of the volume element is independent of time. As a result the the probability density obeys a special equation, with no dilation.

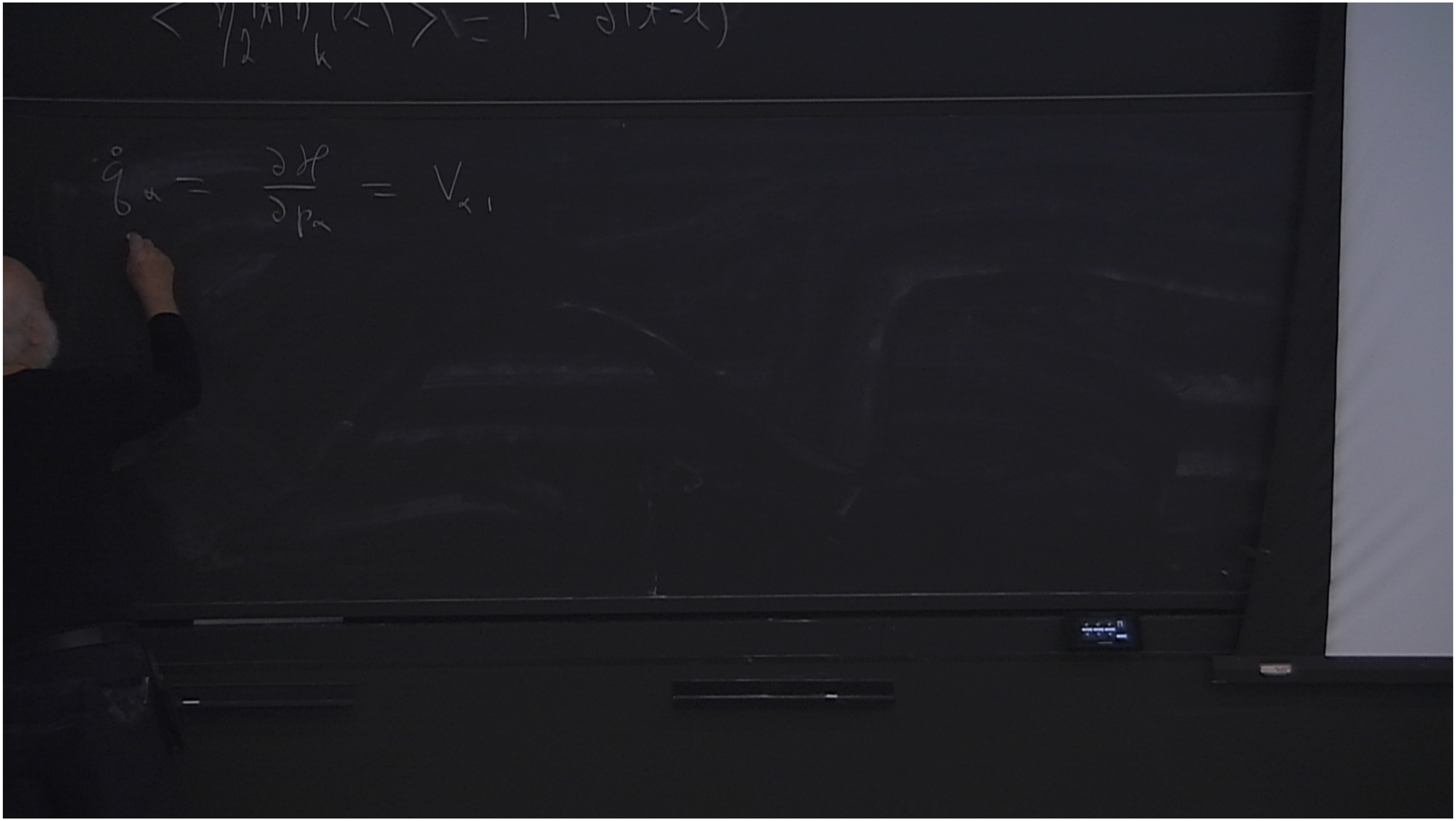
$$\partial_t \rho(p,q,t) + \sum_\alpha [(\partial_{p_\alpha} H)\partial_{q_\alpha} - (\partial_{q_\alpha} H)\partial_{p_\alpha}]\rho(p,q,t) = 0 \qquad \text{v.10}$$

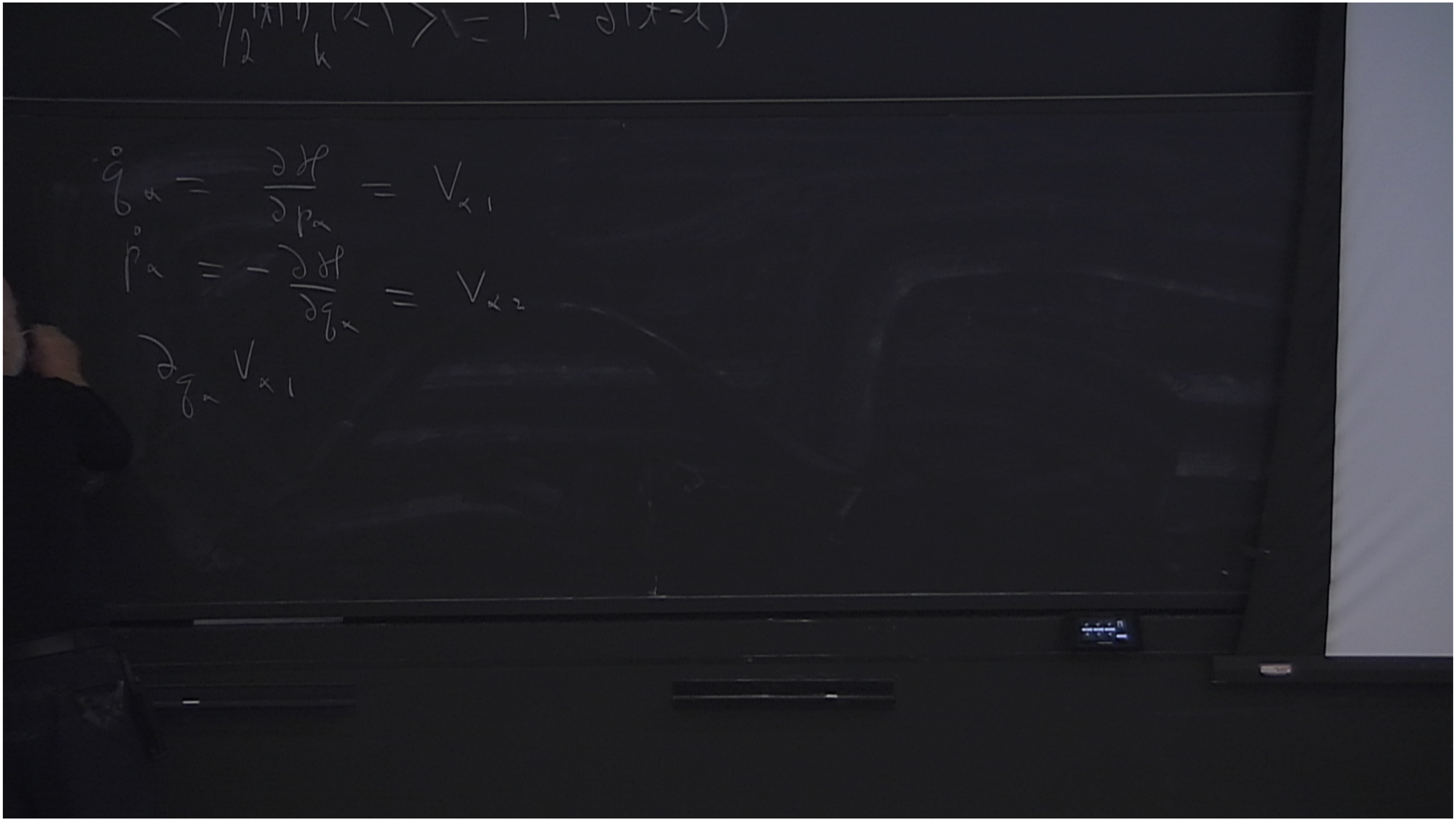
Compare this to the result for a function of *P* and *Q*

$$\frac{dX(P,Q)}{dt} = \sum_\alpha \; [(\partial_{P_\alpha} H)(\partial_{Q_\alpha} X) - (\partial_{Q_\alpha} H)(\partial_{P_\alpha} X)]$$

