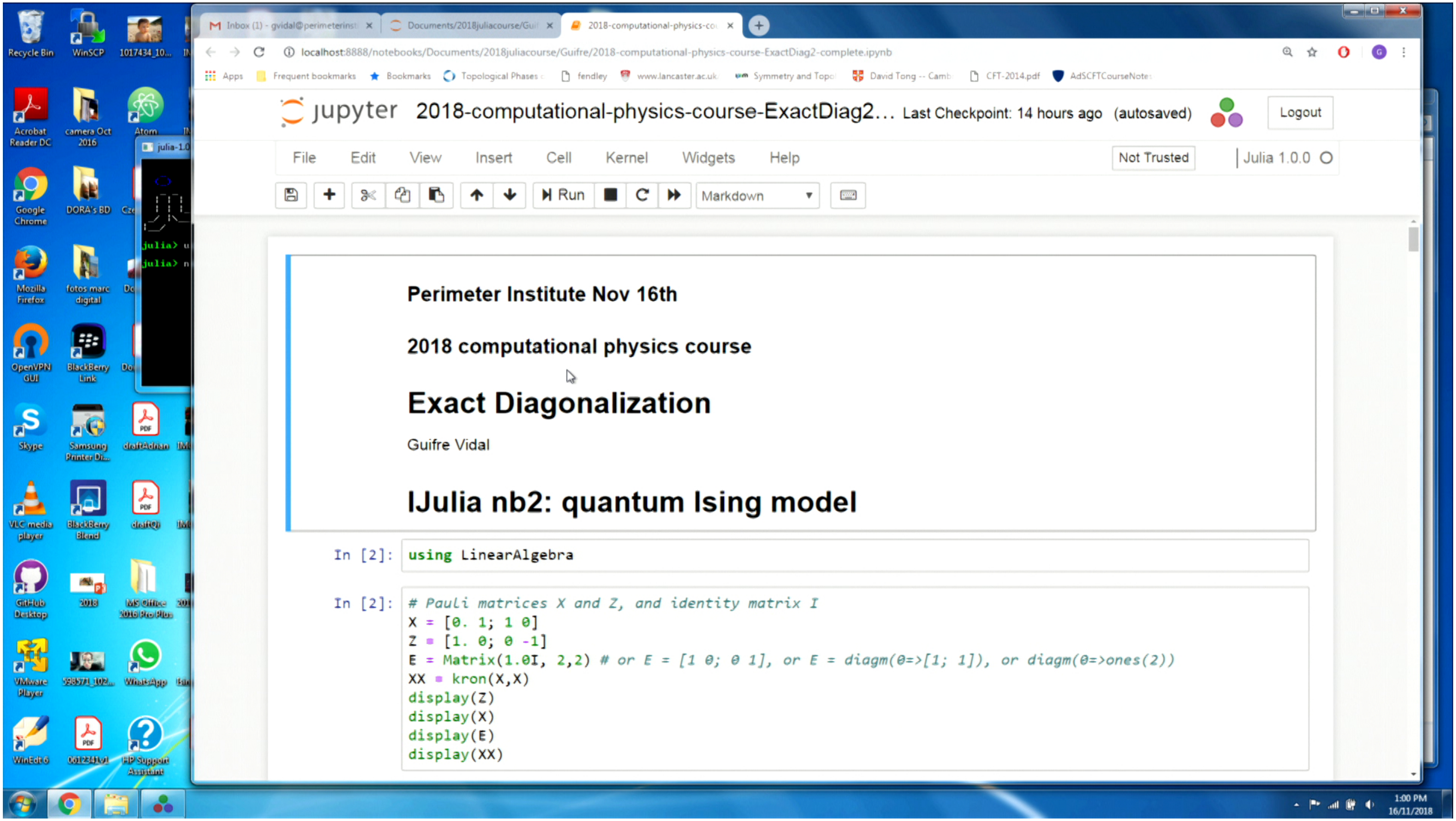
Title: Computational Physics - Lecture 20

Date: Nov 16, 2018 01:00 PM

URL: http://pirsa.org/18110046

Abstract: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Julia 1.0.0
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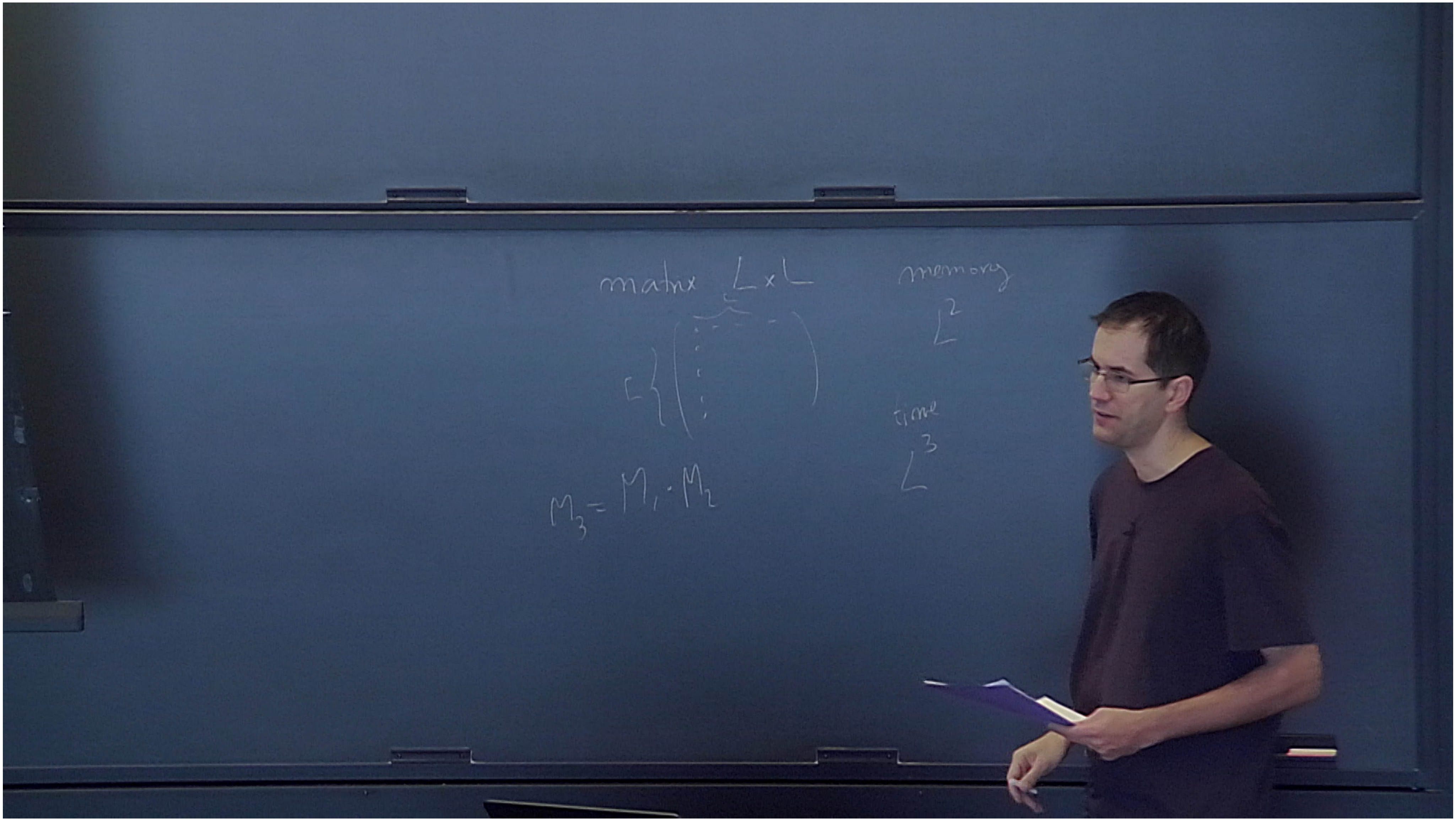
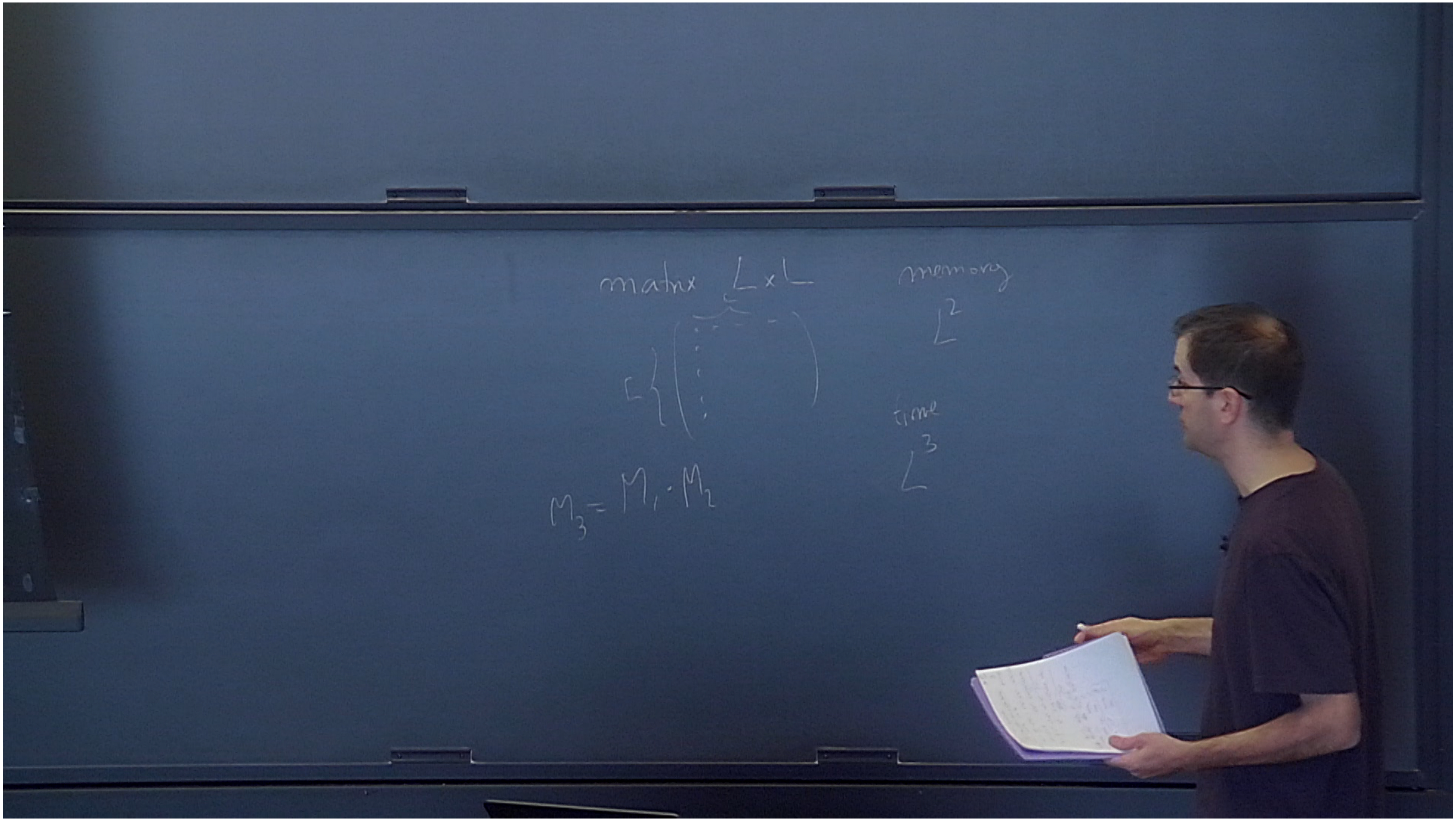
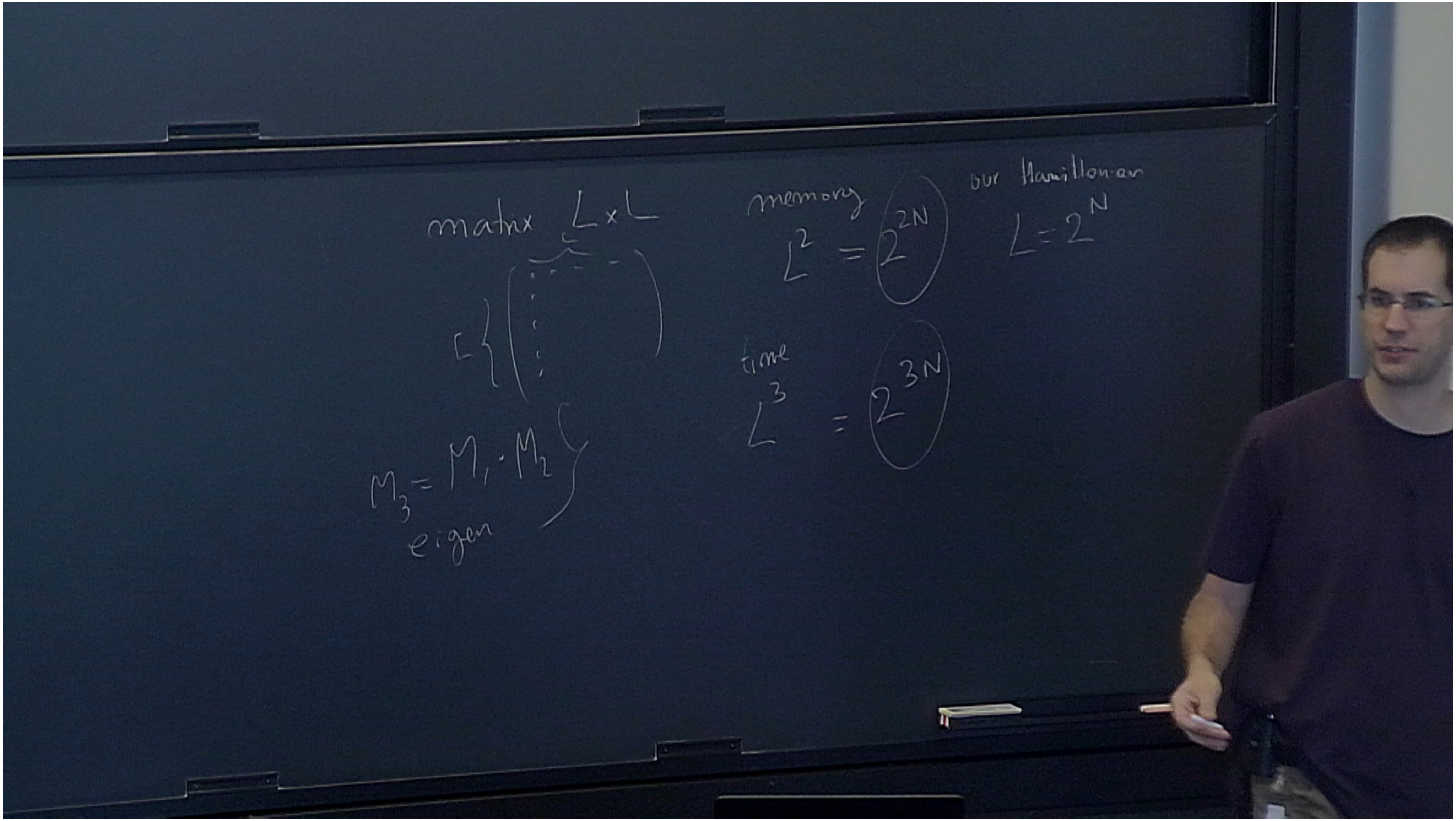
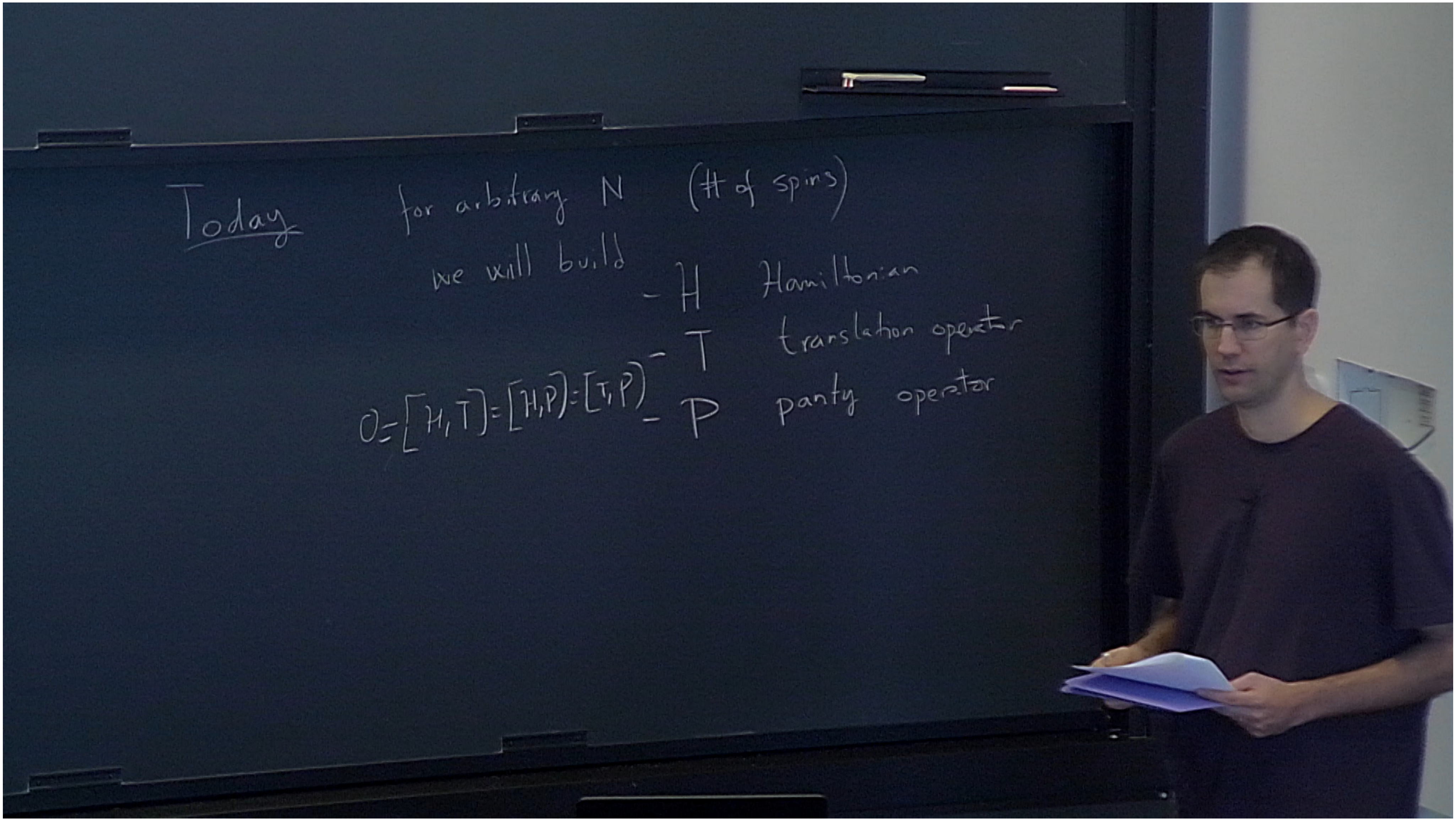
Markdown
Perimeter Institute Nov 16th
2018 computational physics course
Exact Diagonalization
Guifre Vidal
IJulia nb2: quantum Ising model
In [2]: using LinearAlgebra
In [2]: # Pauli matrices X and Z, and identity matrix I
X = [0. 1; 1 0]
Z = [1. 0; 0 -1]
E = Matrix(1.0I, 2,2) # or E = [1 0; 0 1], or E = diagm(0=>[1; 1]), or diagm(0=>ones(2))
XX = kron(X,X)
display(Z)
display(X)
display(E)
display(XX)


matrix L×L
memory
L²
time
L³
M₃ = M₁ · M₂


matrix L×L
memory
L^2
time
L^3
M_3 = M_1 · M_2


matrix L×L
L
memory
L² = 2^2N
our Hamiltonian
L = 2^N
time
L³ = 2^3N
M3 = M1 · M2
eigen


Today
for arbitrary N (# of spins)
we will build
- H Hamiltonian
- T translation operator
- P parity operator
0 = [H, T] = [H, P] = [T, P]

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```julia
display(E)
display(XX)
println(XX)
```

