Title: Explorations in Quantum Information - Lecture 10

Date: Mar 28, 2011 09:00 AM

URL: http://pirsa.org/11030023

Abstract:

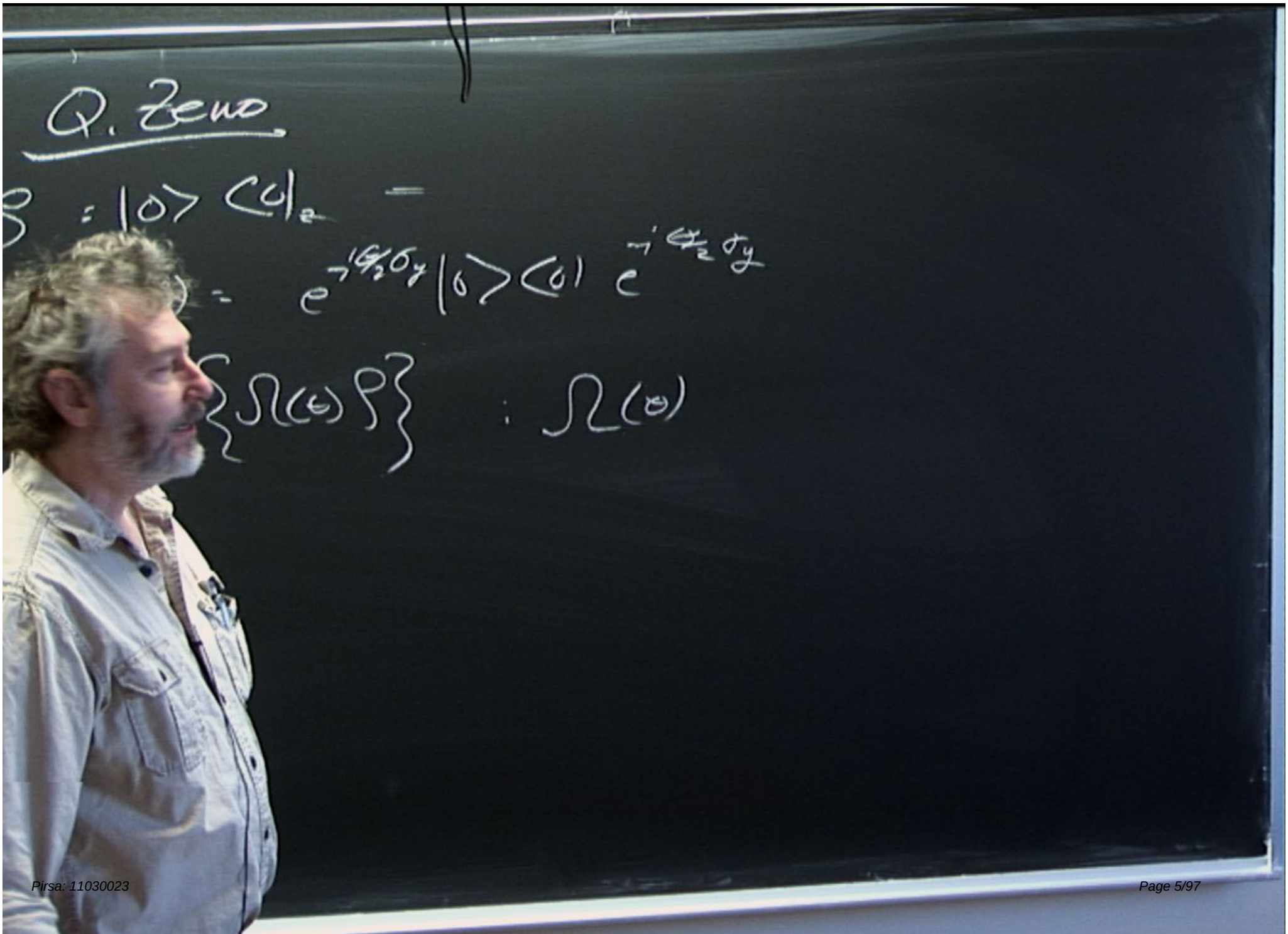
perimeter scholars
international

Q. Zeno

Q. Zeno

$|0\rangle\langle 0| =$

$\Omega =$


Q. Zeno
$\rho = |0\rangle\langle 0|_z$
$= e^{-i\frac{\theta}{2}\sigma_y}|0\rangle\langle 0|\, e^{-i\frac{\theta}{2}\sigma_y}$
$\{\Omega(\theta)\rho\}$: $\Omega(\theta)$

Q. Zeno

$|0\rangle\langle 0| \Rightarrow |1\rangle\langle 1|$

$\rho = |0\rangle\langle 0|$

$$\Omega(\theta) = e^{-i\frac{\theta}{2}\sigma_y}|0\rangle\langle 0|\, e^{-i\frac{\theta}{2}\sigma_y}$$

$$\mathrm{Tr}\{\underbrace{\Omega(\theta)\rho}_{\cos(\theta)}\} : \Omega(\theta)$$

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$$\cos(\pi/n)$$

# of steps

Q. Zeno

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$$\left(\cos\left(\pi/n\right)\right)^n \sim 1$$

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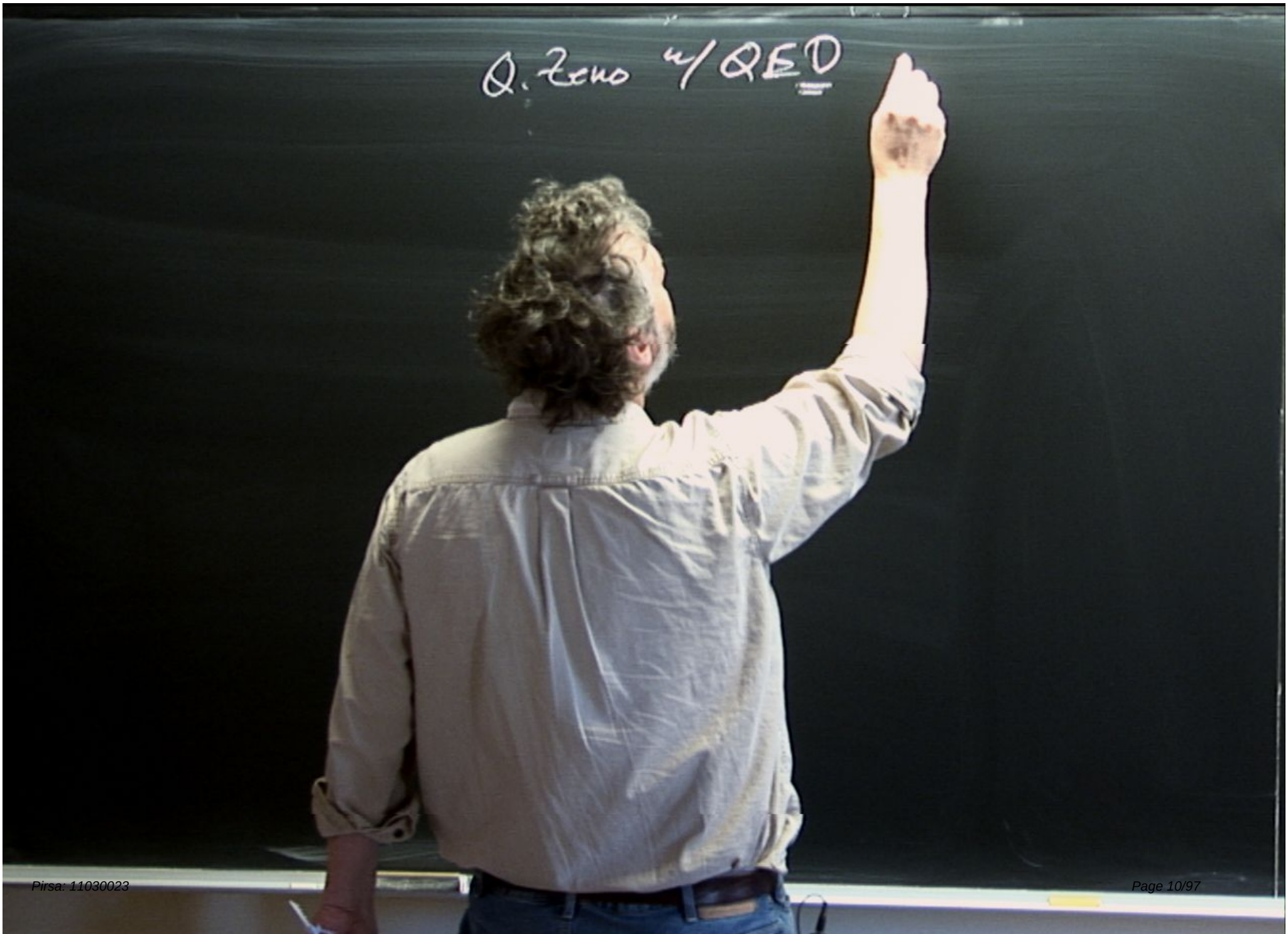
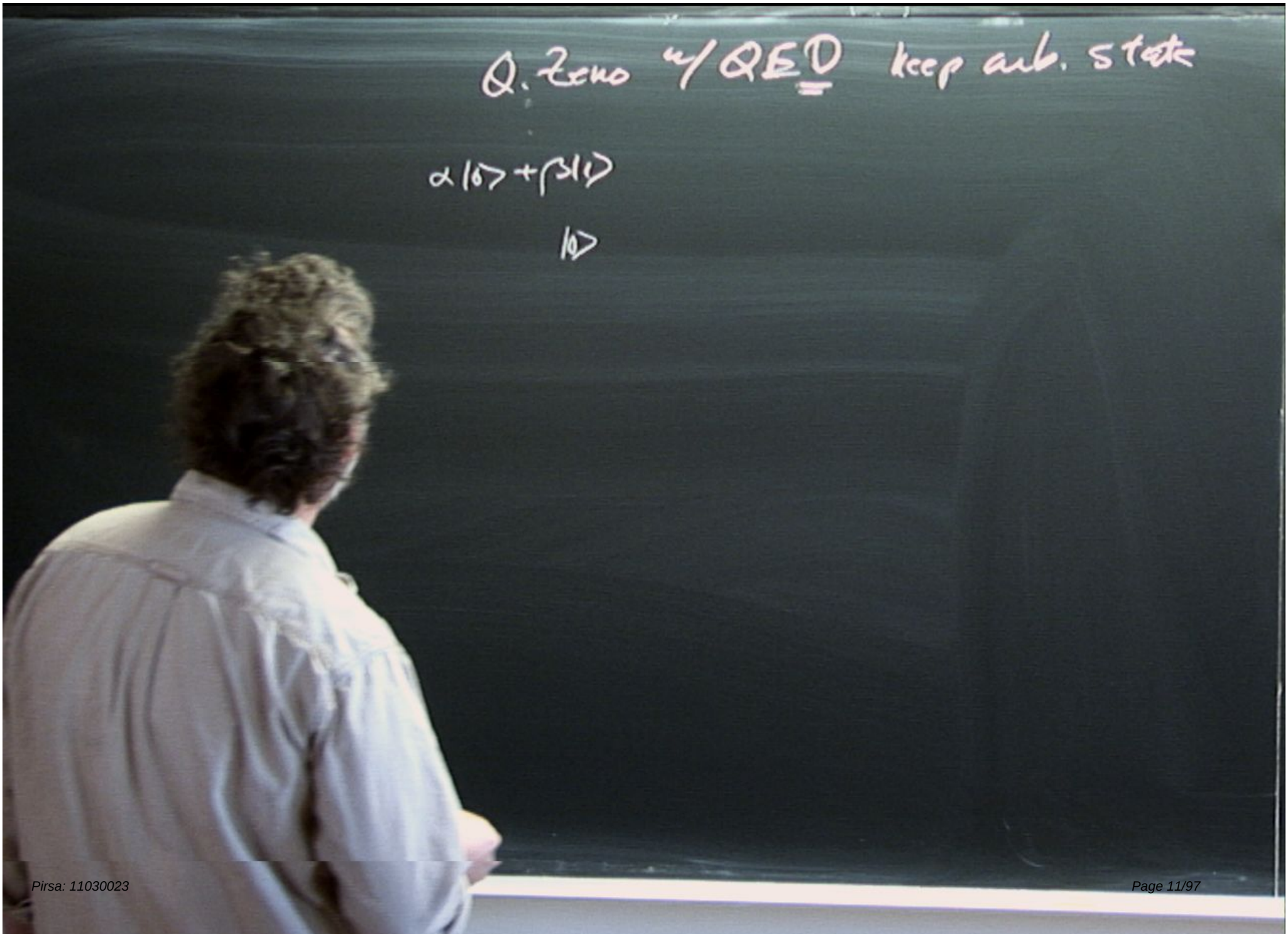
$\mathrm{Tr}\{\underbrace{\Omega(\theta)\rho}_{\cos(\theta)}\} : \Omega(\theta)$

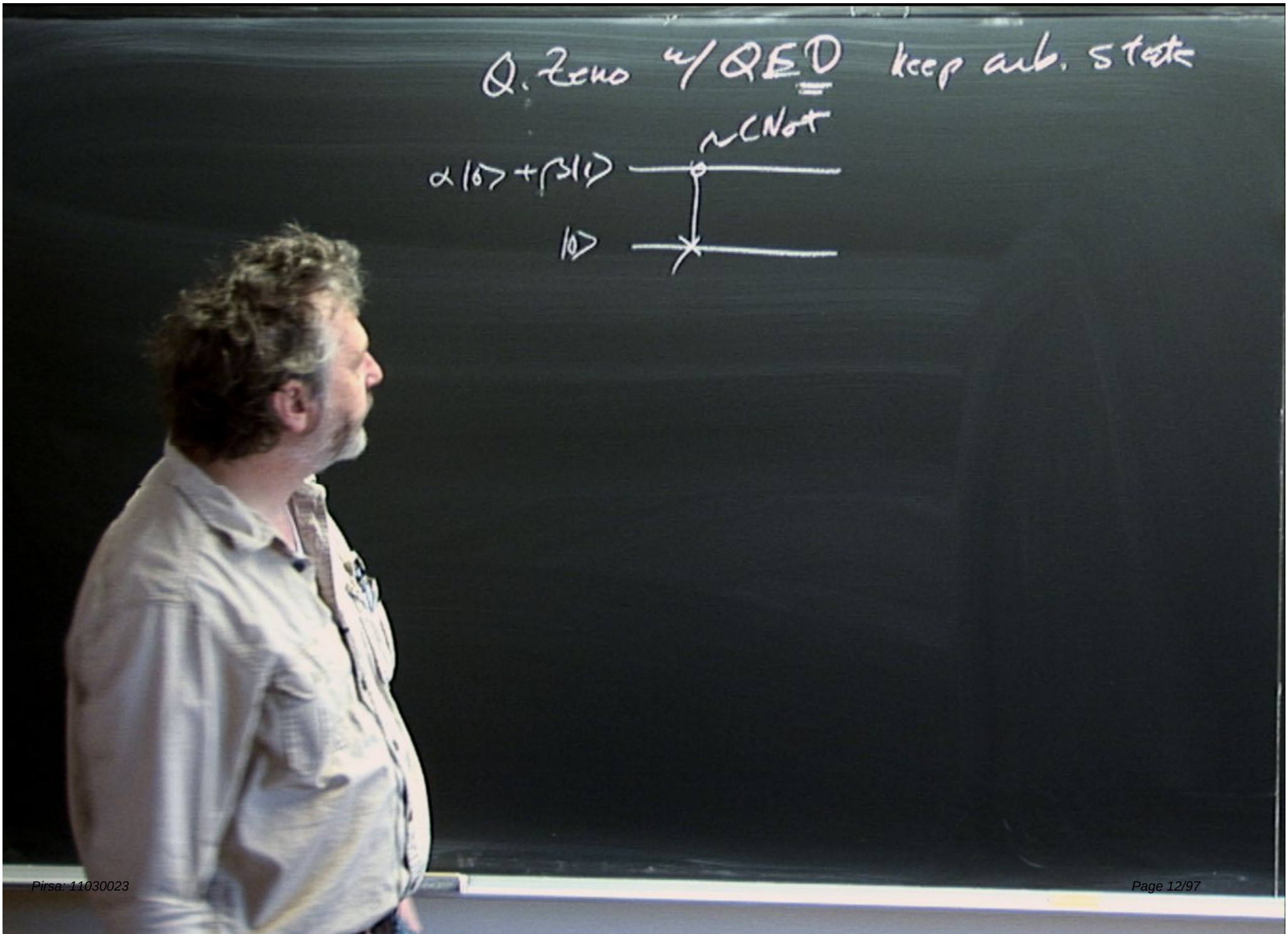
$\left(\cos(\pi/n)\right)^n \sim 1$

n = # of steps

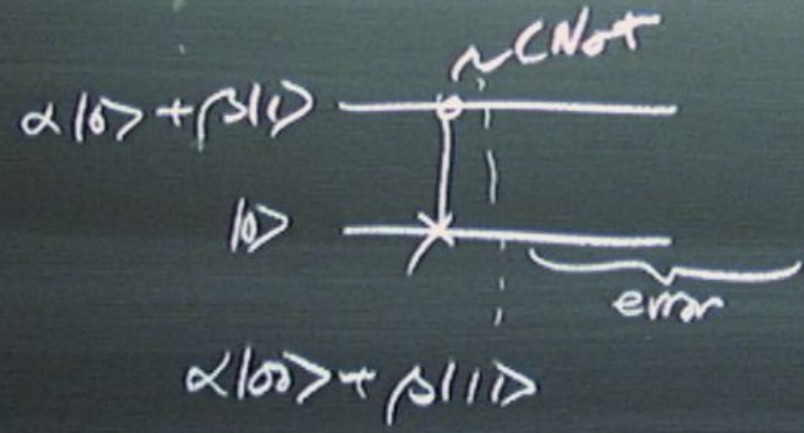
instead of strong meas. apply dephasing about Ω


Q. Zeno w/ QED

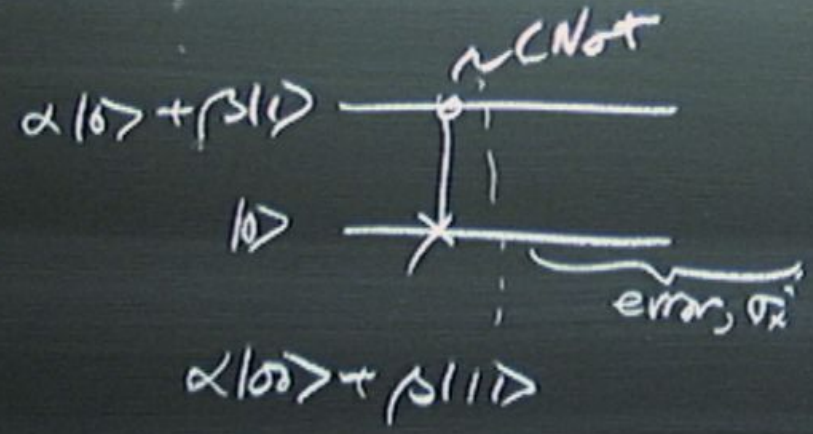

Q. Zeno w/ QED keep arb. state
α|0⟩ + β|1⟩
|0⟩

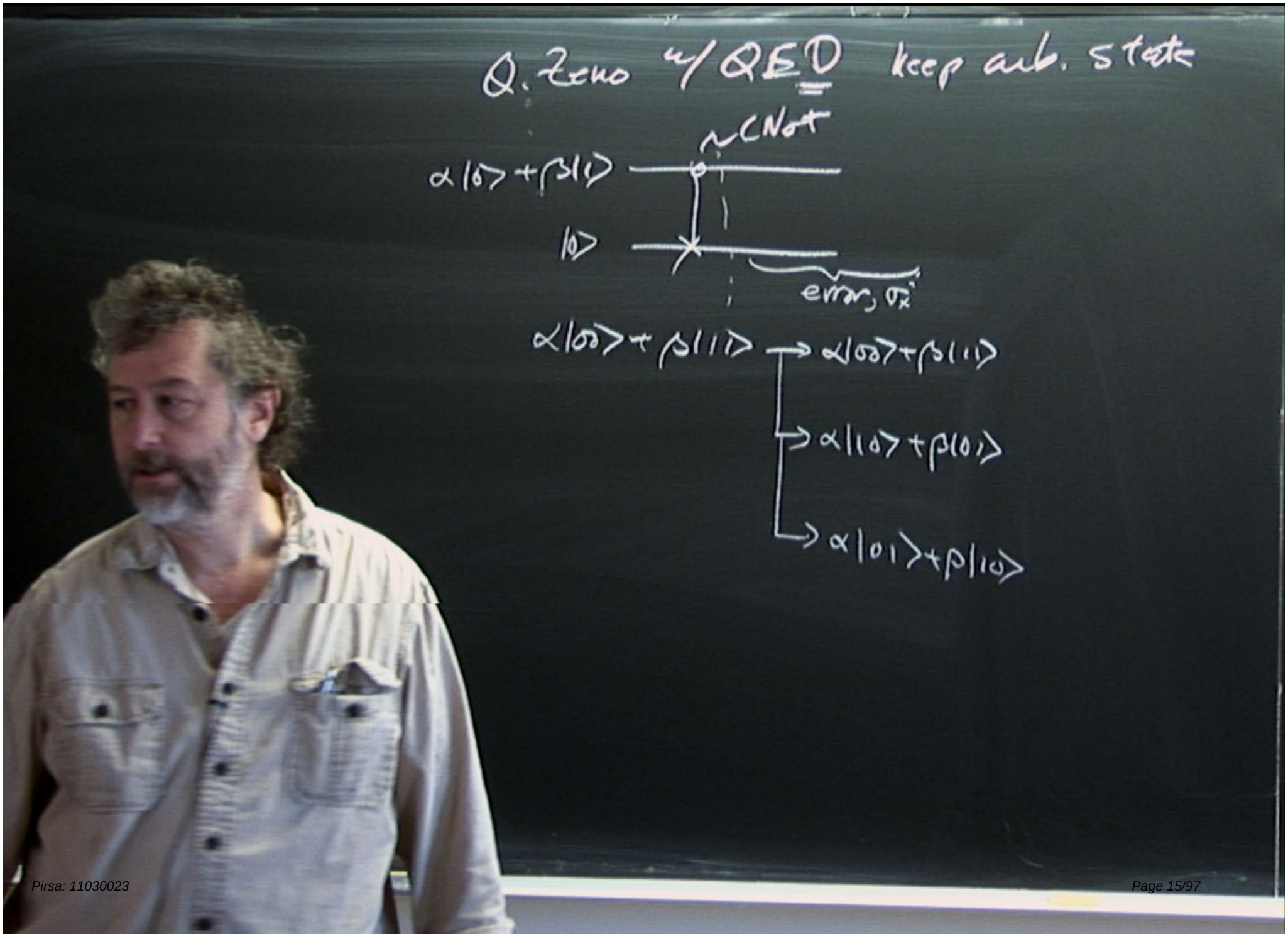

Q. Zeno w/ QED keep arb. state
~CNot
α|0⟩+β|1⟩
|0⟩

Q. Zeno w/ QED keep arb. state

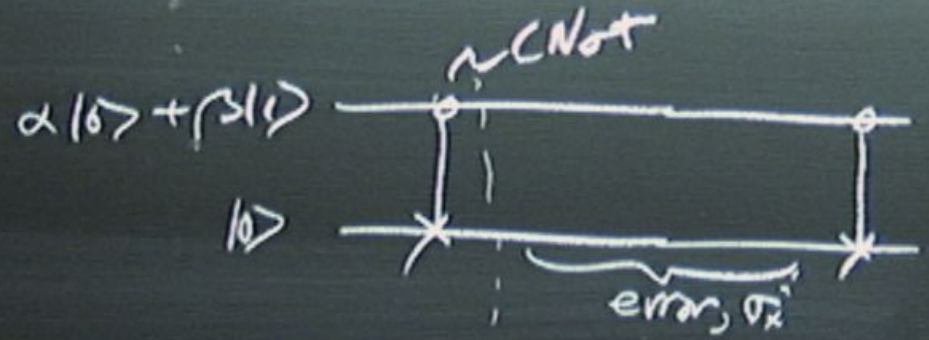


Q. Zeno w/ QED keep arb. state




Q. Zeno w/ QED keep arb. state
~CNot
α|0⟩+β|1⟩
|0⟩
error, σx
α|00⟩+β|11⟩
α|00⟩+β|11⟩
α|10⟩+β|01⟩
α|01⟩+β|10⟩

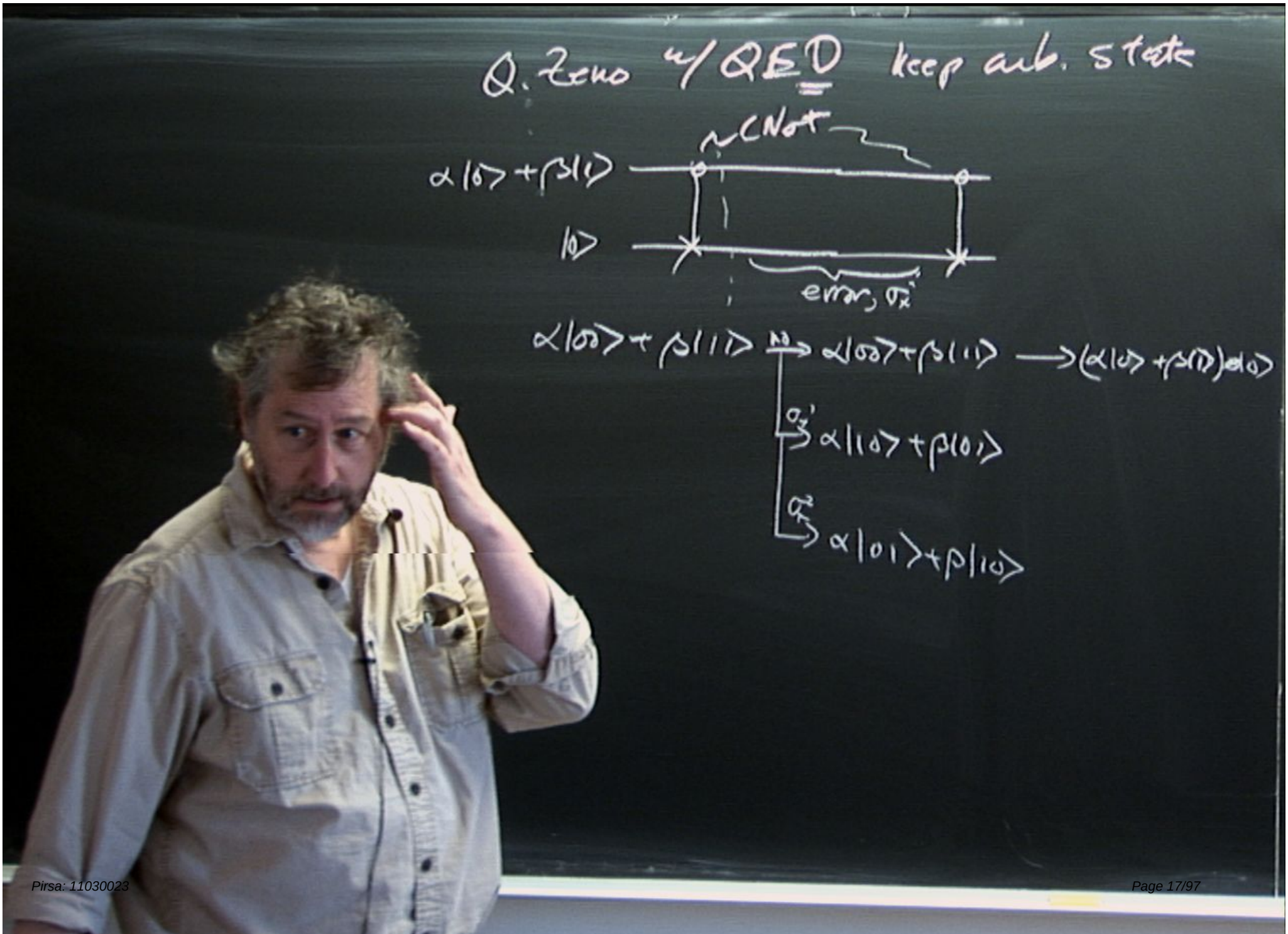
Q. Zeno w/ QED keep arb. state



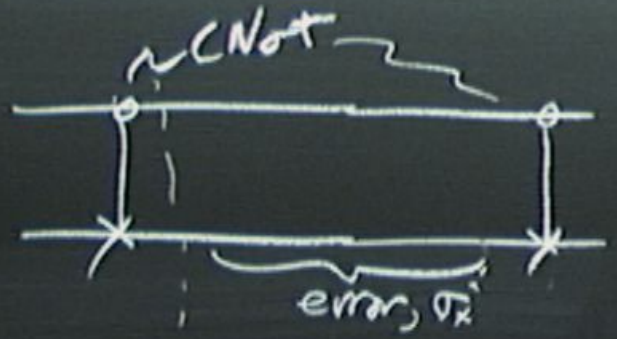
$$\alpha|00\rangle+\beta|11\rangle \xrightarrow{\text{no}} \alpha|00\rangle+\beta|11\rangle$$

$$\xrightarrow{\sigma_x^1} \alpha|10\rangle+\beta|01\rangle$$

$$\xrightarrow{\sigma_x^2} \alpha|01\rangle+\beta|10\rangle$$


Q. Zeno w/ QED keep arb. state
CNot
α|0⟩+β|1⟩
|0⟩
error, σx
α|00⟩+β|11⟩ → α|00⟩+β|11⟩ → (α|0⟩+β|1⟩)⊗|0⟩
σx¹
α|10⟩+β|01⟩
σx²
α|01⟩+β|10⟩

no w/ QED keep arb. state



if ancilla $|0\rangle$ then no error.

$$\alpha|00\rangle+\beta|11\rangle \xrightarrow{\text{no}} \alpha|00\rangle+\beta|11\rangle \longrightarrow (\alpha|0\rangle+\beta|1\rangle)\otimes|0\rangle$$

$$\xrightarrow{\sigma_x^1} \alpha|10\rangle+\beta|01\rangle \longrightarrow (\alpha|1\rangle+\beta|0\rangle)\otimes|1\rangle$$

$$\xrightarrow{\sigma_x^2} \alpha|01\rangle+\beta|10\rangle \longrightarrow (\alpha|0\rangle+\beta|1\rangle)\otimes|1\rangle$$

Q. Zeno

$$\rho = |0\rangle\langle 0|$$

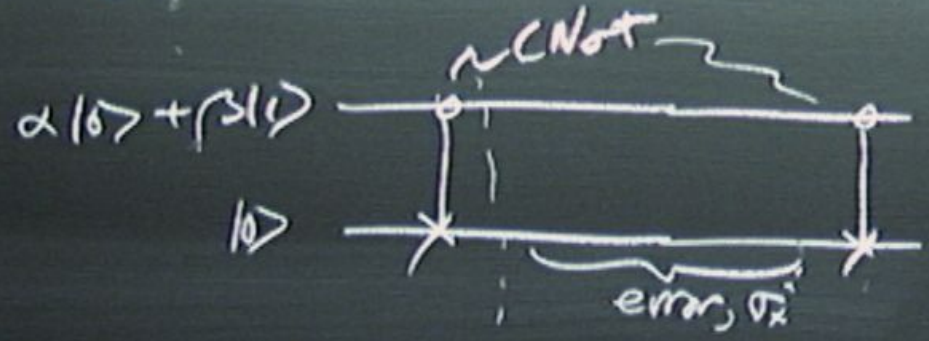
$$\Omega(\theta) = e^{-i\theta/2\,\sigma_y}|0\rangle$$

$$\mathrm{Tr}\{\underbrace{\Omega(\theta)\rho}_{\cos(\theta)}\} :$$

$$(\cos(\pi/n))^n$$

of

Q. Zeno w/ QED keep arb. state



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Q. Z

$\rho = |0$

$\Omega(\theta$

Tr

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QZeno.nb

1-qubit example

▪ Start with a pure state along z

```
input = (PauliMatrix[0] + PauliMatrix[3]) / 2;
```

```
input // MatrixForm
```

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

```
purity[m_] := Tr[m . m]
```

```
purity[input]
```

1

▪ Define measurement

Take the measurement as being in the x, z plane. The angle is that between the +z axis and the measurement.

