Title: LECTURE: Generative Modelling

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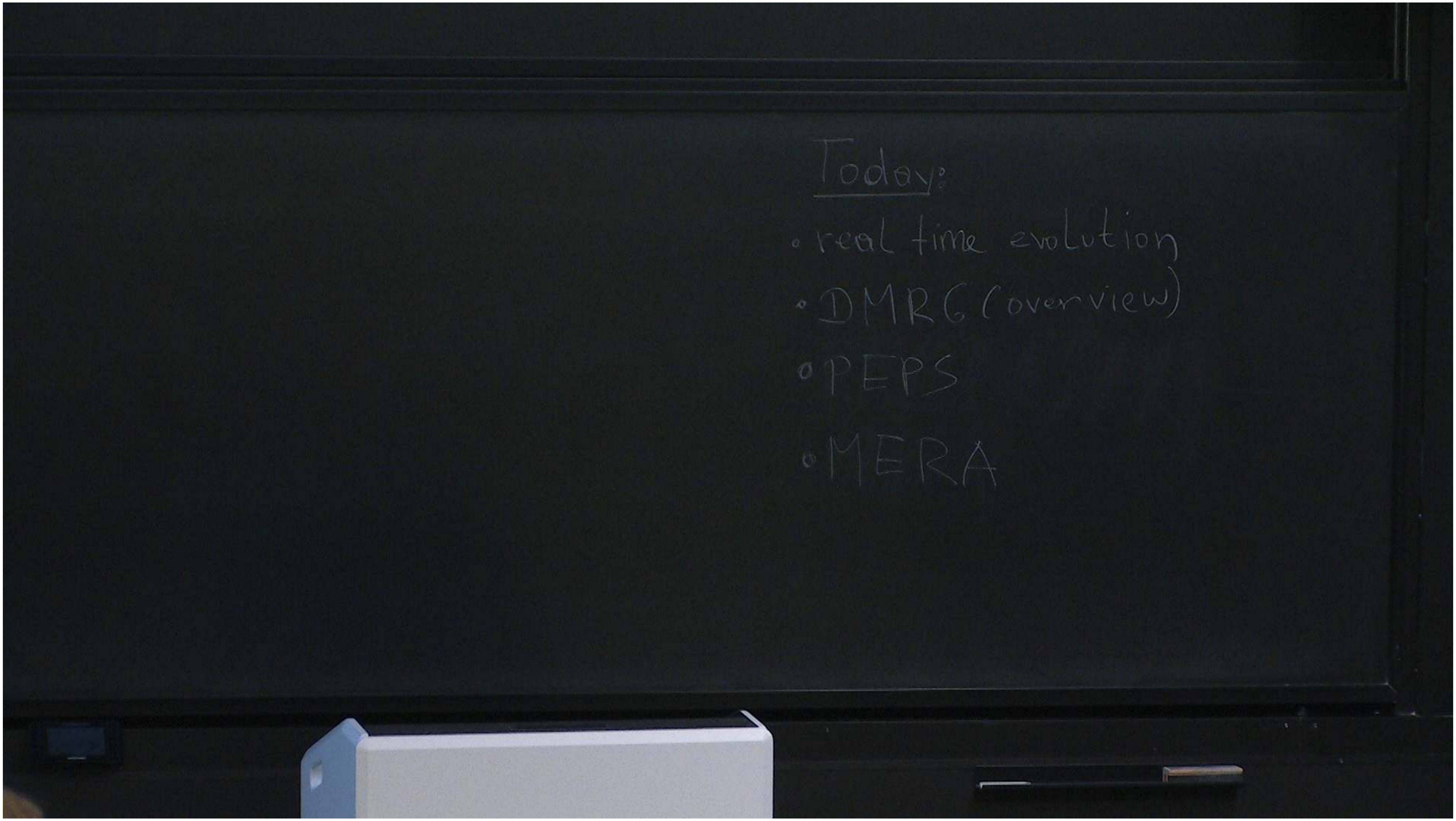
Collection: Quantum and AI Career Trajectories Mini-Course: Computational Methods and their Applications

Date: May 11, 2023 - 11:00 AM

URL: https://pirsa.org/23050096

Abstract: TBC


Today:
• real time evolution
• DMRG (overview)
• PEPS
• MERA

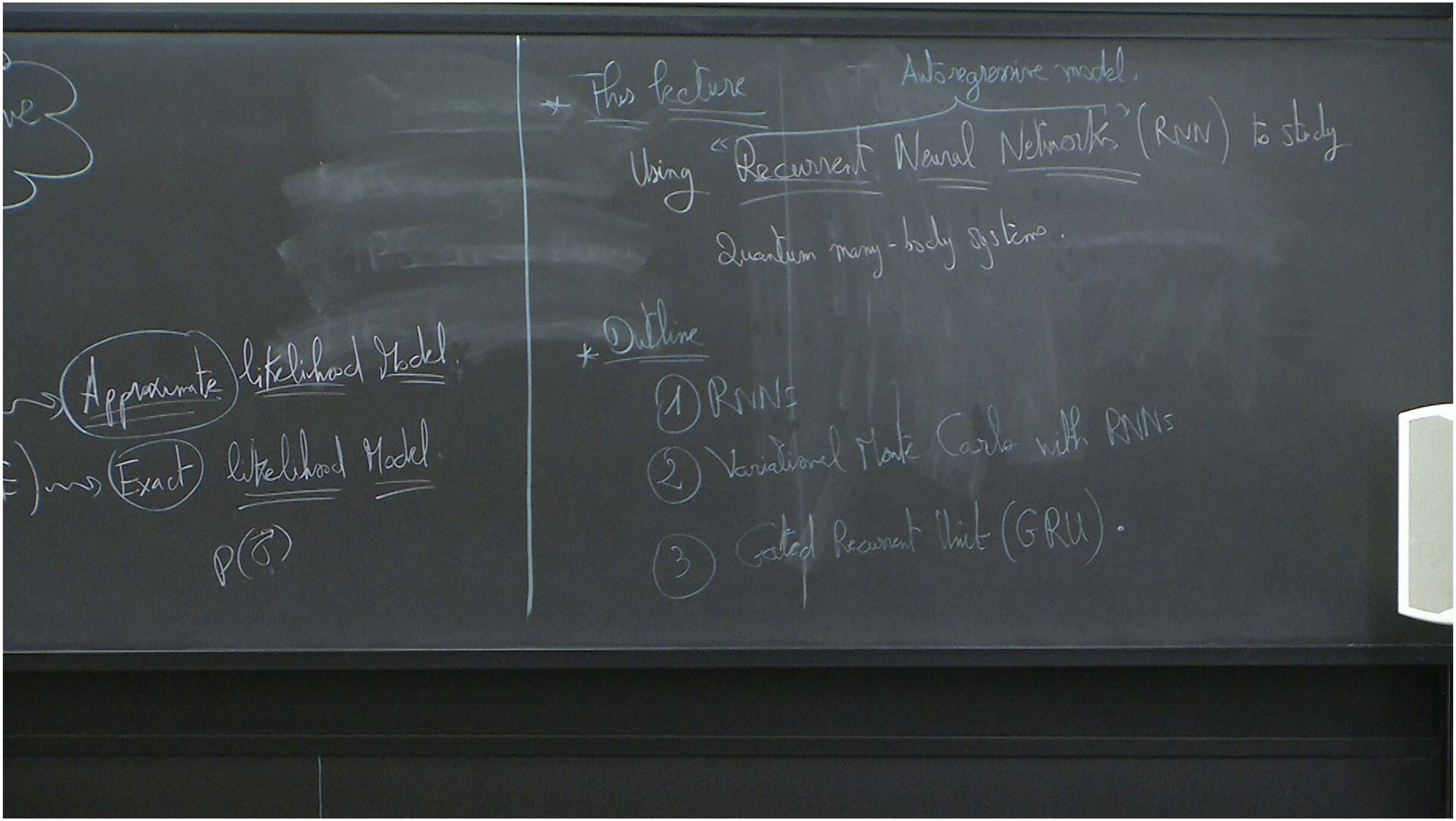
Lecture 4: Generative Models

* Last lectures (Quantum state reconstruction).
  * Restricted Boltzmann Machines (RBM) $\rightsquigarrow$ Approximate likelihood Model.
  * Neural Autoregressive Density Estimator (NADE) $\rightsquigarrow$ Exact likelihood Model.