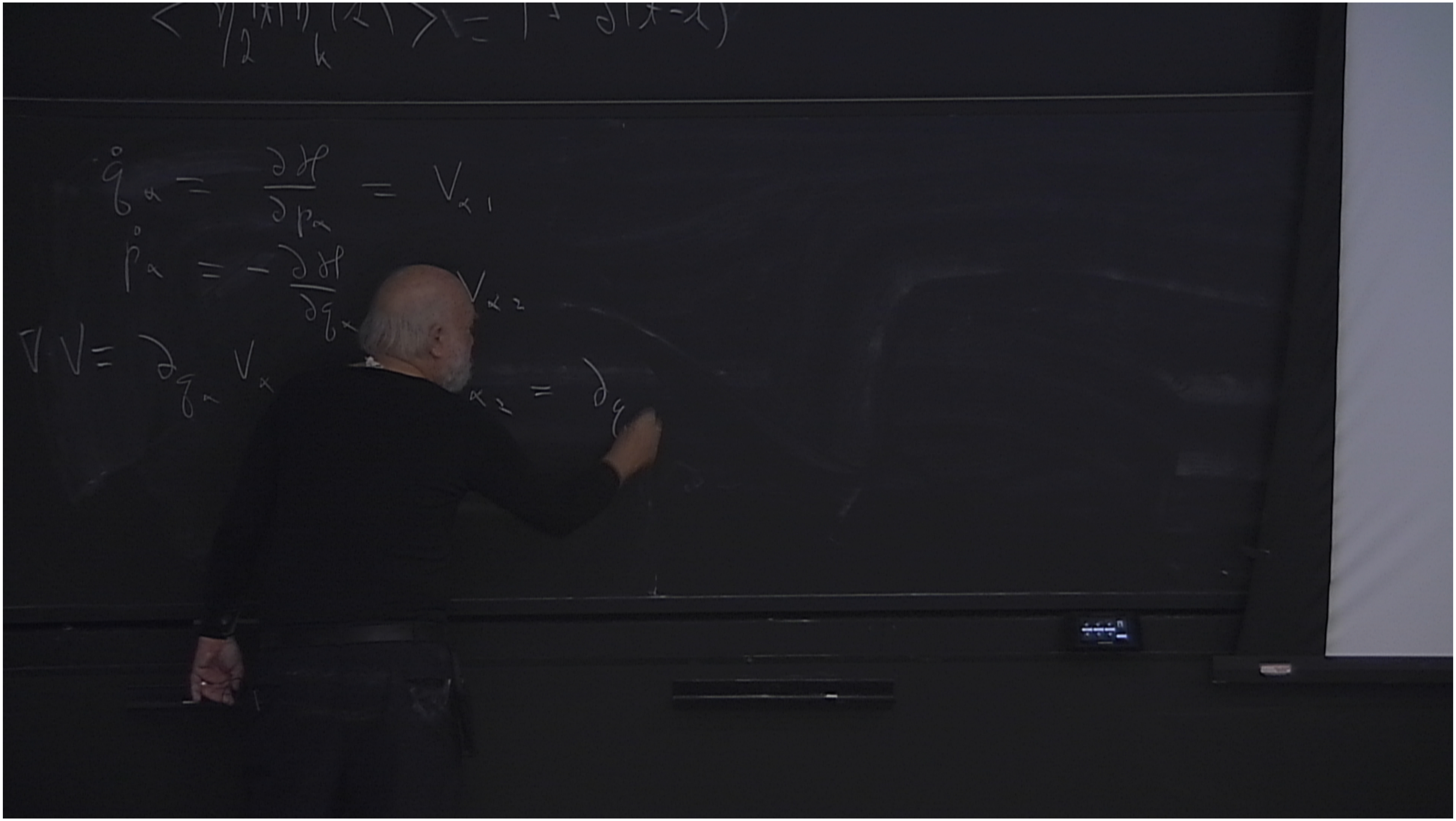
d?

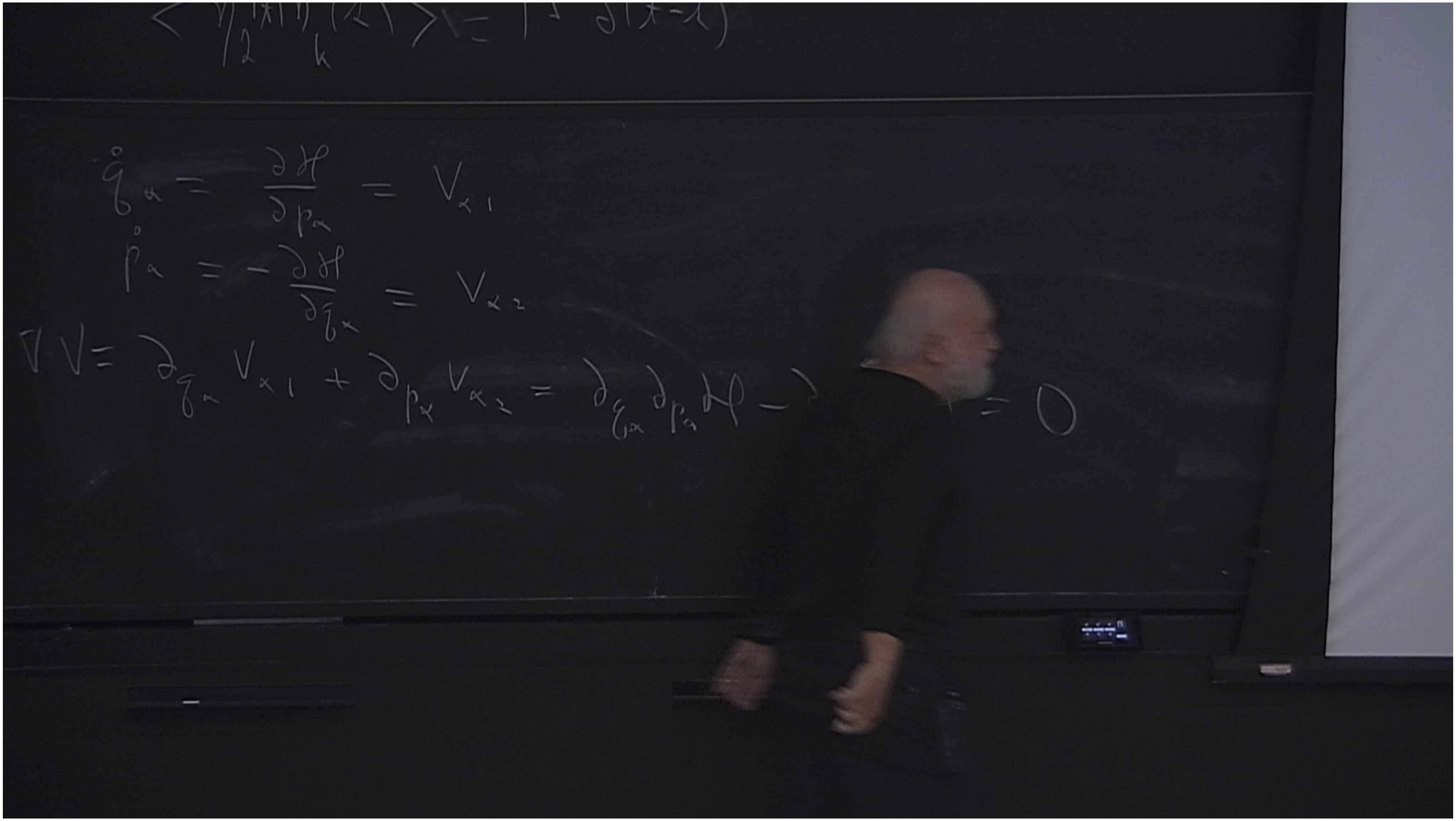
why is there a difference in notation (p,q) versus (P,Q)--
why is there a difference in sign?


