

Title: Quantum Matter Lecture

Speakers: Mohamed Hibat Allah

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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  $T_c$   
superconductor

Quantum  
fluids

Topological  
materials

In certain regimes.  
Very hard to understand  
theoretically & Exp.



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

Use Numerical Tools

① Identify problems with the exact approach.

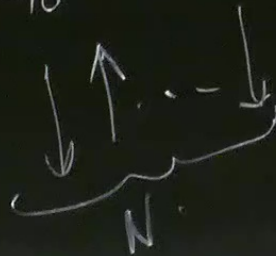
② Variational Principle.

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



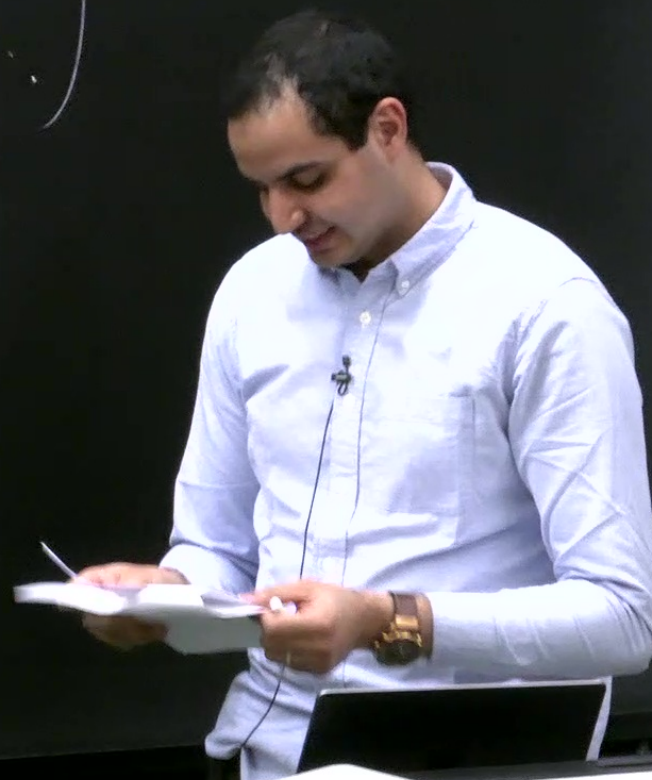
$\rightarrow 2^N$  possibilities

$$\rightarrow |\psi_G\rangle = \begin{pmatrix} \vdots \\ \vdots \\ \vdots \end{pmatrix} \uparrow_{2^N}$$



$$\hat{H} = \underbrace{\begin{pmatrix} - & - & - \\ - & - & - \\ - & - & - \\ - & - & - \end{pmatrix}}_{\mathbb{R}^{2N}} \xrightarrow{\mathbb{R}^{2N}} \text{Diagonalize} \begin{pmatrix} E_0 & & \\ & \ddots & \\ & & 0 \end{pmatrix}$$

$$2^{266} \approx \underline{\underline{10^{80}}}$$



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

“Analytical techniques” “Fractionalization”

Formal Transf.

