

Title: PSI 2015/2016 Explorations in Condensed Matter - Guifre Vidal - 6

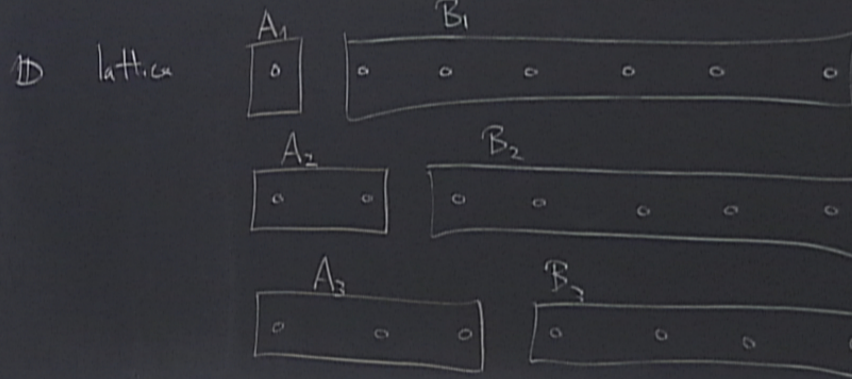
Date: Mar 29, 2016 10:15 AM

URL: <http://pirsa.org/16030013>

Abstract:

LECTURE 6 Entanglement in quantum spin chains

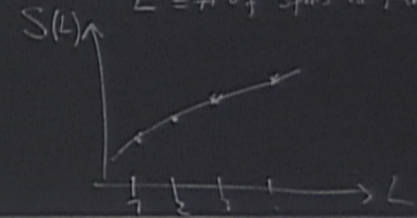
$$|\psi\rangle \in \bigotimes_{n=1}^N \mathbb{C}_2 \quad |\psi\rangle = \sum_{i_1, i_2, \dots, i_N} \psi_{i_1 i_2 \dots i_N} |i_1, i_2, \dots, i_N\rangle$$



for partition $A_n - B_n$

$$S(\rho^{A_n}) = -\text{tr}(\rho^{A_n} \log_2 \rho^{A_n})$$

$L = \# \text{ of spins in } A_n$



Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (autosaved)

File Edit View Insert Cell Kernel Help Julia 0.4.0

```
# pkg.update()
```

**Generate a random state of N qubits,
compute reduced density matrix for first 3 qubits,
then compute its entropy**

```
In [ ]: N=20
Psi = randn(2^N) + im*randn(2^N)
# Psi = rand(2^N) + im*rand(2^N) # do not use rand! x in [0,1]
Psi = Psi/vecnorm(Psi)
A = reshape(Psi, (2^3, 2^(N-3)))
Rho3 = A*A'

function computeEE(Rho) # this function assumes Rho is non-negative defined!
    u,v = eig(Rho)
    chi = size(D,1)
    EE = 0
    for n=1:chi
        if u[n]>0
            EE += -u[n]log2(u[n])
        end
    end
end
```

Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (unsaved changes)

File Edit View Insert Cell Kernel Help Julia 0.4.0

then compute its entropy

```
In [ ]: N=20
Psi = randn(2^N) + im*randn(2^N)
# Psi = rand(2^N) + im*rand(2^N) # do not use rand! x in [0,1]
Psi = Psi/vecnorm(Psi)
A = reshape(Psi, (2^3, 2^(N-3)))
Rho3 = A*A'

function computeEE(Rho) # this function assumes Rho is non-negative defined!
    u,v = eig(Rho)
    chi = size(u,1)
    EE = 0
    for n=1:chi
        if u[n]>0
            EE += -u[n]log2(u[n])
        end
    end
    return EE
end

EE3 = computeEE(Rho3)
```

compute a sequence of Entanglement Spectra and Entanglement entropies

10:26 AM 29/03/2016

Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (autosaved)

File Edit View Insert Cell Kernel Help Julia 0.4.0

compute a sequence of Estanglement Spectra and Entanglement entropies

```
In [ ]: # entanglement entropy
function computeESandEE(Psi) # it assumes  $L = 2^N$  for integer  $N$ . It returns  $p$  ES and  $p$  EEs
    L = length(Psi) # Dimension of the vector space
    N = convert{Int64,log2(L)} # Number of sites
    p = div(N,2) #  $N/2$  or  $(N-1)/2$ 
    EE = zeros(p)
    ES = zeros(2^p,p)
    for n=1:p
        A = reshape(Psi, (2^(n),2^(N-n)))
        rho = A*A'
        u,v = eig(rho)
        u = abs(u) # to make numerical  $\theta$ 's positive
        ES[1:2^n,n] = -sort(-u)
        for m = 1:2^n
            if u[m] > 0
                EE[n] += -u[m]*log2(u[m])
            end
        end
    end
    return ES,EE
end
```