q̇_α = ∂H/∂p_α = V_α ,

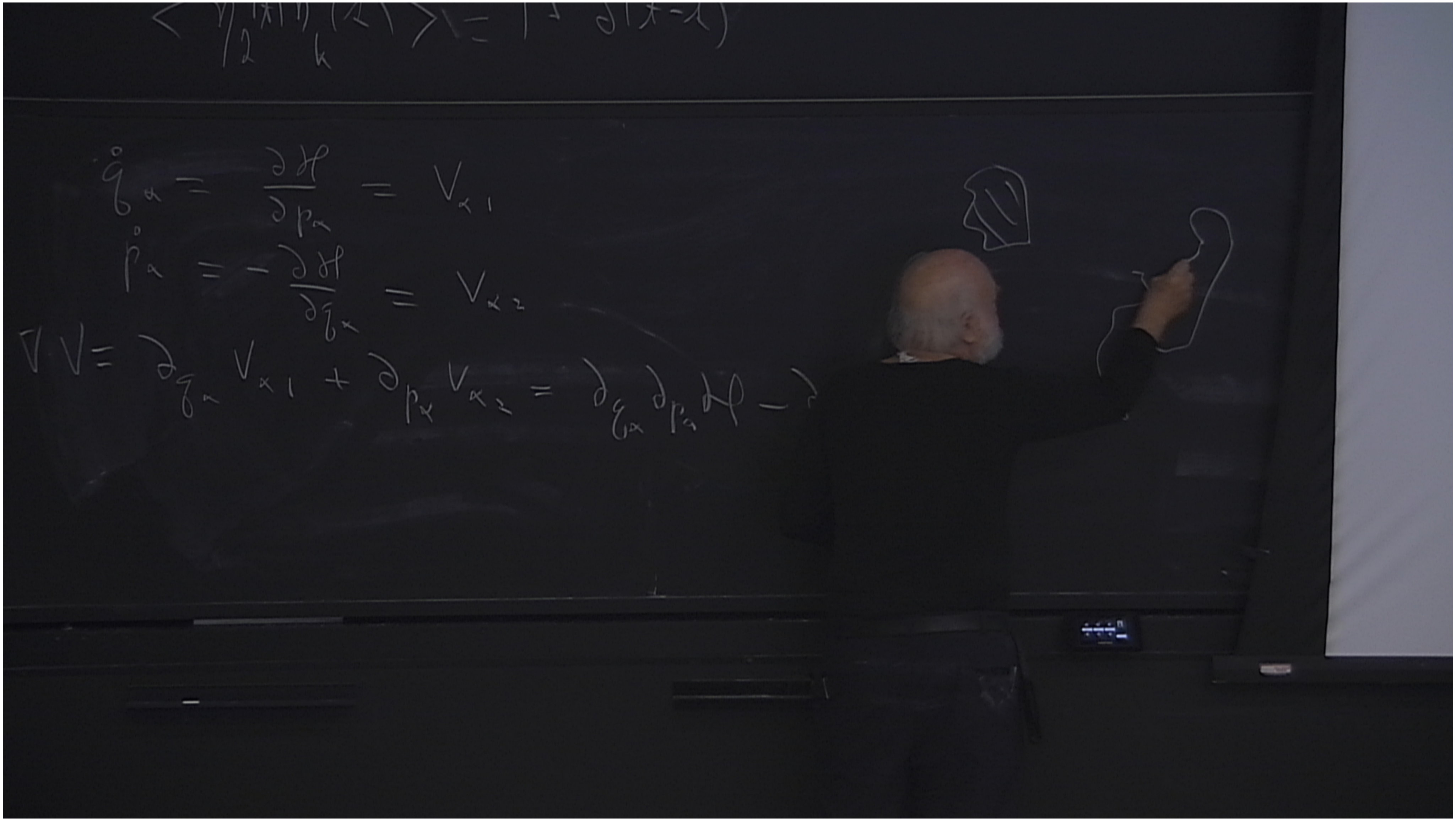


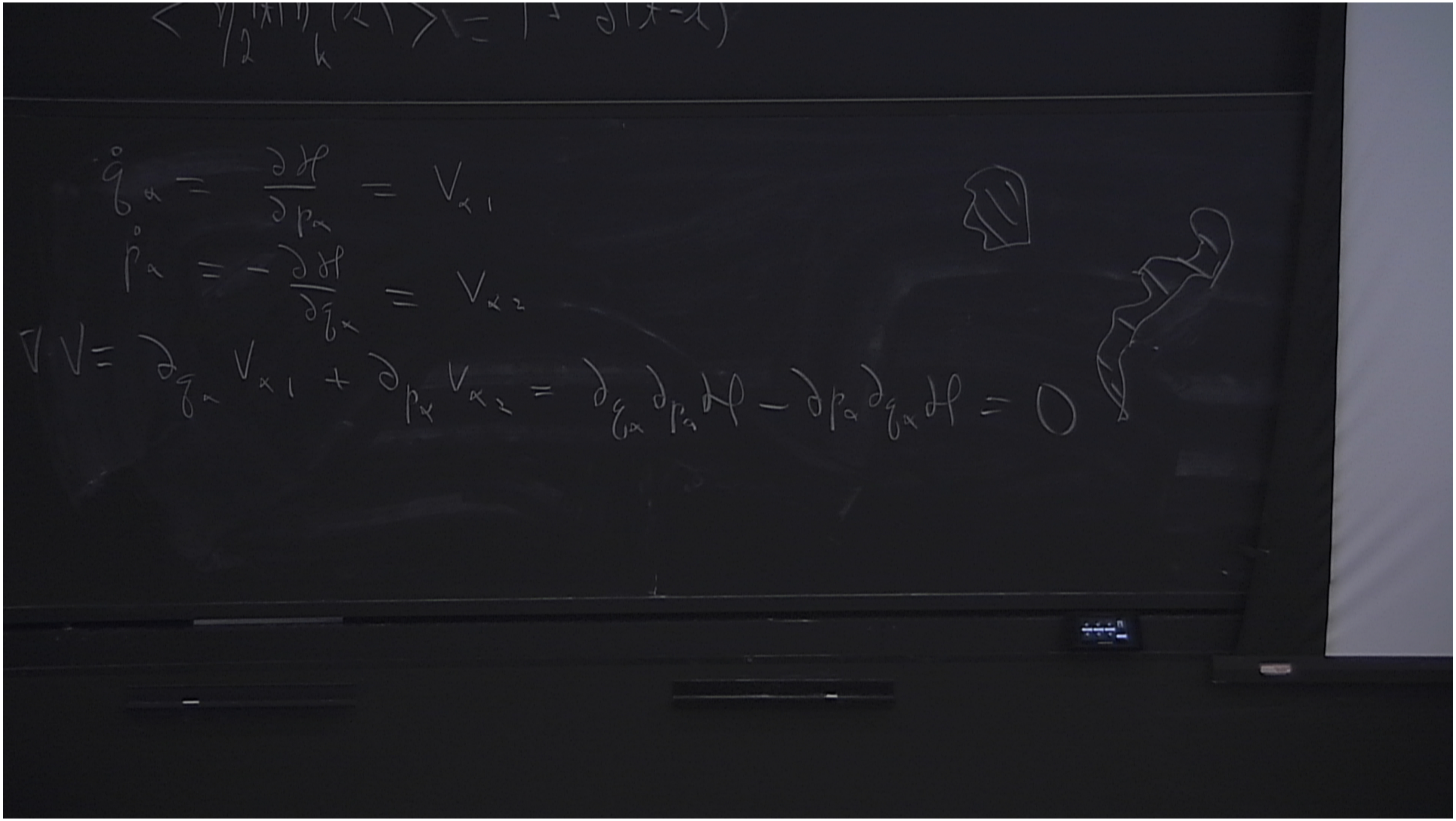
$\dot{q}_\alpha = \frac{\partial H}{\partial p_\alpha} = V_{\alpha 1}$
$\dot{p}_\alpha = -\frac{\partial H}{\partial q_\alpha} = V_{\alpha 2}$
$\partial_{q_\alpha} V_{\alpha 1}$