$p(\vec{\sigma})$

* Th

* D



Approximate likelihood Model.
Exact likelihood Model.
p(σ)
* This lecture
Autoregressive model.
Using « Recurrent Neural Networks » (RNN) to study
Quantum many-body systems.
* Outline
1 RNNs
2 Variational Monte Carlo with RNNs
3 Gated Recurrent Unit (GRU).

① RNNs:

↳ Originally built for language processing.

Application: Machine translation, speech recognition, DNA sequence analysis.
Music generation.

1) RNNs:

↳ Originally built for language processing.

Application: Machine translation, speech recognition, DNA sequence analysis.
Music generation (AIVA)

* Universal approximators. * Can simulate Turing Machines

ce analysis.

hines

* Key idea

↳ We will be using spins instead of words

« Sentence » $\simeq$ « Spin configuration »

« The weather is nice » $\simeq$ $\vec{\sigma} = (\sigma_1, \sigma_2, \dots \sigma_N)$

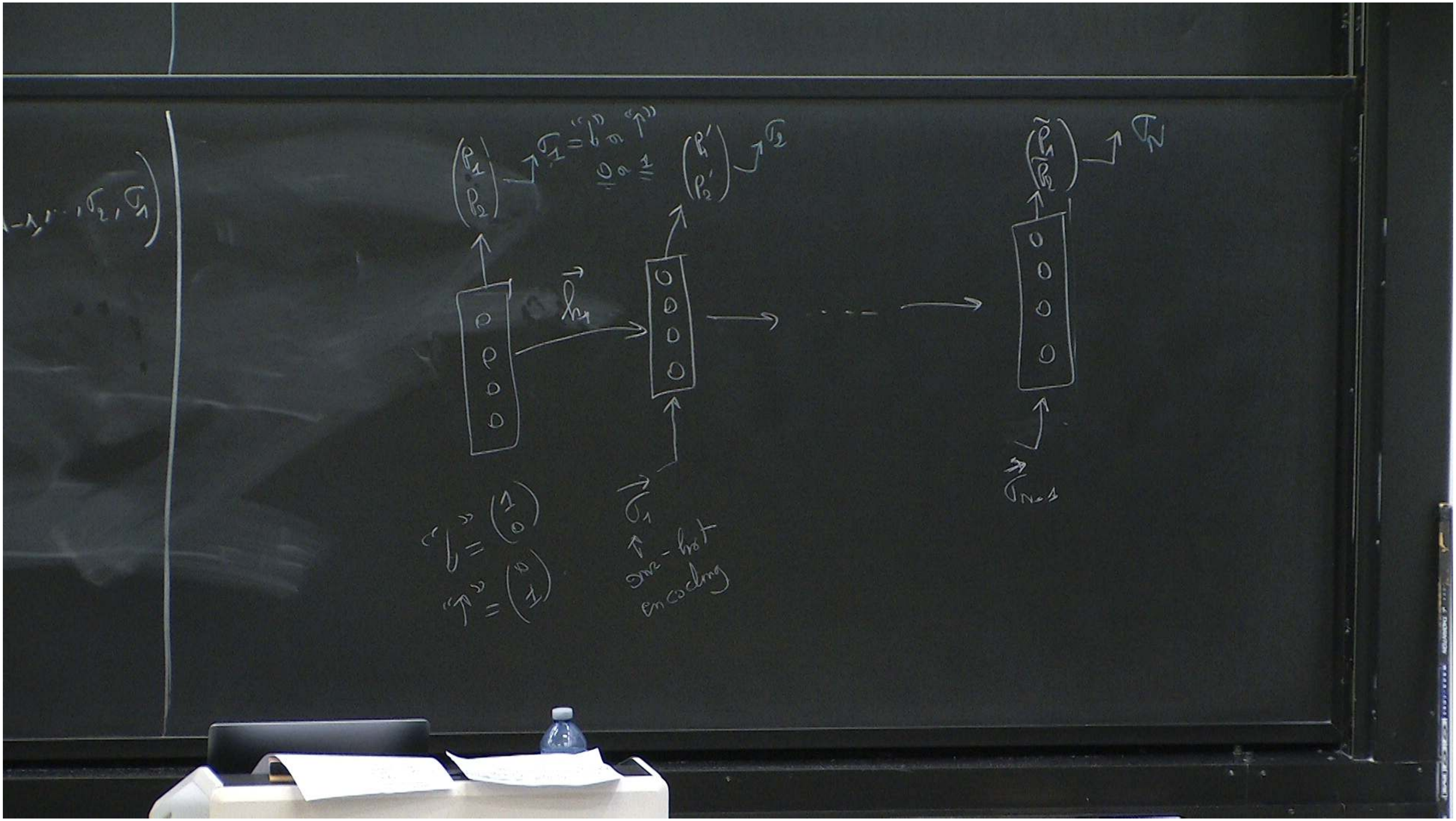
Each word had an ID in a dictionary (10K-1M).