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QZeno.nb

1-qubit example

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Take the measurement as being in the x, z plane. The angle is that between the +z axis and the measurement.

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QZeno.nb

Take the measurement as being in the x, z plane. The angle is that between the +z axis and the measurement.

```
meas[a_] := MatrixExp[-I a PauliMatrix[2] / 2] .
  ((PauliMatrix[0] + PauliMatrix[3]) / 2) .
  MatrixExp[I a PauliMatrix[2] / 2]
```

```
meas[a] // MatrixForm
```

$$\begin{pmatrix} \mathrm{Cos}\left[\frac{a}{2}\right]^2 & \mathrm{Cos}\left[\frac{a}{2}\right] \mathrm{Sin}\left[\frac{a}{2}\right] \\ \mathrm{Cos}\left[\frac{a}{2}\right] \mathrm{Sin}\left[\frac{a}{2}\right] & \mathrm{Sin}\left[\frac{a}{2}\right]^2 \end{pmatrix}$$

Examples

Note that the measurement gives both the projection of the input onto the measurment operator and a new state, which is the meaurement operator

steps of $\pi/100$

```
astep = π / 100;
```

```
output[n_] :=
```

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QZeno.nb

operator and a new state, which is the meaurement operator

steps of $\pi/100$

```
astep = π / 100;

output[n_] :=
 output[n] =
  Tr[meas[n astep] . output[n - 1]] meas[(n - 1) astep] // N

output[1] = input;

output[100]
```

```
{{0.00022375, 0.0142432}, {0.0142432, 0.906674}}
```

```
purity[output[100]]
```

```
0.822464
```

```
pl = ListPlot[Table[purity[output[n]], {n, 1, 100}],
  {PlotRange → {0, 1}, AxesLabel → {step, purity}}]
```

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QZeno.nb

operator and a new state, which is the measurement operator

steps of $\pi/100$

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astep = π / 100;

output[n_] :=
 output[n] =
  Tr[meas[n astep] . output[n - 1]] meas[(n - 1) astep] // N

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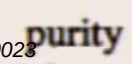
{{0.00022375, 0.0142432}, {0.0142432, 0.906674}}
```

```
purity[output[100]]
```

```
0.822464
```

```
p1 = ListPlot[Table[purity[output[n]], {n, 1, 100}],
  {PlotRange → {0, 1}, AxesLabel → {step, purity}}]
```



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QZeno.nb

```
purity[output[100]]
```

```
0.822464
```

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p1 = ListPlot[Table[purity[output[n]], {n, 1, 100}],
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```

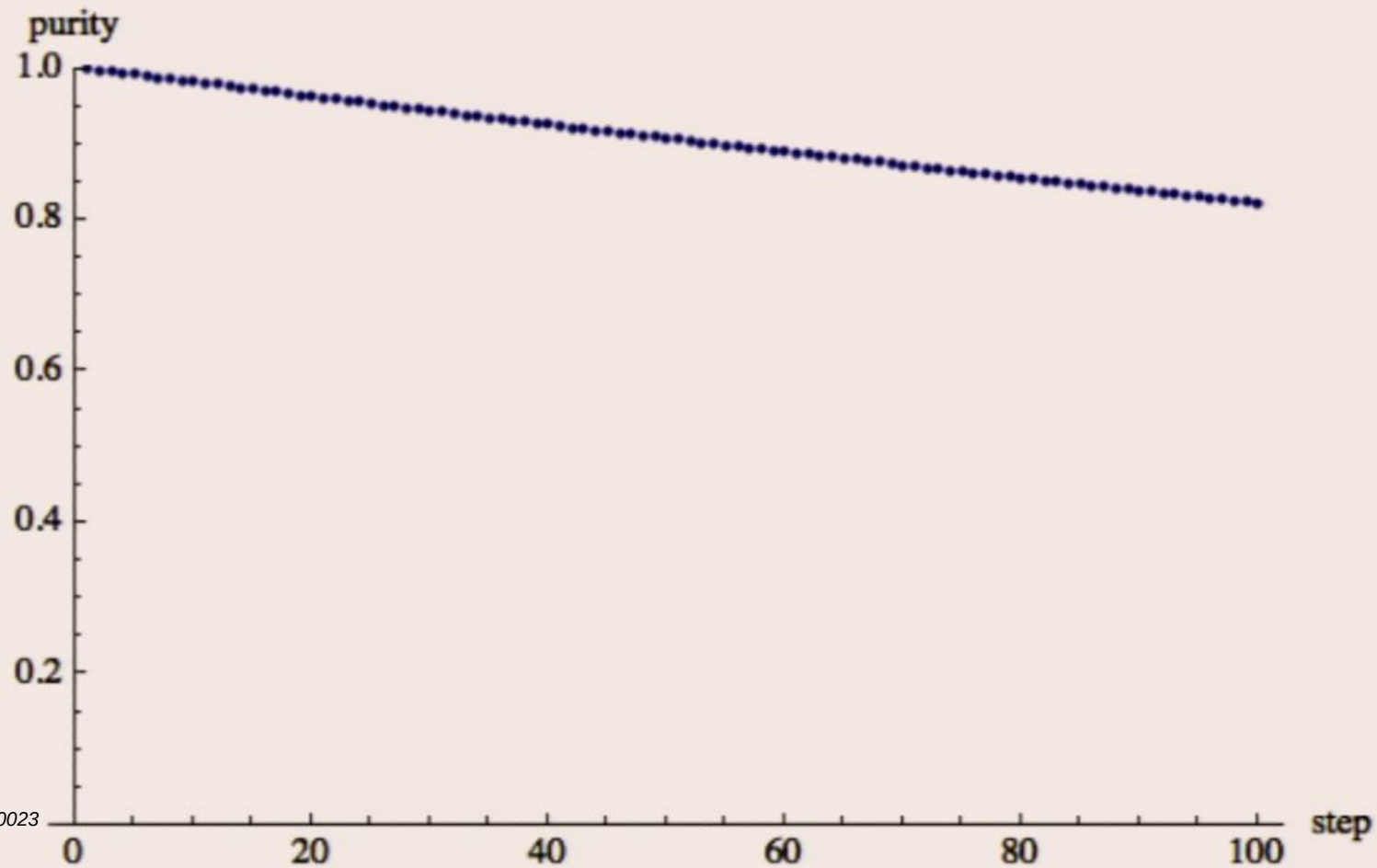

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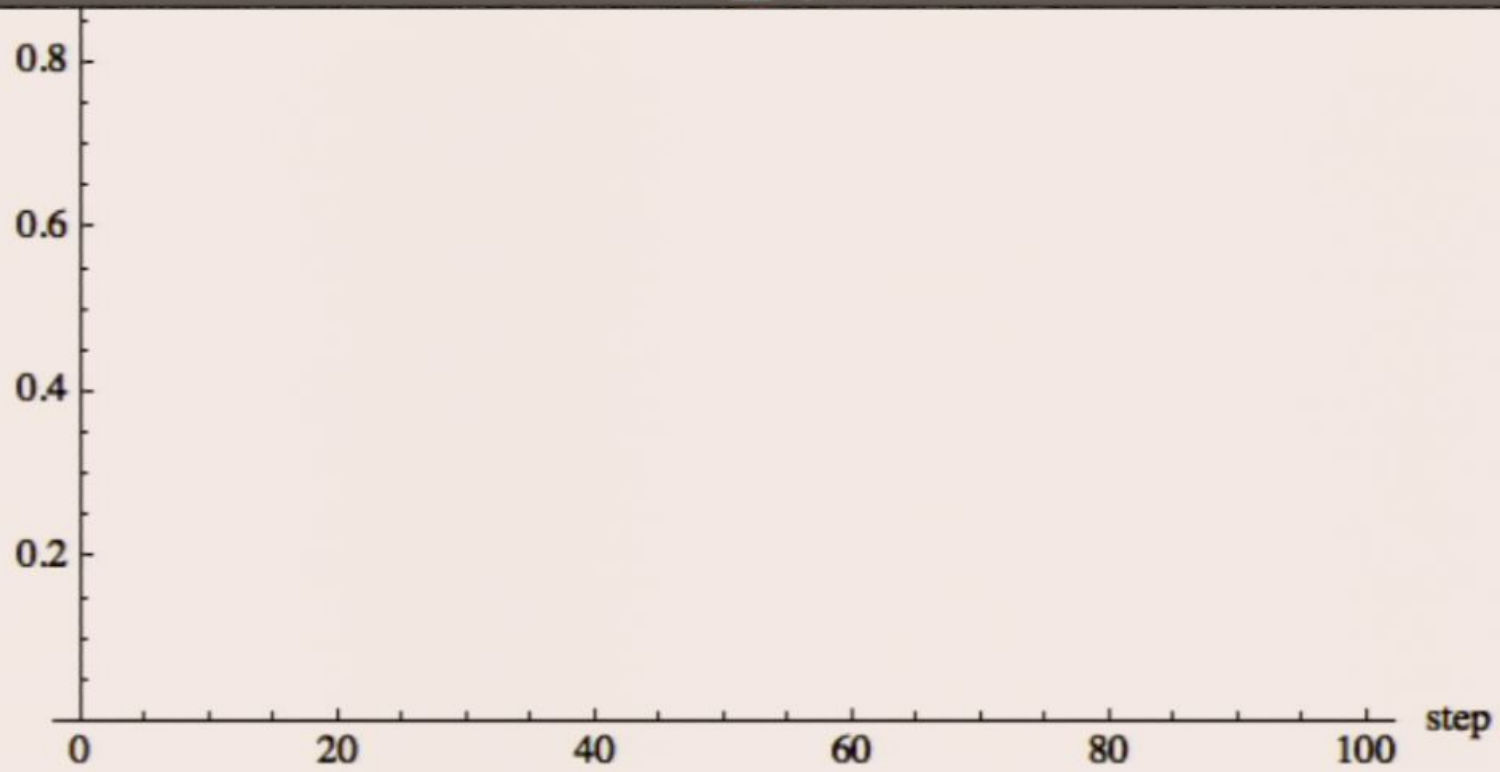
QZeno.nb




```
QZ2 =
  Graphics3D[
   {Thick, Red,
    Line[Table[{Tr[PauliMatrix[1] . output2[n]], 0,
       Tr[PauliMatrix[3] . output2[n]]}, {n, 1, 200}]]}];

Show[sz, sy, sx, QZ2, DisplayFunction → $DisplayFunction]
```

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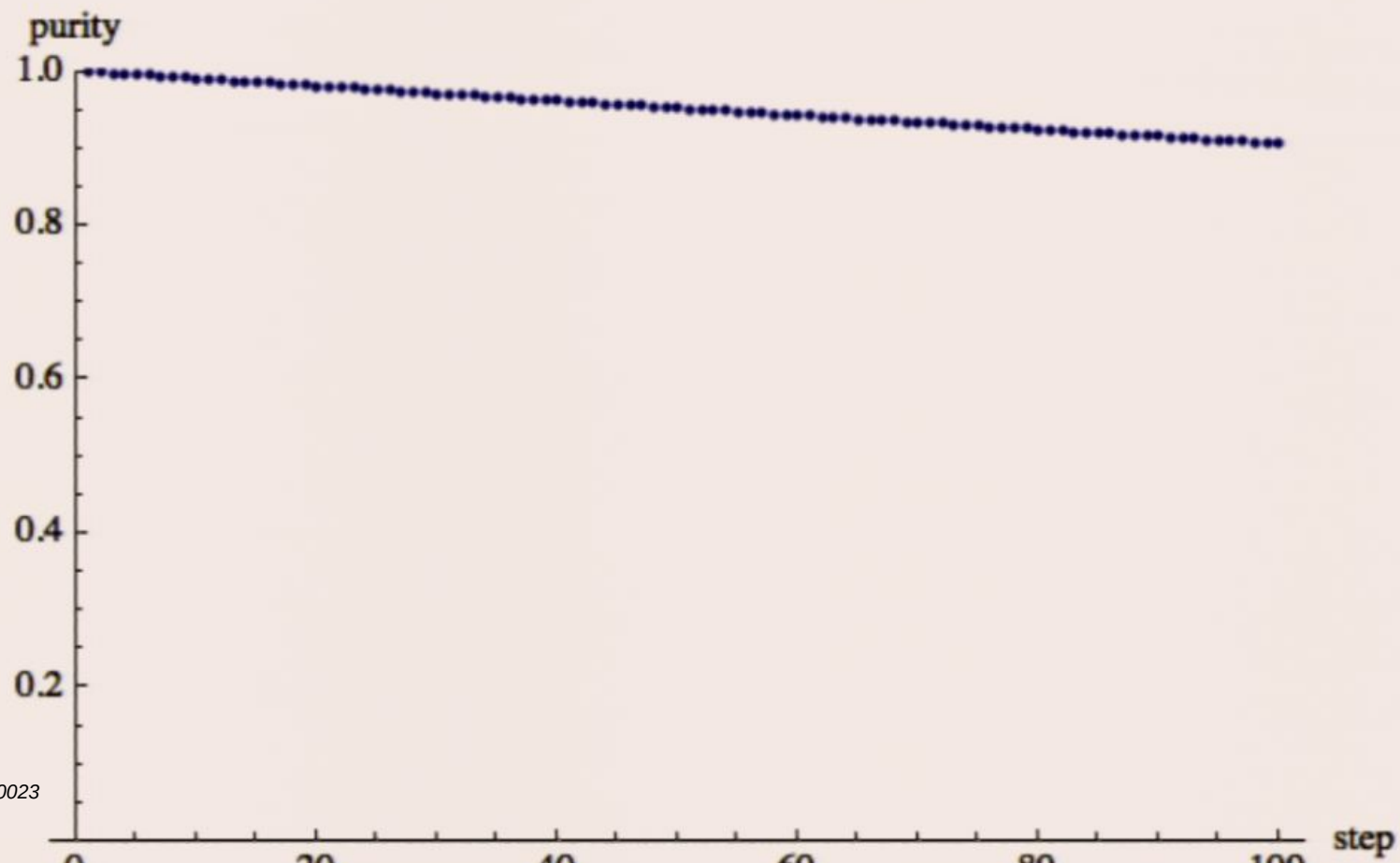
QZeno.nb