```
2×2 Array{Float64,2}:
 1.0   0.0
 0.0  -1.0

2×2 Array{Float64,2}:
 0.0  1.0
 1.0  0.0

2×2 Array{Float64,2}:
 1.0  0.0
 0.0  1.0

4×4 Array{Float64,2}:
 0.0  0.0  0.0  1.0
 0.0  0.0  1.0  0.0
 0.0  1.0  0.0  0.0
 1.0  0.0  0.0  0.0
```

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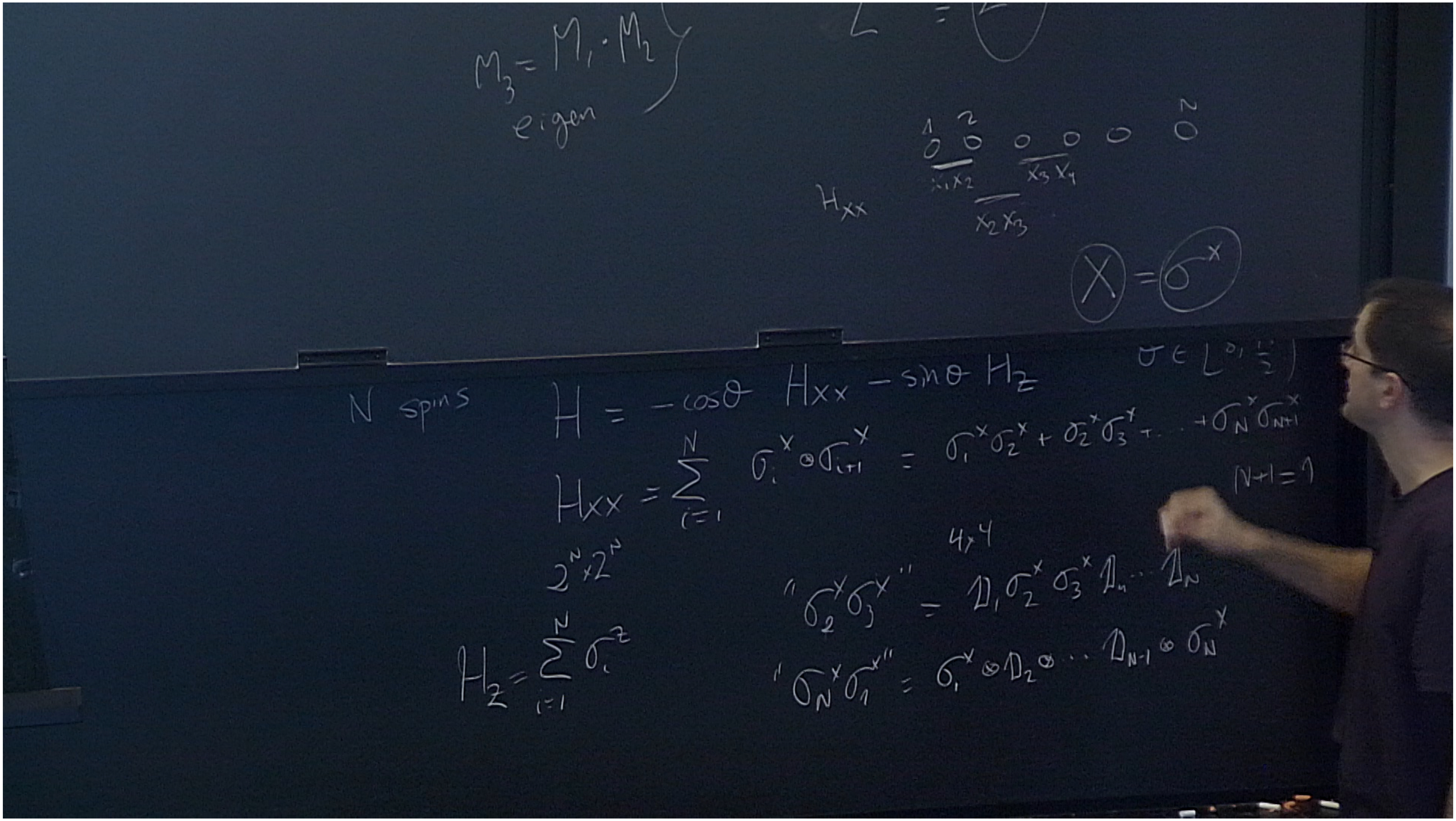
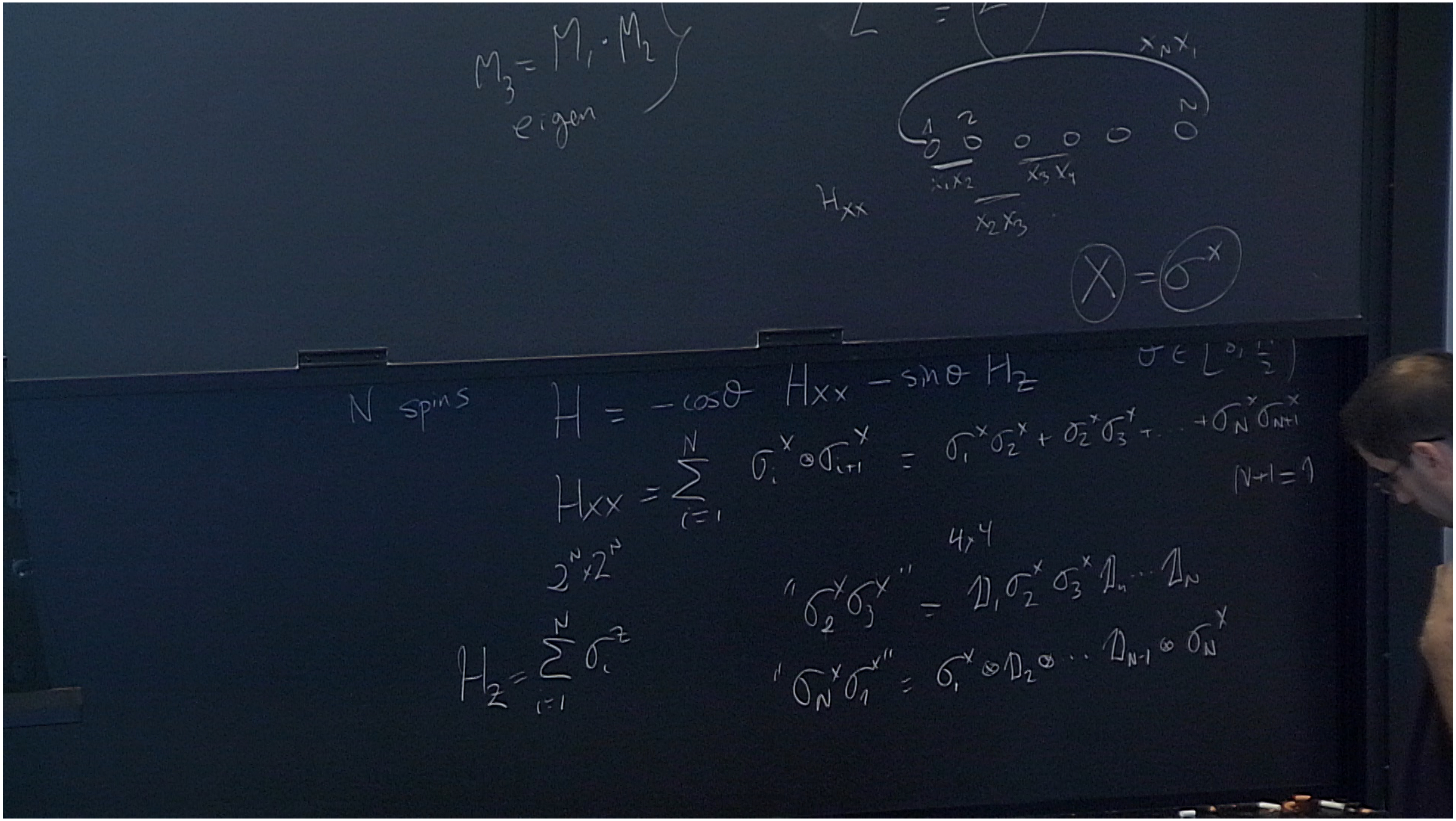
Hamiltonian for N spins (use $N \leq 10$)

In [8]:
```
# Ising Hamiltonian for N spins  with exact diagonalization
N = 3
theta = pi/4 # magnetic field
HXX = XX
HZ = kron(Z,E) + kron(E,Z)
for n = 3:N
    HXX = kron(HXX,E)+kron(diagm(0=>ones(2^(n-2))), XX)
    HZ =  kron(HZ,E) + kron(diagm(0=>ones(2^(n-1))),Z)
end
HXX = HXX + kron(X,kron(diagm(0=>ones(2^(N-2))),X))
H = -cos(theta)*HXX - sin(theta)*HZ

display(H)
```

```
8×8 Array{Float64,2}:
 -2.12132   -0.0        -0.0        …  -0.707107  -0.707107  -0.0
 -0.0       -0.707107   -0.707107      -0.0       -0.0       -0.707107
```


M3 = M1 · M2
eigen
Hxx
x1 x2
x3 x4
x2 x3
X = σx
N spins
H = −cosθ Hxx − sinθ Hz
Hxx = Σ σix ⊗ σi+1x = σ1x σ2x + σ2x σ3x + ... + σNx σN+1x
N+1 = 1
2N × 2N
4×4
"σ2x σ3x" = 1 1 σ2x σ3x 1 4 ... 1 N
"σNx σ1x" = σ1x ⊗ 1 2 ⊗ ... 1 N-1 ⊗ σNx
Hz = Σ σiz


$M_3 = M_1 \cdot M_2$
eigen
$x_N x_1$
1 2 N
$x_1 x_2$
$x_3 x_4$
$x_2 x_3$
H_{xx}
$X = \sigma^x$
$\sigma \in [0, \frac{1}{2})$
N spins
$H = -\cos\theta \, H_{xx} - \sin\theta \, H_Z$
$H_{xx} = \sum_{i=1}^{N} \sigma_i^x \otimes \sigma_{i+1}^x = \sigma_1^x \sigma_2^x + \sigma_2^x \sigma_3^x + \dots + \sigma_N^x \sigma_{N+1}^x$
$N+1 = 1$
$2^N \times 2^N$
4×4
"$\sigma_2^x \sigma_3^x$" $= \mathbb{1}_1 \sigma_2^x \sigma_3^x \mathbb{1}_4 \cdots \mathbb{1}_N$
"$\sigma_N^x \sigma_1^x$" $= \sigma_1^x \otimes \mathbb{1}_2 \otimes \cdots \mathbb{1}_{N-1} \otimes \sigma_N^x$
$H_Z = \sum_{i=1}^{N} \sigma_i^z$

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Hamiltonian for N spins (use $N \leq 10$)

In [8]:

```
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N = 3
theta = pi/4 # magnetic field
HXX = XX
HZ = kron(Z,E) + kron(E,Z)
for n = 3:N
    HXX = kron(HXX,E)+kron(diagm(0=>ones(2^(n-2))), XX)
    HZ =  kron(HZ,E) + kron(diagm(0=>ones(2^(n-1))),Z)
end
HXX = HXX + kron(X,kron(diagm(0=>ones(2^(N-2))),X))
H = -cos(theta)*HXX - sin(theta)*HZ

display(H)
```
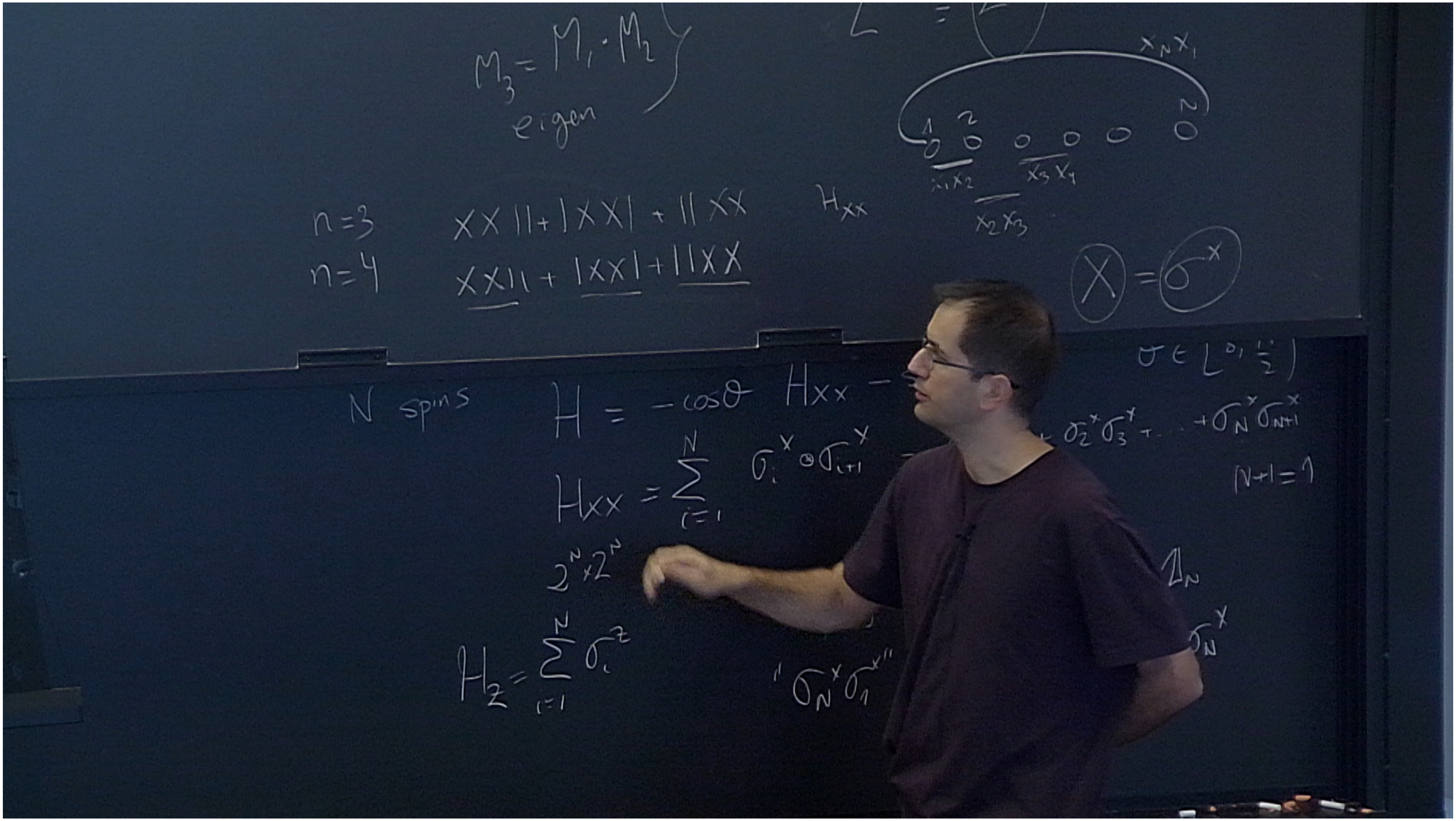

```
8×8 Array{Float64,2}:
 -2.12132   -0.0        -0.0       …  -0.707107  -0.707107  -0.0
 -0.0       -0.707107  -0.707107     -0.0       -0.0       -0.707107
```


M3 = M1 · M2
eigen
n=3 XX11 + 1XX1 + 11XX
n=4 XX11 + 1XX1 + 11XX
Hxx
X = σx
N spins
H = −cosθ Hxx −
Hxx = Σ σix ⊗ σi+1x
2N×2N
Hz = Σ σiz
"σNx σ1x"
N+1 = 1

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Hamiltonian for N spins (use $N \leq 10$)

In [8]:
```julia
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HZ = kron(Z,E) + kron(E,Z)
for n = 3:N
    HXX = kron(HXX,E)+kron(diagm(0=>ones(2^(n-2))), XX)
    HZ =  kron(HZ,E) + kron(diagm(0=>ones(2^(n-1))),Z)
end
HXX = HXX + kron(X,kron(diagm(0=>ones(2^(N-2))),X))
H = -cos(theta)*HXX - sin(theta)*HZ

display(H)
```

```
8×8 Array{Float64,2}:
 -2.12132   -0.0        -0.0        …  -0.707107  -0.707107  -0.0
 -0.0       -0.707107   -0.707107      -0.0       -0.0       -0.707107
```

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Hamiltonian for N spins (use $N \leq 10$)

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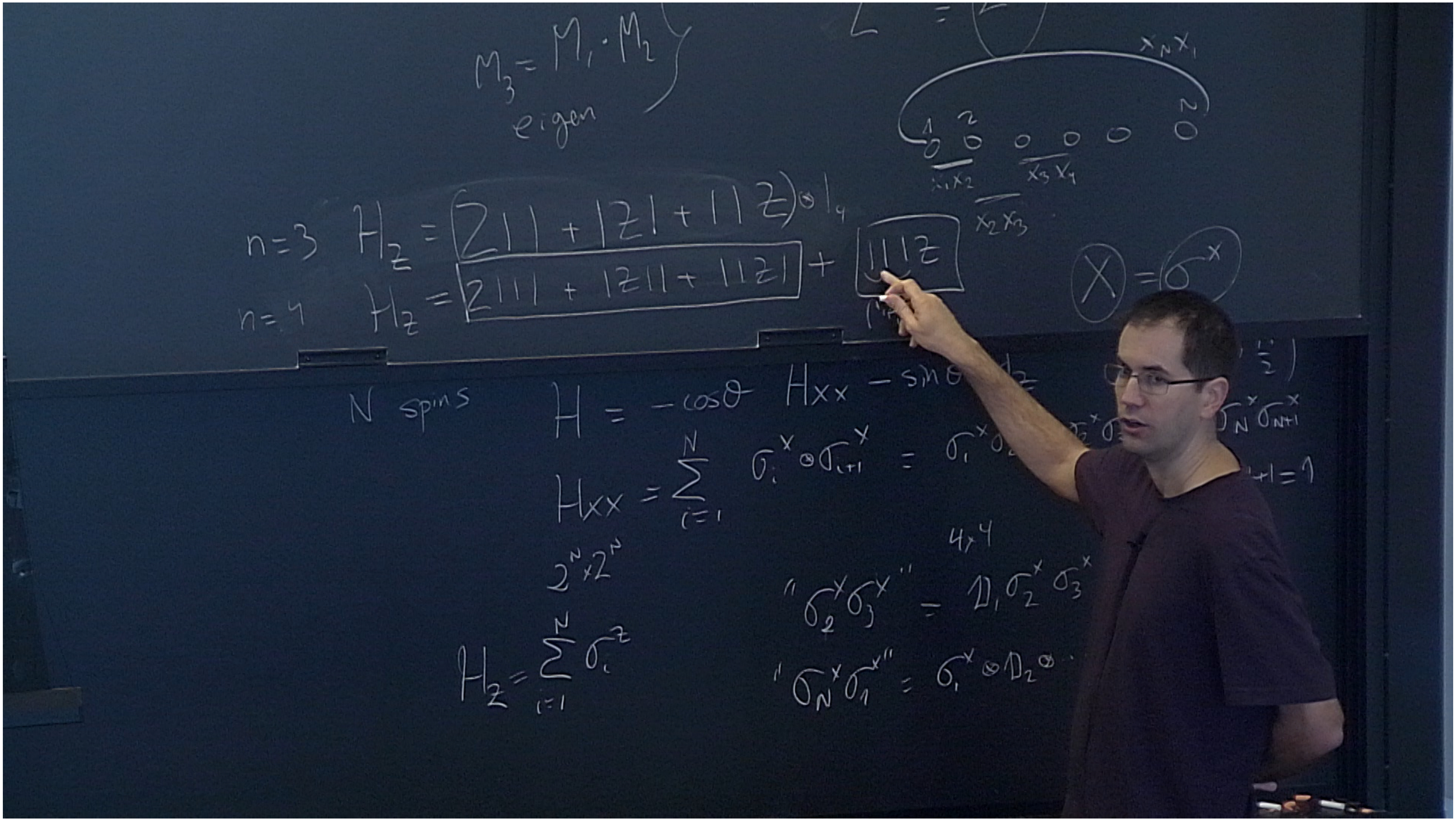
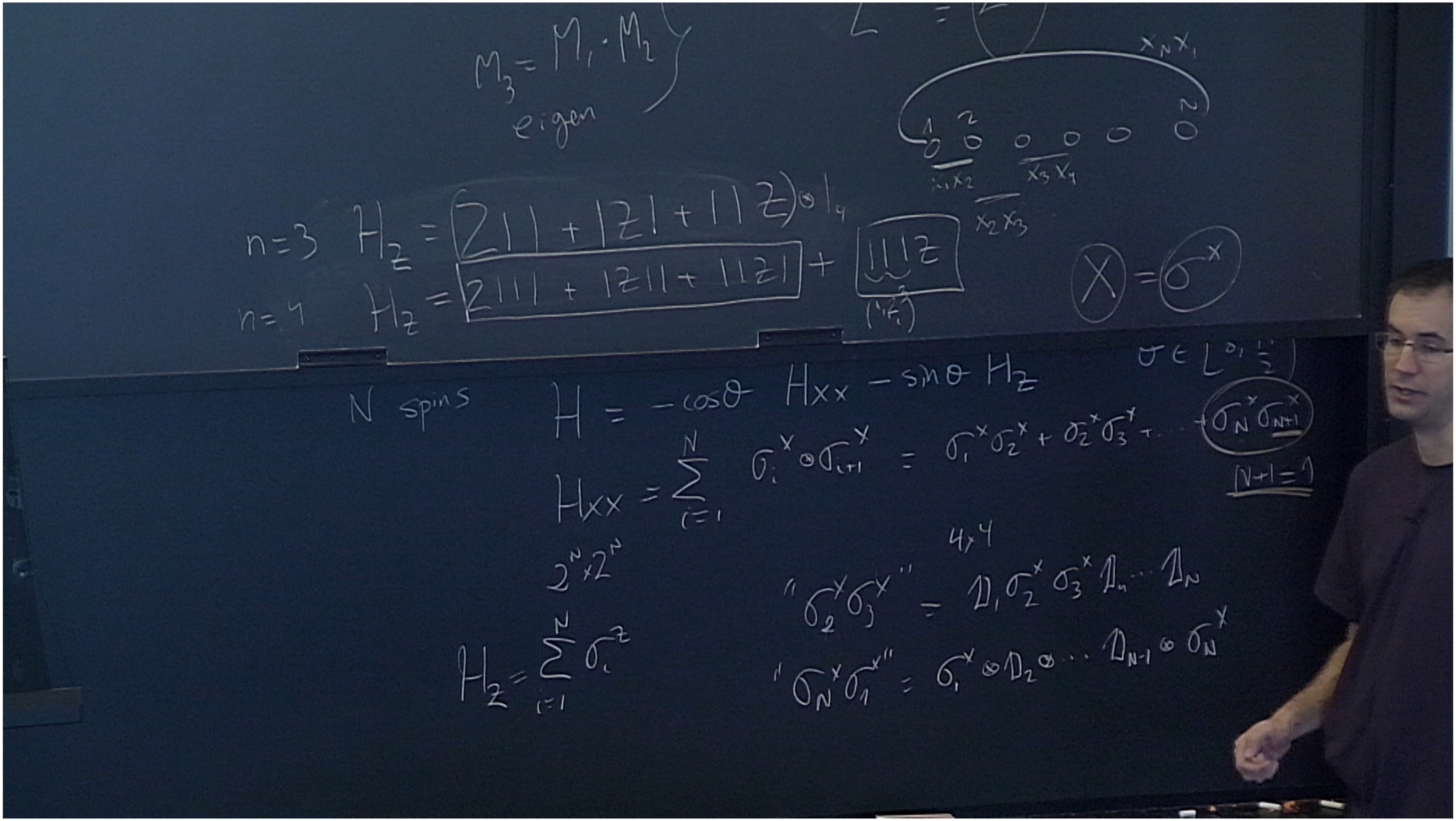
N = 3
theta = pi/4 # magnetic field
HXX = XX
HZ = kron(Z,E) + kron(E,Z)
for n = 3:N
    HXX = kron(HXX,E)+kron(diagm(0=>ones(2^(n-2))), XX)
    HZ =  kron(HZ,E) + kron(diagm(0=>ones(2^(n-1))),Z)
end
HXX = HXX + kron(X,kron(diagm(0=>ones(2^(N-2))),X))
H = -cos(theta)*HXX - sin(theta)*HZ

display(H)
```

```
8×8 Array{Float64,2}:
 -2.12132   -0.0        -0.0       …  -0.707107  -0.707107  -0.0
 -0.0       -0.707107   -0.707107     -0.0       -0.0       -0.707107
```


