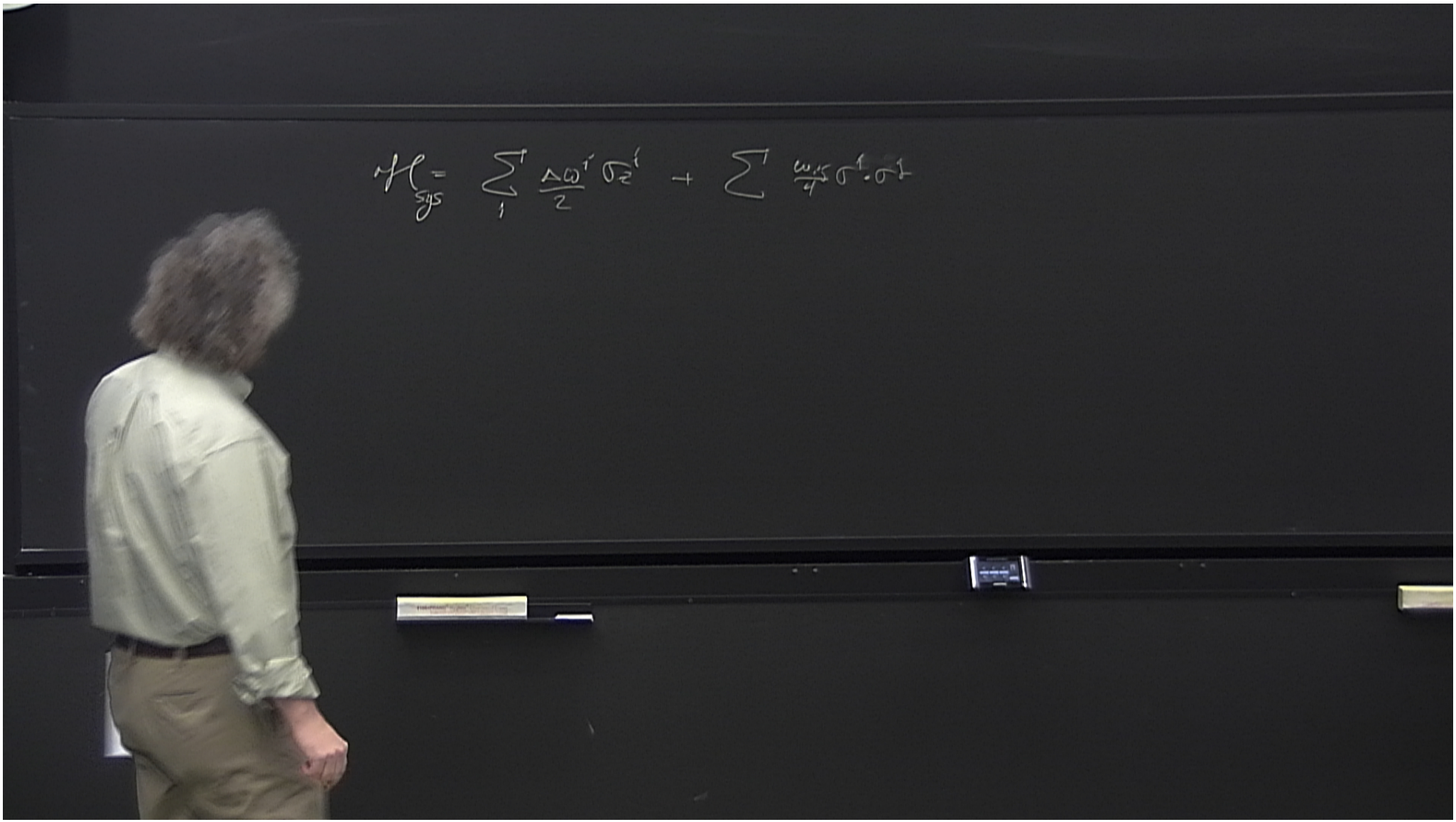
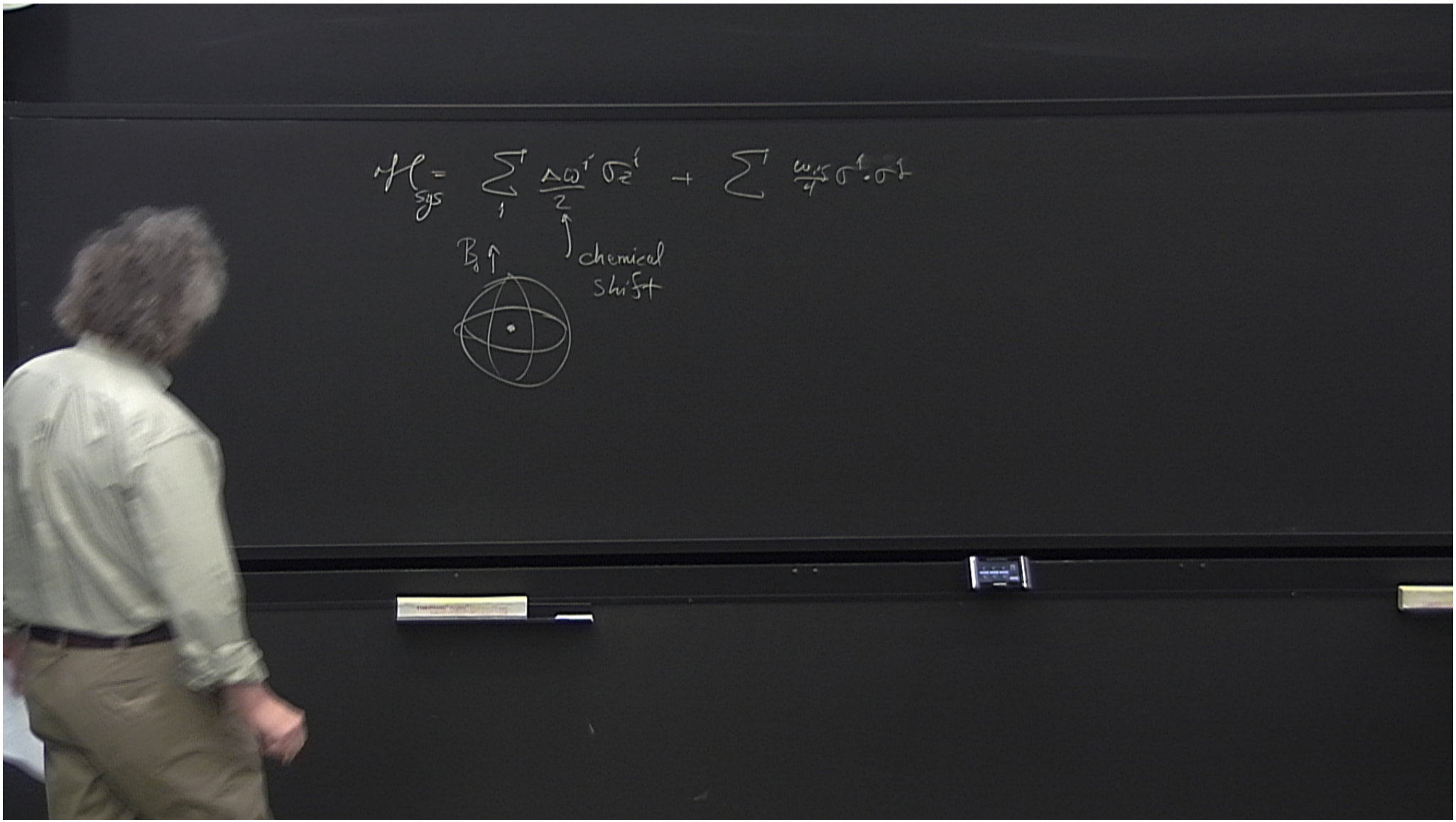
Title: 12/13 PSI - Explorations on Quantum Information Lecture 11

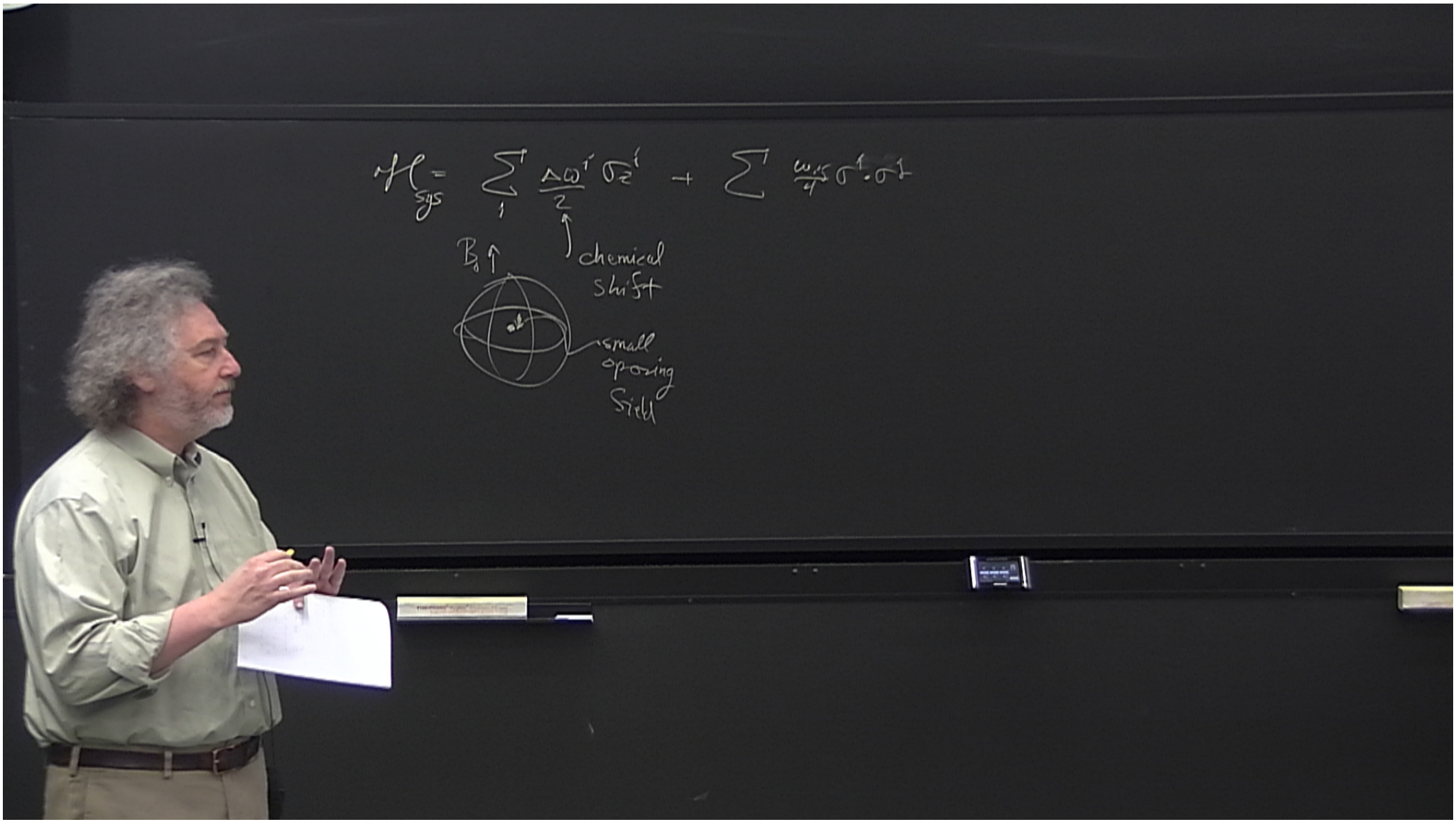
Date: Apr 02, 2013 09:00 AM

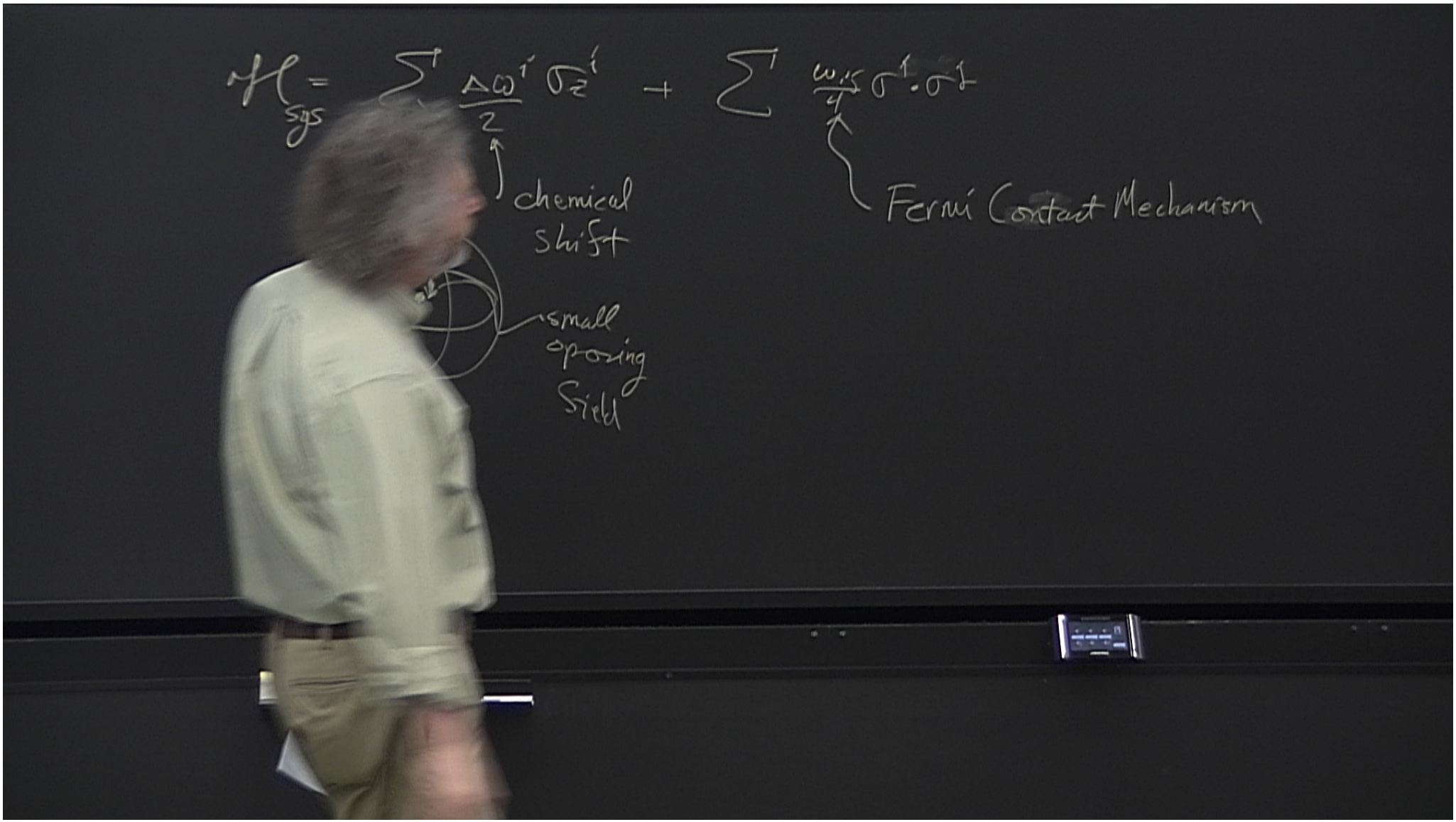
URL: http://pirsa.org/13040034

Abstract:


$\mathcal{H}_{sys} = \sum_i \frac{\Delta\omega^i}{2}\sigma_z^i + \sum \frac{\omega_{ij}}{4}\sigma^i\cdot\sigma^j$


$\mathcal{H}_{sys} = \sum_i \frac{\Delta\omega^i}{2} \sigma_z^i + \sum \frac{\omega_{ij}}{4} \sigma^i \cdot \sigma^j$
B_0
chemical shift


$\mathcal{H}_{sys} = \sum_i \frac{\Delta\omega^i}{2}\sigma_z^i + \sum \frac{\omega_{ij}}{4}\sigma^i\cdot\sigma^j$
B_0
chemical shift
small opposing field


$\mathcal{H}_{sys} = \sum \frac{\Delta\omega^i}{2} \sigma_z^i + \sum \frac{\omega_{ij}}{4} \sigma^i \cdot \sigma^j$
chemical shift
Fermi Contact Mechanism
small opposing field

