Title: Quantum Matter Lecture

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Variational Principle In Quantum Physics

Motivation:

An important mission of modern physics is to uncover the mysteries of Quantum many-body physics.

Exotic phases of matter.

- High T_c superconductors.
- Quantum fluids
- Topological materials

In certain regimes.

Very hard to understand theoretically & Exp.

Use Numerical Tools.

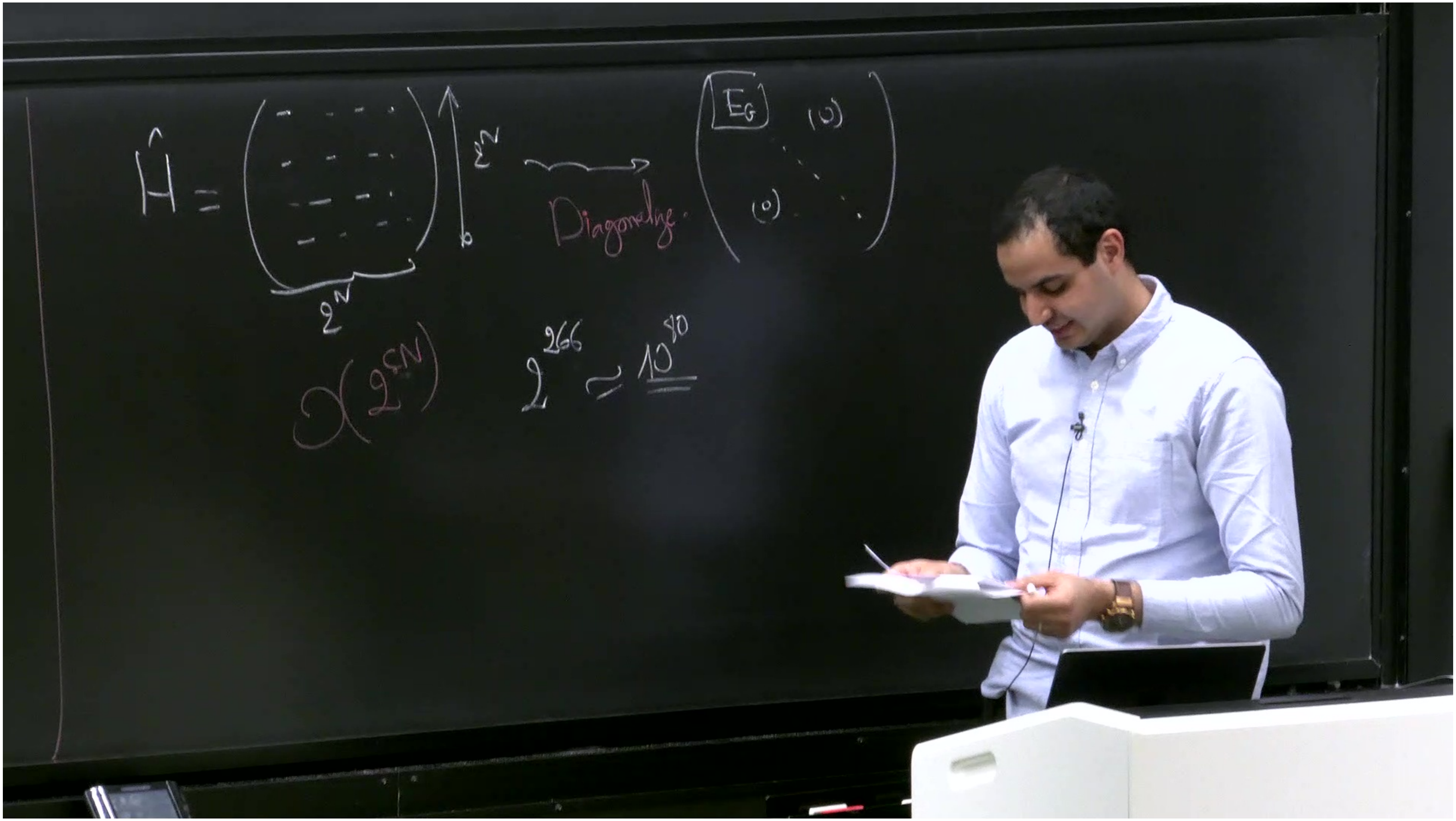
We are interested in finding the GS of the system $|\psi_G\rangle$

1. Identify problems with the exact approach.
2. Variational Principle.
3. Variational Monte Carlo.

How can we find $|\Psi_G\rangle$ given some Hamiltonian $\hat{H}$?