$M_3 = M_1 \cdot M_2$
eigen
$n=3 \quad H_Z = (Z11 + 1Z1 + 11Z) \otimes 1_4$
$n=4 \quad H_Z = Z111 + 1Z11 + 11Z1 + 111Z$
$X = \sigma^x$
N spins
$H = -\cos\theta \, H_{xx} - \sin\theta \, H_Z$
$H_{xx} = \sum_{i=1}^{N} \sigma_i^x \otimes \sigma_{i+1}^x$
$2^N \times 2^N$
$H_Z = \sum_{i=1}^{N} \sigma_i^z$



M3 = M1 · M2
eigen
x1x2
x3x4
x2x3
xNx1
n=3 HZ = (Z11 + 1Z1 + 11Z) ⊗ 14
n=4 HZ = Z111 + 1Z11 + 11Z1 + 111Z
X = σx
N spins
H = −cosθ Hxx − sinθ HZ
Hxx = Σ σix ⊗ σi+1x = σ1xσ2x + σ2xσ3x + ... + σNxσN+1x
N+1 = 1
2N x 2N
4x4
"σ2xσ3x" = 11 σ2x σ3x 14 ... 1N
"σNxσ1x" = σ1x ⊗ 12 ⊗ ... 1N-1 ⊗ σNx
HZ = Σ σiz

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Run Code

```
for n = 3:N
    HXX = kron(HXX,E)+kron(diagm(0=>ones(2^(n-2))), XX)
    HZ =  kron(HZ,E) + kron(diagm(0=>ones(2^(n-1))),Z)
end
HXX = HXX + kron(X,kron(diagm(0=>ones(2^(N-2))),X))
H = -cos(theta)*HXX - sin(theta)*HZ

display(H)
```

```
8×8 Array{Float64,2}:
 -2.12132    -0.0        -0.0       …  -0.707107  -0.707107  -0.0
 -0.0        -0.707107   -0.707107     -0.0       -0.0       -0.707107
 -0.0        -0.707107   -0.707107     -0.0       -0.0       -0.707107
 -0.707107   -0.0        -0.0          -0.707107  -0.707107  -0.0
 -0.0        -0.707107   -0.707107     -0.0       -0.0       -0.707107
 -0.707107   -0.0        -0.0       …   0.707107  -0.707107  -0.0
 -0.707107   -0.0        -0.0          -0.707107   0.707107  -0.0
 -0.0        -0.707107   -0.707107     -0.0       -0.0        2.12132
```

magnetic field angle $\theta \in [0, \pi/2]$

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```
 -0.707107  -0.0       -0.0          -0.707107  -0.707107  -0.0
 -0.0       -0.707107  -0.707107     -0.0       -0.0       -0.707107
 -0.707107  -0.0       -0.0      …    0.707107  -0.707107  -0.0
 -0.707107  -0.0       -0.0          -0.707107   0.707107  -0.0
 -0.0       -0.707107  -0.707107     -0.0       -0.0        2.12132
```

magnetic field angle $\theta \in [0, \pi/2]$

In [4]:

```julia
N_theta=21  # number of values of magnetic field
d_theta = pi/(2*(N_theta-1)) # increments of theta
theta_val = collect(0:d_theta:pi/2) # list of magnetic field angle theta [0, pi/2
Energies = zeros(2^3,N_theta)
for i=1:N_theta
    H = -cos(theta_val[i])*HXX - sin(theta_val[i])*HZ # build the Hamiltonian
    D,U = eigen(H)          # diagonalize the Hamiltonian
    Energies[:,i] = D
end
[theta_val Energies[1,:]]
```

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```
    H = -cos(theta_val[i])*HXX - sin(theta_val[i])*HZ # build the Hamiltonian
    D,U = eigen(H)          # diagonalize the Hamiltonian
    Energies[:,i] = D
end
[theta_val Energies[1,:]]
```

Out[5]:

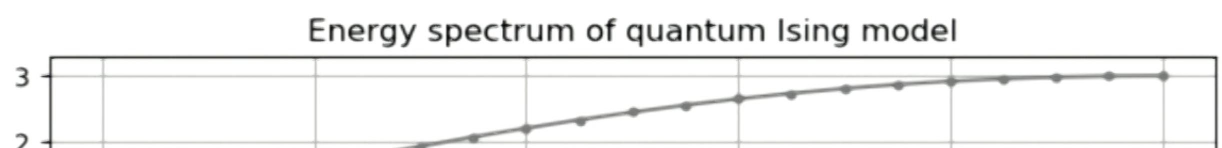
```
21×2 Array{Float64,2}:
 0.0        -3.0
 0.0785398  -2.99557
 0.15708    -2.98314
 0.235619   -2.96423
 0.314159   -2.94068
 0.392699   -2.9146
 0.471239   -2.88836
 0.549779   -2.86443
 0.628319   -2.84521
 0.706858   -2.83275
 0.785398   -2.82843
 0.863938   -2.83275
 0.942478   -2.84521
```

```
1.5708      -3.0
```

Let us plot this!

In [6]:
```
using PyPlot
```

In [7]:
```
figure("My_figure",figsize=(8,3))
grid("on")
for i in 1:2^N
    plot(2*theta_val/pi,vec(Energies[i,:]), marker=".")
end
title("Energy spectrum of quantum Ising model")
xlabel("magnetic field theta")
ylabel("Energy levels");
```



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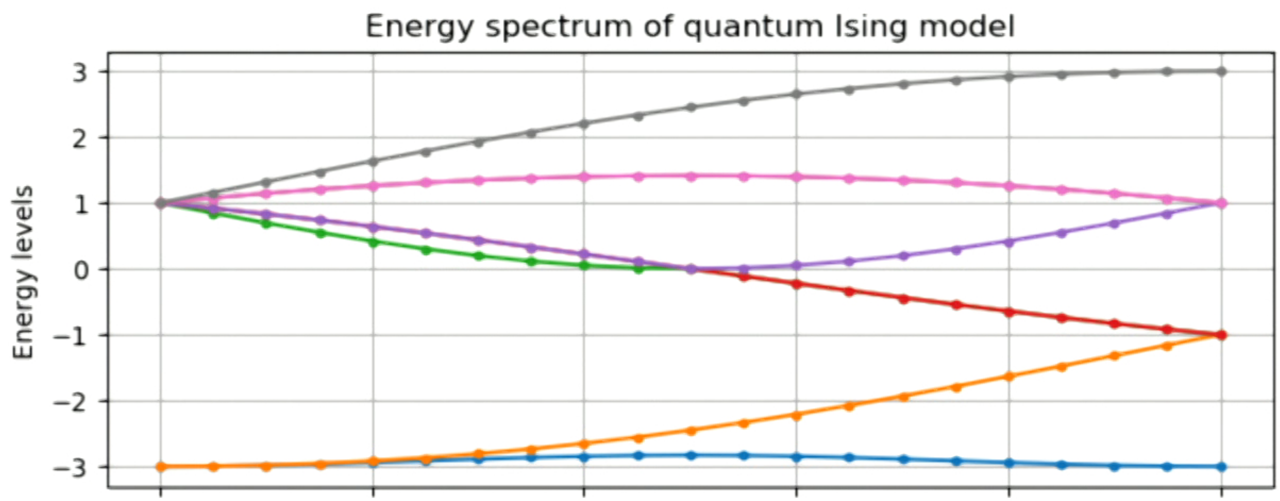
```
for i in 1:2^N
    plot(2*theta_val/pi,vec(Energies[i,:]), marker=".")
end
title("Energy spectrum of quantum Ising model")
xlabel("magnetic field theta")
ylabel("Energy levels");
```



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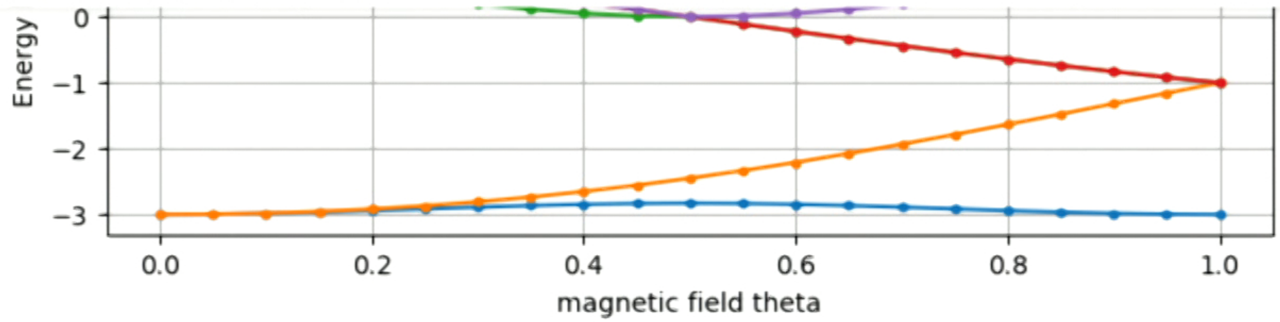

Now it's your turn! (1/3)

1) write a function buildH that builds the Hamiltonian for N spins (use only for $N \leq 10$)

Solution

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Out[3]:

```
8×8 Array{Float64,2}:
 -2.12132    -0.0        -0.0       …  -0.707107  -0.707107  -0.0
 -0.0        -0.707107  -0.707107     -0.0       -0.0       -0.707107
 -0.0        -0.707107  -0.707107     -0.0       -0.0       -0.707107
 -0.707107  -0.0        -0.0          -0.707107  -0.707107  -0.0
 -0.0        -0.707107  -0.707107     -0.0       -0.0       -0.707107
 -0.707107  -0.0        -0.0       …   0.707107  -0.707107  -0.0
 -0.707107  -0.0        -0.0          -0.707107   0.707107  -0.0
 -0.0        -0.707107  -0.707107     -0.0       -0.0        2.12132
```

2) plot the energy spectrum as a function of angle theta, $\theta \in [0, \pi/2]$, for $N = 8$ spins ¶

Solution

In [5]:

```
N=8  # spin chain size N=10 and Nh = 21 takes approx 10 seconds
N_theta=21  # number of values of magnetic field
```

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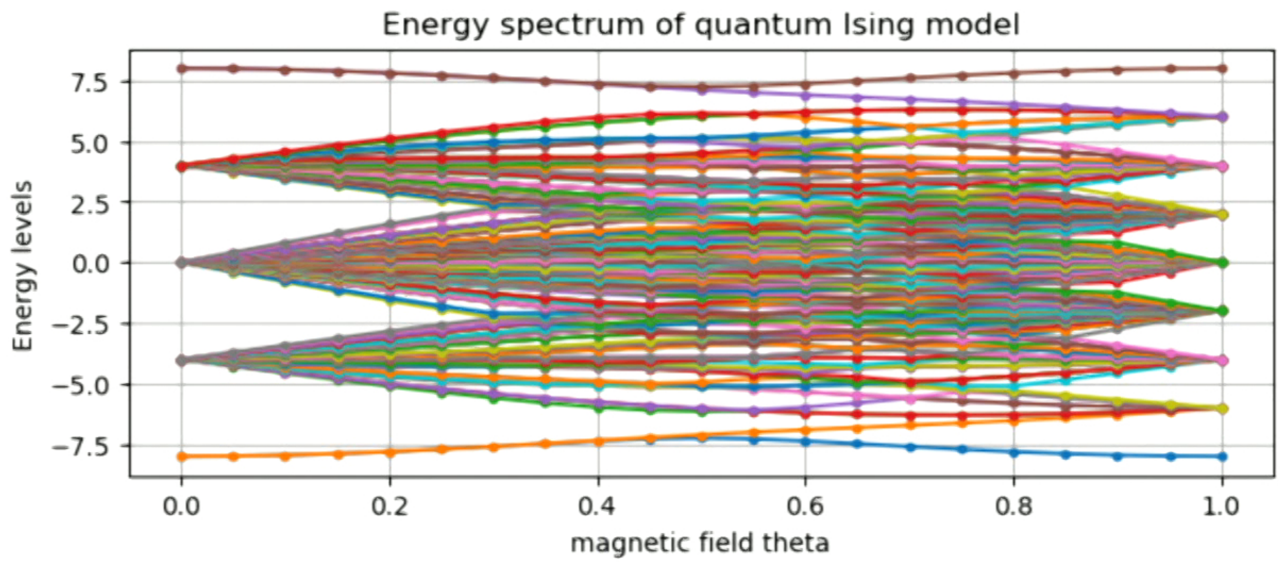
Translation operator T, with $[H, T] = 0$ (translation invariance)

In [43]:

```
# Let us quickly rebuild the Hamiltonian for N=3 spins and magnetic field angle t
EE = kron(E,E)
HZ = kron(Z,EE) + kron(E,kron(Z,E)) + kron(EE,Z)
HXX = kron(XX,E)+kron(E,XX)+kron(X,kron(E,X))
H = -(HXX+HZ)/sqrt(2)

# The translation operator T is
SWAP = [1 0 0 0; 0 0 1 0; 0 1 0 0; 0 0 0 1]
N = 3
T = copy(SWAP)
for n=3:N
    SWAPn = kron(diagm(0=>ones(2^(n-2))), SWAP)
    T =  SWAPn*kron(T,E)
end
#display(SWAP)
#display(SWAP^2)
display(T)
#display(T^3)
```

```
title("Energy spectrum of quantum Ising model")
xlabel("magnetic field theta")
ylabel("Energy levels");
```



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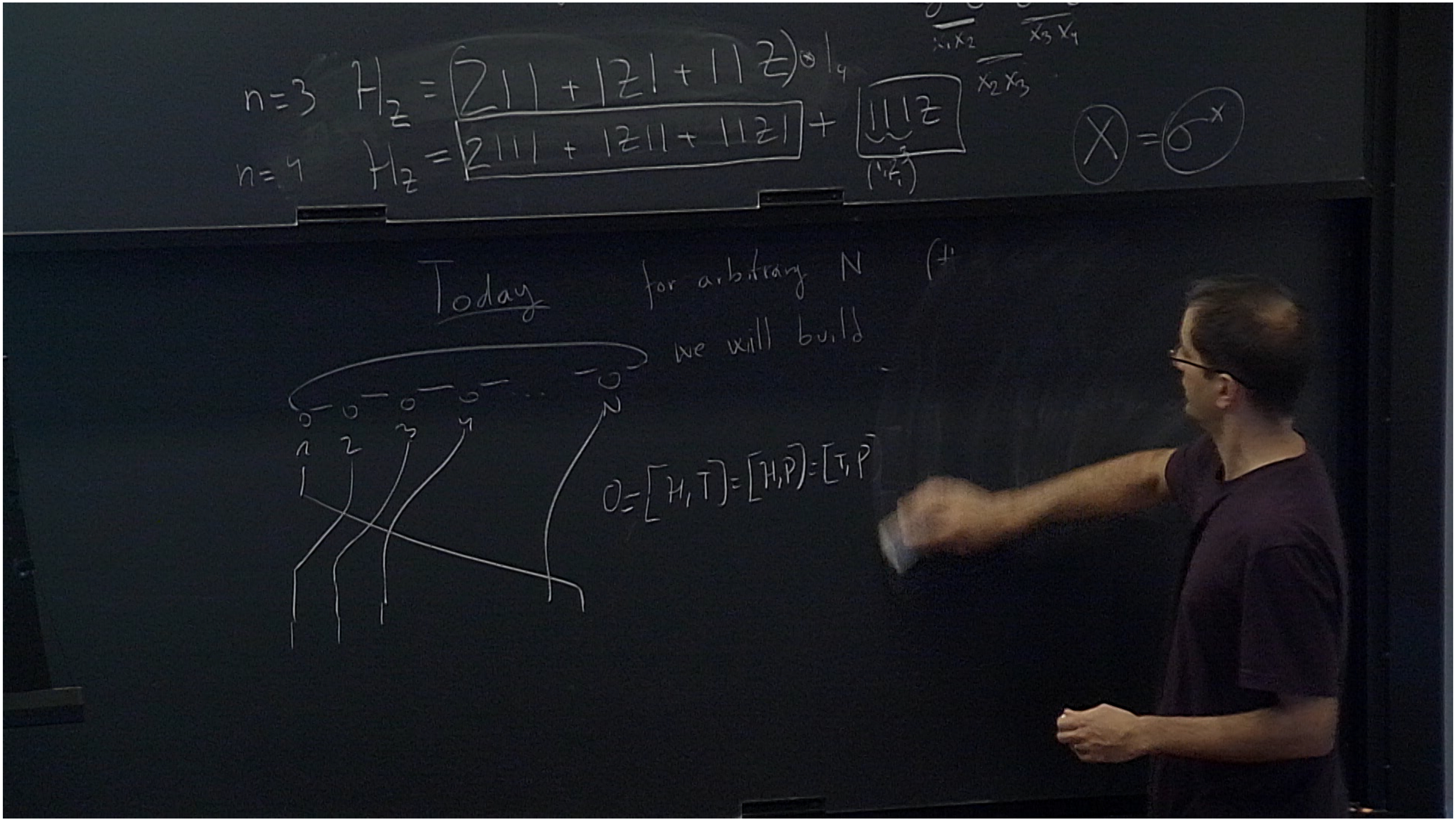
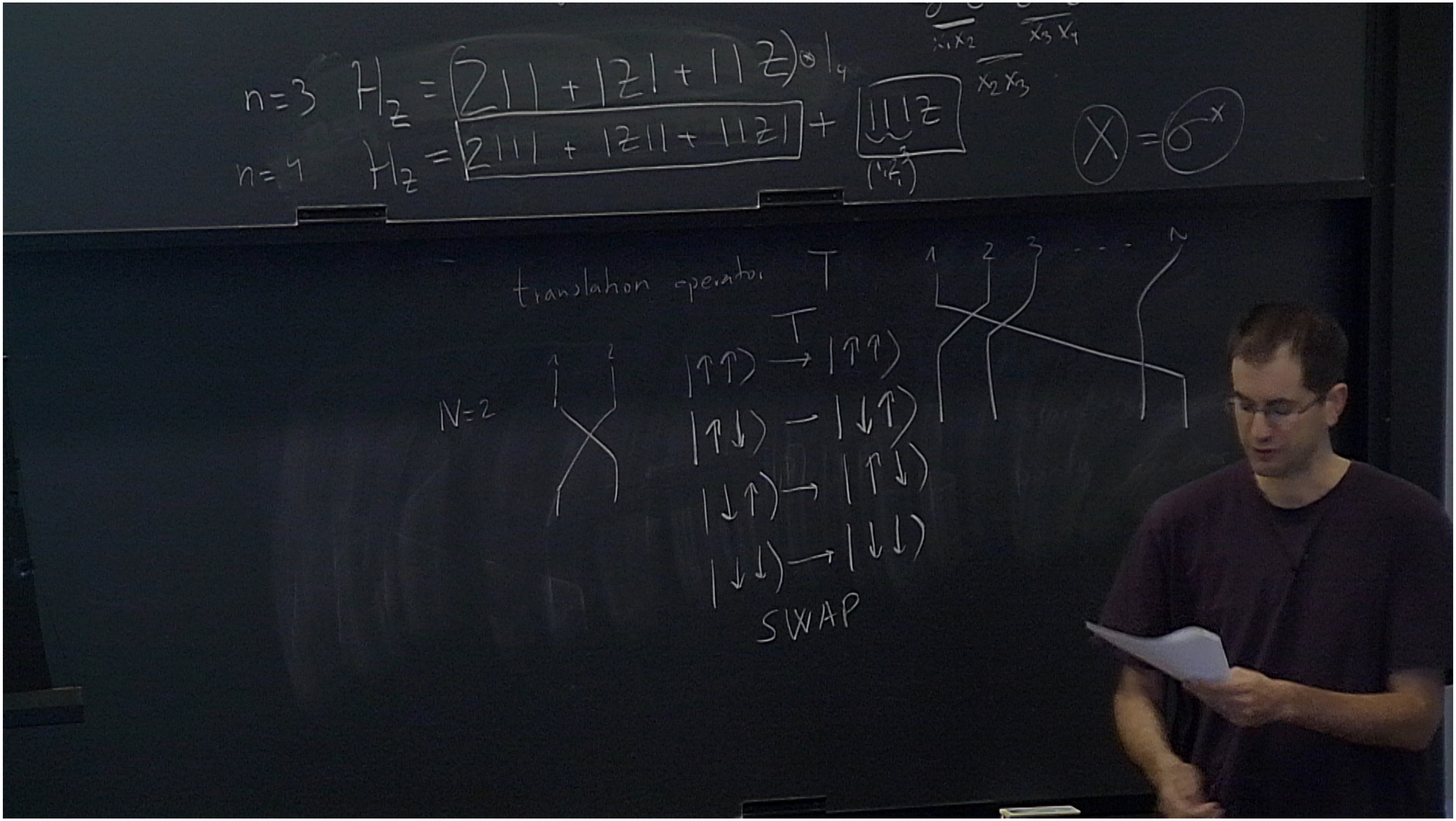
Let us continue:

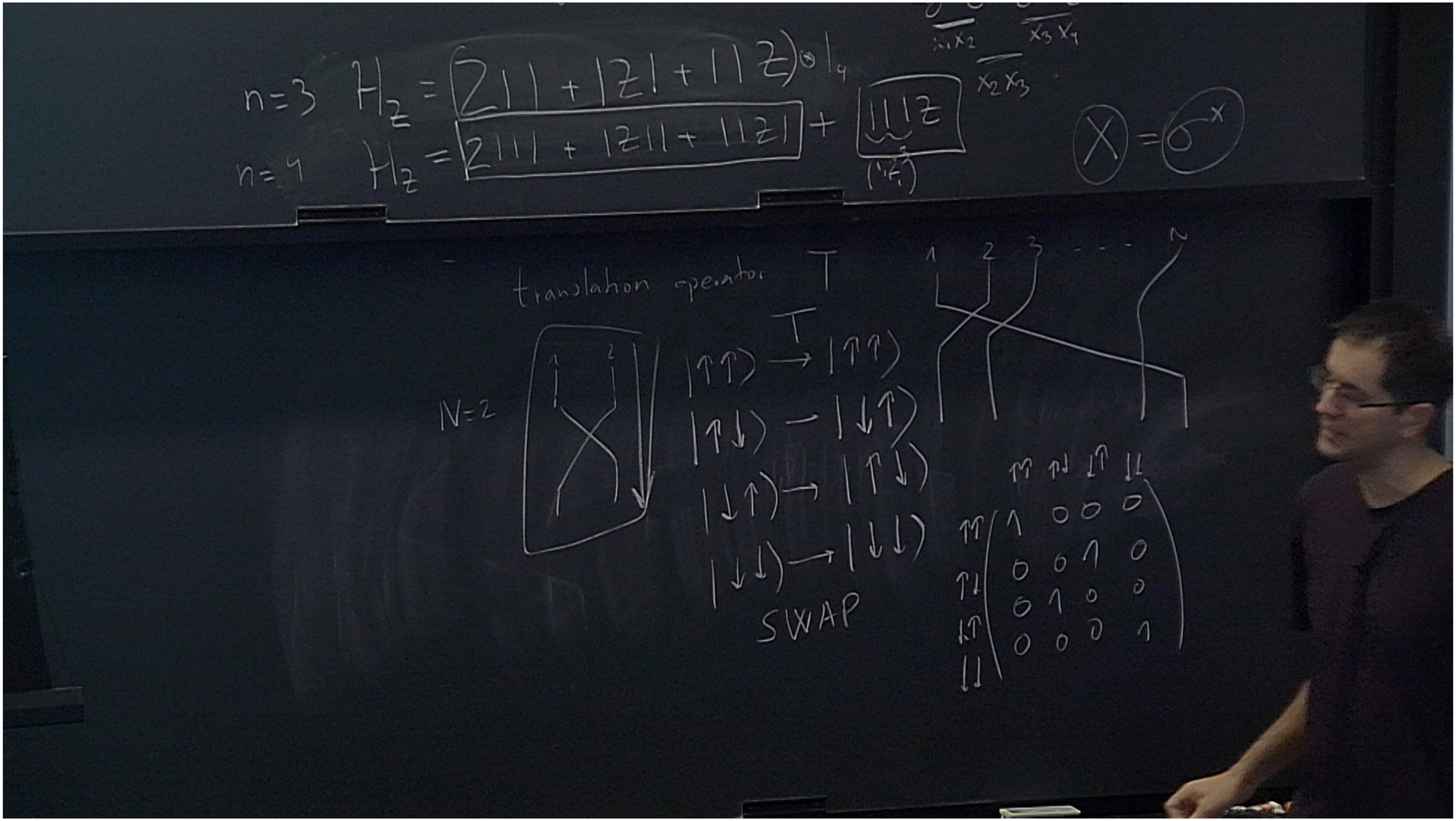
Translation operator T, with $[H,T] = 0$ (translation invariance)

In [43]:
```julia
# Let us quickly rebuild the Hamiltonian for N=3 spins and magnetic field angle t
EE = kron(E,E)
HZ = kron(Z,EE) + kron(E,kron(Z,E)) + kron(EE,Z)
HXX = kron(XX,E)+kron(E,XX)+kron(X,kron(E,X))
H = -(HXX+HZ)/sqrt(2)

# The translation operator T is
SWAP = [1 0 0 0; 0 0 1 0; 0 1 0 0; 0 0 0 1]
N = 3
T = copy(SWAP)
for n=3:N
    SWAPn = kron(diagm(0=>ones(2^(n-2))), SWAP)
    T =  SWAPn*kron(T,E)
end
#display(SWAP)
```


n=3 H_Z = (Z11 + 1Z1 + 11Z) ⊗ 1_4
n=4 H_Z = Z111 + 1Z11 + 11Z1 + 111Z
Today
for arbitrary N
we will build
0 = [H, T] = [H, P] = [T, P]


n=3
n=4
translation operator T
N=2
SWAP


n=3 Hz = (Z11 + 1Z1 + 11Z) ⊗ 1₄
n=4 Hz = Z111 + 1Z11 + 11Z1 + 111Z
X = σ^x
translation operator T
N=2
|↑↑) → |↑↑)
|↑↓) → |↓↑)
|↓↑) → |↑↓)
|↓↓) → |↓↓)
SWAP
1 2 3 . . . N

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Logout

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Run Markdown

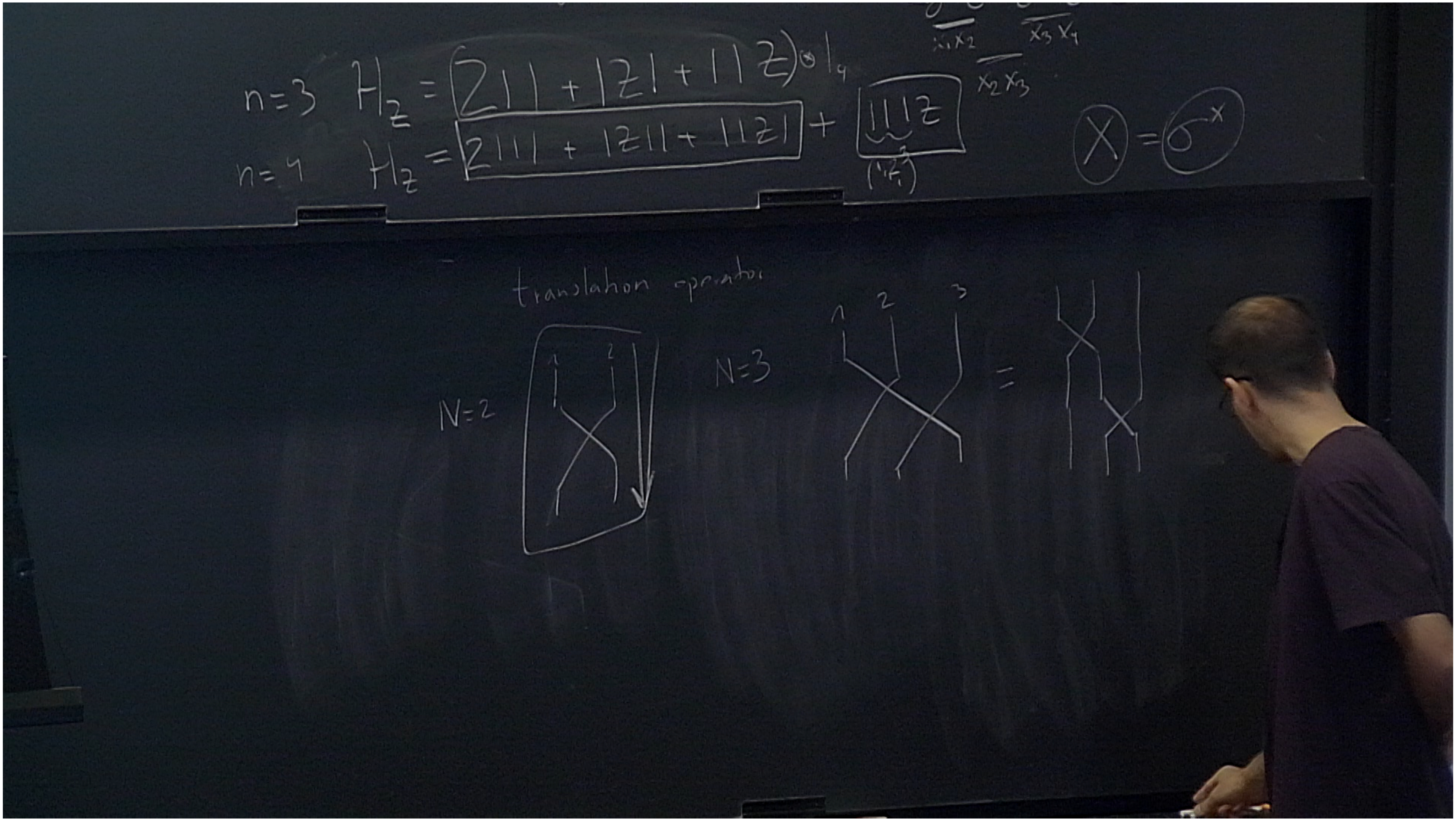
```
end
display(SWAP)
#display(SWAP^2)
#display(T)
#display(T^3)
#display(H3*T-T*H3)
```

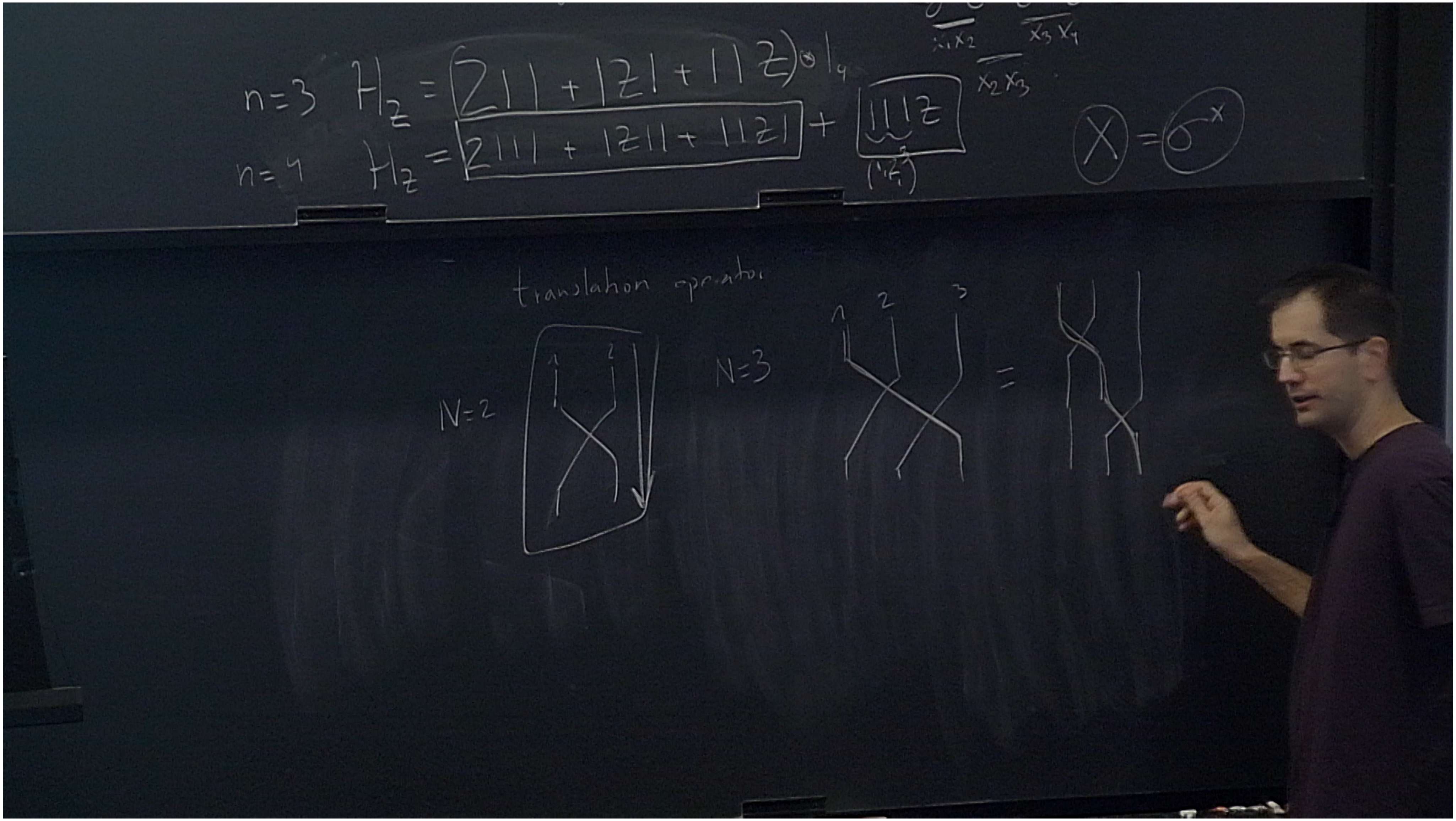
```
4×4 Array{Int64,2}:
 1  0  0  0
 0  0  1  0
 0  1  0  0
 0  0  0  1
```

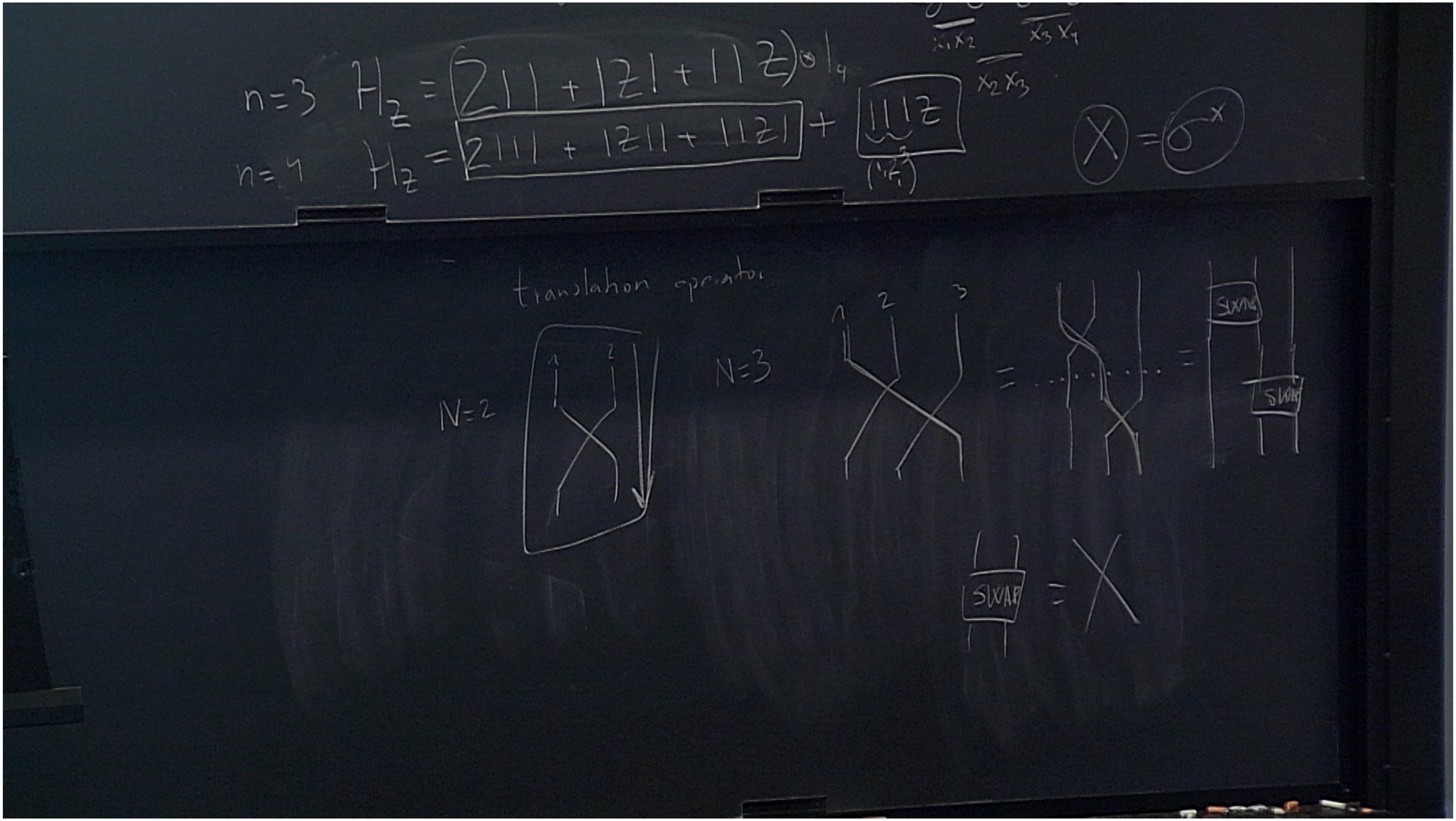
Let us diagonalize H and T simultaneously,

$H|\Psi_i\rangle = e_i|\Psi_i\rangle$ **and** $T|\Psi_i\rangle = \exp(ik_i)|\Psi_i\rangle$

```
In [44]: HT = H + 0.0001*T
```


n=3 $H_Z = (Z11 + 1Z1 + 11Z) \otimes 1_4$
n=4 $H_Z = Z111 + 1Z11 + 11Z1 + 111Z$
$x_1 x_2$
$x_3 x_4$
$x_2 x_3$
X = σ^x
translation operator
N=2
N=3
1 2 3


n=3 Hz = (Z11 + 1Z1 + 11Z) ⊗ 1₄
n=4 Hz = Z111 + 1Z11 + 11Z1 + 111Z
translation operator
N=2
N=3
1 2 3


n=3
n=4
translation operator
N=2
N=3
SWAP
SWAP
SWAP

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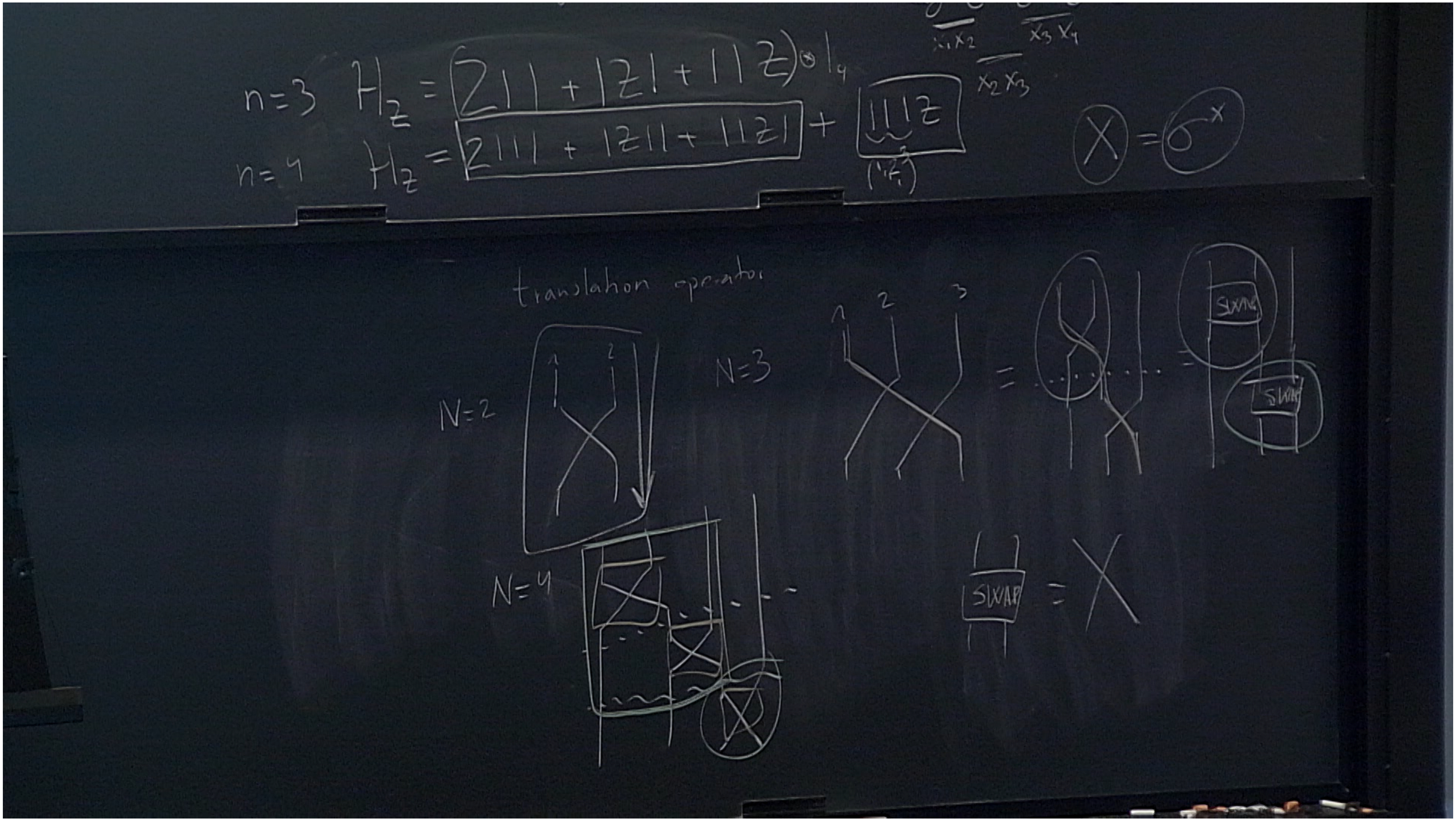
```julia
HZ = kron(Z,EE) + kron(E,kron(Z,E)) + kron(EE,Z)
HXX = kron(XX,E)+kron(E,XX)+kron(X,kron(E,X))
H = -(HXX+HZ)/sqrt(2)

# The translation operator T is
SWAP = [1 0 0 0; 0 0 1 0; 0 1 0 0; 0 0 0 1]
N = 3
T = copy(SWAP)
for n=3:N
    SWAPn = kron(diagm(0=>ones(2^(n-2))), SWAP)
    T =  SWAPn*kron(T,E)
end
display(SWAP)
#display(SWAP^2)
#display(T)
#display(T^3)
#display(H3*T-T*H3)
```

```
4×4 Array{Int64,2}:
 1  0  0  0
 0  0  1  0
```



n=3
n=4
translation operator
N=2
N=3
N=4
SWAP

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```
HZ = kron(Z,EE) + kron(E,kron(Z,E)) + kron(EE,Z)
HXX = kron(XX,E)+kron(E,XX)+kron(X,kron(E,X))
H = -(HXX+HZ)/sqrt(2)

