Title: Scientific Computation (PHYS 608) - Lecture 12

Date: Nov 10, 2009 10:30 AM

URL: http://pirsa.org/09110089

Abstract:

Lanczos Method

Lanczos Method

What to do if $n > 10^4$ $\qquad A^{n \times n}$

Lanczos Method

What to do if $n > 10^4$ $\qquad A^{n \times n}$

Idea

Lanczos Method

$A^{n\times n}$

What to do if $n > 10^4$

Idea :

$\{ v_1 , Hv_1$

Lanczos Method

What to do if $n > 10^4$ $\quad A^{n \times n}$

Idea :

$$\{ v_1 ,\ A v_1 ,\ A^2 v_1 ,\ A^3 v_1 \quad A^{m-1} v_1 \}$$

Lanczos Method

What to do if $n > 10^4$ $\quad A^{n\times n}$

Idea :

$$\mathcal{K} = \text{span}\{ v_1, \mathcal{H} v_1, \mathcal{H}^2 v_1, \mathcal{H}^3 v_1 \ldots \mathcal{H}^{M-1} v_1 \}$$

Krylov subspace

Lanczos Method

What to do if $n > 10^4$ $\quad A^{n\times n}$

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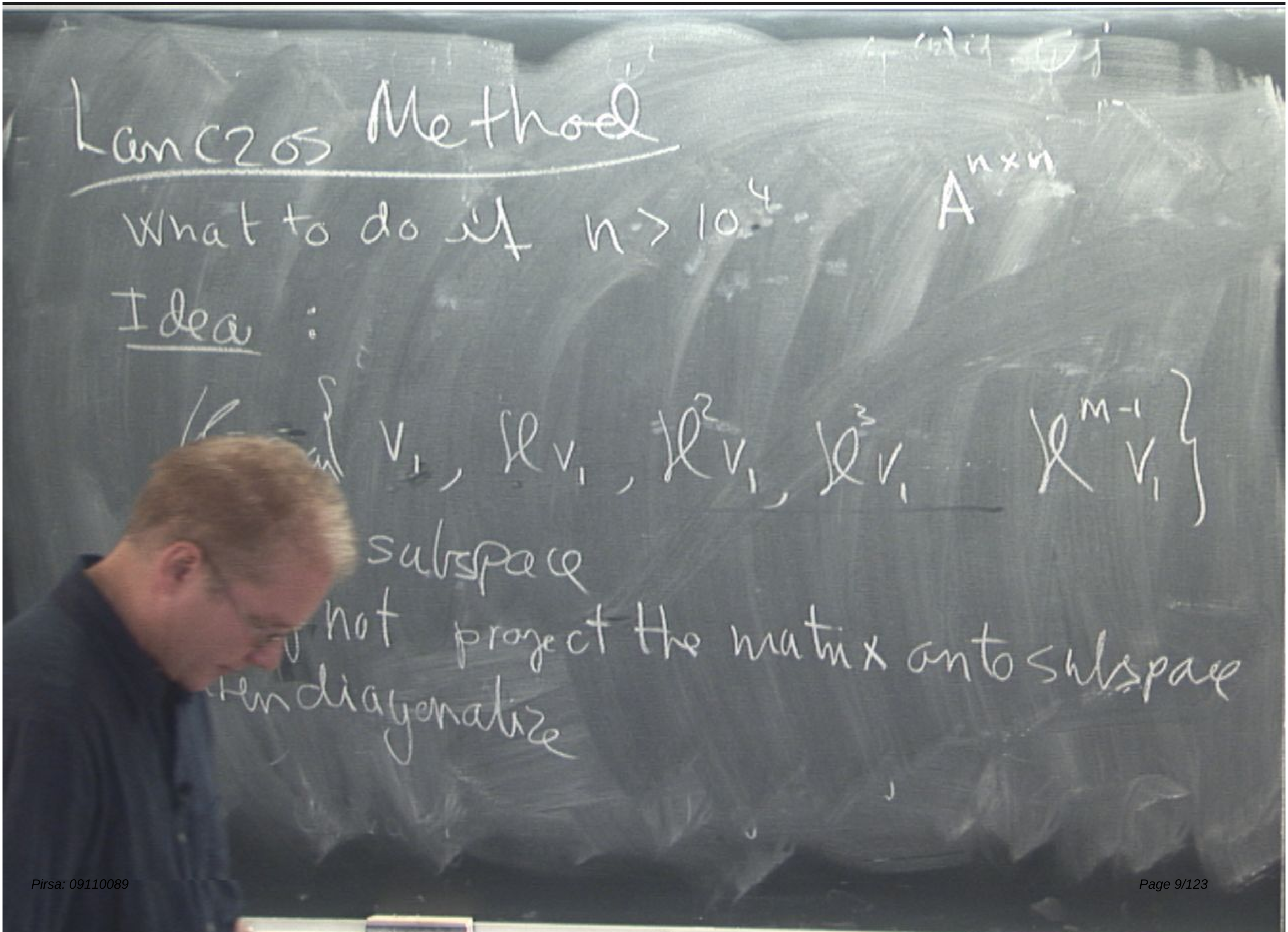
$$K = \text{span}\{ v_1 , A v_1 , A^2 v_1 , A^3 v_1 \quad A^{m-1} v_1 \}$$

Krylov subspace

Why not project the matrix onto subspace


Lanczos Method
What to do if $n > 10^4$
$A^{n \times n}$
Idea :
$\{ v_1, Av_1, A^2v_1, A^3v_1, \ldots A^{m-1}v_1 \}$
subspace
not project the matrix onto subspace
then diagonalize

Lanczos Method

What to do if $n > 10^4$ $A^{n \times n}$

Idea :

$\mathcal{K} = \text{span}\{ v_1, \mathcal{H} v_1, \mathcal{H}^2 v_1, \mathcal{H}^3 v_1 \quad \mathcal{H}^{M-1} v_1 \}$

Krylov subspace

Why not project the matrix onto subspace then diagonalize

We need an orthonormal basis Gramm-Schmidt.

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$|v_1\rangle$

We need an orthonormal basis

Gramm-Schmidt

$$|V_1\rangle = \frac{|U_1\rangle}{\|U_1\|}$$

Then

$|U_2\rangle =$

We need an orthonormal basis   Gramm-Schmidt.

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$$|U_2\rangle = \mathcal{H}|V_1\rangle - \langle V_1|\mathcal{H}|V_1\rangle|V_1\rangle$$

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Then

$$|U_3\rangle = \mathcal{H}|V_2\rangle - \langle V_1|\mathcal{H}|V_2\rangle|V_1\rangle - \langle V_2|\mathcal{H}|V_2\rangle|V_2\rangle$$

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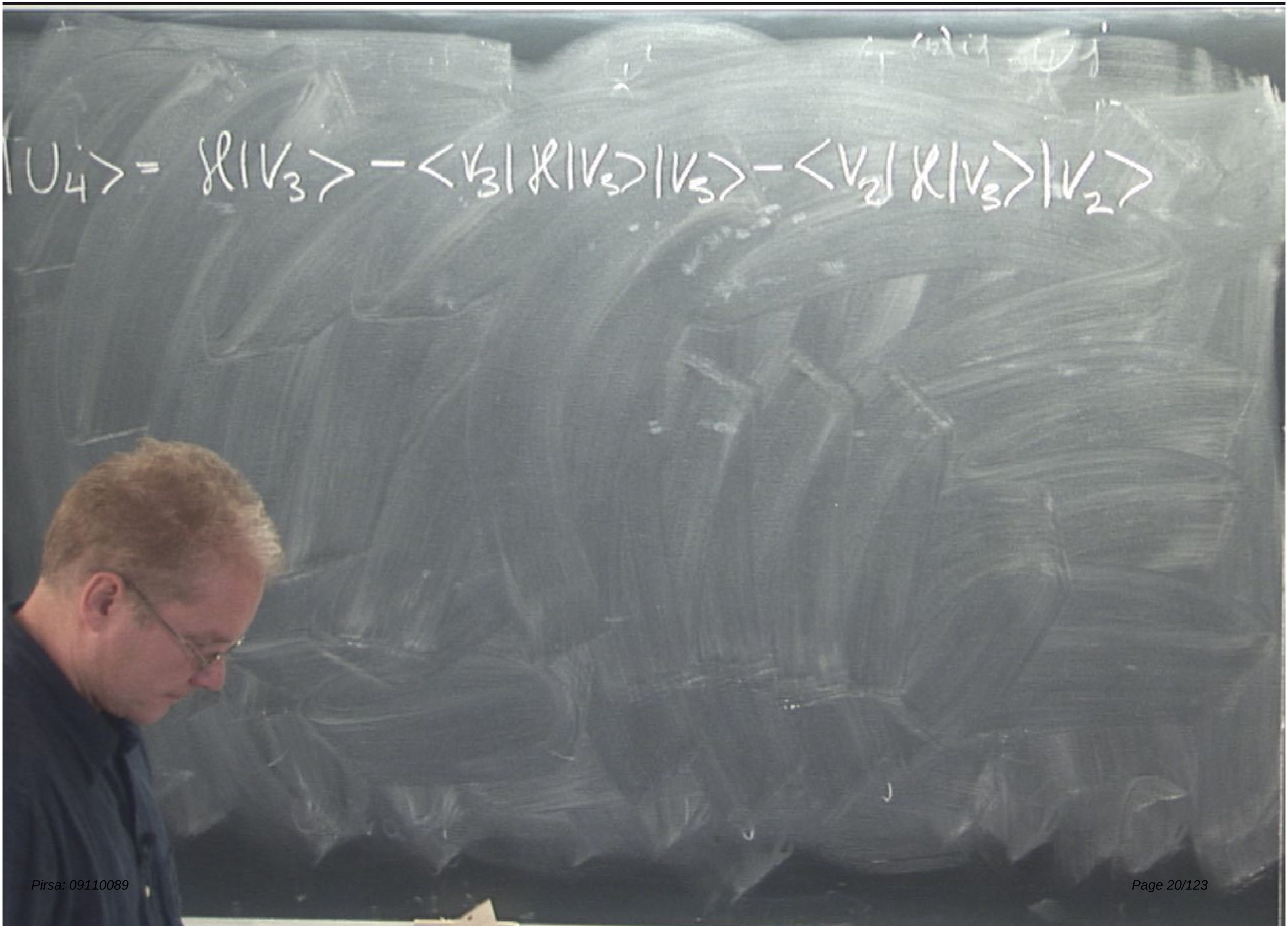
$$|V_3\rangle = \frac{|U_3\rangle}{\|U_3\|}$$

$$\langle V_1|V_3\rangle = \langle V_1|\mathcal{H}|V_2\rangle - \langle V_1|\mathcal{H}|V_2\rangle - 0 = 0$$

V_1, V_2, V_3 are orthogonal


$|U_4\rangle = \mathcal{H}|V_3\rangle - \langle V_3|\mathcal{H}|V_3\rangle|V_3\rangle - \langle V_2|\mathcal{H}|V_3\rangle|V_2\rangle$

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$$- \langle V_1|\mathcal{H}|V_3\rangle|V_1\rangle$$

$$|U_4\rangle = \mathcal{H}|V_3\rangle - \langle V_3|\mathcal{H}|V_3\rangle|V_3\rangle - \langle V_2|\mathcal{H}|V_3\rangle|V_2\rangle$$

$$\underbrace{-\langle V_1|\mathcal{H}|V_3\rangle|V_1\rangle}_{=0}$$

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$$\langle V_1|U_4\rangle = \langle V_1|\mathcal{H}|V_3\rangle - 0 - 0$$

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$$\langle V_1|U_4\rangle = \langle V_1|\mathcal{H}|V_3\rangle - 0 - 0$$

$$= \frac{1}{\|U_3\|}\Big(\langle V_1|\mathcal{H}^2|V_2\rangle - \beta_2\langle V_1|\mathcal{H}|V_1\rangle - \alpha_2\langle V_1|\mathcal{H}|V_2\rangle\Big)$$

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$$|u_4\rangle = \mathcal{H}|v_3\rangle - \langle v_3|\mathcal{H}|v_3\rangle|v_3\rangle - \langle v_2|\mathcal{H}|v_3\rangle|v_2\rangle$$

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$$- \alpha_2\langle v_1|\mathcal{H}|v$$

$$= \frac{1}{\|u_3\|}\Big(\langle v_1|\mathcal{H}^2|v_2\rangle - \beta_2\alpha_1 -$$

$$|U_4\rangle = \mathcal{H}|V_3\rangle - \langle V_3|\mathcal{H}|V_3\rangle|V_3\rangle - \langle V_2|\mathcal{H}|V_3\rangle|V_2\rangle$$