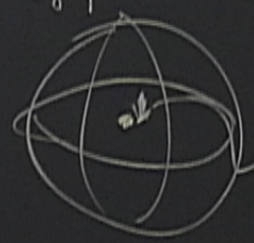
$$\mathcal{H}_{sys} = \sum_i \frac{\Delta\omega^i}{2}\sigma_z^i + \sum \frac{\omega_{ij}}{4}\sigma^i\cdot\sigma^j$$

chemical shift

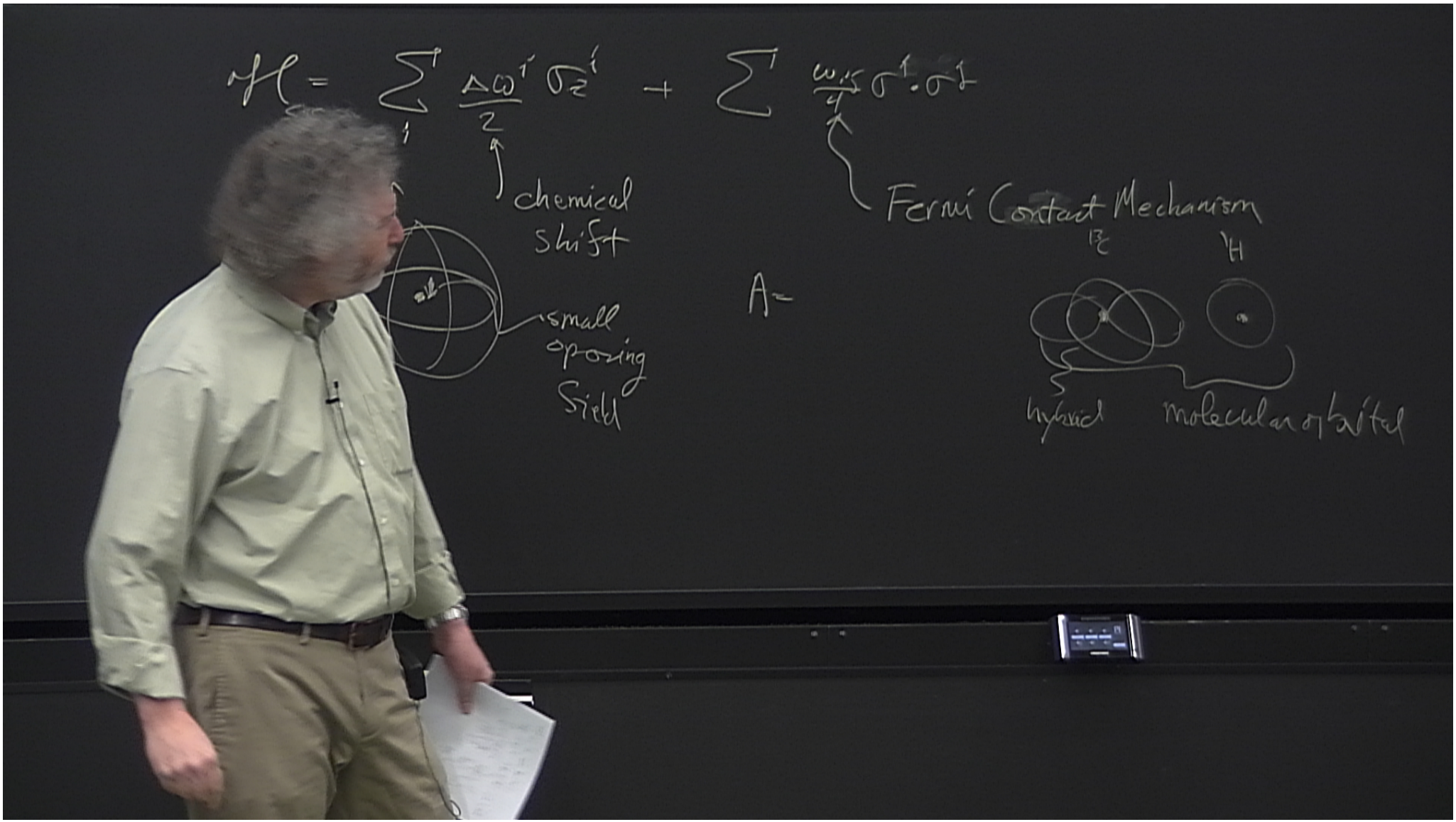
Fermi Contact Mechanism

^{13}C ^{1}H

B_0



small opposing field

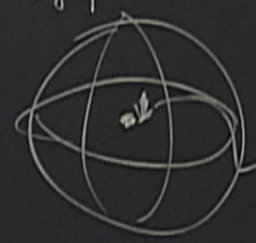

chemical shift
Fermi Contact Mechanism
small opposing field
hybrid
molecular orbital

$$\mathcal{H}_{sys} = \sum_i \frac{\Delta\omega^i}{2}\sigma_z^i + \sum \frac{\omega_{ij}}{4}\sigma^i\cdot\sigma^j$$

chemical shift

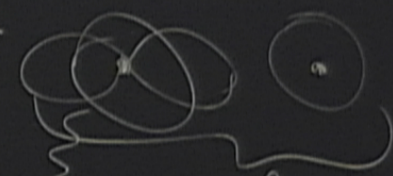
Fermi Contact Mechanism

B_0



small opposing field

$$A = \frac{8}{3}\langle\mu_n\mu_e\rangle|\psi(0)|^2$$



hybrid molecular orbital

$$\mathcal{H}_{sys} = \sum_i \frac{\Delta\omega^i}{2}\sigma_z^i + \sum \frac{\omega_{ij}}{4}\sigma^i\cdot\sigma^j$$

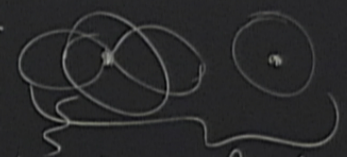
$B_0 \uparrow$

chemical shift

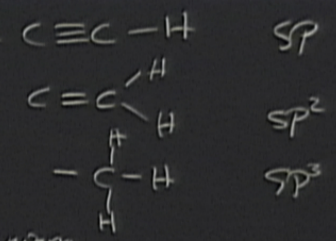
small opposing field

Fermi Contact Mechanism

$$A = \frac{8}{3}\langle\mu_n\mu_e\rangle|\psi(0)|^2$$



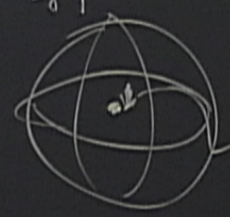
hybrid molecular orbital



$$\mathcal{H}_{sys} = \sum_i \frac{\Delta\omega^i}{2}\sigma_z^i + \sum \frac{\omega_{ij}}{4}\sigma^i\cdot\sigma^j$$

$B_0 \uparrow$

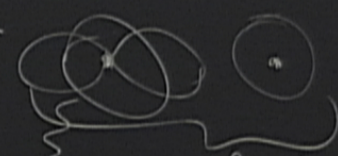
chemical shift



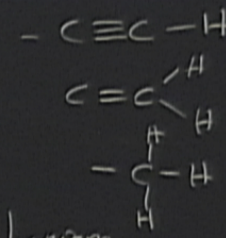
small opposing field

Fermi Contact Mechanism

$$A = \frac{8\pi}{3}\langle\mu_n\mu_e\rangle|\psi(0)|^2$$



hybrid molecular orbital



sp

sp^2

sp^3

$\sigma^1 \cdot \sigma^2$

$-C \equiv C - H$ sp

$C = C$ (H, H) sp^2

$-C$ (H, H) $- H$ sp^3

Fermi Contact Mechanism

^{13}C ^{1}H

$\langle \mu_n \mu_e \rangle |\psi(0)|^2$

hybrid molecular orbital

$$\left[\sigma_z^A + \sigma_z^B , \sigma^A \cdot \sigma^B \right] = 0$$

$$\sigma \cdot \sigma = \sigma_x \sigma_x + \sigma_y \sigma_y + \sigma_z \sigma_z$$

$$\left[\sigma_z^A - \sigma_z^B , \underbrace{\sigma_x^A \sigma_x^B + \sigma_y^A \sigma_y^B}_{\sigma_+^A \sigma_-^B + \sigma_-^A \sigma_+^B} \right] \neq 0$$

AB

E

ω_A

$\sigma^1 \cdot \sigma^2$

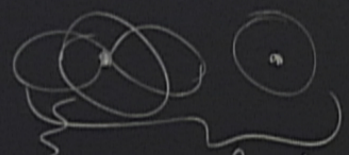
$-C\equiv C-H$ sp

$C=C$ (H, H) sp^2

$-C(H)(H)-H$ sp^3

Fermi Contact Mechanism

$\langle \mu_n \mu_e \rangle |\psi(0)|^2$

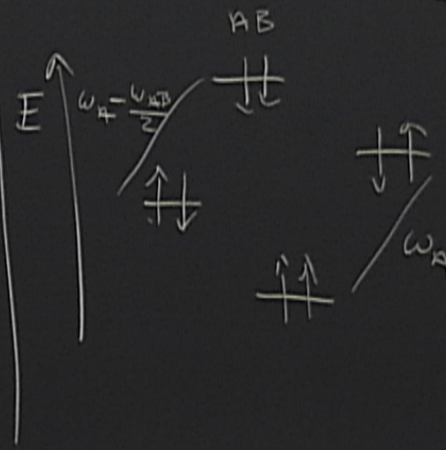


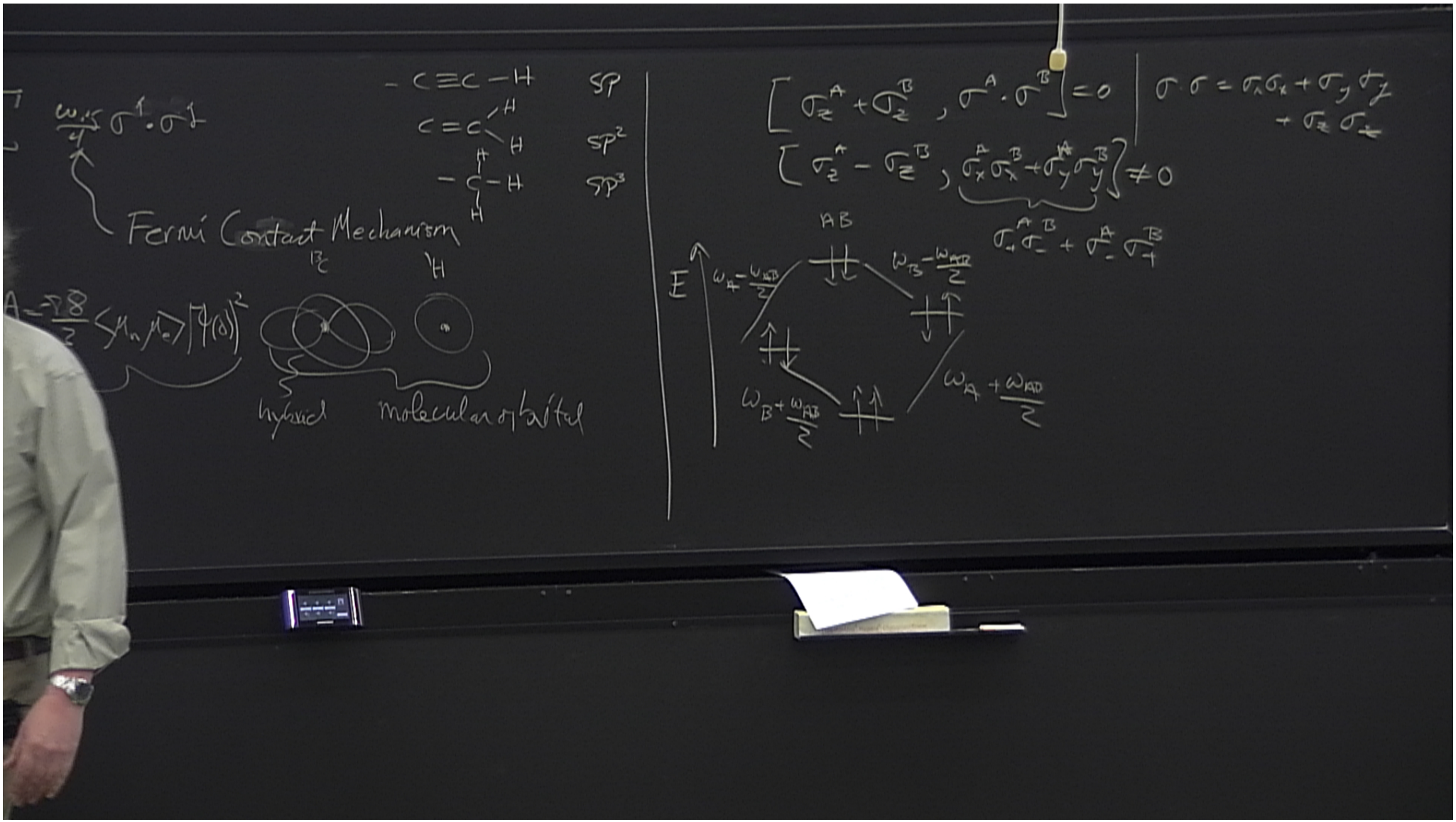
hybrid molecular orbital

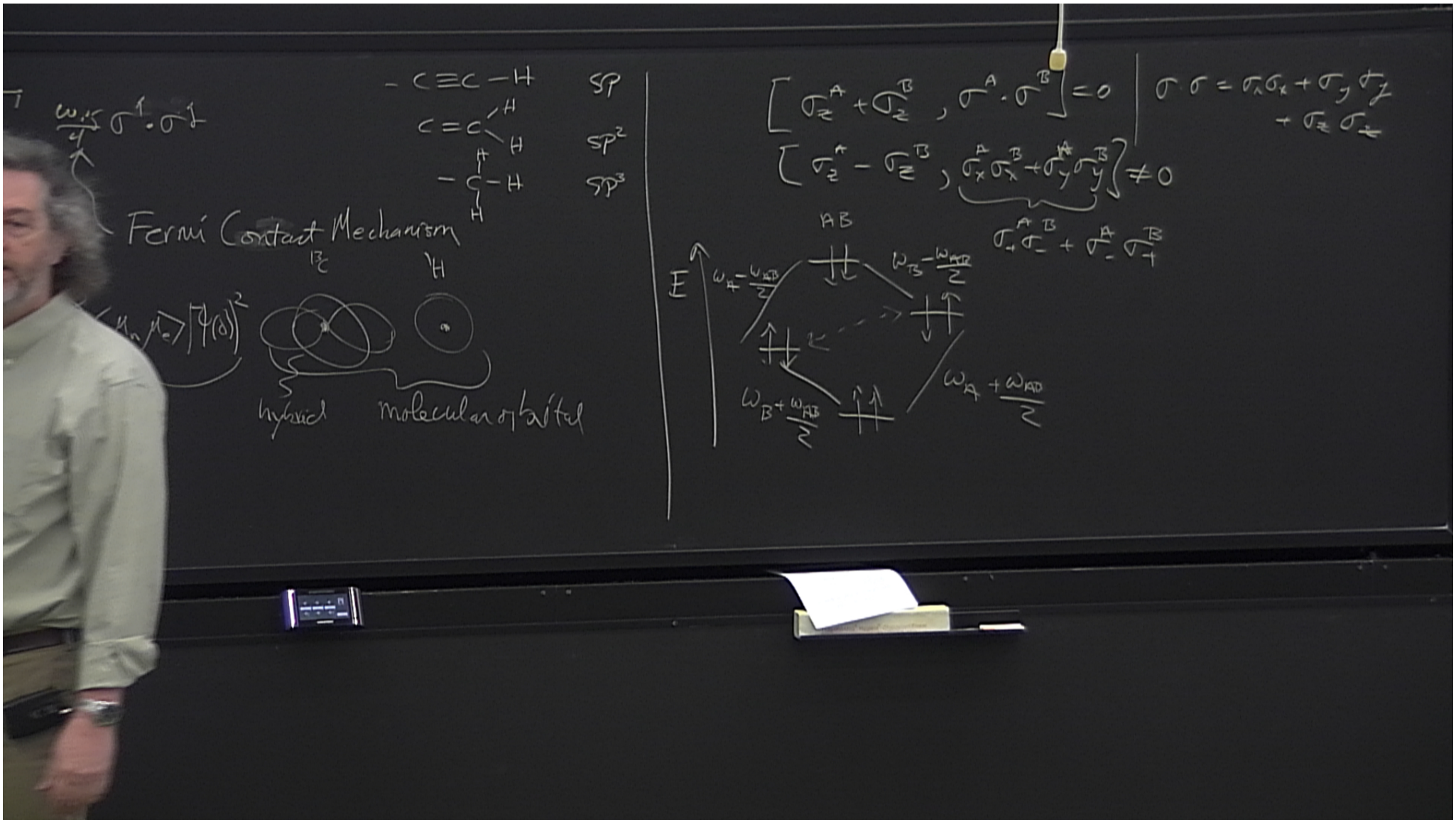
$[\sigma_z^A + \sigma_z^B, \sigma^A \cdot \sigma^B] = 0$

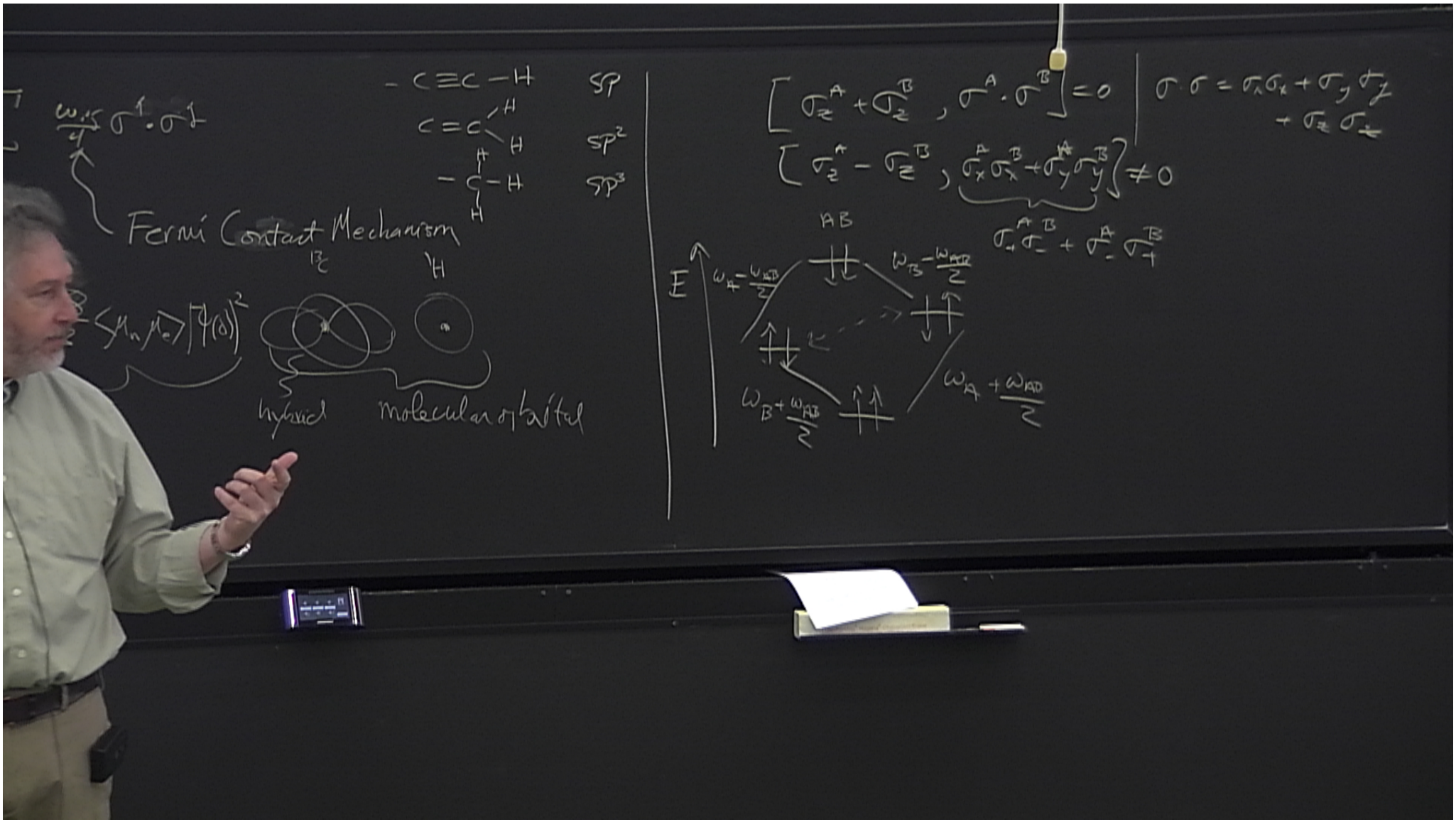
$\sigma \cdot \sigma = \sigma_x \sigma_x + \sigma_y \sigma_y + \sigma_z \sigma_z$