```
purity[output2[200]]
```

```
0.906462
```

```
p2 = ListPlot[Table[purity[output2[n]], {n, 1, 200, 2}],
  {PlotRange → {0, 1}, AxesLabel → {step, purity}}]
```



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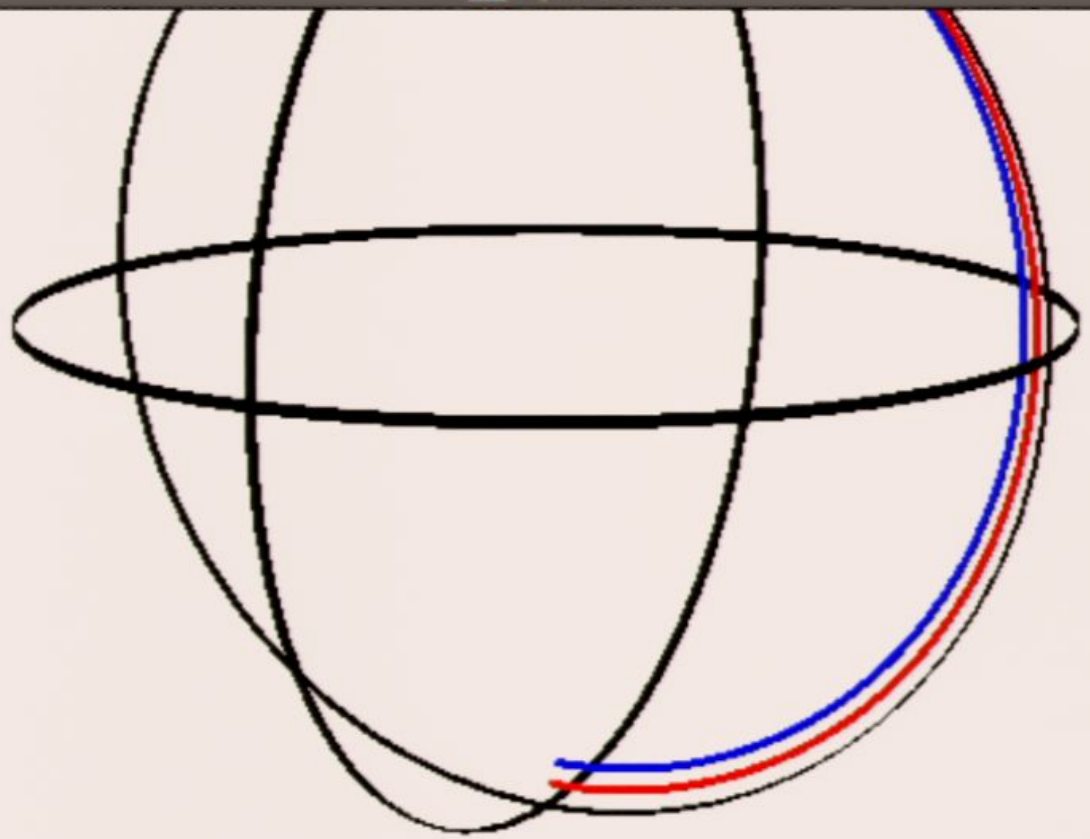
QZeno.nb



In[4]:=
```
ListPlot[Table[Cos[π / n]^n, {n, 1, 200}],
 {PlotRange → {0, 1}, AxesLabel → {steps, overlap}}]
```

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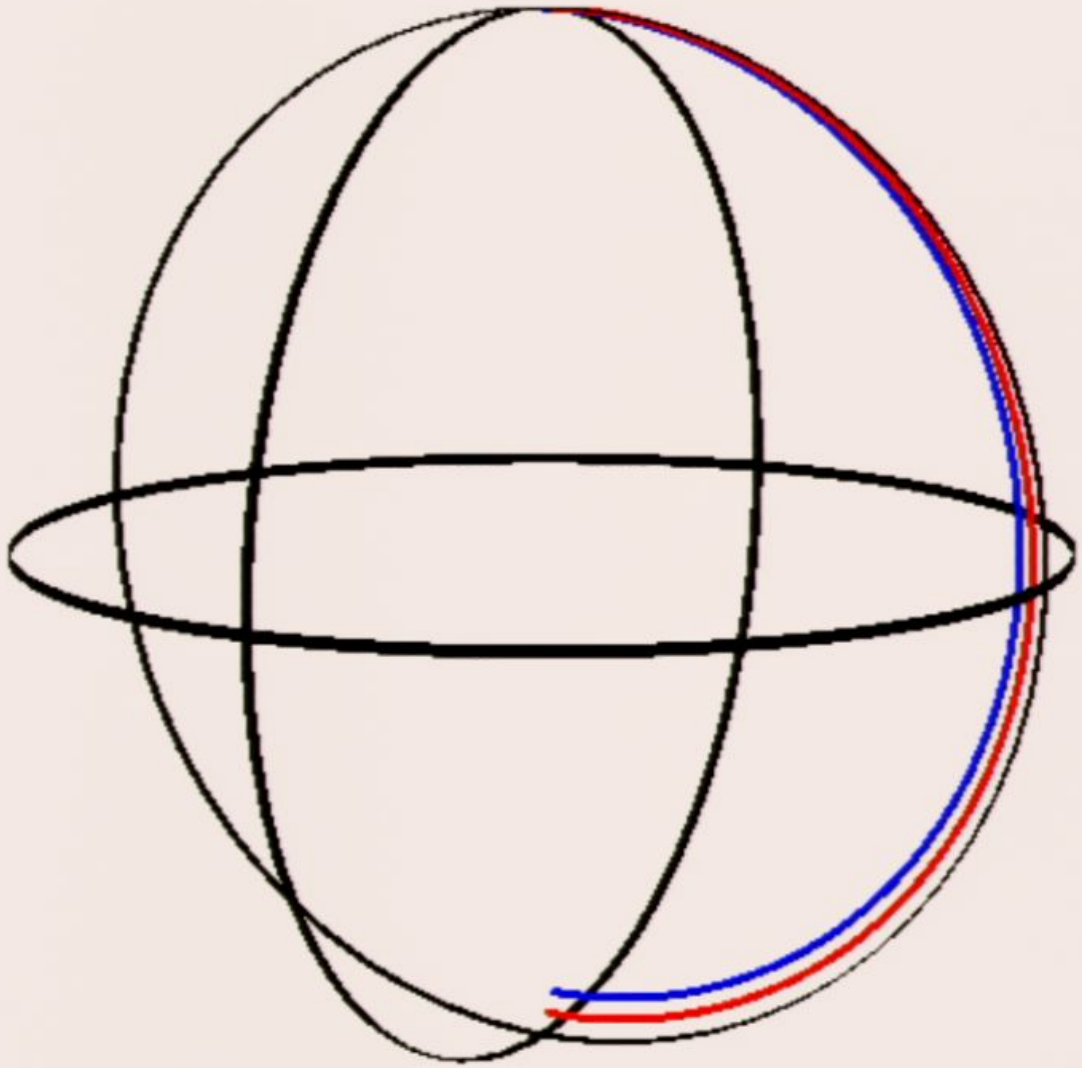
QZeno.nb



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QZeno.nb

In[4]:=
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```

Out[4]=

Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help

QZeno.nb

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```
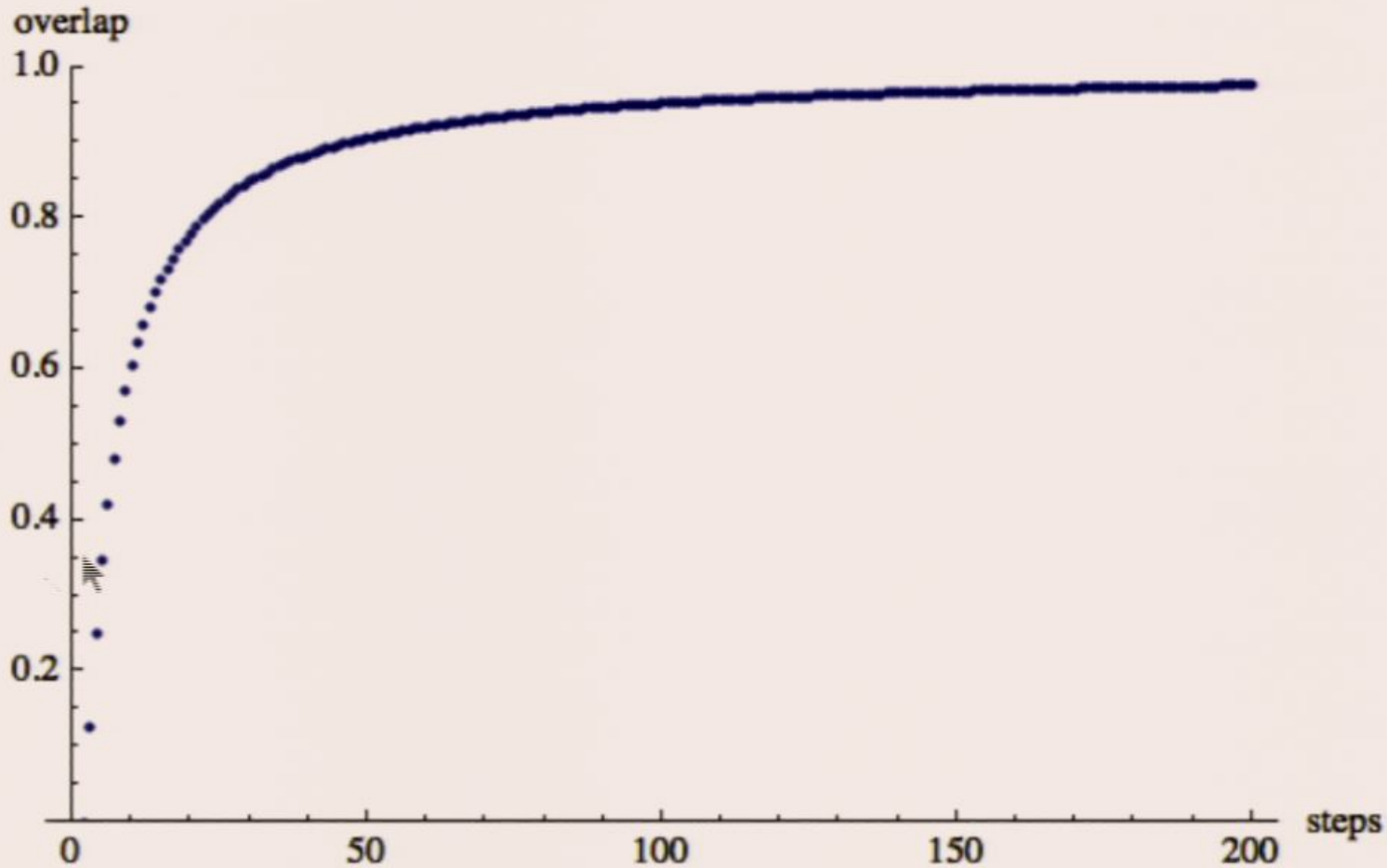
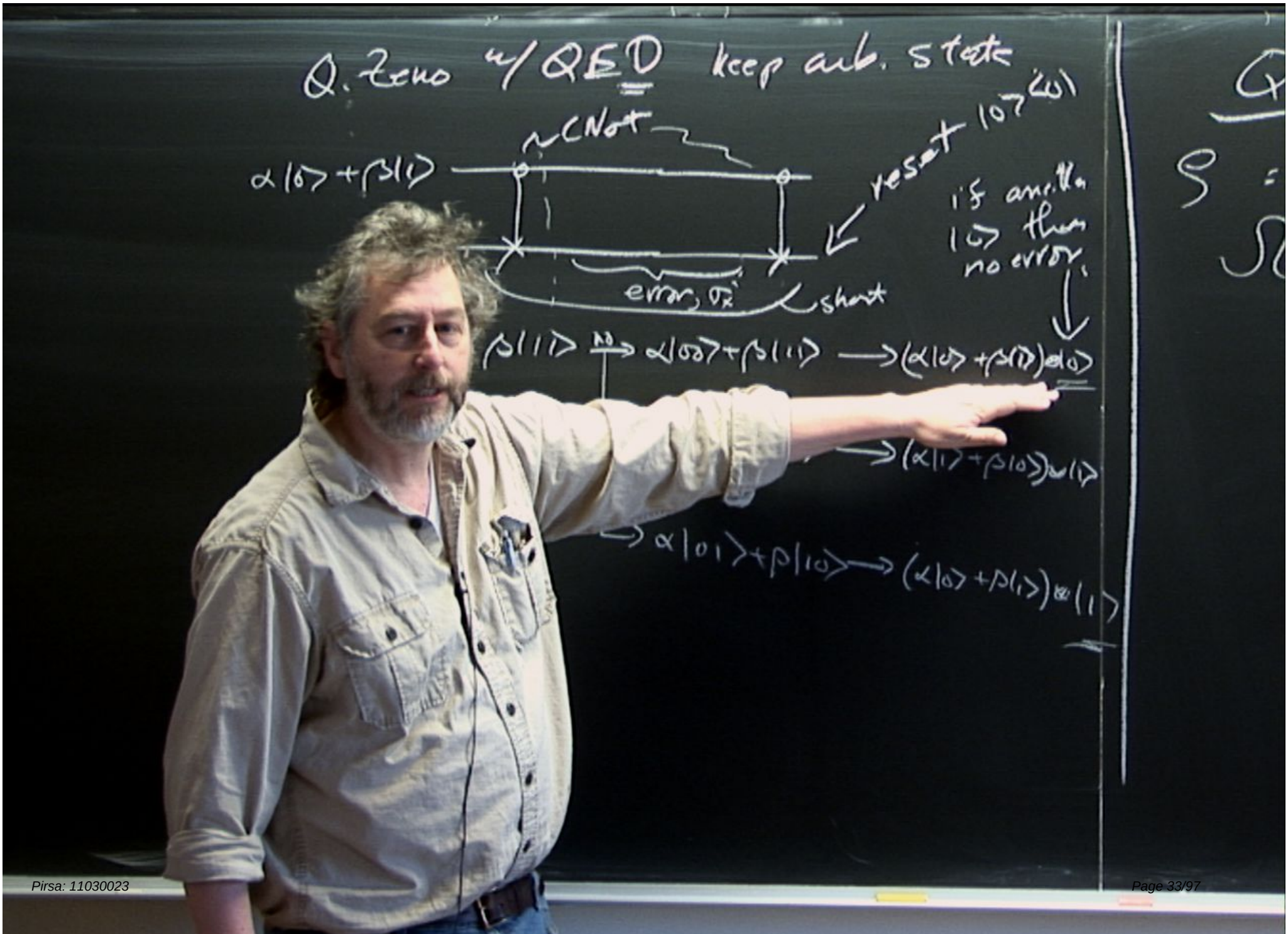
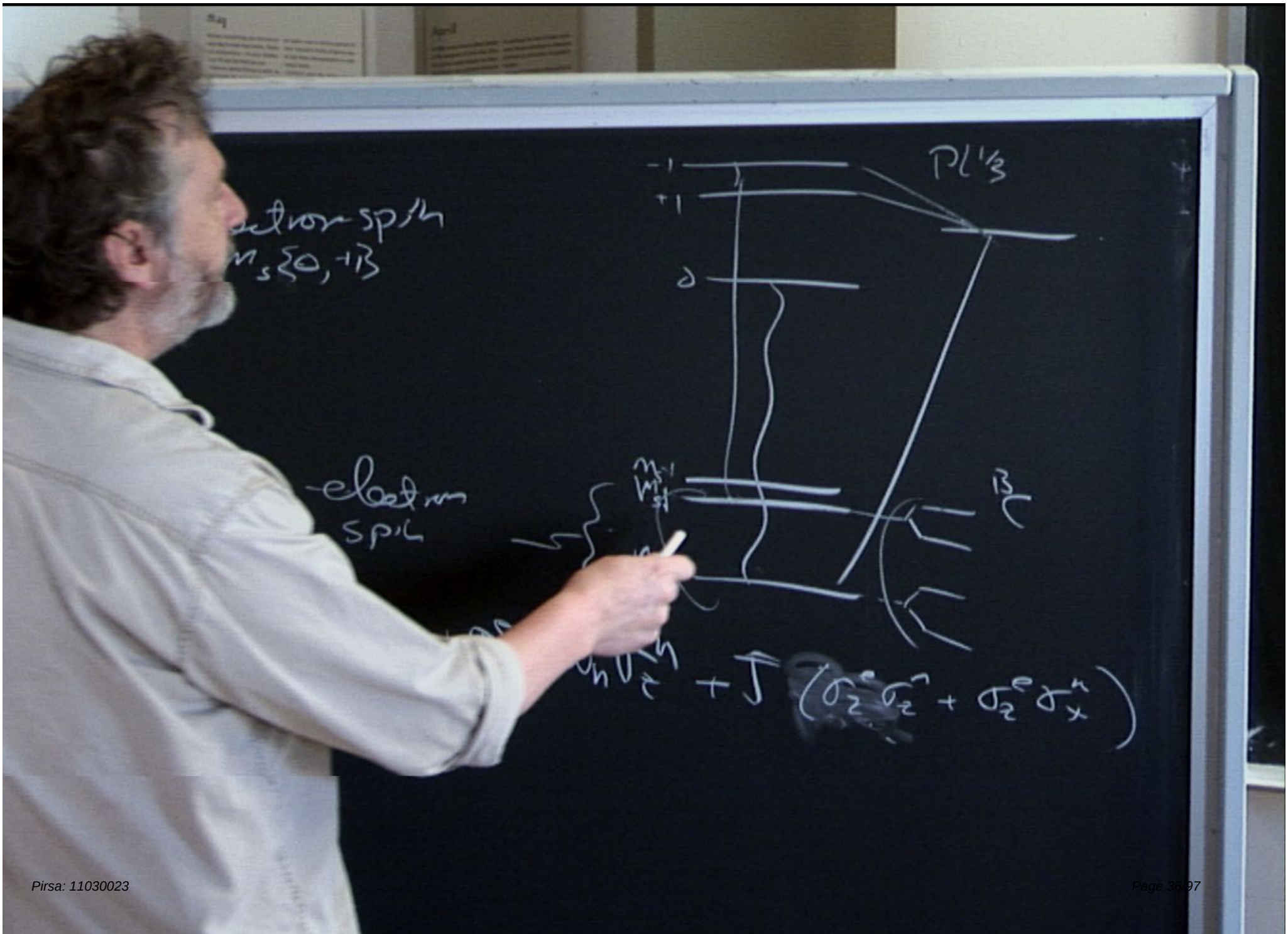

Out[4]=



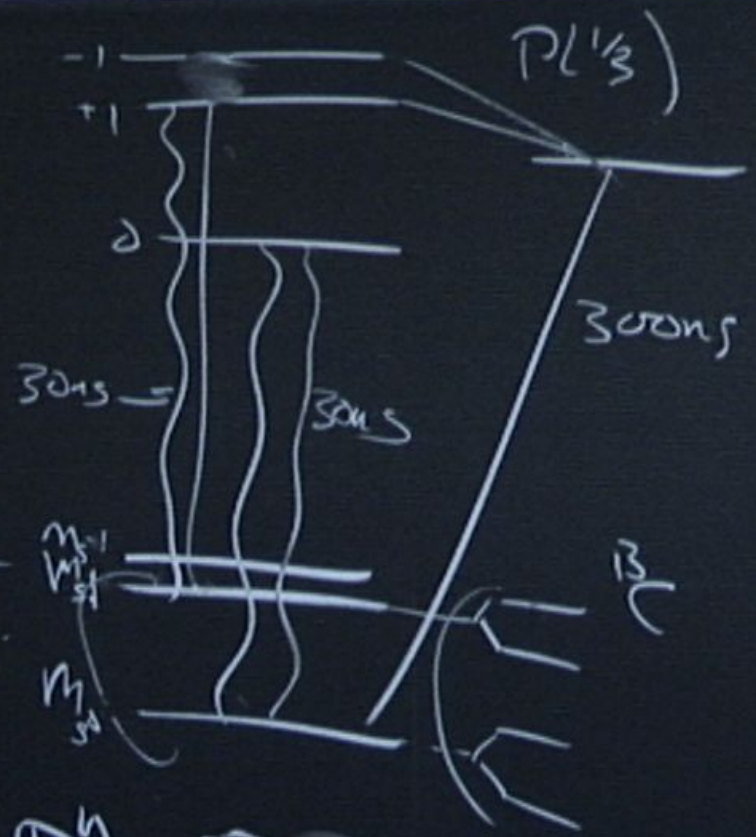

Q. Zeno w/ QED keep arb. state
CNot
α|0⟩+β|1⟩
reset |0⟩ |ω⟩
if ancilla |0⟩ then no error.
error, σx
short
β|11⟩ → α|00⟩+β|11⟩ → (α|0⟩+β|1⟩)⊗|0⟩
→ (α|1⟩+β|0⟩)⊗|1⟩
→ α|01⟩+β|10⟩ → (α|0⟩+β|1⟩)⊗|1⟩

for Atoms
Molecules

-1
+1
0
Pl'13
B


-1
+1
0
Pl 1/3
electron spin
electron
spin
B

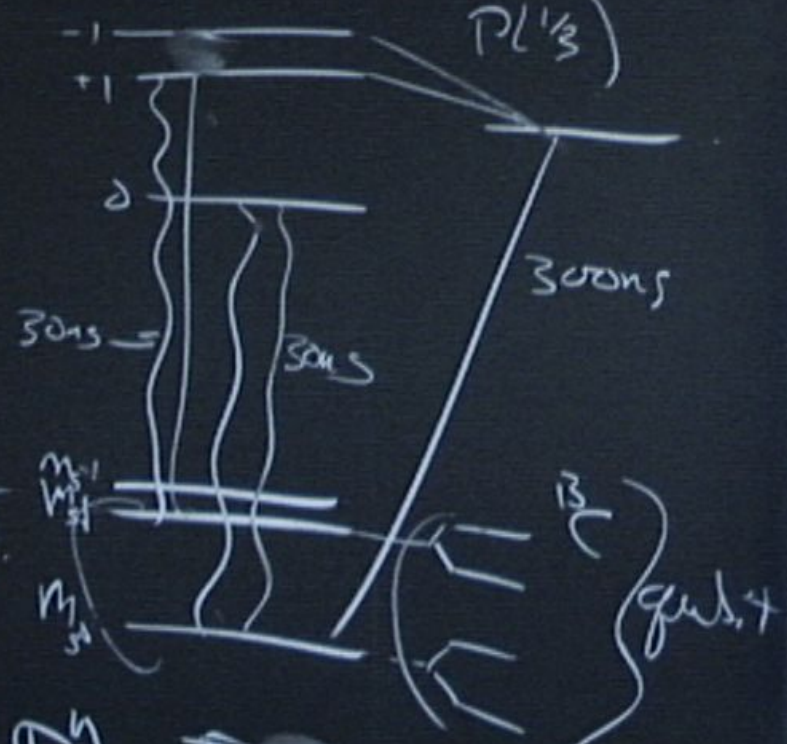
cilla = electron spin
$m_s \{0, \pm 1\}$



electron spin

$$\mathcal{H} = \omega_e \sigma_z^e + \omega_n \sigma_z^n + J\left(\sigma_z^e \sigma_z^n + \sigma_z^e \sigma_x^n\right)$$

ancilla ≡ electron spin
$m_s \in \{0, \pm 1\}$



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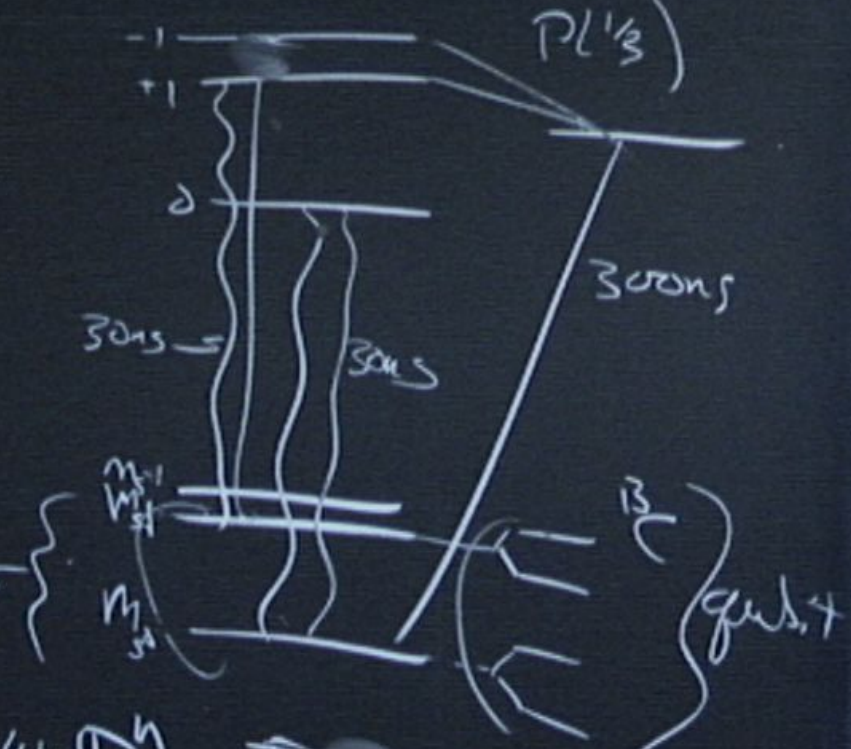
ancilla ≡ electron spin
$m_s \in \{0, +1\}$



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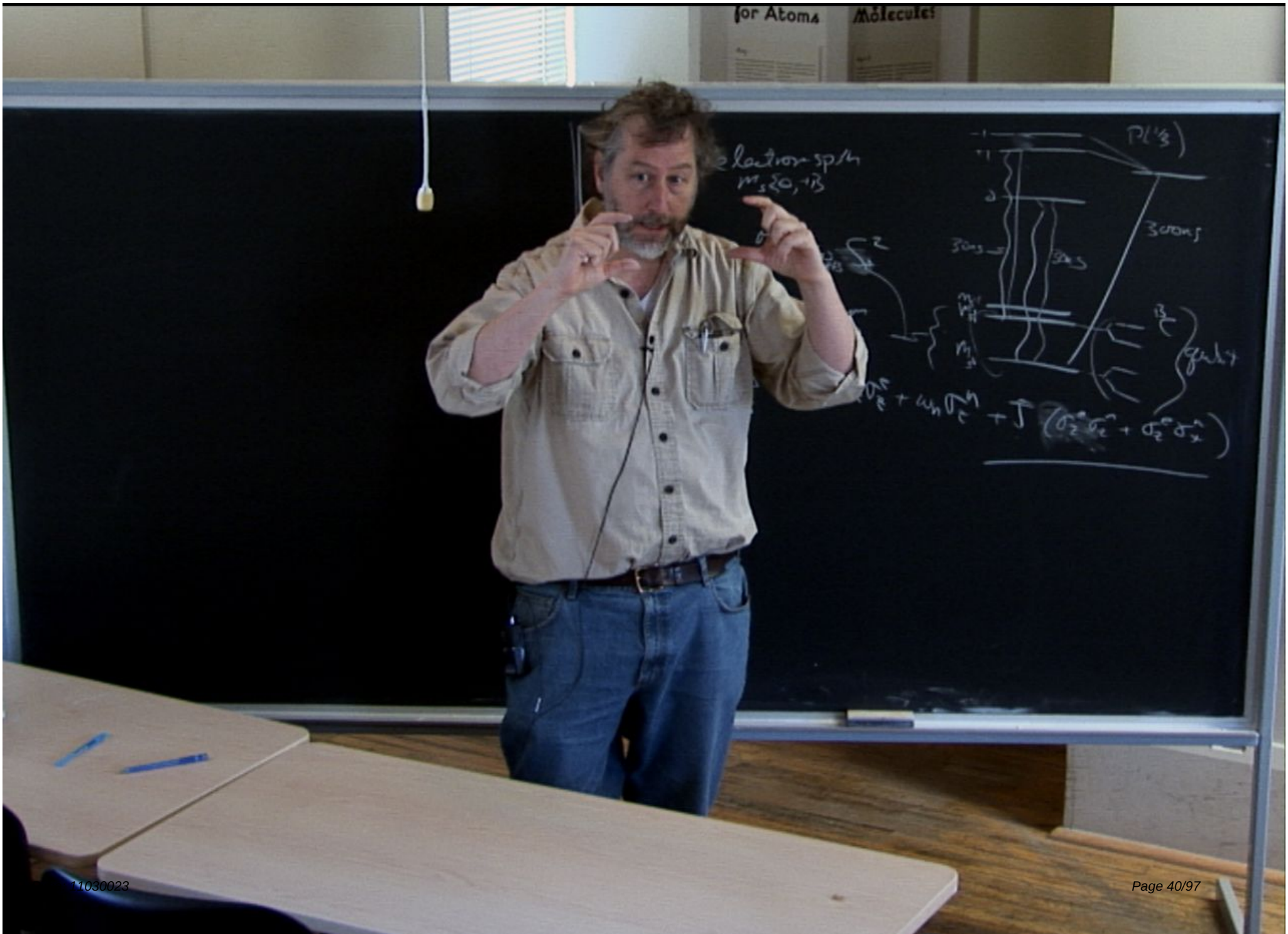
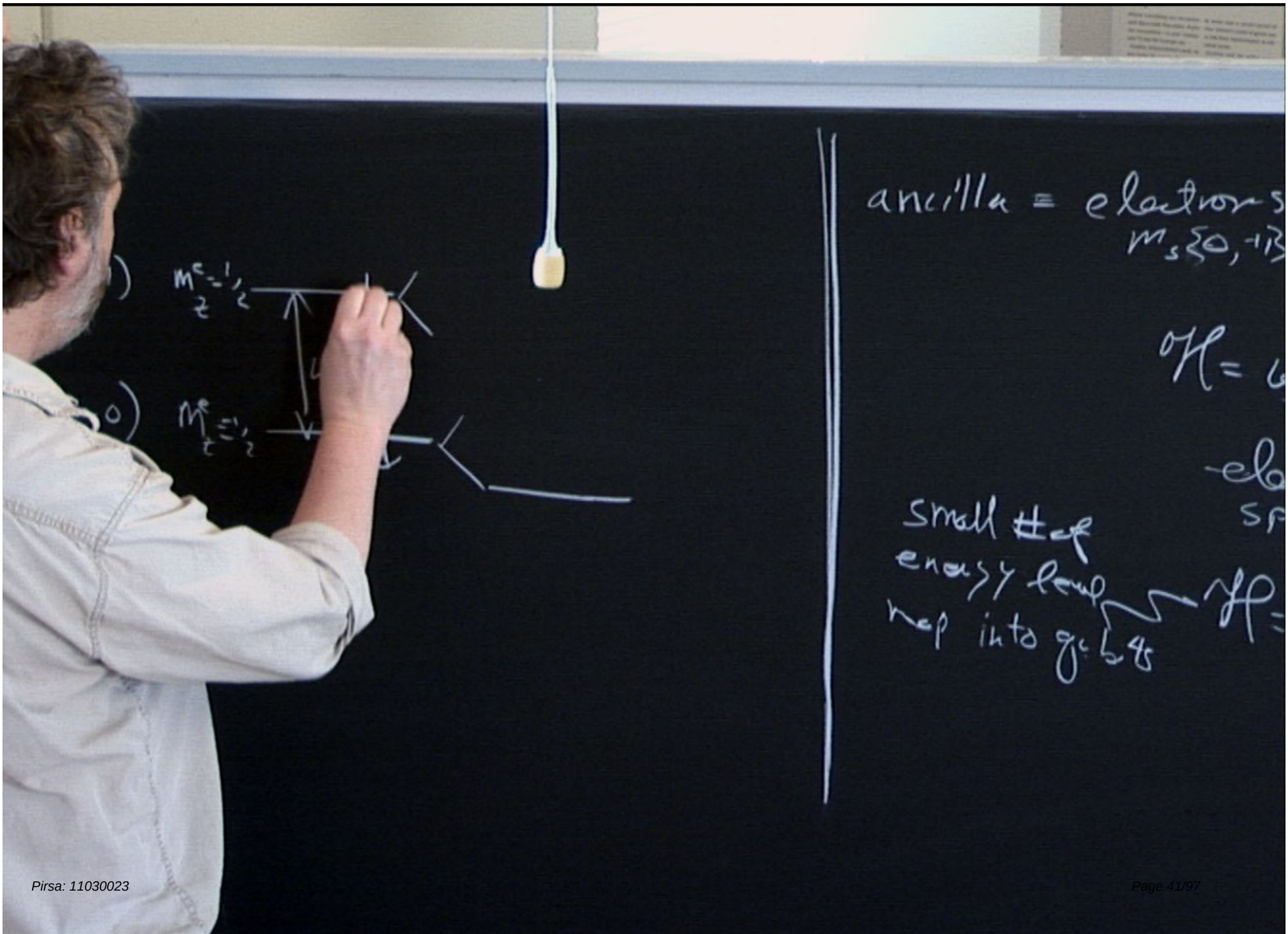
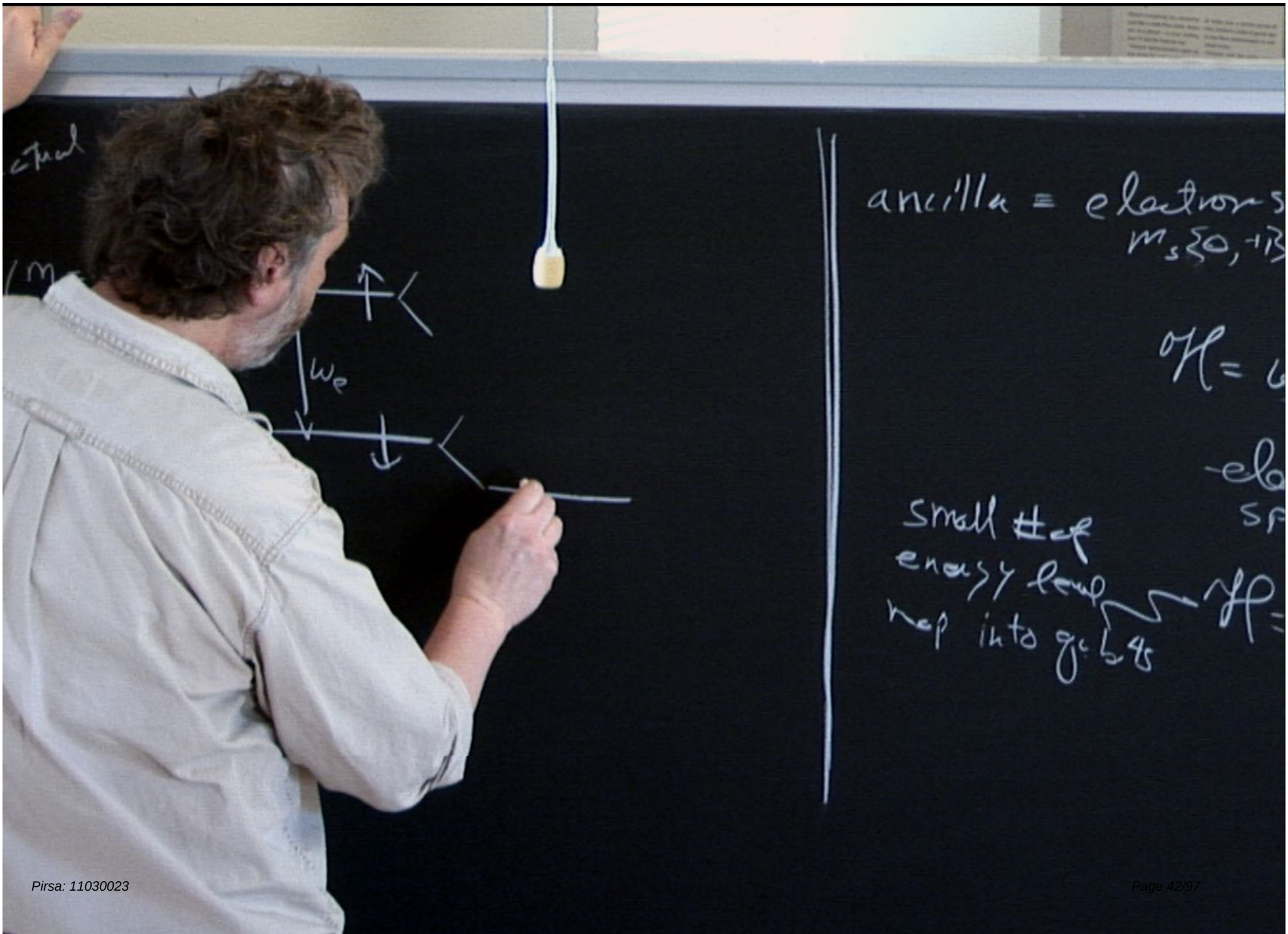

for Atoms
Molecules
electron spin
3 atoms


ancilla = electrons
small # of
energy level
map into qubits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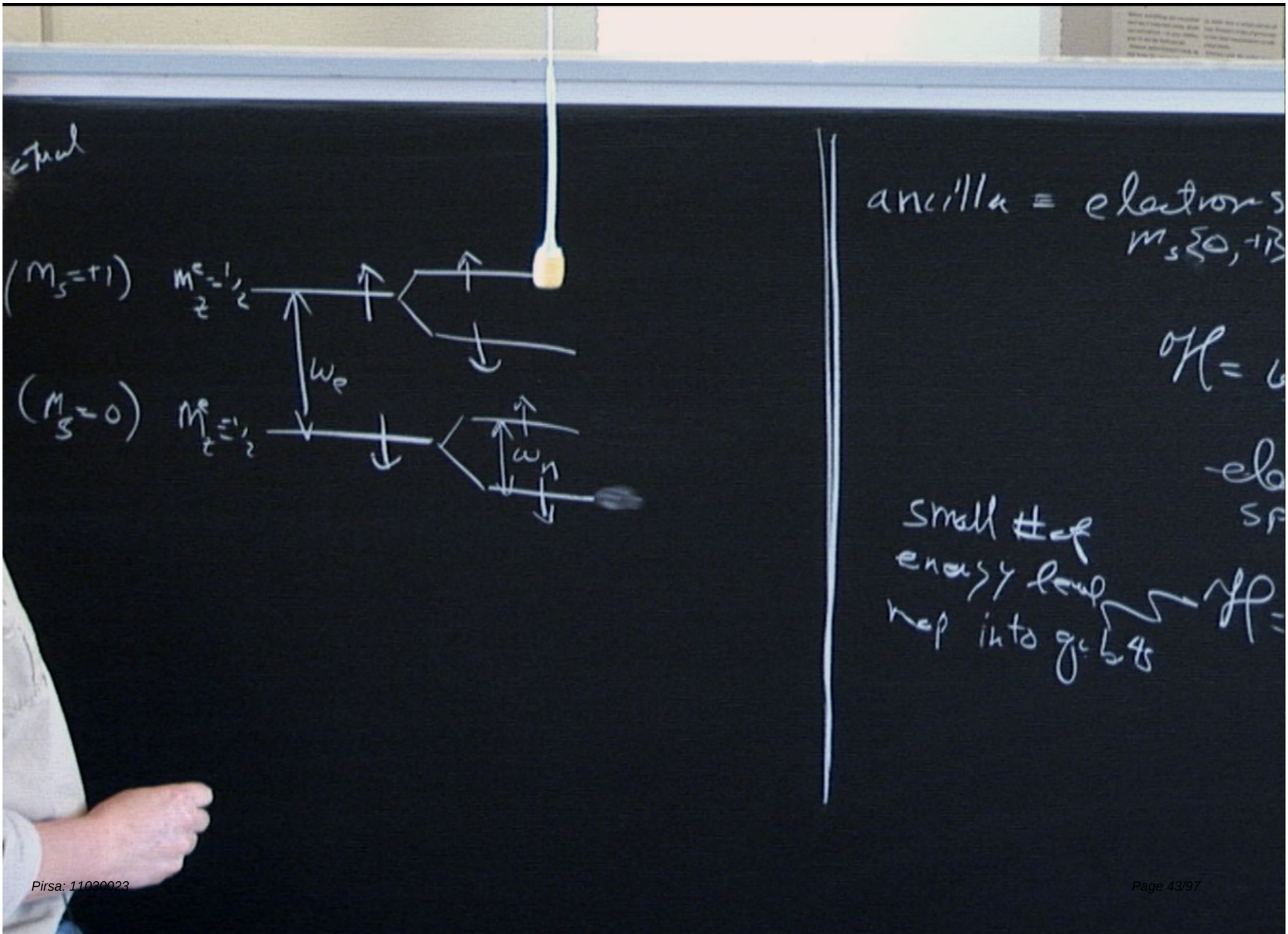
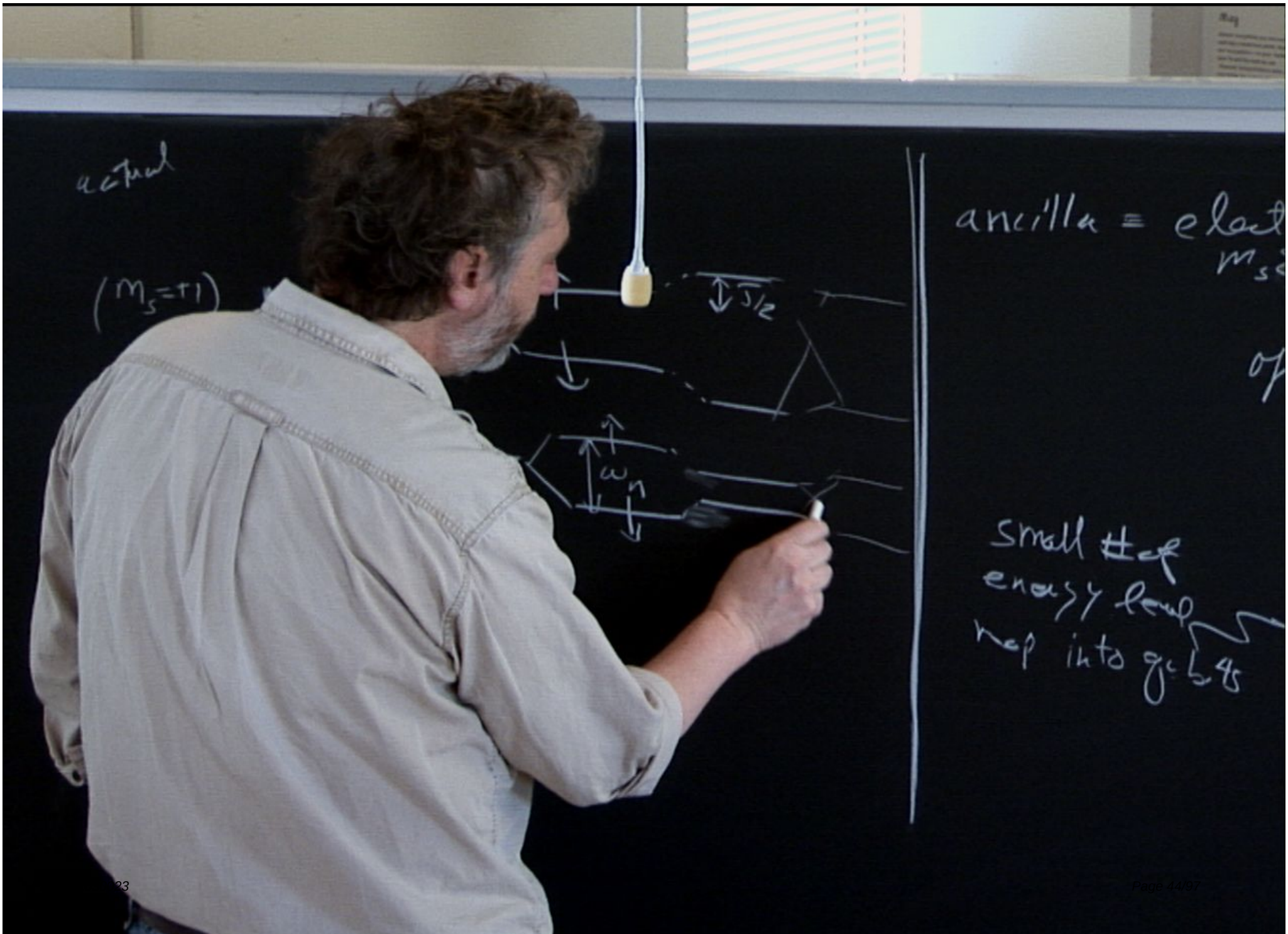
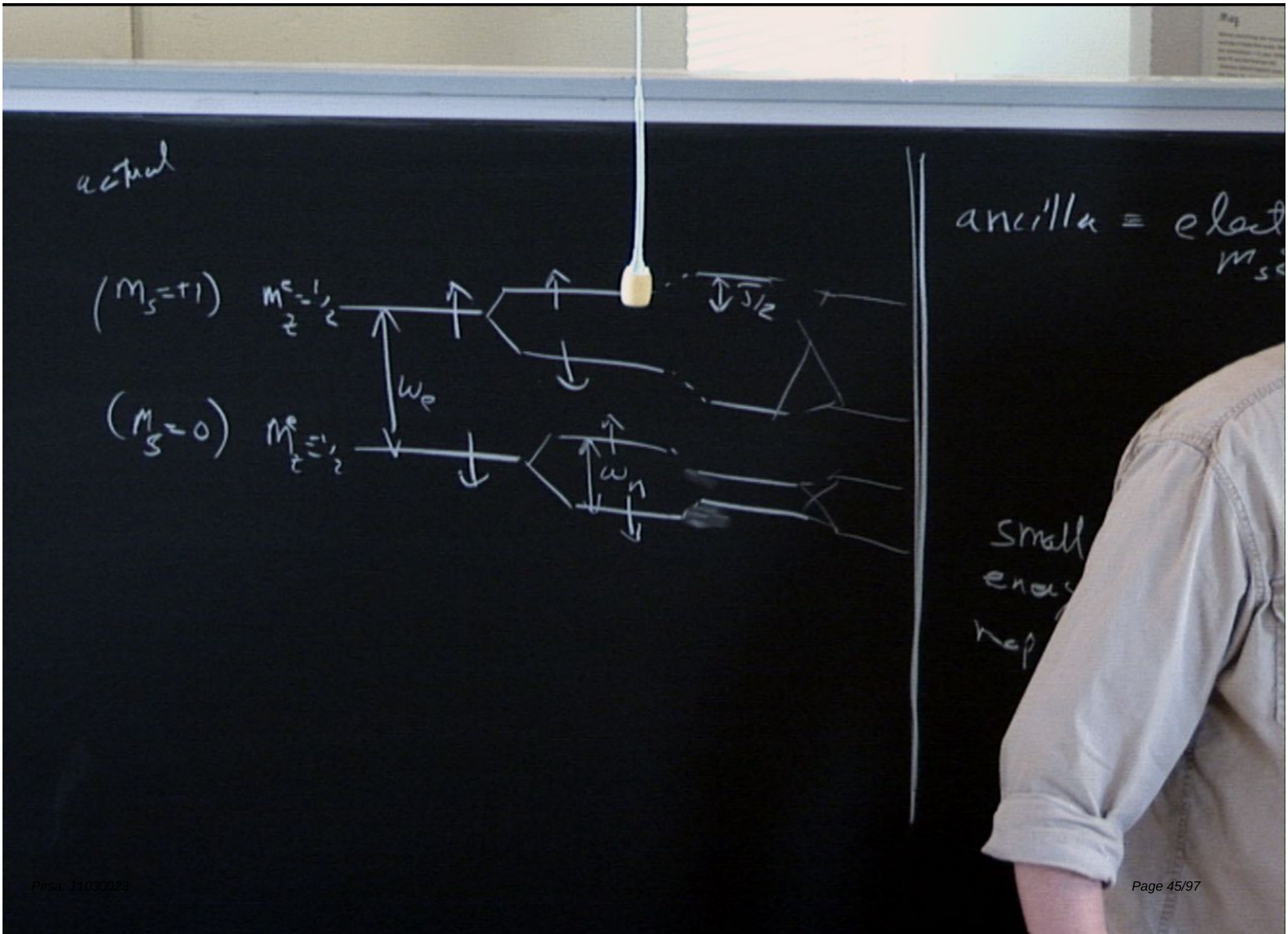
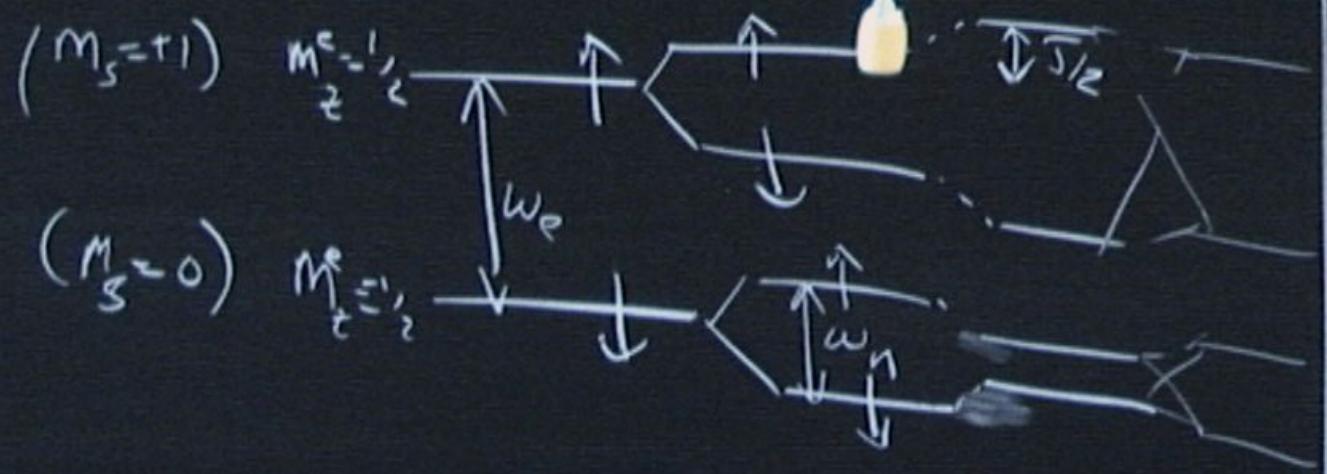

ctual
$(m_s=+1)$ $m_z^e=-1/2$
ω_e
$(m_s=0)$ $m_z^e=-1/2$
ω_n
ancilla = electrons
$m_s \{0,-1\}$
small $\hbar\omega$
energy level
map into qubits


actual
(m_s=+1)
J/2
ω_n
ancilla ≡ elect
small ħω
energy level
map into qubits


actual
$(m_s=+1)$ $m_z^e=-1/2$
$(m_s=0)$ $m_z^e=-1/2$
ω_e
ω_n
$J/2$
ancilla ≡ elect
small

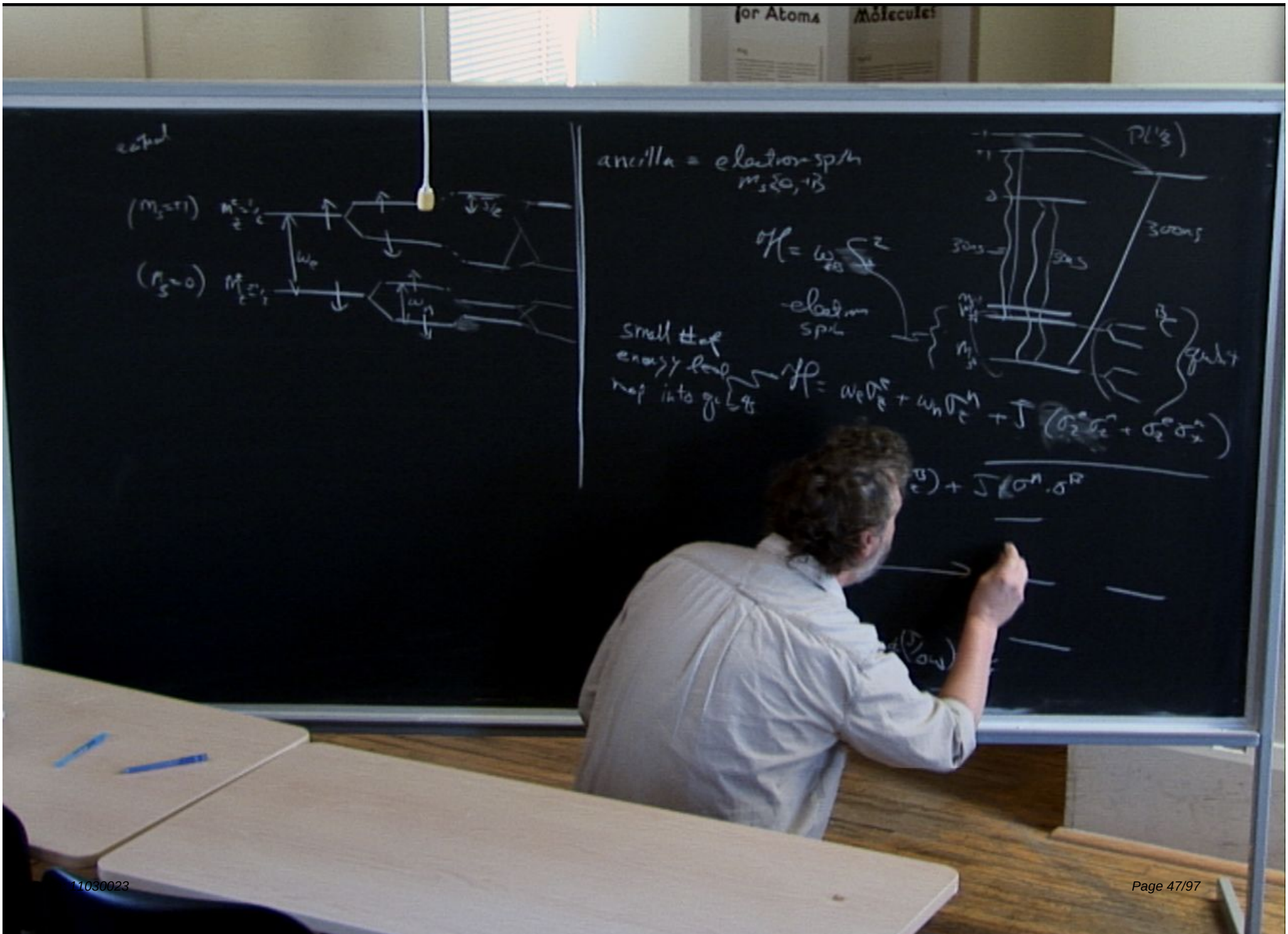
actual

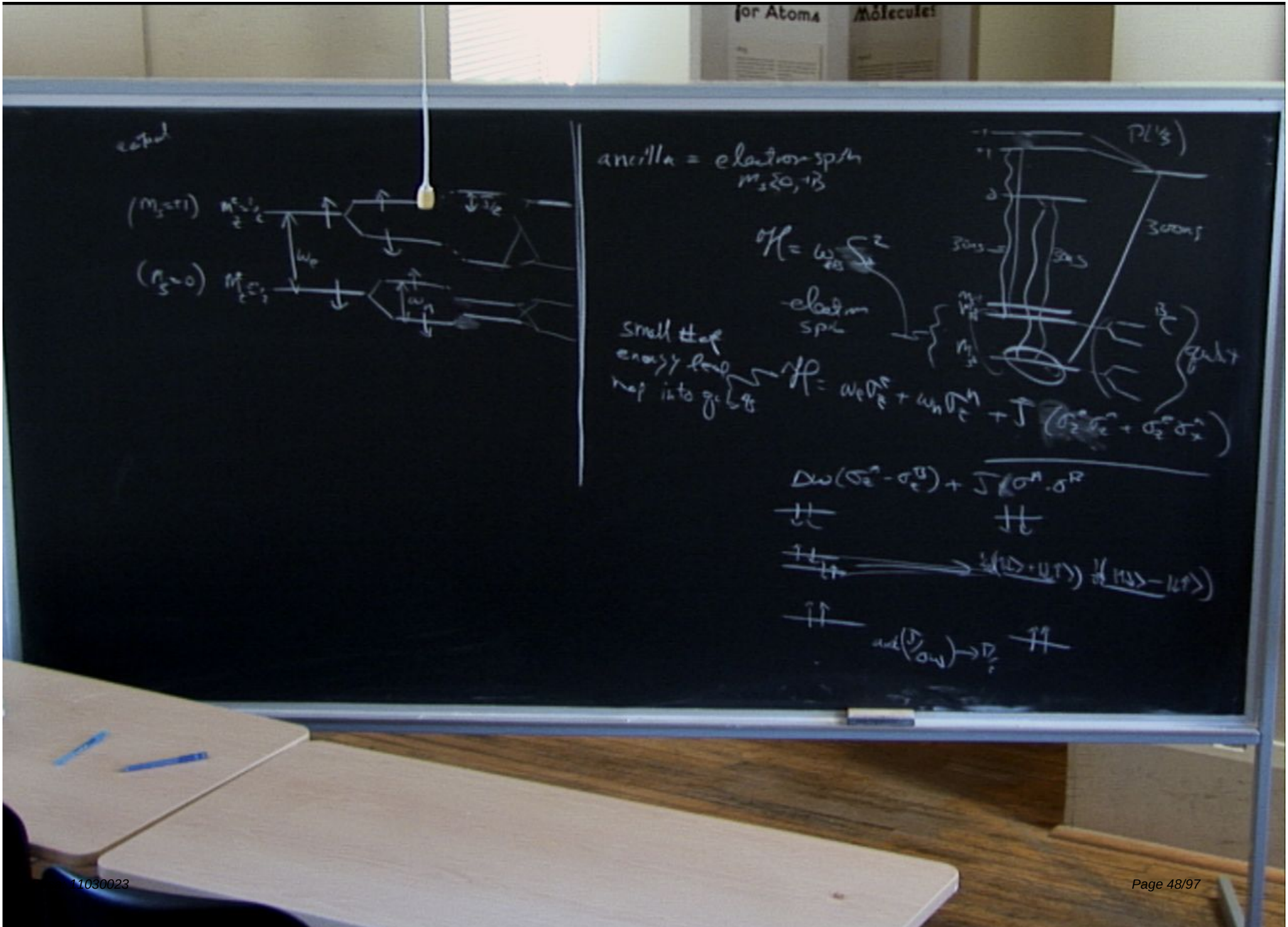


ancilla = elect
m_s

of

small $\hbar\omega$
energy level
map into qubits


ancilla = electron spin
small H of
energy level