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

For N spins $\underbrace{\downarrow\uparrow\cdots\downarrow}_{N} \rightarrow 2^N$ possibilities $\rightarrow |\Psi_G\rangle = \left(\quad\right)\Big\updownarrow 2^N$


Ĥ =
2^N
Diagonalize.
E_G
(0)
(0)
O(2^{SN})
2^266 ≃ 10^80

In 1D TFIM $\longrightarrow$ Jordan-Wigner Tr $\longrightarrow$ Free Fermion

$\downarrow$

Fourier Transf.

« Analytical techniques »   « Fractionalization »

$\swarrow$

Not always possible

$\hookrightarrow$ Quantum Monte Carlo (QMC)

$$\hat{\rho} = \frac{e^{-\beta\hat{H}}}{Z} \qquad Z = \mathrm{Tr}\left(e^{-\beta\hat{H}}\right) = \dots = \mathrm{Tr}\left(e^{-\beta H^{D+1}_{\text{classical}}}\right)$$

TFIM $\longrightarrow$ Jordan - Wiegner Tr $\longrightarrow$ Free Fermion

$\downarrow$

Fourier Transf.

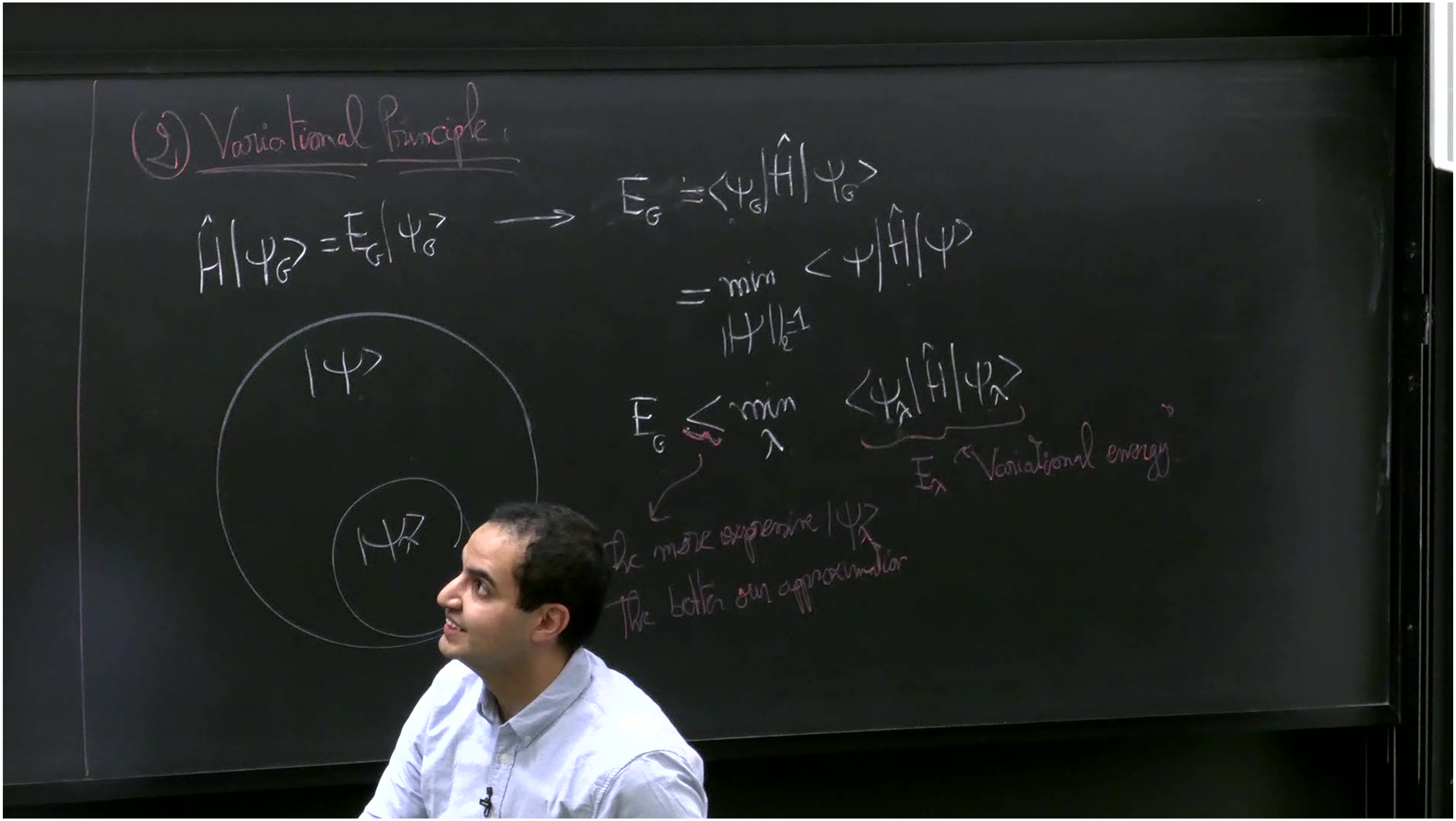
"techniques" "Fractionalization"