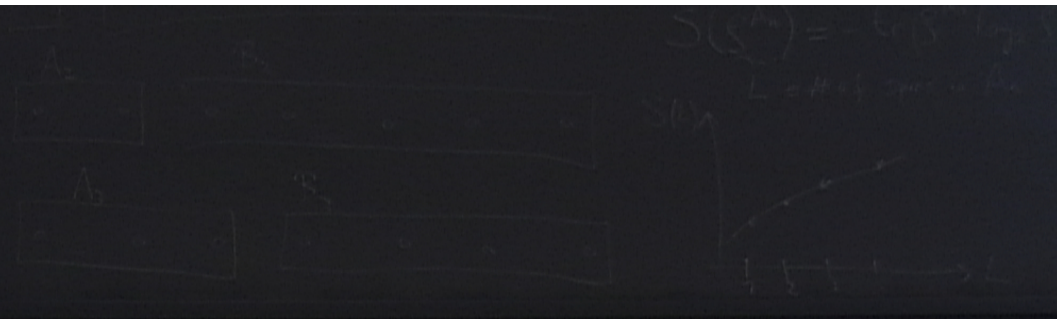
Windows taskbar: 10:31 AM 29/03/2016

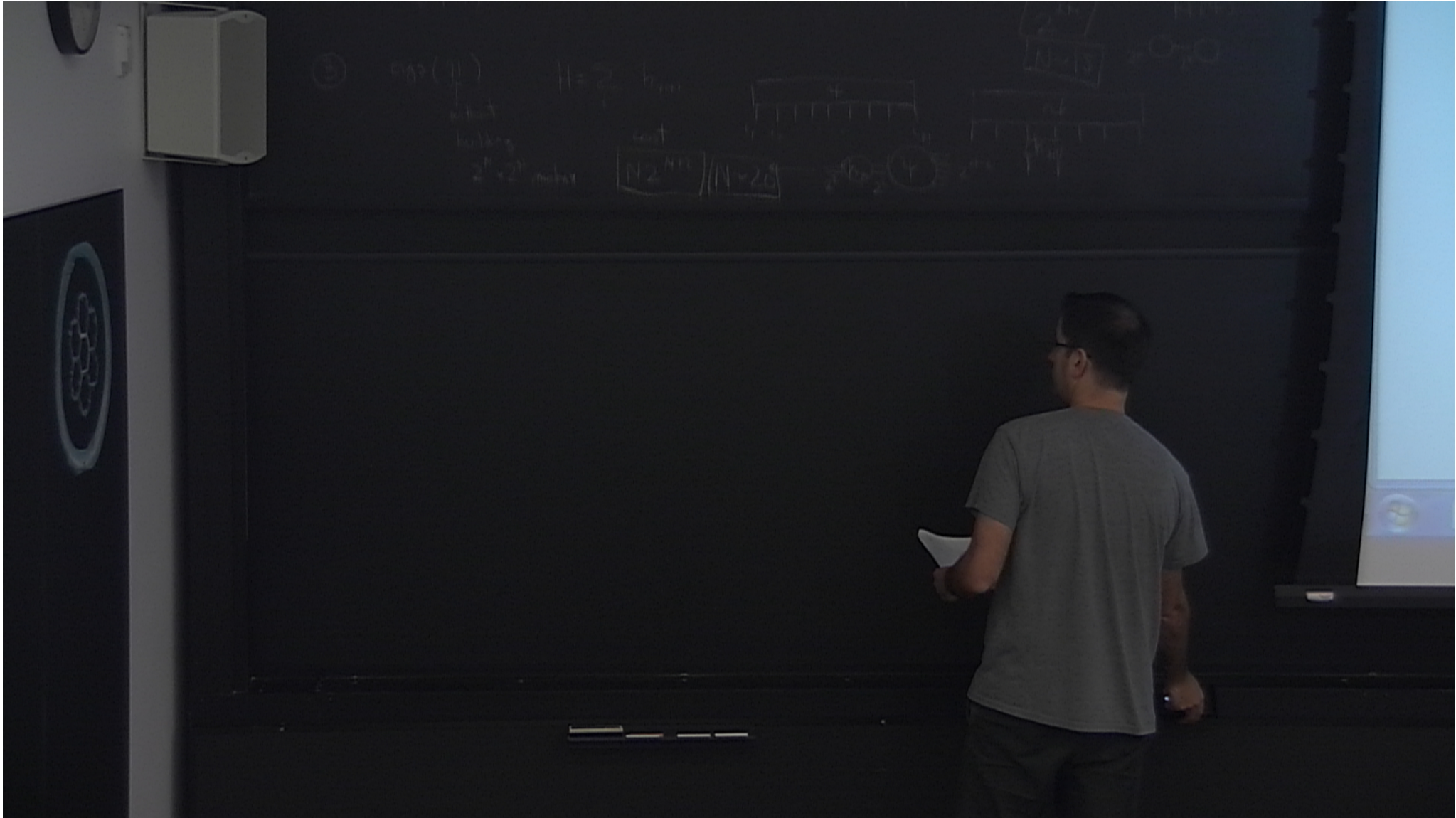
$$\vec{p} = (p_1, p_1, p_2)$$

$$S(\vec{p}) = S\left(\frac{1}{x}, \frac{1}{x}, \frac{1}{x}\right) = -\frac{1}{x} \log_2\left(\frac{1}{x}\right) \times x = \log_2 x$$

$$L=3 \text{ qubits } x=2^L=8$$

$$S(L) \leq S\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = \log_2 2^L = L$$