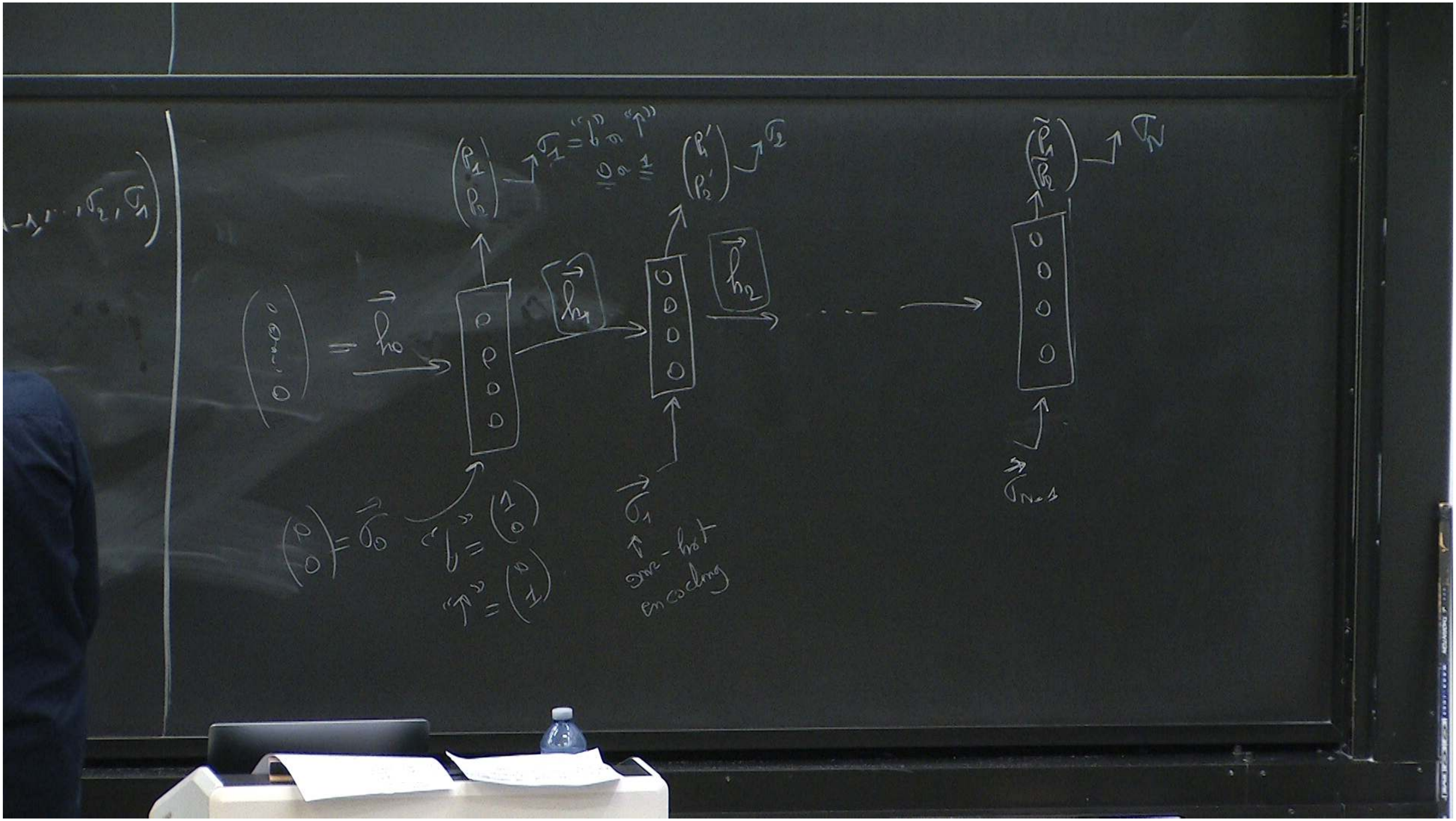
Dictionary size for spins = 2.

* Probability chain rule:

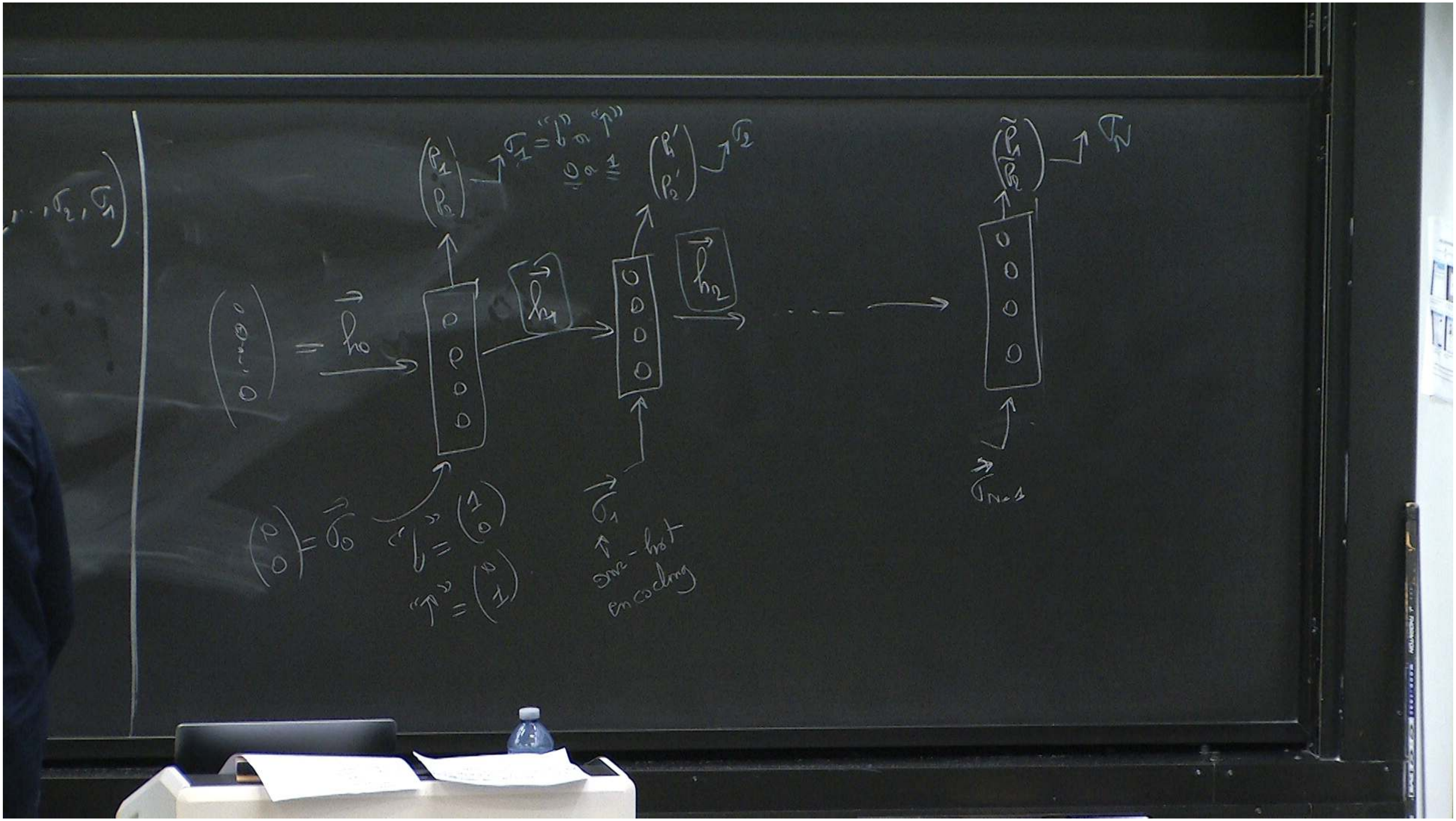
$$P(\sigma_1, \sigma_2, \dots, \sigma_N) = P(\sigma_1)\, P(\sigma_2 | \sigma_1) \dots P(\sigma_N | \sigma_{N-1}, \dots, \sigma_2, \sigma_1)$$