Quantum - Classical mapping

Quantum Monte Carlo (QMC).

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z} \qquad Z = \mathrm{Tr}\left(e^{-\beta \hat{H}}\right) = \dots = \mathrm{Tr}\left(e^{-\beta H^{D+1}_{\text{classical}}}\right).$$

(2) Variational Princ


(2) Variational Principle:
$\hat{H}|\psi_G\rangle = E_G|\psi_G\rangle \longrightarrow E_G = \langle\psi_G|\hat{H}|\psi_G\rangle$
$= \min_{\|\psi\|_2=1} \langle\psi|\hat{H}|\psi\rangle$
$|\psi\rangle$
$|\psi_\lambda\rangle$
$E_G \leq \min_\lambda \underbrace{\langle\psi_\lambda|\hat{H}|\psi_\lambda\rangle}_{E_\lambda}$
Variational energy
The more expensive $|\psi_\lambda\rangle$
The better our approximation

$\rho = \frac{\cdot}{Z}$

How to find the min of E_λ?

$$\partial_\lambda E_\lambda = 0 \longrightarrow \lambda^* = \lambda$$

↳ BCS theory

↳ Laughlin

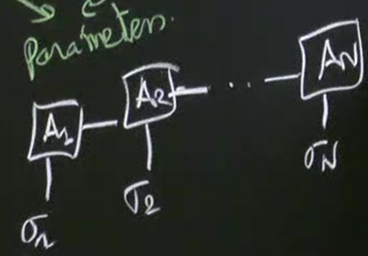
HW1

↳ Mean-field ansatz (MF) and Matrix product states (MPS)

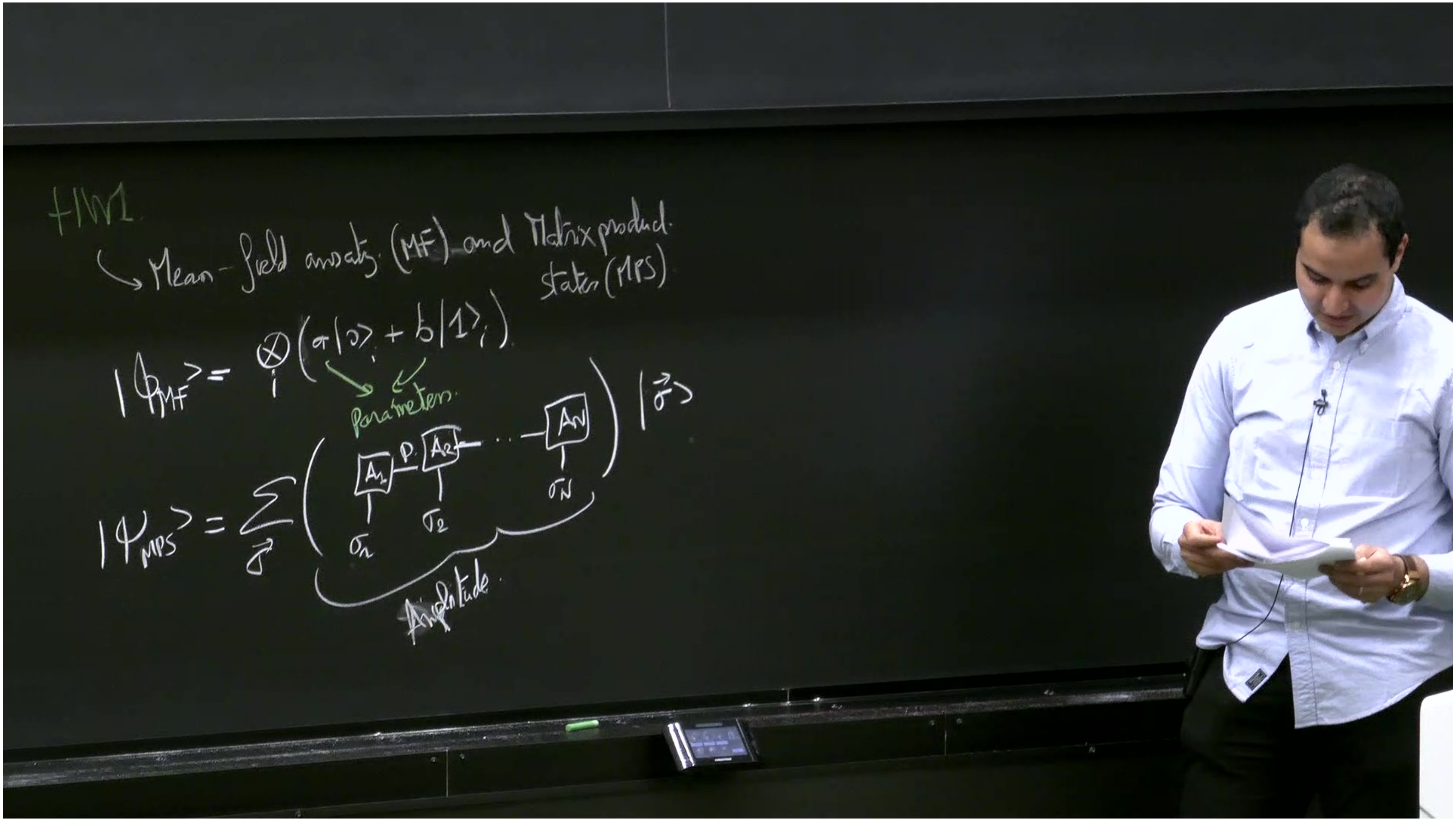
$$|\Psi_{MF}\rangle = \bigotimes_i \left(a|0\rangle_i + b|1\rangle_i \right)$$