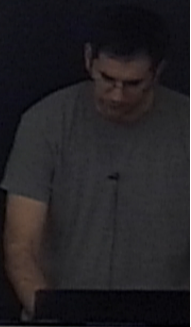


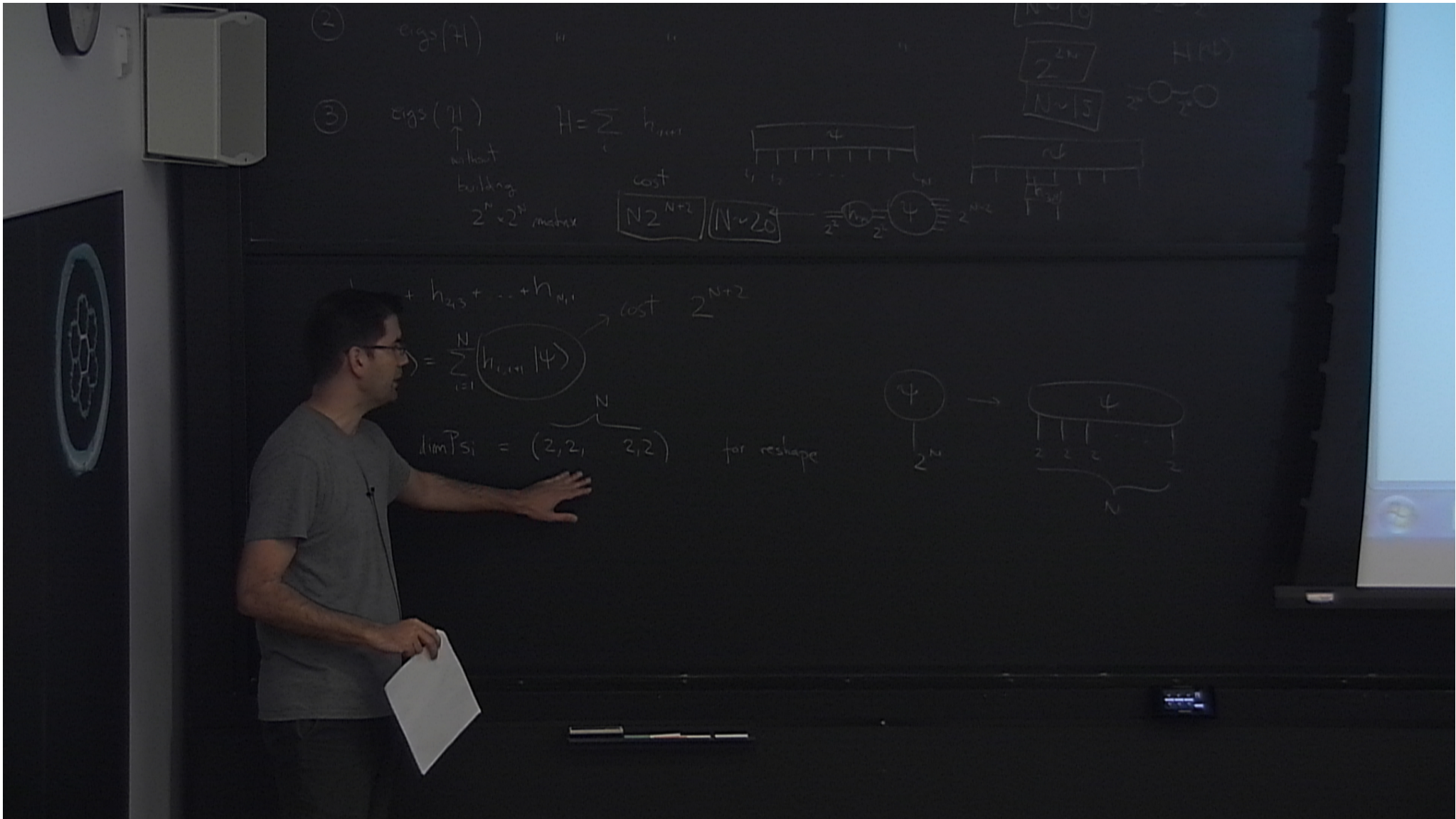



```
localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb
jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (autosaved)
File Edit View Insert Cell Kernel Help
+ -> ← ↻ ↺ ⏪ ⏩ Code CellToolbar

In [ ]: # Ising model using h=1
function buildising(h=1.0) # Ising model with transverse magnetic field h [critical h=1 by default]
    X = [0 1; 1 0]
    Z = [1 0; 0 -1]
    I = eye(2, 2)
    XX = kron(X, X)
    ZZ = kron(Z, Z)
    II = kron(I, I)
    H2_s = (XX + h/2*(ZZ+II))
    return H2
end

# XY model using h=0
function buildXY(h=0.0) # XY model with magnetic field h (h=0 by default)
    X = [0 1; 1 0]
    Y = [0 -1; 1 0] # we avoid using complex numbers
    Z = [1 0; 0 -1]
    I = eye(2, 2)
    XX = kron(X, X)
    YY = kron(Y, Y)
    ZZ = kron(Z, Z)
    H2_s = (kron(X, X) - kron(Y, Y)) + h/2*(ZZ+II) # also called = H2
    return H2
end
```