# The translation operator T is
SWAP = [1 0 0 0; 0 0 1 0; 0 1 0 0; 0 0 0 1]
N = 3
T = copy(SWAP)
for n=3:N
    SWAPn = kron(diagm(0=>ones(2^(n-2))), SWAP)
    T =  SWAPn*kron(T,E)
end
display(SWAP)
#display(SWAP^2)
#display(T)
#display(T^3)
#display(H3*T-T*H3)
```

```
4×4 Array{Int64,2}:
 1  0  0  0
 0  0  1  0
```

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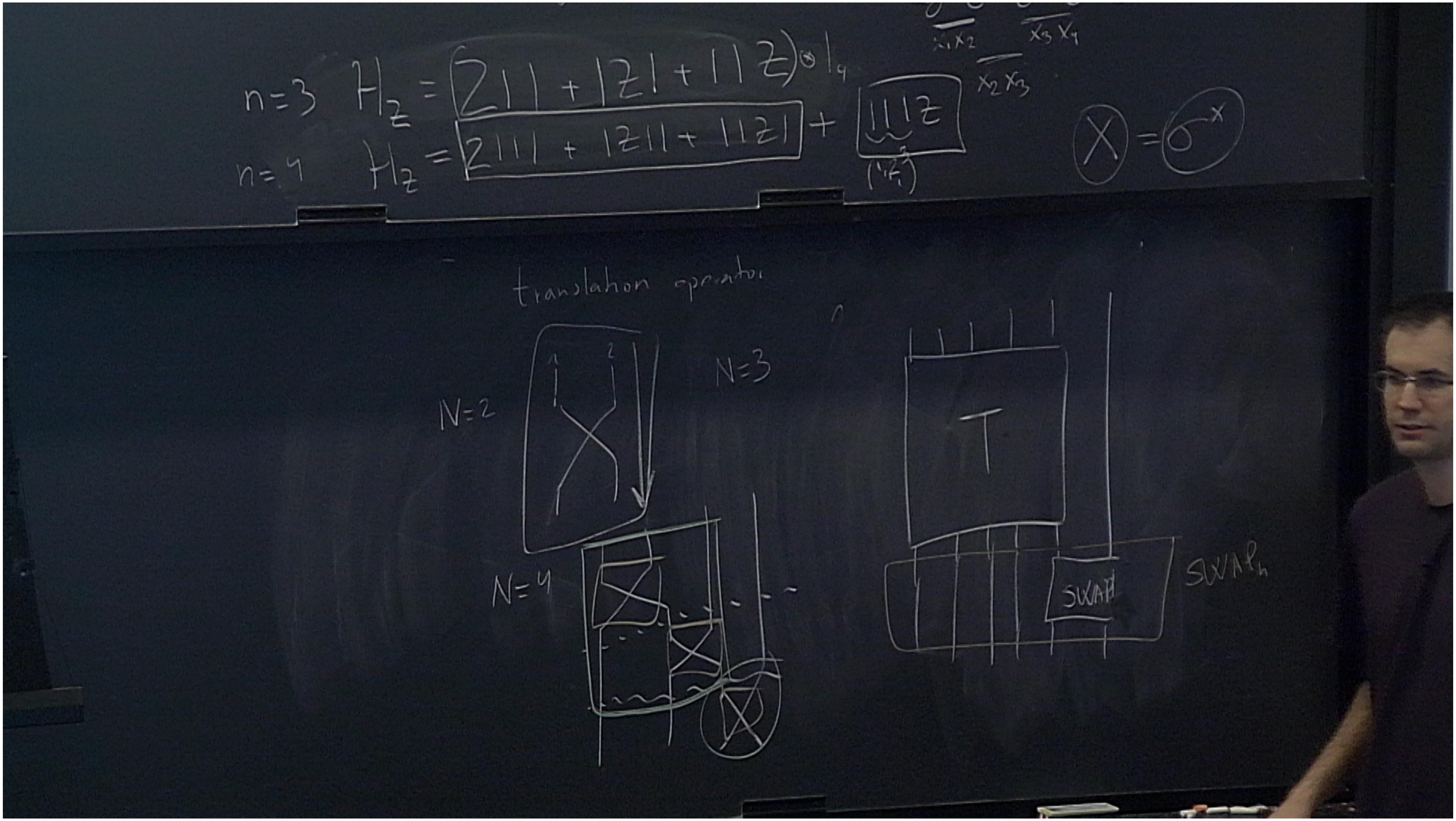
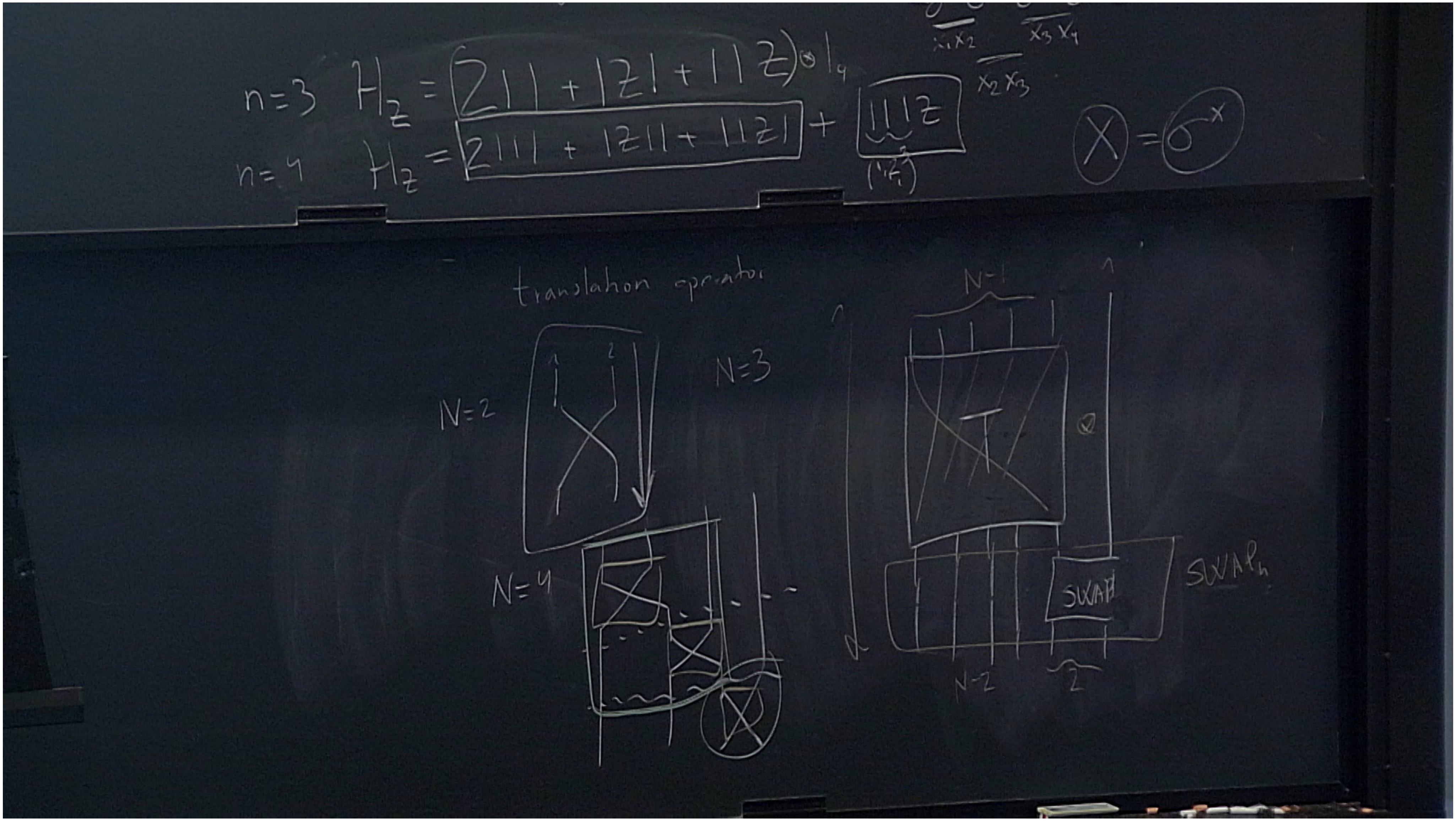
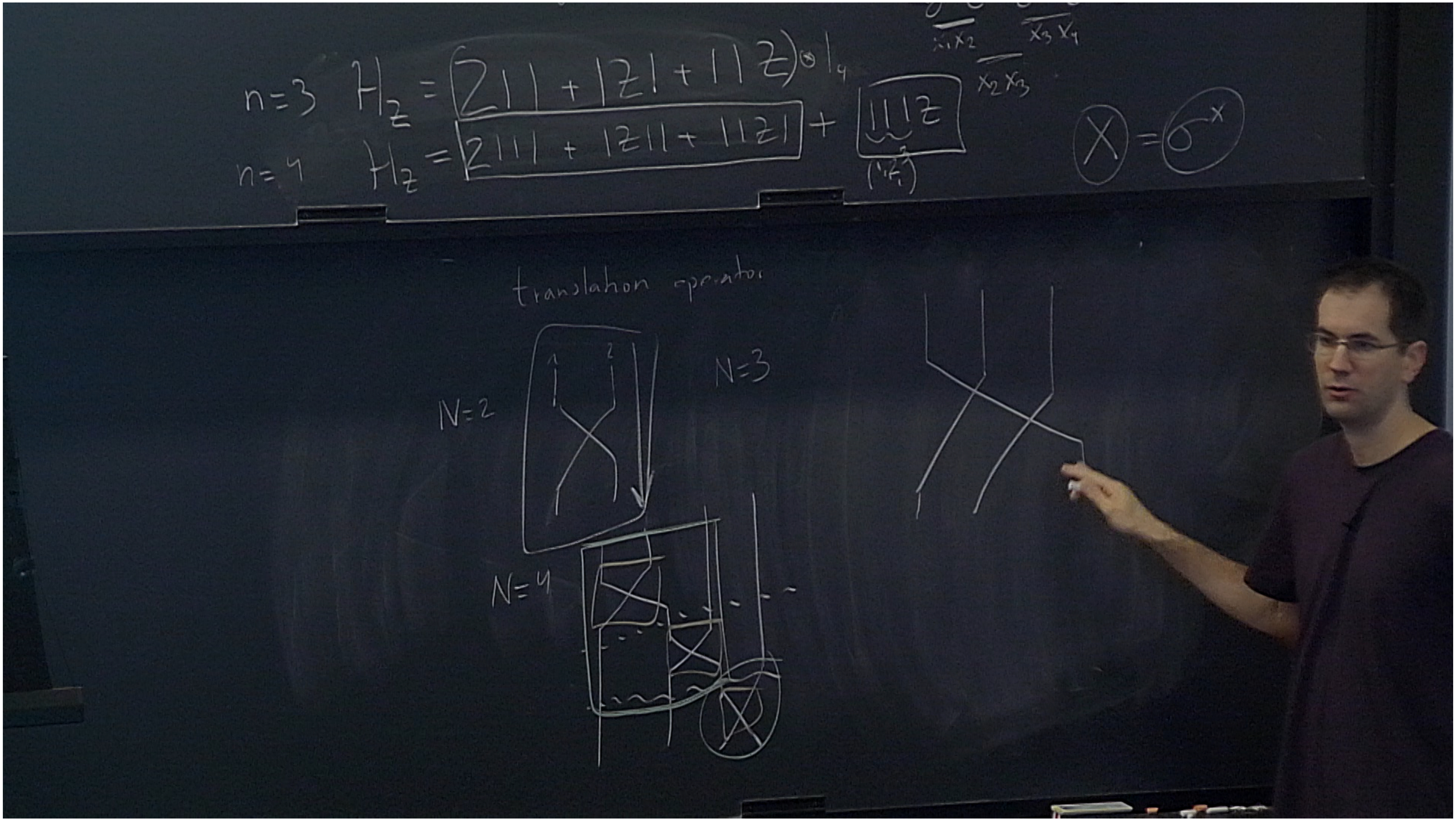
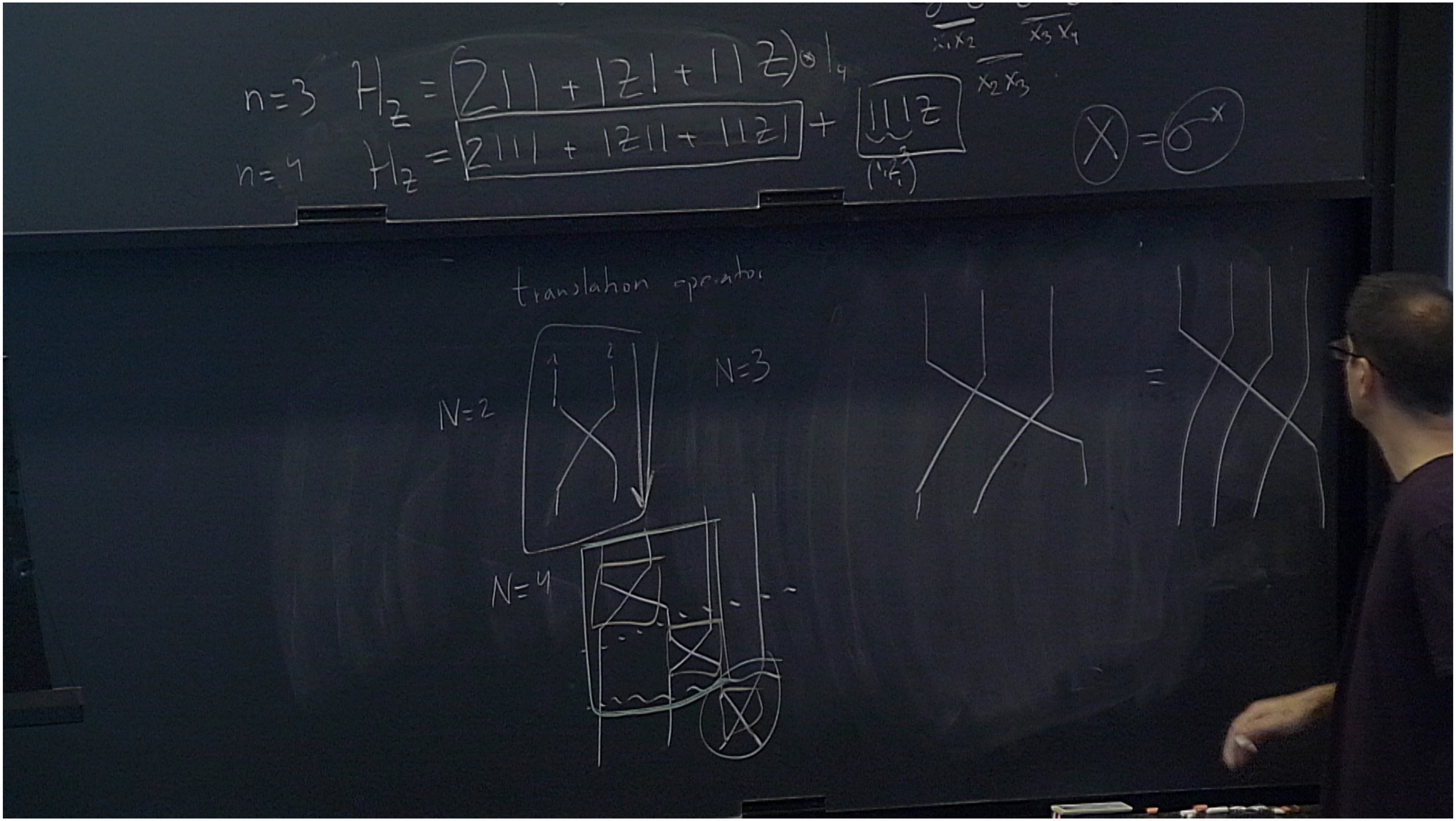
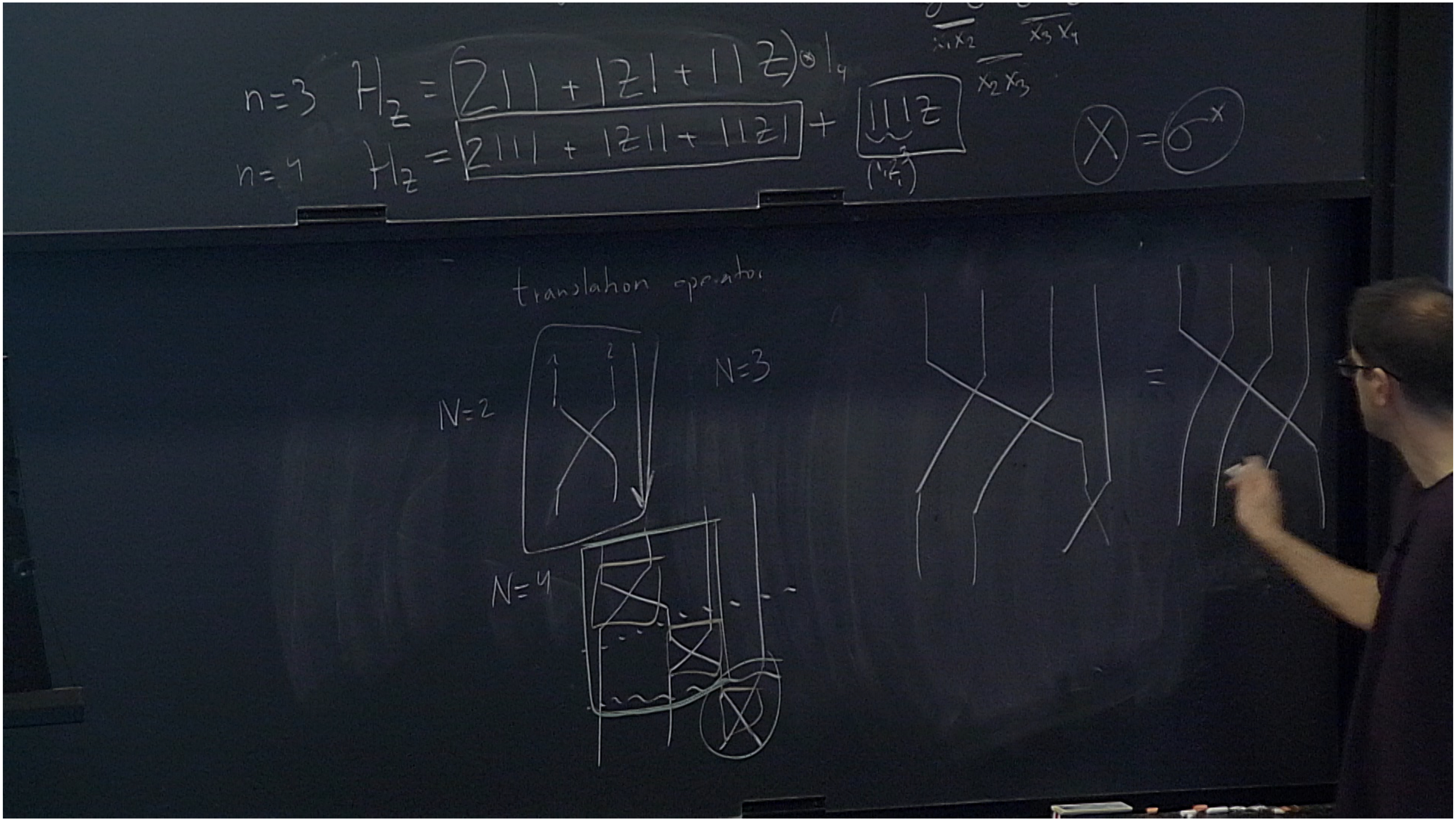

n=3
n=4
translation operator
N=2
N=3
N=4
T
SWAP


n=3 H_Z = (Z11 + 1Z1 + 11Z) ⊗ 1_4
n=4 H_Z = Z111 + 1Z11 + 11Z1 + 111Z
X = σ^x
translation operator
N=2
N=3
N=4
N-1
N-2
SWAP
SWAP_n


n=3 Hz = (Z11 + 1Z1 + 11Z) ⊗ 1₄
n=4 Hz = Z111 + 1Z11 + 11Z1 + 111Z
X = σ^x
translation operator
N=2
N=3
N=4



n=3 Hz = (Z11 + 1Z1 + 11Z) ⊗ 1
n=4 Hz = Z111 + 1Z11 + 11Z1 + 111Z
translation operator
N=2
N=3
N=4


n=3 Hz = (Z11 + 1Z1 + 11Z) ⊗ 1
n=4 Hz = Z111 + 1Z11 + 11Z1 + 111Z
X = σˣ
translation operator
N=2
N=3
N=4

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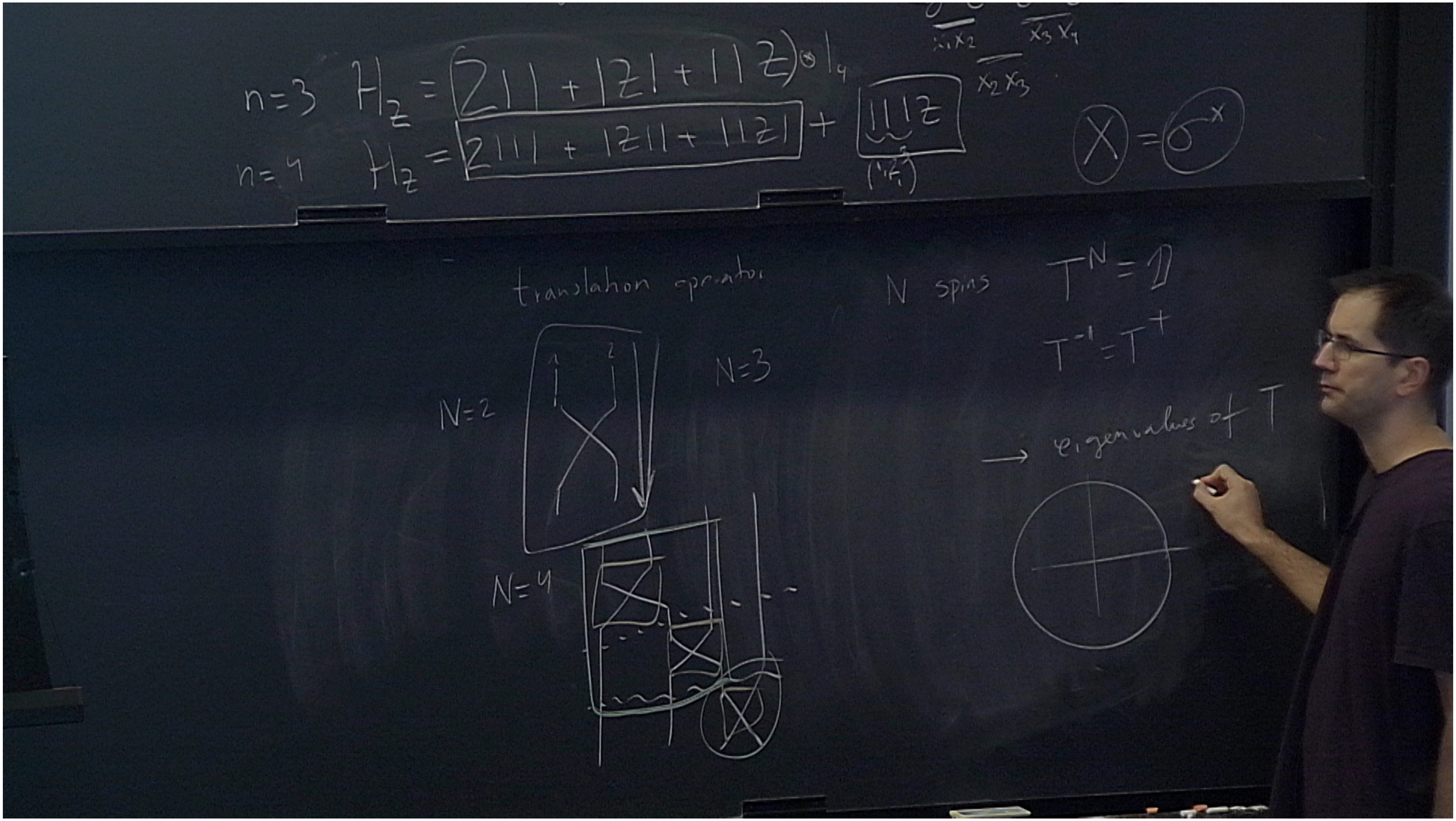
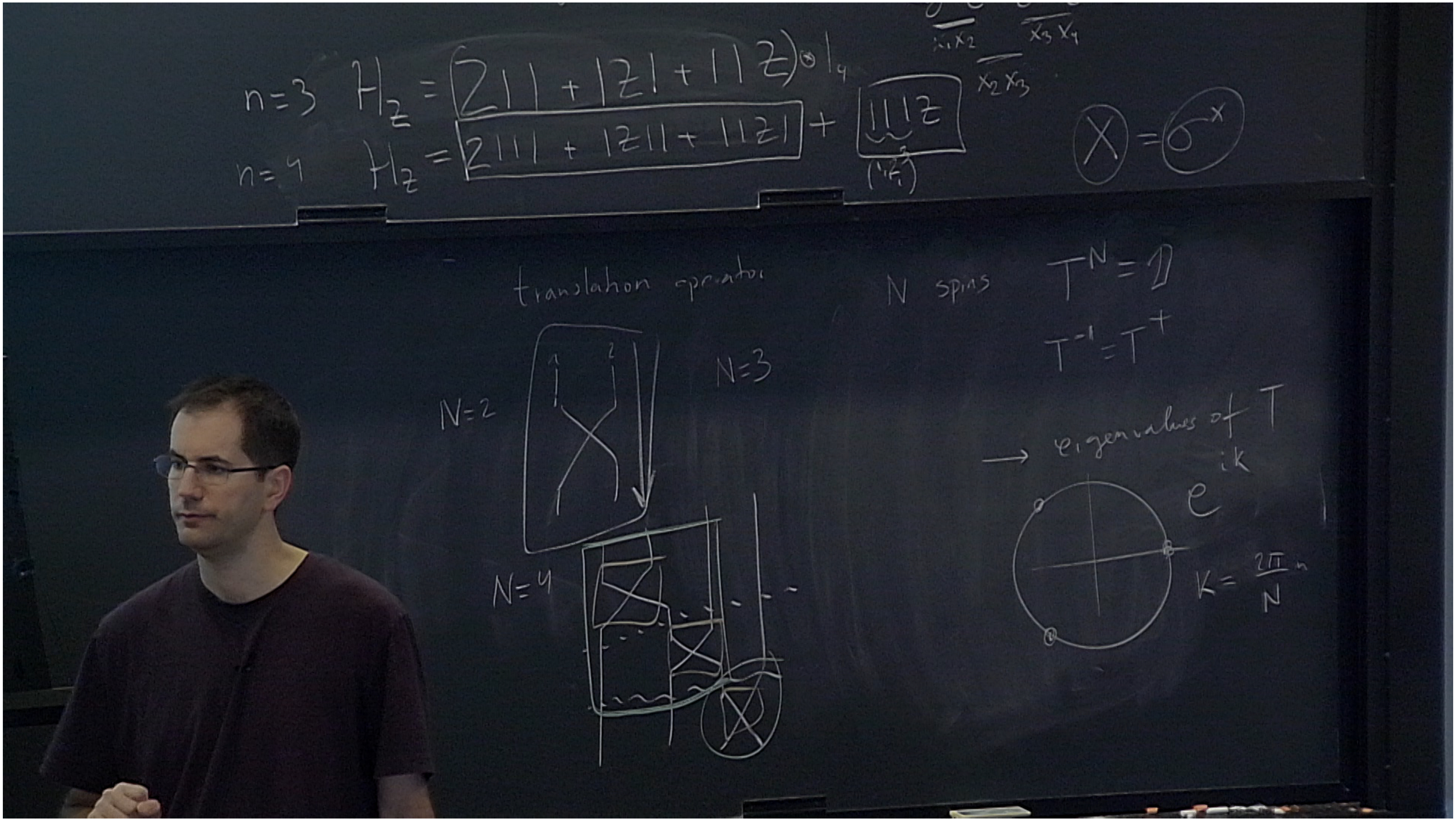
```
display(T^3)
#display(H3*T-T*H3)
```