map into qubits
electron spin
3 atoms
3 atoms
3 atoms

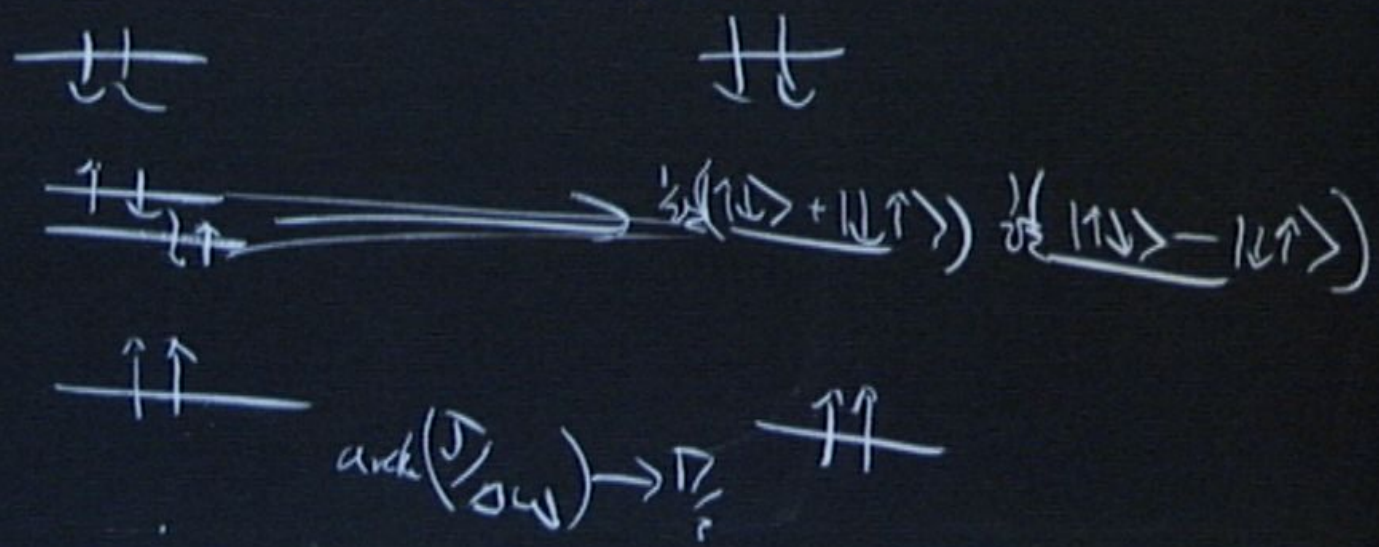

for Atoms
Molecules
ancilla = electron spin
small H of energy level mix into g.s.
3 atoms
3 atoms
3 atoms
gnd st

small # of
energy level
hop into gr. states

electron
spin

$$\mathcal{H} = \omega_e \sigma_z^e + \omega_n \sigma_z^n + J\left(\sigma_z^e \sigma_z^n + \sigma_z^e \sigma_x^n\right)$$

$$\Delta\omega\left(\sigma_z^A - \sigma_z^B\right) + J\,\sigma^A \cdot \sigma^B$$



$$\arctan\left(J/\Delta\omega\right) \to \pi/2$$

ancilla = electron spin
$m_s \in \{0, +1\}$

$\mathcal{H} = \omega_{ESR} S_z^2$

electron spin

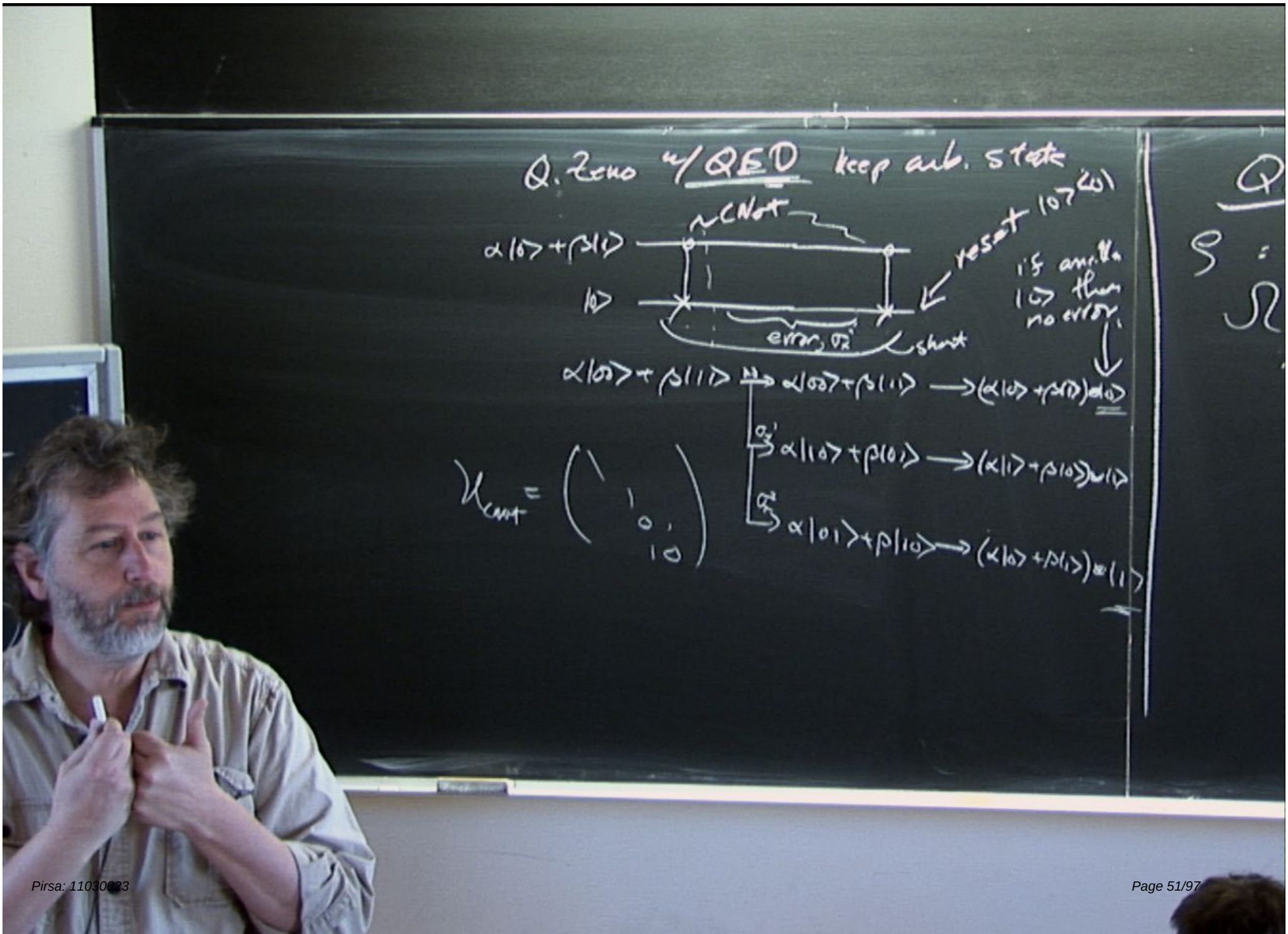
small # of energy level map into qubits

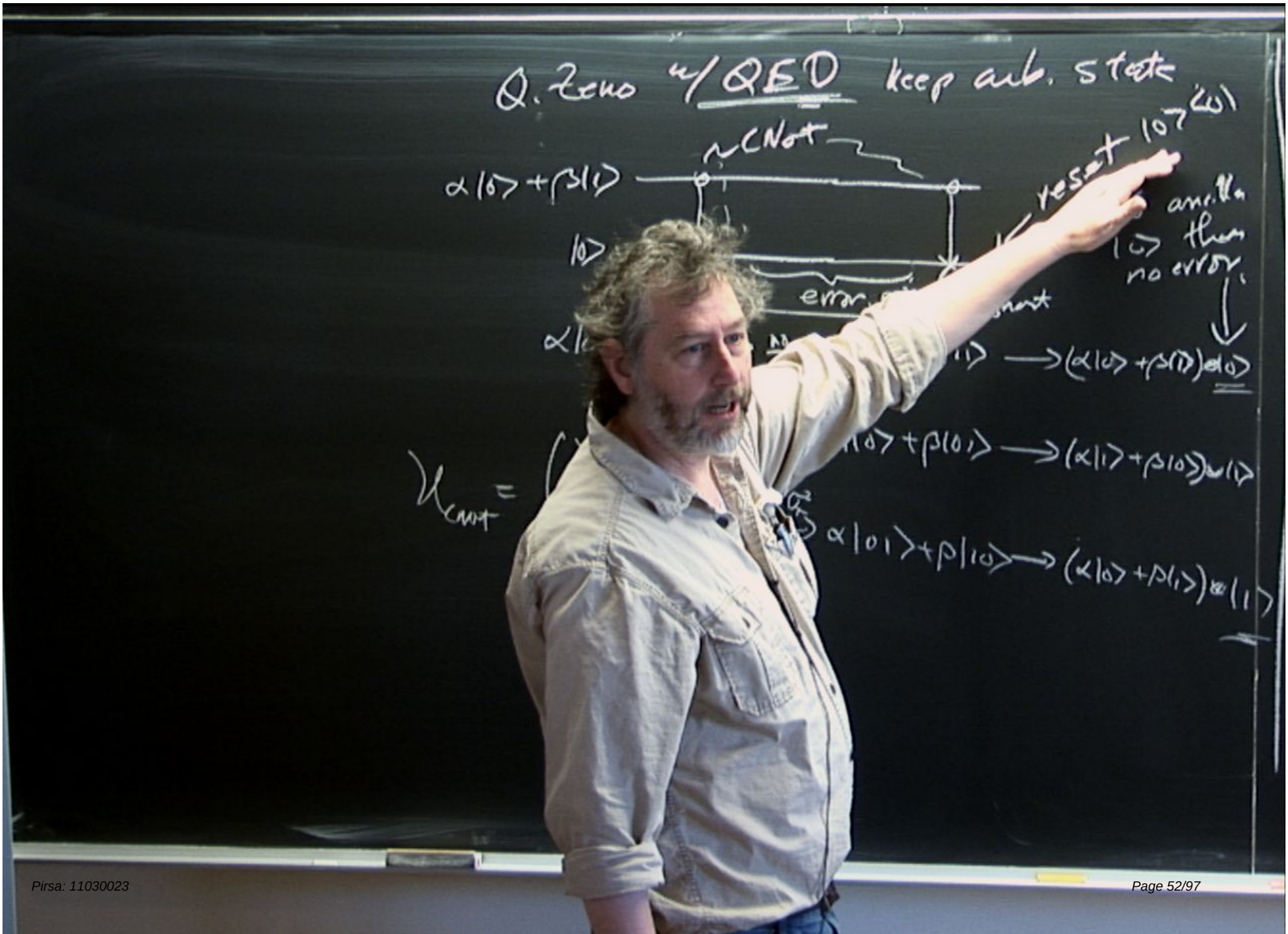
$\mathcal{H} = \omega_e \sigma_z^e + \omega_n \sigma_z^n + J(\sigma_z^e \sigma_z^n + \sigma_z^e \sigma_x^n)$

$\Delta\omega(\sigma_z^n - \sigma_z^B) + J\,\sigma^n \cdot \sigma^B$

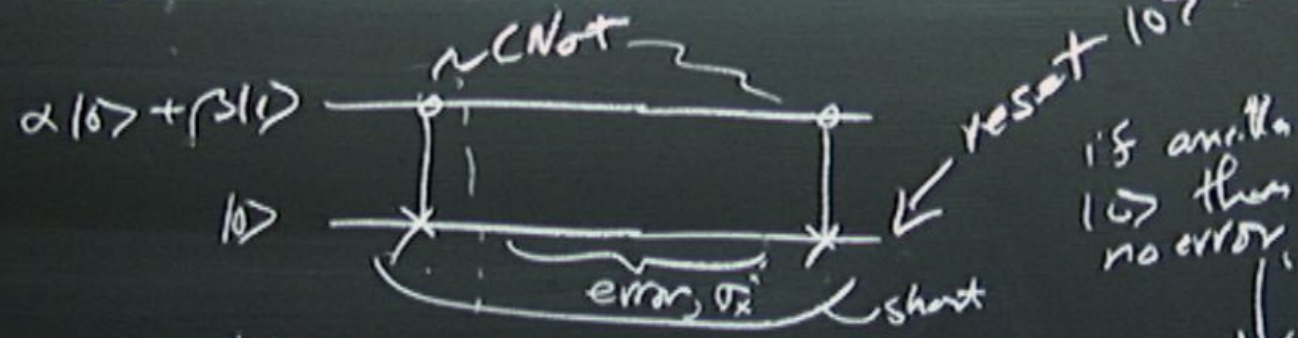
$\frac{1}{\sqrt{2}}(|\downarrow\rangle + |\uparrow\rangle)$ $\frac{1}{\sqrt{2}}(|\downarrow\rangle - |\uparrow\rangle)$

and $(J/\Delta\omega) \to 0$


Q. Zeno w/ QED keep arb. state
CNot
reset $|0\rangle\langle 0|$
$\alpha|0\rangle+\beta|1\rangle$
$|0\rangle$
error, σ_x
short
if ancilla $|0\rangle$ then no error
$\alpha|00\rangle+\beta|11\rangle \to \alpha|00\rangle+\beta|11\rangle \to (\alpha|0\rangle+\beta|1\rangle)\otimes|0\rangle$
σ_x: $\alpha|10\rangle+\beta|01\rangle \to (\alpha|1\rangle+\beta|0\rangle)\otimes|1\rangle$
σ_x: $\alpha|01\rangle+\beta|10\rangle \to (\alpha|0\rangle+\beta|1\rangle)\otimes|1\rangle$
$U_{CNot} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{pmatrix}$


Q. Zeno w/ QED keep arb. state
CNot
reset
error
no error

Q. Zeno w/ QED keep arb. state



if ancilla $|0\rangle$ then no error.

$$\alpha|00\rangle+\beta|11\rangle \xrightarrow{\text{no}} \alpha|00\rangle+\beta|11\rangle \longrightarrow (\alpha|0\rangle+\beta|1\rangle)\otimes|0\rangle$$

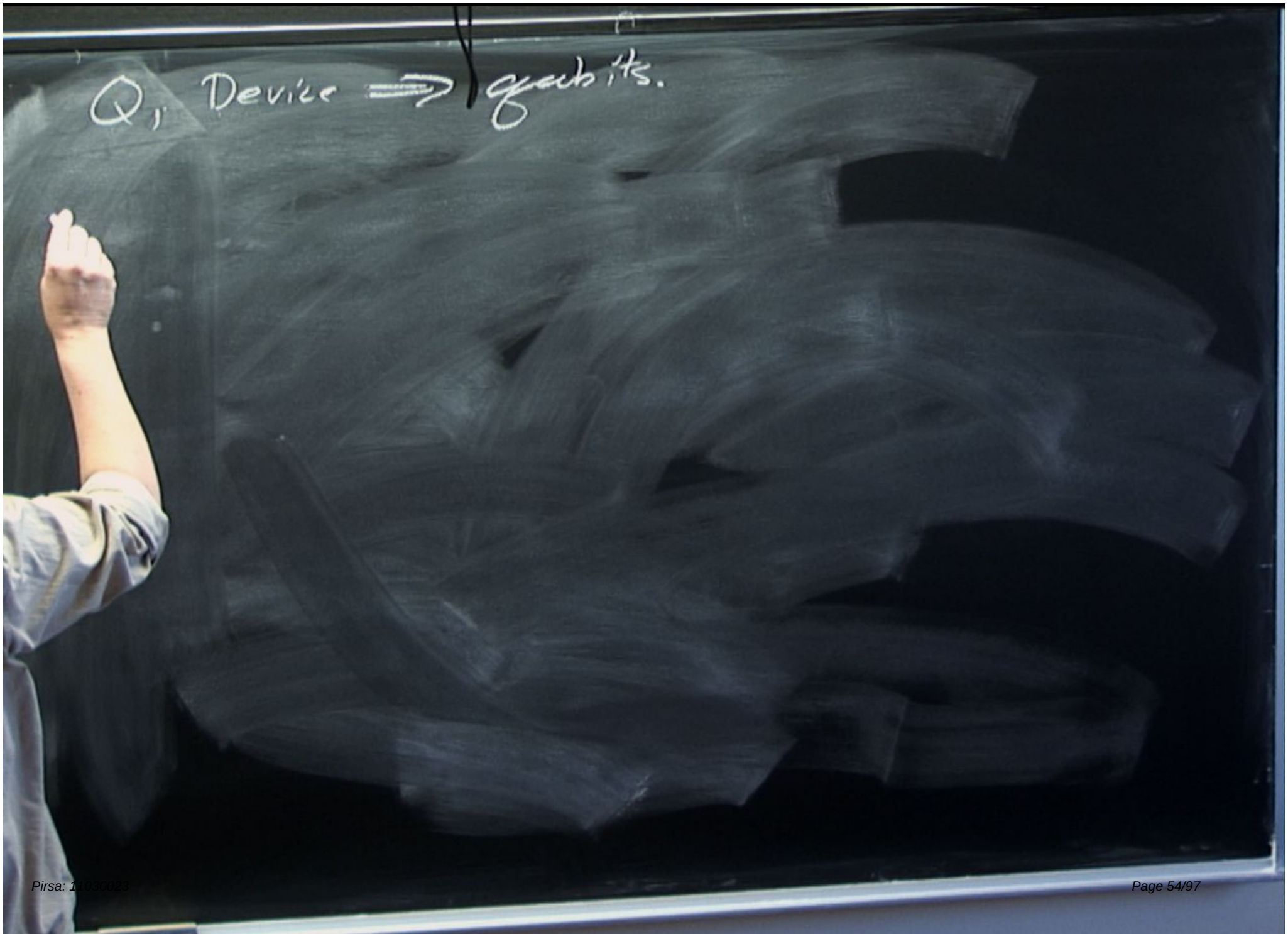
$$\xrightarrow{\sigma_x^1} \alpha|10\rangle+\beta|01\rangle \longrightarrow (\alpha|1\rangle+\beta|0\rangle)\otimes|1\rangle$$

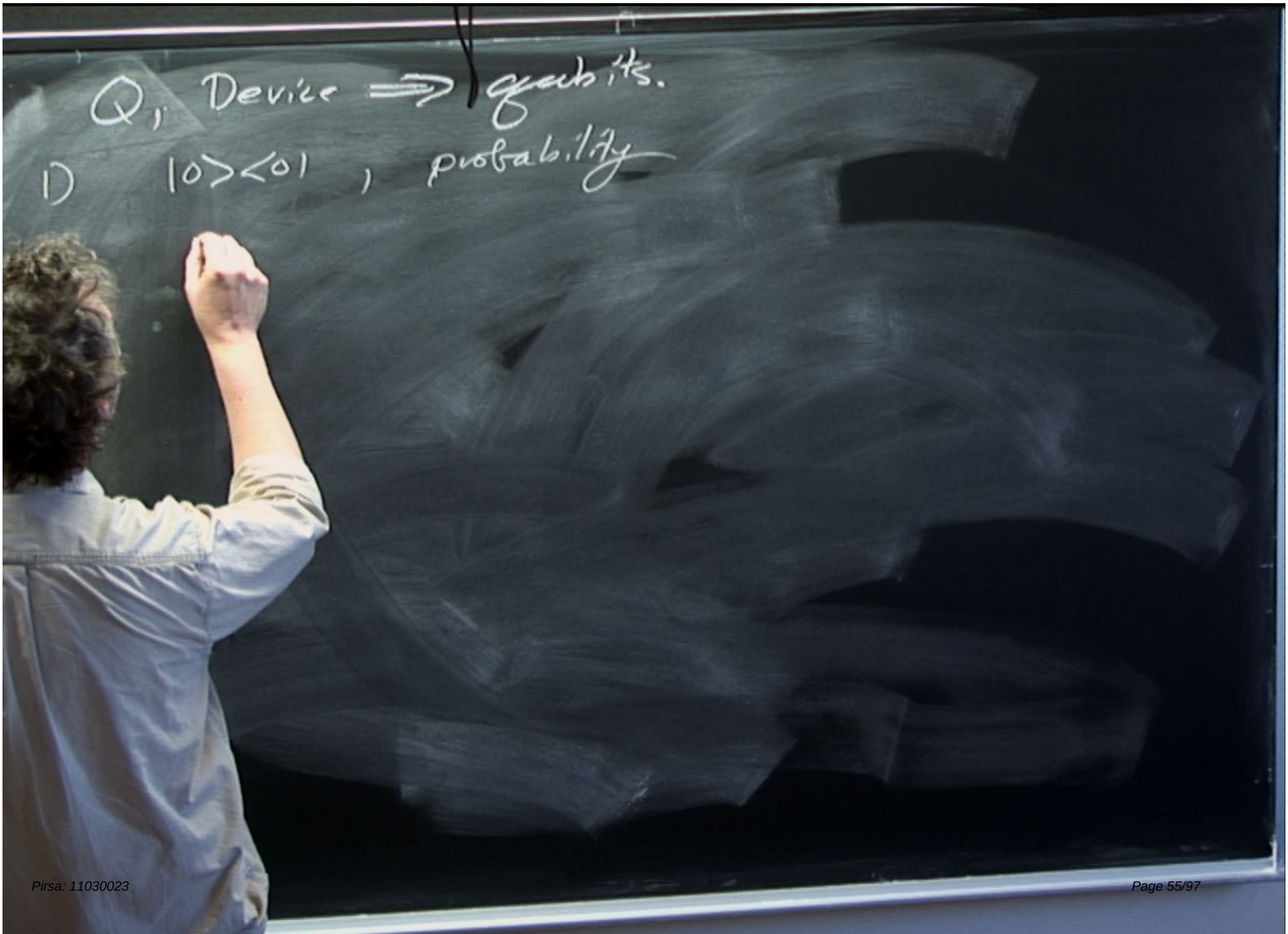
$$\xrightarrow{\sigma_x^2} \alpha|01\rangle+\beta|10\rangle \longrightarrow (\alpha|0\rangle+\beta|1\rangle)\otimes|1\rangle$$

$$U_{CNot} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{pmatrix}$$

$$K_0 = (1-p)^{1/2}\,\mathbb{1}$$

$$K_1 = \left(\frac{\tau}{T_1}\right)^{1/2}\sigma_x$$

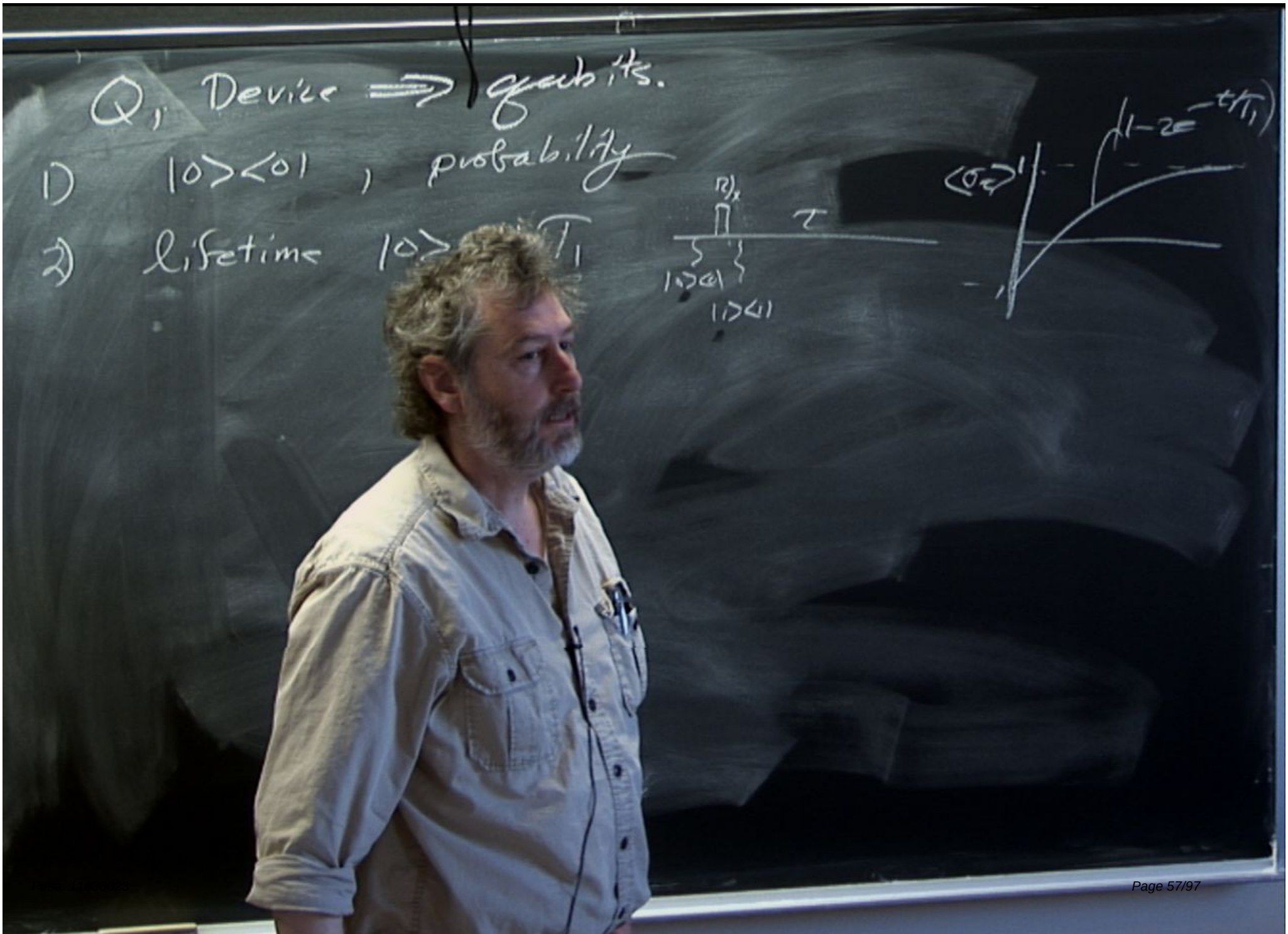

Q, Device ⟹ qubits.


Q, Device ⟹ qubits.
1) |0><0| , probability

Q, Device ⟹ qubits.

1) $|0\rangle\langle 0|$, probability

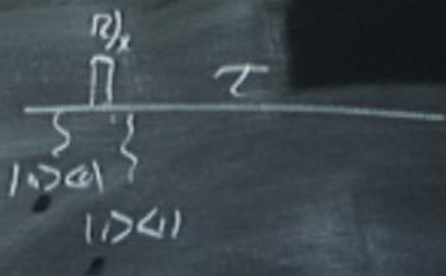