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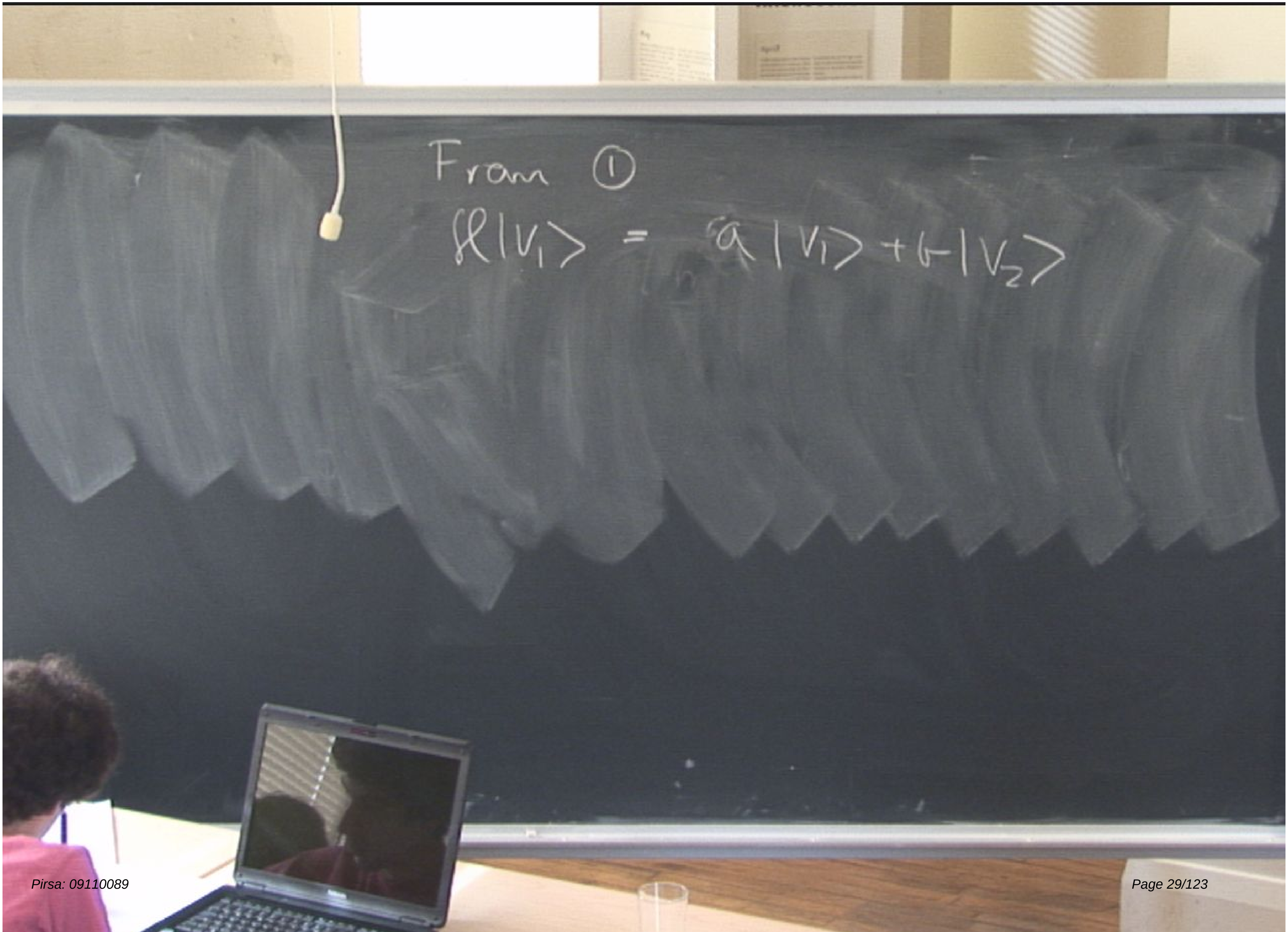
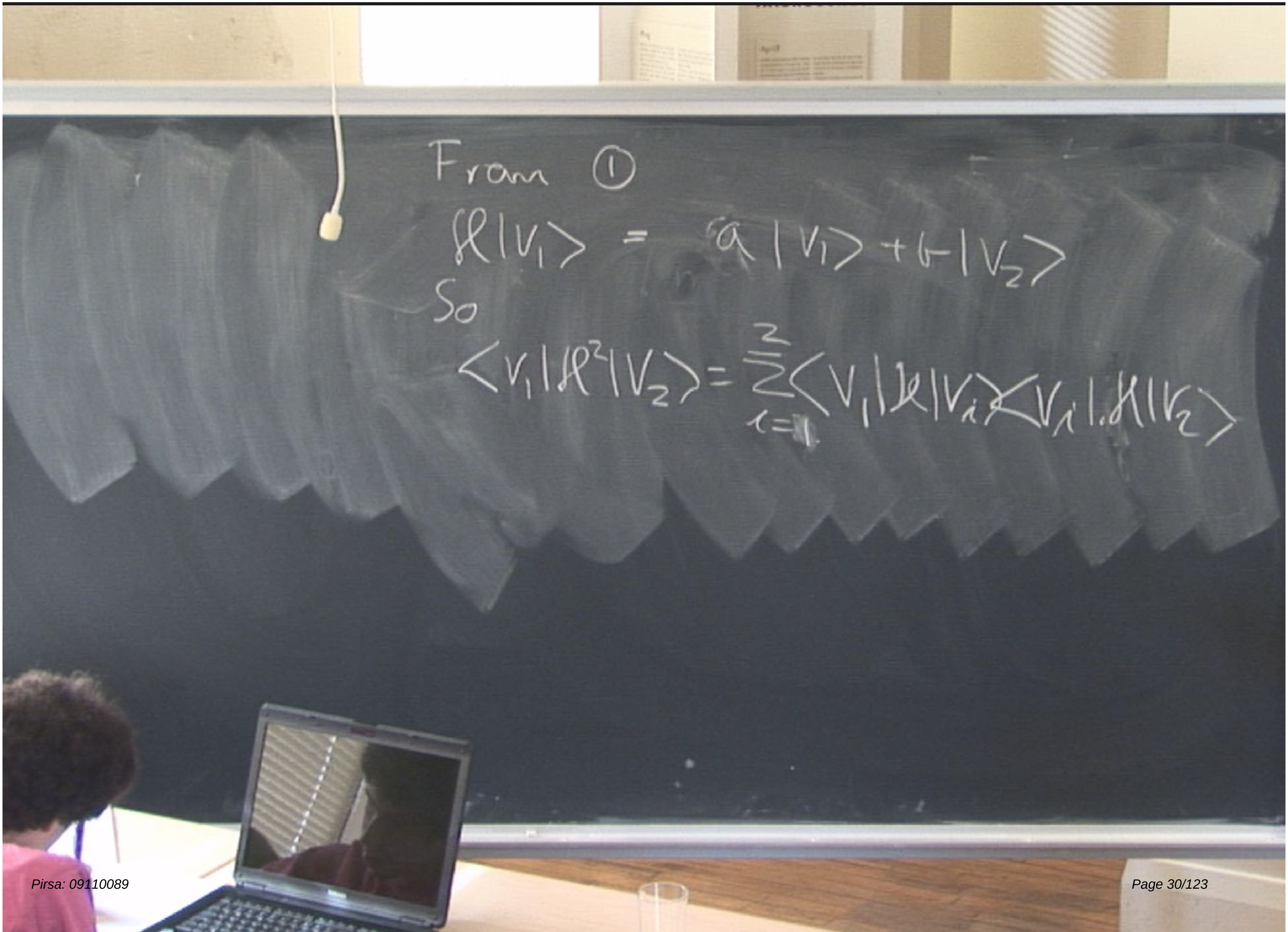
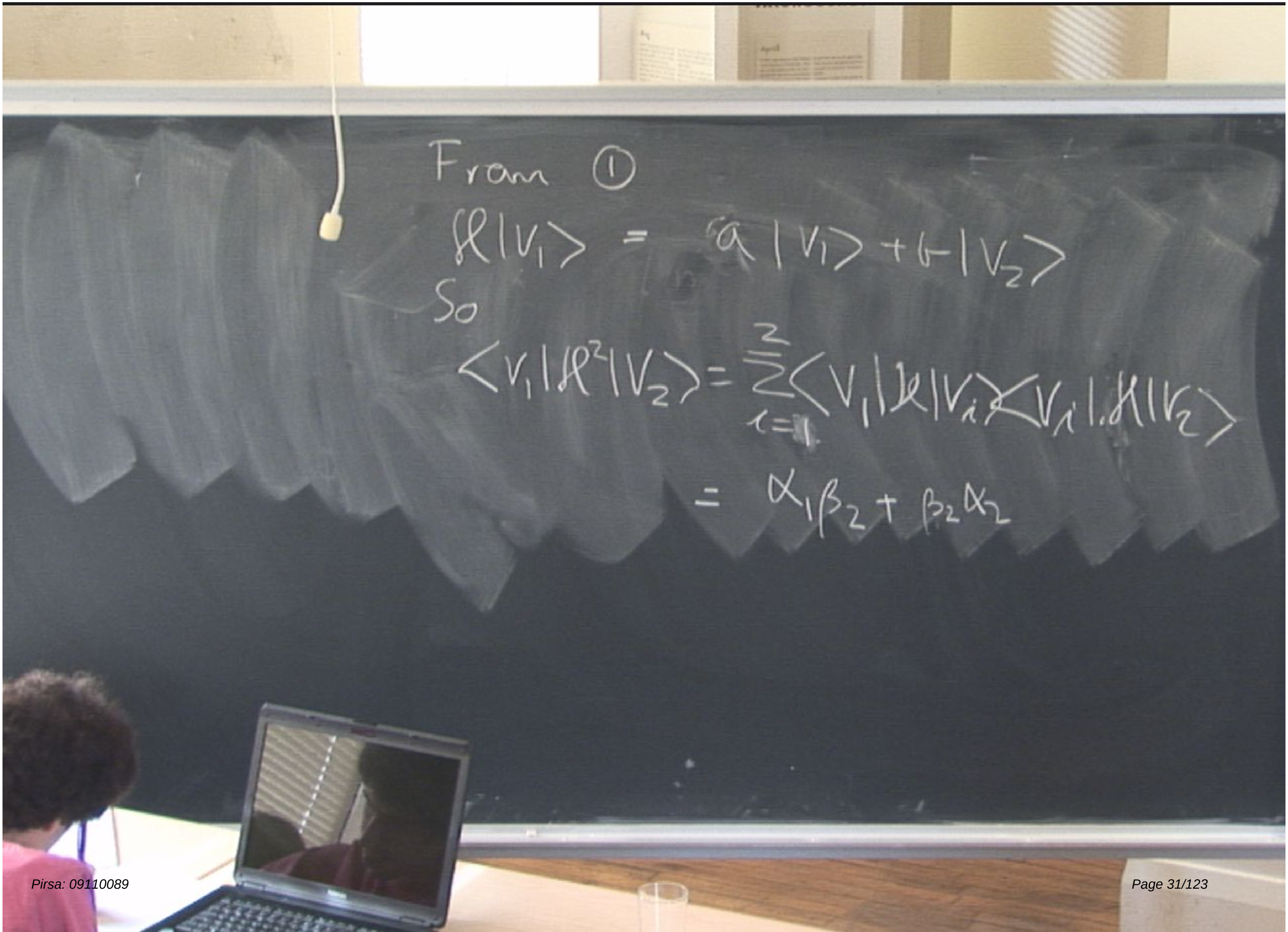
$$- \alpha_2\langle V_1|\mathcal{H}|V_2\rangle\Big)$$

$$= \frac{1}{\|U_3\|}\Big(\langle V_1|\mathcal{H}^2|V_2\rangle - \beta_2\alpha_1 - \alpha_2\beta_2\Big)$$


From 1
$\Omega|v_1\rangle = a|v_1\rangle + b|v_2\rangle$


From ①
$\mathcal{H}|v_1\rangle = a|v_1\rangle + b|v_2\rangle$
So
$\langle v_1|\mathcal{H}^2|v_2\rangle = \sum_{i=1}^{2}\langle v_1|\mathcal{H}|v_i\rangle\langle v_i|\mathcal{H}|v_2\rangle$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$= \alpha_1\beta_2 + \beta_2\alpha_2$

$$|U_4\rangle = \mathcal{H}|V_3\rangle - \langle V_3|\mathcal{H}|V_3\rangle|V_3\rangle - \langle V_2|\mathcal{H}|V_3\rangle|V_2\rangle$$

$$|V_4\rangle = \frac{|U_4\rangle}{\| U_4 \|}$$

$|U_5\rangle$

$$|U_4\rangle = \mathcal{H}|V_3\rangle - \langle V_3|\mathcal{H}|V_3\rangle|V_3\rangle - \langle V_2|\mathcal{H}|V_3\rangle|V_2\rangle$$

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$$\alpha_3 \qquad\qquad\qquad \beta_3$$

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$$\overset{\alpha_3}{} \qquad \overset{\beta_3}{}$$

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$= ($

$$\alpha_3 \qquad\qquad \beta_3$$

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$$\alpha_4 \qquad\qquad |V_4\rangle = \frac{|U_4\rangle}{\| U_4 \|}$$

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$$\beta_4$$

$$\langle V_2|U_5\rangle$$

$$= ($$

$$|U_4\rangle = \mathcal{H}|V_3\rangle - \overbrace{\langle V_3|\mathcal{H}|V_3\rangle}^{\alpha_3}|V_3\rangle - \overbrace{\langle V_2|\mathcal{H}|V_3\rangle}^{\beta_3}|V_2\rangle$$

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$\langle V_2|U_5\rangle = 0$ by construction $\langle V_1|U_5\rangle = 0$

use $\langle V_1|U_4\rangle$

$= ($

$\mathcal{H}$

$V_1 \cdots\cdots V_m$

$n \times n$ $\qquad$ $n \times m$

V_1
V_2
V_m

$\mathcal{H}$

$V_1 \cdots V_m$

$$\begin{pmatrix} \langle v_1|H|v_1\rangle & \langle v_1|H|v_2\rangle & \langle v_1|H|v_3\rangle & \cdots \\ \langle v_2|H|v_1\rangle & \langle v_2|H|v_2\rangle & \cdots & \\ \cdots & & & \end{pmatrix} = \begin{pmatrix} \\ \\ \end{pmatrix}$$

$m \times n$

$$\begin{pmatrix} \alpha_1 & \beta_2 & 0 & \\ \beta_2 & \alpha_2 & \beta_3 & \\ & \beta_3 & \alpha_3 & \beta_4 \end{pmatrix}$$

$$\begin{pmatrix} \langle v_1|H|v_1\rangle & \langle v_1|H|v_2\rangle & \langle v_1|H|v_3\rangle & \cdots \\ \langle v_2|H|v_1\rangle & \langle v_2|H|v_2\rangle & \cdots & \\ \cdots & & & \end{pmatrix} = \overset{m\times n}{\left(\quad \right.}$$

$$\begin{pmatrix} \alpha_1 & \beta_2 & 0 & 0 & \cdots & 0 \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \beta_4 & & \\ & & \ddots & \ddots & \ddots & \end{pmatrix}$$

$$\begin{pmatrix} \langle v_1|\mathcal{H}|v_1\rangle & \langle v_1|\mathcal{H}|v_2\rangle & \langle v_1|\mathcal{H}|v_3\rangle & \cdots \\ \langle v_2|\mathcal{H}|v_1\rangle & \langle v_2|\mathcal{H}|v_2\rangle & \cdots & \\ \cdots & & & \end{pmatrix} = \begin{pmatrix} \\ \\ \end{pmatrix}$$

$m \times n$

$$\begin{pmatrix} \alpha_1 & \beta_2 & 0 & 0 & \cdots & 0 \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \beta_4 & & \\ & & \ddots & \ddots & \ddots & \end{pmatrix}$$