```
8×8 Array{Float64,2}:
 1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0
 0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0
 0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  1.0  0.0
 0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  1.0

8×8 Array{Float64,2}:
 1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  1.0  0.0
```


n=3 H_Z = (Z11 + 1Z1 + 11Z) ⊗ 1_4
n=4 H_Z = Z111 + 1Z11 + 11Z1 + 111Z
X = σ^x
translation operator
N spins
T^N = 1
T^-1 = T^+
→ eigenvalues of T
N=2
N=3
N=4


n=3 Hz = (Z11 + 1Z1 + 11Z) ⊗ 1_4
n=4 Hz = Z111 + 1Z11 + 11Z1 + 111Z
X = σ^x
translation operator
N spins
T^N = 1
T^-1 = T^+
N=2
N=3
N=4
→ eigenvalues of T
e^ik
K = 2π/N n

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```
    SWAPn = kron(diagm(0=>ones(2^(n-2))), SWAP)
    T =  SWAPn*kron(T,E)
end
#display(SWAP)
#display(SWAP^2)
#display(T)
#display(T^3)
display(H*T-T*H)
```

```
8×8 Array{Float64,2}:
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
```

Let us diagonalize H and T simultaneously

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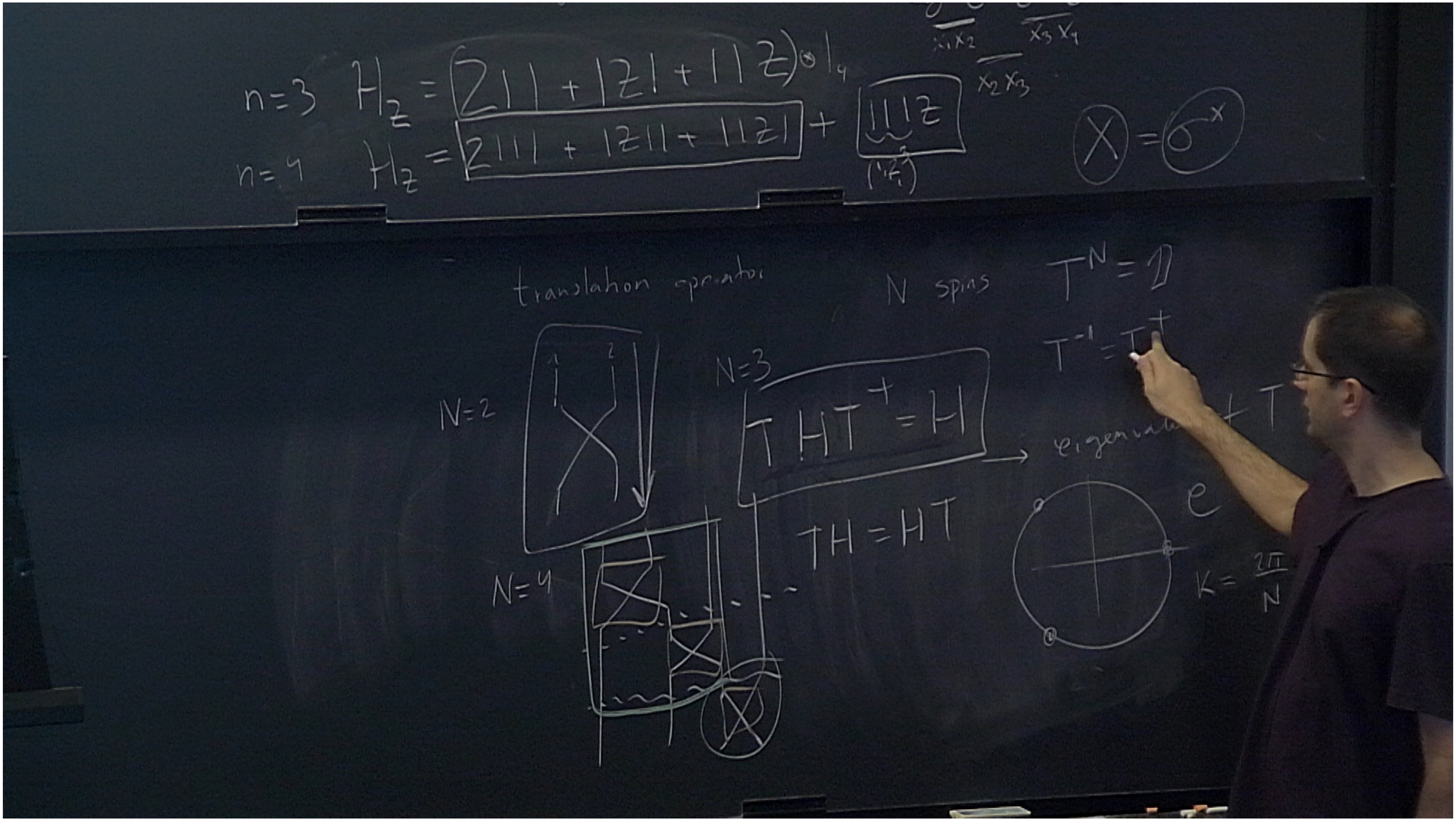
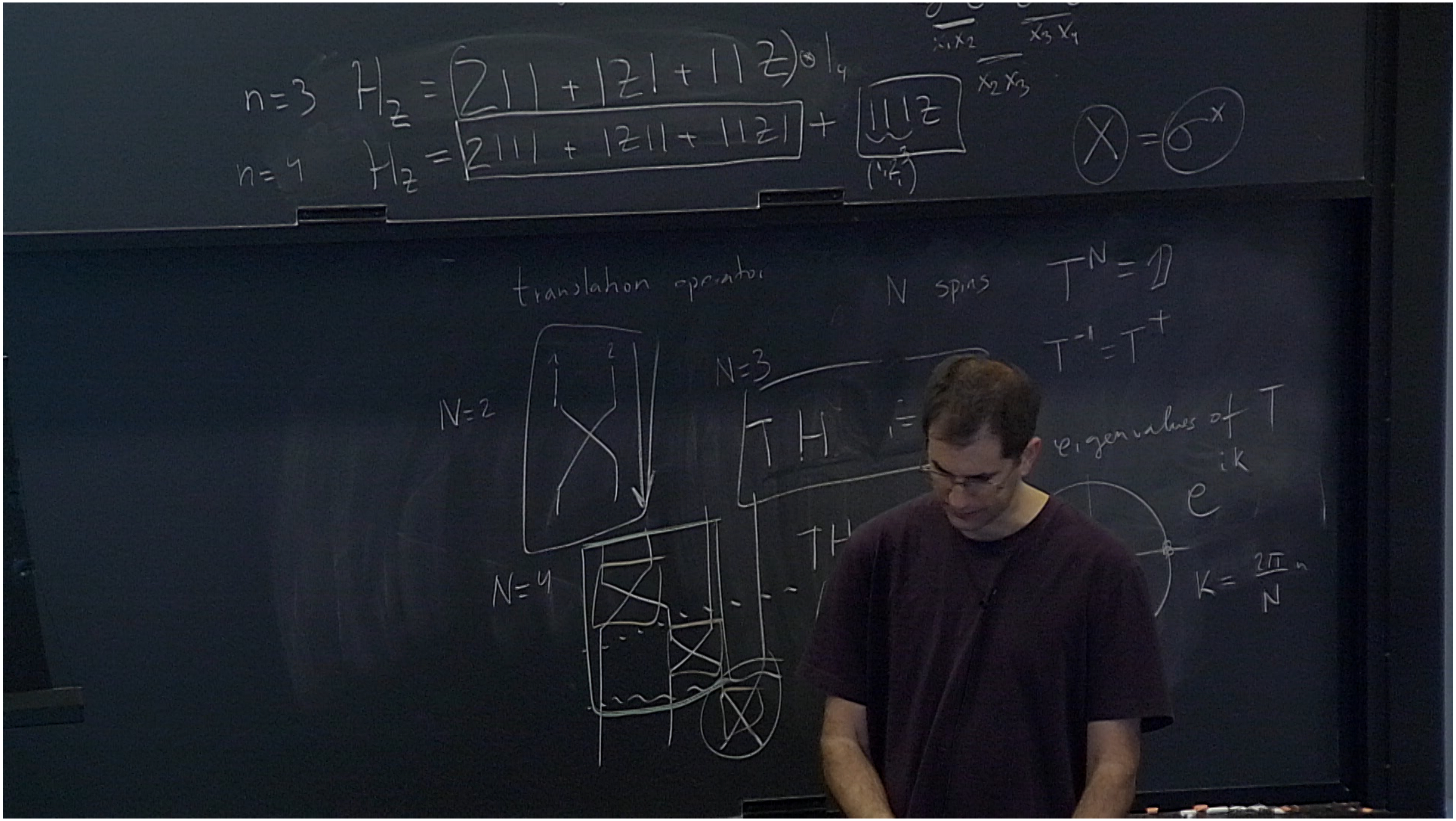

n=3 Hz = (Z11 + 1Z1 + 11Z) ⊗ 1
n=4 Hz = Z111 + 1Z11 + 11Z1 + 111Z
X = σ^x
translation operator
N spins
T^N = 1
T^-1 = T^†
N=2
N=3
THT^† = H
TH = HT
eigenval
N=4
K = 2π/N


n=3 Hz = (Z11 + 1Z1 + 11Z) ⊗ 1
n=4 Hz = Z111 + 1Z11 + 11Z1 + 111Z
X = σ^x
translation operator
N spins T^N = 1
T^-1 = T^†
N=2
N=3
N=4
TH
eigenvalues of T
e^ik
K = 2π/N n

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Let us diagonalize H and T simultaneously,

$$H|\Psi_i\rangle = e_i|\Psi_i\rangle \text{ and } T|\Psi_i\rangle = \exp(ik_i)|\Psi_i\rangle$$

In [44]:
```
HT = H + 0.0001*T
D,U = eigen(HT);
```

Let us compute and plot energies e_i as a function of momenta k_i

In [45]:
```
e = real(diag(U'*H*U))
k = angle.(diag(U'*T*U))

perm = sortperm(e) # re-order eigenvalues according to increasing energies e
e = e[perm]
k = k[perm]
```

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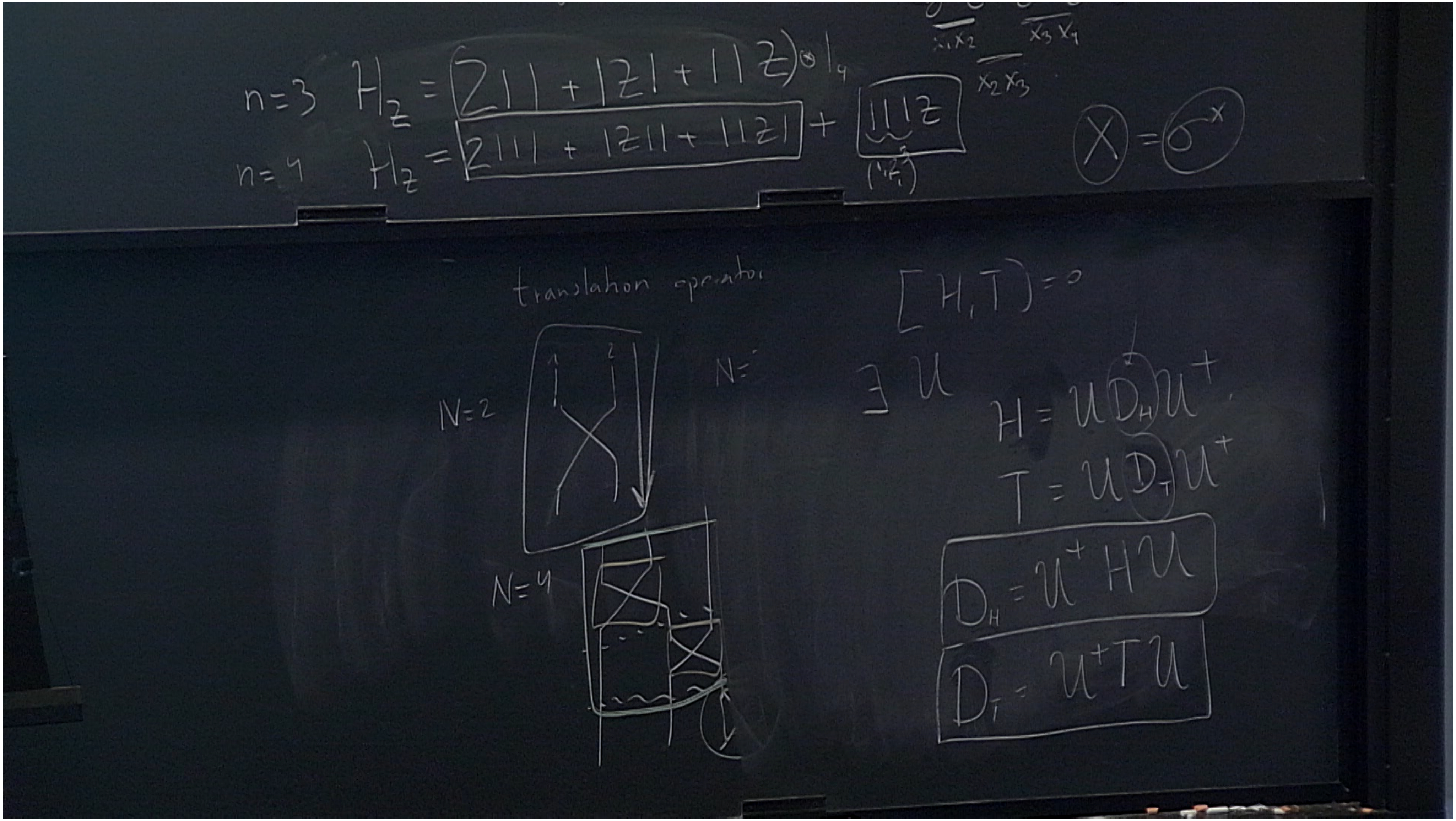
In [13]:
```julia
e = real(diag(U'*H*U))
k = angle.(diag(U'*T*U))

perm = sortperm(e) # re-order eigenvalues according to increasing energies e
e = e[perm]
k = k[perm]

[e k]
```