2) lifetime $|0\rangle\langle 0|$, T_1

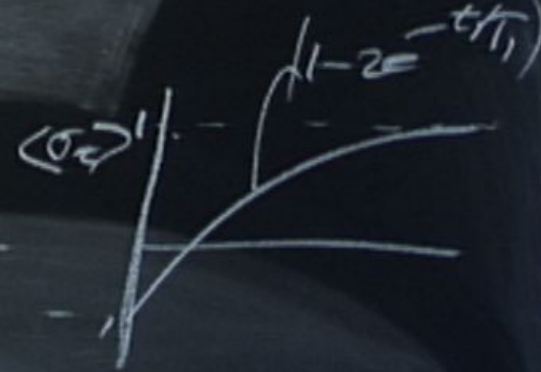

Q, Device ⟹ qubits.
1) |0><0| , probability
2) lifetime |0> T1
τ
|0><0|
|1><1|
<σz>
1
(1-2e^-t/T1)

Q: Device $\Rightarrow$ qubits.

1) $|0\rangle\langle 0|$, probability

2) lifetime $|0\rangle\langle 0|$, T_1



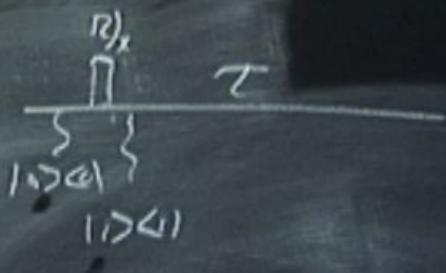


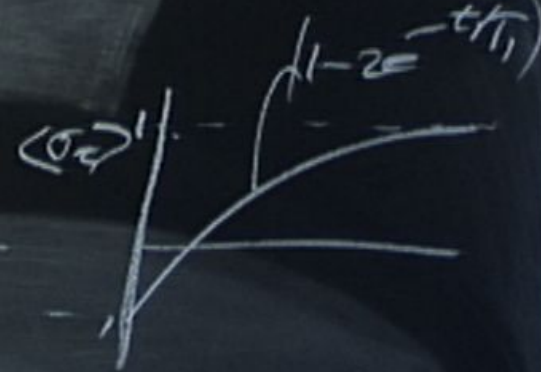
Q: Device $\Rightarrow$ qubits.

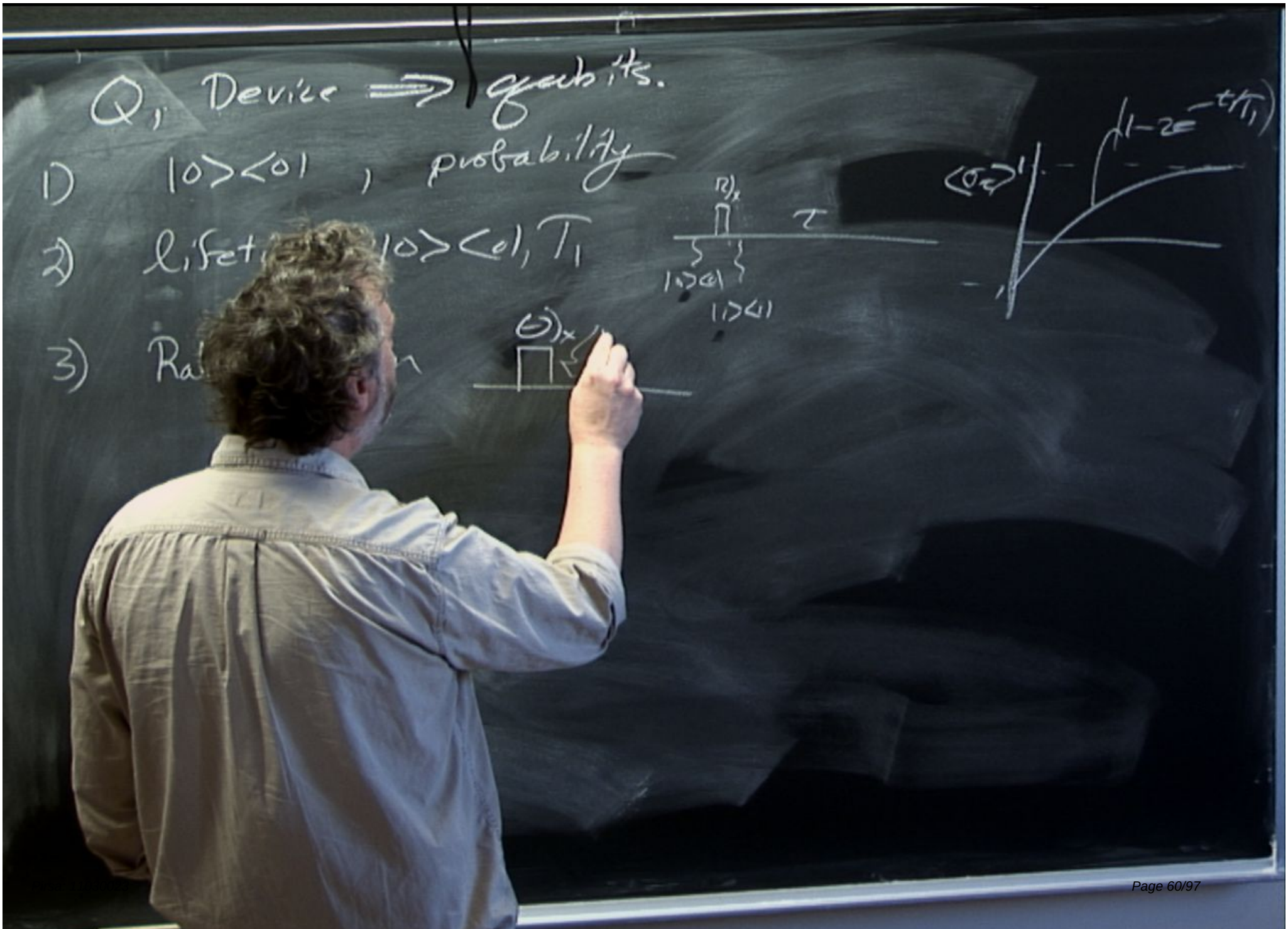
1) $|0\rangle\langle 0|$, probability

2) lifetime $|0\rangle\langle 0|$, T_1

3) Rabi oscillation



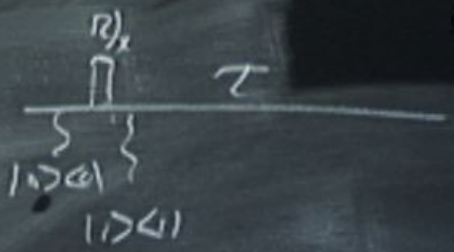


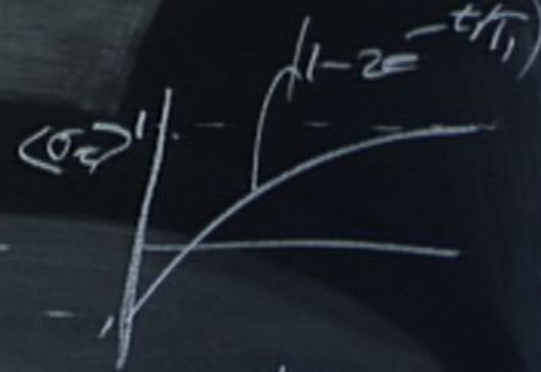

Q, Device ⟹ qubits.
1) |0><0| , probability
2) lifet |0><0|, T1
3) Ra
τ
|1><1|
|1><1|
<σz>
(1-2e^-t/T1)

Q: Device ⟹ qubits.

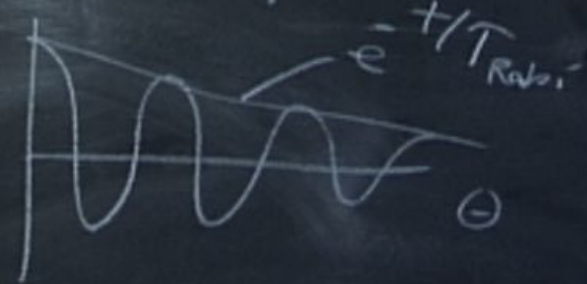
1) $|0\rangle\langle 0|$, probability

2) lifetime $|0\rangle\langle 0|$, T_1





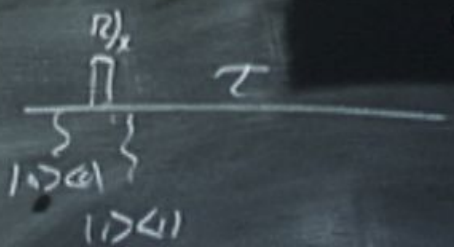
3) Rabi oscillation

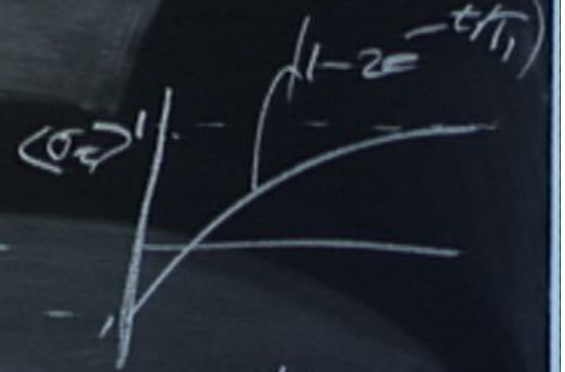


Q, Device ⟹ qubits.

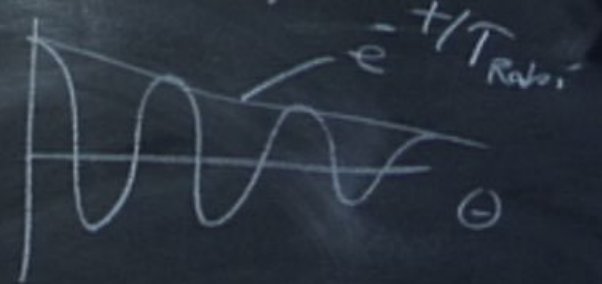
1) $|0\rangle\langle 0|$, probability

2) lifetime $|0\rangle\langle 0|$, T_1

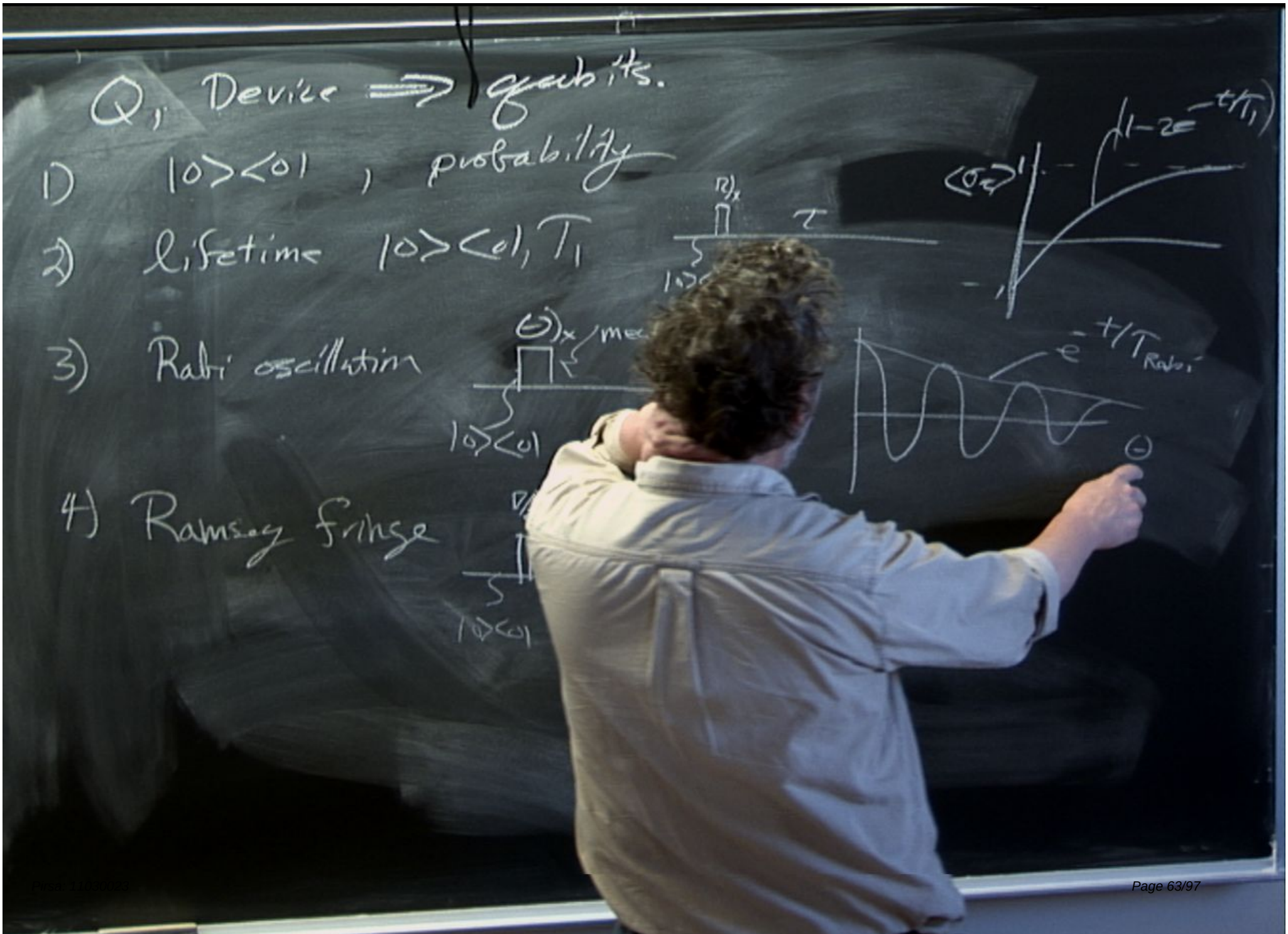




3) Rabi oscillation



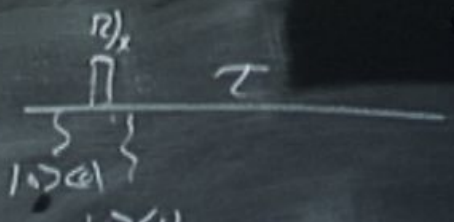
4) Ramsey fringe

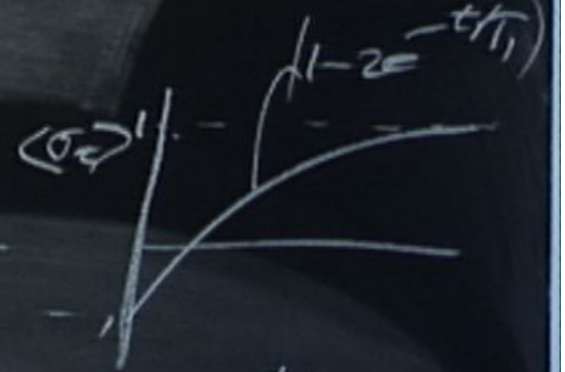

Q, Device ⟹ qubits.
1) |0><0| , probability
2) lifetime |0><0|, T1
3) Rabi oscillation
4) Ramsey fringe
τ
|0><0|
<σz>
(1-2e^-t/T1)
e^-t/T_Rabi
θ

Q: Device ⟹ qubits.

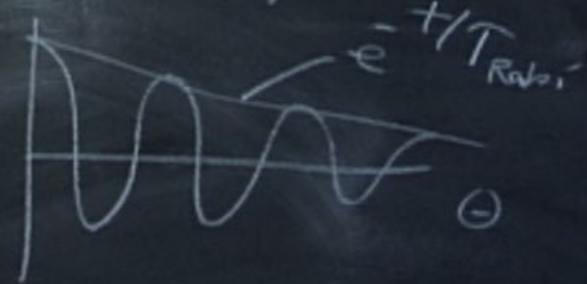
1) $|0\rangle\langle 0|$, probability

2) lifetime $|0\rangle\langle 0|$, T_1

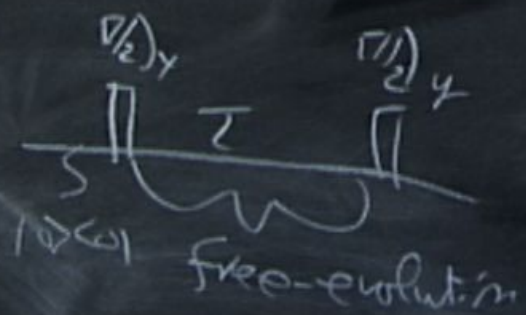




3) Rabi oscillation



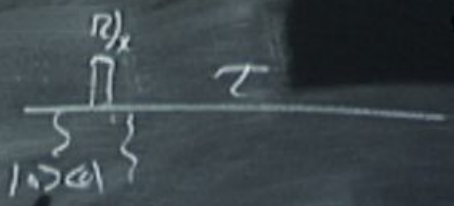
4) Ramsey fringe

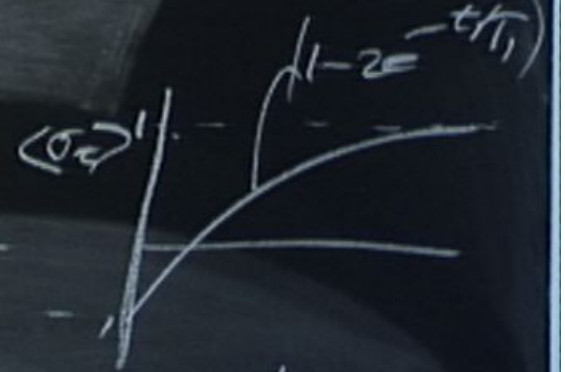


Q: Device ⟹ qubits.

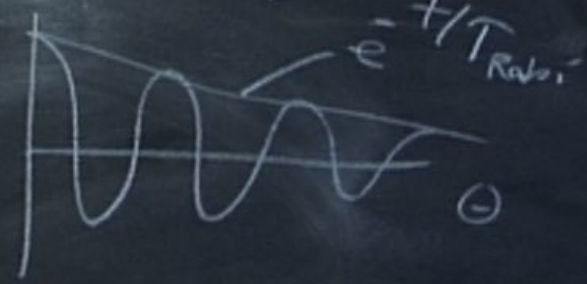
1) $|0\rangle\langle 0|$, probability

2) lifetime $|0\rangle\langle 0|$, T_1





3) Rabi oscillation

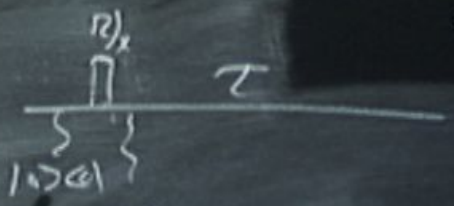


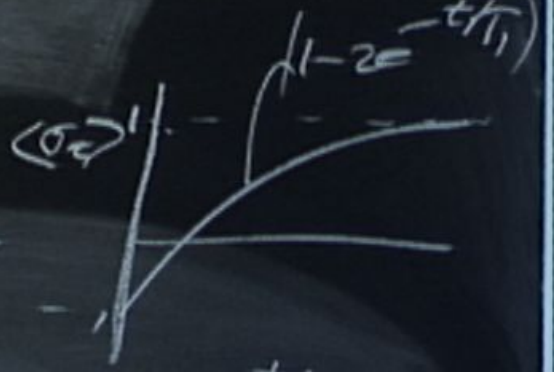
4) Ramsey fringe

Q: Device ⟹ qubits.

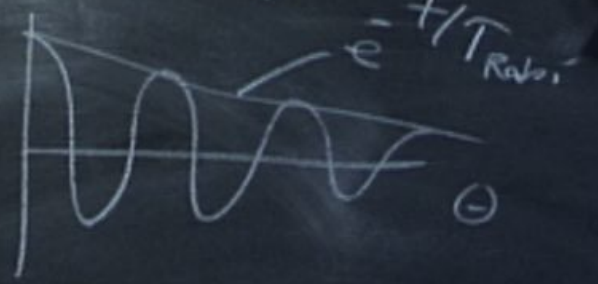
1) $|0\rangle\langle 0|$, probability

2) lifetime $|0\rangle\langle 0|$, T_1





3) Rabi oscillation



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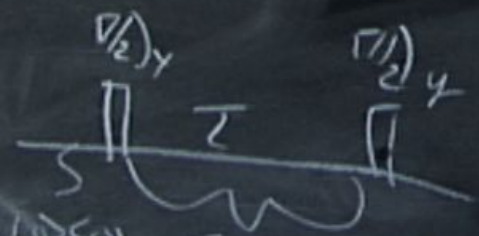
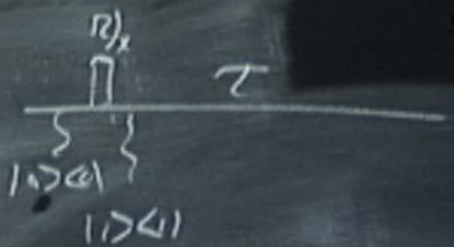
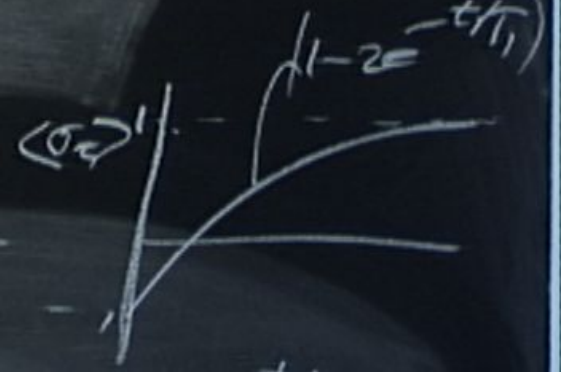


Q: Device ⟹ qubits.

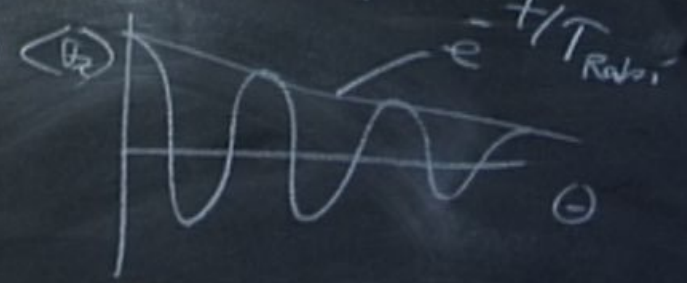
1) $|0\rangle\langle 0|$, probability

2) lifetime $|0\rangle\langle 0|$, T_1

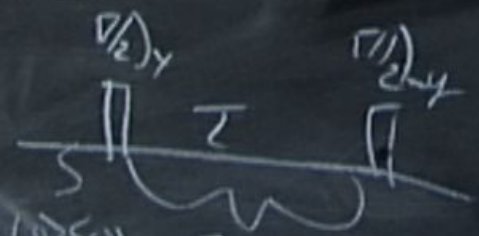


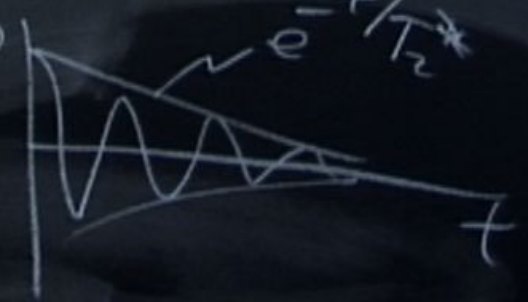


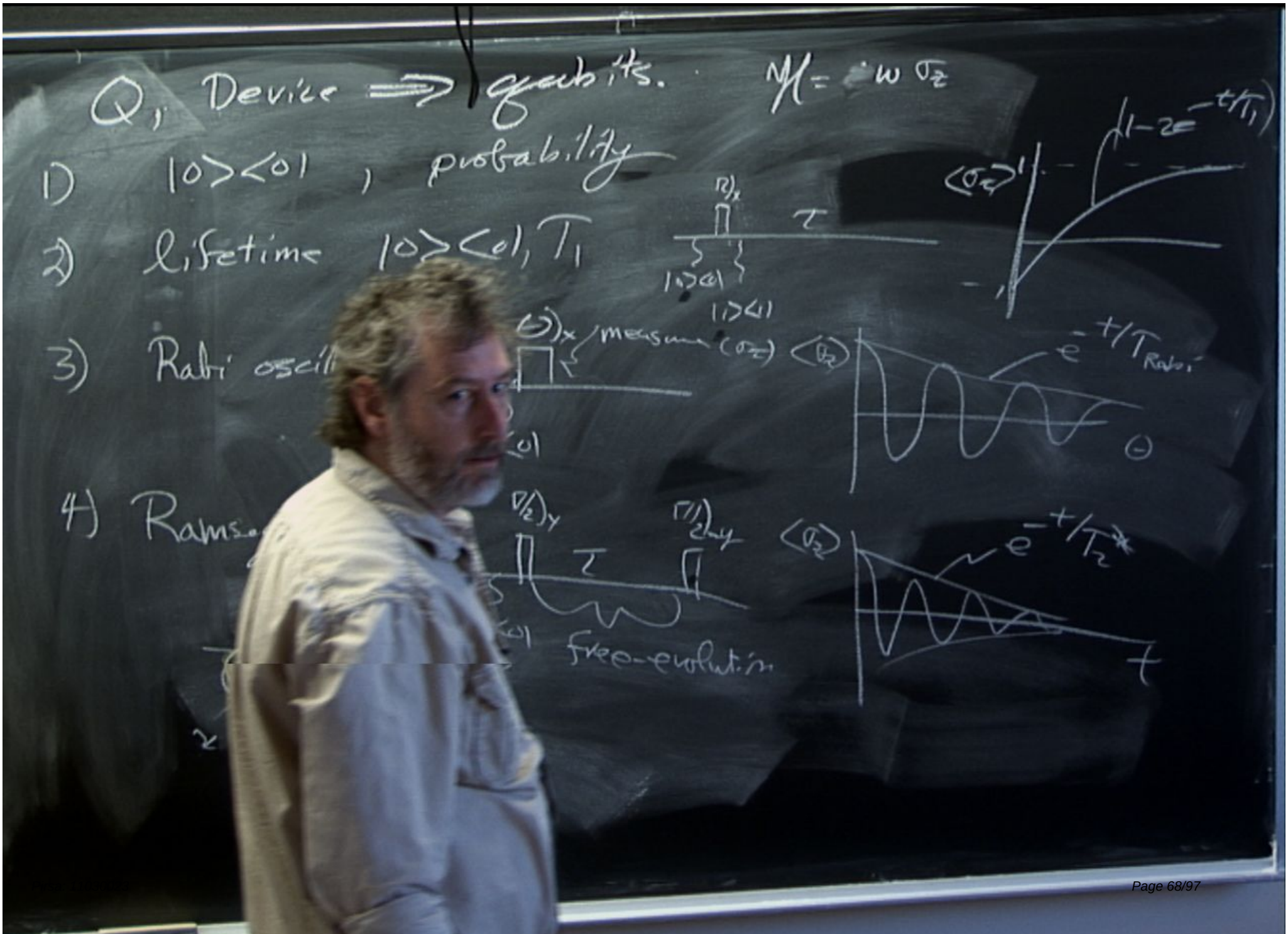
3) Rabi oscillation