② $\text{eigs}(H)$

③ $\text{eigs}(H)$ without building $2^N \times 2^N$ matrix

$H = \sum_i h_{i,i+1}$

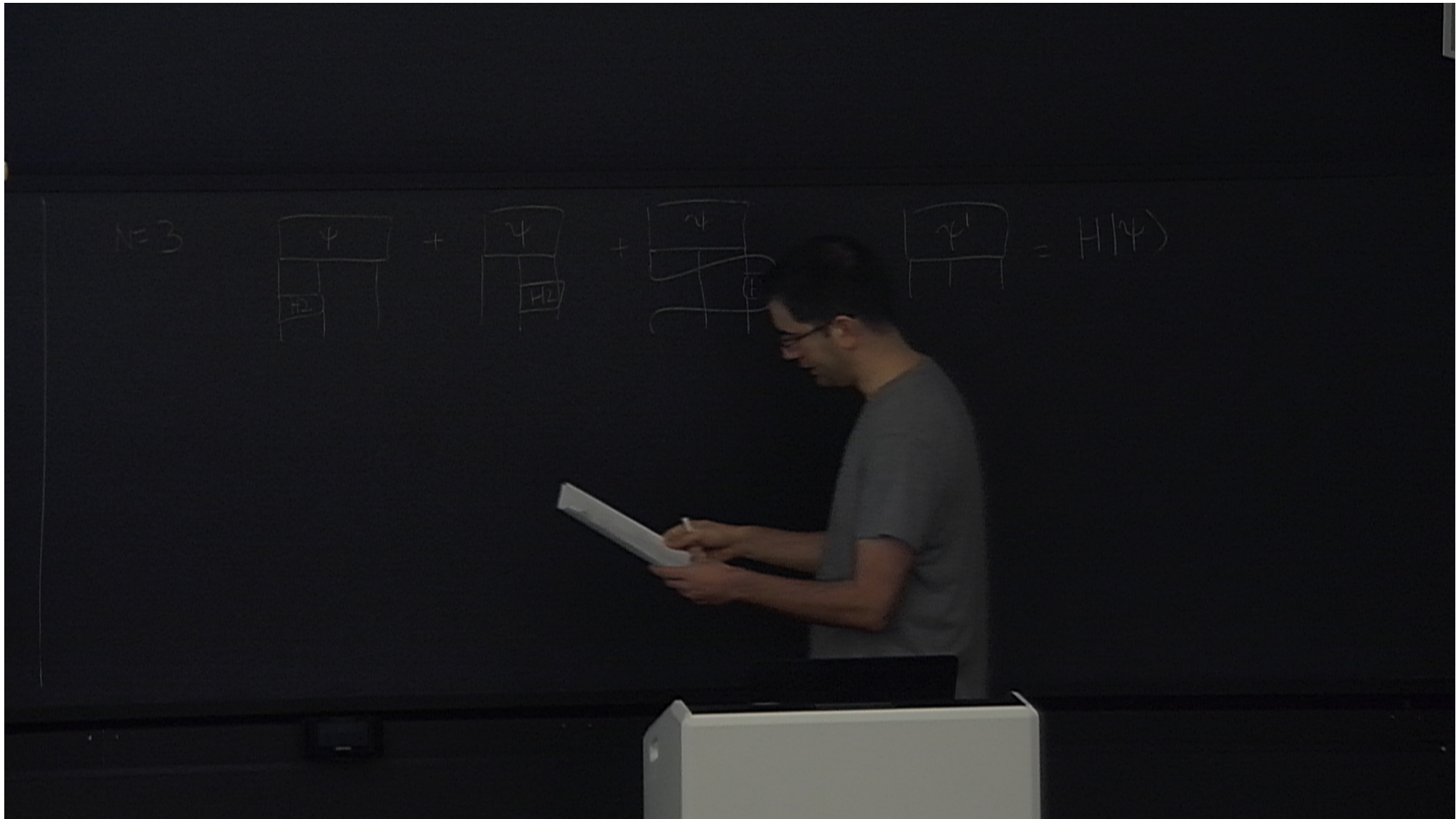
cost $N \cdot 2^{N+2}$ $(N \sim 20)$

$h_{1,2} + h_{2,3} + \dots + h_{N,N+1}$

$H|\psi\rangle = \sum_{i=1}^N (h_{i,i+1}|\psi\rangle)$ cost 2^{N+2}

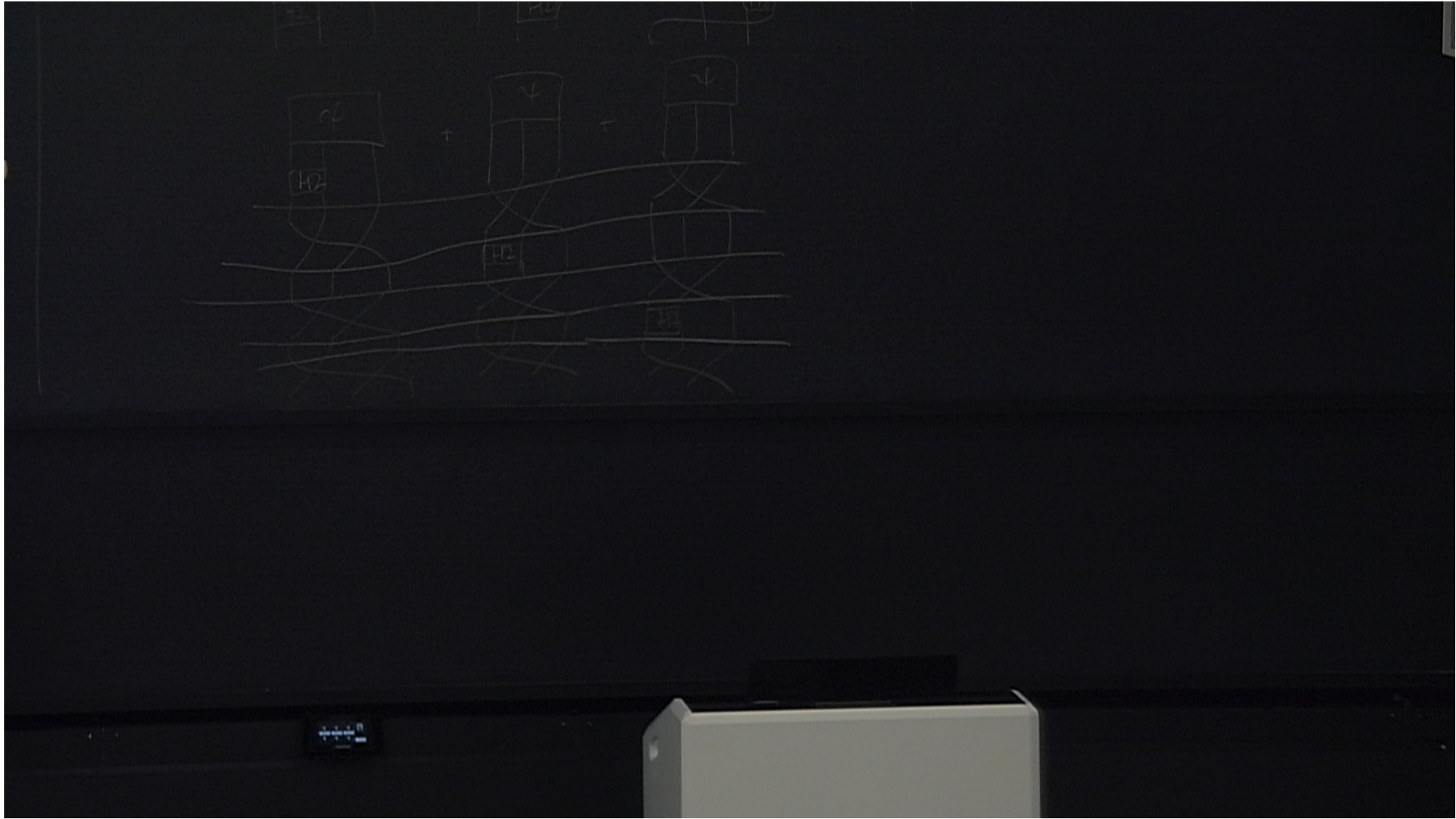
$\dim \psi_i = (2, 2, \dots, 2, 2)$ for reshape