Out[13]:
```
8×2 Array{Float64,2}:
 -2.82843       0.0
 -2.44949       0.0
  0.0           0.0
  2.34557e-31   2.0944
  2.34557e-31  -2.0944
  1.41421       2.0944
  1.41421      -2.0944
  2.44949       0.0
```


n=3 Hz = (Z11 + 1Z1 + 11Z) ⊗ 1_4
n=4 Hz = Z111 + 1Z11 + 11Z1 + 111Z
x1 x2
x3 x4
x2 x3
X = σ^x
translation operator
[H, T] = 0
∃ U
N=2
N=4
H = U D_H U^+
T = U D_T U^+
D_H = U^+ H U
D_T = U^+ T U

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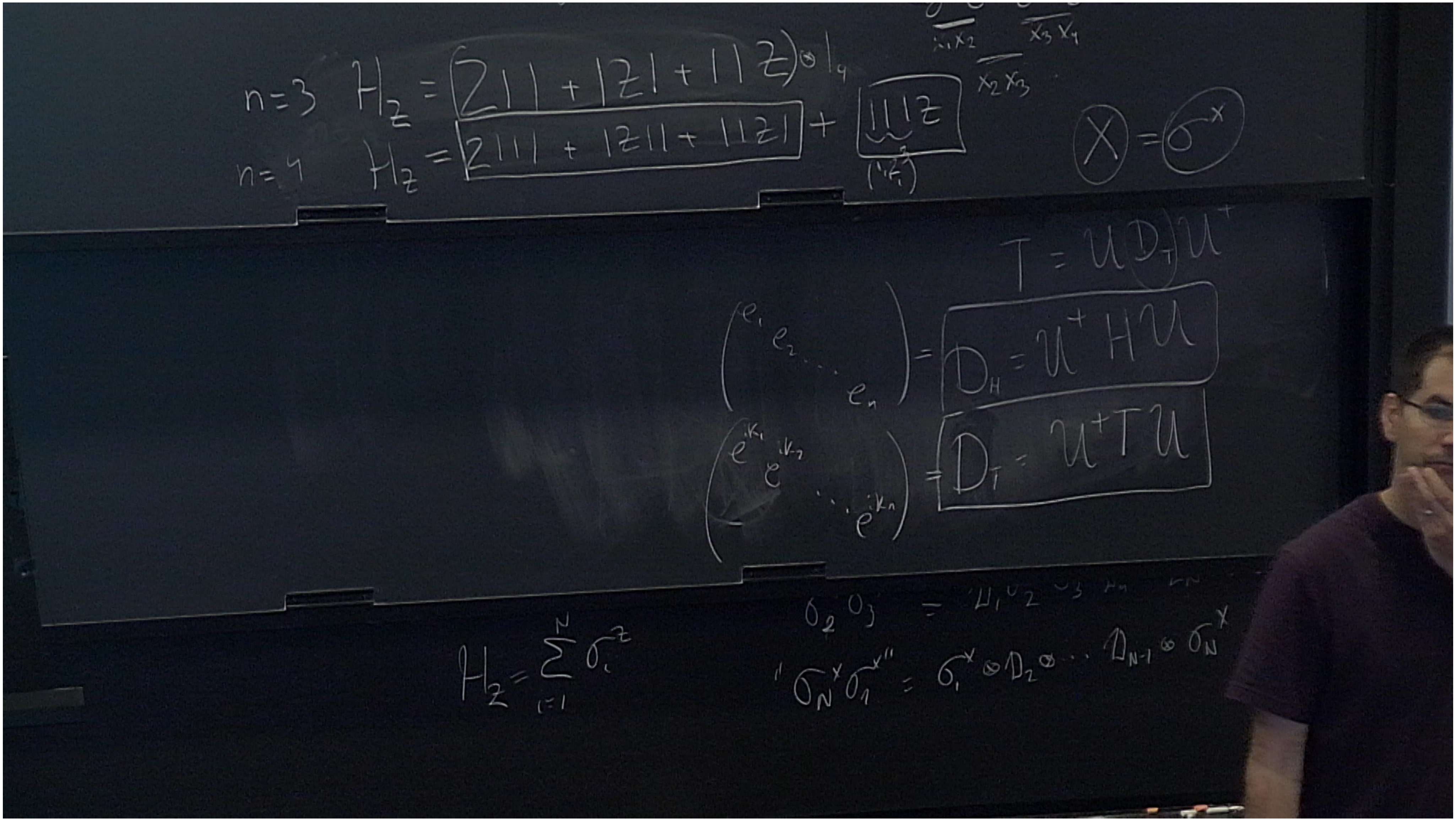
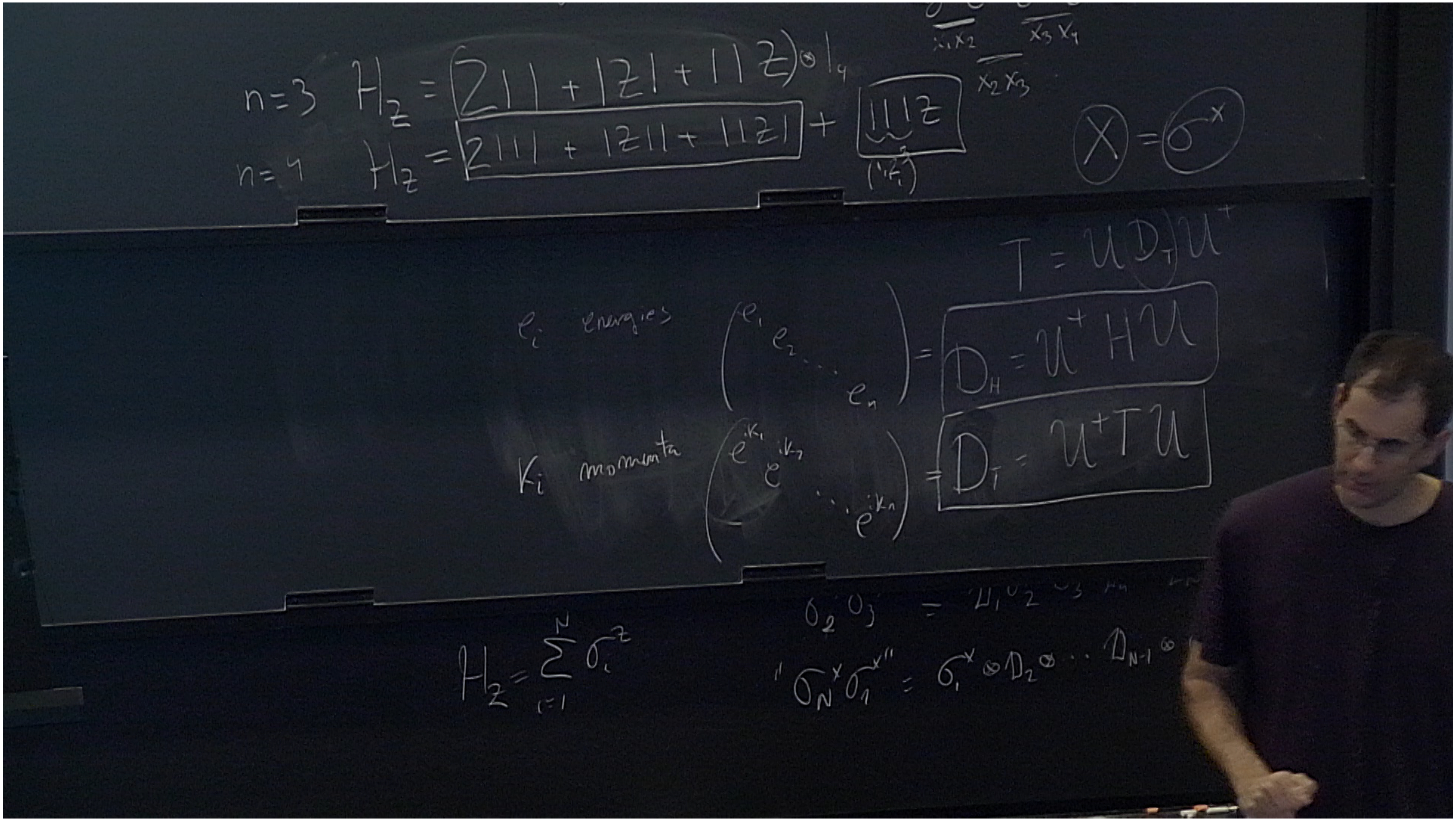
In [13]:

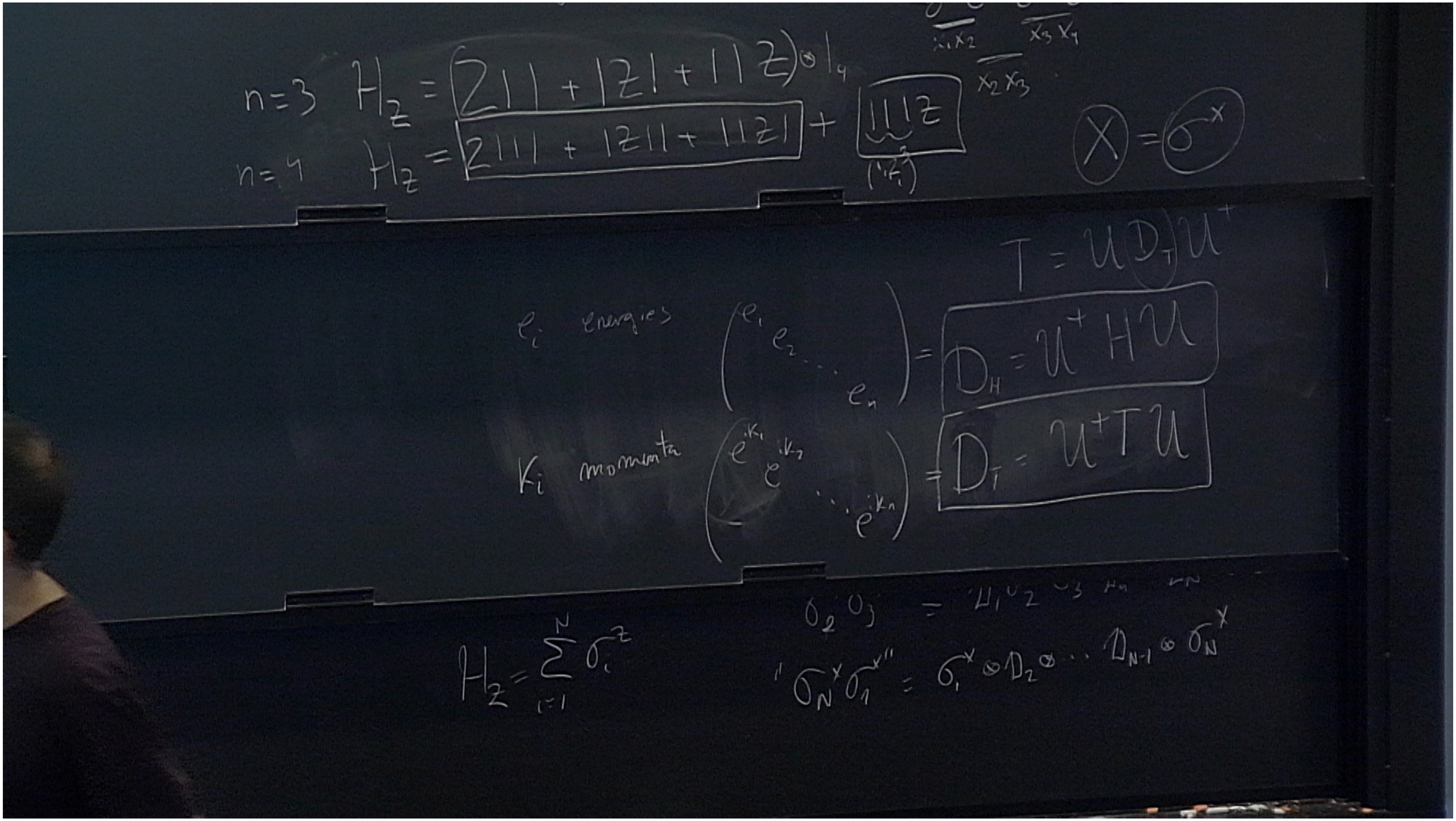
```
e = real(diag(U'*H*U))
k = angle.(diag(U'*T*U))

perm = sortperm(e) # re-order eigenvalues according to increasing energies e
e = e[perm]
k = k[perm]

[e k]
```

Out[13]:

```
8×2 Array{Float64,2}:
 -2.82843       0.0
 -2.44949       0.0
  0.0           0.0
  2.34557e-31   2.0944
  2.34557e-31  -2.0944
  1.41421       2.0944
  1.41421      -2.0944
  2.44949       0.0
```


n=3 H_Z = (Z11 + 1Z1 + 11Z) ⊗ 1_4
n=4 H_Z = Z111 + 1Z11 + 11Z1 + 111Z
X = σ^x
T = U D_T U^†
D_H = U^† H U
D_T = U^† T U
H_Z = Σ_{i=1}^N σ_i^z
"σ_N^x σ_1^x" = σ_1^x ⊗ D_2 ⊗ ... D_{N-1} ⊗ σ_N^x


n=3 Hz = (Z11 + 1Z1 + 11Z) ⊗ 14
n=4 Hz = Z111 + 1Z11 + 11Z1 + 111Z
T = U DT U+
ei energies
DH = U+ H U
Ki momenta
DT = U+ T U
Hz = Σ σiz


n=3 Hz = (Z11 + 1Z1 + 11Z) ⊗ 1_4
n=4 Hz = Z111 + 1Z11 + 11Z1 + 111Z
X = σ^x
T = U D_T U^+
e_i energies
D_H = U^+ H U
k_i momenta
D_T = U^+ T U
Hz = Σ_{i=1}^N σ_i^z
"σ_N^x σ_1^x" = σ_1^x ⊗ D_2 ⊗ ... D_{N-1} ⊗ σ_N^x

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In [13]:

```julia
e = real(diag(U'*H*U))
k = angle.(diag(U'*T*U))

perm = sortperm(e) # re-order eigenvalues according to increasing energies e
e = e[perm]
k = k[perm]

[e k]
```

Out[13]:

```
8×2 Array{Float64,2}:
 -2.82843       0.0
 -2.44949       0.0
  0.0           0.0
  2.34557e-31   2.0944
  2.34557e-31  -2.0944
  1.41421       2.0944
  1.41421      -2.0944
  2.44949       0.0
```

```
In [13]: e = real(diag(U'*H*U))
         k = angle.(diag(U'*T*U))

         perm = sortperm(e) # re-order eigenvalues according to increasing energies e
         e = e[perm]
         k = k[perm]

         [e k]

Out[13]: 8×2 Array{Float64,2}:
          -2.82843       0.0
          -2.44949       0.0
           0.0           0.0
           2.34557e-31   2.0944
           2.34557e-31  -2.0944
           1.41421       2.0944
           1.41421      -2.0944
           2.44949       0.0
```

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```
e = e[perm]
k = k[perm]

[e k]
perm
```

Out[15]:

```
8-element Array{Int64,1}:
 1
 3
 2
 5
 6
 7
 8
 4
```

In [46]:

```
figure("low_energies",figsize=(8,3))

grid("on") # Create a grid on the axis
title("low energies spin chain")
```

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Run Code

```
[e k]
```

Out[16]:
```
8×2 Array{Float64,2}:
 -2.82843       0.0
 -2.44949       0.0
  0.0           0.0
  2.34557e-31   2.0944
  2.34557e-31  -2.0944
  1.41421       2.0944
  1.41421      -2.0944
  2.44949       0.0
```

In [46]:
```
figure("low_energies",figsize=(8,3))

grid("on") # Create a grid on the axis
title("low energies spin chain")
#ax = gca()
#ax[:set_xlim]([-3,3])
#ax[:set_ylim]([-0.2,2.8])
```

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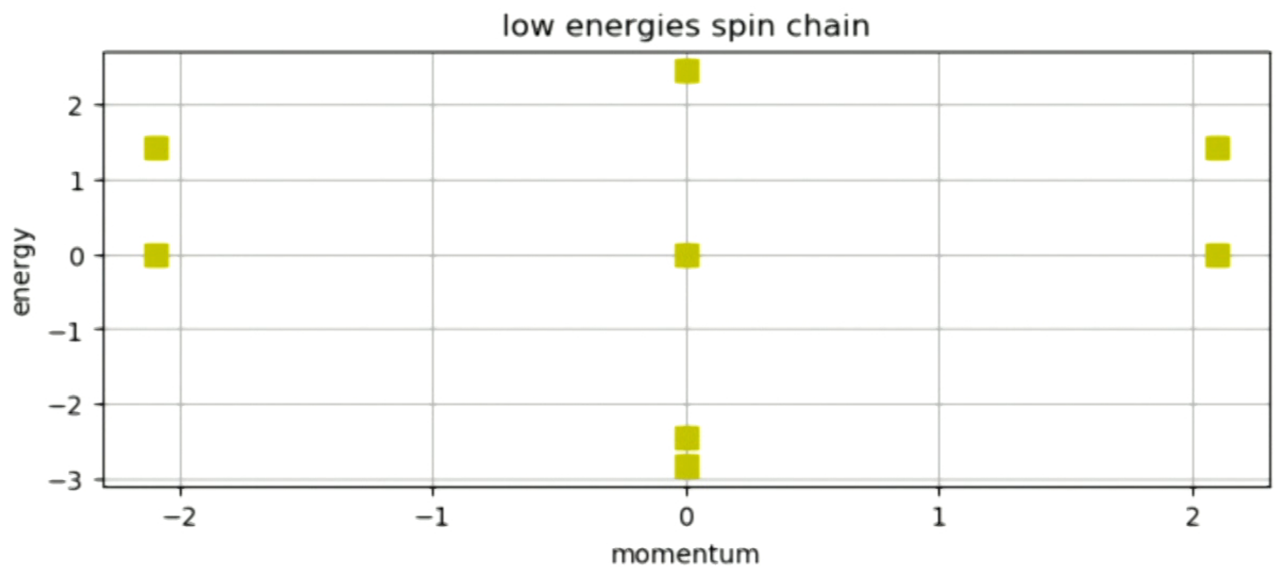
```
    plot(k[i],e[i], marker = "s", markersize = 8, color = "y")
end
```



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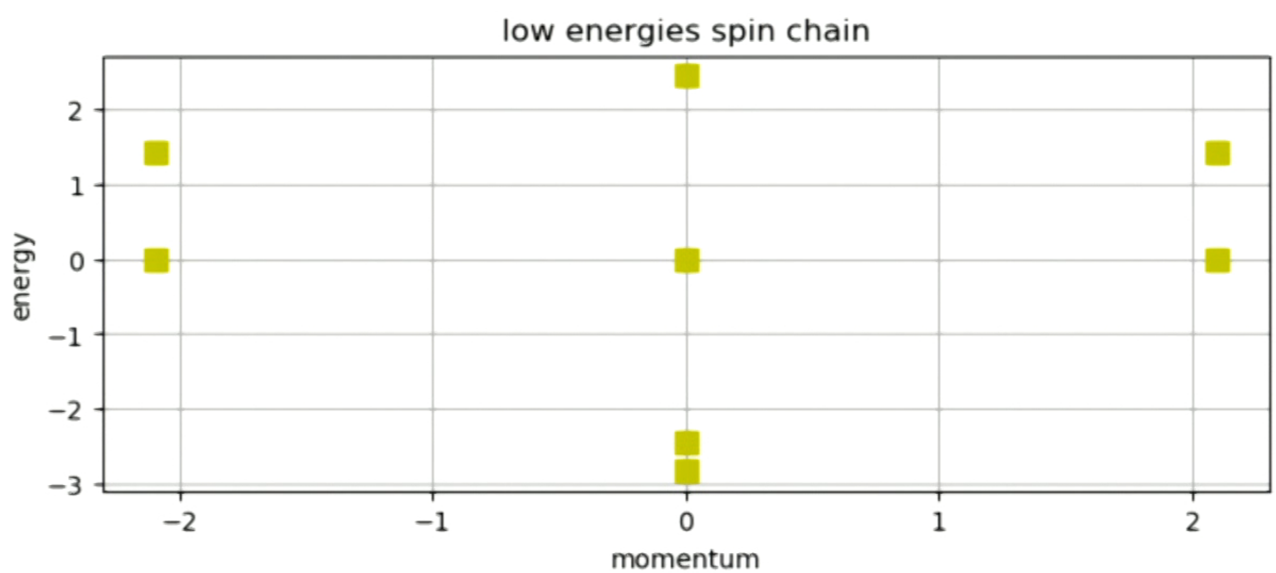
```
    plot(k[i],e[i], marker = "s", markersize = 8, color = "y")
end
```



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```
[e k]
```

```
8-element Array{Complex{Float64},1}:
   -2.8284271247461885 + 0.0im
                   0.0 + 0.0im
    -2.449489742783178 + 0.0im
    2.4494897427831788 + 0.0im
  2.345571399448979e-31 + 3.799215150296093 5e-33im
  2.345571399448979e-31 - 3.7992151502960935e-33im
     1.414213562373095 + 8.338914357139747e-18im
     1.414213562373095 - 8.338914357139747e-18im
```