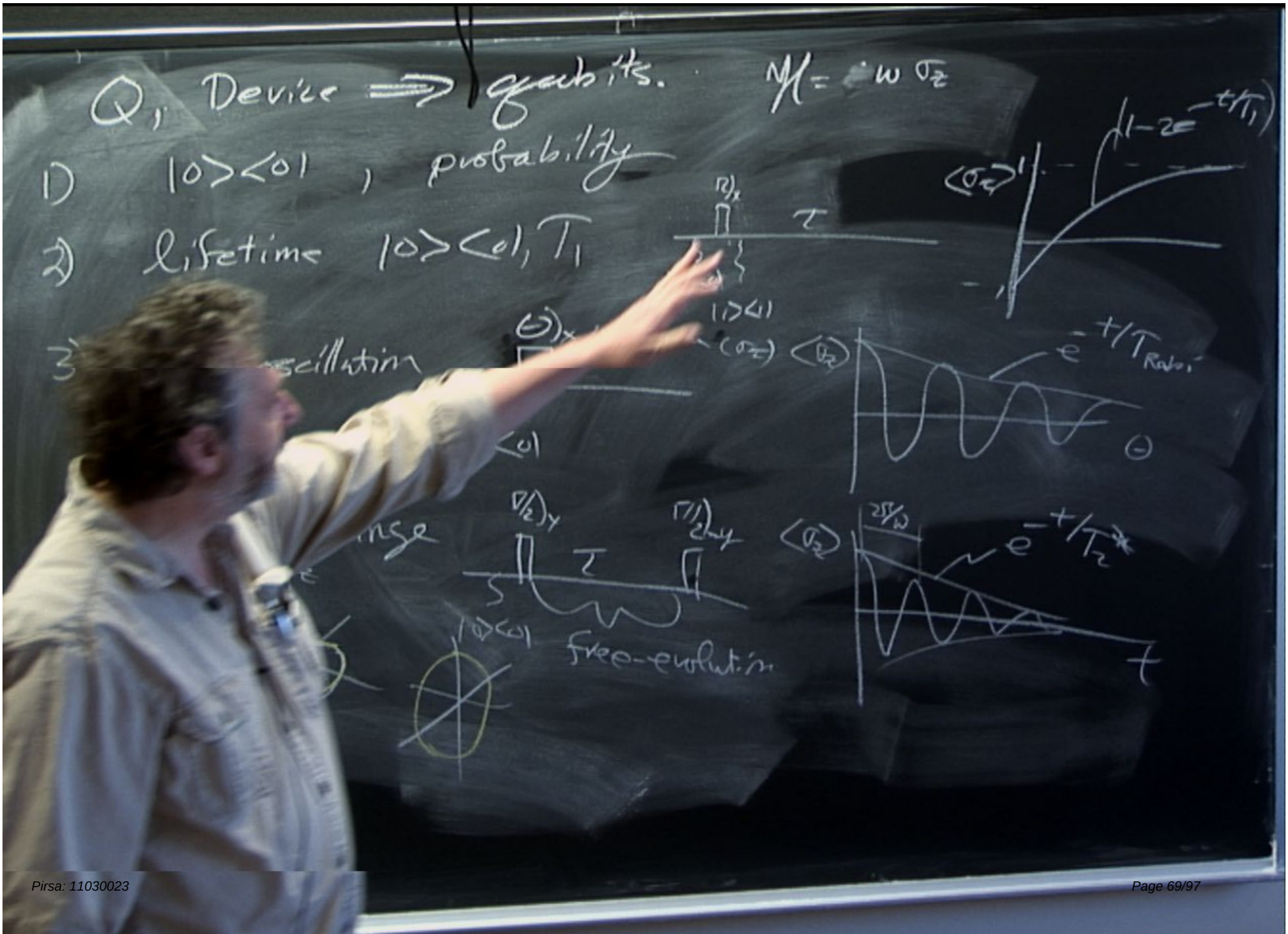


4) Ramsey fringe





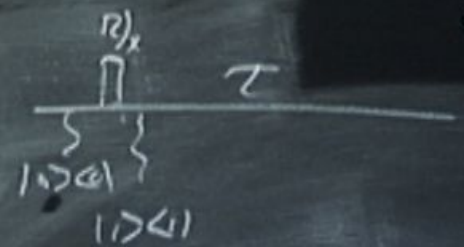

Q, Device ⟹ qubits.
1) |0><0| , probability
2) lifetime |0><0|, T1
3) Rabi oscill
4) Ramse
measure
free-evolution

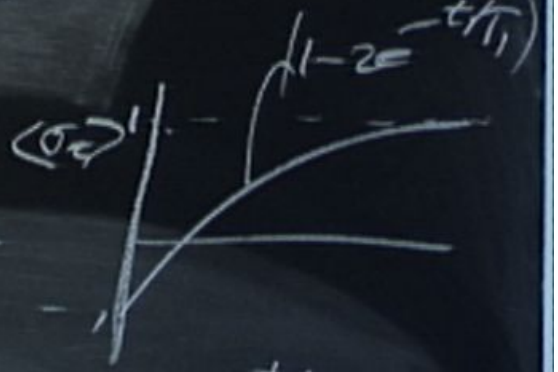

Q, Device ⟹ qubits.
1) |0><0| , probability
2) lifetime |0><0|, T1
free-evolution

Q, Device ⟹ qubits. $\mathcal{H} = \omega \sigma_z$

1) $|0\rangle\langle 0|$, probability

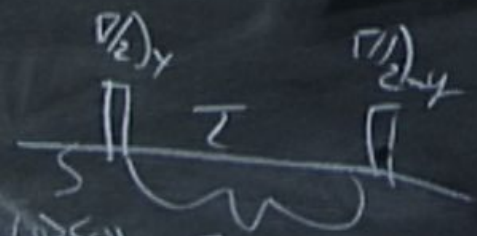
2) lifetime $|0\rangle\langle 0|$, T_1

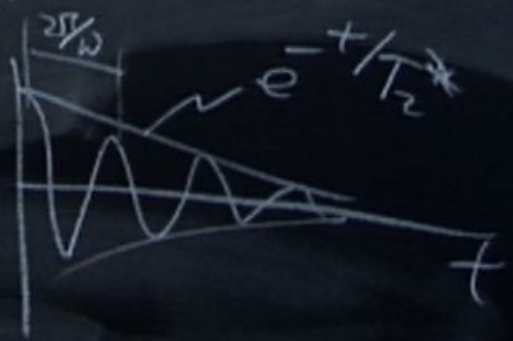


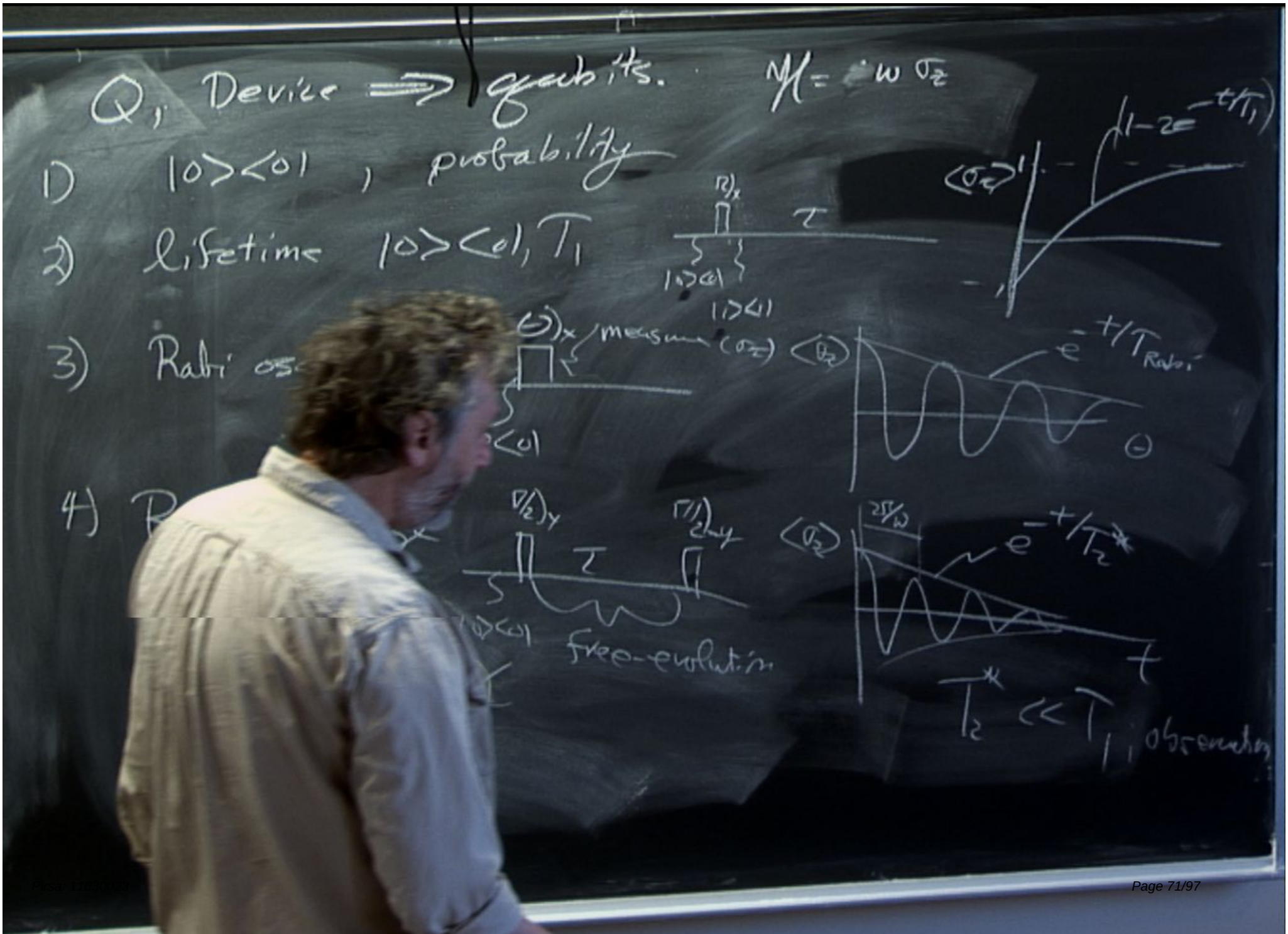


3) Rabi oscillation

4) Ramsey fringe



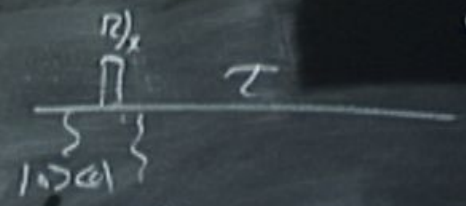


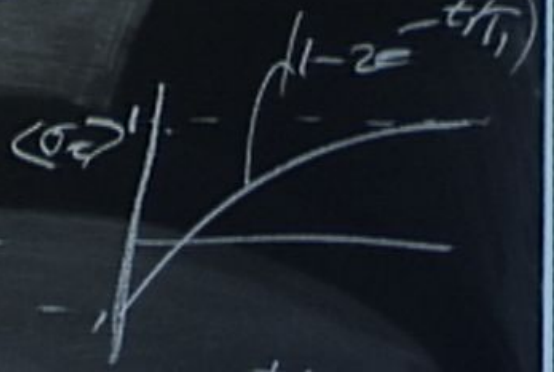

Q, Device ⟹ qubits.
1) |0><0| , probability
2) lifetime |0><0|, T1
3) Rabi os
measure
4)
free-evolution
T2* << T1, observation

Q: Device ⟹ qubits. $\mathcal{H} = \omega \sigma_z$

1) $|0\rangle\langle 0|$, probability

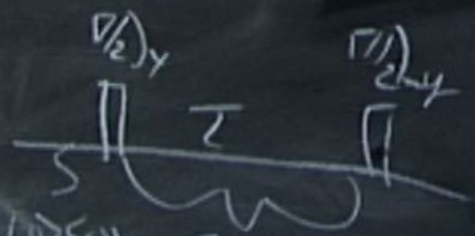
2) lifetime $|0\rangle\langle 0|$, T_1

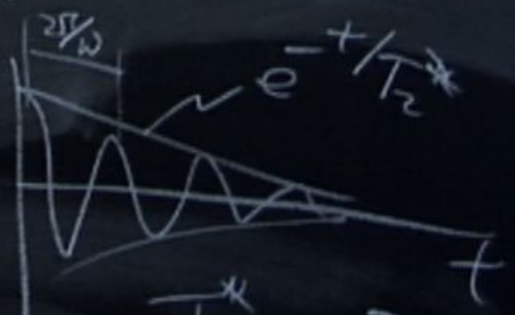




3) Rabi oscillation

4) Ramsey fringe



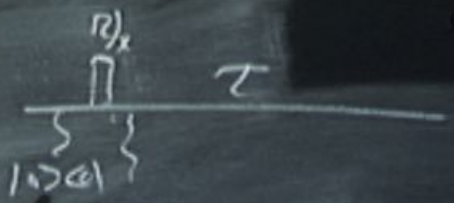


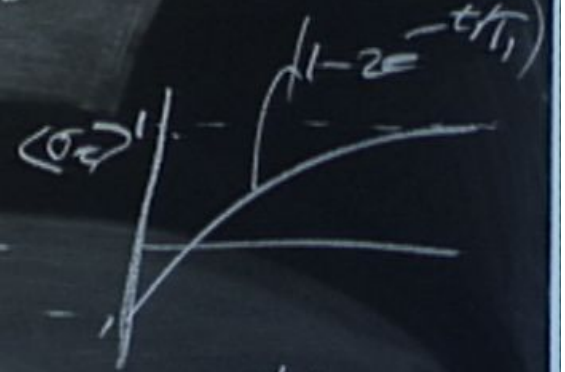
$T_2^* \ll T_1$, typical observation

Q: Device ⟹ qubits. $\mathcal{H} = \omega \sigma_z$

1) $|0\rangle\langle 0|$, probability

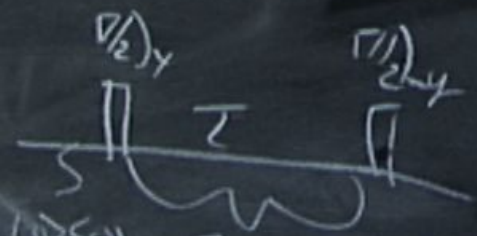
2) lifetime $|0\rangle\langle 0|$, T_1

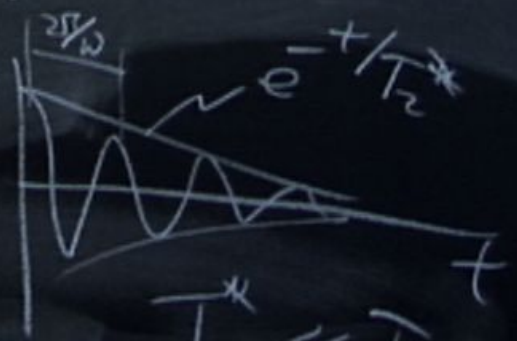




3) Rabi oscillation

4) Ramsey fringe



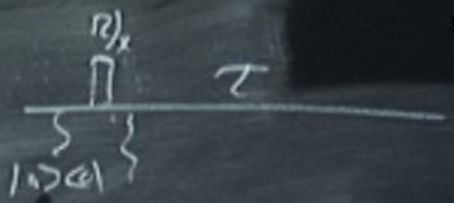


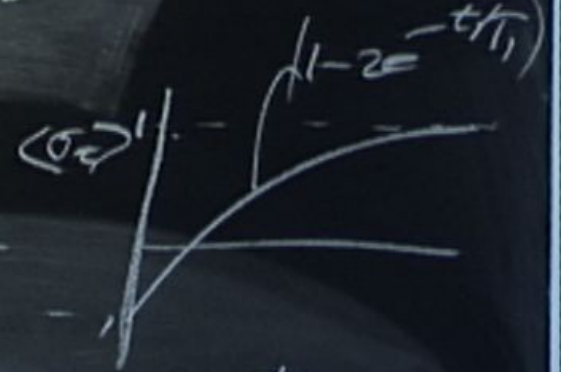
$T_2^* \ll T_1$, typical observation

Q, Device ⟹ qubits. $\mathcal{H} = \omega \sigma_z$

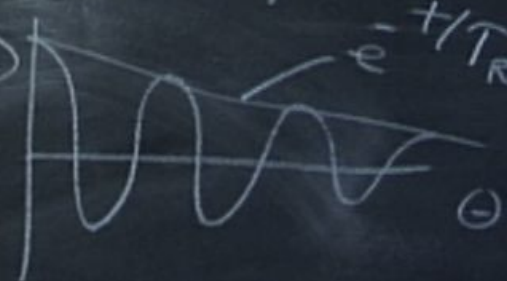
1) $|0\rangle\langle 0|$, probability

2) lifetime $|0\rangle\langle 0|$, T_1

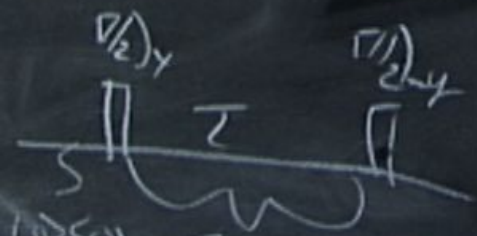


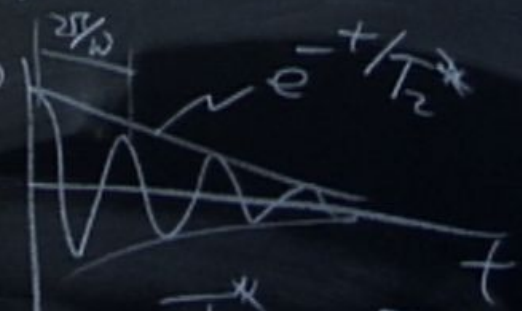


3) Rabi oscillation



4) Ramsey fringe





free-evolution

$T_2^* \ll T_1$, typical observation

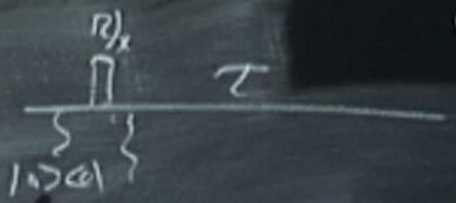
$T_2 = T_1$

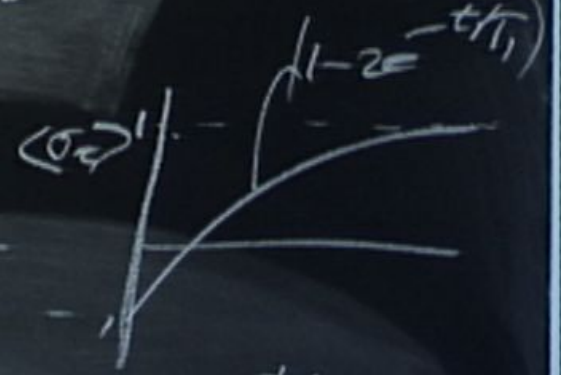
Pla. 4

Q: Device ⟹ qubits. $\mathcal{H} = \omega \sigma_z$

1) $|0\rangle\langle 0|$, probability

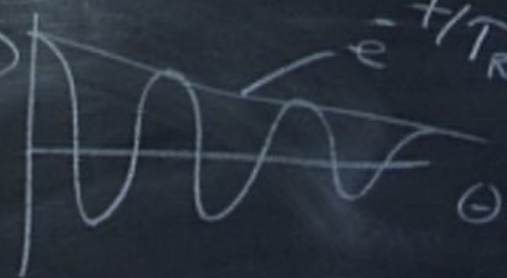
2) lifetime $|0\rangle\langle 0|$, T_1



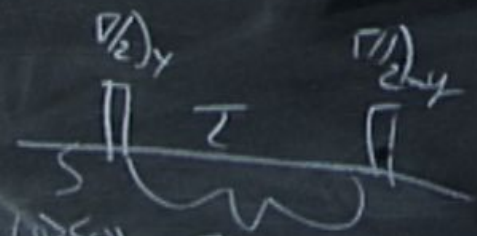


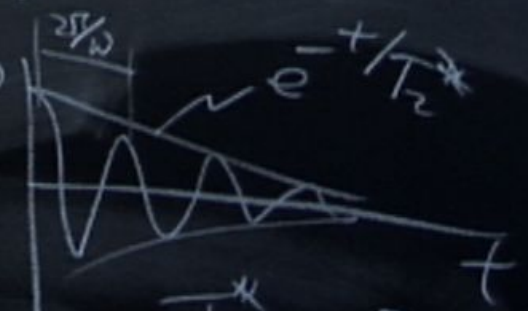
3) Rabi oscillation

$$\frac{1}{T_{Rabi}} = \frac{1}{T_2} + \frac{1}{T_1}$$



4) Ramsey fringe





$T_2^* \ll T_1$, typical observation

$$\boxed{T_2 = T_1}$$

Pla. 4

Q, Device ⟹ qubits. $\mathcal{H} = \omega \sigma_z$

1) $|0\rangle\langle 0|$, probability

2) lifetime $|0\rangle\langle 0|$, T_1