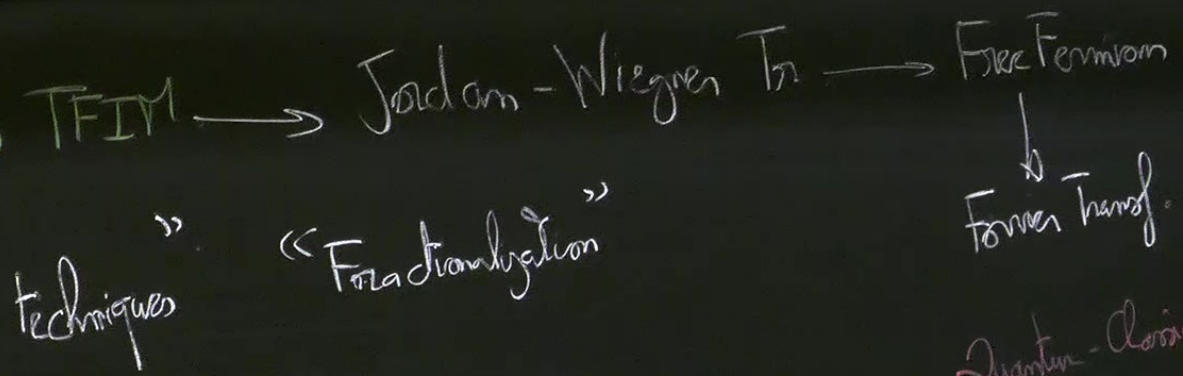
Not always possible

Quantum Monte Carlo (QMC)

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z}$$

$$Z = \text{Tr}(e^{-\beta \hat{H}}) = \dots = \text{Tr}(e^{-\beta H_{\text{classical}}})$$

N



Quantum-classical mapping

↓

Quantum Monte Carlo (QMC)

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z}$$

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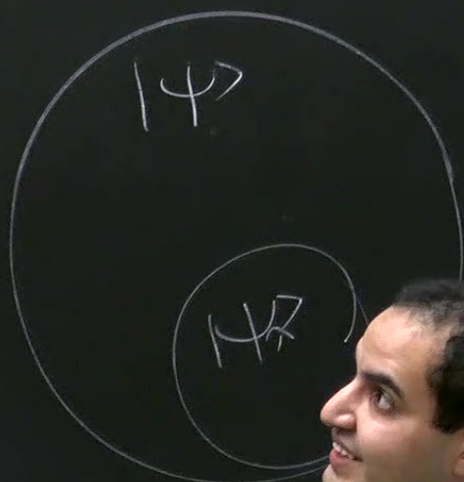
② Variational Part



## ② Variational Principle

$$\hat{H}|\psi_0\rangle = E_0|\psi_0\rangle \rightarrow$$

$$E_0 = \langle \psi_0 | \hat{H} | \psi_0 \rangle$$
$$= \min_{\|\psi\|_2=1} \langle \psi | \hat{H} | \psi \rangle$$



$$E_0 \leq \min_{\lambda} \underbrace{\langle \psi_\lambda | \hat{H} | \psi_\lambda \rangle}_{E_\lambda \text{ Variational energy}}$$

The more expensive  $|\psi_\lambda\rangle$   
The better our approximation



$$P = Z$$

How to find the min of  $E_n$ ?

$$\partial_{\lambda} E_n = 0 \rightarrow \lambda^* = \lambda$$

$\rightarrow$  BCS Theory  
 $\rightarrow$  Laughlin

FWL

$\rightarrow$  Mean-field ansatz (MF) and Matrix product states (MPS)

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

$\swarrow \quad \nwarrow$   
Parameters

$$|\Psi_{MPS}\rangle = \sum_{\vec{\sigma}} \left( \begin{array}{c} \boxed{A_1} \text{---} \boxed{A_2} \text{---} \dots \text{---} \boxed{A_N} \\ \sigma_1 \quad \sigma_2 \quad \quad \quad \sigma_N \end{array} \right)$$