Tridiagona

$\langle v_1|\mathcal{H}|v_2\rangle \langle v_1|\mathcal{H}|v_3\rangle \ldots$

$\langle v_2|\mathcal{H}|v_2\rangle$

$\beta_2 \; 0 \; 0$

$\alpha_2 \; \beta_3$

$\beta_3 \; \alpha_3 \; \beta_4$

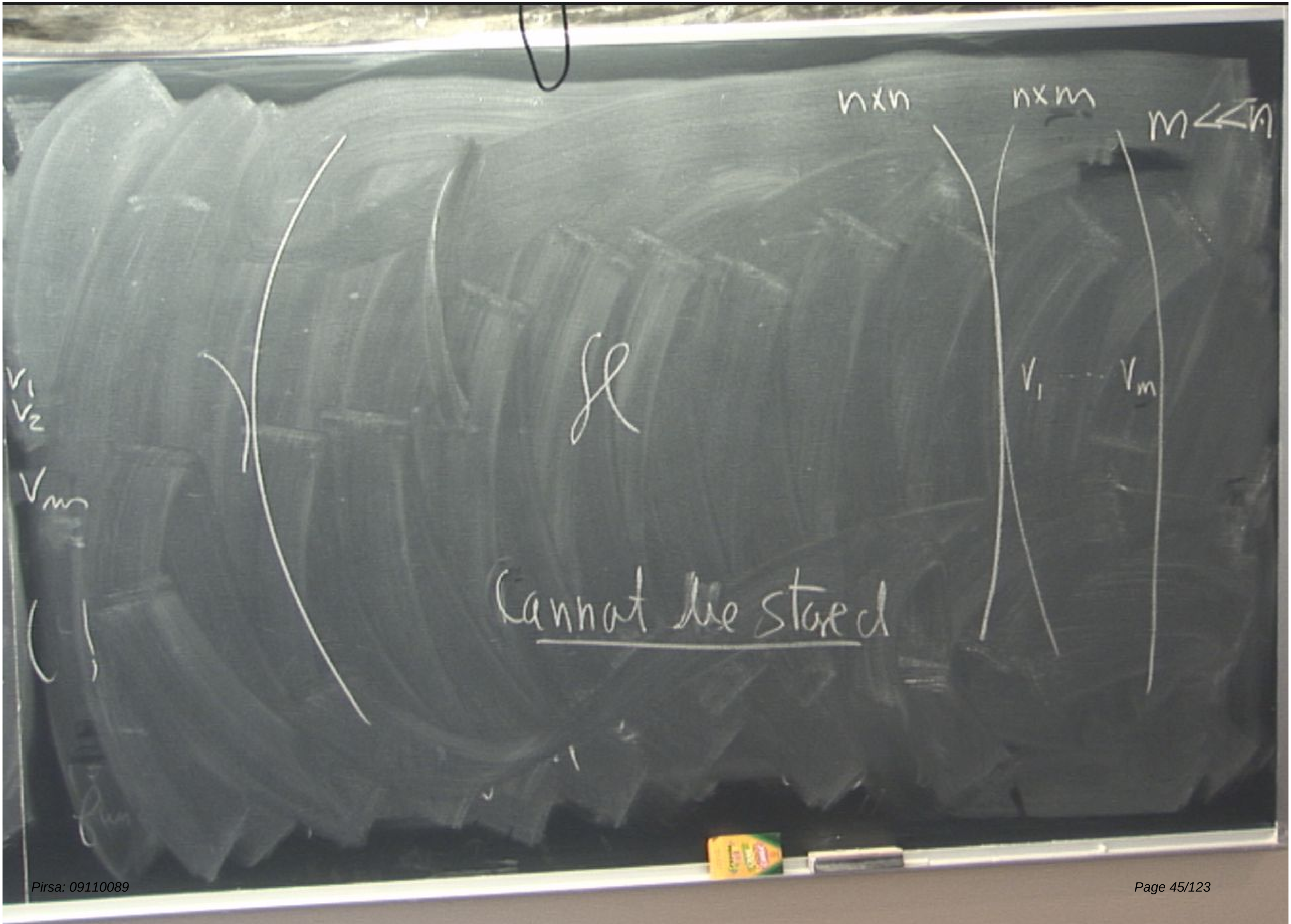
Propertian

$= \underset{m \times n}{(\;\;)}$

v_1
v_2
v_m

Tridiagona (


n x n
n x m
m << n
V1 ...... Vm
V1
V2
Vm



n×n
n×m
m<<n
V_1
V_2
V_m
$V_1 \cdots V_m$
Cannot be stored

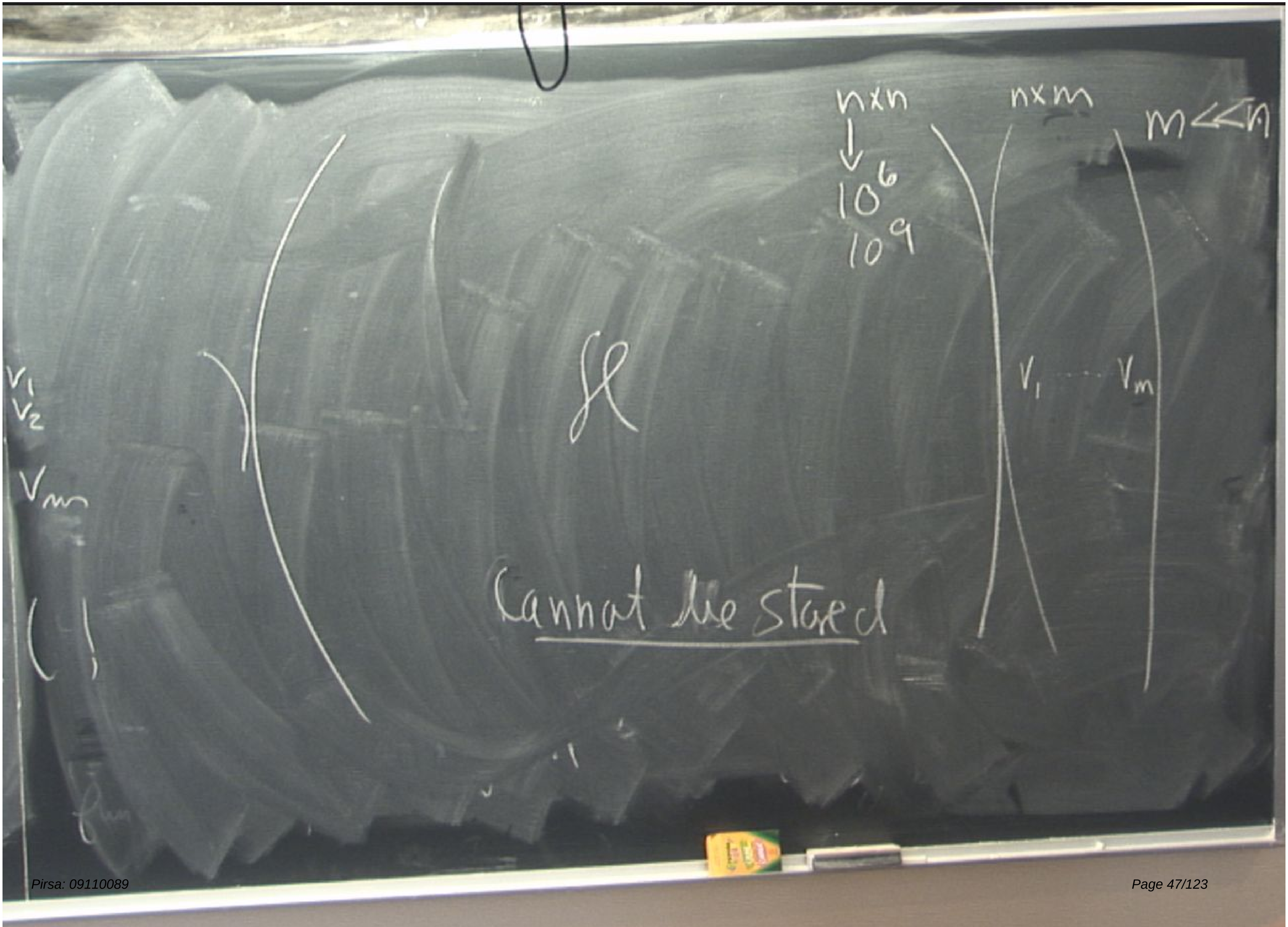
Projection

$m = 200-500$

$$\begin{pmatrix} \langle v_1|H|v_1\rangle & \langle v_1|H|v_2\rangle & \langle v_1|H|v_3\rangle & \cdots \\ \langle v_2|H|v_1\rangle & \langle v_2|H|v_2\rangle & \cdots & \\ \cdots & & & \end{pmatrix} = \underset{m\times n}{\left(\right.}$$

$$\begin{pmatrix} \alpha_1 & \beta_2 & 0 & 0 & \cdots & 0 \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \beta_4 & & \\ & & \ddots & \ddots & \ddots & \end{pmatrix}$$

Tridiagona


n x n
10^6
10^9
n x m
m << n
v_1 ...... v_m
v_1
v_2
v_m
Cannot be stored

v_1
v_2
v_m

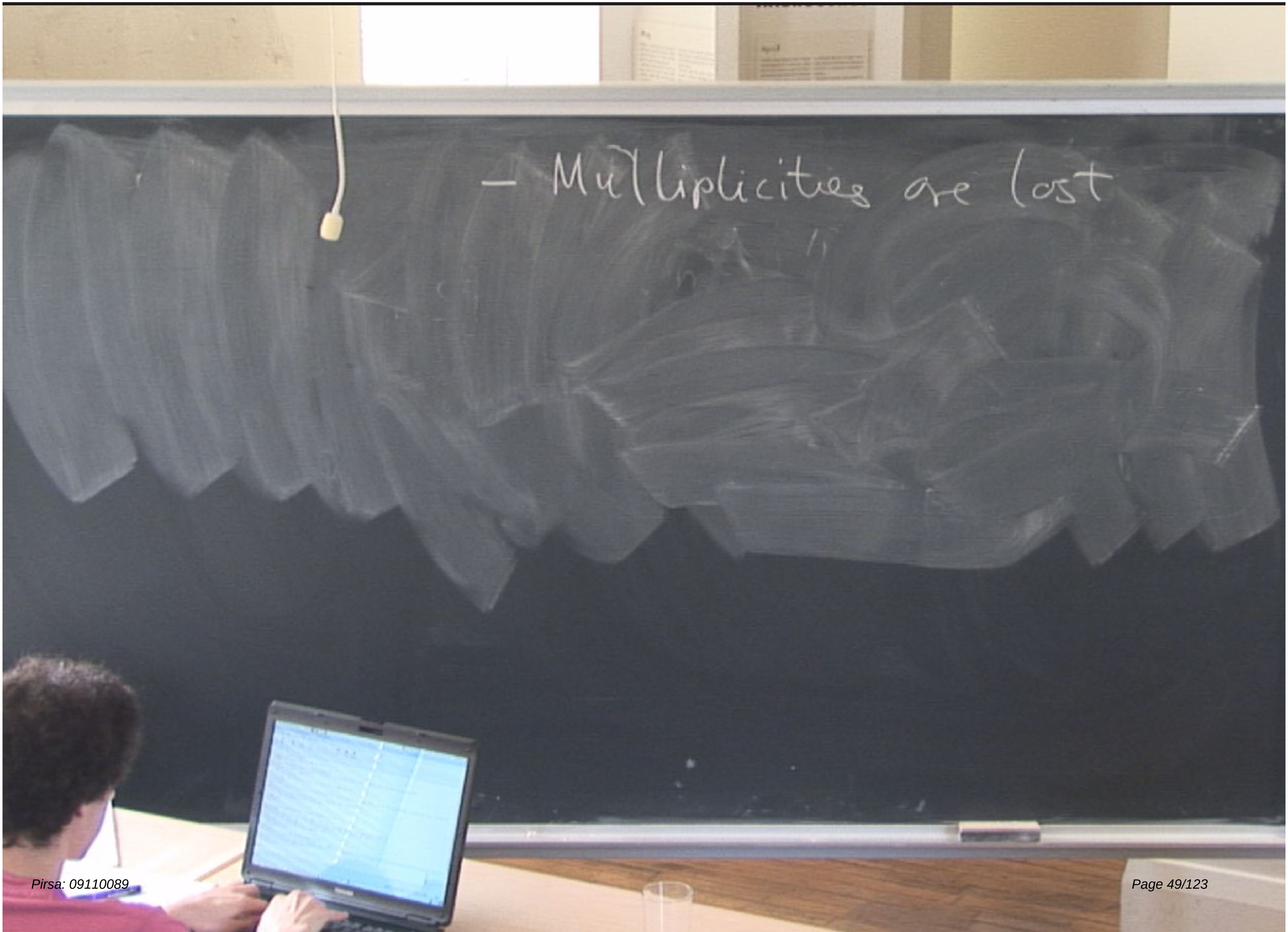
$n \times n$
$\downarrow$
10^6
10^9

$n \times m$ $\quad m \ll n$

$\mathcal{H}$

$v_1 \cdots v_m$

Cannot be stored


– Multiplicities are lost

Tridiagonal

$m \times n$

$L = \Big($

all eigenvalues / eigenvectors

Tridiagonal

$m \times n$

$L = ($

V_1
V_2

V_m

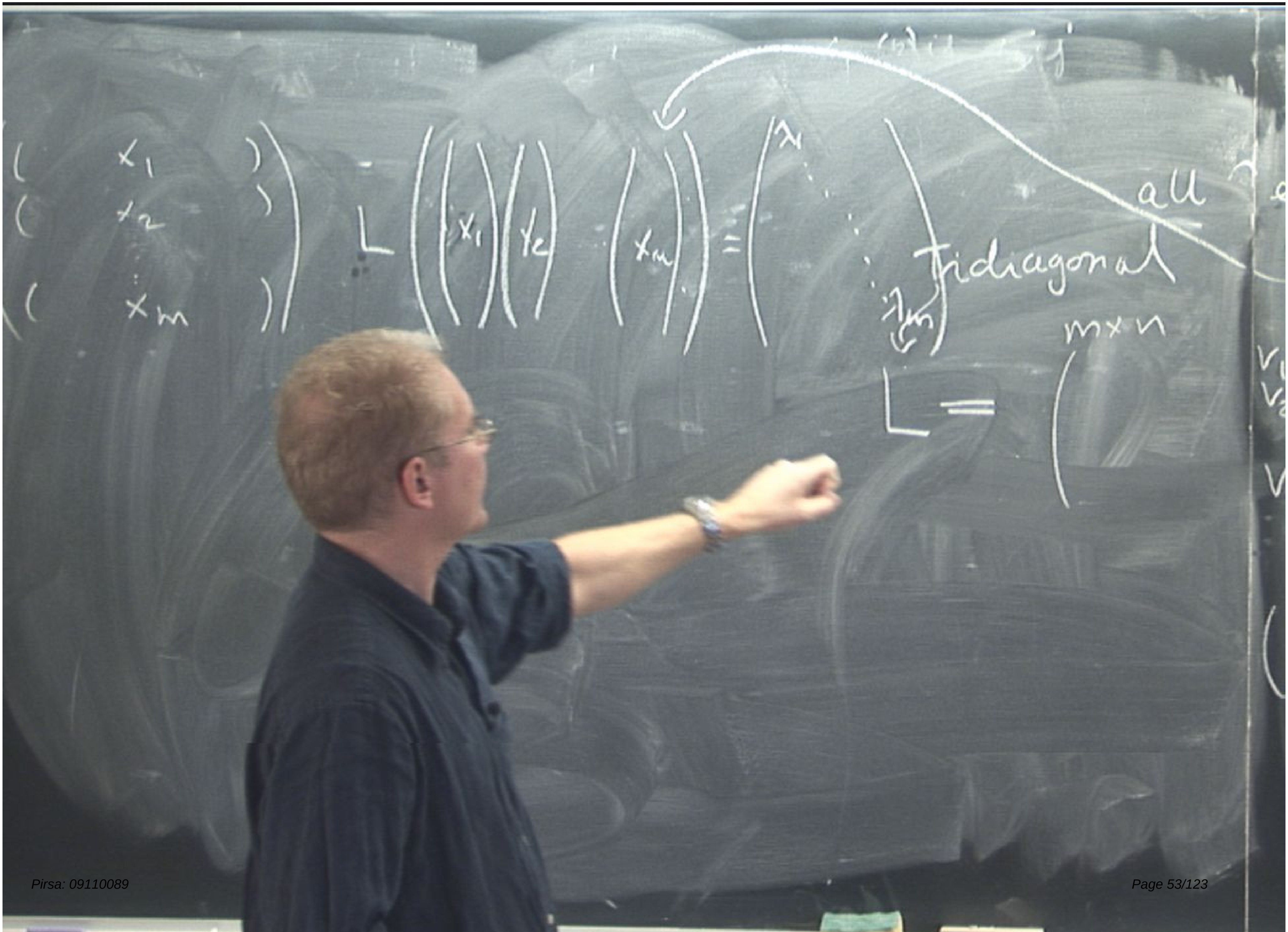
$$\begin{pmatrix} (& x_1 &) \\ (& x_2 &) \\ & \vdots & \\ (& x_m &) \end{pmatrix} = L\left(\begin{pmatrix} x_1 \end{pmatrix} \begin{pmatrix} x_2 \end{pmatrix} \cdots \begin{pmatrix} x_m \end{pmatrix} \right)$$

all

Tridiagonal

$m \times n$

$L = \Big($


x_1
x_2
x_m
L
x_1
x_2
x_m
$=$
λ_1
λ_m
Tridiagonal
all
$m \times n$
$L =$

$$\begin{pmatrix} (& x_1 &) \\ (& x_2 &) \\ & \vdots & \\ (& x_m &) \end{pmatrix}$$