* Autoregressive sampling

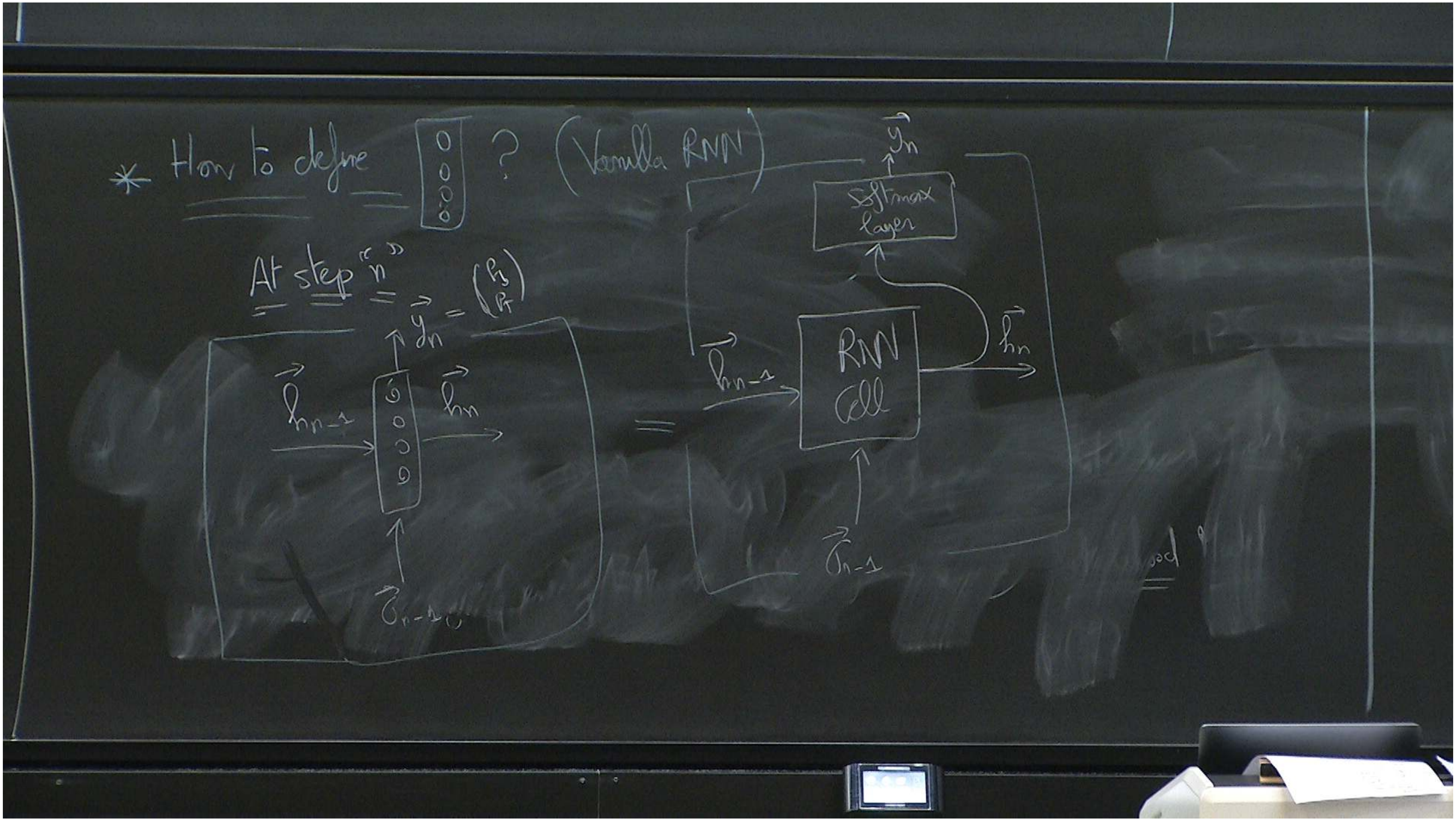

one - hot
encoding

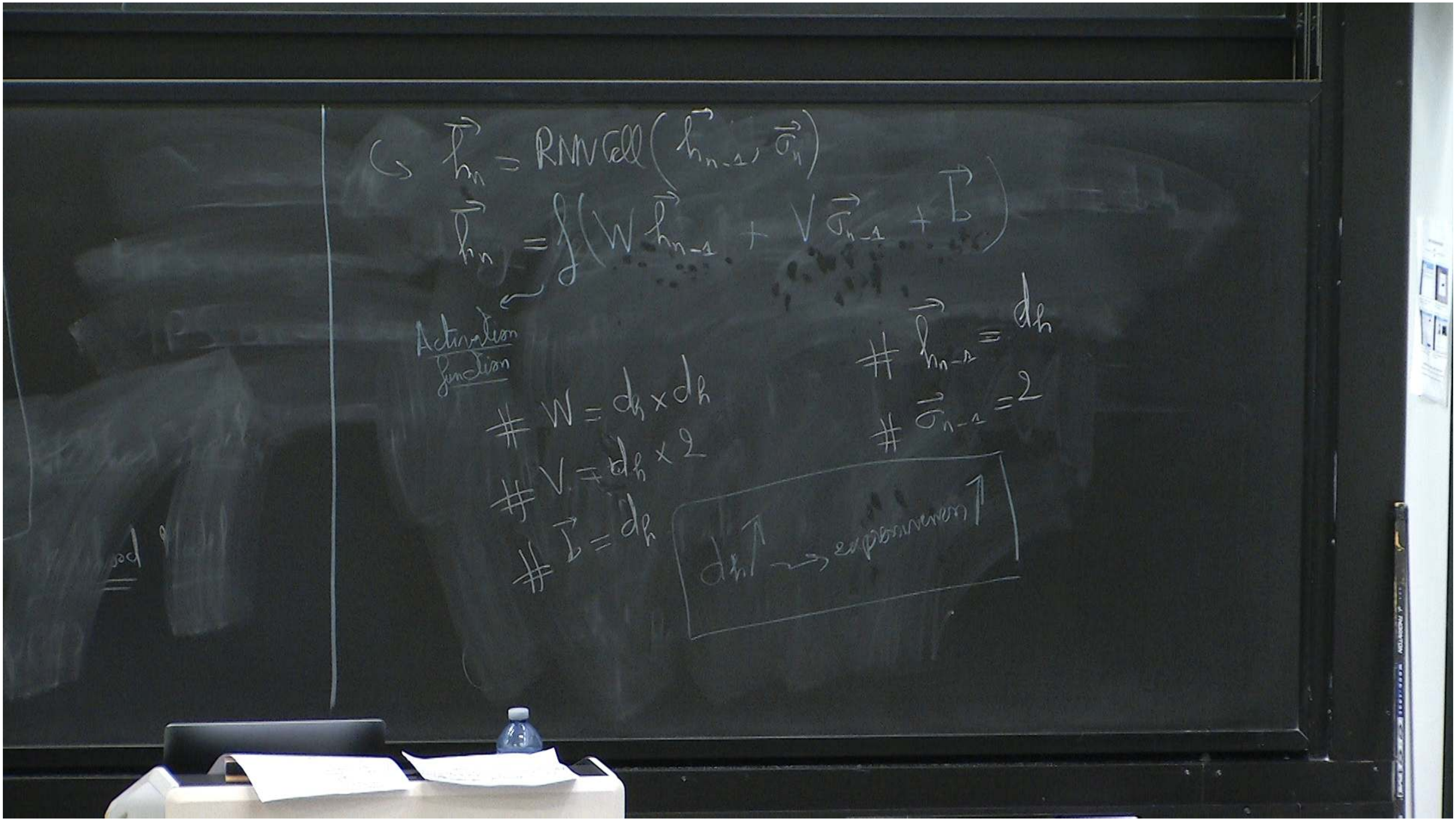


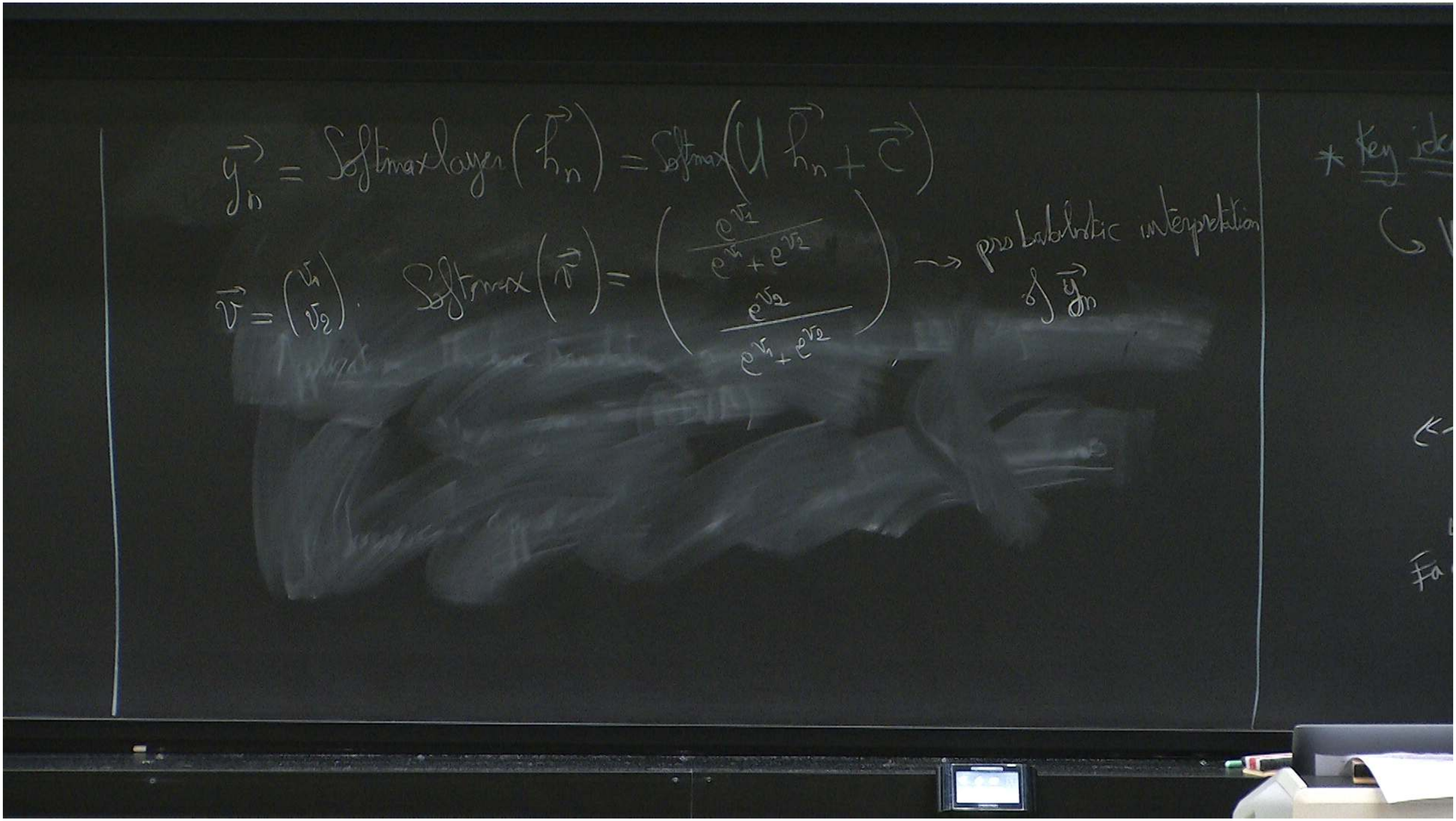
$\vec{h}_0$
$\vec{h}_1$
$\vec{h}_2$
one-hot
encoding



σ_1 = "↓" or "↑"
0 or 1
one-hot encoding
encoding


* How to define ? (Vanilla RNN)
At step "n"
yn
hn-1
hn
σn-1
Softmax layer
RNN Cell
hn-1
hn
yn
σn-1


$\hookrightarrow \vec{h}_n = \mathrm{RNNCell}(\vec{h}_{n-1}, \vec{\sigma}_n)$
$\vec{h}_n = f(W \vec{h}_{n-1} + V \vec{\sigma}_{n-1} + \vec{b})$
Activation function
$W = d_h \times d_h$
$V = d_h \times 2$
$\vec{b} = d_h$
$\vec{h}_{n-1} = d_h$
$\vec{\sigma}_{n-1} = 2$
$d_h \uparrow \rightarrow$ expressiveness $\uparrow$


$\vec{y}_n = \text{Softmaxlayer}(\vec{h}_n) = \text{Softmax}(U\vec{h}_n + \vec{c})$
$\vec{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$. $\text{Softmax}(\vec{v}) = \begin{pmatrix} \frac{e^{v_1}}{e^{v_1}+e^{v_2}} \\ \frac{e^{v_2}}{e^{v_1}+e^{v_2}} \end{pmatrix} \rightsquigarrow$ probabilistic interpretation of $\vec{y}_n$

$$\vec{y}_n = \text{Softmaxlayer}(\vec{h}_n) = \text{Softmax}(U\vec{h}_n + \vec{c})$$

$$\vec{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}. \quad \text{Softmax}(\vec{v}) = \begin{pmatrix} \dfrac{e^{v_1}}{e^{v_1}+e^{v_2}} \\[2ex] \dfrac{e^{v_2}}{e^{v_1}+e^{v_2}} \end{pmatrix} \longrightarrow \text{probabilistic interpretation of } \vec{y}_n$$