$\text{cycperm} = (2, 3, \dots, N, 1)$ for permutedims



$N=3$

$$\begin{array}{c} \begin{array}{|c|} \hline \psi \\ \hline \end{array} + \begin{array}{|c|} \hline \psi \\ \hline \end{array} + \begin{array}{|c|} \hline \psi \\ \hline \end{array} \\ \begin{array}{|c|} \hline \psi \\ \hline \end{array} + \begin{array}{|c|} \hline \psi \\ \hline \end{array} + \begin{array}{|c|} \hline \psi \\ \hline \end{array} \end{array} = \begin{array}{|c|} \hline \psi \\ \hline \end{array} = H|\psi\rangle$$



Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

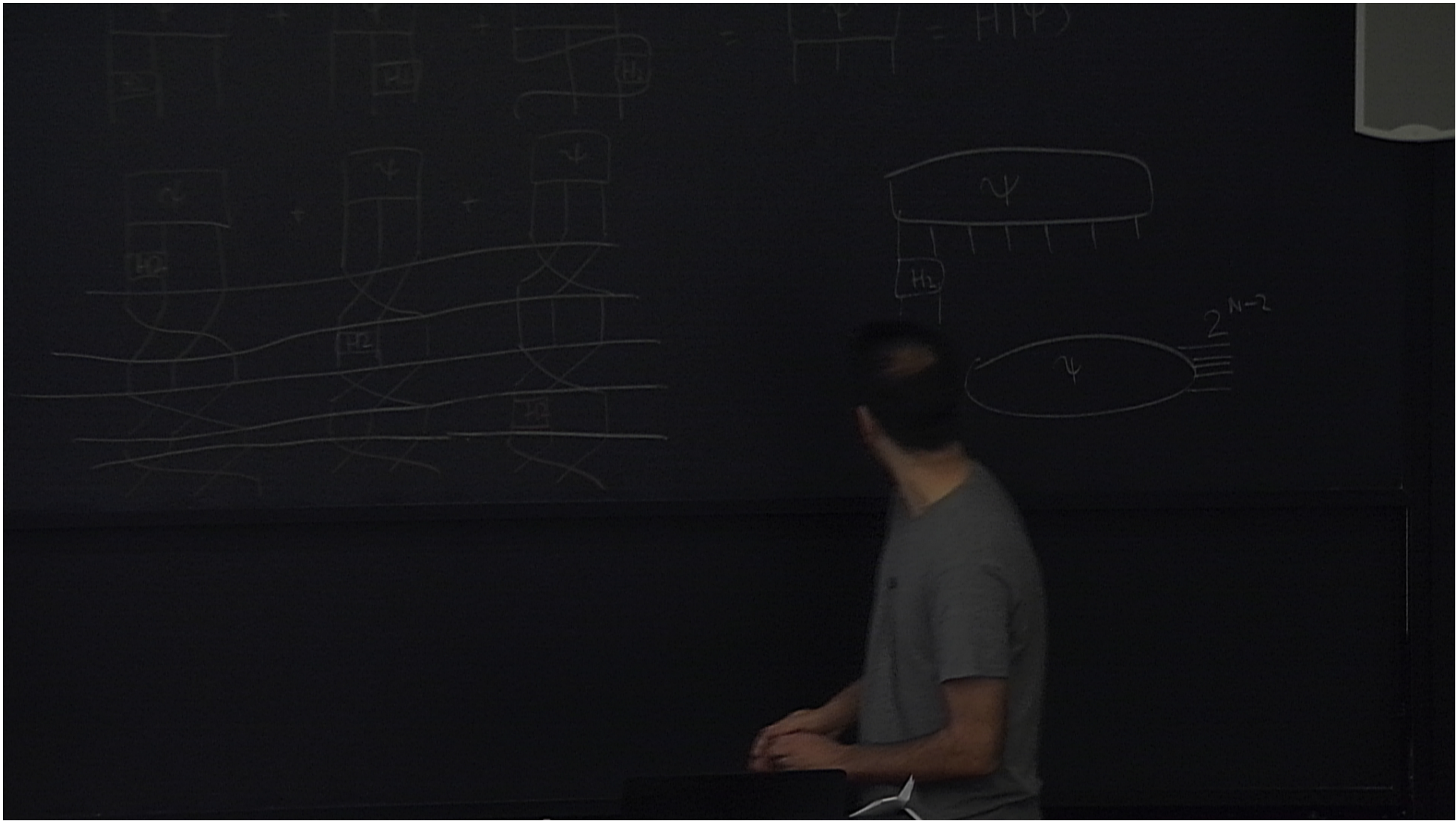
jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (autosaved)