$[\sigma_z^A - \sigma_z^B, \underbrace{\sigma_x^A \sigma_x^B + \sigma_y^A \sigma_y^B}_{\sigma_+^A \sigma_-^B + \sigma_-^A \sigma_+^B}] \neq 0$




Fermi Contact Mechanism
hybrid
molecular orbital
sp
sp2
sp3
AB
E


Fermi Contact Mechanism
hybrid
molecular orbital
sp
sp2
sp3
E


Fermi Contact Mechanism
hybrid
molecular orbital
sp
sp2
sp3
AB
E

$\frac{\omega_{AB}}{4}\,\sigma^1\cdot\sigma^2$

Fermi Contact Mechanism

$-C\equiv C-H$ sp

$C=C$ (H, H) sp^2

$-C$ (H, H) $-H$ sp^3

$A = \frac{8\pi}{3}\langle\mu_n\mu_e\rangle|\psi(0)|^2$

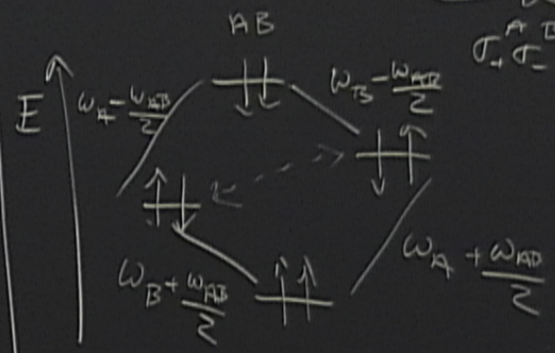
^{13}C ^{1}H

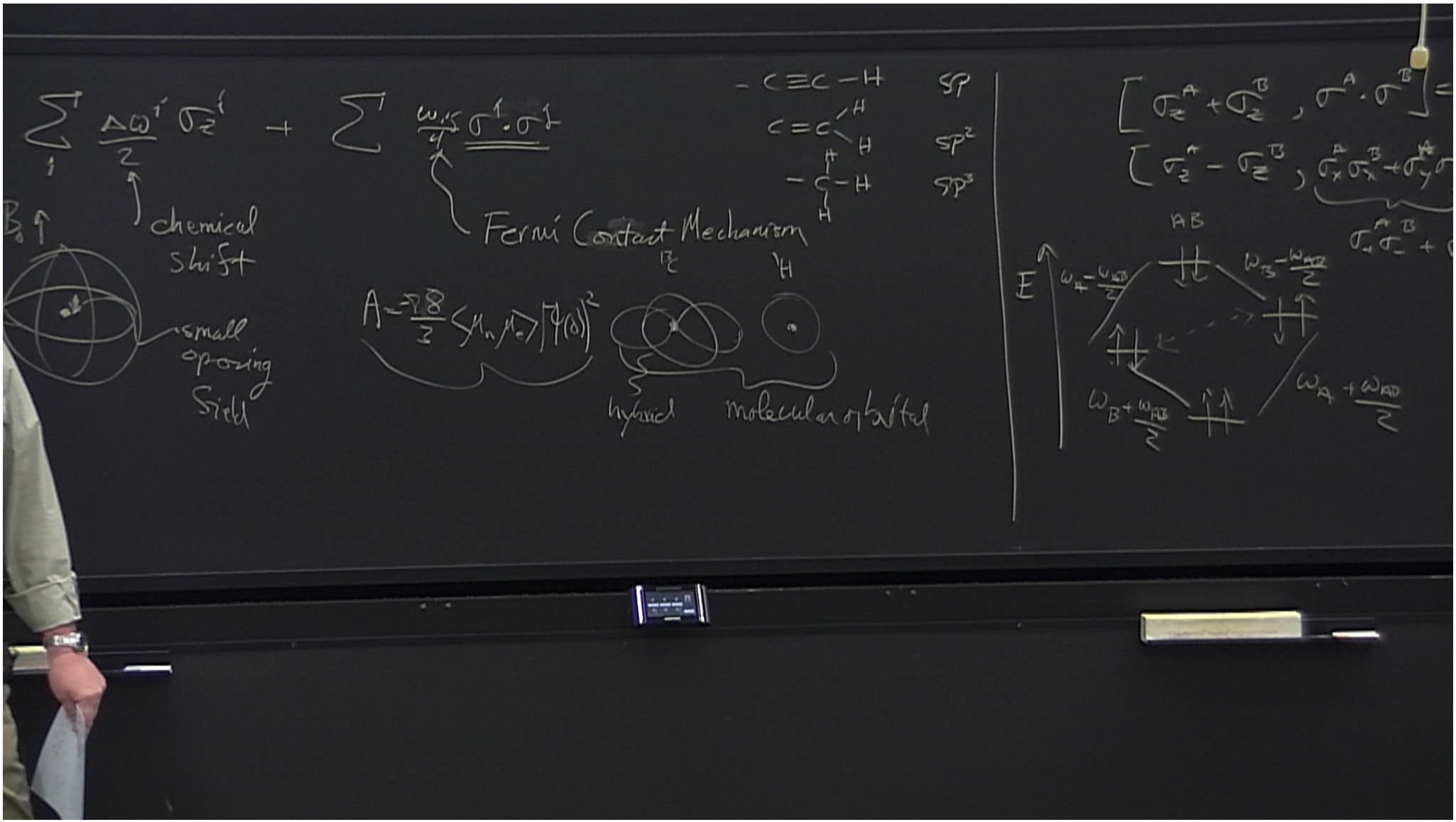
hybrid molecular orbital

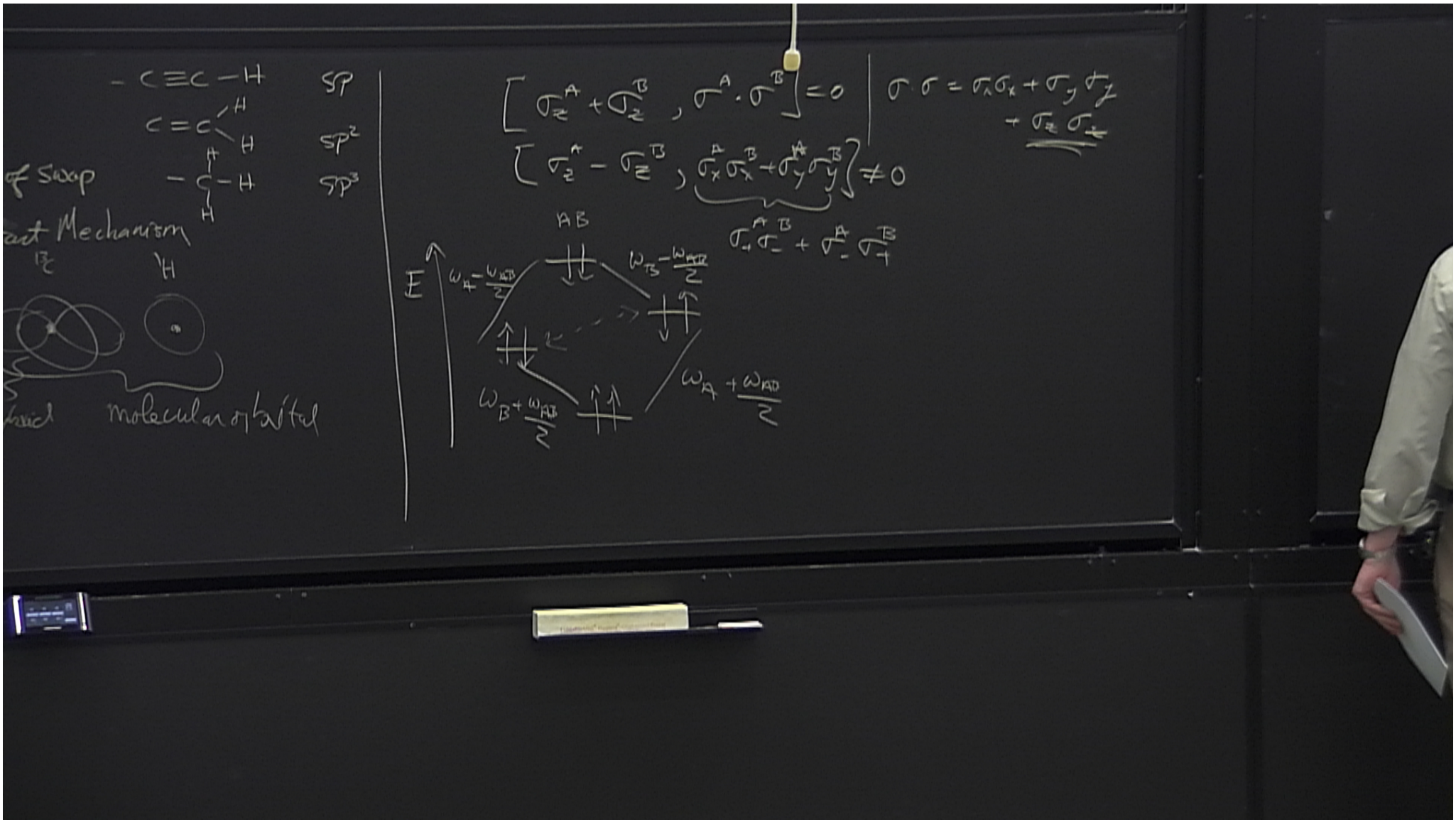
$[\sigma_z^A+\sigma_z^B,\ \sigma^A\cdot\sigma^B]=0$

$\sigma\cdot\sigma=\sigma_x\sigma_x+\sigma_y\sigma_y+\sigma_z\sigma_z$

$[\sigma_z^A-\sigma_z^B,\ \underbrace{\sigma_x^A\sigma_x^B+\sigma_y^A\sigma_y^B}_{\sigma_+^A\sigma_-^B+\sigma_-^A\sigma_+^B}]\neq 0$




chemical shift
small opposing field
Fermi Contact Mechanism
hybrid
molecular orbital
sp
sp2
sp3
E


- C≡C - H sp
C=C sp²
- C - H sp³
of swap
act Mechanism
molecular orbital
$[\sigma_z^A + \sigma_z^B, \sigma^A \cdot \sigma^B] = 0$
$\sigma \cdot \sigma = \sigma_x \sigma_x + \sigma_y \sigma_y + \sigma_z \sigma_z$
$[\sigma_z^A - \sigma_z^B, \sigma_x^A \sigma_x^B + \sigma_y^A \sigma_y^B] \neq 0$
$\sigma_+^A \sigma_-^B + \sigma_-^A \sigma_+^B$
AB
E
$\omega_A - \frac{\omega_{AB}}{2}$
$\omega_B - \frac{\omega_{AB}}{2}$
$\omega_B + \frac{\omega_{AB}}{2}$
$\omega_A + \frac{\omega_{AB}}{2}$

$$\mathcal{H}_{sys} = \sum_i \frac{\Delta\omega^i}{2}\sigma_z^i + \sum \frac{\omega_{ij}}{4}\,\sigma^i\cdot\sigma^j$$

given, fixed in time.

chemical shift

generator of swap

Fermi Contact Mechanism

B_0

small opposing field

$A = \frac{8\pi}{3}\langle\mu_n\mu_e\rangle|\psi(0)|^2$

hybrid

molecular orbital

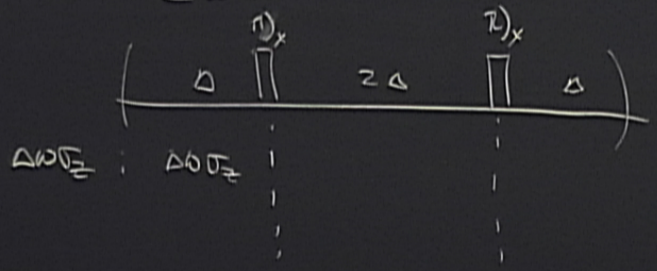
$-C\equiv C-H$ sp

$C=C$ (H, H) sp^2

$-C$ (H, H) $-H$ sp^3

E

Carr Purcell



Carr Purcell

$\pi)_x^{A,B}$ $\pi)_x^{A,B}$

Δ 2Δ Δ

$\Delta\omega\sigma_z$: $\Delta\omega\sigma_z$: $-\Delta\omega\sigma_z$: $\Delta\omega\sigma_z$: $\langle\ \rangle = 0$

$\omega_{AB}\sigma_z^A\sigma_z^B$: $+$: $-$: $+$

$\langle\ \rangle = \omega_{AB}\sigma_z^A\sigma_z^B$

on average over this cycle: the effective off $= 0$

Carr Purcell

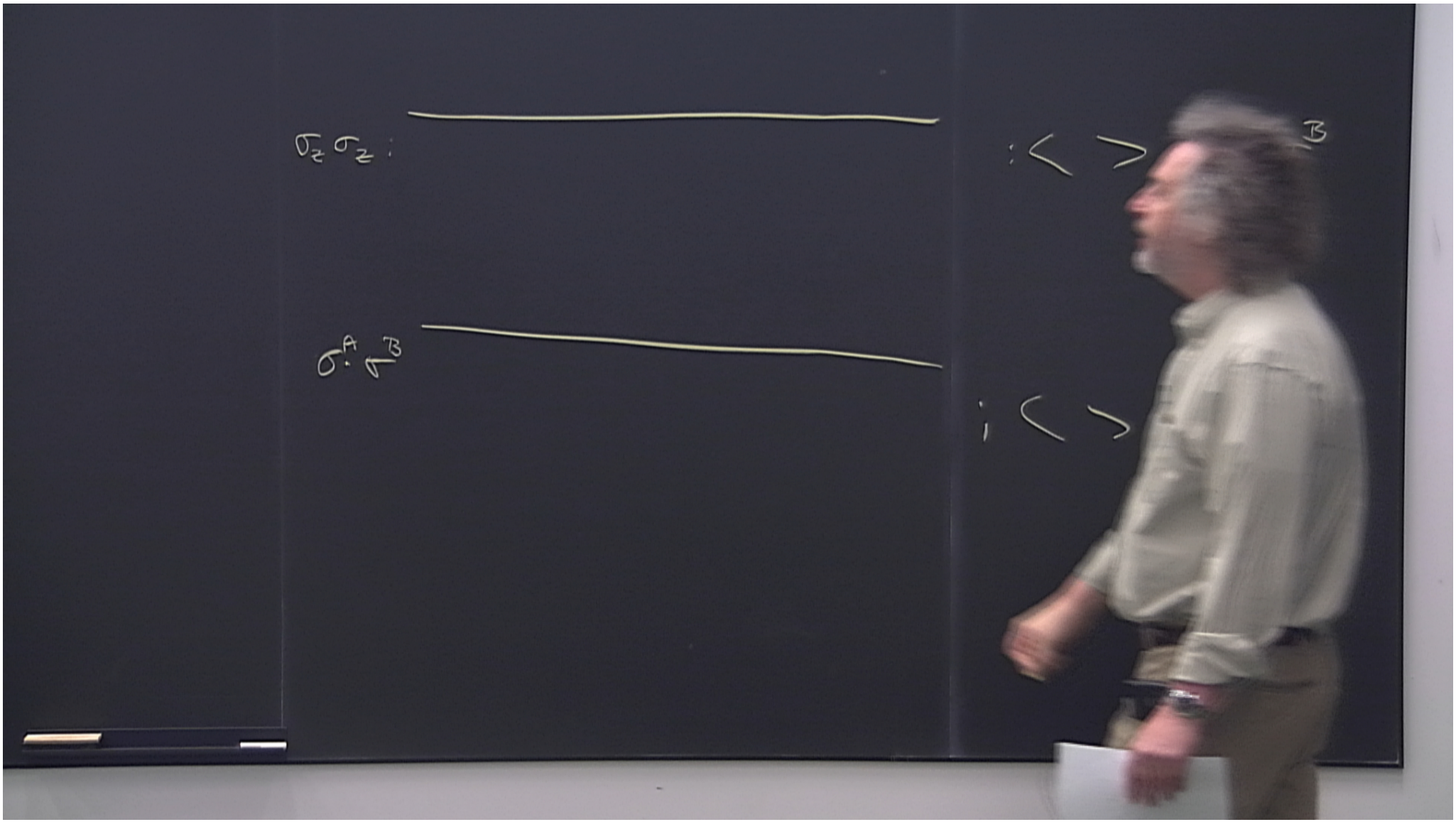
$\pi)_x^{A,B}$ $\pi)_x^{A,B}$

	Δ		2Δ		Δ
$\Delta\omega\sigma_z$	$\Delta\omega\sigma_z$		$-\Delta\omega\sigma_z$		$\Delta\omega\sigma_z$
$\omega_{AB}\sigma_z^A\sigma_z^B$	$+$		$-$		$+$