parameters

$$|\Psi_{MPS}\rangle = \sum_{\vec{\sigma}} \Big($$



$$\Big)$$


HW1
Mean-field ansatz (MF) and Matrix product states (MPS)
$|\psi_{MF}\rangle = \bigotimes_i (a|0\rangle_i + b|1\rangle_i)$
Parameters
$|\psi_{MPS}\rangle = \sum_{\vec{\sigma}} (\dots) |\vec{\sigma}\rangle$
A_1 A_2 A_N D
σ_1 σ_2 σ_N
Amplitude

* Solving $\partial_\lambda E_\lambda = 0$ is not always possible.

$$\lambda \leftarrow \lambda - \overbrace{\underbrace{\varepsilon}_{\substack{>0 \\ \text{learning rate}}} \partial_\lambda \bar{E}_\lambda}^{\delta\lambda}$$

$$E_{\lambda+\delta\lambda} = \bar{E}_\lambda + \delta\lambda\, \partial_\lambda E_\lambda + O\left((\delta\lambda)^2\right)$$

$$= E_\lambda - \underbrace{\varepsilon\left(\partial_\lambda E_\lambda\right)^2} + \dots$$

* Calculating E_λ and its gradients exactly is not always possible.

* Ex. Jastrow factor:

$$|\psi_{jf}\rangle = \sum_{\sigma} \exp\left(\sum_{ij} \overset{\lambda}{\tilde{J}_{ij}}\, \sigma_i \sigma_j \right) |\sigma\rangle$$

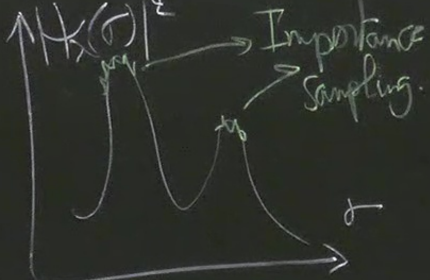
$\langle \psi_{jf} | \hat{H} | \psi_{jf} \rangle$ not efficient $\psi_{jf}(\sigma)$.