$(\pi)_x$ τ $|1\rangle\langle 1|$ $|0\rangle\langle 0|$

$\langle\sigma_z\rangle$ $(1-2e^{-t/T_1})$

3) Rabi oscillation

$(\theta)_x$ measure (σ_z) $|0\rangle\langle 0|$

$\langle\sigma_z\rangle$ $e^{-t/T_{Rabi}}$ θ

$$\frac{1}{T_{Rabi}} = \frac{1}{2}\frac{1}{T_2} + \frac{1}{2}\frac{1}{T_1}$$

4) Ramsey fringe

$(\pi/2)_y$ τ $(\pi/2)_{-y}$ $|0\rangle\langle 0|$ free-evolution

$\langle\sigma_z\rangle$ $2\pi/\omega$ e^{-t/T_2^*} t

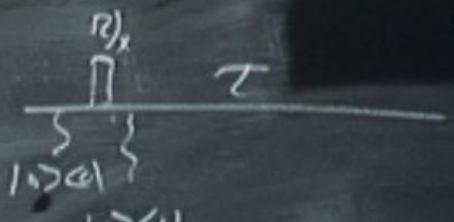
$T_2^* \ll T_1$, typical observation

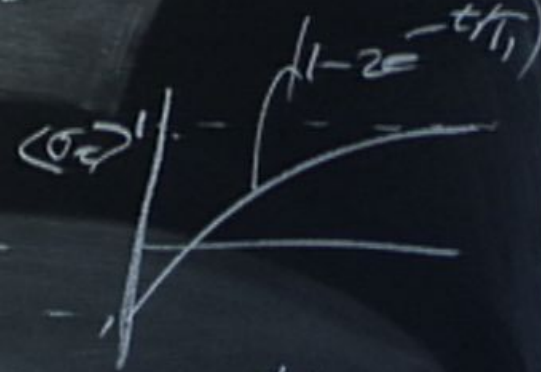
$T_2 = T_1$ Pla. 4

Q: Device ⟹ qubits. $\mathcal{H} = \omega \sigma_z$

1) $|0\rangle\langle 0|$, probability

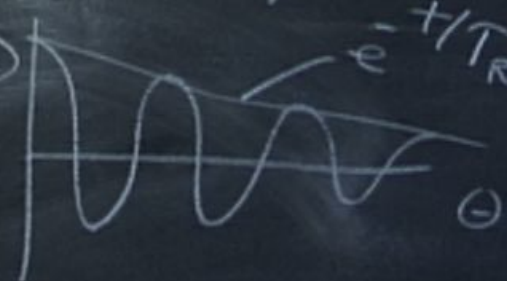
2) lifetime $|0\rangle\langle 0|$, T_1



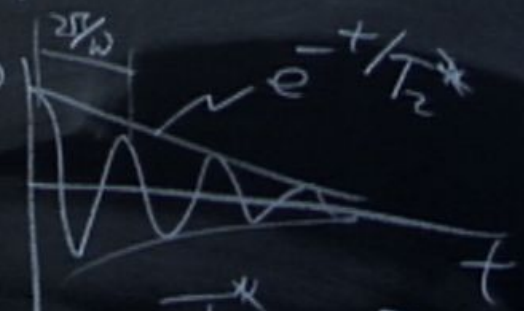


3) Rabi oscillation

$$\boxed{\frac{1}{T_{Rabi}} = \frac{1}{2}\frac{1}{T_2} + \frac{1}{2}\frac{1}{T_1}}$$



4) Ramsey fringe



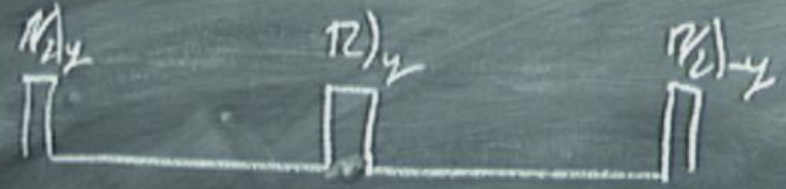
$T_2^* \ll T_1$, typical observation

$$\boxed{T_2 = T_1}$$

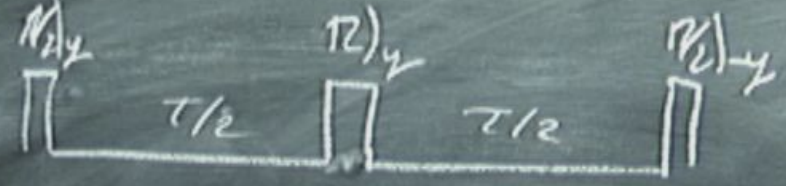
Pla. 4

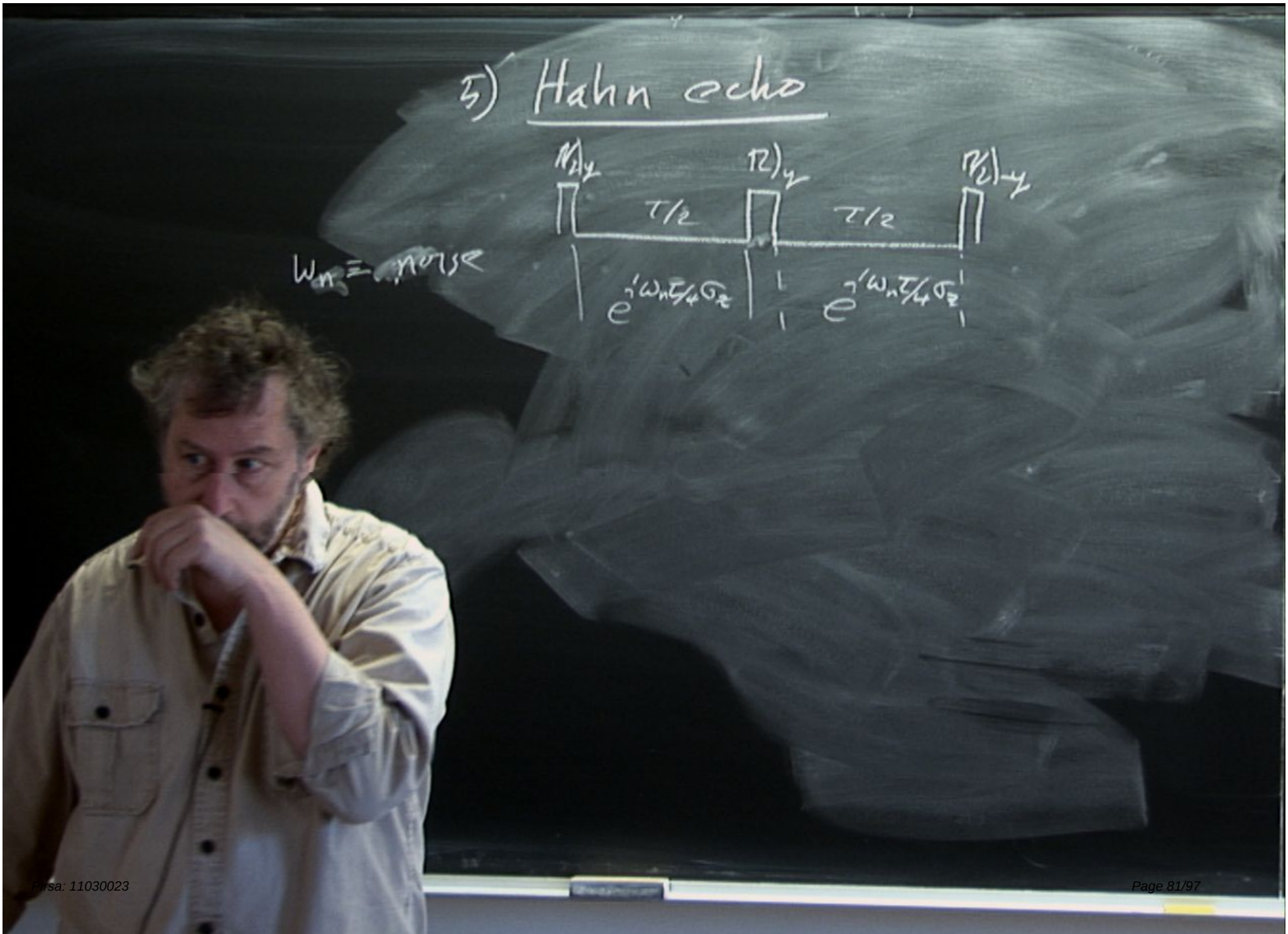
5) Hahn echo

5) Hahn echo

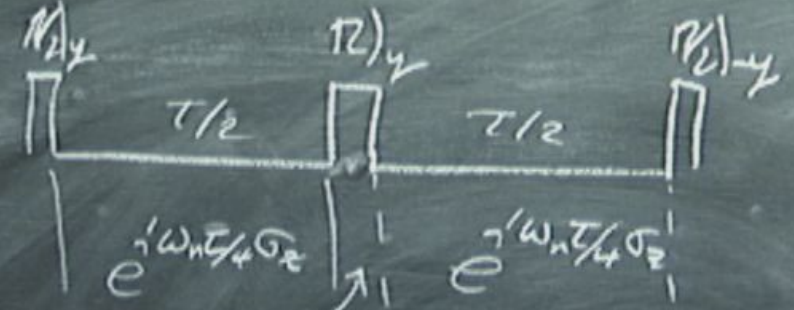


5) Hahn echo



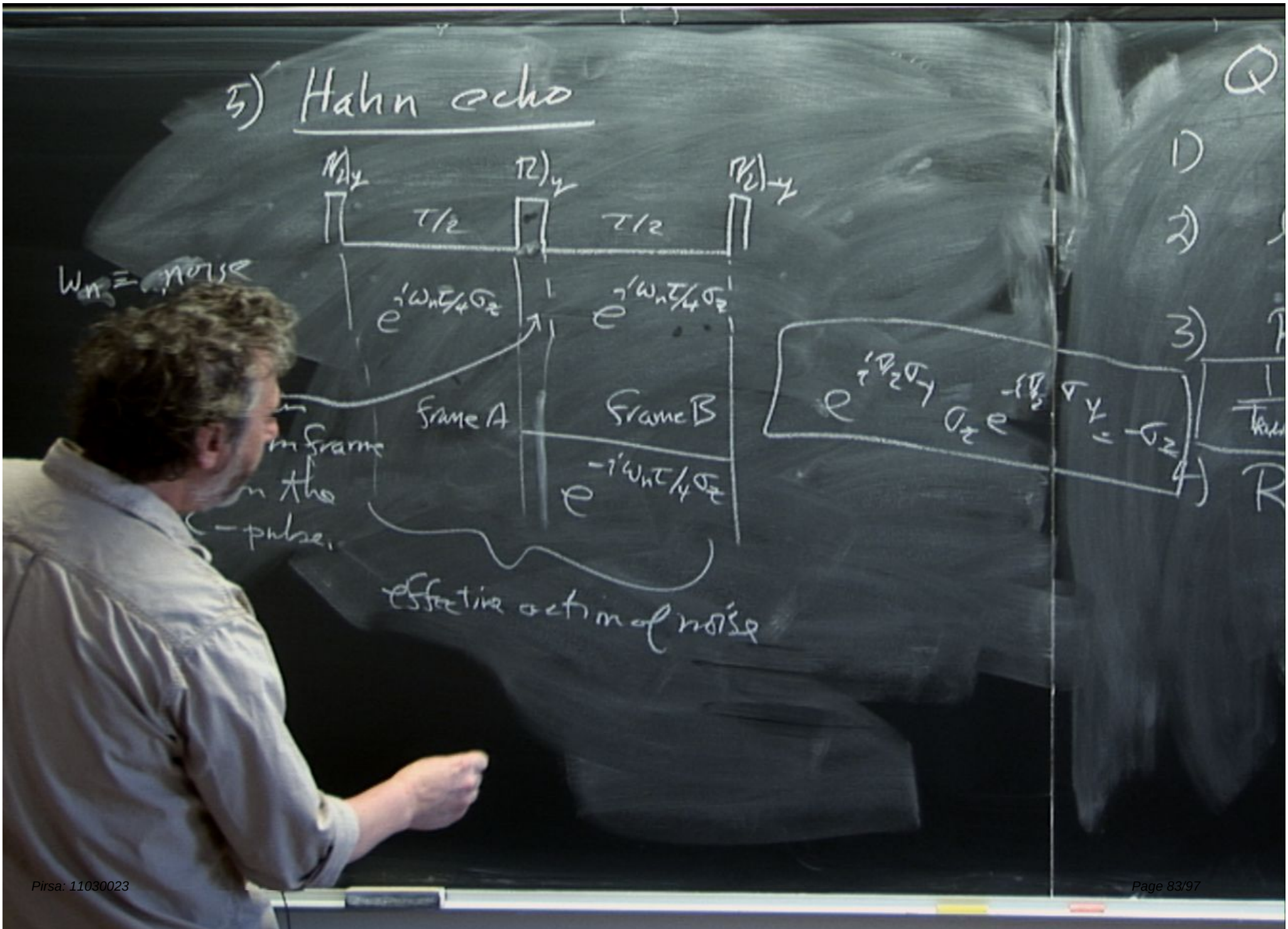

3) Hahn echo
π/2 y
π y
π/2 -y
τ/2
τ/2
$e^{i\omega_n \tau/4 \sigma_z}$
$e^{i\omega_n \tau/4 \sigma_z}$
ω_n = noise

5) Hahn echo

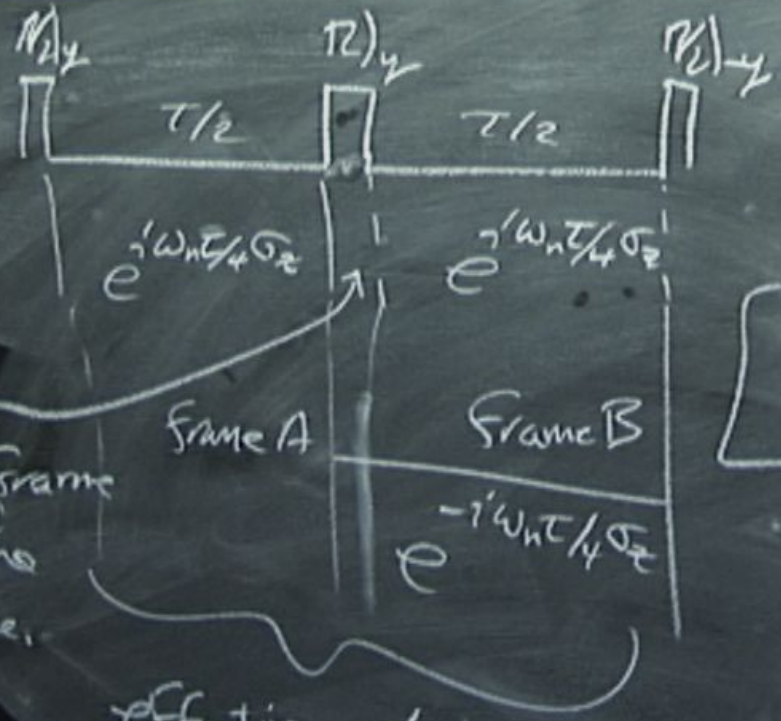


$\omega_n \equiv$ noise

define an interaction frame based on the π-pulse.


5) Hahn echo
π/2 y
π y
π/2 -y
τ/2
τ/2
$e^{-i\omega_n \tau/4 \sigma_z}$
$e^{-i\omega_n \tau/4 \sigma_z}$
Frame A
Frame B
$e^{-i\omega_n \tau/4 \sigma_z}$
$e^{i\pi/2 \sigma_y} \sigma_z e^{-i\pi/2 \sigma_y} = -\sigma_z$
effective action of noise
1)
2)
3)
4)

5) Hahn echo



ω_n = noise

define an interaction frame based on the π-pulse.

effective action of noise

$$e^{i\omega_n \tau/4 \sigma_z} e^{-i\omega_n \tau/4 \sigma_z}$$

$$e^{i\frac{\pi}{2}\sigma_y} \sigma_z e^{-i\frac{\pi}{2}\sigma_y} = -\sigma_z$$

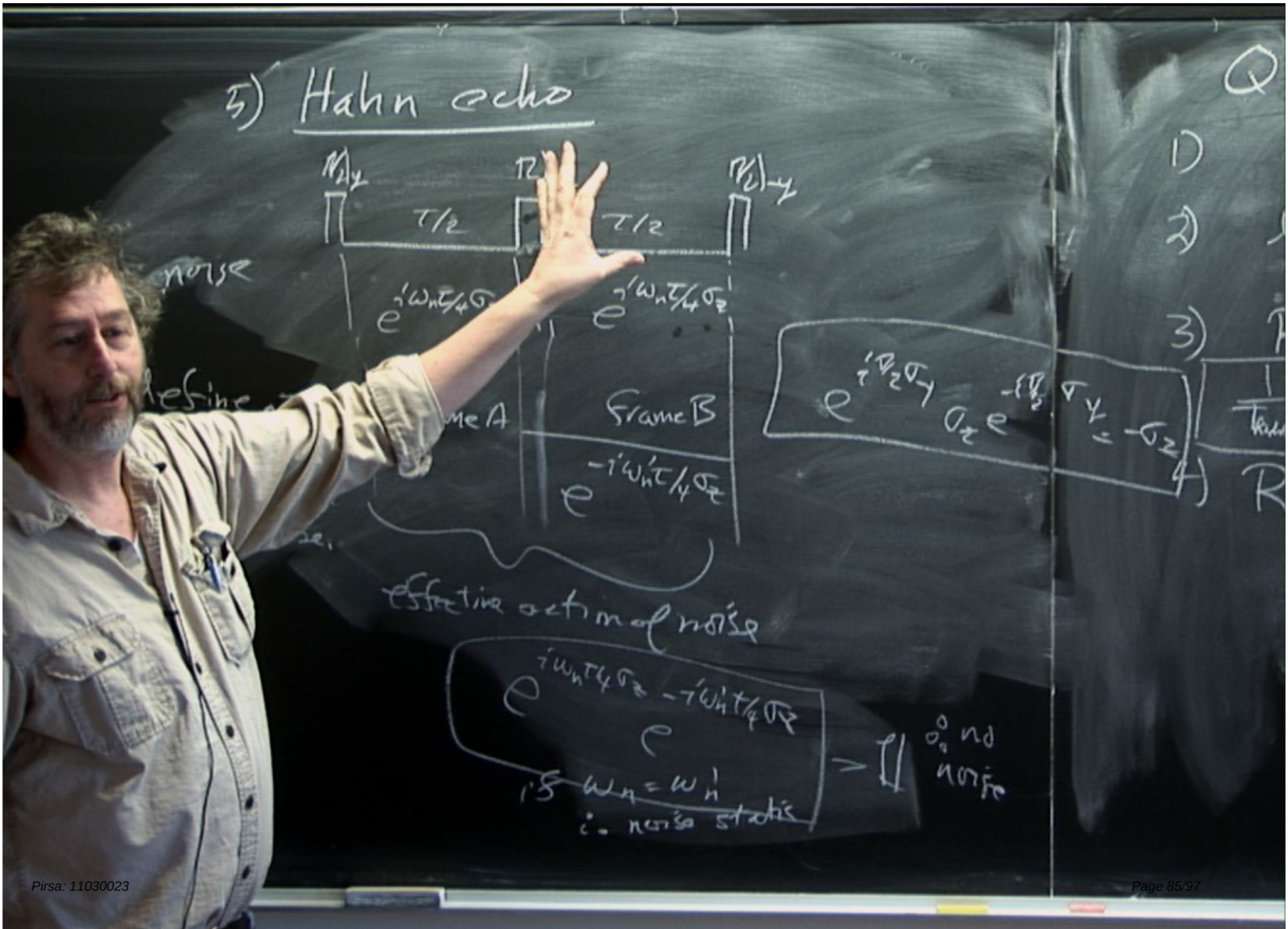
Q

1)

2)

3)

4)


5) Hahn echo
π/2 y
π
π/2 -y
τ/2
τ/2
noise
$e^{i\omega_n \tau/4 \sigma_z}$
$e^{i\omega_n \tau/4 \sigma_z}$
Frame A
Frame B
$e^{-i\omega_n' \tau/4 \sigma_z}$
$e^{i\pi/2 \sigma_y} \sigma_z e^{-i\pi/2 \sigma_y} = -\sigma_z$
effective action of noise
$e^{i\omega_n \tau/4 \sigma_z - i\omega_n' \tau/4 \sigma_z}$
if $\omega_n = \omega_n'$
i.e. noise static
no noise
Q
1)
2)
3)
4)

5) Hahn echo

$\pi/2)_y$ — $\tau/2$ — $\pi)_y$ — $\tau/2$ — $(\pi/2)_{-y}$

$e^{-i\omega_n \tau/4 \sigma_z}$ $\quad$ $e^{-i\omega_n' \tau/4 \sigma_z}$

Frame A $\quad$ Frame B

$e^{-i\omega_n' \tau/4 \sigma_z}$

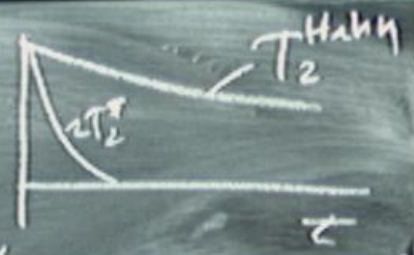