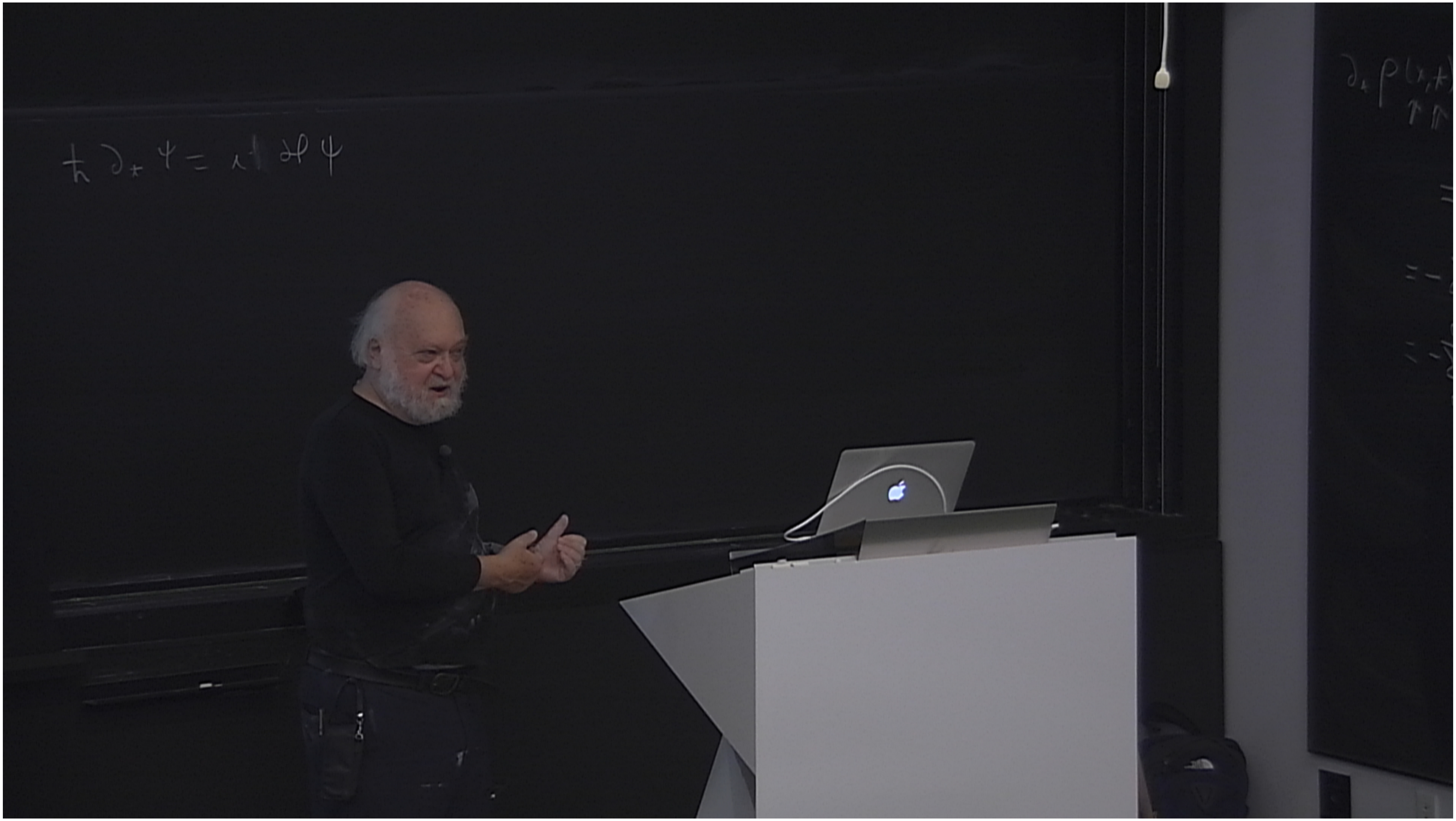


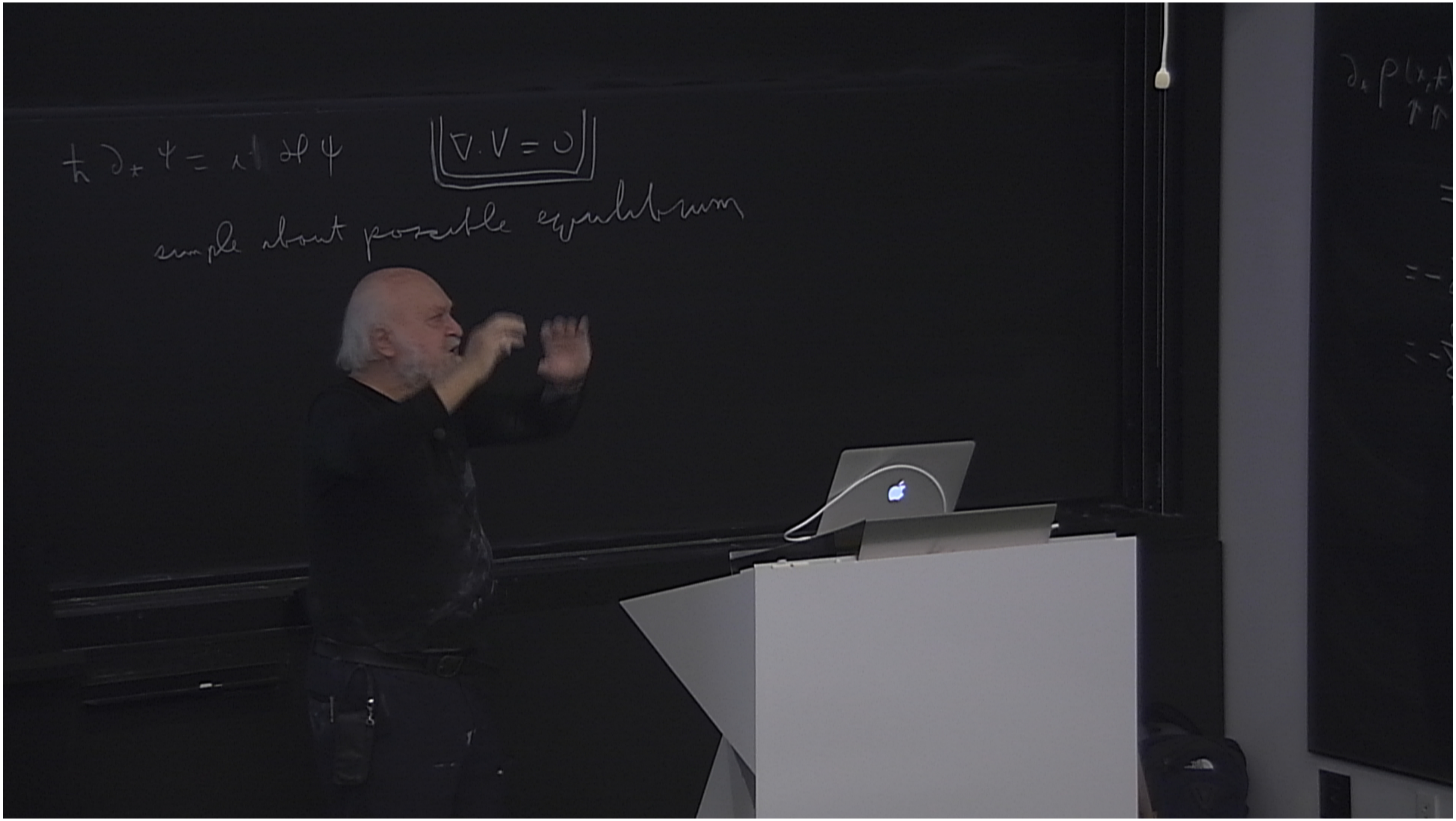


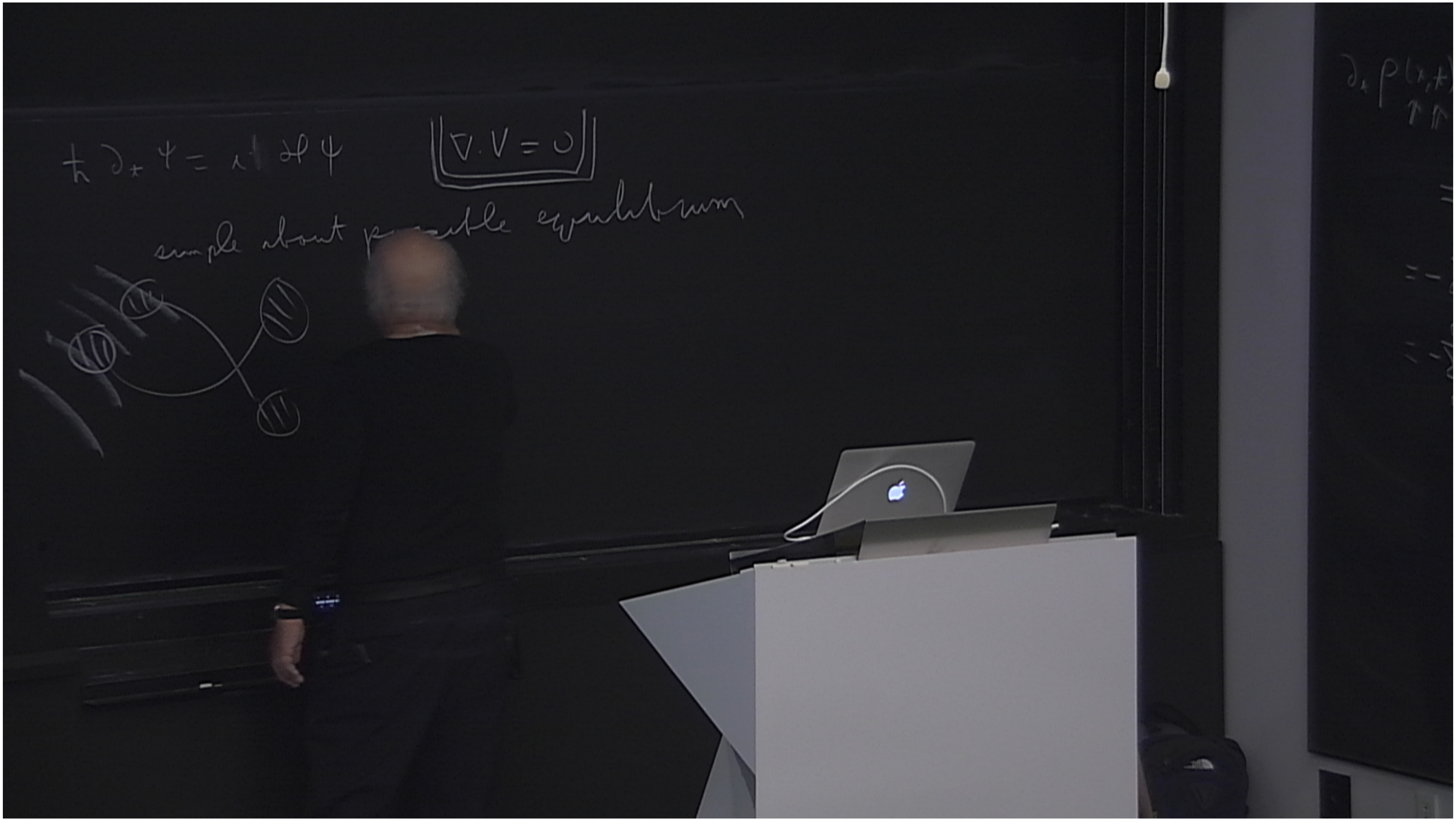
$\dot{q}_\alpha = \frac{\partial H}{\partial p_\alpha} = V_{\alpha 1}$
$\dot{p}_\alpha = -\frac{\partial H}{\partial q_\alpha} = V_{\alpha 2}$
$\nabla \cdot V = \partial_{q_\alpha} V_{\alpha 1} + \partial_{p_\alpha} V_{\alpha 2} = \partial_{q_\alpha} \partial_{p_\alpha} H -$
$= 0$