3. Variational Monte Carlo (VMC)

Let $|\psi_\lambda\rangle = \sum_\sigma \psi_\lambda(\sigma)\,|\sigma\rangle$.

$$E_\lambda = \langle\psi_\lambda|\hat{H}|\psi_\lambda\rangle = \sum_\sigma \sum_{\sigma'} \psi^*_\lambda(\sigma)\langle\sigma|\hat{H}|\sigma'\rangle\,\psi_\lambda(\sigma') \times \frac{\psi_\lambda(\sigma)}{\psi_\lambda(\sigma)}$$

$2^N \times 2^N$ (exp).



$$= \sum_\sigma \underbrace{|\psi_\lambda(\sigma)|^2}_{\text{Prob.}} \underbrace{\left(\sum_{\sigma'} \langle\sigma|H|\sigma'\rangle \cdot \frac{\psi_\lambda(\sigma')}{\psi_\lambda(\sigma)}\right)}_{\text{Local energy } E_{loc}(\sigma)}$$

$$\simeq \frac{1}{M}\sum_{i=1}^{M} E_{loc}(\sigma^{(i)})$$

$\{\sigma^{(i)}\}_{i=1}^{M}$ $(\ll 2^N)$

$\sim |\psi_\lambda(\sigma)|^2$

Metropolis - Hasting Scheme

$$\tilde{\sigma}_1 \longrightarrow \tilde{\sigma}_2 \longrightarrow \cdots \longrightarrow \tilde{\sigma}_{\underline{M\times N}}$$

$$A(\sigma_i \to \sigma_{i+1}) = \min\left(1, \frac{|\psi_\lambda(\sigma_{i+1})|^2}{|\psi_\lambda(\sigma_i)|^2}\right)$$

N times (sweep)

Prob.

Local energy $E_{loc}(\sigma)$.

$$\#\{\sigma' / \langle\sigma|\hat{H}|\sigma'\rangle \neq 0\} = O(N)$$ for local (Physical) Hamiltonians

$$\hat{H} = \sum_{i=1}^{L} \sigma_i^z \sigma_{i+1}^z - g \sum_{i=1}^{N} \sigma_i^x$$

$$\hat{H}|\downarrow\downarrow\downarrow\rangle = -3|\downarrow\downarrow\downarrow\rangle - g|\uparrow\downarrow\downarrow\rangle - g|\downarrow\uparrow\downarrow\rangle - g|\downarrow\downarrow\uparrow\rangle$$

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Local energy $E_{loc}(\sigma)$.