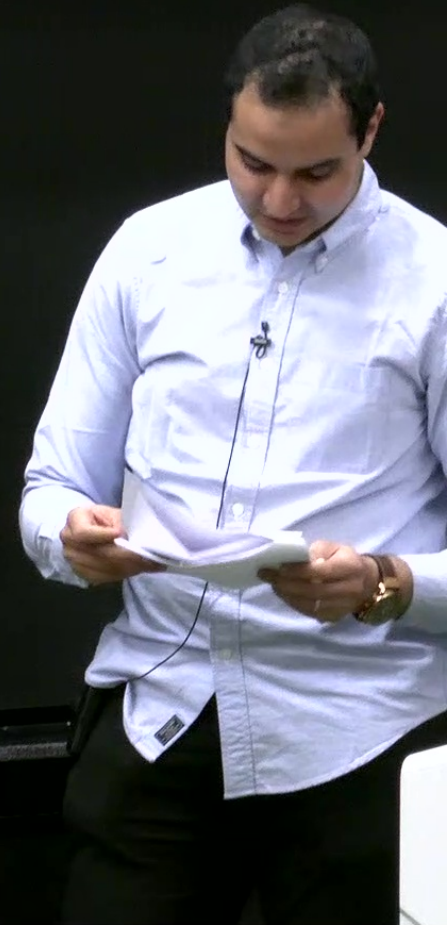
HW1

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

$$|\psi_{MF}\rangle = \bigotimes_i (a|\uparrow\rangle_i + b|\downarrow\rangle_i)$$

Parameters

$$|\psi_{MPS}\rangle = \sum_{\vec{\sigma}} \left( \underbrace{\left[ \begin{array}{c} \boxed{A_1} \text{---} \boxed{A_2} \text{---} \dots \text{---} \boxed{A_N} \\ \sigma_1 \quad \sigma_2 \quad \quad \quad \sigma_N \end{array} \right]}_{\text{Amplitude}} \right) |\vec{\sigma}\rangle$$



\* Lösung  $\partial_{\lambda} E_{\lambda} = 0$  is not always possible.

$$\lambda \leftarrow \lambda - \underbrace{\epsilon}_{\substack{> 0 \\ \text{learning rate}}} \partial_{\lambda} E_{\lambda}$$

$$\begin{aligned} E_{\lambda + S\lambda} &= \bar{E}_{\lambda} + S\lambda \partial_{\lambda} E_{\lambda} + O((S\lambda)^2) \\ &= \bar{E}_{\lambda} - \underbrace{\epsilon}_{\substack{> 0 \\ \text{learning rate}}} (\partial_{\lambda} E_{\lambda})^2 + \dots \end{aligned}$$





\* Calculating  $E_\lambda$  and its gradients exactly is not always possible.

\* Ex: Jastrow factor:  $\hat{H}$  

$$|\Psi_{JP}\rangle = \sum_{\sigma} \exp\left(\sum_{ij} J_{ij} \sigma_i \sigma_j\right) |\sigma\rangle$$

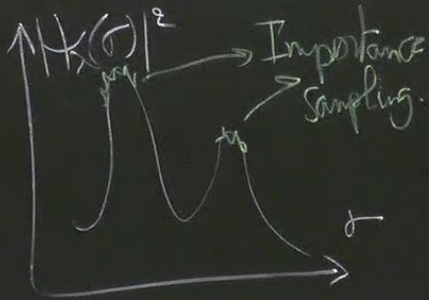
$\langle \Psi_{JP} | \hat{H} | \Psi_{JP} \rangle$  not efficient  $\Psi_{JP}(\sigma)$ .

### ③ Variational Monte Carlo (VMC)

$$\text{Let } |\Psi\rangle = \sum_{\sigma} \Psi_{\lambda}(\sigma) |\sigma\rangle$$

$$E_{\lambda} = \langle \Psi | \hat{H} | \Psi \rangle = \sum_{\sigma} \sum_{\sigma'} \underbrace{\Psi_{\lambda}^*(\sigma) \langle \sigma | \hat{H} | \sigma' \rangle \Psi_{\lambda}(\sigma')}_{\substack{\Psi_{\lambda}^*(\sigma) \\ \Psi_{\lambda}(\sigma')}} \underbrace{\Psi_{\lambda}(\sigma')}_{\Psi_{\lambda}(\sigma)}$$

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



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

$$\left\{ \sigma^{(i)} \right\}_{i=1}^M \approx \frac{1}{M} \sum_{i=1}^M E_{\text{loc}}(\sigma^{(i)})$$

$$\sim |\Psi_{\lambda}(\sigma)|^2$$

Metropolis-Hastings Scheme

$$\tilde{\sigma}_1 \rightarrow \tilde{\sigma}_2 \rightarrow \dots \rightarrow \tilde{\sigma}_{M \times N}$$

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

N Times (Sweep)



Prob.