* $P_{RNN} = P_1 \times P_2 \times \dots \times P_N$

↳ Normalized probability distribution

* $P_{RNN} = |\psi_{RNN}|^2$

↳ RNN wave function

② Variational Monte Carlo with RNNs

* Variational principle

$$\hat{H}|\Psi_G\rangle = E_G|\Psi_G\rangle$$

2^N

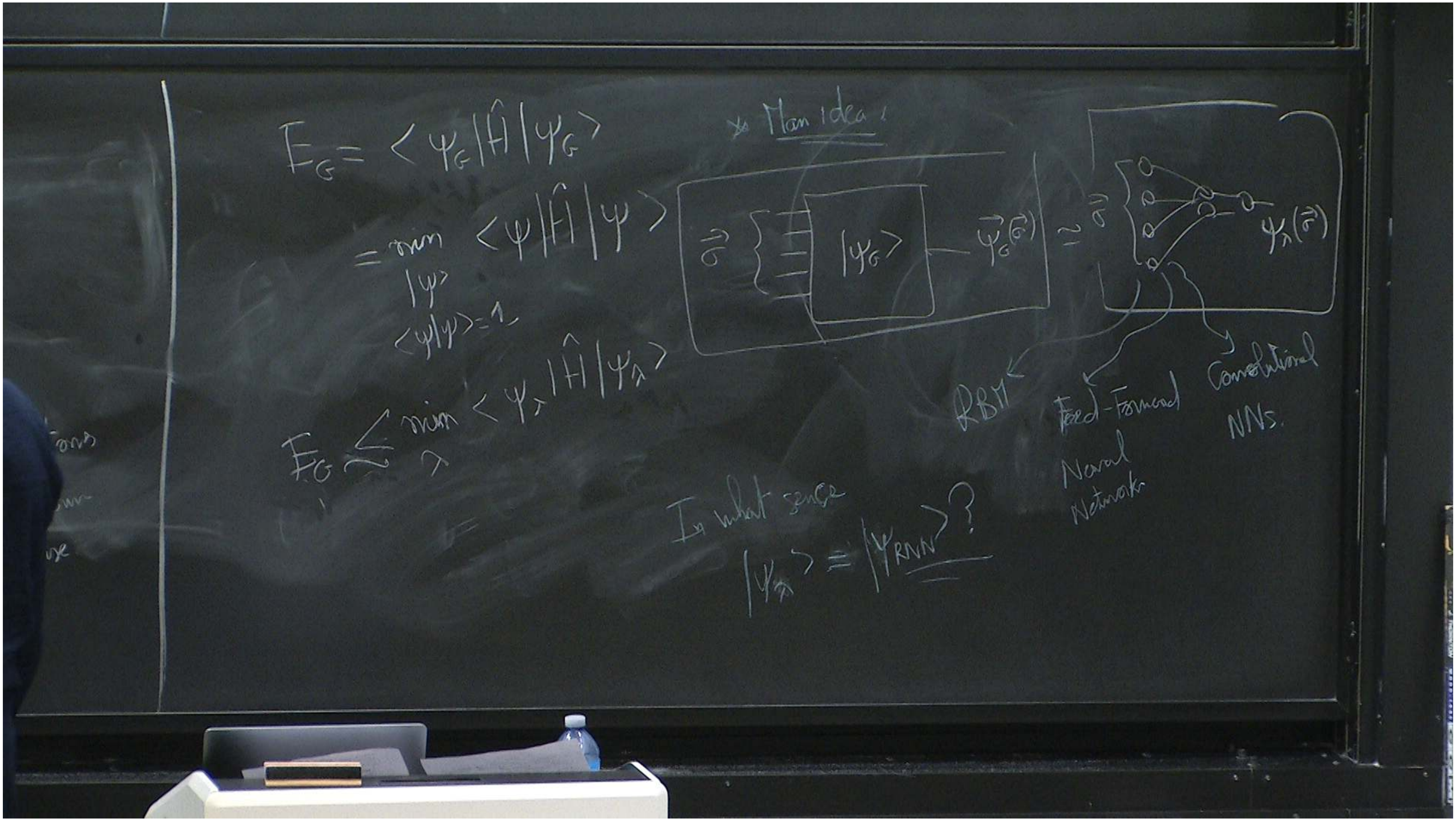
2^N

Diagonalize

$$\begin{pmatrix} E_G & & \\ & \ddots & \\ & & \ddots \end{pmatrix}$$

$O(2^{cN})$

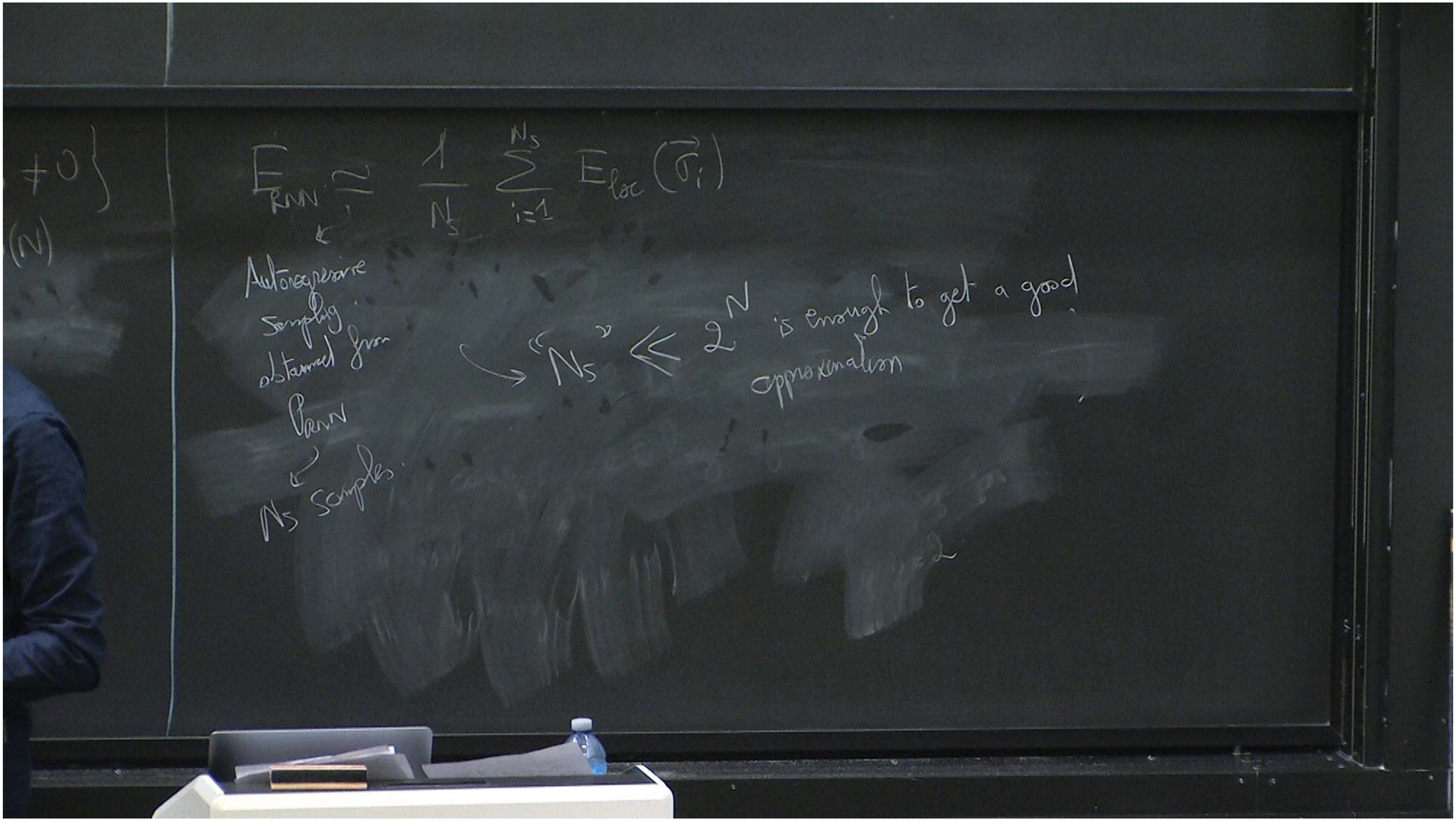
$2^{266} \simeq 10^{80} \sim$ # Atoms in known universe