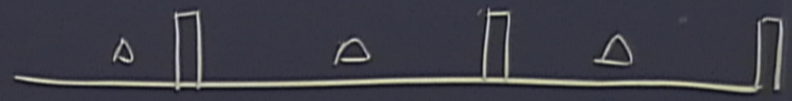
$\langle\ \rangle = 0$

on average over this cycle: the effective $\mathcal{H} = 0$

$\langle\ \rangle = \omega_{AB}\sigma_z^A\sigma_z^B$

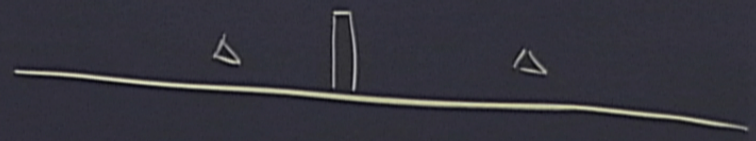

$\sigma_z \sigma_z$:
: < >
B
$\sigma^A \cdot \sigma^B$
; < >

$\sigma_z \sigma_z$:

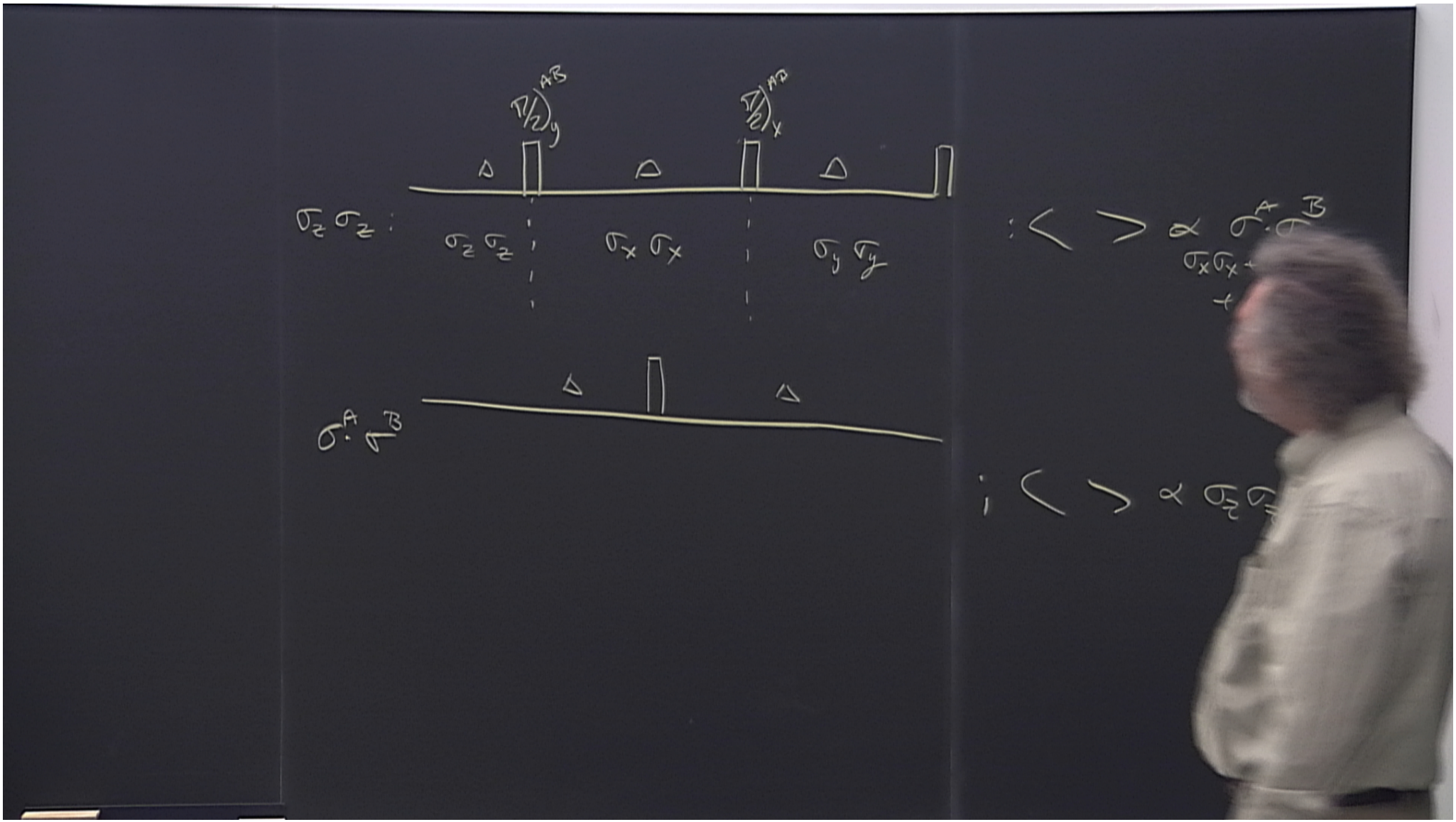


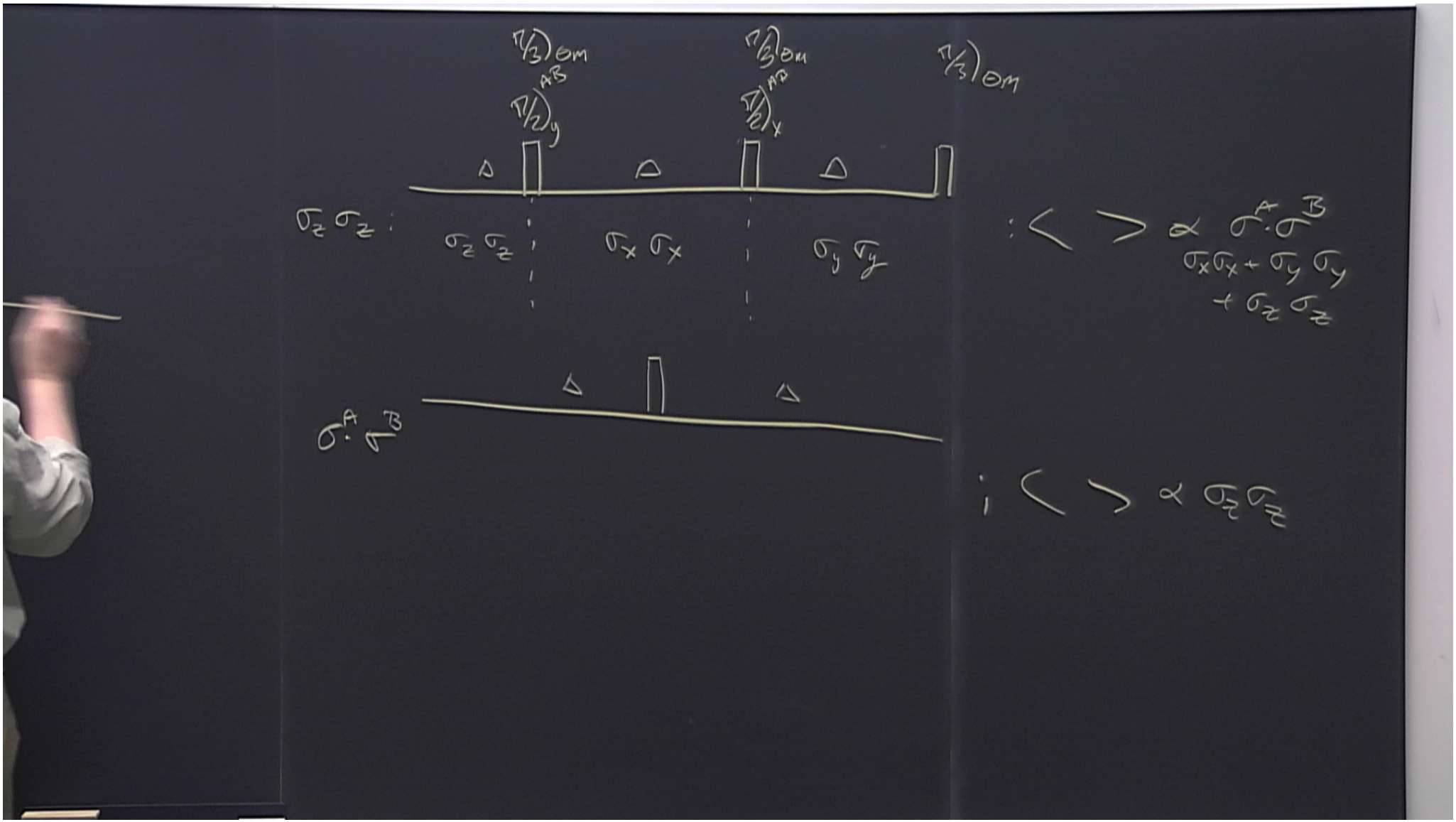
$: \langle \; \rangle \propto \sigma^A \cdot \sigma^B$

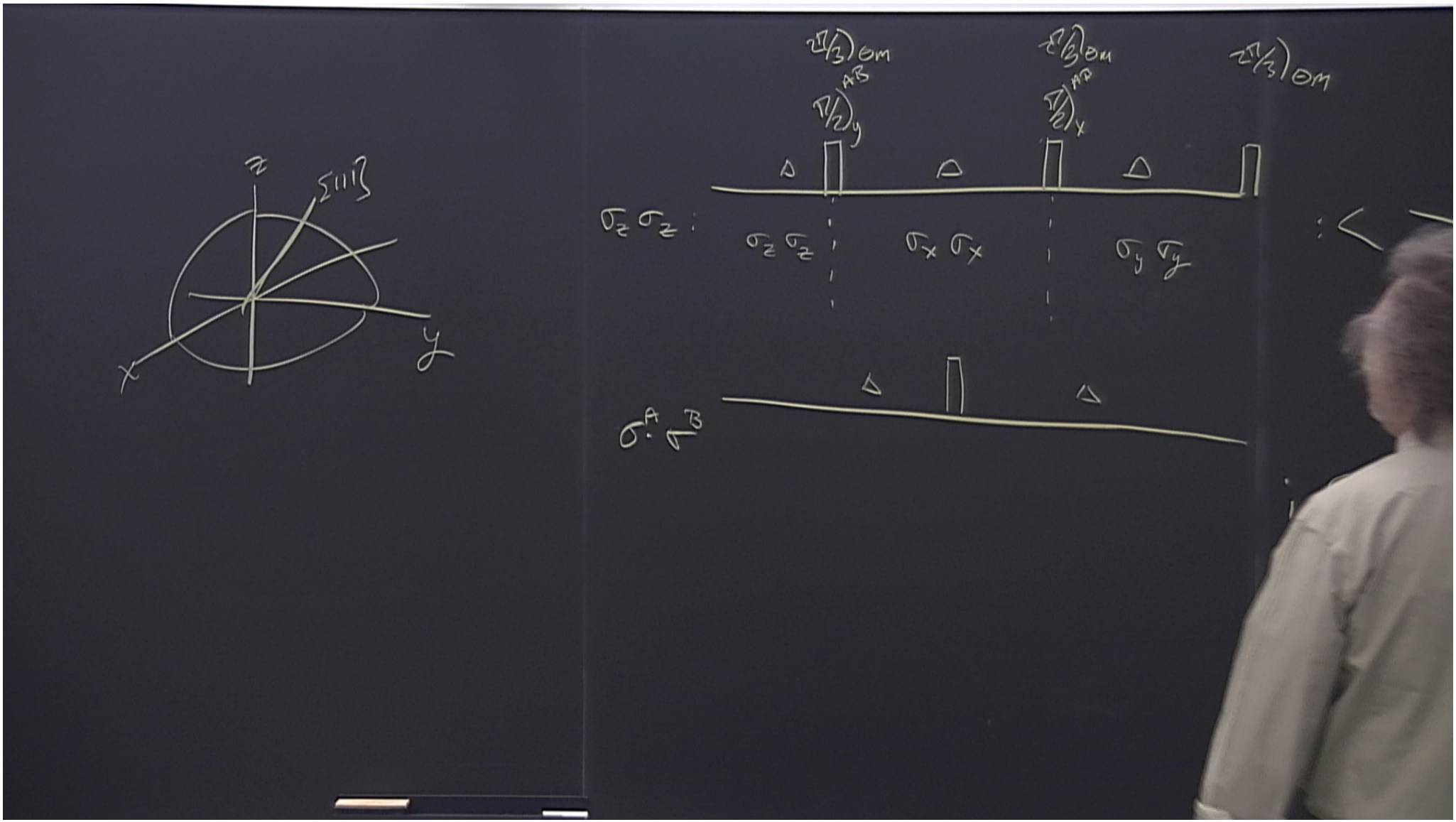
$\sigma^A \cdot \sigma^B$

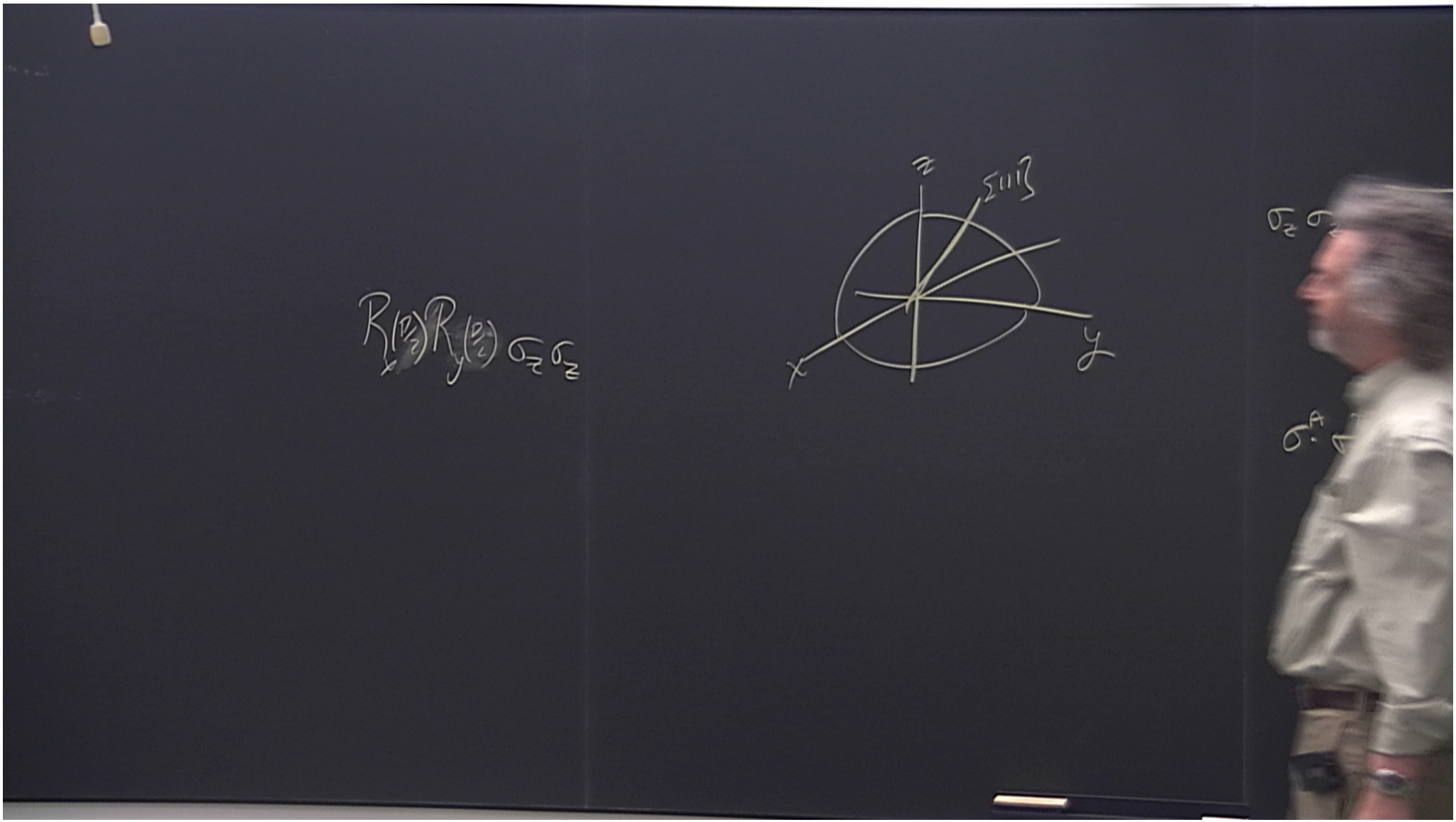


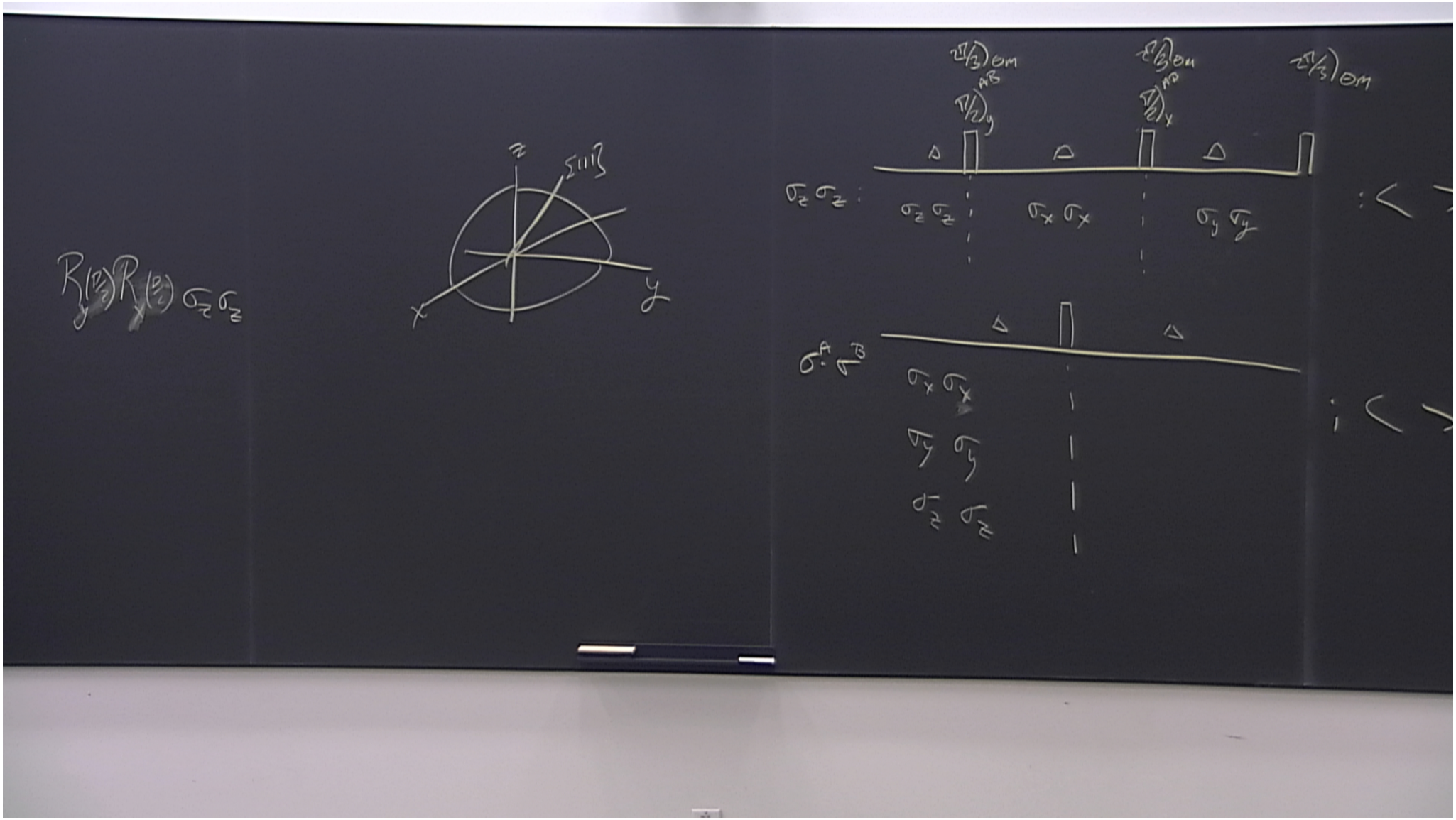
$; \langle \; \rangle \propto \sigma_z \sigma_z$