$n \times m$

$$L \left((x_1)(x_2) \cdots (x_m) \right) = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_m \end{pmatrix}$$

all

tridiagonal

$m \times n$

$$L = \Big(\quad \Big)$$

$$\begin{pmatrix} v_1 & \cdots & v_m \end{pmatrix}_{n \times m} \left((x_1)(x_2) \cdots (x_m) \right)_{m \times m}$$

give eigenvectors of $\mathcal{H}$

$$\begin{pmatrix} (& x_1 &) \\ (& x_2 &) \\ & \vdots & \\ (& x_m &) \end{pmatrix} \quad L \left((x_1)(x_2) \cdots (x_m) \right) = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_m \end{pmatrix}$$

all

tridiagonal

$n \times m$

$m \times n$

$$L = \Big($$

$m \times m$

$$\begin{pmatrix} v_1 & \cdots & v_m \end{pmatrix} \left((x_1)(x_2) \cdots (x_m) \right)$$

give eigenvectors of H

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{pmatrix} L \begin{pmatrix} x_1 & x_2 & \cdots & x_m \end{pmatrix} = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_m \end{pmatrix}$$

all

tridiagonal

$n \times m$

$m \times n$

$L =$

$$\begin{pmatrix} v_1 & \cdots & v_m \end{pmatrix} \begin{pmatrix} x_1 & x_2 & \cdots & x_m \end{pmatrix}$$

$m \times m$

give eigenvectors of $\mathcal{H}$

$$= \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_m \end{pmatrix}$$

all eigenvalues / eigenvectors

tridiagonal

$x_1 \ldots x_m$

$m \times n$

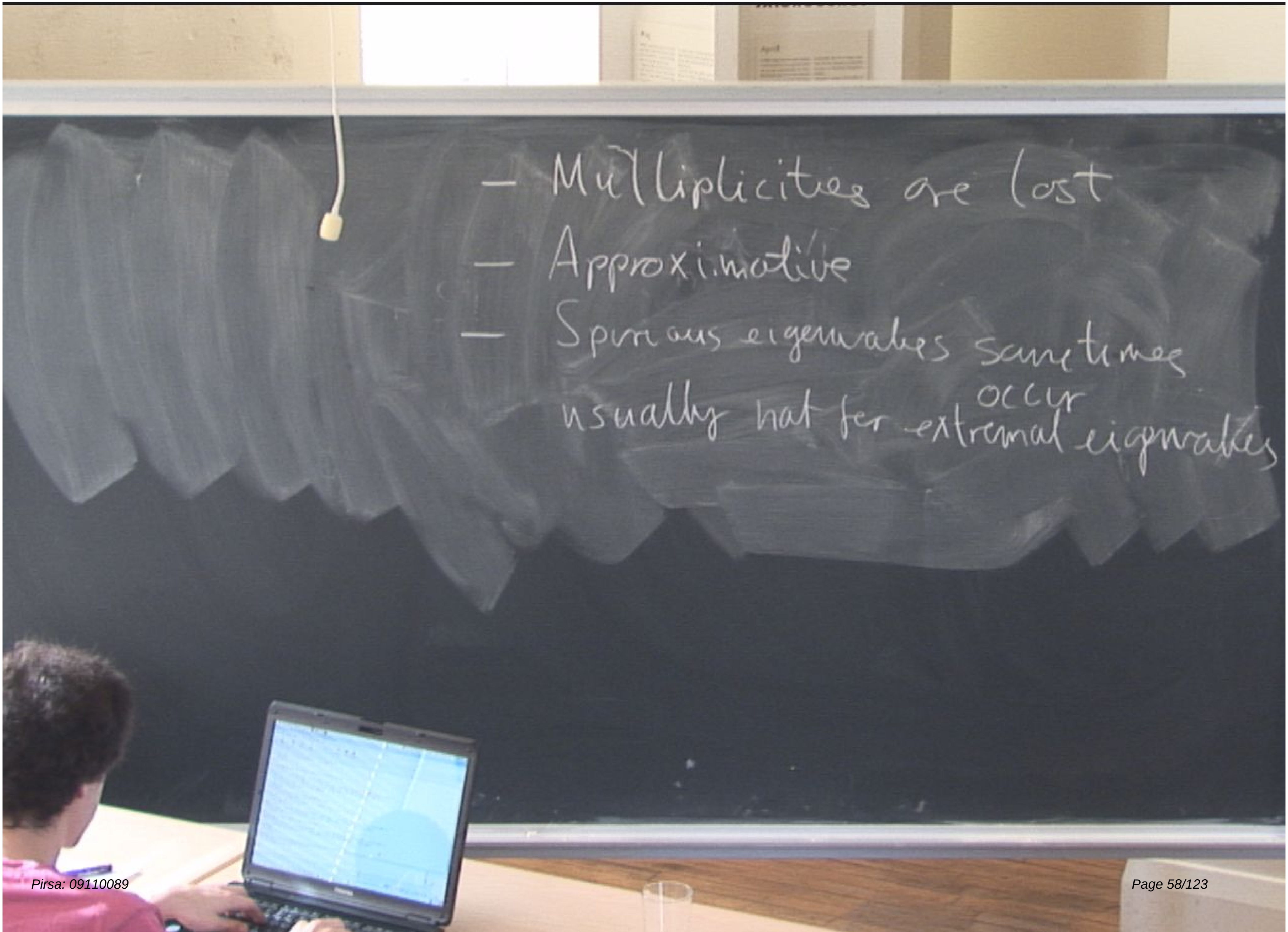
$L =$

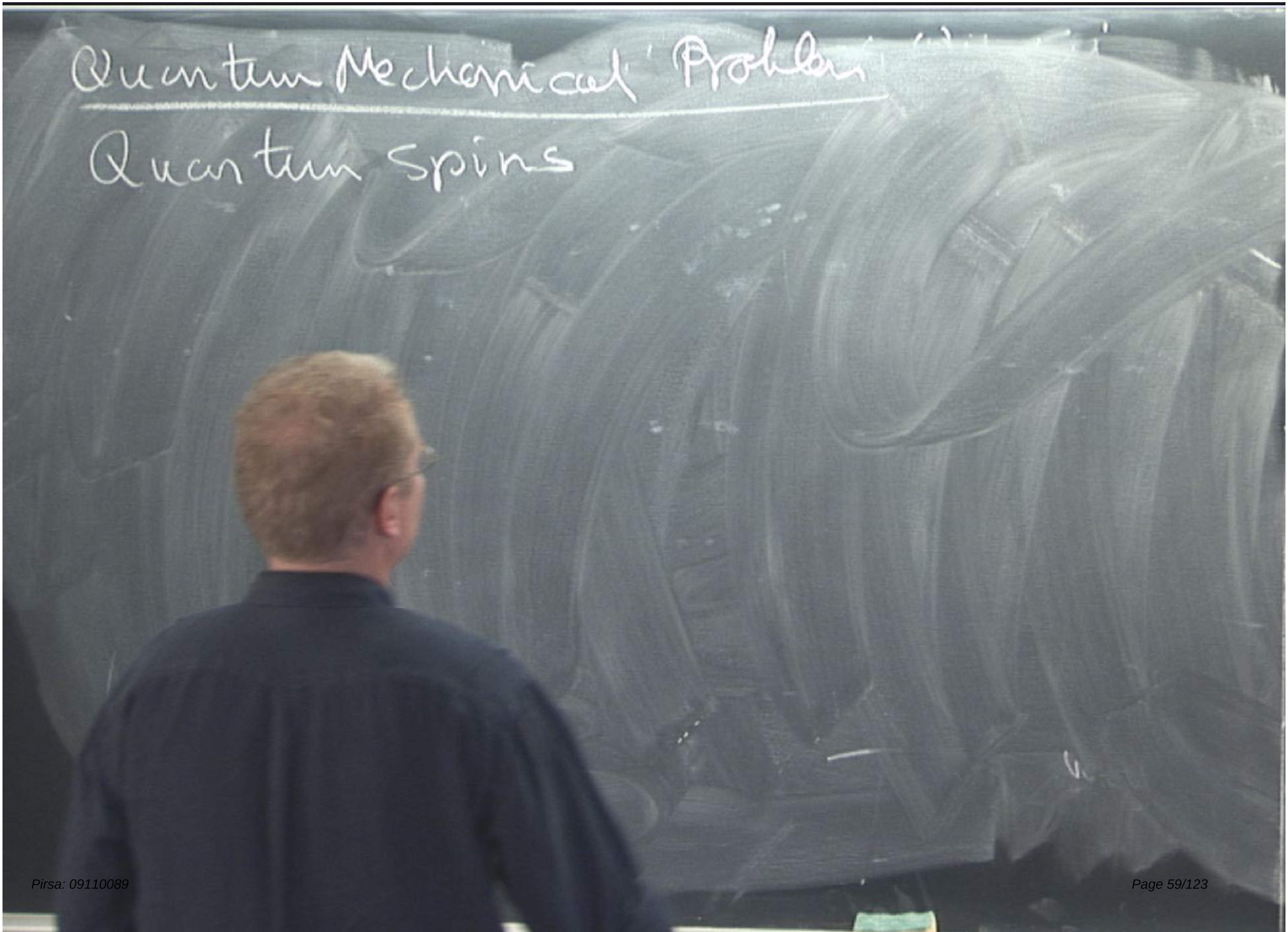
v_1
v_2
v_m

give eigenvectors of H

works well for extremal eigenvectors

Can


— Multiplicities are lost
— Approximative
— Spurious eigenvalues sometimes occur
usually not for extremal eigenvalues


Quantum Mechanical Problem
Quantum spins

Quantum Mechanical Problem

Quantum spins $\quad \hbar = 1$

$$\vec{S} = \frac{1}{2}\{\sigma^x, \sigma^y, \sigma^z\}$$

Quantum Mechanical Problem

Quantum spins $\hbar = 1$

$$\vec{S} = \frac{1}{2}\{\sigma^x, \sigma^y, \sigma^z\}$$

written S_z basis

Quantum Mechanical Problem

Quantum spins $\quad \hbar = 1, \quad S = 1/2$

$$\vec{S} = \frac{1}{2}\{\sigma^x, \sigma^y, \sigma^z\}$$

written S_z basis

S_z basis $\quad |\uparrow\rangle \quad |\downarrow\rangle$

Quantum Mechanical Problem

Quantum spins $\hbar = 1$, $S = 1/2$

$$\vec{S} = \frac{1}{2}\{\sigma^x, \sigma^y, \sigma^z\}$$

written S_z basis

S_z basis $|\uparrow\rangle$, $|\downarrow\rangle$

Intracting spins

Quantum Mechanical Problem

Quantum spins $\hbar = 1$, $S = 1/2$

$$\vec{S} = \frac{1}{2}\{\sigma^x, \sigma^y, \sigma^z\}$$

written S_z basis

S_z basis $|\uparrow\rangle$ $|\downarrow\rangle$

Intracting spins Heisenberg $\sum_{\langle i,j \rangle} S_i \cdot S_j$

Quantum Mechanical Problem

Quantum spins $\hbar = 1$, $S = 1/2$

$$\vec{S} = \frac{1}{2}\{\sigma^x, \sigma^y, \sigma^z\}$$

written S_z basis

S_z basis $|\uparrow\rangle$ $|\downarrow\rangle$

Intracting spins Heisenberg $\sum_{\langle i,j\rangle} S_i \cdot S_j$

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S_z basis $|\uparrow\rangle$, $|\downarrow\rangle$

Intracting spins

Heisenberg $J\sum_{\langle i,j\rangle} S_i \cdot S_j$

product basis $|\uparrow\uparrow\rangle$ $|\uparrow\downarrow\rangle$ $|\downarrow\uparrow\rangle$ $|\downarrow\downarrow\rangle$

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S_z basis $|\uparrow\rangle$: $|\downarrow\rangle$

Intracting spins Heisenberg $J \sum_{\langle i,j \rangle} S_i \cdot S_j$

product basis $|\overset{i}{\uparrow}\overset{j}{\uparrow}\rangle$ $|\uparrow\downarrow\rangle$ $|\downarrow\uparrow\rangle$ $|\downarrow\downarrow\rangle$

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S_z basis $|\uparrow\rangle$ $|\downarrow\rangle$ 2 states

Intracting spins Heisenberg $J\sum_{\langle i,j\rangle} S_i \cdot S_j$

product basis $|\overset{i}{\uparrow}\overset{j}{\uparrow}\rangle$ $|\uparrow\downarrow\rangle$ $|\downarrow\uparrow\rangle$ $|\downarrow\downarrow\rangle$ 2^2