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

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

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

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

Prob.

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

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Zero-Variance  
principle

$$\text{Var}(E_{loc}(\sigma)) \rightarrow 0 \text{ (Near convergence)}$$

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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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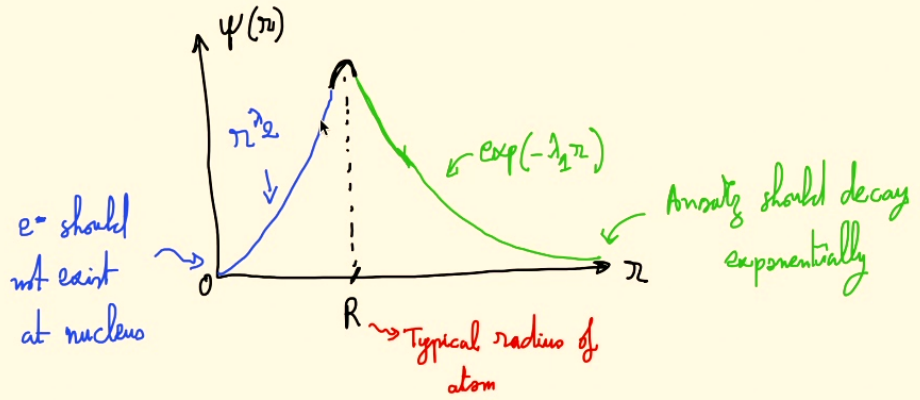
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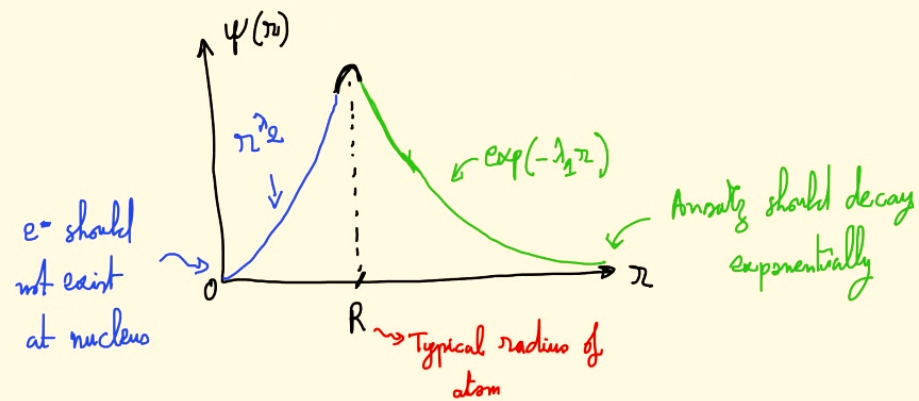
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### 1. Define the variational wave function (ansatz)



# 1. Define the variational wave function (ansatz)



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

Initial Guess:





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Run Code

The top plot shows the 'Variator' on the y-axis (ranging from -0.5 to 0.5) against 'Gradient descent step' on the x-axis (ranging from 0 to 2000). The data points, represented by blue and red dots, start at approximately 0.5 and rapidly descend, crossing the 0.0 line around step 100. They continue to decrease, reaching a stable plateau at approximately -0.5 after about 1200 steps. A dashed horizontal line is drawn at y = -0.5.

The bottom plot shows 'Energy Variance' on a logarithmic y-axis (ranging from  $10^{-21}$  to  $10^{-1}$ ) against 'Gradient descent step' on the x-axis (ranging from 0 to 2000). The data points, represented by blue and red dots, start at approximately  $10^{-1}$  and decrease rapidly, reaching a plateau around  $10^{-10}$  after about 1000 steps. After this plateau, the variance continues to decrease linearly on the log scale, reaching approximately  $10^{-21}$  by step 2000.

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