$\pi/2)_y^{AB}$
$\pi/2)_x^{AB}$
$\sigma_z\sigma_z$:
$\sigma_z\sigma_z$
$\sigma_x\sigma_x$
$\sigma_y\sigma_y$
: $\langle\ \rangle \propto \sigma^A\cdot\sigma^B$
$\sigma_x\sigma_x +$
$+$
$\sigma^A\cdot\sigma^B$
; $\langle\ \rangle \propto \sigma_z\sigma_z$

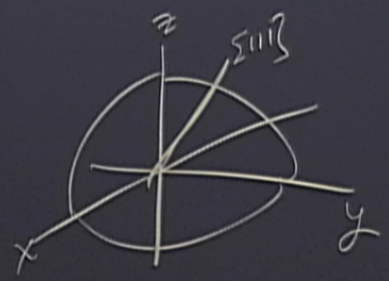

π/3 om
π/3 om
π/3 om
π/2 y AB
π/2 x AB
Δ
Δ
Δ
σz σz :
σz σz
σx σx
σy σy
: < > ∝ σA · σB
σx σx + σy σy
+ σz σz
Δ
Δ
σA · σB
; < > ∝ σz σz

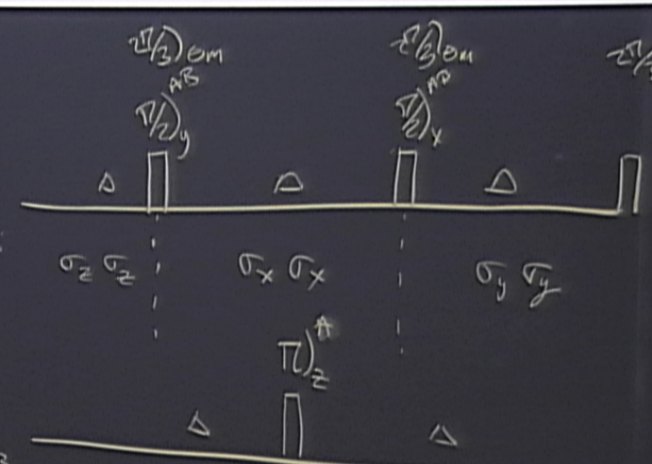

z
{111}
x
y
π/3 om
π/2 y
AB
π/3 om
π/2 x
AB
π/3 om
σz σz :
σz σz
σx σx
σy σy
σA σB

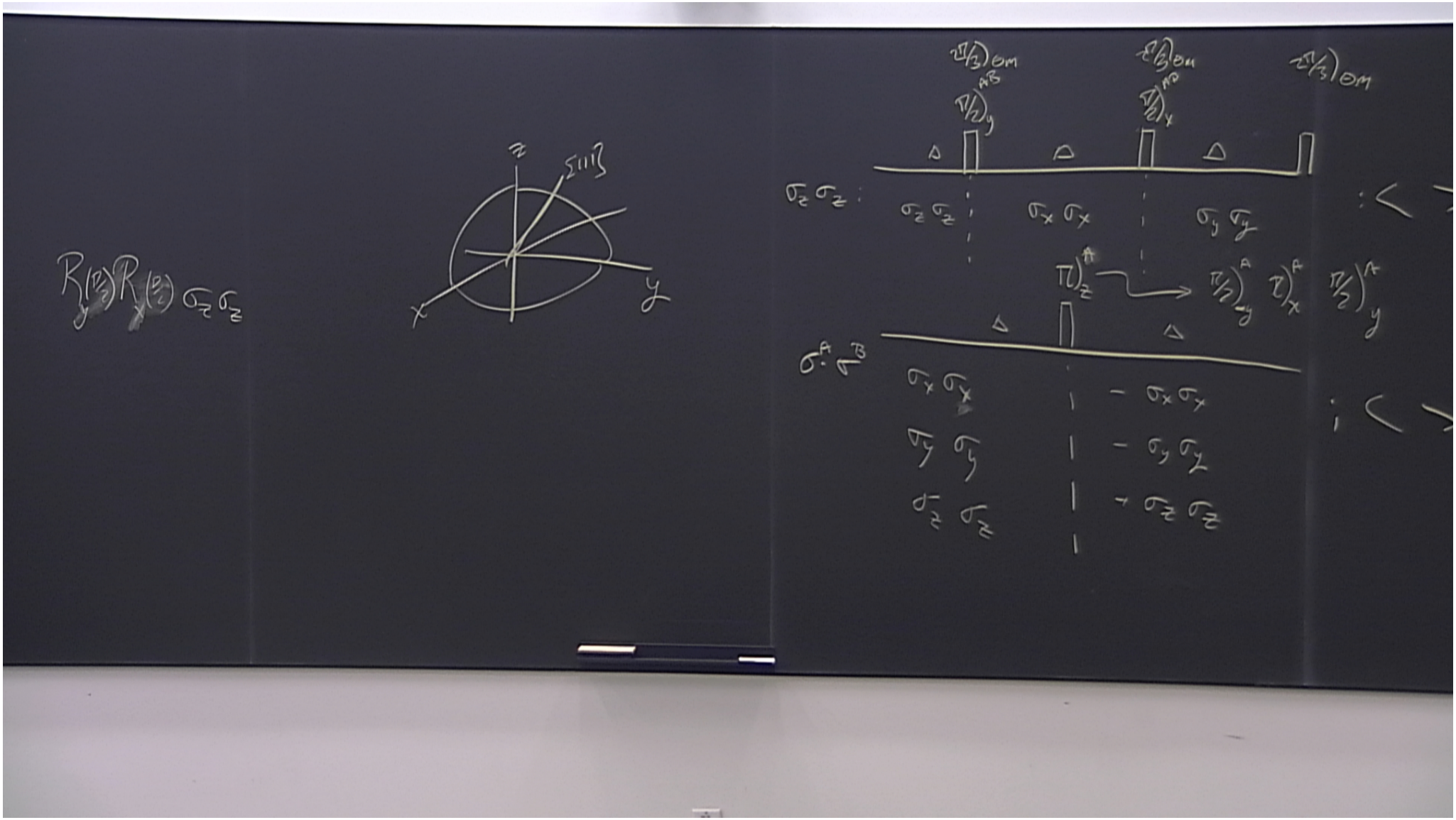

$R_x(\frac{\pi}{2}) R_y(\frac{\pi}{2}) \sigma_z \sigma_z$
z
[111]
x
y
$\sigma_z \sigma_z$
σ^A

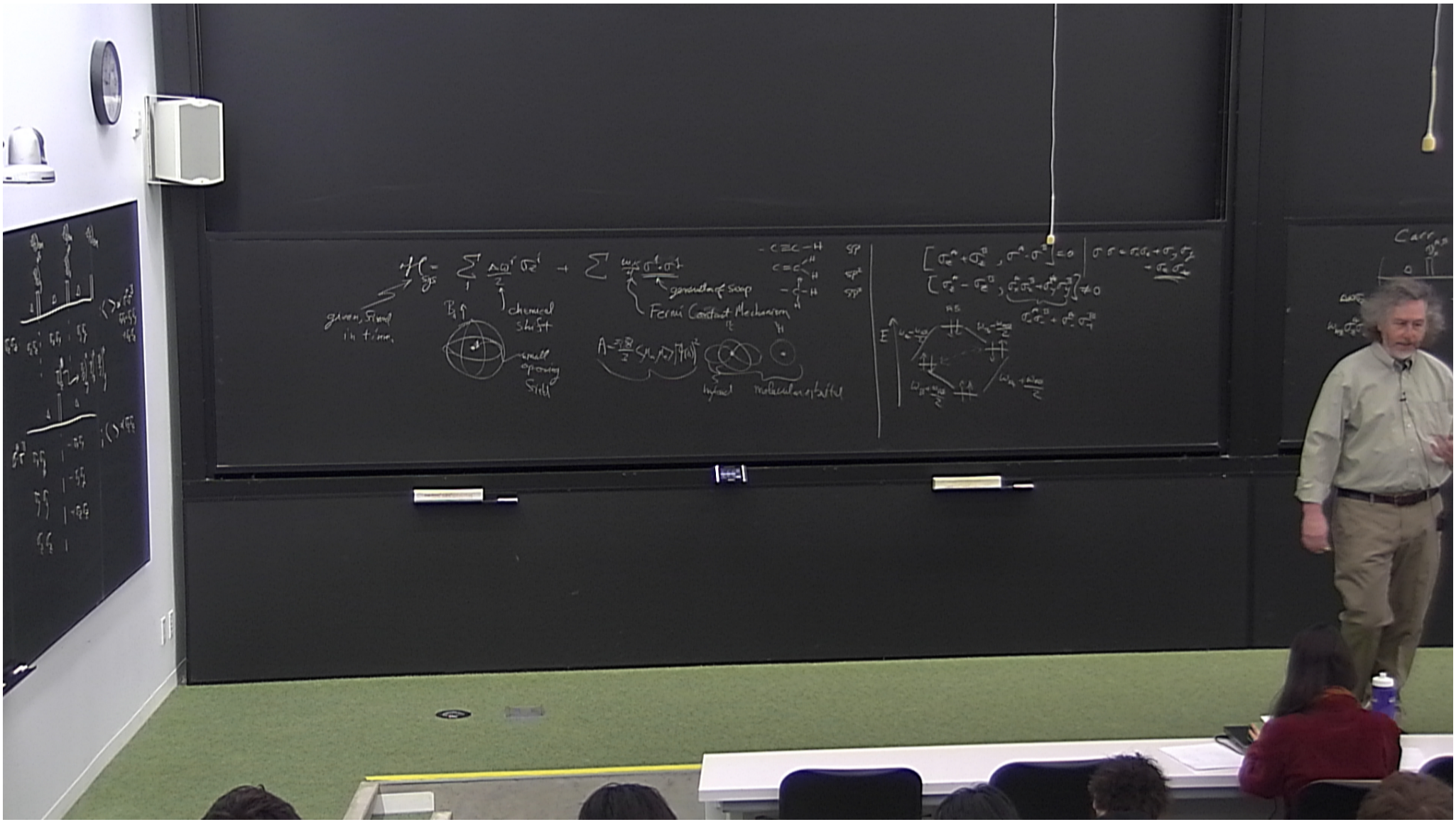

$R_y(\frac{\pi}{2}) R_x(\frac{\pi}{2})\, \sigma_z \sigma_z$
z
{111}
x
y
$\sigma_z \sigma_z$:
$\sigma_z \sigma_z$
$\sigma_x \sigma_x$
$\sigma_y \sigma_y$
$\sigma^A \cdot \sigma^B$
$\sigma_x \sigma_x$
$\sigma_y \sigma_y$
$\sigma_z \sigma_z$

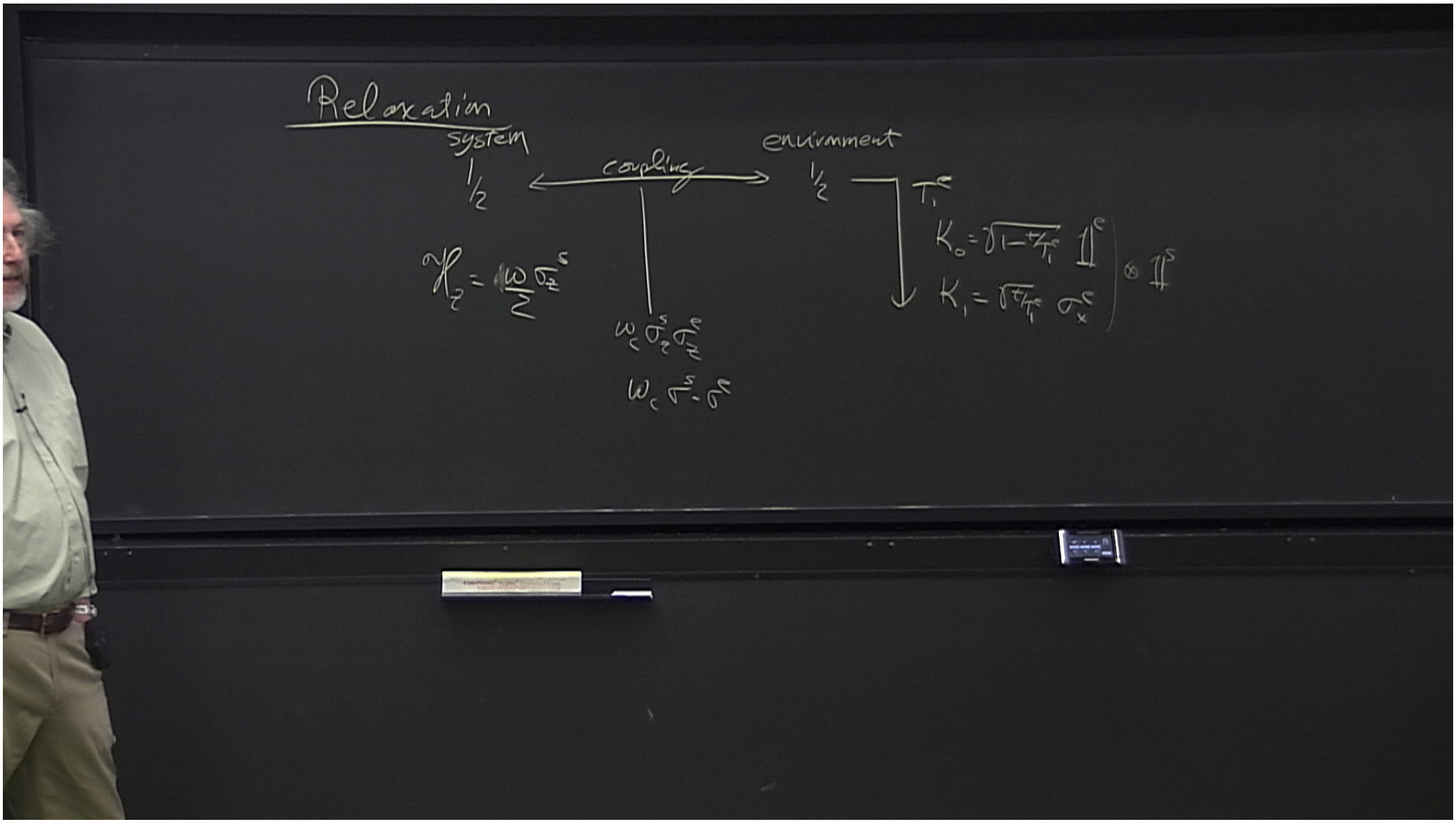
$R_y(\pi/3) R_x(\pi/2)\, \sigma_z \sigma_z$