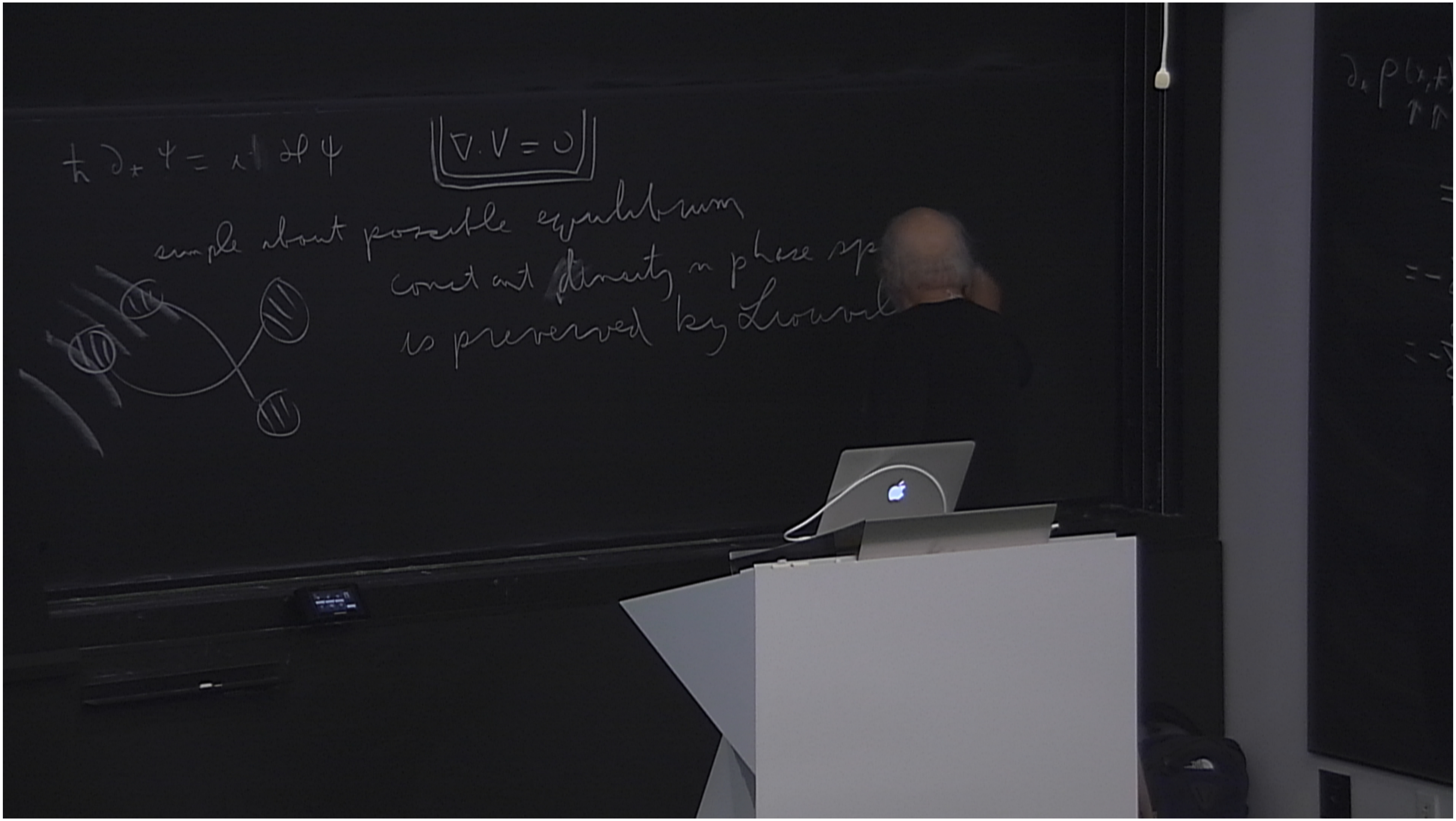

q̇α = ∂H/∂pα = Vα1
ṗα = −∂H/∂qα = Vα2
∇·V = ∂qα Vα1 + ∂pα Vα2 = ∂qα ∂pα H − ∂

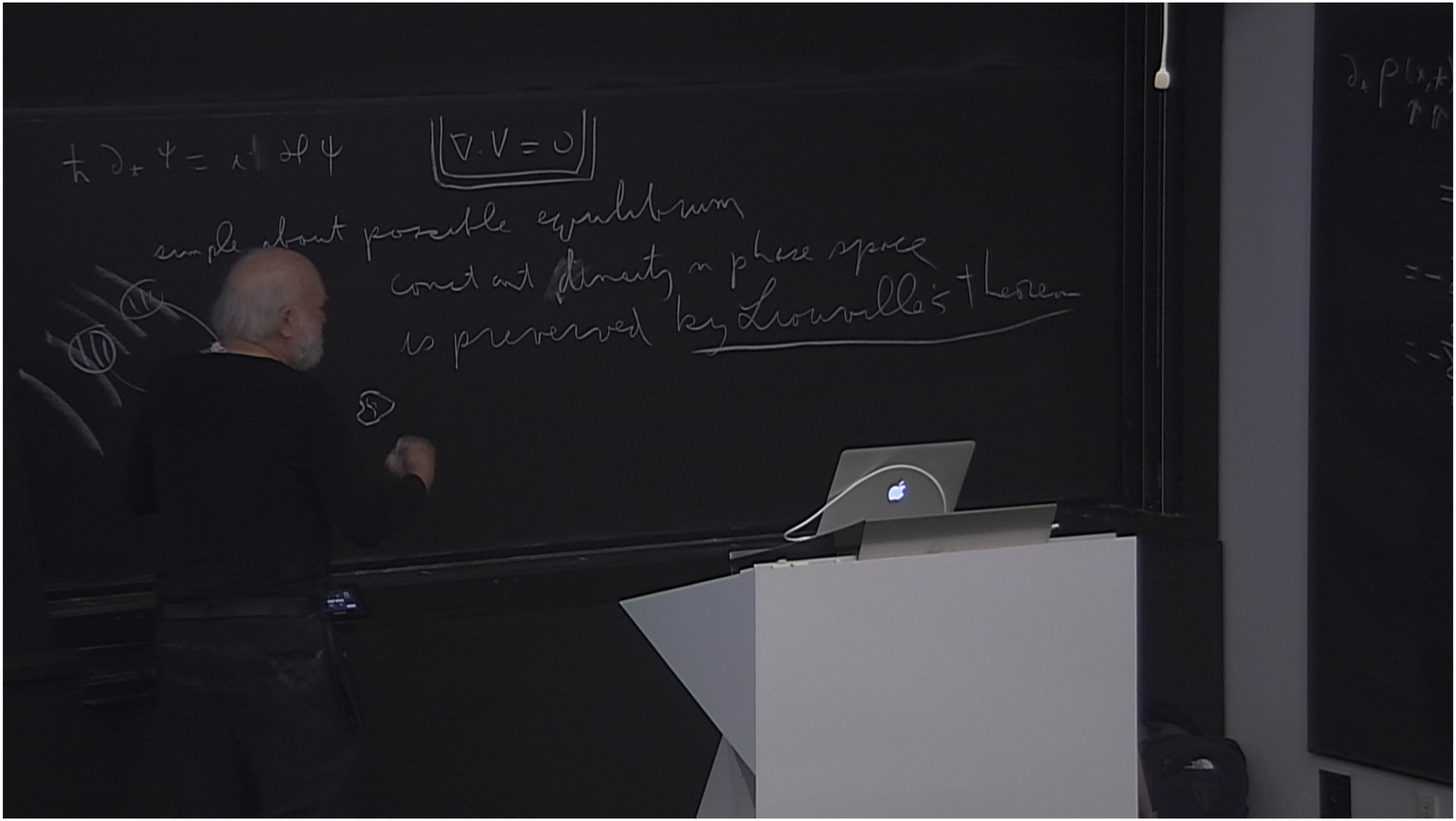

$\dot{q}_\alpha = \frac{\partial H}{\partial p_\alpha} = V_{\alpha 1}$
$\dot{p}_\alpha = -\frac{\partial H}{\partial q_\alpha} = V_{\alpha 2}$
$\nabla \cdot V = \partial_{q_\alpha} V_{\alpha 1} + \partial_{p_\alpha} V_{\alpha 2} = \partial_{q_\alpha}\partial_{p_\alpha} H - \partial_{p_\alpha}\partial_{q_\alpha} H = 0$

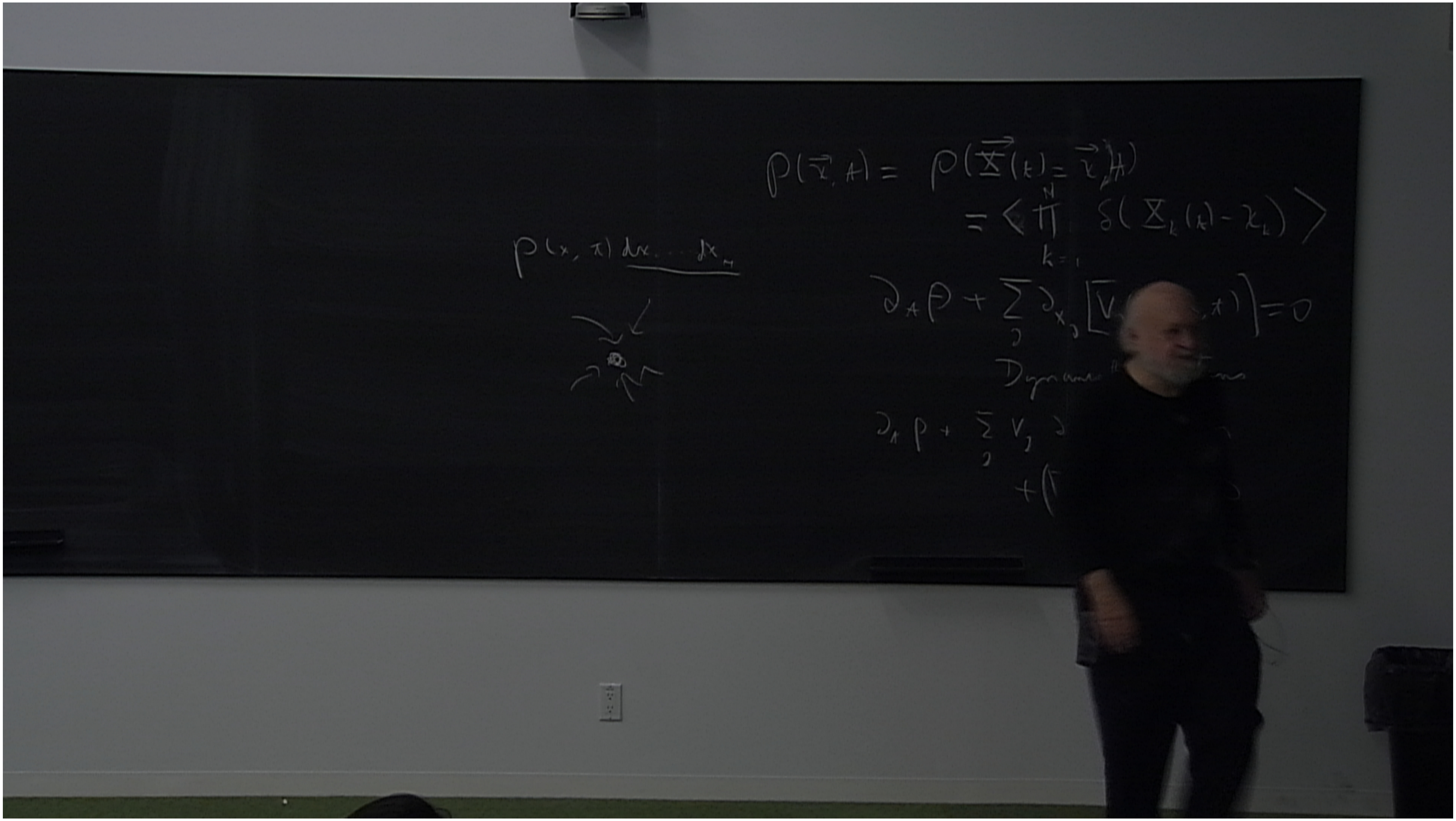

ħ ∂ₜ ψ = i ℋ ψ


∇ · V = 0


∇ · V = 0


∇·V = 0
constant density in phase
is preserved by


∇·V = 0
constant density in phase space
is preserved by Liouville's theorem



Poisson Bracket

The Poisson Bracket is Defined by

$$\{f,g\} = \sum_{\alpha} \left[\frac{\partial f}{\partial q_\alpha} \frac{\partial g}{\partial p_\alpha} - \frac{\partial g}{\partial q_\alpha} \frac{\partial f}{\partial p_\alpha} \right]$$

It then follows immediately that the probability density obeys $\partial_t \rho = \{H, \rho\}$

Also, for any, $X(\mathbf{p},\mathbf{q})$, that is a function of p's and q's, with no explicit time-dependence, the time-dependence of X is given by

$$dX/dt = \{X,H\}$$

These Poisson brackets are rather like the commutators of quantum mechanics. For example they satisfy the identities

$\{f,g\} = -\{g,f\}$

Leibnitz rule $\{fg,h\} = f\{g,h\} + \{f,h\}g$

and also Bianchi identity $\{\{f,g\},h\} + \{\{h,f\},g\} + \{\{g,h\},f\} = 0$.