Quantum Mechanical Problem

Quantum spins $\hbar = 1$, $S = 1/2$

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← written S_z basis

S_z basis $|\uparrow\rangle$: $|\downarrow\rangle$ 2 states

Interacting spins Heisenberg $J\sum_{\langle i,j\rangle} S_i \cdot S_j$

product basis $|\overset{i}{\uparrow}\overset{j}{\uparrow}\rangle$ $|\uparrow\downarrow\rangle$ $|\downarrow\uparrow\rangle$ $|\downarrow\downarrow\rangle$ 2^2

In general for L spins I get 2^L states

Linear Chain $\quad J \sum S_i \cdot S_{i+1}$

Linear Chain $J \sum S_i \cdot S_{i+1}$

Trick generate "on the fly"

Linear Chain $J \sum S_i \cdot S_{i+1}$

Trick generate "on the fly"

$$4\, S_1 \cdot S_2 = \begin{pmatrix} 1 & & & \\ & -1 & 2 & \\ & 2 & -1 & \\ & & & 1 \end{pmatrix}$$

Linear Chain $J \sum S_i \cdot S_{i+1}$

Trick generate "on the fly"

permutation matrix

$$4\, S_1 \cdot S_2 = \begin{pmatrix} 1 & & & \\ & -1 & 2 & \\ & 2 & -1 & \\ & & & 1 \end{pmatrix} = 4\, \mathcal{H}_{ij}$$

$$\mathcal{H}' = 2\,\mathcal{H}_{ij} + \tfrac{1}{2} I = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Quantum Mechanical Problem

Coding for the states

$\uparrow\uparrow$	0 0
$\uparrow\downarrow$	0 1
$\downarrow\uparrow$	1,0
$\downarrow\downarrow$	1 1

Quantum Mechanical 'Problem'

Coding for the states

$\uparrow\uparrow$	0 0
$\uparrow\downarrow$	0 1
$\downarrow\uparrow$	1,0
$\downarrow\downarrow$	1 1

$\mathcal{R}'\Big($

Quantum Mechanical Problem

Coding for the states

$\uparrow\uparrow$	0 0
$\uparrow\downarrow$	0 1
$\downarrow\uparrow$	1,0
$\downarrow\downarrow$	1 1

$$\mathcal{L}' \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} =$$

Quantum Mechanical Problem

Coding for the states

$\uparrow\uparrow$ 0 0

$\uparrow\downarrow$ 0 1

$\downarrow\uparrow$ 1, 0

$\downarrow\downarrow$ 1 1

$$\ell' \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} a_0 \\ a_2 \\ a_1 \\ a_3 \end{pmatrix}$$

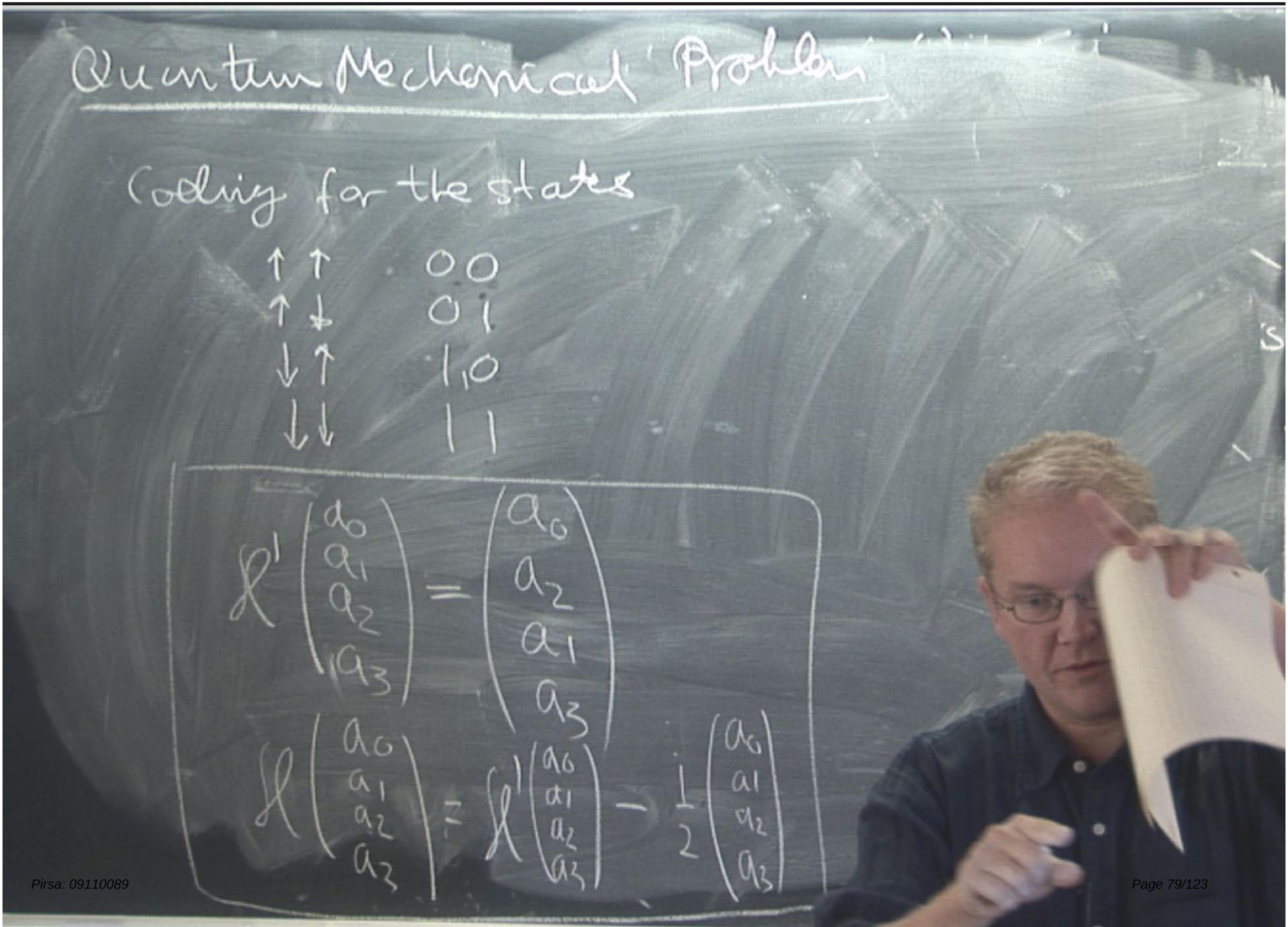
Quantum Mechanical Problem

Coding for the states

$\uparrow\uparrow$	0 0
$\uparrow\downarrow$	0 1
$\downarrow\uparrow$	1 0
$\downarrow\downarrow$	1 1

$$\mathcal{H}'\begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} a_0 \\ a_2 \\ a_1 \\ a_3 \end{pmatrix}$$

$$\mathcal{H}\begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \mathcal{H}'\begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} - \frac{1}{2}\begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix}$$


Quantum Mechanical 'Problem'
Coding for the states
↑↑ 00
↑↓ 01
↓↑ 1,0
↓↓ 11
$\mathcal{L}' \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} a_0 \\ a_2 \\ a_1 \\ a_3 \end{pmatrix}$
$\mathcal{L} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \mathcal{L}' \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix}$

```
IMPLICIT NONE
real (dbl),intent(in)          :: x(N)
real (dbl)                     :: y(N)
integer,intent(in)             :: L,N
integer                        :: i,j,k,jm

  y = 0.0_dbl
  do i = 0,N-1
    if (abs(x(i+1)).gt.EPSILON(1.0_dbl)) then
      do j=1,L-1
        jm = j-1
        k=i
        if (btest(i,j)) then
          k=ibset(k,jm)
        else
          k=ibclr(k,jm)
        end if
        if (btest(i,jm)) then
          k=ibset(k,j)
        else
          k=ibclr(k,j)
        end if
        y(k+1)=y(k+1)+x(i+1)
      end do
    end if
  end do
  y=(y-(L-1)/2.0_dbl*x)/2.0_dbl
end function hv
```

Linear Chain $\quad J\sum_i S_i \cdot S_{i+1}$

Trick generate "on the fly"

$$4\, S_1 \cdot S_2 = \begin{pmatrix} 1 & & & \\ & -1 & 2 & \\ & 2 & -1 & \\ & & & 1 \end{pmatrix} = 4\, h_{ij}$$

permutation matrix

$$h' = 2\, h_{ij} + \tfrac{1}{2} I = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Linear Chain $J\sum_i S_i \cdot S_{i+1}$ Bethe

Trick generate "on the fly"

$$4\, S_1 \cdot S_2 = \begin{pmatrix} 1 & & & \\ & -1 & 2 & \\ & 2 & -1 & \\ & & & 1 \end{pmatrix} = 4\, h_{ij}$$

permutation matrix

$$h' = 2\, h_{ij} + \tfrac{1}{2} I = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Linear Chain $J \sum_i S_i \cdot S_{i+1}$

Bethe Ansatz

<u>Trick</u> generates "on the fly"

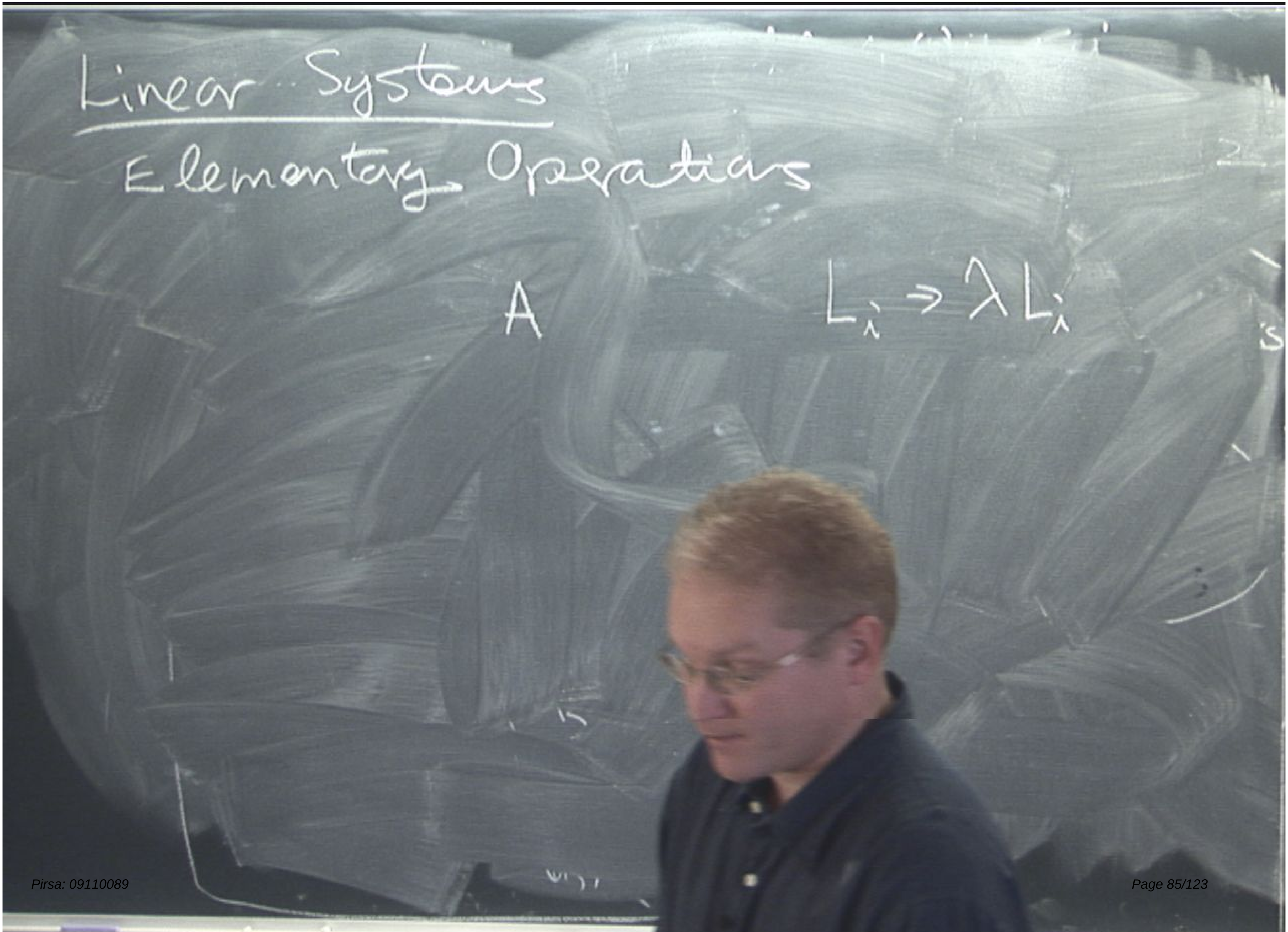
$$4\, S_1 \cdot S_2 = \begin{pmatrix} 1 & & & \\ & -1 & 2 & \\ & 2 & -1 & \\ & & & 1 \end{pmatrix} = 4\, h_{ij}$$

permutation matrix

$$h' = 2\, h_{ij} + \frac{1}{2} I = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Linear Systems

Elementary Operations


Linear Systems
Elementary Operations
A
$L_i \Rightarrow \lambda L_i$

Linear Systems

Elementary Operations

$$\begin{pmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & \lambda & & & & \\ & & & 1 & & & \\ & & & & 1 & & \\ & & & & & 1 & \\ & & & & & & 1 \end{pmatrix} A \qquad L_i \Rightarrow \lambda L_i$$

J_1

Linear Systems

Elementary Operations

1 $\begin{pmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & \lambda & & & & \\ & & & 1 & & & \\ & & & & 1 & & \\ & & & & & \ddots & \\ & & & & & & 1 \end{pmatrix} A$ $\qquad L_i \Rightarrow \lambda L_i$

J_1

2

Linear Systems

Elementary Operations

① $\begin{pmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & \lambda & & & \\ & & & 1 & & \\ & & & & \ddots & \\ & & & & & 1 \end{pmatrix} A$ $\qquad L_i \Rightarrow \lambda L_i$

J_1

② $\qquad L_i \Leftrightarrow L_i + \lambda L_j$

Linear Systems

Elementary Operations

① $\begin{pmatrix} 1 & & & & & \\ & 1 & & & & \\ & & \lambda & & & \\ & & & 1 & & \\ & & & & 1 & \\ & & & & & 1 \end{pmatrix} A$ $\qquad L_i \Rightarrow \lambda L_i$

J_1

② $\begin{pmatrix} & & \\ & & \\ & & \end{pmatrix} A$ $\qquad L_i \Leftrightarrow L_i + \lambda L_j$

Linear Systems

Elementary Operations

(1) $\begin{pmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & \lambda & & & & \\ & & & 1 & & & \\ & & & & 1 & & \\ & & & & & 1 & \\ & & & & & & 1 \end{pmatrix} A \qquad L_i \Rightarrow \lambda L_i$