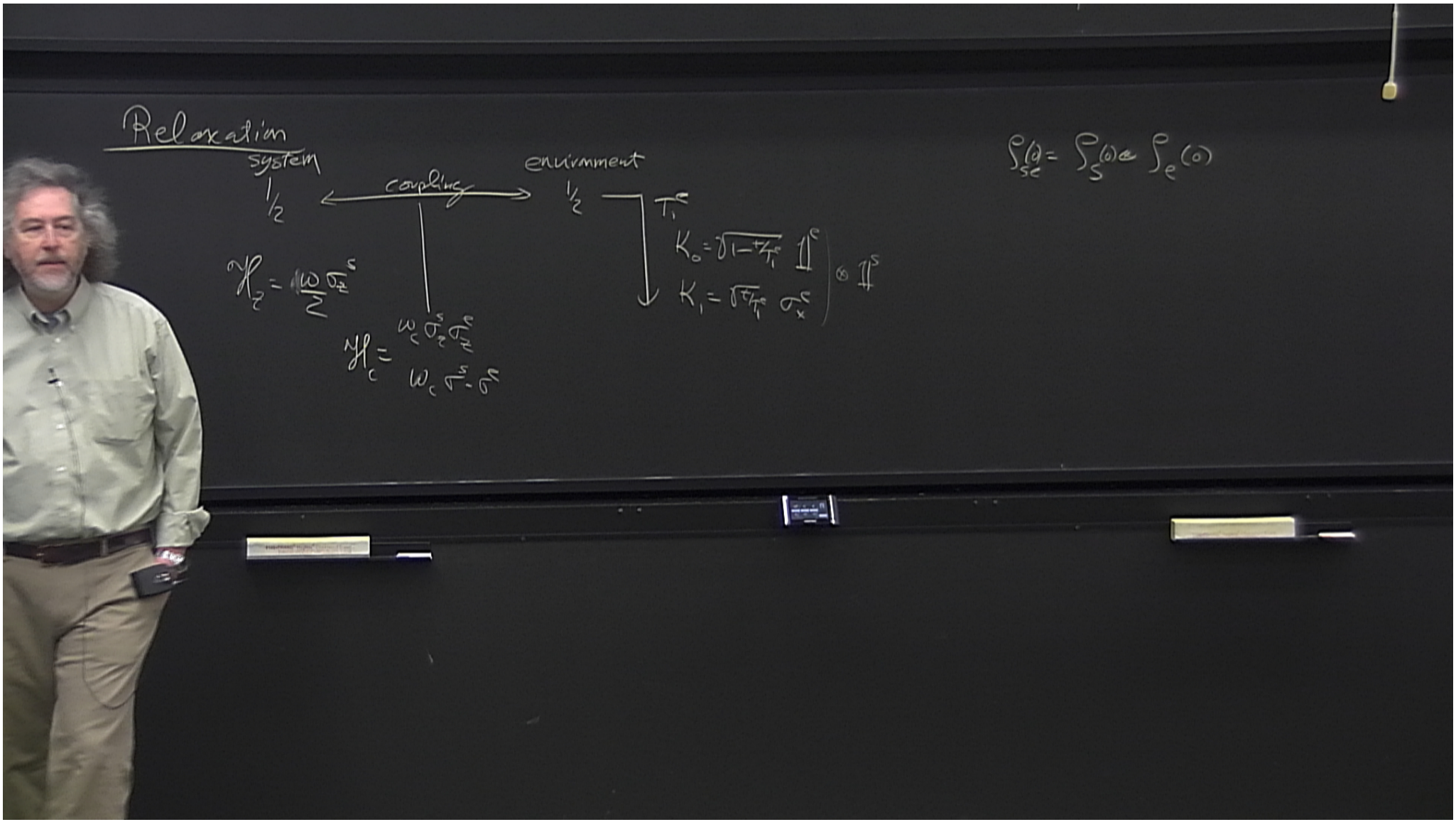





$R_y(\frac{\pi}{2}) R_x(\frac{\pi}{2})\, \sigma_z \sigma_z$
z
{111}
x
y
$\sigma_z \sigma_z$:
$\sigma_z \sigma_z$
$\sigma_x \sigma_x$
$\sigma_y \sigma_y$
$\sigma^A \cdot \sigma^B$
$\sigma_x \sigma_x$
$\sigma_y \sigma_y$
$\sigma_z \sigma_z$
$-\sigma_x \sigma_x$
$-\sigma_y \sigma_y$
$+\sigma_z \sigma_z$


given, Stimulus in time.
chemical shift
small opening Still
generation of scalp
Fermi Contact Mechanism
Hybrid
Molecular orbitals


Relaxation
system
1/2
coupling
environment
1/2
T_1^e
$\mathcal{H}_z = \frac{\omega}{2}\sigma_z^s$
$K_0 = \sqrt{1-t/T_1^e}\,\mathbb{1}^e$
$K_1 = \sqrt{t/T_1^e}\,\sigma_x^e$
$\otimes\,\mathbb{1}^s$
$\omega_c\,\sigma_z^s\sigma_z^e$
$\omega_c\,\sigma^s\cdot\sigma^e$


Relaxation
system
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1/2
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$\mathbb{1}^s$
$\rho_{se}(0) = \rho_s(0) \otimes \rho_e(0)$

electron induced relaxation.cdf

0.5.1 decoherence, zz coupling

Superoperator with coherent precession and decoherenc. Here we look at the effective map in just the system space.

```
In[•]:= Sz[w_, wc_, t_, T1_] :=
  Table[Tr[KroneckerProduct[PauliMatrix[i], PauliMatrix[0]] . U[w, wc, t] .
      Sum[Kx[k, t, T1] . KroneckerProduct[PauliMatrix[j], PauliMatrix[0]] .
        ConjugateTranspose[Kx[k, t, T1]], {k, 1, 2}] .
      Uinv[w, wc, t]] / 4, {i, 0, 3}, {j, 0, 3}];
```

Of course for t=0 the map is the identity.

```
In[•]:= Chop[Sz[0, 0, 0, 0.2]] // MatrixForm
```

Out[•]=
$$\begin{pmatrix} 1. & 0 & 0 & 0 \\ 0 & 1. & 0 & 0 \\ 0 & 0 & 1. & 0 \\ 0 & 0 & 0 & 1. \end{pmatrix}$$

We add the Zeeman interaction and coupling to the environment we see the normal combination of precession and dephasing.

```
In[•]:= Chop[Sz[(2 π) 20, (2 π) 100 , .001, 0.1]] // MatrixForm
```

Out[•]=
$$\begin{pmatrix} 1. & 0 & 0 & 0 \\ 0 & 0.943557 & 0.119199 & 0 \\ 0 & -0.119199 & 0.943557 & 0 \\ 0 & 0 & 0 & 1. \end{pmatrix}$$

Notice that the action of a T1 on the environment combined with a zz coupling leads to T2 relaxation of the system. However there is no T1 processes on the system.

```
In[•]:= Chop[Sz[0, (2 π) 200 , .0001, 1000]] // MatrixForm
```

Out[•]=
$$\begin{pmatrix} 1. & 0 & 0 & 0 \\ 0 & 0.998027 & 0 & 0 \\ 0 & 0 & 0.998027 & 0 \\ 0 & 0 & 0 & 1. \end{pmatrix}$$

Superoperator in full space

It is instructive to look at the full system/environment map. In this way we can see the effects of memory left in the environment.

200%

electron induced relaxation.cdf

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Superoperator in full space

It is instructive to look at the full system/environment map. In this way we can see the effects of memory left in the environment.

```
Szfull[w_, wc_, t_, T1_] := Table[
    Tr[PauliSU4[i] . U[w, wc, t] . Sum[Kx[k, t, T1] . PauliSU4[j] . ConjugateTranspose[
          Kx[k, t, T1]], {k, 1, 2}] . Uinv[w, wc, t]] / 4, {i, 0, 15}, {j, 0, 15}];
```

When the coupling of the system/environment is set to zero then we recover simple precession.

```
Chop[Szfull[2 π 20, 0 , .001, 1000]] // MatrixForm
```

$$\begin{pmatrix} 1. & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1. & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.999999 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.999999 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.992115 & 0 & 0 & 0 & 0.125333 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.992115 & 0 & 0 & 0 & 0.125333 \\ 0 & 0 & 0 & 0 & & & & & & \end{pmatrix}$$

200%

Relaxation

system $\frac{1}{2}$ $\xleftrightarrow{\text{coupling}}$ environment $\frac{1}{2}$

$$\mathcal{H}_z = \frac{\omega}{2}\sigma_z^s$$

$$\mathcal{H}_c = \omega_c \sigma_z^s \sigma_z^e$$

$$\mathcal{H}_c = \omega_c \sigma^s \cdot \sigma^e$$

T_1^e

$$\left.\begin{aligned} K_0 &= \sqrt{1-t/T_1^e}\,\mathbb{1}^e \\ K_1 &= \sqrt{t/T_1^e}\,\sigma_x^e \end{aligned}\right) \otimes \mathbb{1}^s$$

$$\rho_{se}(0) = \rho_s(0) \otimes \underbrace{\rho_e(0)}_{\mathbb{1}}$$

Relaxation

system $\frac{1}{2}$ $\xleftrightarrow{\text{coupling}}$ environment $\frac{1}{2}$

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$$\mathcal{H}_c = \omega_c \vec{\sigma}^s \cdot \vec{\sigma}^e$$

T_2^s

$T_1^s = \infty$

T_1^e

$$\left.\begin{array}{l} K_0 = \sqrt{1 - t/T_1^e}\ \mathbb{1}^e \\ K_1 = \sqrt{t/T_1^e}\ \sigma_x^e \end{array}\right) \otimes \mathbb{1}^s$$

$$\rho_{se}(0) = \rho_s(0) \otimes \underbrace{\rho_e(0)}_{\mathbb{1}}$$

electron induced relaxation.cdf

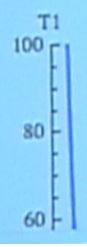
When we add the environment coupling then the dynamics become more complex
The precession case is x -> y
The environment introduces x -> yz
So all together the system operator x -> {y, yz, xz}

```
Chop[Szfull[(2 π) 20, (2 π) 40 , 0.001, .001]] // MatrixForm
```

1.	0	0	0	0	0	0	0	0
0	0.992115	0	0	0	0	0	0	0
0	0	0.364979	0	0	0	0	0	0
0	0	0	0.367879	0	0	0	0	0
0	0	0	0	0.984292	0	0	-0.0057788	0.124
0	0	0	0	0	0.992115	0	0	0
0	0	0	0	0	0	0.364979	0	0
0	0	0	0	-0.0157084	0	0	0.362101	0.124
0	0	0	0	-0.124345	0	0	-0.0457439	0.984
0	0	0	0	0	-0.125333	0	0	0
0	0	0	0	0	0	-0.0461075	0	0
0	0	0	0	-0.124345	0	0	-0.0457439	-0.015
0	0	0	0	0	0	0	0	0
0	0	0.0461075	0	0	0	0	0	0
0	-0.125333	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0

The amplitude of the coherence decays as Exp[-t/T2] so the effective T2 is -t/Log[amplitude]

```
Plot[- 0.0001 / Log[Sz[0, (2 π) f , .0001, 0.1][[2, 2]]],
 {f, 0, 200}, {PlotRange → {0, 100},
  PlotStyle → {Thickness[0.005], RGBColor[0, 0, 2]}, AxesLabel → {coupling, T1}}]
```



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sys T_2

$\sigma_x^s \mathbb{1} \longrightarrow \sigma_x^s \mathbb{1}$

Zeeman $\sigma_x^s \mathbb{1} \rightarrow \sigma_y^s \mathbb{1}, \sigma_x^s \mathbb{1}$

sys T_2

$\sigma_x^s \mathbb{1} \longrightarrow \sigma_x^s \mathbb{1}$

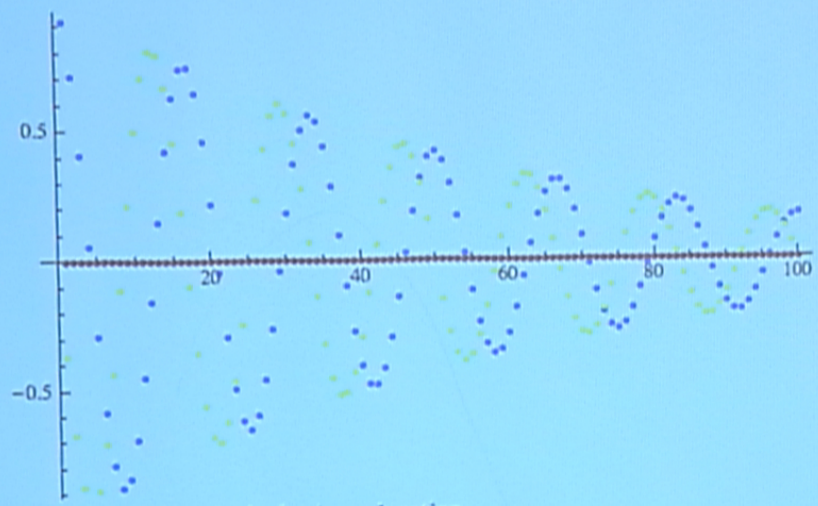
Zeeman $\sigma_x^s \mathbb{1} \rightarrow \sigma_y^s \mathbb{1}, \sigma_x^s \mathbb{1}$

sys/env $\sigma_x^s \mathbb{1} \rightarrow \sigma_y^s \sigma_z^e, \sigma_x^s \sigma_z^e$

$\sigma_x^s \mathbb{1}^e, \sigma_y^s \mathbb{1}^e$

electron induced relaxation.cdf

```
        DisplayFunction → Identity}],
    ListPlot[Table[pm2[n][[9]], {n, 1, 100, 1}],
        {PlotStyle → {RGBColor[0, 1, 0], Thickness[0.003]},
         DisplayFunction → Identity}],
    ListPlot[Table[pm2[n][[13]], {n, 1, 100, 1}],
        {PlotStyle → {RGBColor[1, 0, 0], Thickness[0.003]},
         DisplayFunction → Identity}]}, DisplayFunction → $DisplayFunction]
```



As we expect there is dephasing relaxation

Now the coupling to the environment can introduce a correlation to the environment. In this case that correlation would show up in the yz operator (#12)

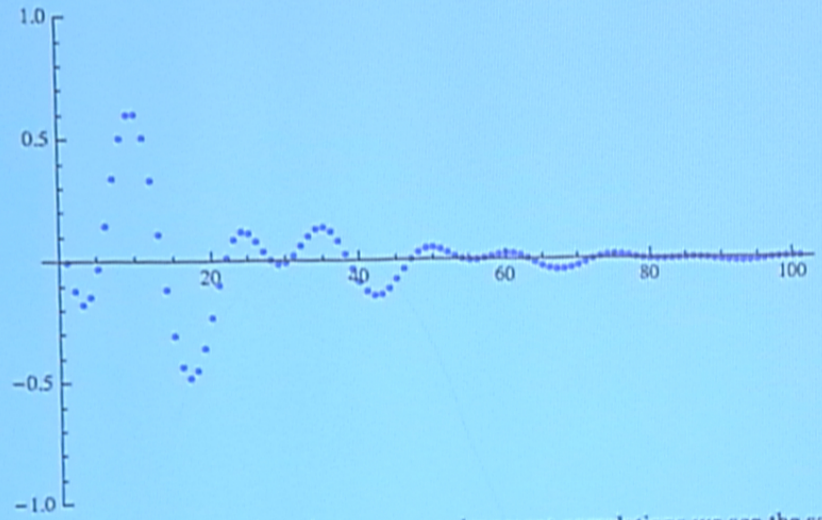
```
ListPlot[Table[pm2[n][[12]], {n, 0, 100, 1}],
    {PlotRange → {-1, 1}, PlotStyle -> {RGBColor[0, 0, 1], Thickness[0.003]}}]
```

200%

electron induced relaxation.cdf

Now we see that the system is strongly effected by the memory of the environment.
Now the coupling to the environment can introduce a correlation to the environment. In this case that correlation would show up in the yz operator (#12)

```
ListPlot[Table[pm3[n][[12]], {n, 0, 100, 1}],
    {PlotRange → {-1, 1}, PlotStyle -> {RGBColor[0, 0, 1], Thickness[0.003]}}]
```



Of course when we look at the system environment correlations we see the same thing.