effective action of noise

$$e^{i\omega_n \tau/4 \sigma_z - i\omega_n' \tau/4 \sigma_z}$$

if $\omega_n = \omega_n'$

i.e. noise static

$\Rightarrow$ no noise



$$T_2^{Hahn} = T_1$$

$$e^{i\pi/2 \sigma_y} \sigma_z e^{-i\pi/2 \sigma_y} = -\sigma_z$$

Q, Device

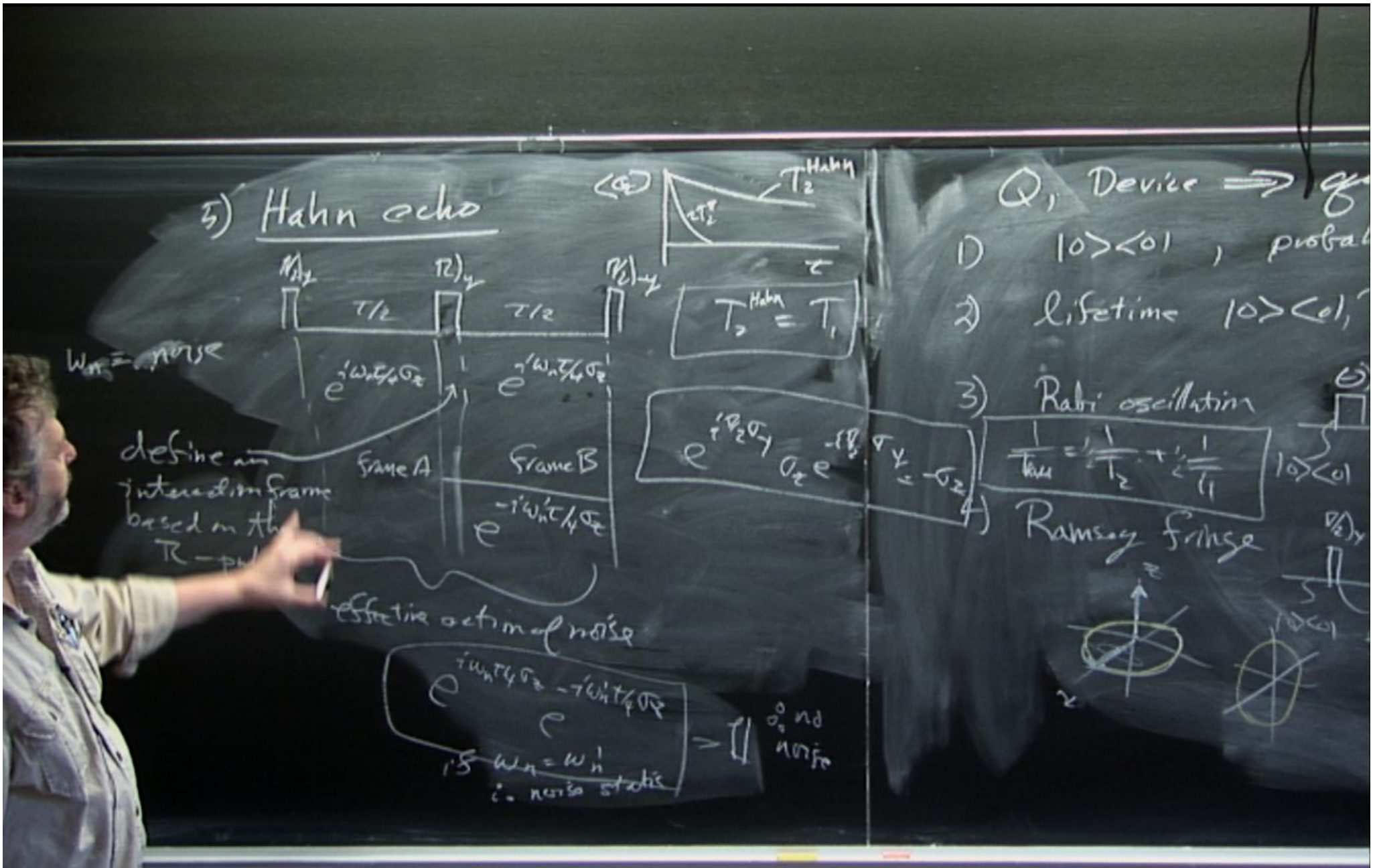
1) $|0\rangle\langle 0|$

2) lifetime

3) Rabi oscill

$$\frac{1}{T_{Hahn}} = \frac{1}{T_2} + \frac{1}{T_2}$$

4) Ramsey fr


3) Hahn echo
$T_2^{Hahn} = T_1$
$\tau/2$
$\tau/2$
$e^{i\omega_n \tau/4 \sigma_z}$
$e^{-i\omega_n \tau/4 \sigma_z}$
Frame A
Frame B
define an interaction frame based on the
effective action of noise
$e^{i\omega_n \tau/4 \sigma_z - i\omega_n' \tau/4 \sigma_z}$
if $\omega_n = \omega_n'$
i.e. noise static
$e^{i\pi/2 \sigma_y} \sigma_z e^{-i\pi/2 \sigma_y} = -\sigma_z$
$\frac{1}{T_{Hahn}} = \frac{1}{2}\frac{1}{T_2} + \frac{1}{2}\frac{1}{T_1}$
Q, Device
1) $|0\rangle\langle 0|$, probab
2) lifetime $|0\rangle\langle 0|$,
3) Rabi oscillation
4) Ramsey fringe

3) Hahn echo

$\langle\sigma_z\rangle$ T_2^{Hahn} τ

$\boxed{T_2^{Hahn} = T_1}$

$\pi/2)_x$ $\pi)_y$ $\pi/2)_{-y}$

$\tau/2$ $\tau/2$

W_n = noise

$e^{i\omega_n\tau/4\sigma_z}$ $e^{i\omega_n\tau/4\sigma_z}$

define an interaction frame based on the π-pulse.

Frame A Frame B

$e^{-i\omega_n'\tau/4\sigma_z}$

$\boxed{e^{i\pi/2\sigma_y}\sigma_z e^{-i\pi/2\sigma_y} = -\sigma_z}$

effective action of noise

$\boxed{e^{i\omega_n\tau/4\sigma_z - i\omega_n'\tau/4\sigma_z}}$ $\Rightarrow$ $\mathbb{1}$ no noise

if $\omega_n = \omega_n'$

i.e. noise static

Q, Device $\Rightarrow$ q

1) $|0\rangle\langle 0|$, probal

2) lifetime $|0\rangle\langle 0|$,

3) Rabi oscillation

$\boxed{\frac{1}{T_{Rabi}} = \frac{1}{2}\frac{1}{T_2} + \frac{1}{2}\frac{1}{T_1}}$

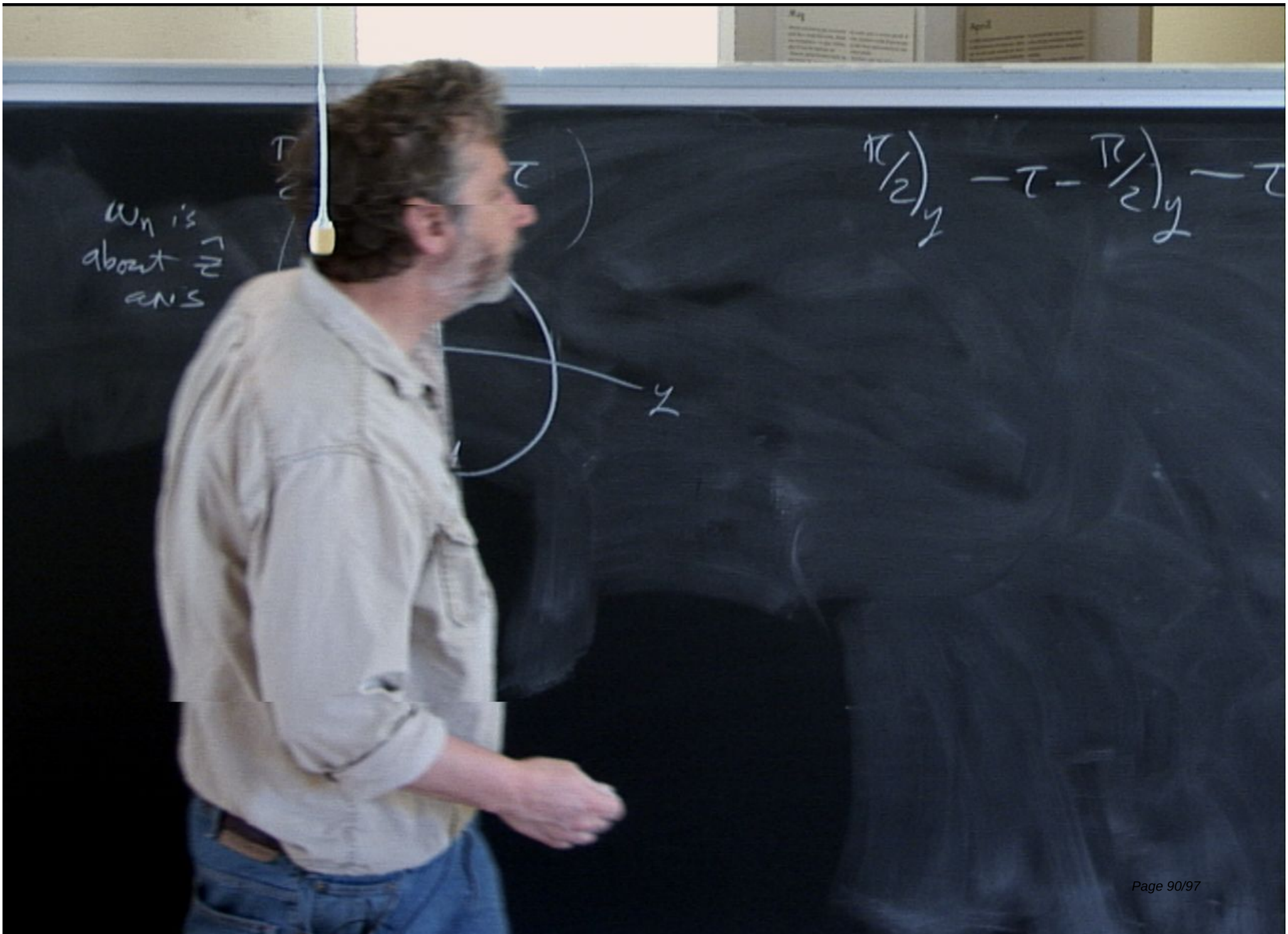
$|0\rangle\langle 0|$

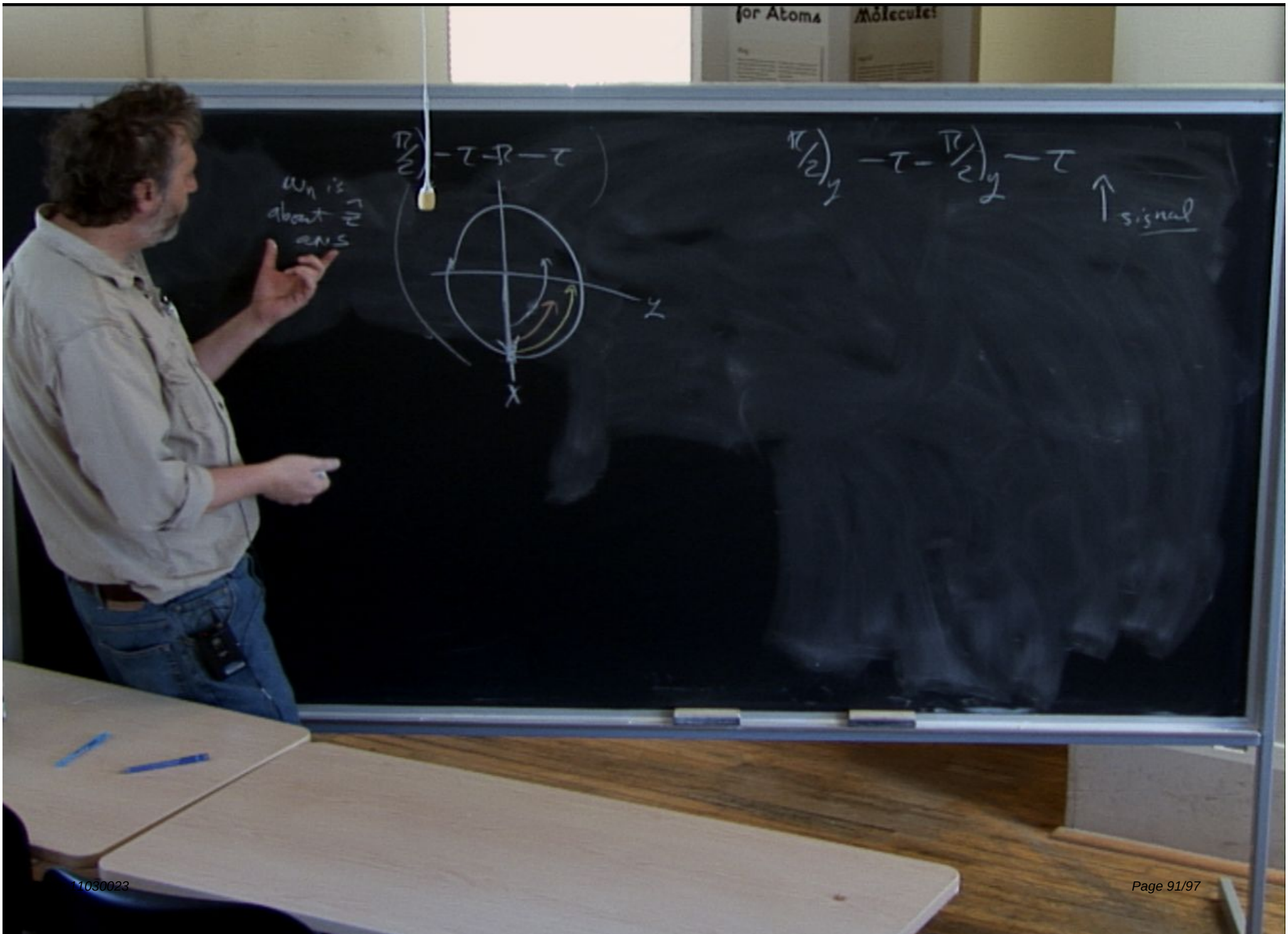
4) Ramsey fringe

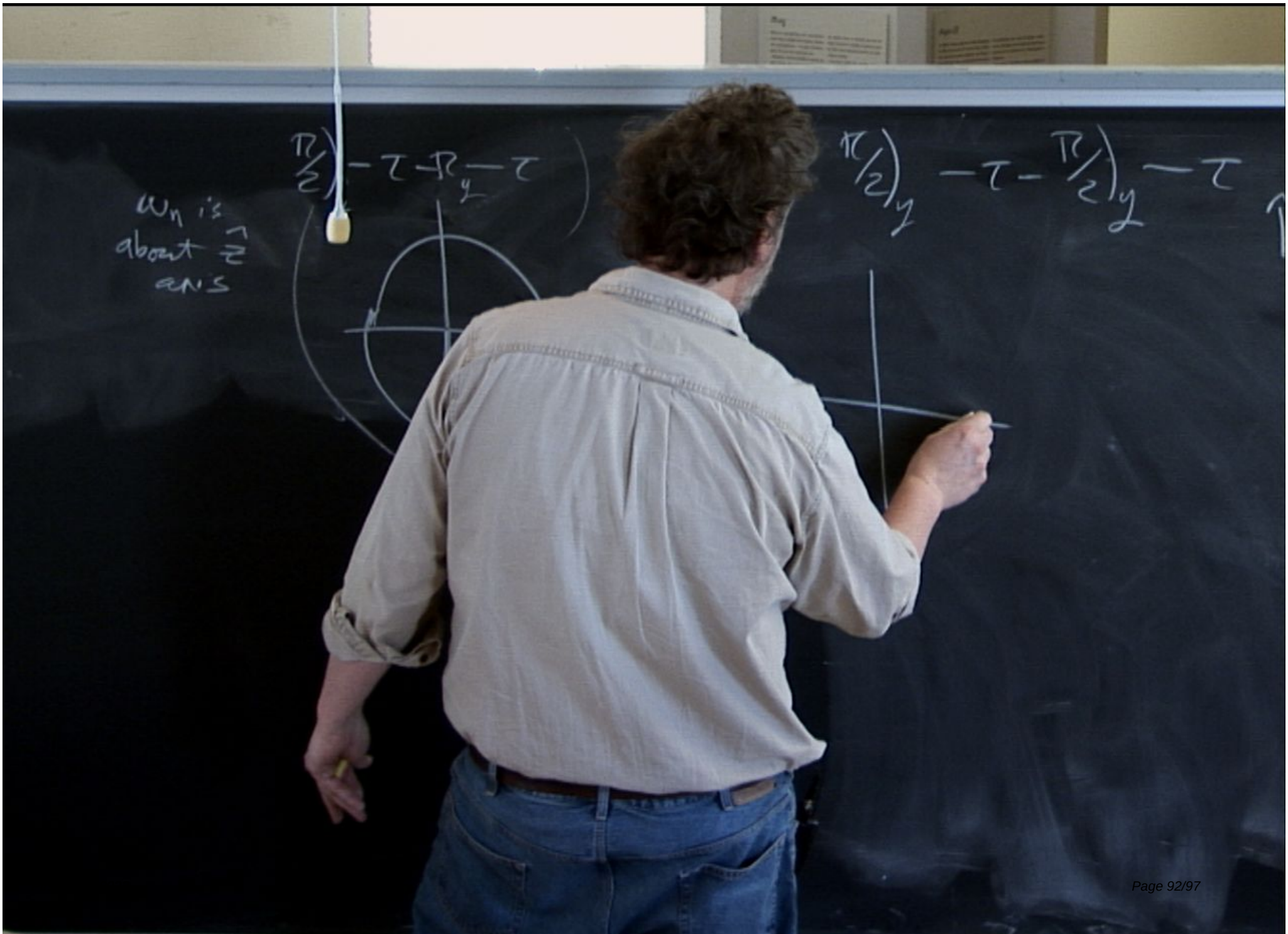
$\pi/2)_x$

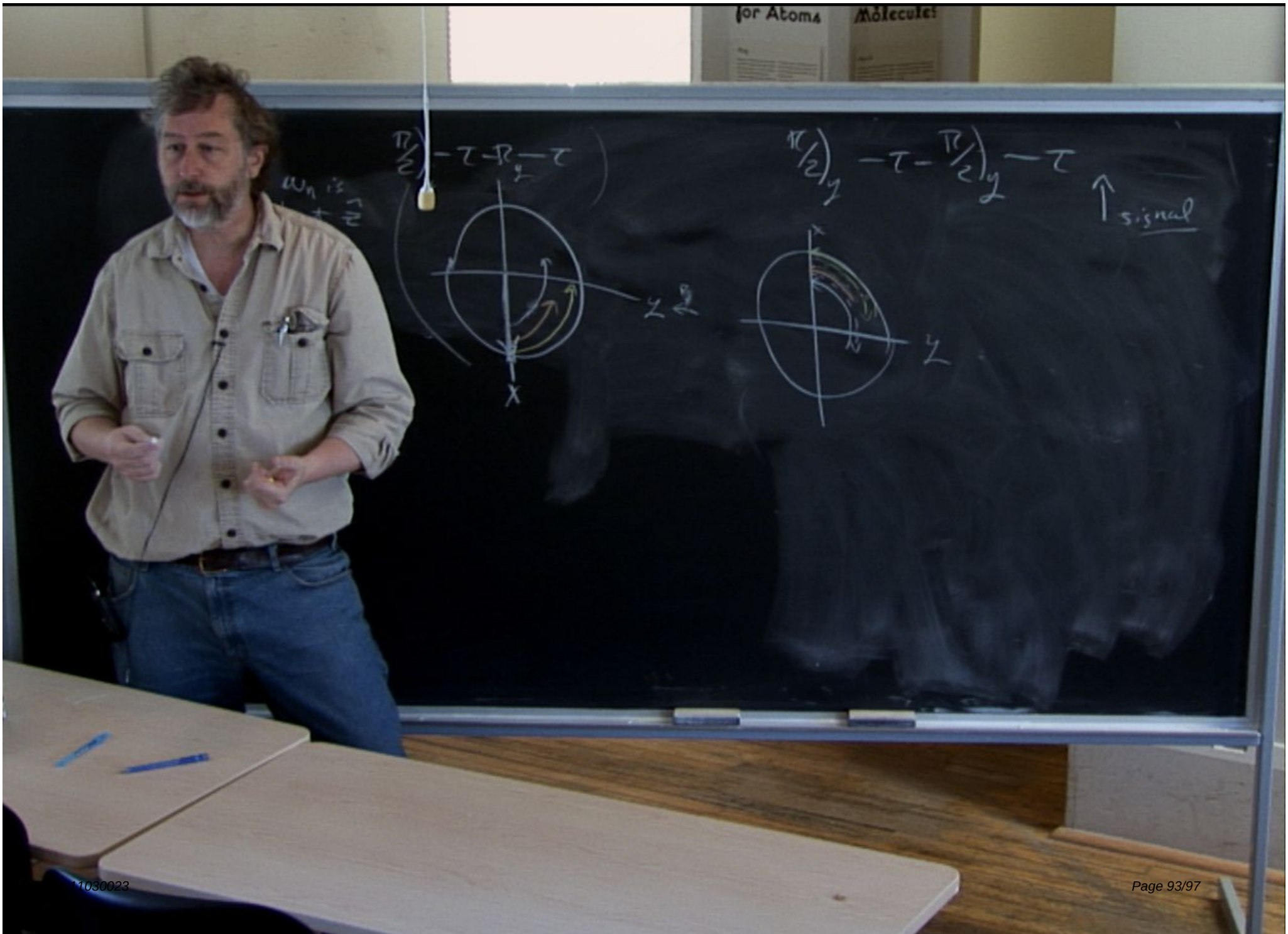
$|0\rangle\langle 0|$

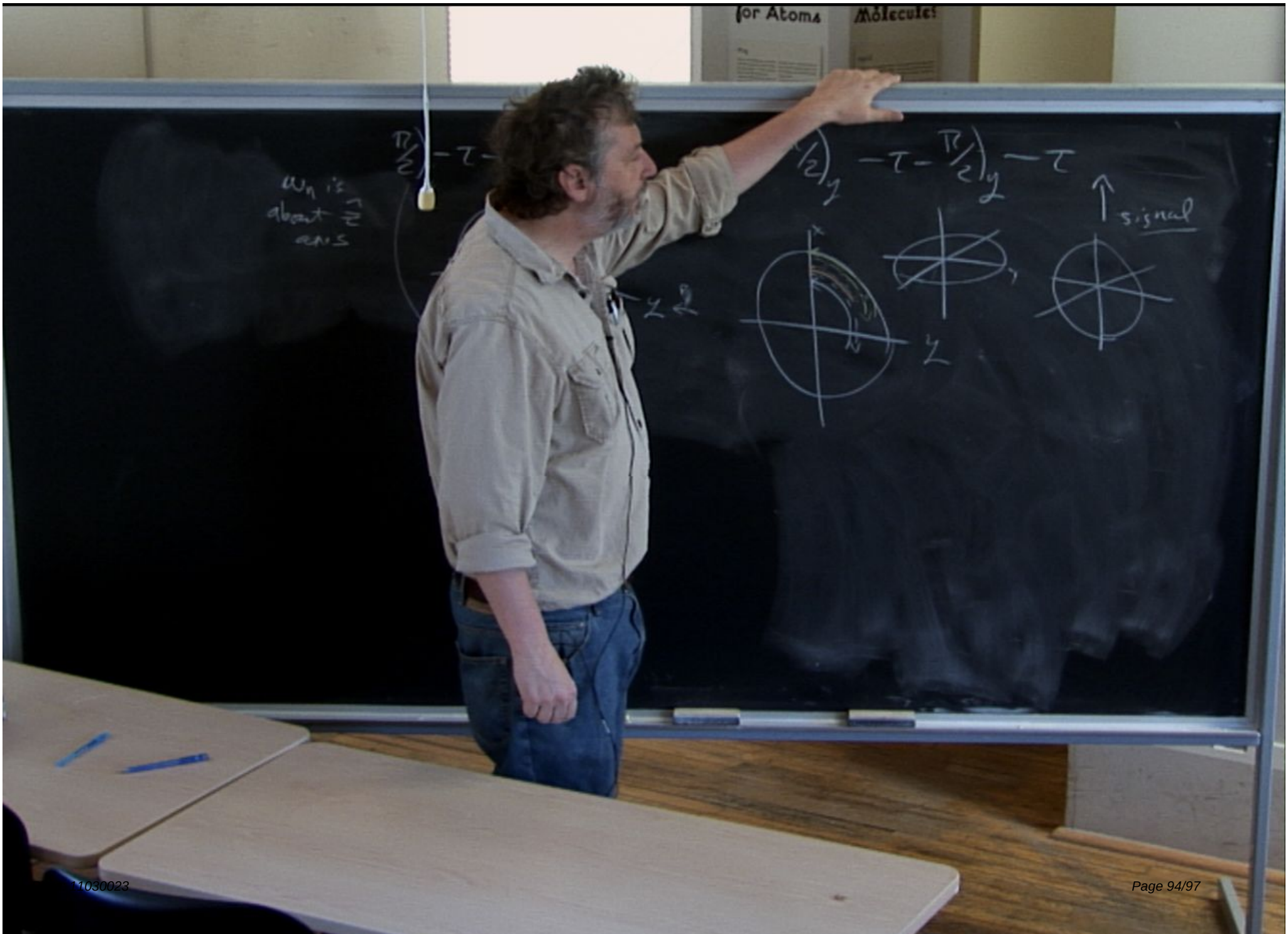
for Atoms
Molecules
π/2 — τ — π — τ
π/2)y — τ — π/2)y — τ
signal

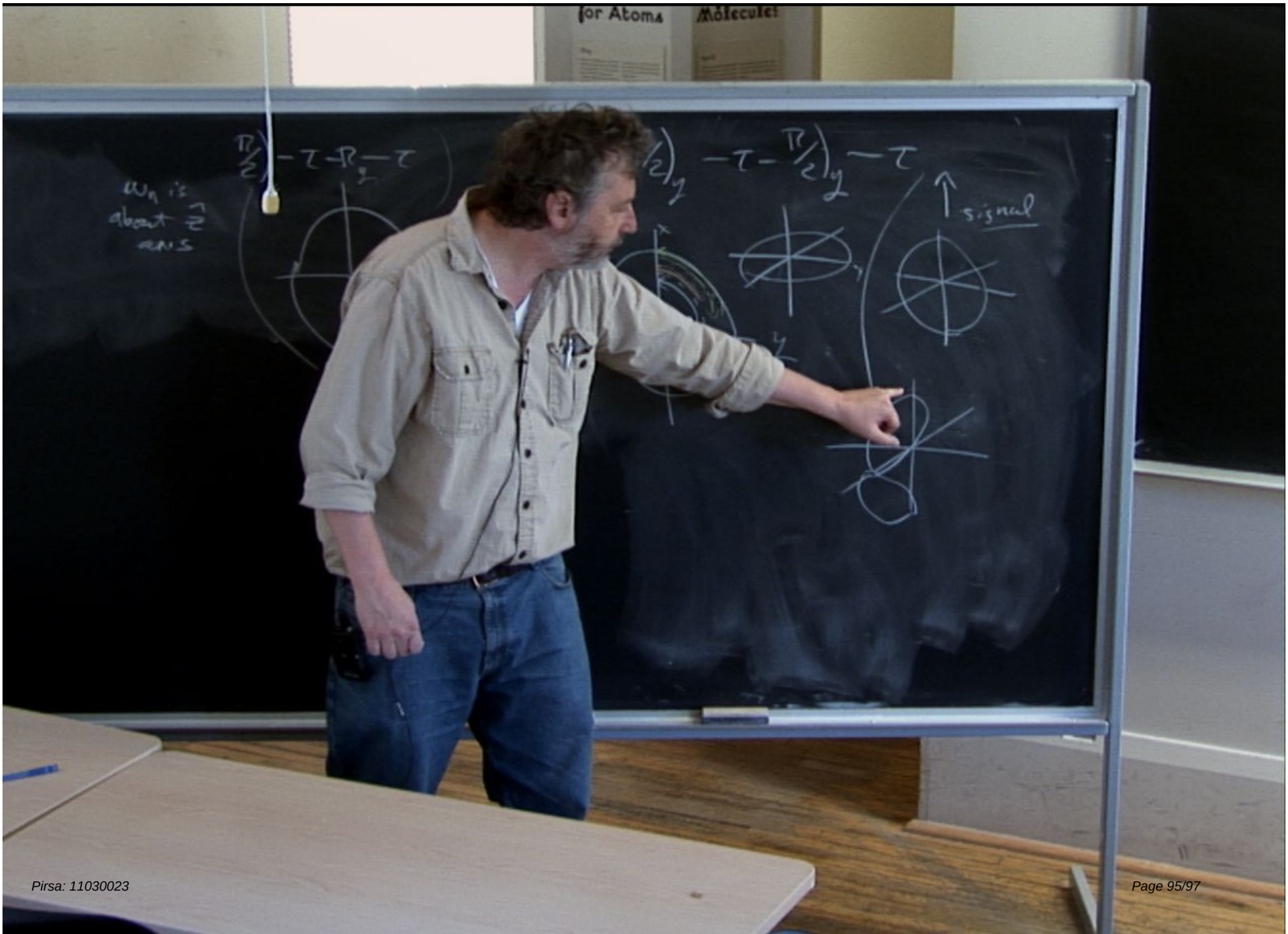

ω_n is
about $\hat{z}$
axis
y
$\pi/2)_y - \tau - \pi/2)_y - \tau$


for Atoms
Molecules
ω_n is about ẑ axis
π/2 — τ — π — τ
y
x
π/2 — τ — π/2 — τ
signal


ω_n is
about $\hat{z}$
axis


for Atoms
Molecules
signal


for Atoms
Molecules
signal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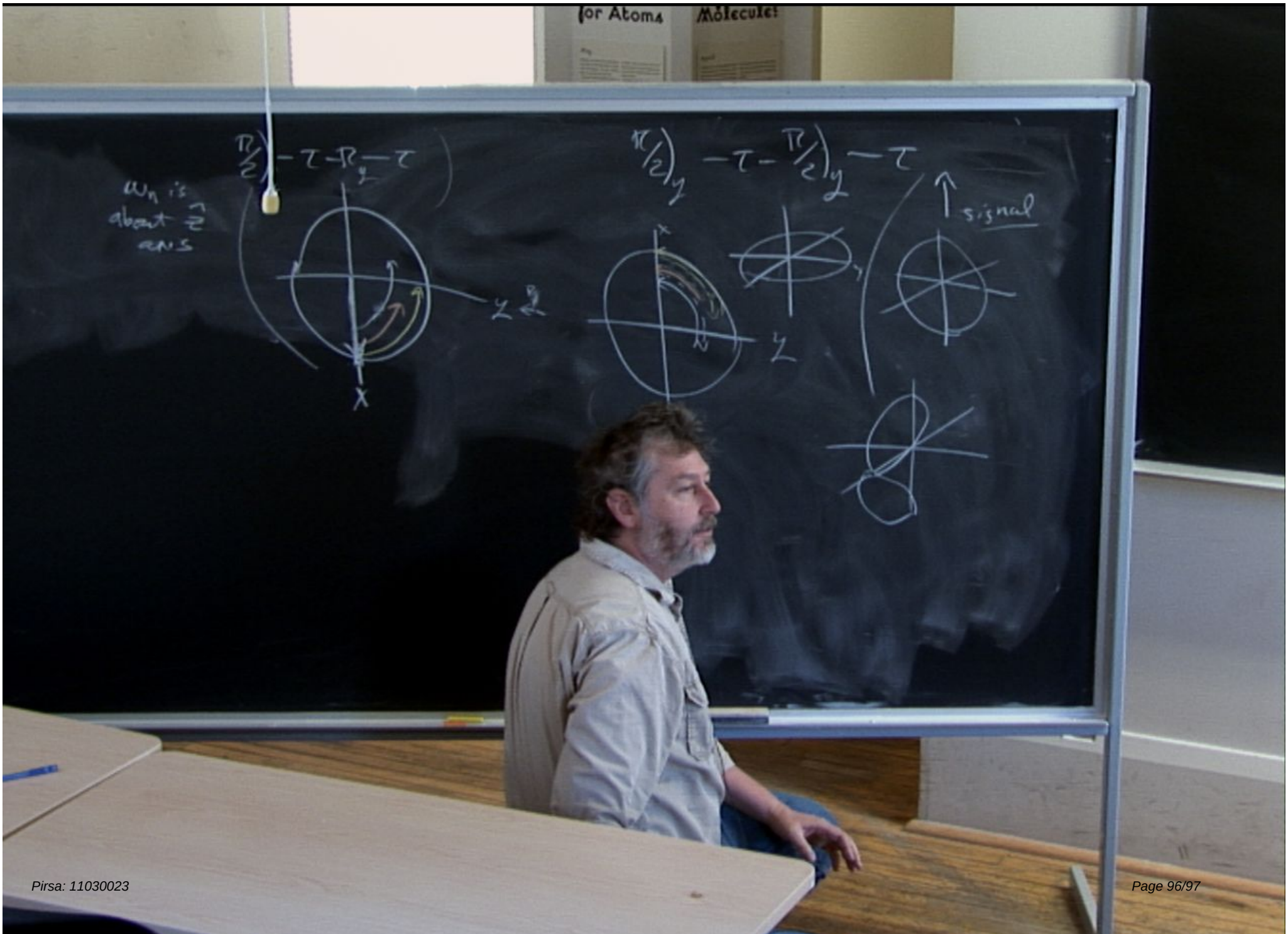
for Atoms
Molecules
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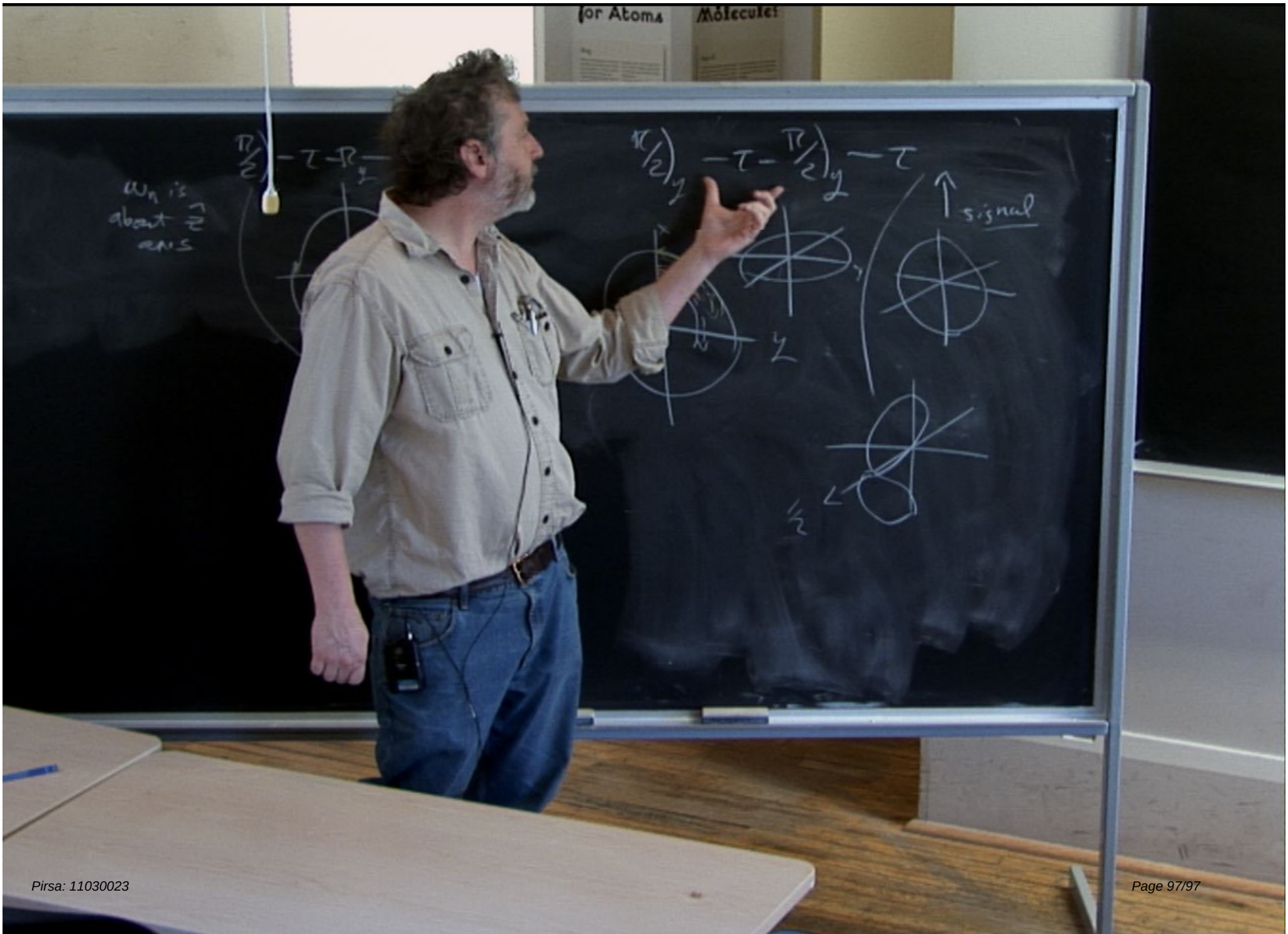
for Atoms
Molecules
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