File Edit View Insert Cell Kernel Help Julia 0.4.0

multiply H and PSI --> COST $N2^{(N+2)}$

```
In [ ]: function multiplyHPsi!(nPsi::Vector, Psi::Vector) # requires H2 to have been defined
    length(nPsi)==length(Psi) || throw(DimensionMismatch())
    dimN = length(Psi) # Dimension of the vector space
    N = convert{Int64,log2(dimN)} # Number of spins
    dimPsi = tuple(fill{Int,1,N}...) # dimsPsi =(2,2,2, ..., 2)
    a = collect{2:N}
    a = [a;1]
    cyclperm = tuple{a...} #tuple for cyclic permutation cyclperm = (2, 3, ... N, 1)
    Psi = reshape{Psi,dimPsi}
    nPsi = zeros{dimPsi}
    for n=1:N
        Psi = reshape{Psi,(4,2^(N-2))}
        nPsi = reshape{nPsi,(4,2^(N-2))}
        nPsi += H2*Psi
        Psi = reshape{Psi,dimPsi}
        nPsi = reshape{nPsi,dimPsi}
        Psi = permutedims{Psi,cyclperm}
        nPsi = permutedims{nPsi,cyclperm}
    end
    nPsi = reshape{nPsi,dimN}
    # return nPsi
end
```

10:58 AM 29/03/2016



Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (autosaved)

File Edit View Insert Cell Kernel Help Julia 0.4.0

multiply n and Ψ --> $\text{cost } N^2 \cdot (N+2)$

```
In [ ]: function multiplyHPsi!(nPsi::Vector, Psi::Vector) # requires H2 to have been defined
    length(nPsi)==length(Psi) || throw(DimensionMismatch())
    dimN = length(Psi) # Dimension of the vector space
    N = convert{Int64,log2(dimN)} # Number of spins
    dimPsi = tuple(fill{Int,1,N}...) # dimsPsi =(2,2,2, ..., 2)
    a = collect{2:N}
    a = [a;1]
    cyclperm = tuple(a...) #tuple for cyclic permutation cyclperm = (2, 3, ... N, 1)
    Psi = reshape(Psi,dimPsi)
    nPsi = zeros(dimPsi)
    for n=1:N
        Psi = reshape(Psi,(4,2^(N-2)))
        nPsi = reshape(nPsi,(4,2^(N-2)))
        nPsi += H2*Psi
        Psi = reshape(Psi,dimPsi)
        nPsi = reshape(nPsi,dimPsi)
        Psi = permutedims(Psi,cyclperm)
        nPsi = permutedims(nPsi,cyclperm)
    end
    nPsi = reshape(nPsi,dimN)
    # return nPsi
end
```

10:59 AM 29/03/2016

Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (unsaved changes)

File Edit View Insert Cell Kernel Help

Code CellToolbar

Choose Hamiltonian H2, N, and initialize Psi

```
In [ ]: h = 1
H2 = buildIsing(h) # Hamiltonian
H2 = buildXX()
D,U = eig(H2)
shiftE = D[end]
H2 = H2 - shiftE*eye(4) # remember to re-shift the energy later on!

N = 10 # number of spins
Psi = rand(2^N)
nPsi = rand(2^N)
Psi = Psi/vecnorm(Psi)

init_steps = 1
energy = ones(0)
initial_step=1
Nsteps = 0

@time nPsi = multiplyHPsi!(nPsi, Psi) # N = 20 took 4 seconds
;
```

11:00 AM
29/03/2016

(4)

$$H = \sum_{n=0}^{2^N-1} E_n |E_n\rangle\langle E_n|$$

$$E_0 < E_1 \leq E_2 \leq \dots \leq E_{2^N-1}$$

$$|\psi\rangle = \sum_{n=0}^{2^N-1} \psi_n |E_n\rangle \quad H = \sum_{n=0}^{2^N-1} E_n |E_n\rangle \langle E_n|$$

$$E_0 < E_1 \leq E_2 \leq \dots \leq E_{2^N-1}$$

$$H|\psi\rangle = \sum_n \psi_n E_n |\psi_n\rangle$$

$$|E_0\rangle > |E_1\rangle$$

$$H^p |\psi\rangle = \sum_n \psi_n (E_n)^p |\psi_n\rangle = \psi_0 E_0^p |E_0\rangle + \frac{\psi_1}{\psi_0} \left(\frac{E_1}{E_0}\right)^p |E_1\rangle + \dots$$

$$\left| \frac{E_1}{E_0} \right|^p$$

Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

Apps Frequent bookmarks ★ Bookmarks kitaev Rahul Roy Topological Phases of fendley www.lancaster.ac.uk/ KITP Events | KITP KITP Conference: From Other bookmarks

jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (unsaved changes)

File Edit View Insert Cell Kernel Help Julia 0.4.0

0.002551 seconds (52.97 k allocations: 1.174 MB)

Apply power method to Psi

```
In [ ]: initial_step += Nsteps
Nsteps = 10
final_step = initial_step + Nsteps-1

for n=initial_step:final_step
    nPsi = multiplyHPsi!(nPsi,Psi)
    newenergy = real(Psi'*nPsi)[1] + shiftE*N
    energy = [energy; newenergy]
    Psi = nPsi/vecnorm(nPsi)
    print(n-initial_step+1, ":", Nsteps, " ")
end

figure("Power_method",figsize=(14,4))

subplot(121) # Create the 1st axis of a 2x2 array of axes
grid("on") # Create a grid on the axis
title("Power method")
ax = gca()
```