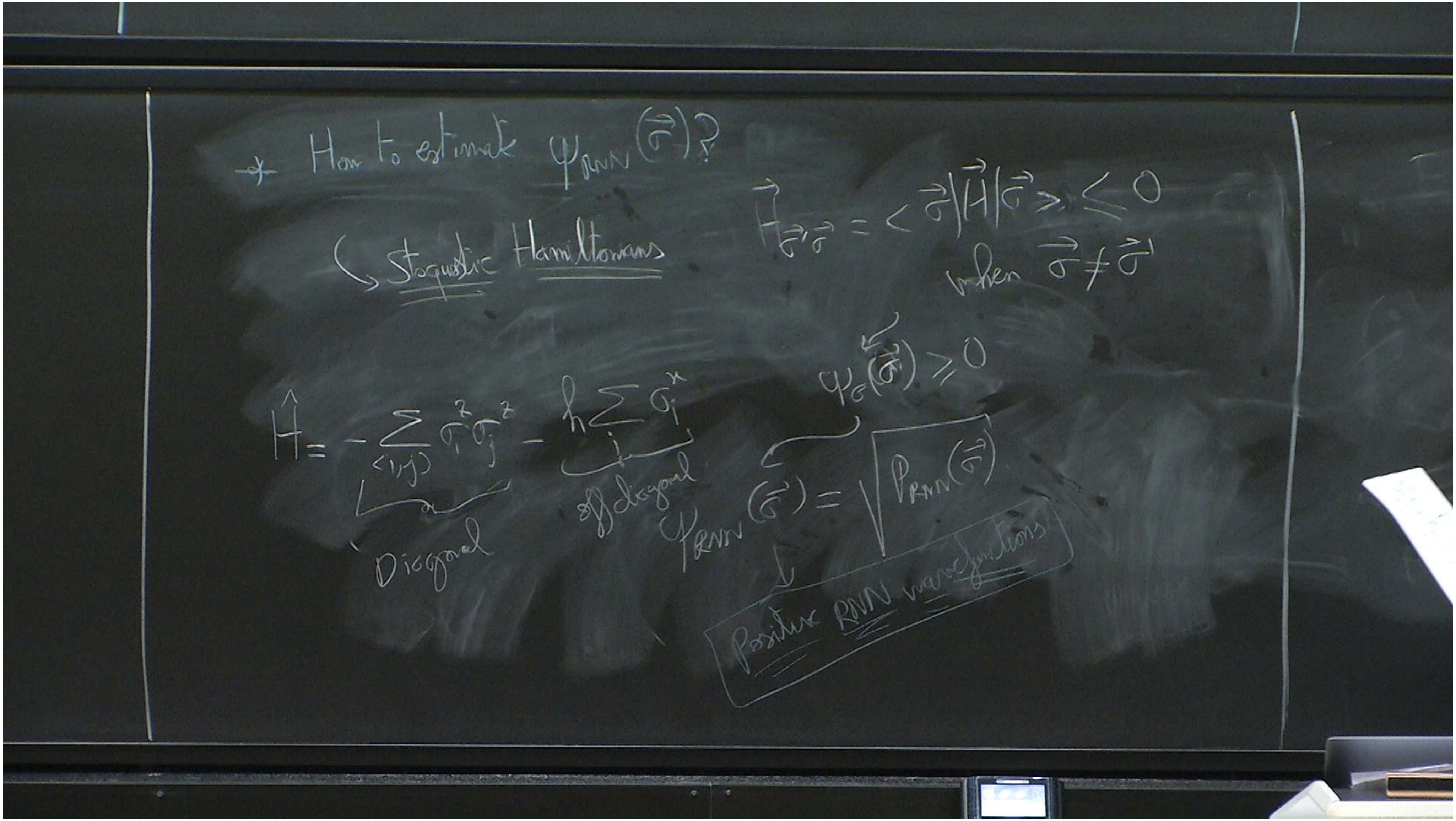

$E_G = \langle \psi_G | \hat{H} | \psi_G \rangle$
$= \min_{|\psi\rangle, \langle\psi|\psi\rangle = 1} \langle \psi | \hat{H} | \psi \rangle$
$E_G \lesssim \min_{\lambda} \langle \psi_\lambda | \hat{H} | \psi_\lambda \rangle$
Main idea:
$\vec{\sigma}$
$|\psi_G\rangle$
$\psi_G(\vec{\sigma})$
$\simeq$
$\psi_\lambda(\vec{\sigma})$
RBM
Feed-Forward Neural Network
Convolutional NNs.
In what sense
$|\psi_\lambda\rangle \simeq |\psi_{RNN}\rangle$?

$$E_{RNN} = \langle \Psi_{RNN} | \hat{H} | \Psi_{RNN} \rangle$$

$$= \sum_{\vec{\sigma}, \vec{\sigma}'} \Psi^*_{RNN}(\vec{\sigma}) \, H_{\vec{\sigma}\vec{\sigma}'} \, \Psi_{RNN}(\vec{\sigma}')$$

$$= \sum_{\vec{\sigma}} \underbrace{|\Psi_{RNN}(\vec{\sigma})|^2}_{P_{RNN}(\vec{\sigma})} \underbrace{\left(\sum_{\vec{\sigma}'} H_{\vec{\sigma}\vec{\sigma}'} \frac{\Psi_{RNN}(\vec{\sigma}')}{\Psi_{RNN}(\vec{\sigma})} \right)}_{\text{Local energy } E_{loc}(\vec{\sigma})}$$


$E_{RNN} \simeq \frac{1}{N_s} \sum_{i=1}^{N_s} E_{loc}(\vec{\sigma}_i)$
Autoregressive sampling obtained from P_{RNN}
N_s samples
"N_s" $\ll 2^N$ is enough to get a good approximation


* How to estimate $\psi_{RNN}(\vec{\sigma})$?
↳ Stoquastic Hamiltonians
$H_{\vec{\sigma}',\vec{\sigma}} = \langle \vec{\sigma}' | \hat{H} | \vec{\sigma} \rangle \leq 0$
when $\vec{\sigma} \neq \vec{\sigma}'$
$\psi_G(\vec{\sigma}) \geq 0$
$\hat{H} = -\sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x$
Diagonal
off diagonal
$\psi_{RNN}(\vec{\sigma}) = \sqrt{P_{RNN}(\vec{\sigma})}$
Positive RNN wavefunctions

* How to estimate $\psi_{RNN}(\vec{\sigma})$?

↳ Stoquastic Hamiltonians

$$H_{\vec{\sigma}',\vec{\sigma}} = \langle \vec{\sigma}' | \hat{H} | \vec{\sigma} \rangle \leq 0$$