The same relations are true for operators in quantum theory with { and } replaced by [and]. Why are these relations important?

The bracket relations for classical time-dependence are very much like the time-dependence of operators and density matrices in quantum theory, and also of Lie derivatives. This relation between quantum mechanics and the canonical version of classical mechanics is quite surprising and turns out to be quite deep.

$$(fg)' = f'g + g'f$$

$$\rho(\vec{x}, t) = \rho(\vec{X}(t) = \vec{x}, t)$$

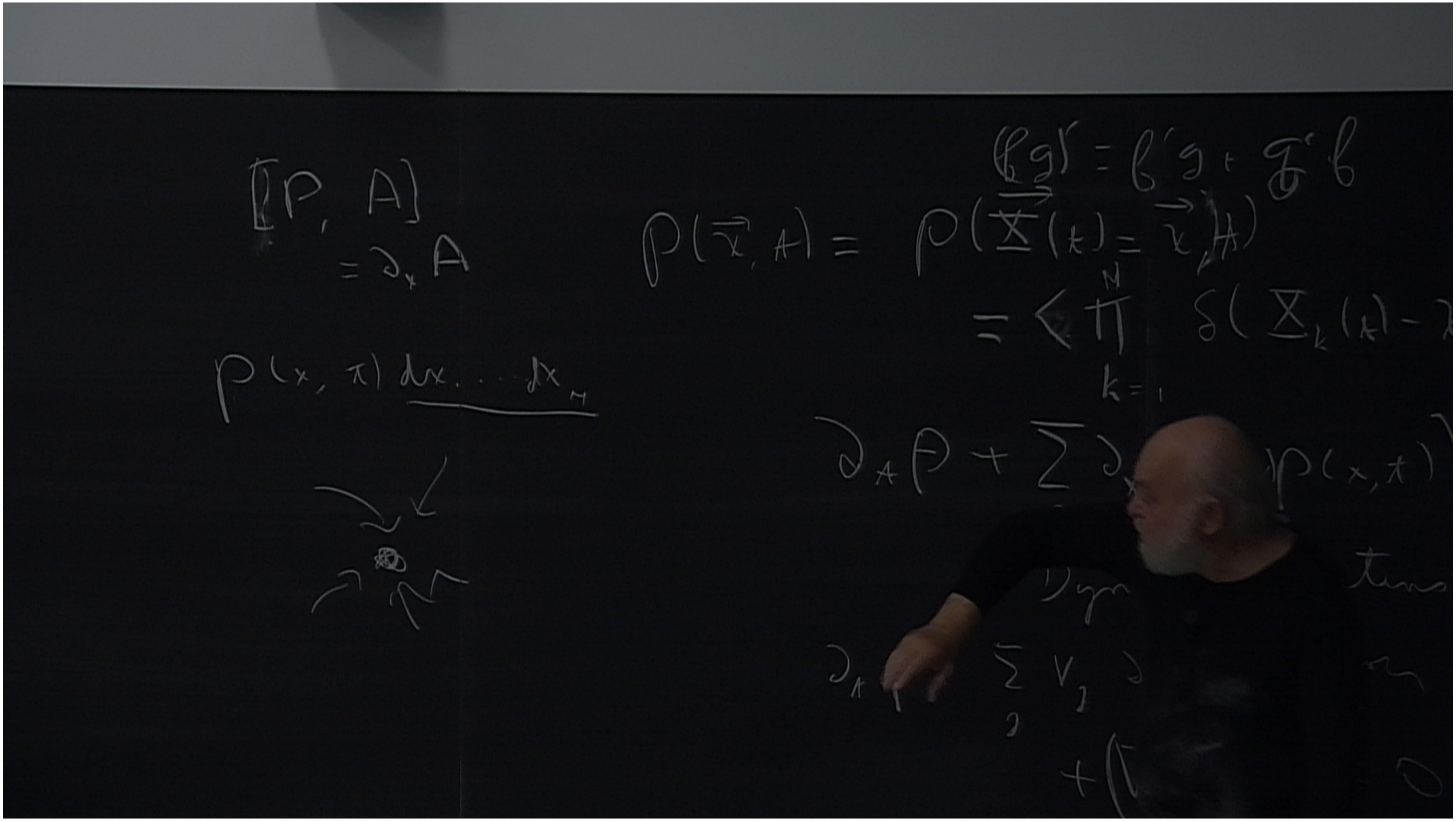
$$= \left\langle \prod_{k=1}^{M} \delta(X_k(t) - x_k) \right\rangle$$

$$\ldots dx_M$$

$$\partial_t \rho + \sum_j \partial_{x_j} \left[V_j(x) \rho(x, t) \right] = 0$$

Dynamical Systems Theory

$$\partial_t \rho + \sum_j V_j \partial_{x_j} \rho + (\nabla \cdot V) \rho = 0$$



Why are brackets important

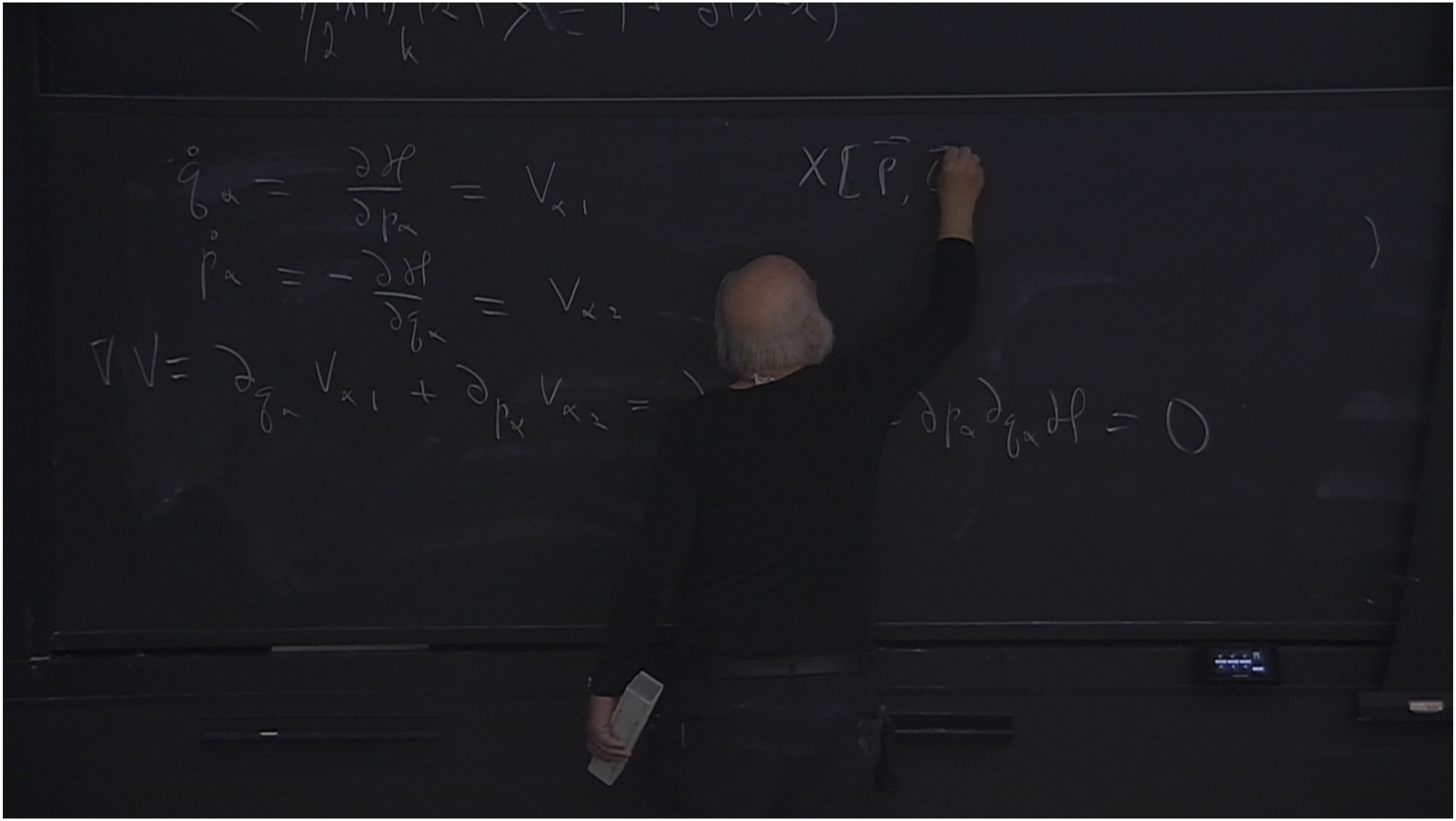
Brackets can be used to describe symmetries. For example the total momentum, P, acts as the translation operator within the brackets
$\{P, X(P,Q)\} = \Sigma_i \, (d/dx_i) \, X(P,Q)$
Similarly the center of mass coordinate is a displacement operator for the momentumn. Similarly the angular momentum operators serve to rotate the coordinates and the momenta. Similarly the Hamiltonian serves as a time translation operator
We have