11:06 AM
29/03/2016

Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (unsaved changes)

File Edit View Insert Cell Kernel Help Julia 0.4.0

Apply power method to Psi

```
In [ ]: initial_step += Nsteps
Nsteps = 10
final_step = initial_step + Nsteps-1

for n=initial_step:final_step
    nPsi = multiplyHPsi!(nPsi,Psi)
    newenergy = real(Psi'*nPsi)[1] + shiftE*N
    energy = [energy; newenergy]
    Psi = nPsi/vecnorm(nPsi)
    print(n-initial_step+1, ":", Nsteps, " ")
end

figure("Power_method",figsize=(14,4))

subplot(121) # Create the 1st axis of a 2x2 array of axes
grid("on") # Create a grid on the axis
title("Power method")
ax = gca()
xlabel("all iterations")
ylabel("Energy")
```

11:06 AM
29/03/2016

Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (unsaved changes)

File Edit View Insert Cell Kernel Help | Julia 0.4.0

```
ylab("Energy")
plot(initial_step:final_step, energy[initial_step:final_step], marker = "o")
```

1

Energy

Power method

all iterations

Energy

Power method

most recent iterations

Out[12]: 1-element Array{Any,1}:
PyObject <matplotlib.lines.Line2D object at 0x00000000F202320>

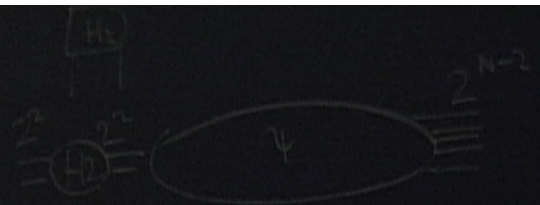
11:07 AM
29/03/2016

$$|\psi\rangle = \sum_{n=0}^{2^N-1} \psi_n |E_n\rangle \quad H = \sum_{n=0}^{2^N-1} E_n |E_n\rangle \langle E_n|$$

$$E_0 < E_1 \leq E_2 \leq \dots \leq E_{2^N-1}$$

$$H|\psi\rangle = \sum_n \psi_n E_n |\psi_n\rangle$$

$$H^p |\psi\rangle = \sum_n \psi_n E_n^p |\psi_n\rangle = \psi_0 E_0^p |E_0\rangle + \psi_1 E_1^p |E_1\rangle + \dots$$



Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (unsaved changes)

File Edit View Insert Cell Kernel Help | Julia 0.4.0

```

1000 909:1000 910:1000 911:1000 912:1000 913:1000 914:1000 915:1000 916:1000 917:1000 918:1000 919:100
0 920:1000 921:1000 922:1000 923:1000 924:1000 925:1000 926:1000 927:1000 928:1000 929:1000 930:1000 9
31:1000 932:1000 933:1000 934:1000 935:1000 936:1000 937:1000 938:1000 939:1000 940:1000 941:1000 942:
1000 943:1000 944:1000 945:1000 946:1000 947:1000 948:1000 949:1000 950:1000 951:1000 952:1000 953:100
0 954:1000 955:1000 956:1000 957:1000 958:1000 959:1000 960:1000 961:1000 962:1000 963:1000 964:1000 9
65:1000 966:1000 967:1000 968:1000 969:1000 970:1000 971:1000 972:1000

```

Energy

all iterations

Energy

most recent iterations

Out[14]: 1-element Array{Any,1}:
PyObject <matplotlib.lines.Line2D object at 0x0000000020A0C080>

11:08 AM
29/03/2016

Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (unsaved changes)

File Edit View Insert Cell Kernel Help | Julia 0.4.0

```

yiaoe1(energy)
plot(initial_step:final_step, energy[initial_step:final_step], marker = "o")

```

1

Power method

Energy

all iterations

$1e-7-1.2784905e1$ Power method

Energy

most recent iterations

Out[15]: 1-element Array{Any,1}:
 PyObject <matplotlib.lines.Line2D object at 0x00000000F245908>

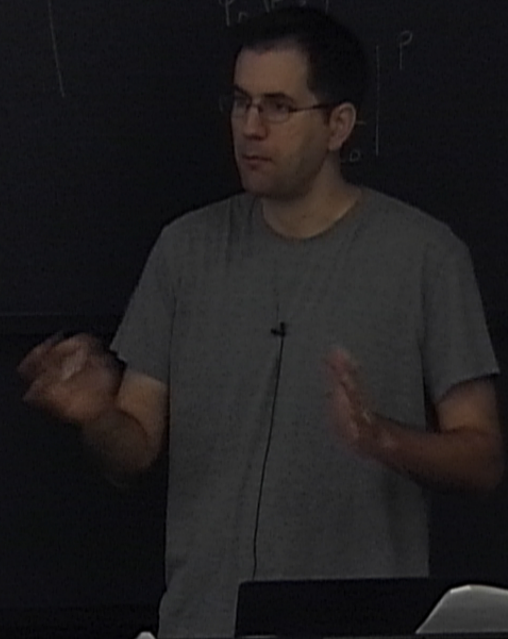
Windows taskbar: 11:09 AM, 29/03/2016

$$H|\psi\rangle = \sum_n \psi_n E_n |\psi_n\rangle$$

$$H^P |\psi\rangle = \sum_n \psi_n E_n^P |\psi_n\rangle = \psi_0 E_0^P |E_0\rangle + \frac{\psi_1}{\psi_0} \left(\frac{E_1^P}{E_0^P} |E_1\rangle + \dots \right)$$