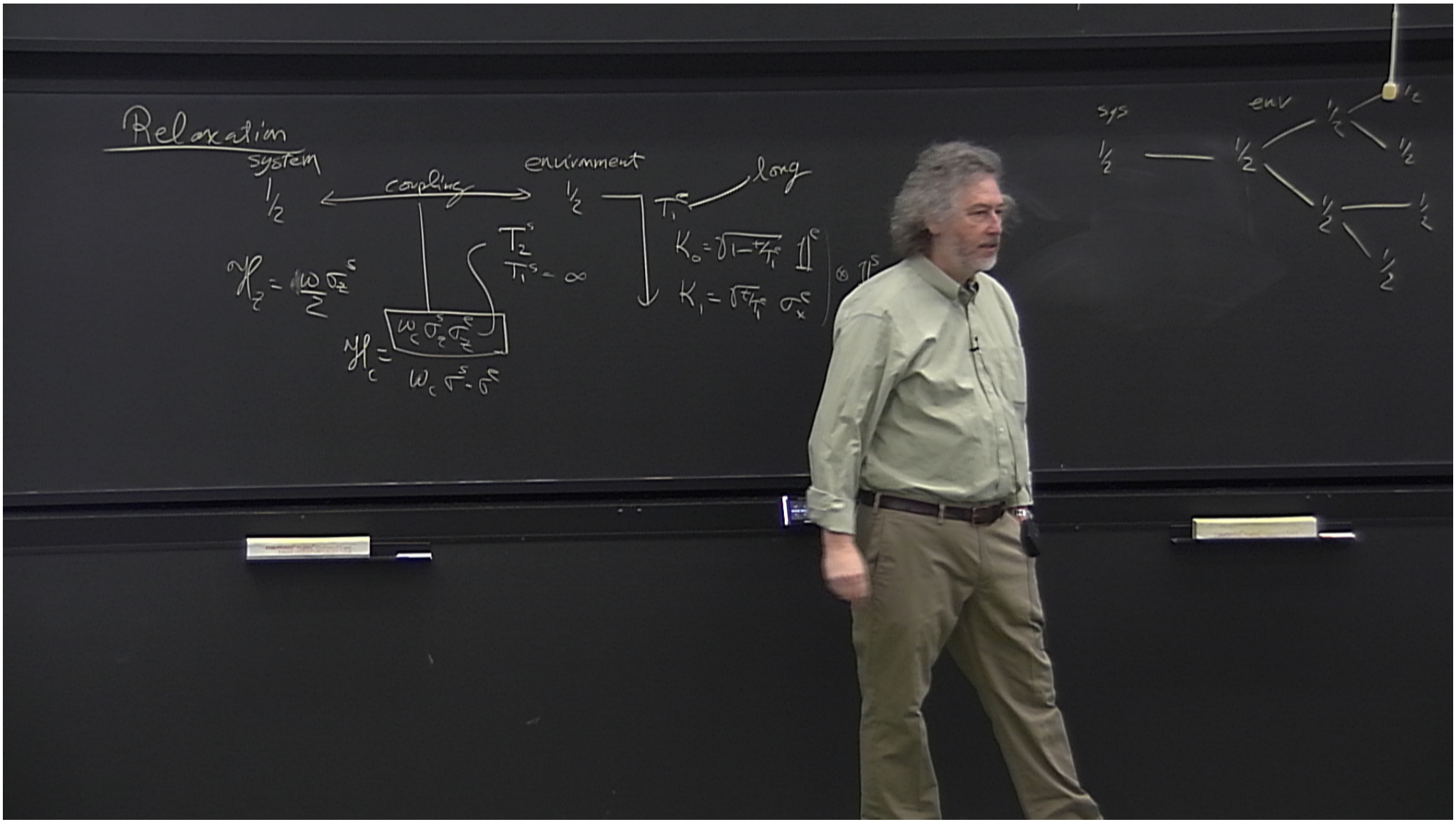
0.5.3 decoherence, xx + yy + zz coupling

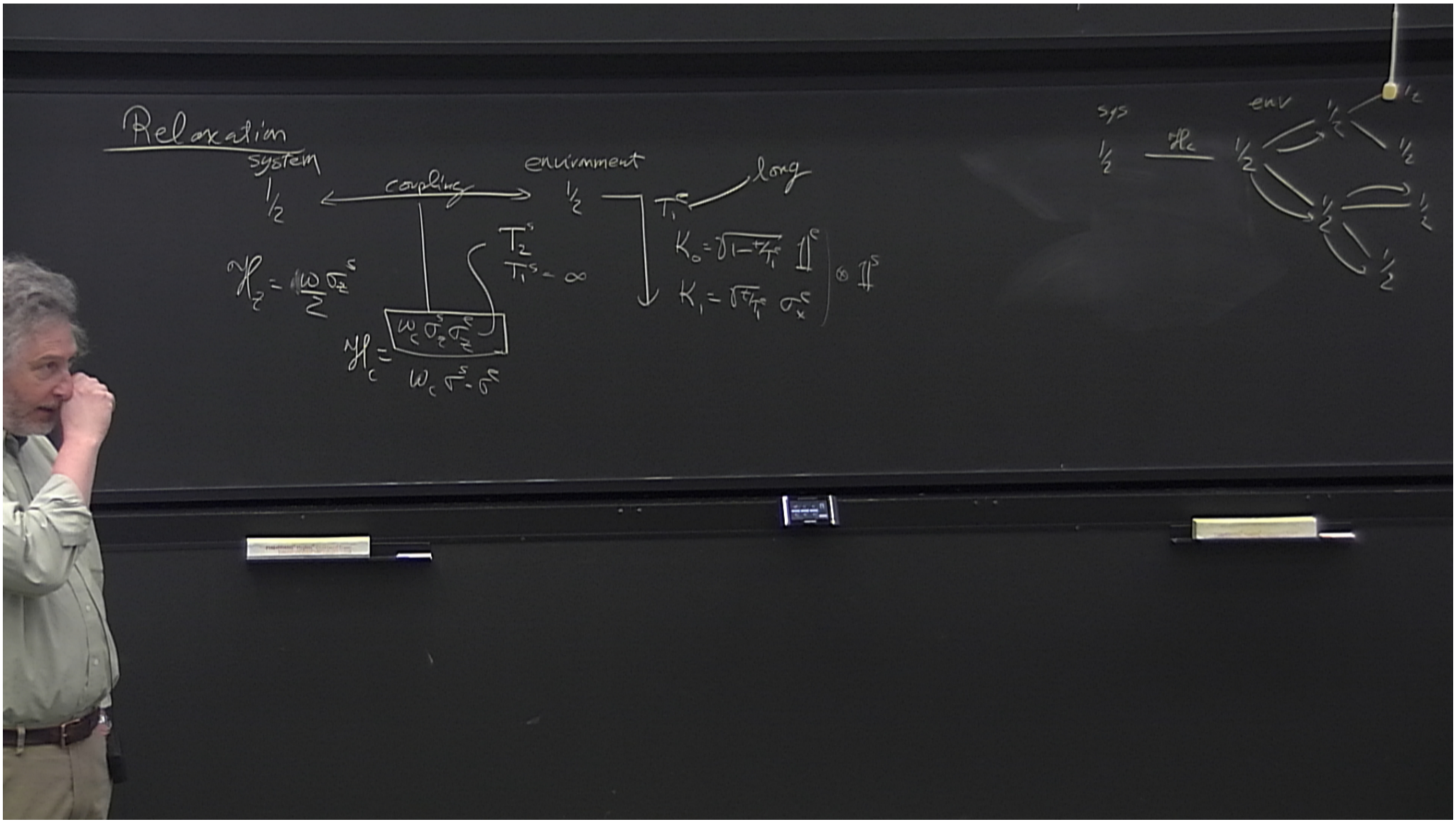
By making the system environment coupling isotropic then we introduce a T1 process to the system.

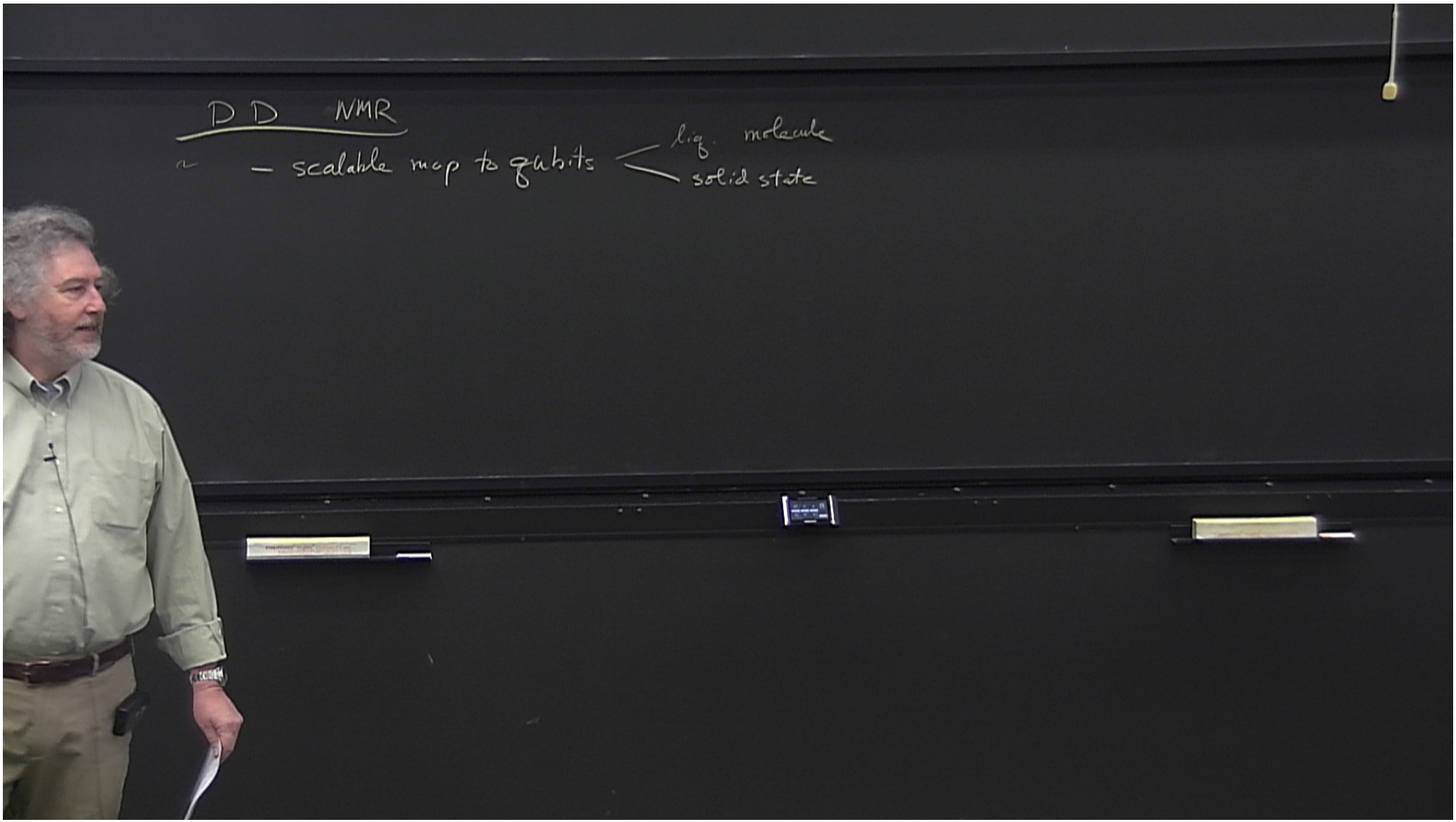
```
S2[w_, wc_, t_, T1_] :=
  Table[Tr[KroneckerProduct[PauliMatrix[i], PauliMatrix[0]] . U2[w, wc, t] .
      Sum[Kx[k, t, T1] . KroneckerProduct[PauliMatrix[j], PauliMatrix[0]] .
        ConjugateTranspose[Kx[k, t, T1]], {k, 1, 2}] .
      U2inv[w, wc, t]] / 4, {i, 0, 3}, {j, 0, 3}];
```