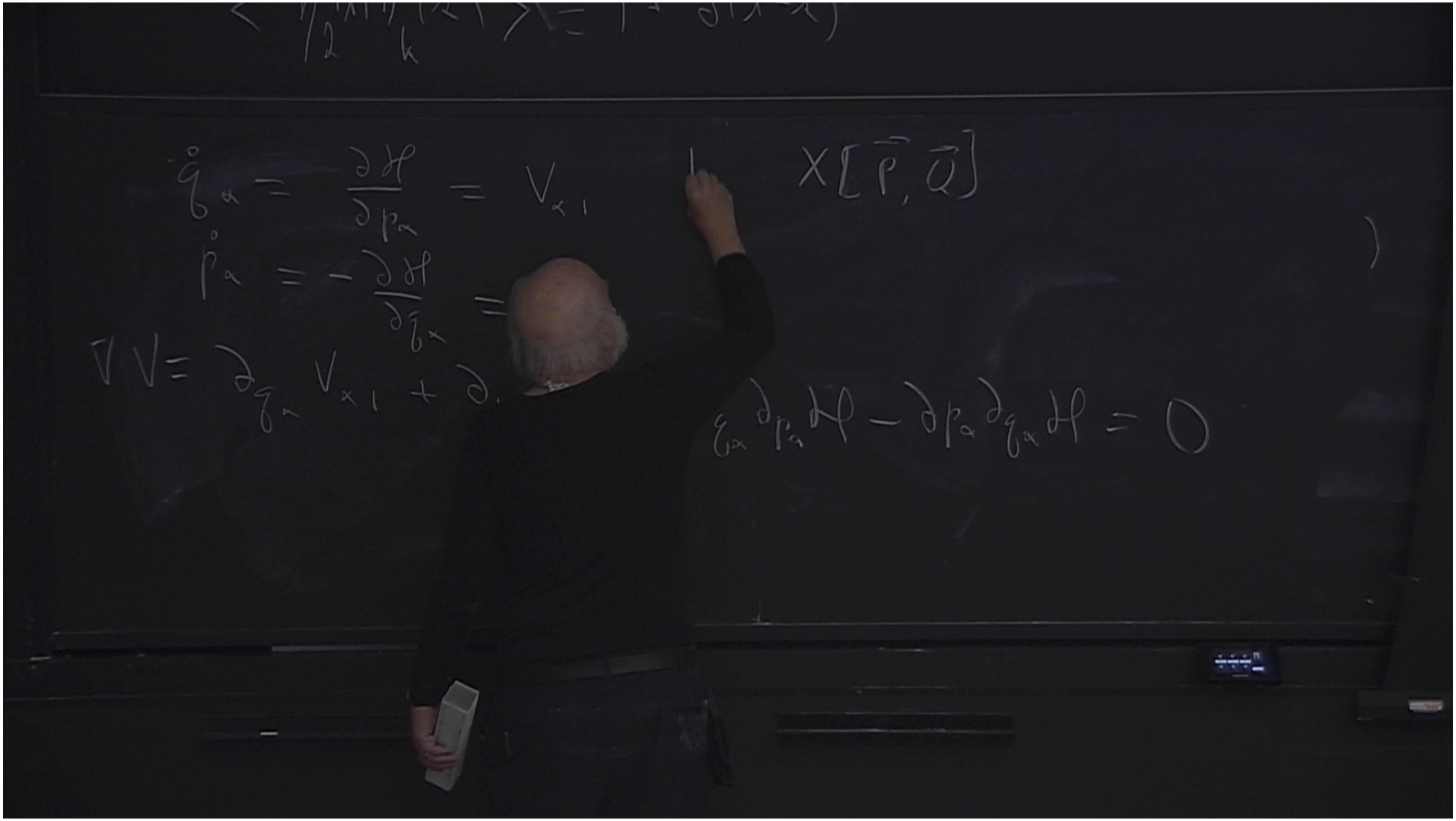
$\{P,L\} = -\{L, P\}$ Operations of symmetries upon one another is as in quantum theory. e.g. $\{P_2,L_3\}=\partial_y \, (p_x \, y - p_y \, x) \sim p_x$

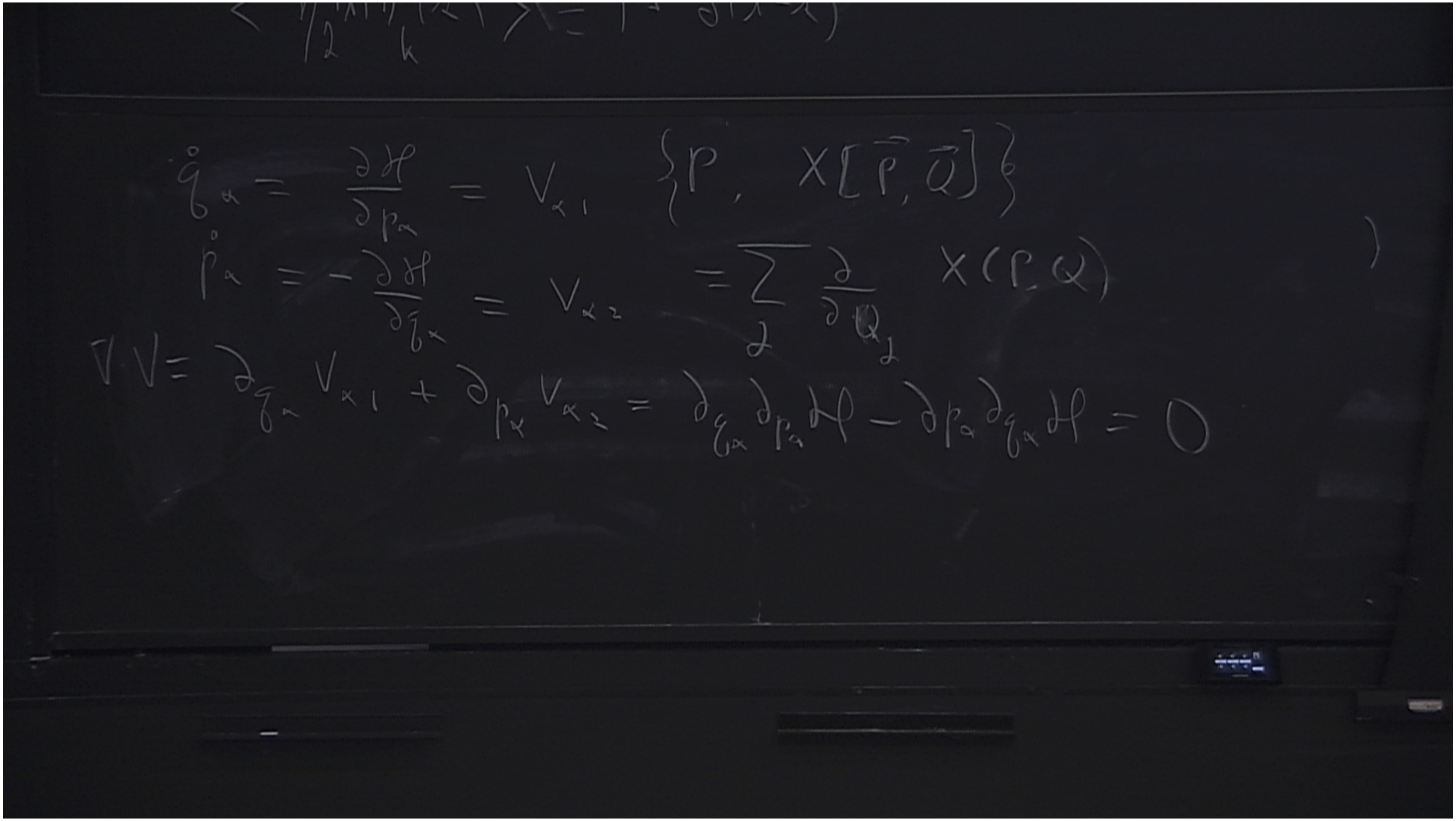
Leibnitz rule $\{H,XY\}=\{H,X\}Y + X\,\{H,Y\}$ XY is a product. H is a symmetry operation. H acts like a derivative operator. We can talk about symmetry operations applied to products

and also Bianchi identity $\{\{X,Y\},H\}+\{\{H,X\},Y\}+\{\{Y,H\},X\}=0.$
H also acts like a derivative when applied to a bracket therefore we can talk about symmetry operations applied to brackets. e.g other symmtry operations.