$$H|\psi\rangle$$

$$|E_0\rangle > |E_1\rangle > |E_2\rangle$$



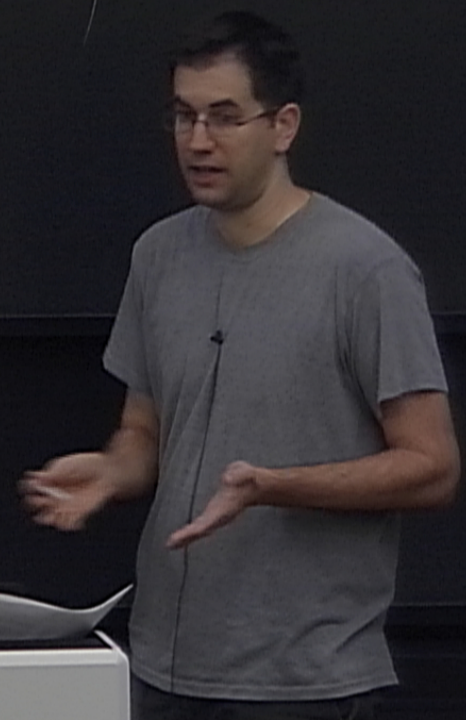
$$\hat{H}|\psi\rangle = \sum_n \psi_n E_n |\psi_n\rangle$$

$$\hat{H}^P |\psi\rangle = \sum_n \psi_n E_n^P |\psi_n\rangle = \psi_0 E_0^P (|E_0\rangle + \frac{\psi_1 (E_1)^P}{\psi_0 (E_0)^P} |E_1\rangle + \dots)$$

$|\psi\rangle, \hat{H}|\psi\rangle, \hat{H}^2|\psi\rangle, \hat{H}^P|\psi\rangle$
 P+1

$$|E_0\rangle > |E_1\rangle > |E_2\rangle$$

$$\frac{|E_1\rangle^P}{|E_0\rangle^P}$$



Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (autosaved)

File Edit View Insert Cell Kernel Help Julia 0.4.0

Out[15]: 1-element Array{Any,1}:
PyObject <matplotlib.lines.Line2D object at 0x000000000F245908>
:10 2:10 3:10 4:10 5:10 6:10 7:10 8:10 9:10 10:10

Lanczos

```
In [ ]: using LinearMaps

N = 14 # N=14 took 4.5 sec; N=16 took 35 sec; N=18 took 122 sec
m = 1 # how many states?

# this produces a linear map H that can be called from eigs
H = LinearMap(multiplyHPsi!, 2^N, isreal=true, ismutating=true) # use this for real symmetric H
#H = LinearMap(multiplyHPsi!, 2^N, isreal=false, ismutating=true, ishermitian=true) # use this for complex hermitian H

@time u, v = eigs(H; nev=m, which=:SR) #:SR stands for smallest real part

Energy = real(u[1]+ shiftE*N) # let us undo the shift in energy

Psi = v
E = Energy
```

11:11 AM
29/03/2016

Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (autosaved)

File Edit View Insert Cell Kernel Help | Julia 0.4.0

7.541662 seconds (298.53 M allocations: 5.183 GB, 5.61% gc time)

Saving the result in a file

```
In [ ]: using JLD
save("myfile.jld", "Psi", Psi, "E", E)
```

Loading data from the file

```
In [ ]: Psi2 = load("myfile.jld", "Psi")

In [ ]: ES,EE = computeESandEE(Psi2)
N = convert{Int64,log2(size(Psi2,1))}
Lmax = div(N,2)
L = collect(1:Lmax)
subplot(221)
semilogy(L,ES', "o") # semilogy plot (y-axis in logarithmic scale)
subplot(222)
plot(L,EE, marker = "o") # regular plot
```

11:13 AM 29/03/2016

Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (autosaved)

File Edit View Insert Cell Kernel Help

Code CellToolbar

```
Energy = real(u[1] + shift(E)) # let us undo the shift in energy
Psi = v
E = Energy
```

Out[17]: -17.862808540760923
7.541662 seconds (298.53 M allocations: 5.183 GB, 5.61% gc time)

Saving the result in a file

```
In [ ]: using JLD
save("myfile.jld", "Psi", Psi, "E", E)
```

Loading data from the file

```
In [ ]: Psi2 = load("myfile.jld", "Psi")
In [ ]: ES, EE = computeESandEE(Psi2)
```

11:13 AM
29/03/2016

Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (unsaved changes)

File Edit View Insert Cell Kernel Help Julia 0.4.0

```
subplot(221)
semilogy(L,ES', "o") # semilogy plot (y-axis in logarithmic scale)
subplot(222)
plot(L,EE, marker = "o") # regular plot
```

Out[21]: 1-element Array{Any,1}:
PyObject <matplotlib.lines.Line2D object at 0x0000000022117F28>

11:15 AM 29/03/2016

Documents/PSI 2016/ x PSI2016JuliaV x

localhost:8888/notebooks/Documents/PSI%202016/PSI2016JuliaV.ipynb

jupyter PSI2016JuliaV Last Checkpoint: 2 hours ago (unsaved changes)

File Edit View Insert Cell Kernel Help | Julia 0.4.0

Code CellToolbar

Out[21]: 1-element Array{Any,1}:
PyObject <matplotlib.lines.Line2D object at 0x000000022117F28>

```
In [ ]: # In the tutorial, you will be ask to Load the ground states of the Ising and XX chain for N=18 spins
Psi1 = load("Ising.jld", "Psi")
Psi2 = load("XX.jld", "Psi")
```

In []:

In []:

11:16 AM
29/03/2016