J_1

(2) $\begin{pmatrix} 1 & & & & & & & \\ & 1 & & & & & & \\ & & 1 & & & & & \\ & & & 1 & & & & \\ & & & & 1 & & & \\ & & & & & 1 & & \\ & & & & & & 1 & \\ & & & & & & & 1 \end{pmatrix} A \qquad L_i \Leftrightarrow L_i + \lambda L_j$

Linear Systems

Elementary Operations

(1) $\begin{pmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & \lambda & & & & \\ & & & 1 & & & \\ & & & & 1 & & \\ & & & & & 1 & \\ & & & & & & 1 \end{pmatrix} A$ $\qquad L_i \Rightarrow \lambda L_i$

$J_i \qquad j$

(2) $\begin{pmatrix} 1 & & & & & & & \\ & 1 & & & & & & \\ & & 1 & & & & & \\ & & & 1 & & & & \\ & & & & 1 & & & \\ & & & & & 1 & & \\ & & & & & & 1 \; \lambda & \\ & & & & & & & 1 \end{pmatrix} A$ $\qquad L_i \Leftrightarrow L_i + \lambda L_j$


3
$L_i \Leftrightarrow L_j$

$$3 \qquad \begin{array}{ccccccccc} & & i & & & j & & & \\ \end{array}$$

$$\begin{pmatrix} 1 & & & & & & & \\ & 1 & & & & & & \\ & & 0 & & 1 & & & \\ & & & 1 & & & & \\ & & & & 1 & & & \\ & & 1 & & 0 & & & \\ & & & & & 1 & & \\ & & & & & & 1 & \\ & & & & & & & 1 \end{pmatrix} A$$

$$L_i \leftrightarrow L_j$$

$L_i \leftrightarrow L_j$

$$3 \quad \begin{array}{c} \begin{array}{ccccccc} & & i & & j & & \end{array} \\ \begin{pmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & 0 & & 1 & & \\ & & & 1 & & & \\ & & 1 & & 0 & & \\ & & & & & 1 & \\ & & & & & & 1 \end{pmatrix} \end{array} \quad A$$

I_3

Matrix Inversion

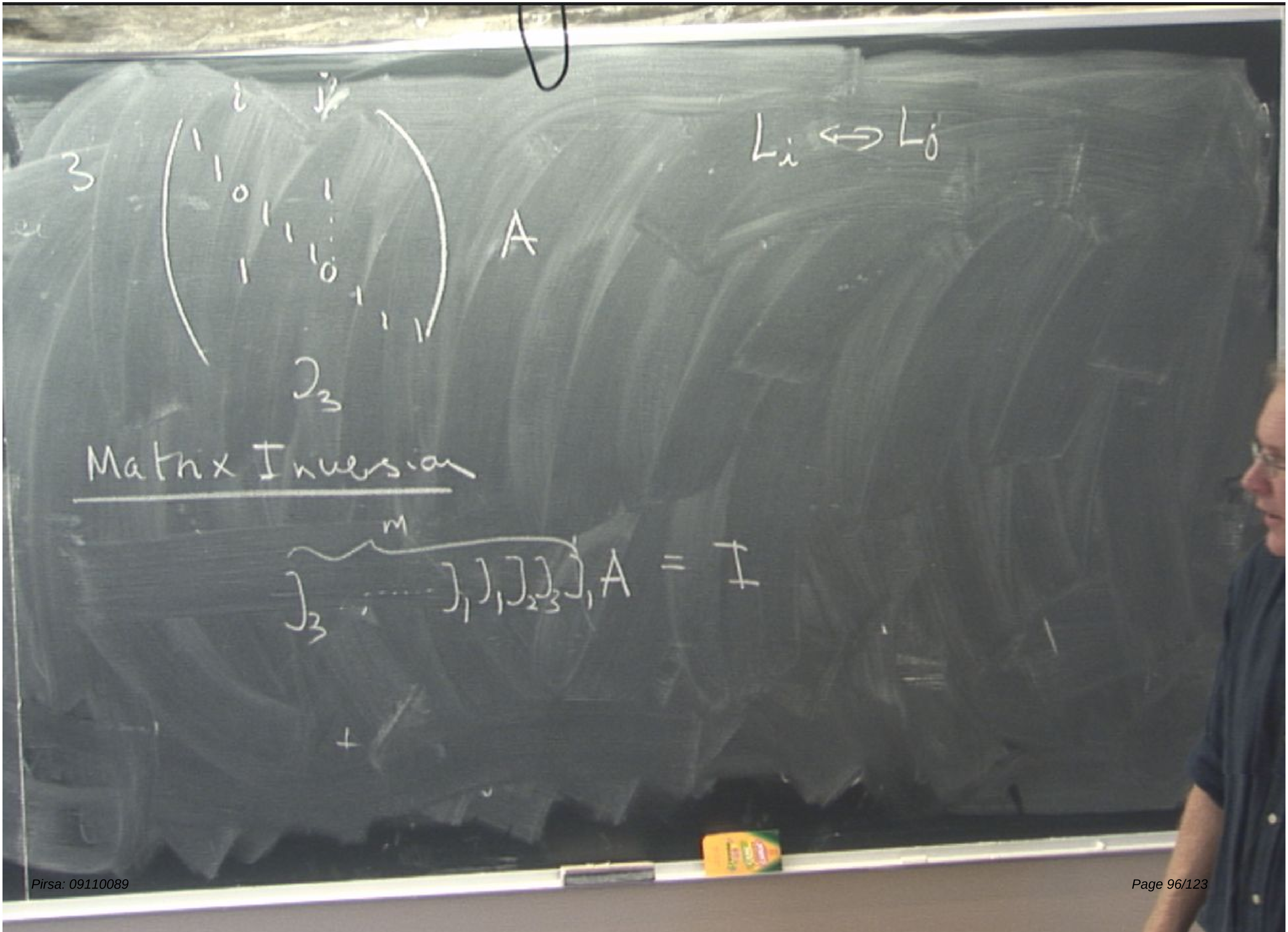
$$3 \quad \begin{array}{c} \begin{array}{ccccccc} & & i & & j & & \end{array} \\ \begin{pmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & 0 & & 1 & & \\ & & & 1 & & & \\ & & 1 & & 0 & & \\ & & & & & 1 & \\ & & & & & & 1 \end{pmatrix} \end{array} \quad A$$

$$\mathcal{J}_3$$

$$L_i \Leftrightarrow L_j$$

Matrix Inversion

$$\mathcal{J}_3 \cdots\cdots \mathcal{J}_1 \mathcal{J}_1 \mathcal{J}_2 \mathcal{J}_3 \mathcal{J}_1 A$$



$L_i \Leftrightarrow L_j$
A
J_3
Matrix Inversion
$\overbrace{J_3 \cdots\cdots J_1 J_1 J_2 J_3 J_1}^{m} A = I$

$$\begin{array}{c} \quad\quad\quad\quad i \quad\quad\quad j \\ J_3 = \begin{pmatrix} 1 & & & & & & & \\ & 1 & & & & & & \\ & & 0 & & & 1 & & \\ & & & 1 & & & & \\ & & & & 1 & & & \\ & & 1 & & & 0 & & \\ & & & & & & 1 & \\ & & & & & & & 1 \end{pmatrix} \end{array} \quad A$$

$$L_i \Leftrightarrow L_j$$

Matrix Inversion

$$\overbrace{J_3 \cdots\cdots J_1 J_1 J_2 J_3 J_1}^{m} A = I$$

$$\Downarrow$$

$$J_3 \cdots\cdots J_1 = A^{-1}$$

$$\begin{array}{cc} & \begin{array}{ccccccccc} & & i & & & j & & & \end{array} \\ 3 & \begin{pmatrix} 1 & & & & & & & & \\ & 1 & & & & & & & \\ & & 0 & & & 1 & & & \\ & & & 1 & & & & & \\ & & & & 1 & & & & \\ & & & & & 1 & & & \\ & & 1 & & & 0 & & & \\ & & & & & & 1 & & \\ & & & & & & & 1 & \\ & & & & & & & & 1 \end{pmatrix} A \end{array}$$

J_3

$L_i \leftrightarrow L_j$

$J_1 \; J_2 \; J_3$ are all invertible

Matrix Inversion

$$\overbrace{J_3 \cdots\cdots J_1 J_1 J_2 J_3 J_1}^{m} A = I$$

$$\Downarrow$$

$$J_3 \cdots\cdots J_1 = A^{-1}$$

$$3 \quad \begin{array}{c} \begin{array}{ccccccccc} & & i & & & j & & & \end{array} \\ \begin{pmatrix} 1 & & & & & & & & \\ & 1 & & & & & & & \\ & & 0 & & & 1 & & & \\ & & & 1 & & & & & \\ & & & & 1 & & & & \\ & & 1 & & & 0 & & & \\ & & & & & & 1 & & \\ & & & & & & & 1 & \\ & & & & & & & & 1 \end{pmatrix} \\ J_3 \end{array} \quad A$$

$L_i \leftrightarrow L_j$

$J_1 \ J_2 \ J_3$ are all invertible

Matrix Inversion

$$\overbrace{J_3 \cdots\cdots J_1 J_1 J_2 J_3 J_1}^{m} A = I$$

$$\Downarrow$$

$$J_3 \cdots\cdots J_1 = A^{-1}$$

$$3 = \begin{array}{c} \begin{array}{cccccc} & i & & j & & \end{array} \\ \begin{pmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & 0 & & 1 & & \\ & & & 1 & & & \\ & & 1 & & 0 & & \\ & & & & & 1 & \\ & & & & & & 1 \end{pmatrix} \end{array} A$$

J_3

$L_i \leftrightarrow L_j$

$J_1 \; J_2 \; J_3$ are all invertible

Matrix Inversion

$$\overbrace{J_3 \cdots J_1 J_1 J_2 J_3 J_1}^{m} A = I$$

$$\Downarrow$$

$$J_3 \cdots J_1 = A^{-1}$$

$$\begin{array}{c} \\ J_3 = \end{array} \begin{array}{c} \begin{array}{ccccccc} & & i & & j & & \end{array} \\ \begin{pmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & 0 & & 1 & & \\ & & & 1 & \vdots & & \\ & & 1 & & 0 & & \\ & & & & & 1 & \\ & & & & & & 1 \end{pmatrix} \end{array} \quad A$$

$$L_i \leftrightarrow L_j$$

$J_1 \; J_2 \; J_3$ are all invertible

Matrix Inversion

$$\overbrace{J_3 \cdots\cdots J_1 J_1 J_2 J_3 J_1}^{m} A = I$$

$$\Downarrow$$

$$J_3 \cdots\cdots J_1 = A^{-1}$$

Don't miss
— Column and row operations

Linear Systems

$$a_{11}x_1 + a_{12}x_2 \quad \cdots \quad a_{1n}x_n = b_1$$

Linear Systems

$$a_{11}x_1 + a_{12}x_2 \quad \cdots \quad a_{1n}x_n = b_1$$

$$\vdots$$

$$a_{n1}x_1 + a_{n2}x_2 \quad \cdots \quad a_{nn}x_n = b_n$$

Linear Systems

$$a_{11}x_1 + a_{12}x_2 \quad \cdots \quad a_{1n}x_n = b_1$$
$$a_{21}x_1 \quad \vdots$$
$$a_{n1}x_1 + a_{n2}x_2 \quad \cdots \quad a_{nn}x_n = b_n$$