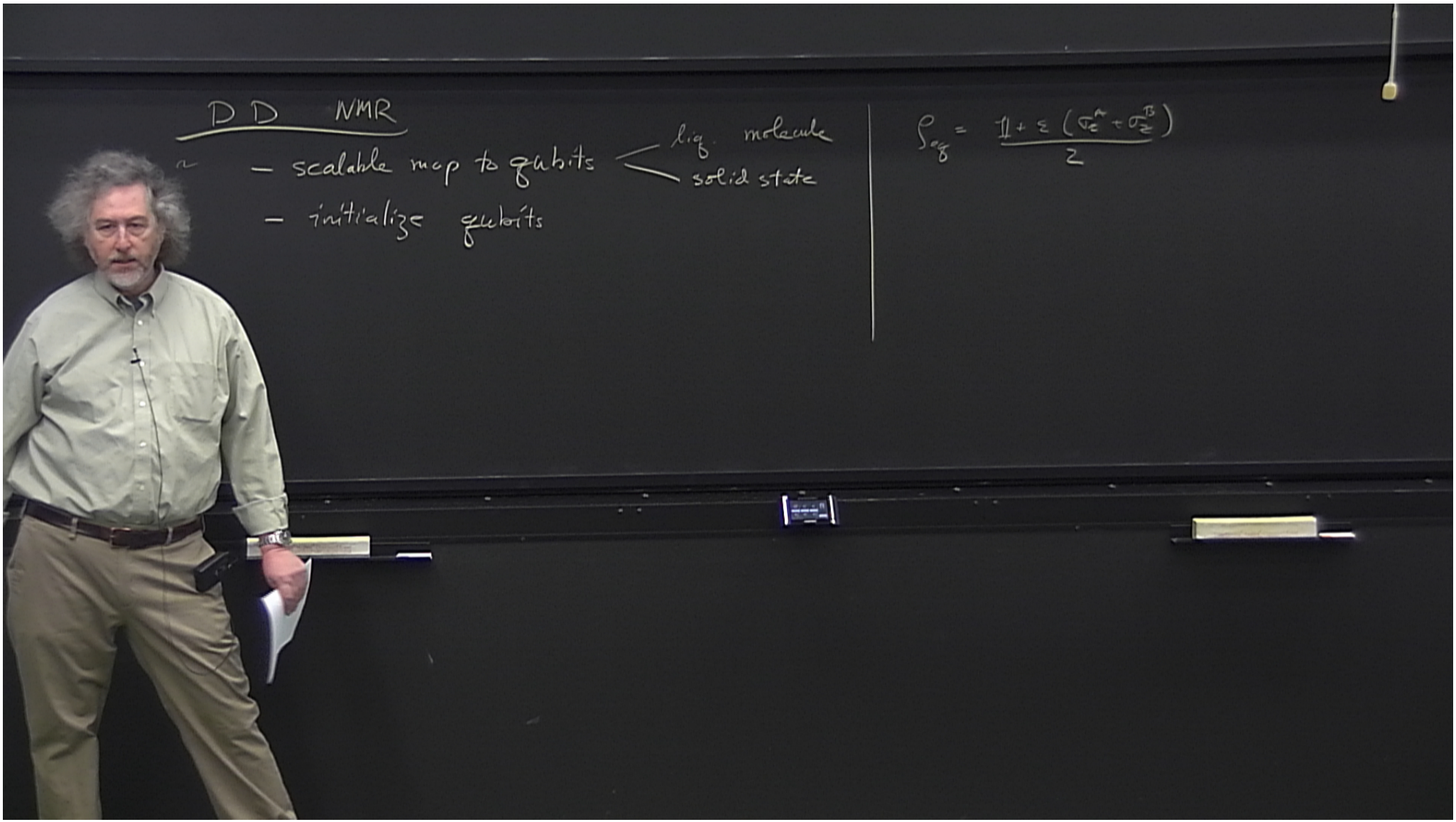
```
S2[0, 0, 0, 0.2] // MatrixForm
```

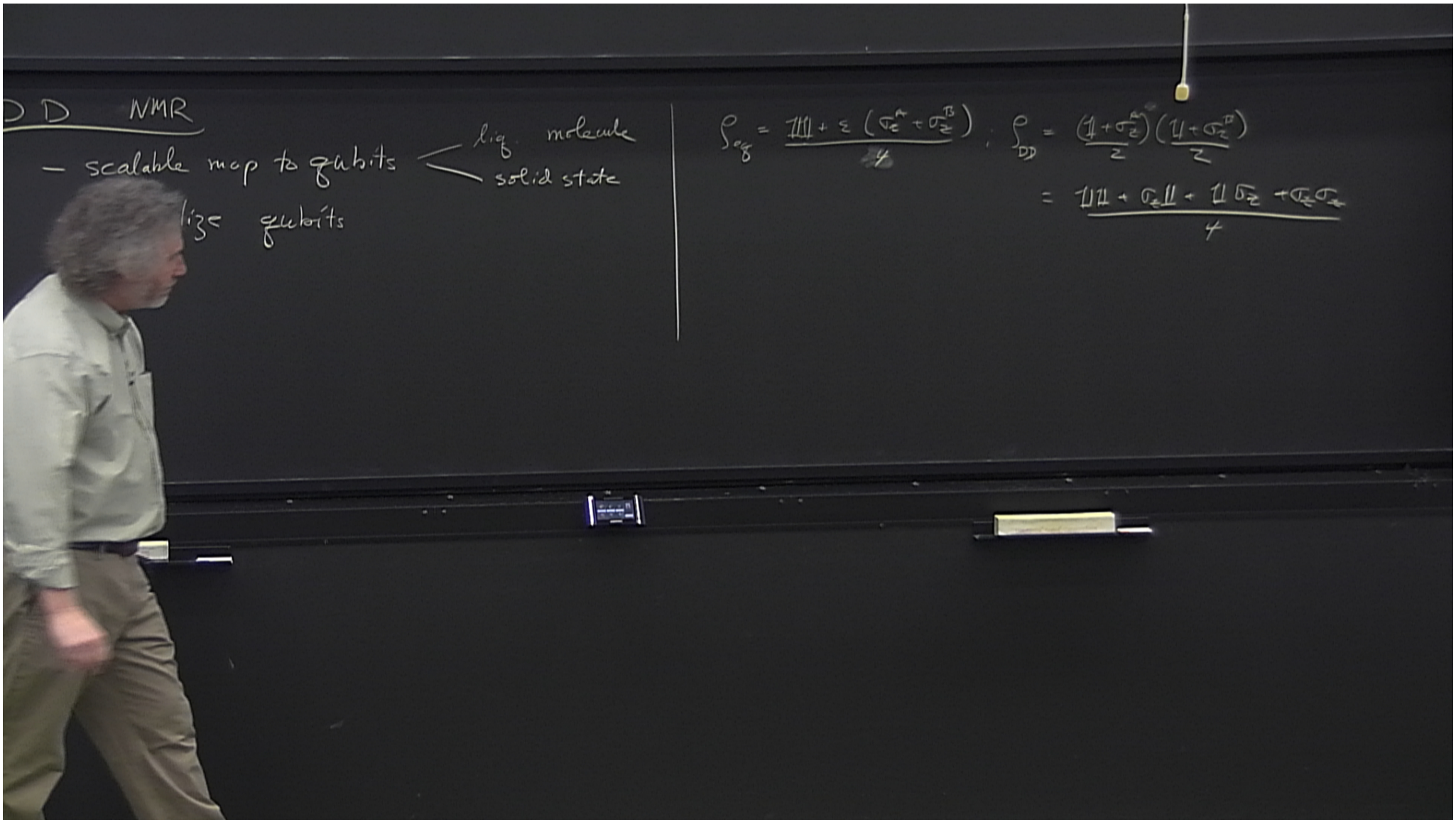
200%

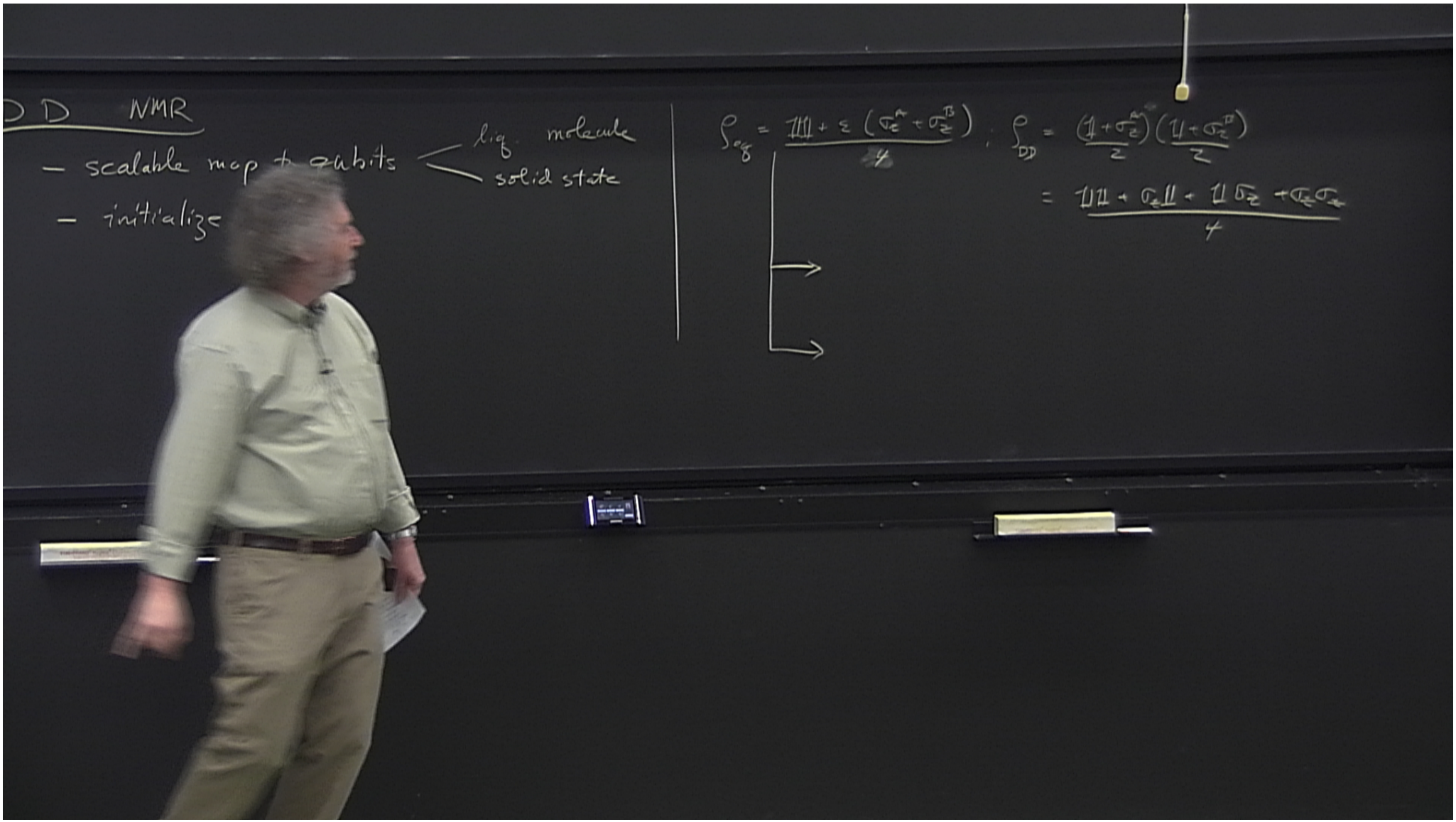

Relaxation
system
environment
coupling
long
sys
env


Relaxation
system
environment
coupling
long
sys
env


DD NMR
– scalable map to qubits
liq. molecule
solid state


DD NMR
– scalable map to qubits
liq. molecule
solid state
– initialize qubits
$\rho_{eq} = \frac{\mathbb{1} + \varepsilon(\sigma_z^A + \sigma_z^B)}{2}$


D D NMR
– scalable map to qubits
liq. molecule
solid state
lize qubits
$\rho_{eq} = \frac{\mathbb{1}\mathbb{1} + \varepsilon(\sigma_z^A + \sigma_z^B)}{4}$; $\rho_{DD} = \left(\frac{\mathbb{1} + \sigma_z^A}{2}\right)\left(\frac{\mathbb{1} + \sigma_z^B}{2}\right)$
$= \frac{\mathbb{1}\mathbb{1} + \sigma_z\mathbb{1} + \mathbb{1}\sigma_z + \sigma_z\sigma_z}{4}$


D D NMR
– scalable map to qubits
liq. molecule
solid state
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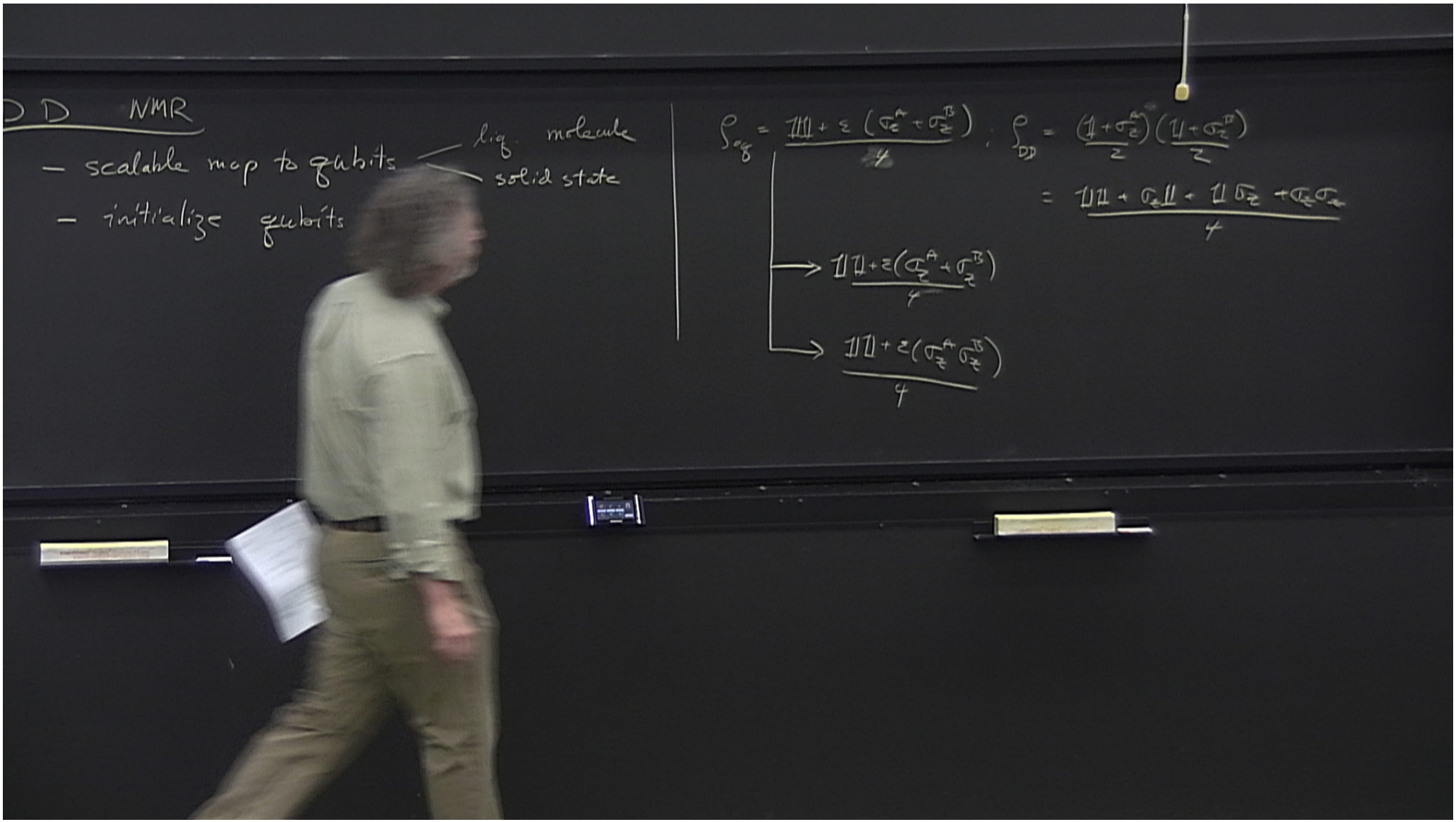
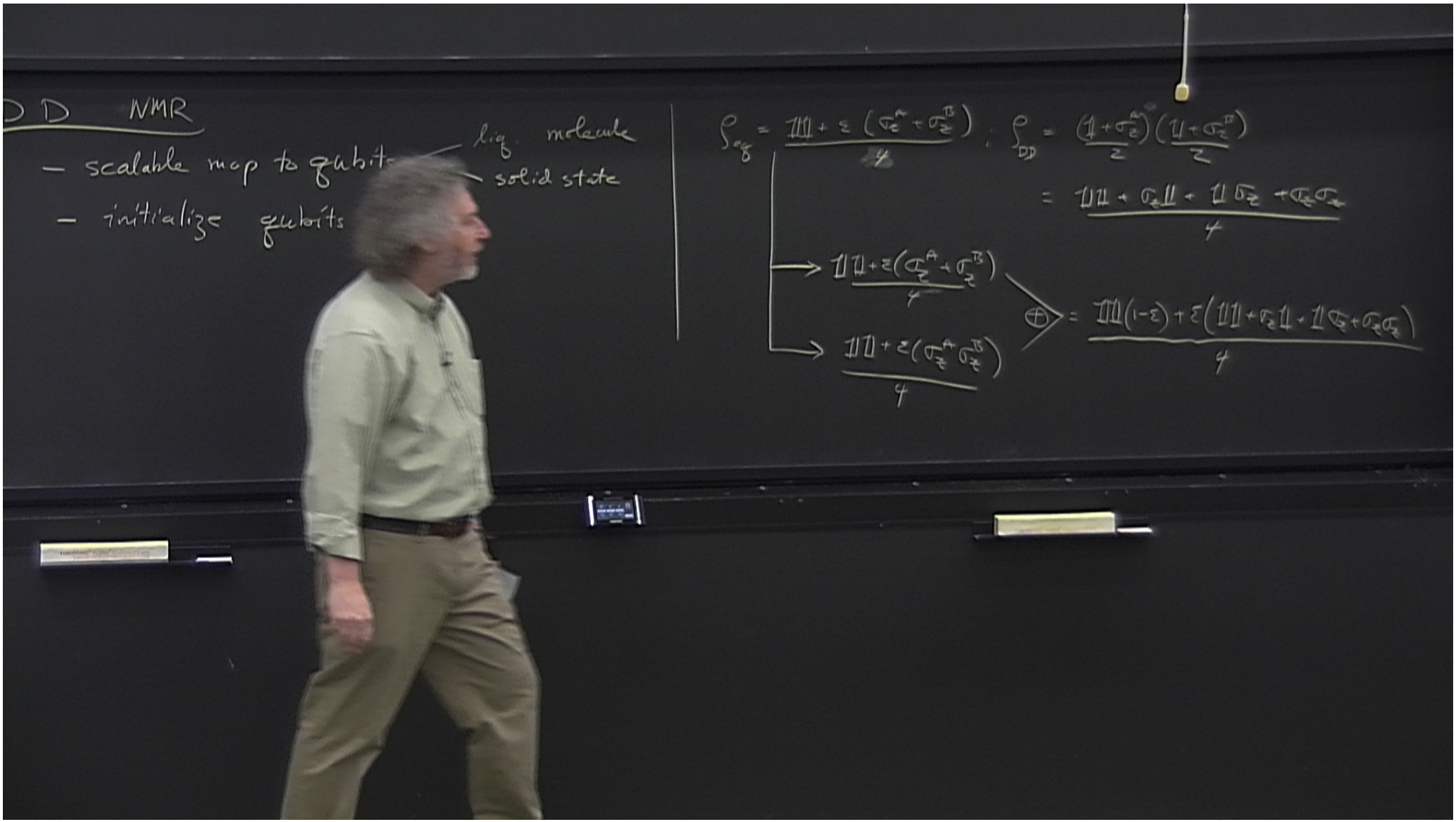
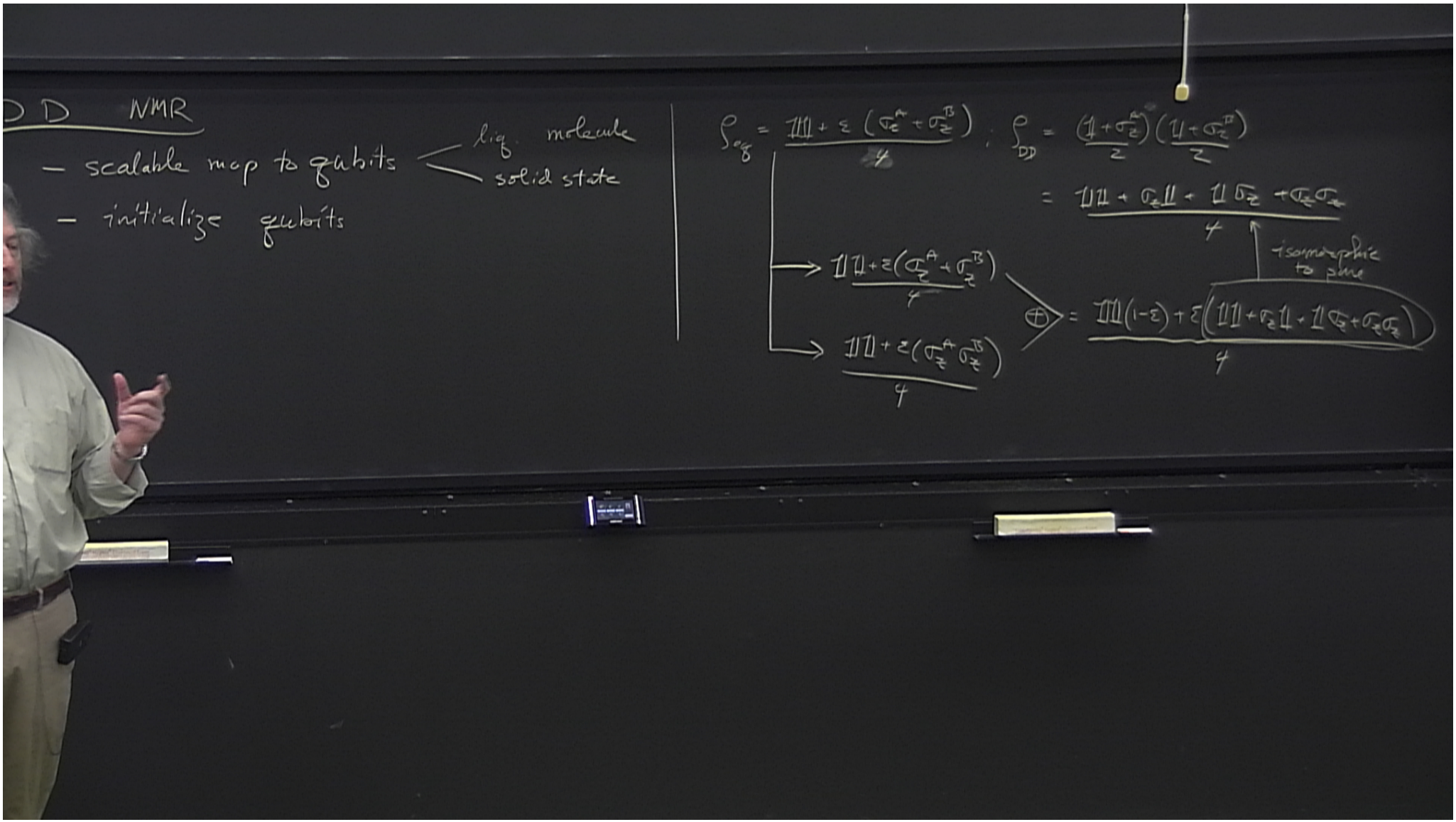

D D NMR
– scalable map to qubits
liq. molecule
solid state
– initialize qubits
$\rho_{eq} = \frac{\mathbb{1}\mathbb{1} + \varepsilon(\sigma_z^A + \sigma_z^B)}{4}$; $\rho_{DD} = \frac{(\mathbb{1} + \sigma_z^A)}{2}\frac{(\mathbb{1} + \sigma_z^B)}{2}$
$= \frac{\mathbb{1}\mathbb{1} + \sigma_z\mathbb{1} + \mathbb{1}\sigma_z + \sigma_z\sigma_z}{4}$
$\frac{\mathbb{1}\mathbb{1} + \varepsilon(\sigma_z^A + \sigma_z^B)}{4}$
$\frac{\mathbb{1}\mathbb{1} + \varepsilon(\sigma_z^A \sigma_z^B)}{4}$


D D NMR
– scalable map to qubits
liq. molecule
solid state
– initialize qubits


D D NMR
- scalable map to qubits
liq. molecule
solid state
- initialize qubits
isomorphic to pure

DD NMR

- ~ — scalable map to qubits < liq. molecule / solid state
- X — initialize qubits
- ✓ — universal control
- ✓ — qubit specific measurement
- ✓ — control noise

$$\rho_{eq} = \frac{\mathbb{1}\mathbb{1} + \varepsilon(\sigma_z^A + \sigma_z^B)}{4} \; ; \; \rho_{DD} = \frac{(\mathbb{1} + \sigma_z^A)}{2}\frac{(\mathbb{1} + \sigma_z^B)}{2}$$

$$= \frac{\mathbb{1}\mathbb{1} + \sigma_z\mathbb{1} + \mathbb{1}\sigma_z + \sigma_z\sigma_z}{4}$$

$$\frac{\mathbb{1}\mathbb{1} + \varepsilon(\sigma_z^A + \sigma_z^B)}{4}$$

$$\frac{\mathbb{1}\mathbb{1} + \varepsilon(\sigma_z^A \sigma_z^B)}{4}$$

$$\oplus = \frac{\mathbb{1}\mathbb{1}(1-\varepsilon) + \varepsilon(\mathbb{1}\mathbb{1} + \sigma_z\mathbb{1} + \mathbb{1}\sigma_z}{4}$$

isomorph to pa