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Zero-Variance principle

$$\mathrm{Var}(E_{loc}(\sigma)) \longrightarrow 0 \text{ (Near convergence).}$$

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```
In [ ]: from optimization import *
```

Hamiltonian of the Hydrogen *Atom*

$$\hat{H} = -\frac{1}{2}\frac{\partial^2}{\partial^2 r} + \frac{l(l+1)}{2r^2} - \frac{1}{r}$$

We consider $n = 0$ (principal quantum number), $l = 0$ (angular momentum) to get the ground state. Physical constants are absorbed in `r`.

- Ground state energy: $E_G = -\frac{1}{2}$

- Ground state: $\psi_G(r) = r\exp(-r)$

1. Define the variational wave function (ansatz)

$\psi(r)$

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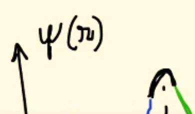

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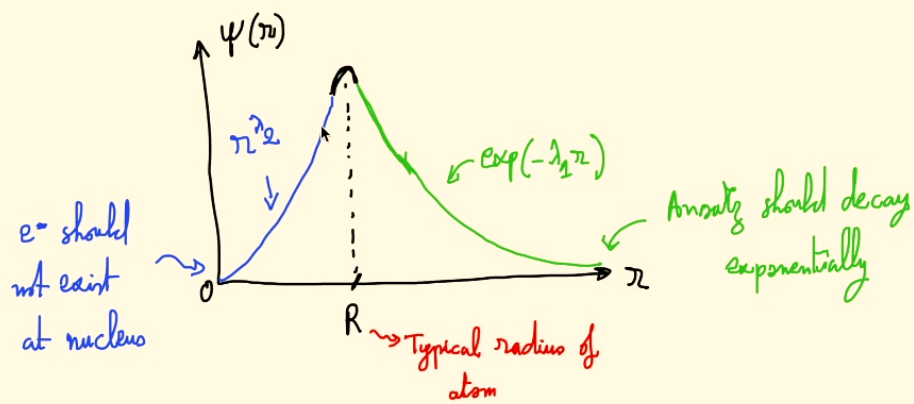

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Trusted | Python 3 (ipykernel)

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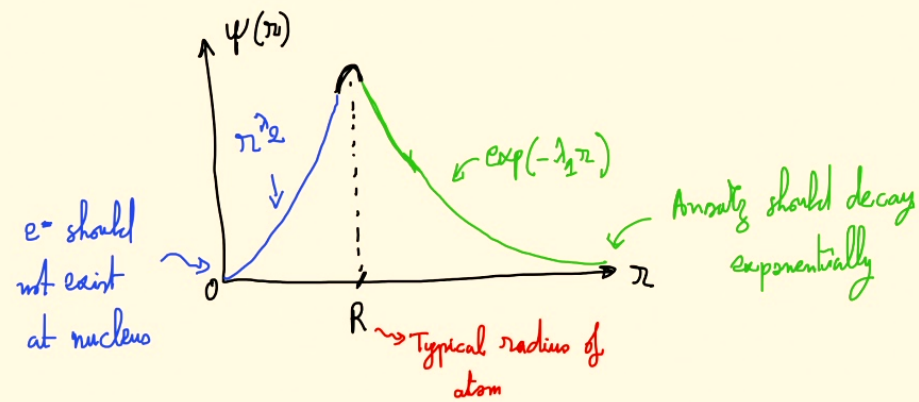
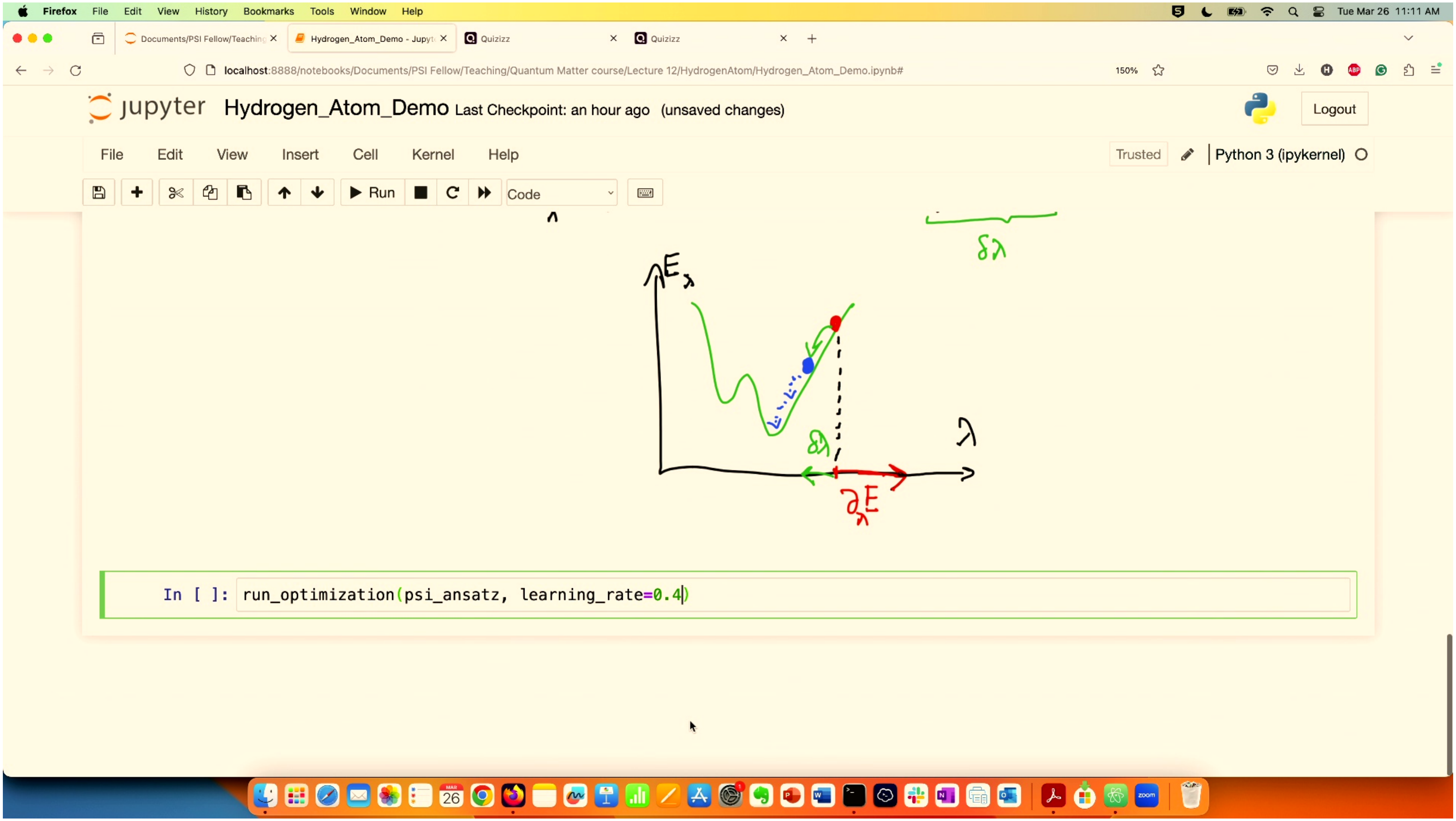


$$\psi_{\lambda_1,\lambda_2}(r) = r^{\lambda_2}\exp(-\lambda_1 r)$$