Linear Systems

$$a_{11}x_1 + a_{12}x_2 \quad \cdots \quad a_{1n}x_n = b_1$$

$$a_{21}x_1 \quad \vdots$$

$$a_{n1}x_1 + a_{n2}x_2 \quad \cdots \quad a_{nn}x_n = b_n$$

$$L_2 \rightarrow L_2 - a_{21}\frac{L_1}{a_{11}}$$

Linear Systems

pivot

$$a_{11}x_1 + a_{12}x_2 \quad \cdots \quad a_{1n}x_n = b_1$$

$$a_{21}x_1 \quad \vdots$$

$$a_{n1}x_1 + a_{n2}x_2 \quad \cdots \quad a_{nn}x_n = b_n$$

$$L_2 \to L_2 - a_{21}\frac{L_1}{a_{11}}$$

Linear Systems

pivot

$$a_{11}x_1 + a_{12}x_2 \quad \cdots \quad a_{1n}x_n = b_1$$

$$a_{21}x_1$$

$$\vdots$$

$$a_{n1}x_1 + a_{n2}x_2 \quad \cdots \quad a_{nn}x_n = b_n$$

$$L_2 \to L_2 - a_{21}\frac{L_1}{a_{11}}$$

$$\downarrow$$

$$a_{11}x_1 + a_{12}x_2 + \quad \cdots \quad a_{1n}x_n = b_1$$

$$0 \quad a_{22}x_2$$

$$\vdots \quad 0 \quad a_{33}x_3$$

$$0 \quad 0$$

$$a_{nn}x_n = b_n$$

Linear Systems

pivot

$$a_{11}x_1 + a_{12}x_2 \quad \cdots \quad a_{1n}x_n = b_1$$

$$a_{21}x_1 \qquad \vdots$$

$$a_{n1}x_1 + a_{n2}x_2 \quad \cdots \quad a_{nn}x_n = b_n$$

$$L_2 \rightarrow L_2 - a_{21}\frac{L_1}{a_{11}}$$

$$\downarrow$$

$$a_{11}x_1 + a_{12}x_2 + \cdots a_{1n}x_n = b_1$$

$$0 \quad a_{22}x_2$$

$$\vdots \quad 0 \quad a_{33}x_3$$

$$0 \quad 0 \qquad a_{nn}x_n = b_n$$

Linear Systems

pivot

$$a_{11}x_1 + a_{12}x_2 \quad \cdots \quad a_{1n}x_n = b_1$$

$$a_{21}x_1 \quad \vdots$$

$$a_{n1}x_1 + a_{n2}x_2 \quad \cdots \quad a_{nn}x_n = b_n$$

$$L_2 \to L_2 - a_{21}\frac{L_1}{a_{11}}$$

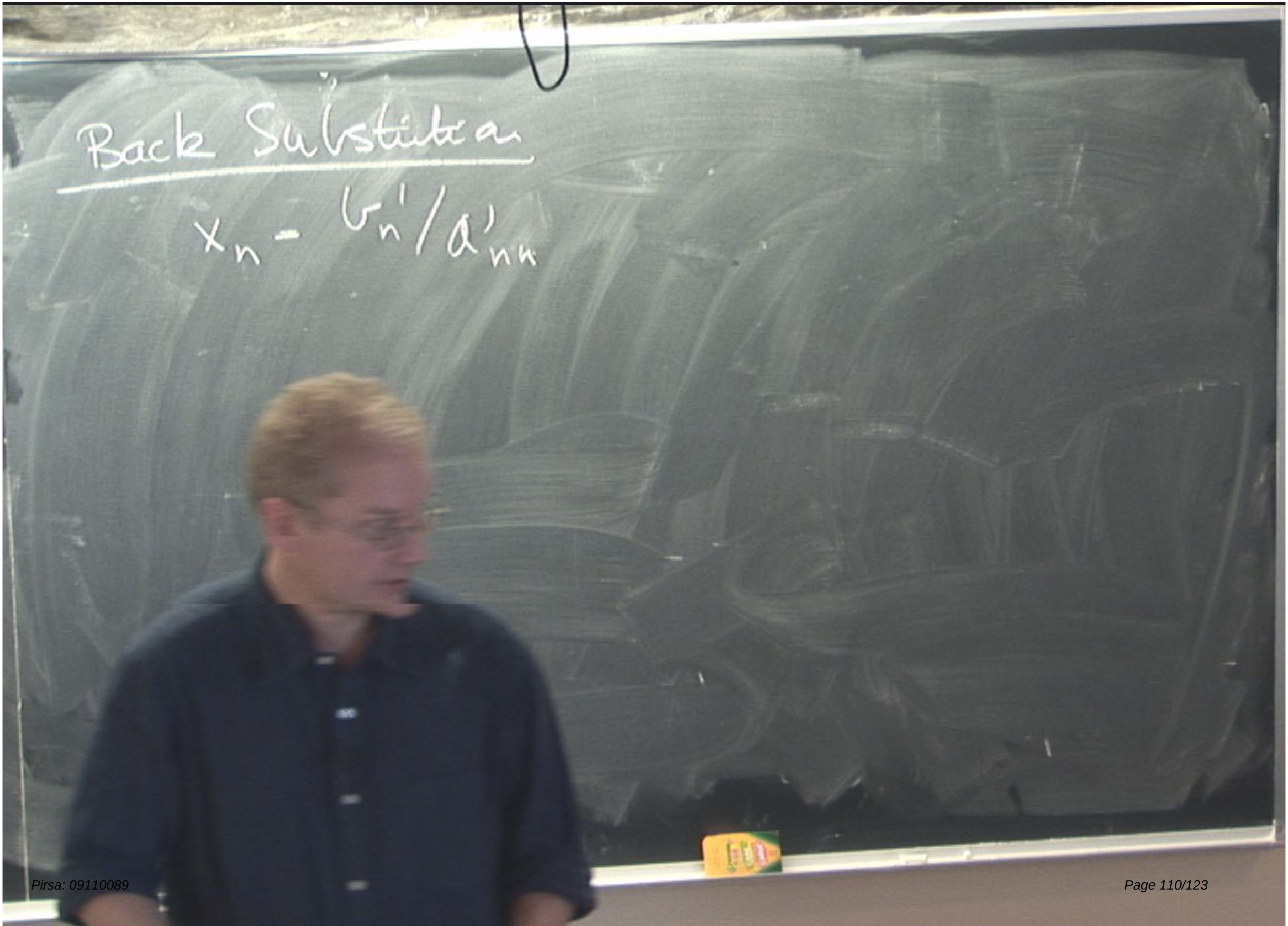
$$\downarrow$$

$$a_{11}x_1 + a_{12}x_2 + \quad \cdots \quad a_{1n}x_n = b_1$$

$$0 \quad a'_{22}x_2$$

$$\vdots \quad 0 \quad a'_{33}x_3$$

$$0 \quad 0 \quad \cdots \quad a'_{nn}x_n = b'_n$$


Back Substitution
$x_n = b'_n / a'_{nn}$

Back Substitution

$$x_n = b'_n / a'_{nn}$$

$$x_{n-1} = (b'_{n-1}$$

Back Substitution

$$x_n = b'_n / a'_{nn}$$

$$x_{n-1} = \left(b'_{n-1} - a'_{n-1,n}\, x_n \right) / a'_{n-1,n-1}$$

Back Substitution

$$x_n = b'_n / a'_{nn}$$

$$x_{n-1} = \left(b'_{n-1} - a'_{n-1,n} x_n \right) / a'_{n-1,n-1}$$

$$x_i = \left(b'_i - \sum_{k=i+1}^{n} a'_{ki} x_k \right) / a'_{ii}$$

Linear Systems

pivot

$$a_{11}x_1 + a_{12}x_2 \quad \cdots \quad a_{1n}x_n = b_1$$

$$a_{21}x_1 \quad \vdots$$

$$a_{n1}x_1 + a_{n2}x_2 \quad \cdots \quad a_{nn}x_n = b_n$$

$$\downarrow$$

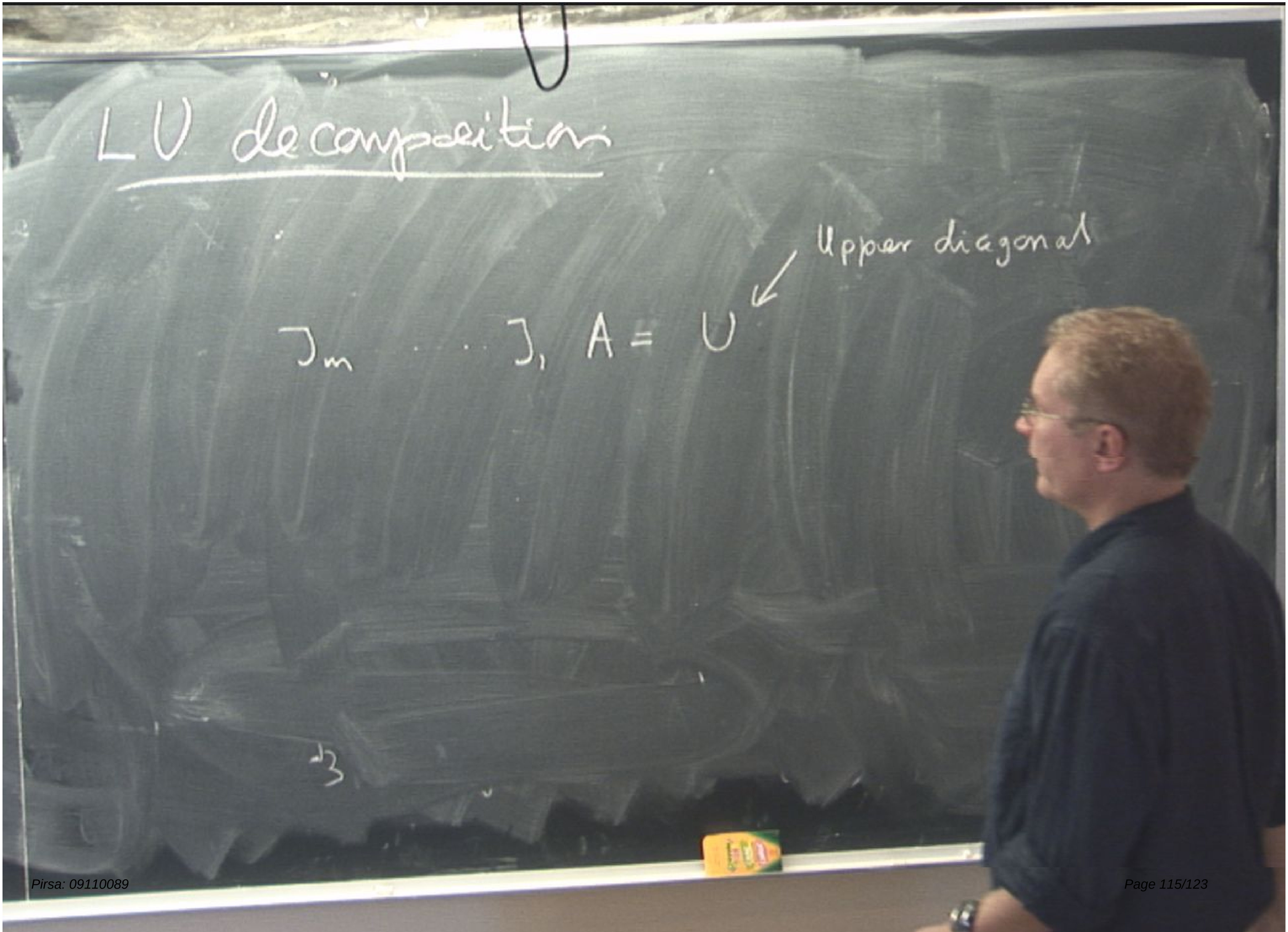
$$a_{11}x_1 + a_{12}x_2 + \quad \cdots \quad a_{1n}x_n = b_1$$

$$0 \quad a'_{22}x_2$$

$$\vdots \quad 0 \quad a'_{33}x_3$$

$$0 \quad 0 \quad a'_{nn}x_n = b'_n$$

$$L_2 \to L_2 - a_{21}\frac{L_1}{a_{11}}$$


LU decomposition
Upper diagonal
$J_m \cdots J_1 A = U$

LU decomposition

Upper diagonal

$$\left\{\begin{array}{l} \underbrace{J_m \cdots J_1}_{\text{Lower diagonal}}\, A = U \\ \text{Invertible} \\ J_i^{-1} \text{ is also lower diagonal} \end{array}\right.$$