Out[18]:
```
8×2 Array{Float64,2}:
 -2.82843       0.0
 -2.44949       0.0
  0.0           0.0
  2.34557e-31   2.0944
  2.34557e-31  -2.0944
  1.41421       2.0944
  1.41421      -2.0944
```

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In [12]:
```julia
HT = H + 0.0001*T
D,U = eigen(HT);
```

Let us compute and plot energies e_i as a function of momenta k_i

In [18]:
```julia
display(diag(U'*H*U))
e = real(diag(U'*H*U))
k = angle.(diag(U'*T*U))

perm = sortperm(e) # re-order eigenvalues according to increasing energies e
e = e[perm]
k = k[perm]

[e k]
```

```
8-element Array{Complex{Float64},1}:
  2.8284271247461885 + 0.0im
```

jupyter 2018-computational-physics-course-ExactDiag2-co... (autosaved)

```
In [12]: HT = H + 0.0001*T
         D,U = eigen(HT);
```

Let us compute and plot energies e_i as a function of momenta k_i

```
In [18]:
         e = real(diag(U'*H*U))
         k = angle.(diag(U'*T*U))

         perm = sortperm(e) # re-order eigenvalues according to increasing energies e
         e = e[perm]
         k = k[perm]

         [e k]
```

```
8-element Array{Complex{Float64},1}:
 -2.8284271247461885 + 0.0im
```

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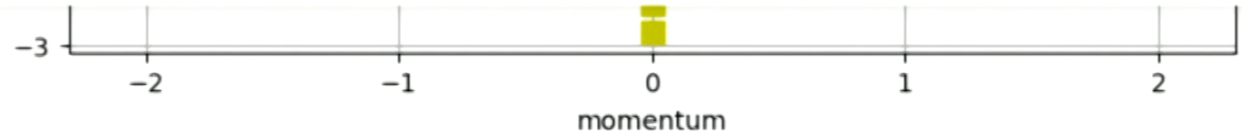
```
In [19]: HT = H + 0.0001*T
         D,U = eigen(HT);
         D
```

```
Out[19]: 8-element Array{Complex{Float64},1}:
             -2.8283271247461896 + 0.0im
            9.999999999987796e-5 + 0.0im
             -2.4493897427831772 + 0.0im
              2.4495897427831794 + 0.0im
          -4.9999999999968974e-5 + 8.66025403783867e-5im
          -4.9999999999968974e-5 - 8.66025403783867e-5im
              1.4141635623730955 + 8.660254037823334e-5im
              1.4141635623730955 - 8.660254037823334e-5im
```

Let us compute and plot energies e_i as a function of momenta k_i

```
In [18]: e = real(diag(U'*H*U))
         k = angle.(diag(U'*T*U))
```



It's your turn again! (2/3)

3) write a function buildT that builds the translation operator T for N spins (use only for $N \leq 10$)

In [9]:
```
# function buildT takes as input N (number of spins) and outputs T (translatio op
function buildT(N::Int64)::Array{Float64,2}
    SWAP = [1 0 0 0; 0 0 1 0; 0 1 0 0; 0 0 0 1]
    E = diagm(0=>ones(2))
    T = copy(SWAP)
    for n=3:N
        SWAPn = kron(diagm(0=>ones(2^(n-2))), SWAP)
        T = SWAPn*kron(T,E)
```

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```
0.0  0.0  0.0  0.0  0.0  0.0  0.0  1.0
```

4) compute and plot energies e_i as a function of momenta k_i for $N = 8$ spins and $\theta = \pi/4$

In [10]:
```
N=8
H = buildH(N,pi/4)
T = buildT(N)
HT = H + 0.0001*T
D,U = eigen(HT);
```

In [13]:
```
e = real(diag(U'*H*U))
k = angle.(diag(U'*T*U))

perm = sortperm(e) # re-order eigenvalues according to increasing energies e
e = e[perm]
k = k[perm]
[e k];
```

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```
end

buildT(3) # test for N=3 and critical angle pi/4
```

Out[9]:

```
8×8 Array{Float64,2}:
 1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0
 0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0
 0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  1.0  0.0
 0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  1.0
```

4) compute and plot energies e_i as a function of momenta k_i for $N = 8$ spins and $\theta = \pi/4$

In [10]:

```
N=8
H = buildH(N,pi/4)
```

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Run Markdown

spins (use only for $N \le 10$)

In [20]:

```julia
# function buildT takes as input N (number of spins) and outputs T (translatio op
function buildT(N::Int64)::Array{Float64,2}
    SWAP = [1 0 0 0; 0 0 1 0; 0 1 0 0; 0 0 0 1]
    E = diagm(0=>ones(2))
    T = copy(SWAP)
    for n=3:N
        SWAPn = kron(diagm(0=>ones(2^(n-2))), SWAP)
        T =  SWAPn*kron(T,E)
    end
    return T
end

buildT(3) # test for N=3 and critical angle pi/4
```

Out[20]:

```
8×8 Array{Float64,2}:
 1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0
 0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0
```

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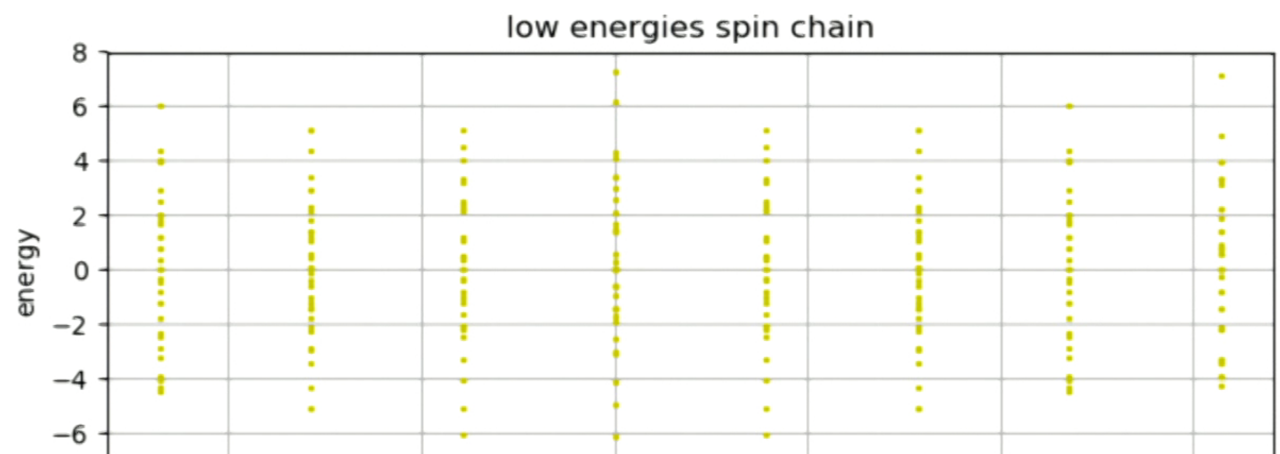
```
#ax = gca()
#ax[:set_xlim]([-3,3])
#ax[:set_ylim]([-0.2,2.8])
xlabel("momentum")
ylabel("energy")
for i in 1:size(e,1)
    plot(k[i],e[i], marker = "s", markersize = 2, color = "y")
end
```



Let us continue:

We add the parity operator P, with $[H, P] = [T, P] = 0$ (parity conservation)

In [23]:
```
# Let us quickly rebuild the Hamiltonian for N=3 spins and magnetic field angle t
EE = kron(E,E)
HZ = kron(Z,EE) + kron(E,kron(Z,E)) + kron(EE,Z)
HXX = kron(XX,E)+kron(E,XX)+kron(X,kron(E,X))
H = -(HXX+HZ)/sqrt(2)
# ...and the translation operator for N=3
T = kron(E,SWAP)*kron(SWAP,E)

# The parity operator P is
Z = [1 0; 0 -1]
N=3
P = copy(Z)
```

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```
display(P)
#display(P^2)
#display(norm(H3*P-P*H3))
#display(norm(T*P-P*T))
```

```
8×8 Array{Int64,2}:
 1   0   0  0   0  0  0   0
 0  -1   0  0   0  0  0   0
 0   0  -1  0   0  0  0   0
 0   0   0  1   0  0  0   0
 0   0   0  0  -1  0  0   0
 0   0   0  0   0  1  0   0
 0   0   0  0   0  0  1   0
 0   0   0  0   0  0  0  -1
```

Let us diagonalize H, T, and P simultaneously,

$H|\Psi_i\rangle = e_i|\Psi_i\rangle$, $T|\Psi_i\rangle = \exp(ik_i)|\Psi_i\rangle$, **and** $Z|\Psi_i\rangle = (-1)^p|\Psi_i\rangle$

```
0   0   0  0   0  0  0  -1
```

Let us diagonalize H, T, and P simultaneously,

$$H|\Psi_i\rangle = e_i|\Psi_i\rangle, \quad T|\Psi_i\rangle = \exp(ik_i)|\Psi_i\rangle, \text{ and } \quad Z|\Psi_i\rangle = (-1)^p|\Psi_i\rangle$$

In [48]:
```
HTP = H + 0.0001*T + im*0.01*P
D,U = eigen(HTP)
```

Out[48]:
```
Eigen{Complex{Float64},Complex{Float64},Array{Complex{Float64},2},Array{Complex
{Float64},1}}
eigenvalues:
8-element Array{Complex{Float64},1}:
      -2.82832712474619 + 0.01im
   9.999999999990363e-5 + 0.010000000000000002im
     -2.4493897427831812 - 0.009999999999999998im
      2.4495897427831794 - 0.01im
  -4.999999999980888e-5 - 0.010086602540378445im
```

localhost:8888/notebooks/Documents/2018juliacourse/Guifre/2018-computational-physics-course-ExactDiag2-complete.ipynb

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Let us compute and plot energies e_i, momenta k_i, and parity p_i

In [50]:

```
e = real(diag(U'*H*U))
k = angle.(diag(U'*T*U))
p = real(diag(U'*P*U))
p = round.((1 .- p)/2)
perm = sortperm(e) # re-order eigenvalues according to E
e = e[perm]
k = k[perm]
p = p[perm]
[e k p]
```

Out[50]:

```
8×3 Array{Float64,2}:
 -2.82843        0.0          0.0
 -2.44949        0.0          1.0
 -1.13883e-31    2.0944       1.0
 -5.54732e-32    0.0          0.0
```

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Let us compute and plot energies e_i, momenta k_i, and parity p_i

In [50]:

```
e = real(diag(U'*H*U))
k = angle.(diag(U'*T*U))
p = real(diag(U'*P*U))
p = round.((1 .- p)/2)
perm = sortperm(e) # re-order eigenvalues according to E
e = e[perm]
k = k[perm]
p = p[perm]
[e k p]
```

Out[50]:

```
8×3 Array{Float64,2}:
 -2.82843      0.0       0.0
 -2.44949      0.0       1.0
 -1.13883e-31  2.0944    1.0
 -5.54732e-32  0.0       0.0
```

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```
DimensionMismatch("matrix A has dimensions (256,256), matrix B has dimensions (8,8)")

Stacktrace:
 [1] _generic_matmatmul!(::Array{Complex{Float64},2}, ::Char, ::Char, ::Array{Complex{Float64},2}, ::Array{Float64,2}) at C:\cygwin\home\Administrator\buildbot\worker\package_win64\build\usr\share\julia\stdlib\v1.0\LinearAlgebra\src\matmul.jl:588
 [2] generic_matmatmul!(::Array{Complex{Float64},2}, ::Char, ::Char, ::Array{Complex{Float64},2}, ::Array{Float64,2}) at C:\cygwin\home\Administrator\buildbot\worker\package_win64\build\usr\share\julia\stdlib\v1.0\LinearAlgebra\src\matmul.jl:578
 [3] mul! at C:\cygwin\home\Administrator\buildbot\worker\package_win64\build\usr\share\julia\stdlib\v1.0\LinearAlgebra\src\matmul.jl:290 [inlined]
 [4] * at C:\cygwin\home\Administrator\buildbot\worker\package_win64\build\usr\share\julia\stdlib\v1.0\LinearAlgebra\src\matmul.jl:141 [inlined]
 [5] *(::Adjoint{Complex{Float64},Array{Complex{Float64},2}}, ::Array{Float64,2}, ::Array{Complex{Float64},2}) at .\operators.jl:502
 [6] top-level scope at In[28]:1
```

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```
Out[31]: 8×3 Array{Float64,2}:
 -2.82843       0.0           0.0
 -2.44949       0.0           1.0
 -1.13883e-31   2.0944        1.0
 -5.54732e-32   0.0           0.0
 -4.32111e-32  -2.0944        1.0
  1.41421       2.0944        0.0
  1.41421      -2.0944       -0.0
  2.44949      -3.85186e-32   1.0
```

```
In [56]: figure("low_energies",figsize=(8,3))

subplot(121) # Create the 1st axis of a 2x2 arrax of axes
grid("on") # Create a grid on the axis
title("Even Parity, p=0")
xlabel("momentum")
ylabel("energy")

subplot(122) # Create the 1st axis of a 2x2 arrax of axes
grid("on") # Create a grid on the axis
title("Even Parity, p=1")
```

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```julia
subplot(121) # Create the 1st axis of a 2x2 arrax of axes
grid("on") # Create a grid on the axis
title("Even Parity, p=0")
xlabel("momentum")
ylabel("energy")

subplot(122) # Create the 1st axis of a 2x2 arrax of axes
grid("on") # Create a grid on the axis
title("Even Parity, p=1")
xlabel("momentum")
ylabel("energy")

for i in 1:size(e,1)
    if p[i] == 0
        subplot(121)
        plot(k[i],e[i], marker = "s", color = "b")
    elseif p[i] == 1
        subplot(122)
        plot(k[i],e[i], marker = "s", color = "k")
    end
end
```

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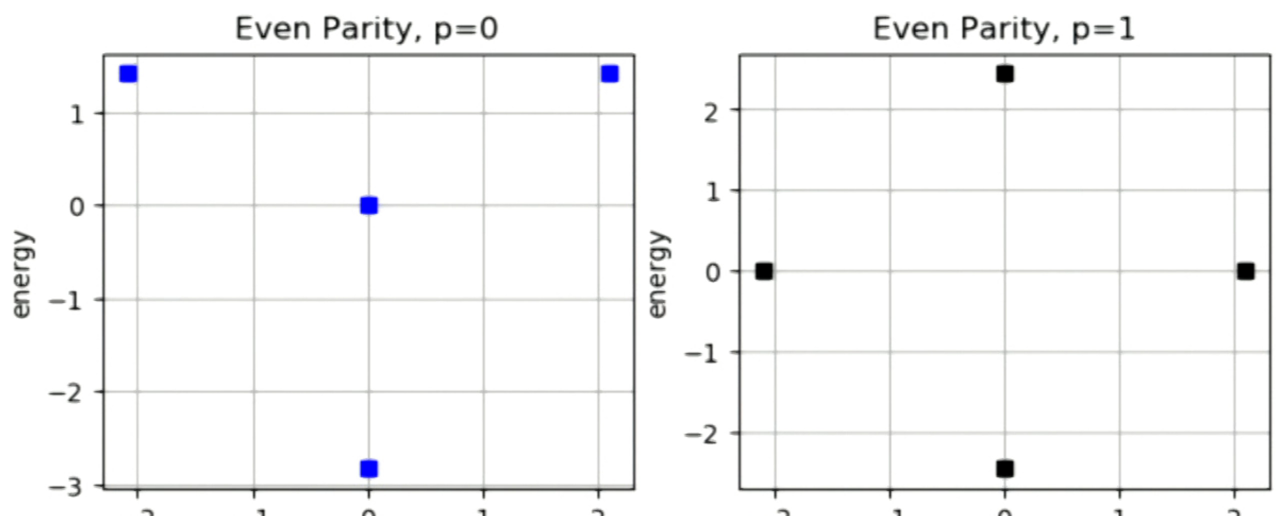
```
        plot(k[i],e[i], marker = "s", color = "b")
    elseif p[i] == 1
        subplot(122)
        plot(k[i],e[i], marker = "s", color = "k")
    end
end
```



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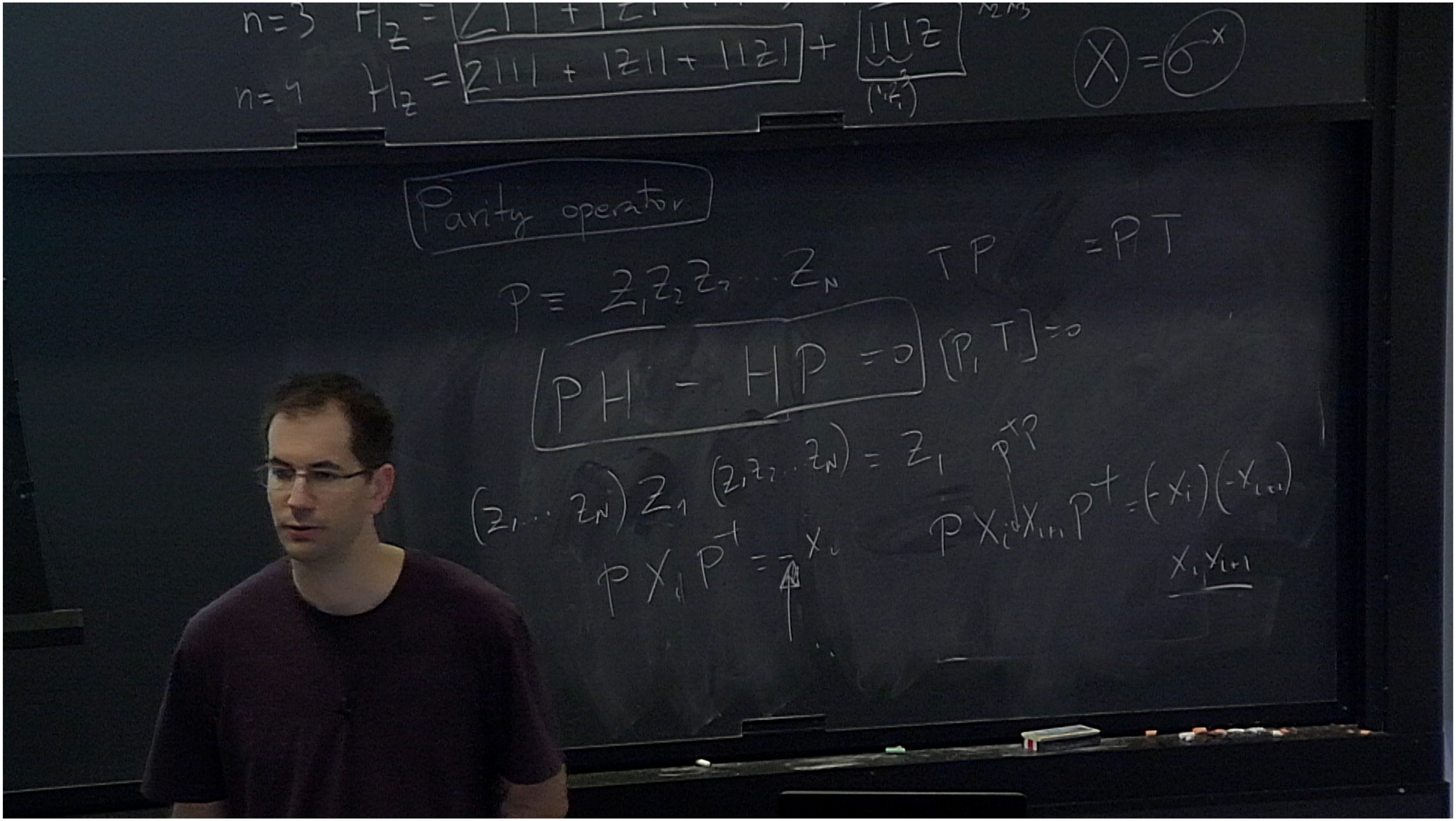
It's your turn for the last time! (3/3)

5) write a function buildP that builds the parity operator P for N spins (use only for $N \leq 10$)

In [20]:
```
# function buildP takes as input N (number of spins) and outputs P (parity operat
function buildP(N::Int64)::Array{Float64,2}
    Z = [1 0; 0 -1]
    P = copy(Z)
    for i=2:N
        P = kron(P,Z)
    end
    return P
```


Parity operator
P ≡ Z1 Z2 Z3 ... ZN
PH - HP = 0
[P, T] = 0
TP = PT
X = σ^x