Initial Guess: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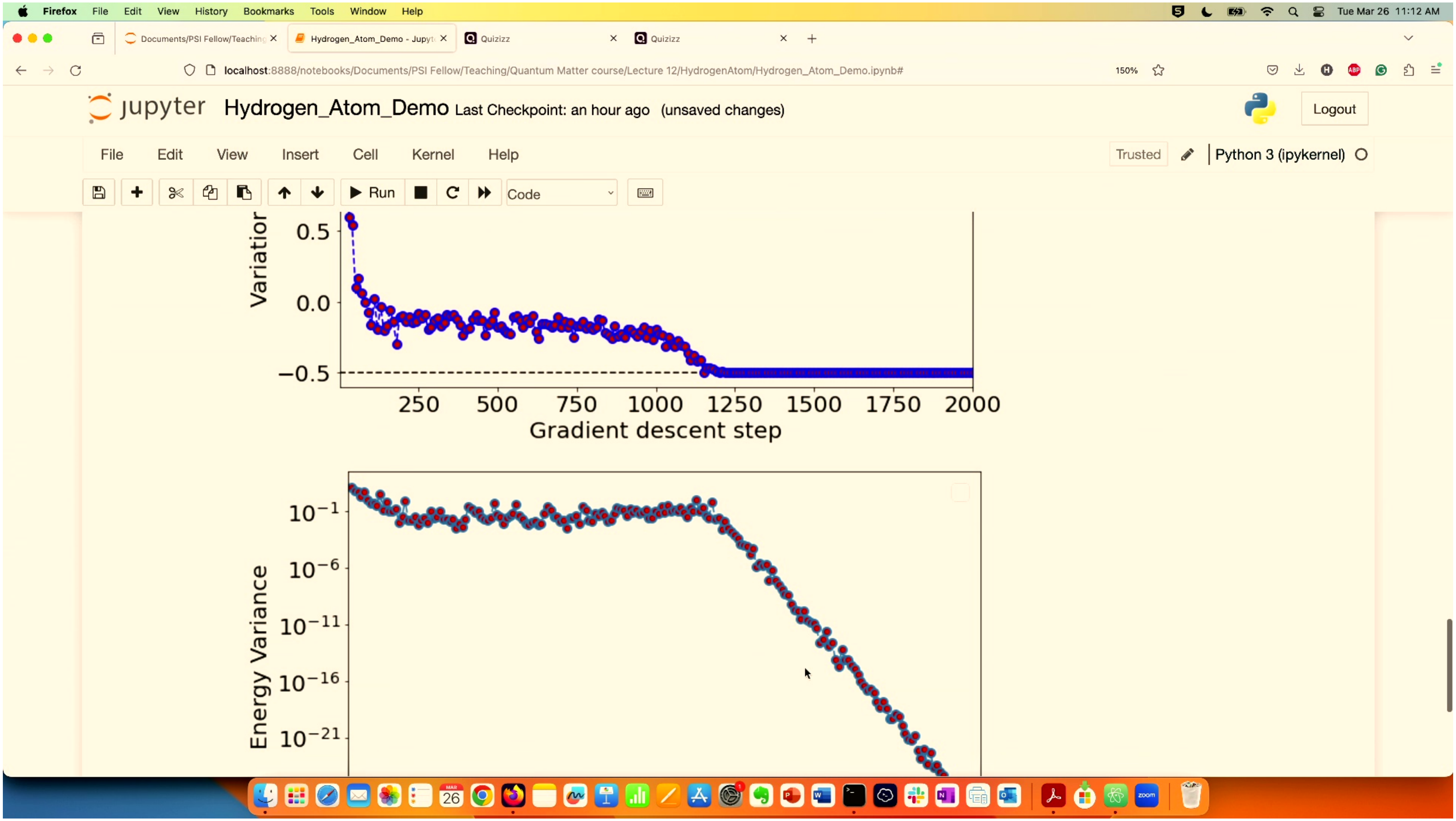
Trusted
Python 3 (ipykernel)
Run
Code
δλ
E_λ
λ
δλ
$\partial_\lambda E$
In [ ]: run_optimization(psi_ansatz, learning_rate=0.4)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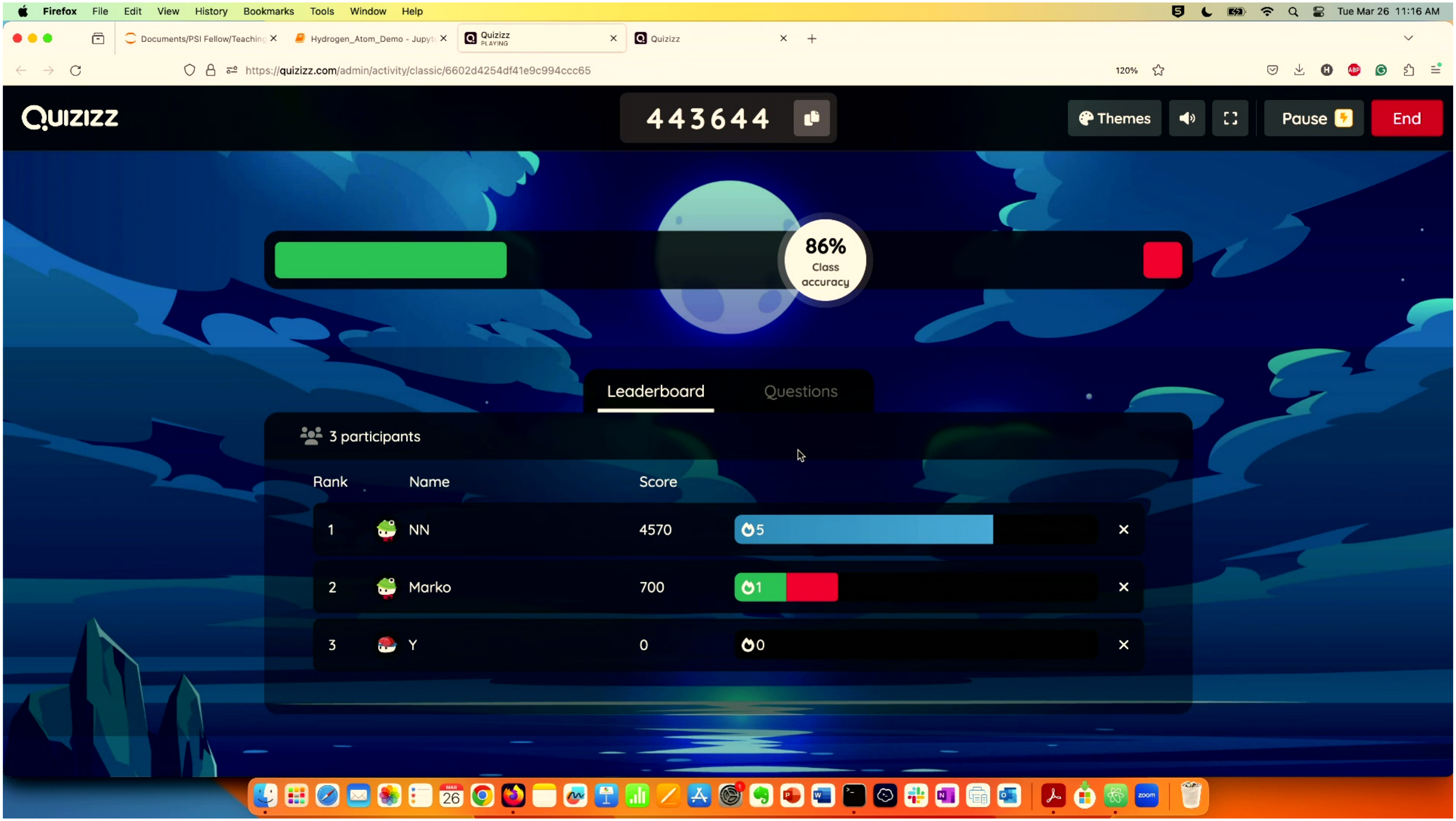
Trusted
Python 3 (ipykernel)
Run
Code
Variation
0.5
0.0
−0.5
250 500 750 1000 1250 1500 1750 2000
Gradient descent step
Energy Variance
10^−1
10^−6
10^−11
10^−16
10^−21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