$$\Downarrow$$

$$A = J_1^{-1} \cdots J_m^{-1} U = LU$$

LU decomposition

Upper diagonal

$$\underbrace{J_m \cdots\cdots J_1}_{\text{Lower diagonal}} A = U$$

Lower diagonal

Invertible

J_i^{-1} is also lower diagonal

$$\Downarrow$$

$$A = J_1^{-1} \cdots\cdots J_m^{-1} U = LU$$

LU decomposition

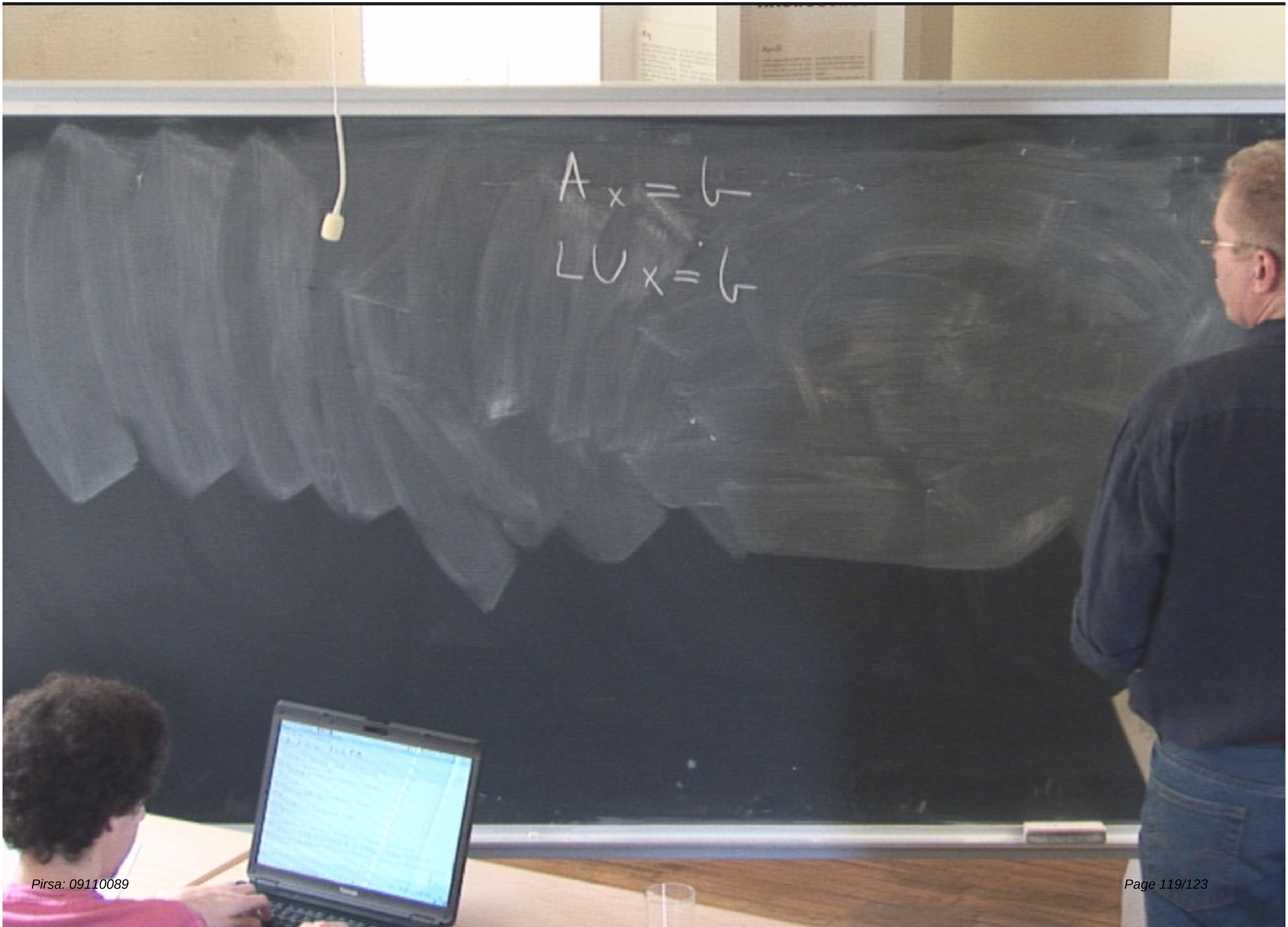
Upper diagonal

$$\underbrace{J_m \cdots\cdots J_1}_{\text{Lower diagonal}} A = U$$

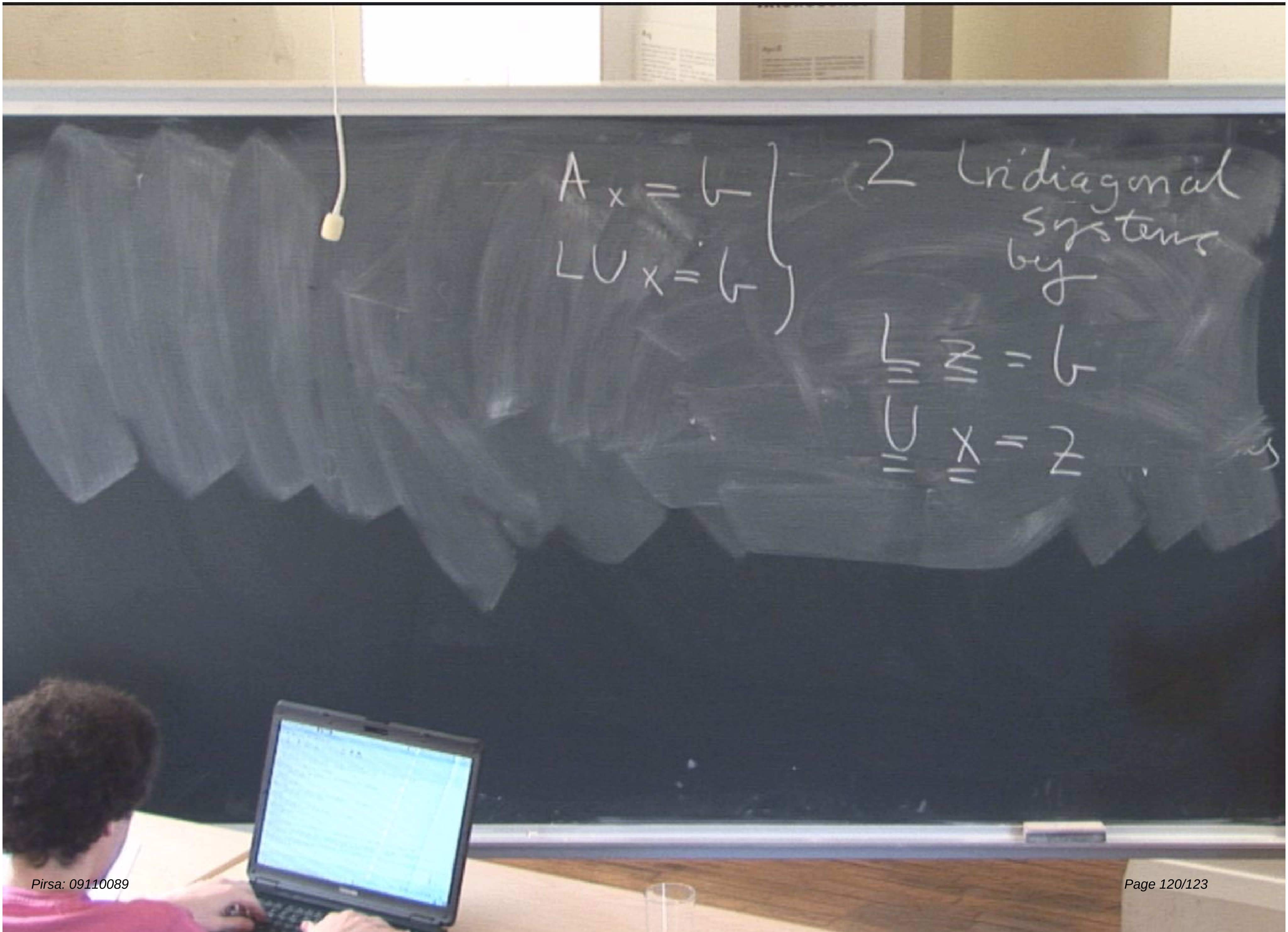
Lower diagonal
Invertible
J_i^{-1} is also lower diagonal

$$\Downarrow$$

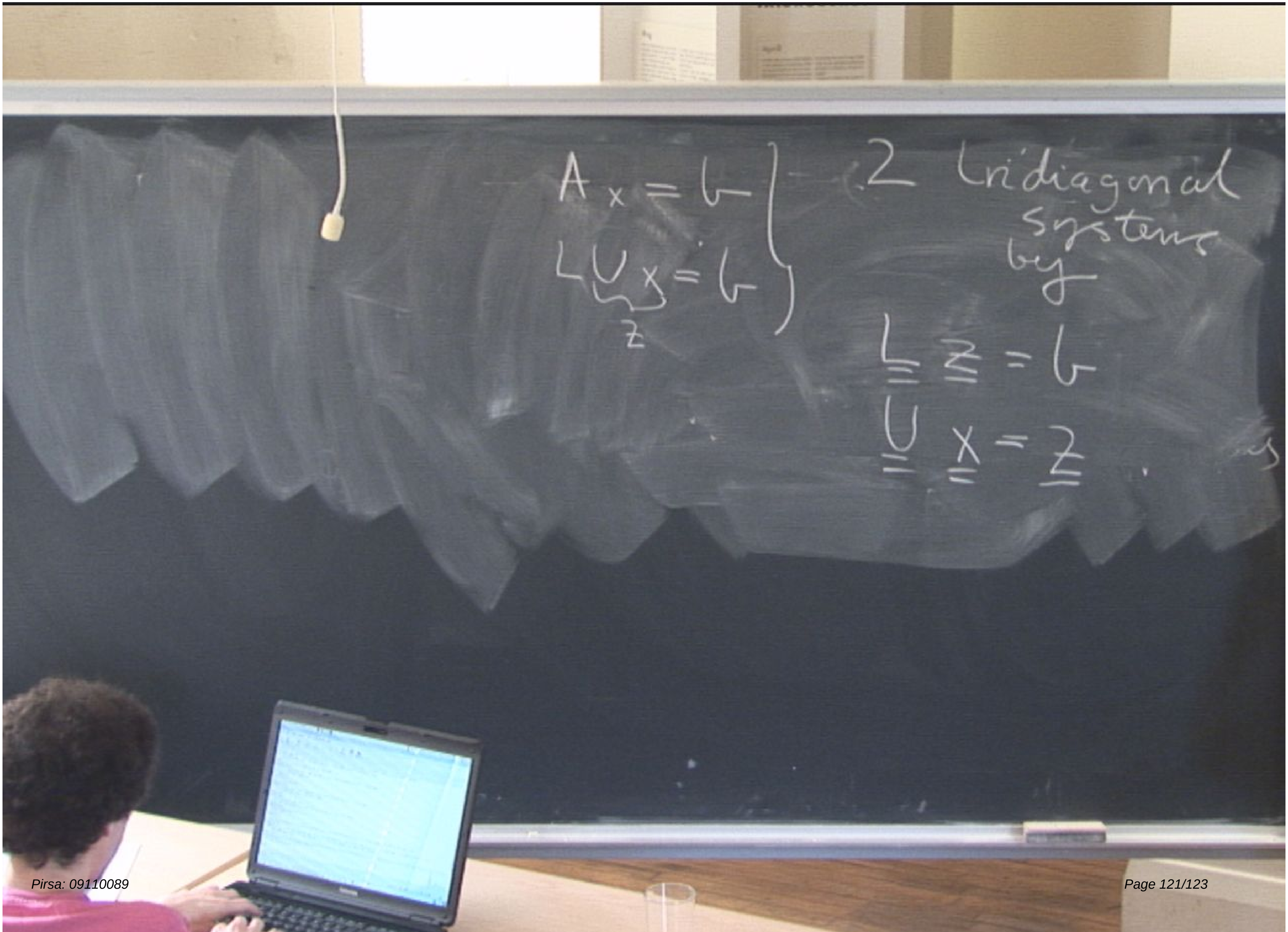
$$A = J_1^{-1} \cdots\cdots J_m^{-1} U = \underline{\underline{LU}}$$



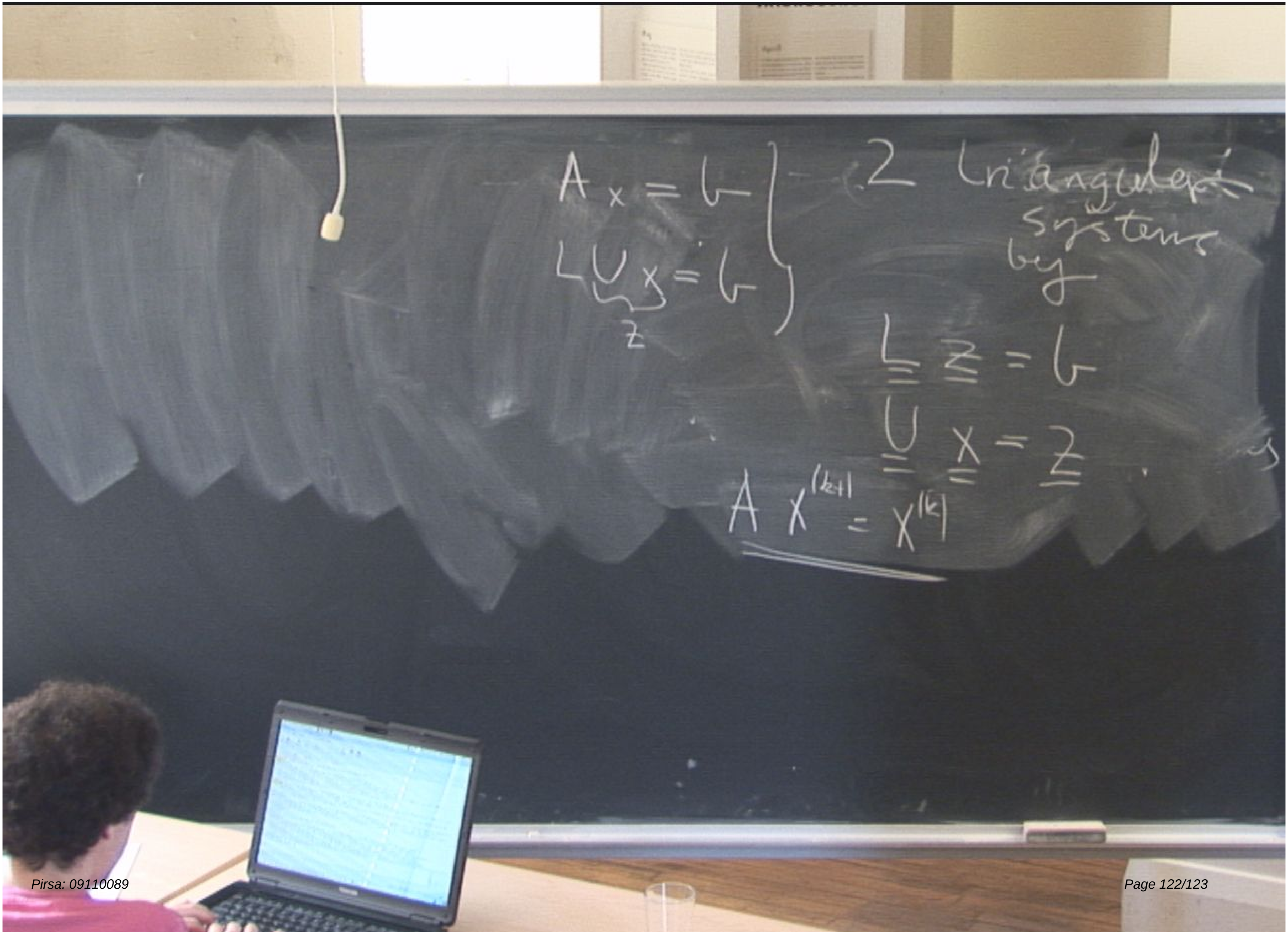
$Ax = b$
$LUx = b$

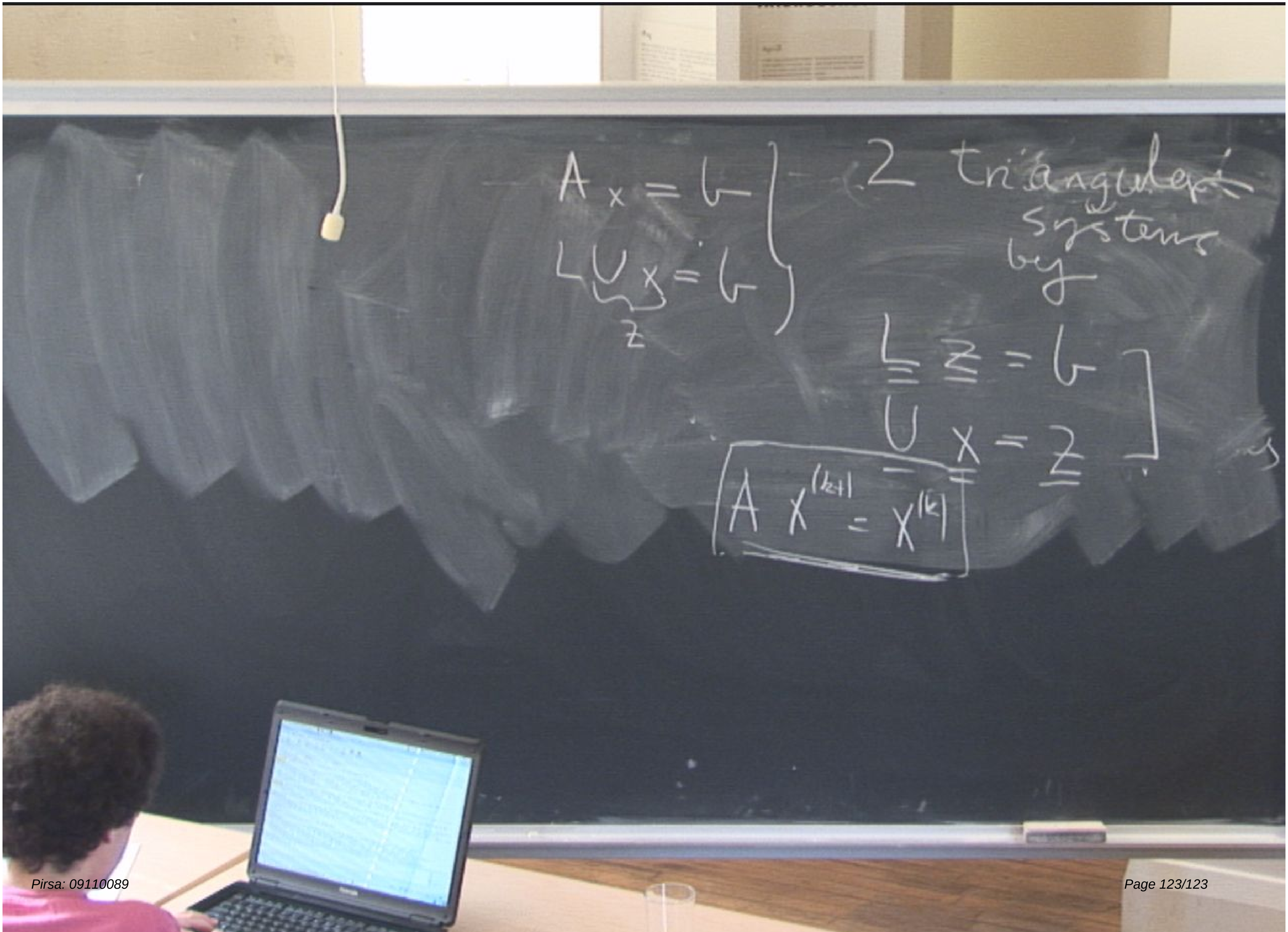


Ax = b
LUx = b
2 tridiagonal systems by
L z = b
U x = z



Ax = b
LUx = b
z
2 tridiagonal systems by
Lz = b
Ux = z


Ax = b
LUx = b
z
2 triangular systems by
Lz = b
Ux = z
Ax^(k+1) = x^(k)


$Ax = b$
$LUx = b$
z
2 triangular systems by
$Lz = b$
$Ux = z$
$Ax^{(k+1)} = x^{(k)}$