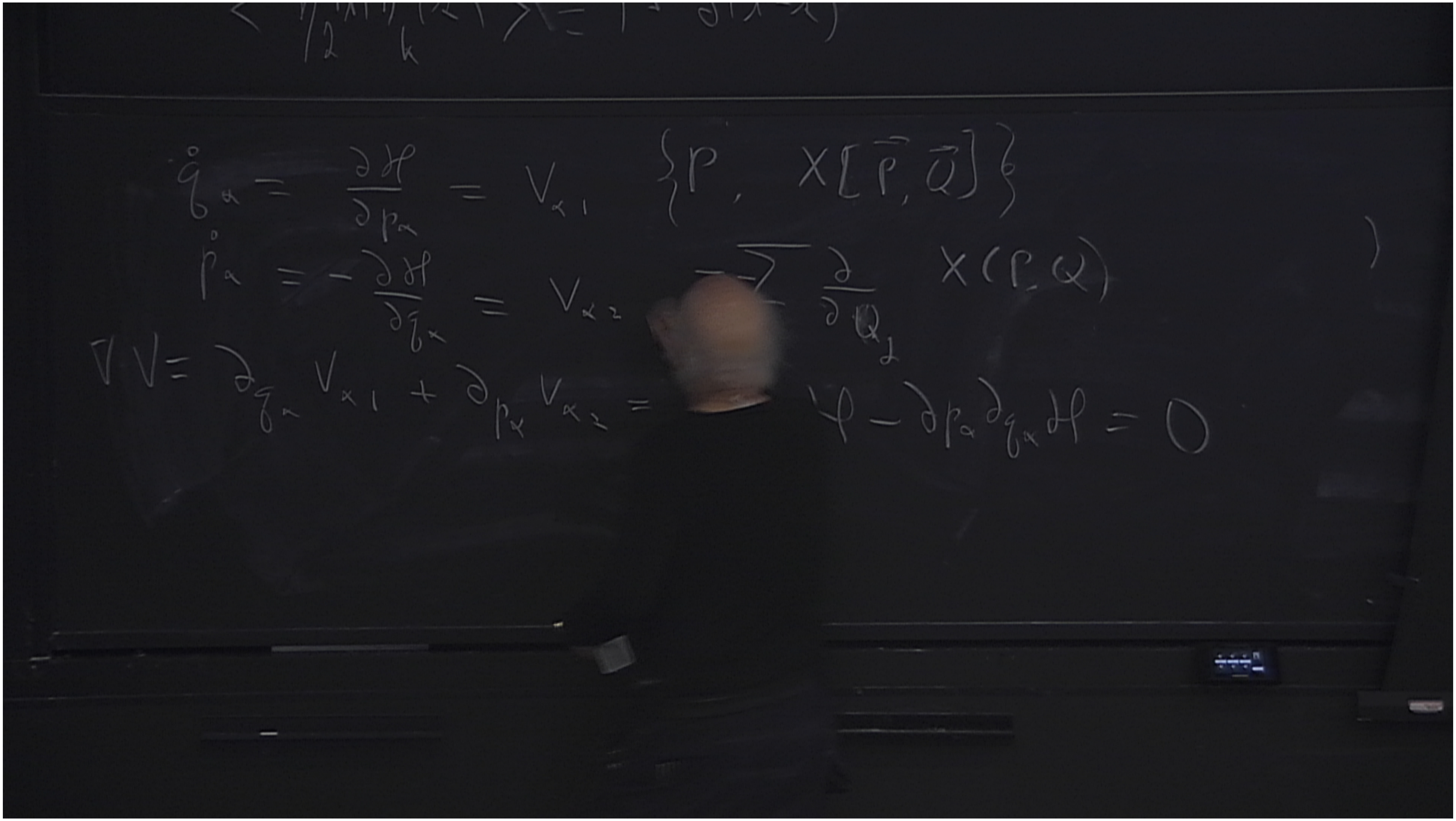
These identities mean we have a complete algebra of symmetries.


$\dot{q}_\alpha = \frac{\partial H}{\partial p_\alpha} = V_{\alpha 1}$
$\dot{p}_\alpha = -\frac{\partial H}{\partial q_\alpha} = V_{\alpha 2}$


q̇α = ∂H/∂pα = Vα1
ṗα = − ∂H/∂qα =
∇V = ∂qα Vα1 + ∂
X[P, Q]
qα ∂pα H − ∂pα ∂qα H = 0



$\dot{q}_\alpha = \frac{\partial H}{\partial p_\alpha} = V_{\alpha 1}$
$\{P, \; X[\vec{P}, \vec{Q}]\}$
$\dot{p}_\alpha = -\frac{\partial H}{\partial q_\alpha} = V_{\alpha 2}$
$= \sum_{d} \frac{\partial}{\partial Q_d} X(P, Q)$
$\nabla V = \partial_{q_\alpha} V_{\alpha 1} + \partial_{p_\alpha} V_{\alpha 2} = \partial_{q_\alpha} \partial_{p_\alpha} H - \partial_{p_\alpha} \partial_{q_\alpha} H = 0$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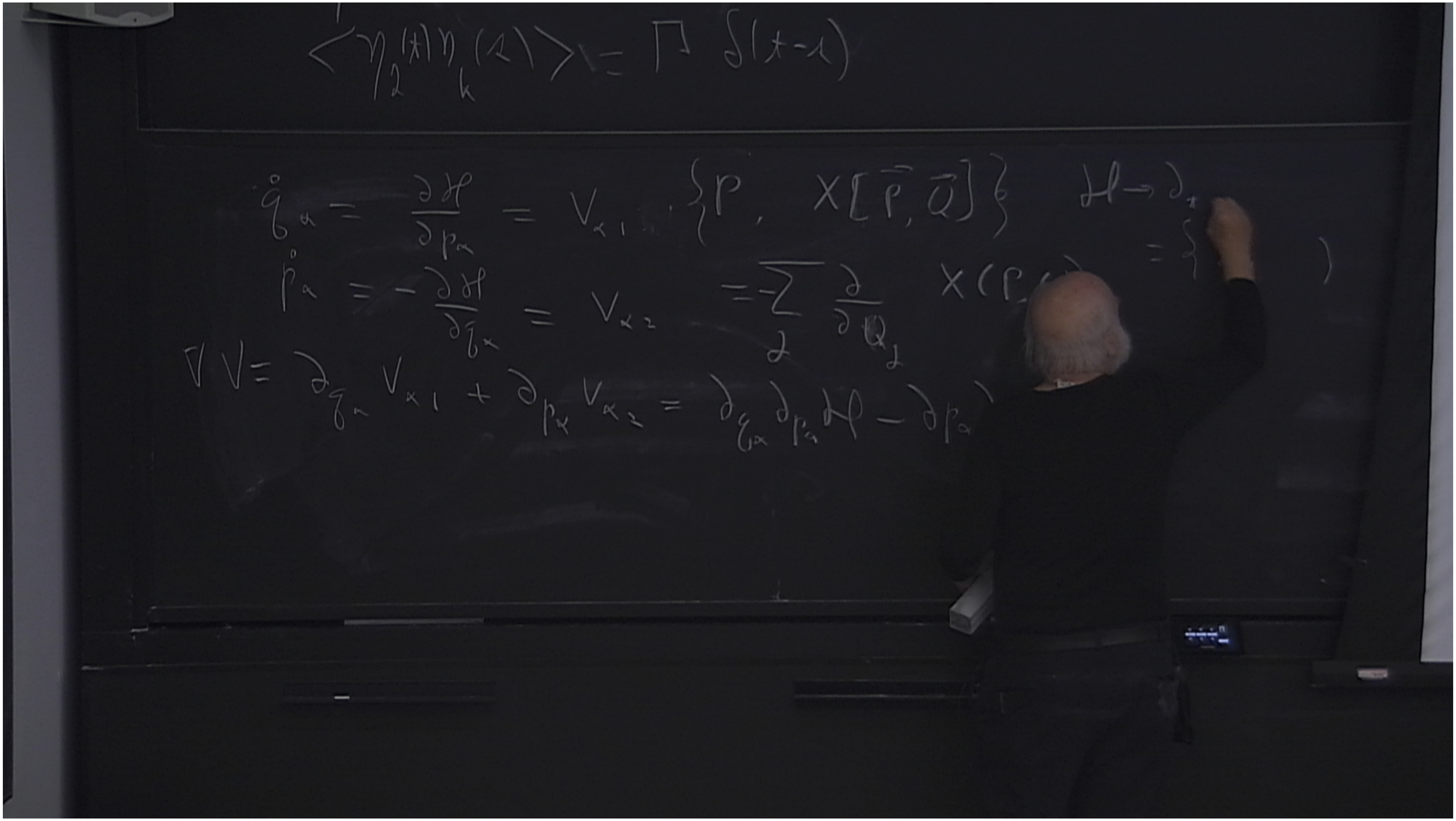
$\langle \eta_i(t)\eta_k(s)\rangle = \Gamma\,\delta(t-s)$
$\dot{q}_\alpha = \frac{\partial H}{\partial p_\alpha} = V_{\alpha 1}$
$\{P, X[\vec{P},\vec{Q}]\}$
$H \to \partial_t$
$\dot{p}_\alpha = -\frac{\partial H}{\partial q_\alpha} = V_{\alpha 2}$
$= -\sum_l \frac{\partial}{\partial Q_l}$
$\nabla V = \partial_{q_\alpha} V_{\alpha 1} + \partial_{p_\alpha} V_{\alpha 2} = \partial_{q_\alpha}\partial_{p_\alpha} H - \partial_{p_\alpha}$

Poisson Bracket

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Liouville's Theorem and conservation of functions of the energy

$$\partial_t \rho(p,q,t) + \sum_\alpha [(\partial_{p_\alpha} H)\partial_{q_\alpha} - (\partial_{q_\alpha} H)\partial_{p_\alpha}]\rho(p,q,t) = 0$$

If $\rho(p,q,0)$ is any function of the Hamiltonian, e.g. $\rho(p,q,0) = Z^{-1}\exp[-\beta H(p,q)]$ then this same functional form will hold for all times, assuming that the Hamiltonian has no explicit time dependence. $\rho(p,q,0)=f(H(p,q))$ implies that $\rho(p,q,t)=f(H(p,q))$ for any f.

Further, if ρ is any function of a time-independent H and of any other conserved functions of p and q, with no explicit time-dependence, then ρ will be a solution of our equation. Thus, not only is the Maxwell- Boltzmann distribution function a solution describing the equilibrium time-dependence of a Hamiltonian system, there are many other solutions as well.

Classical mechanics is not enough to specify a unique equilibrium probability density in a classical system. Something else is needed in addition.

Give some examples of functions of H with and without explicit time-dependence.