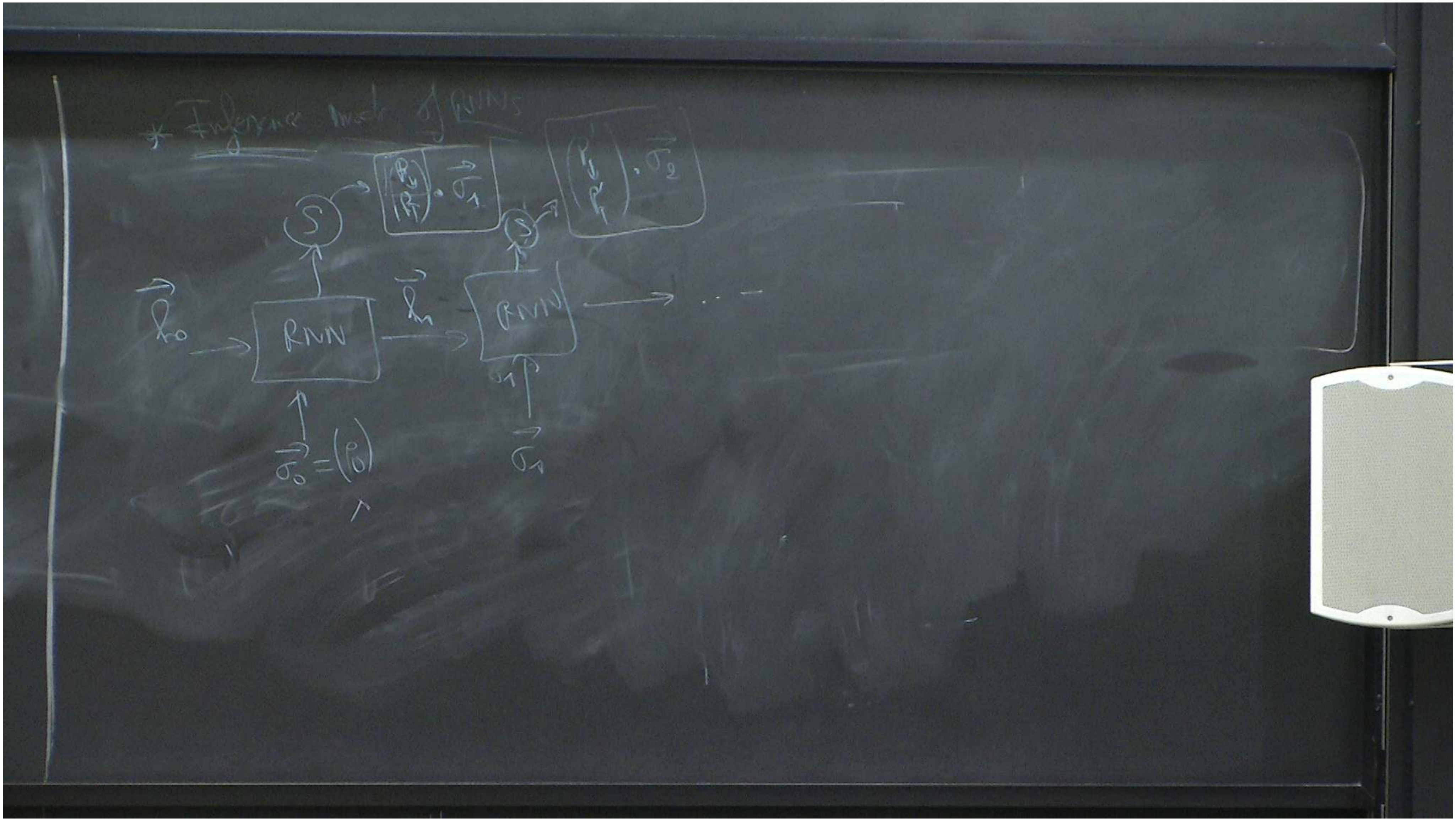
when $\vec{\sigma} \neq \vec{\sigma}'$

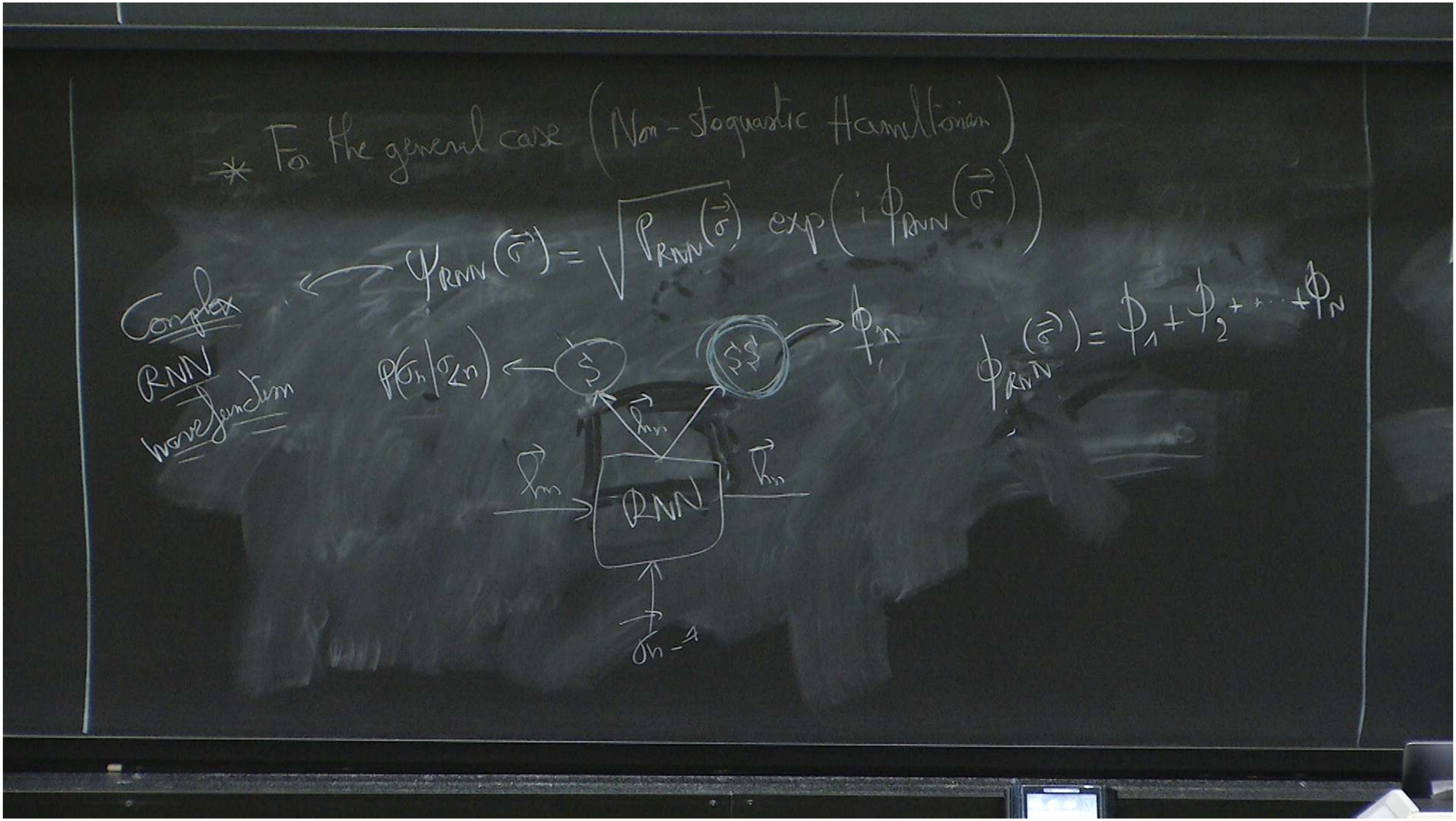
$$\psi_G(\vec{\sigma}) \geq 0$$

$$\hat{H} = \underbrace{-\sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z}_{\text{Diagonal}} \underbrace{- h \sum_i \sigma_i^x}_{\text{off diagonal}}$$

$$\psi_{RNN}(\vec{\sigma}) = \sqrt{P_{RNN}(\vec{\sigma})}$$

$\boxed{\text{Positive RNN wavefunctions}}$


* Inference mode of RNNs
RNN
RNN


* For the general case (Non-stoquastic Hamiltonian)
$\psi_{RNN}(\vec{\sigma}) = \sqrt{P_{RNN}(\vec{\sigma})}\ \exp\left(i\,\phi_{RNN}(\vec{\sigma})\right)$
Complex RNN wavefunction
$\phi_{RNN}(\vec{\sigma}) = \phi_1 + \phi_2 + \cdots + \phi_N$
$P(\sigma_n|\sigma_{<n})$
$
$$
ϕ_n
$\vec{h}_n$
RNN
$\vec{h}_{n-1}$
σ_{n-1}

$$\vec{\phi}_n = \mathcal{S}\left(\vec{h}_n\right) = \pi\, \mathrm{Softsign}\left(U'\,\vec{h}_n + \vec{c}\,'\right)$$

$$\mathrm{Softsign}(x) = \frac{x}{1+|x|} \in (-1,1)$$