My Background

UNIVERSIDAD NACIONAL DE COLOMBIA
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Bachelor in Physics (2013)

MSc in Physics (2015)

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Speeding up Variational Quantum Monte Carlo by Machine Learning.

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My Background

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Pedro Alvares (MSc student)
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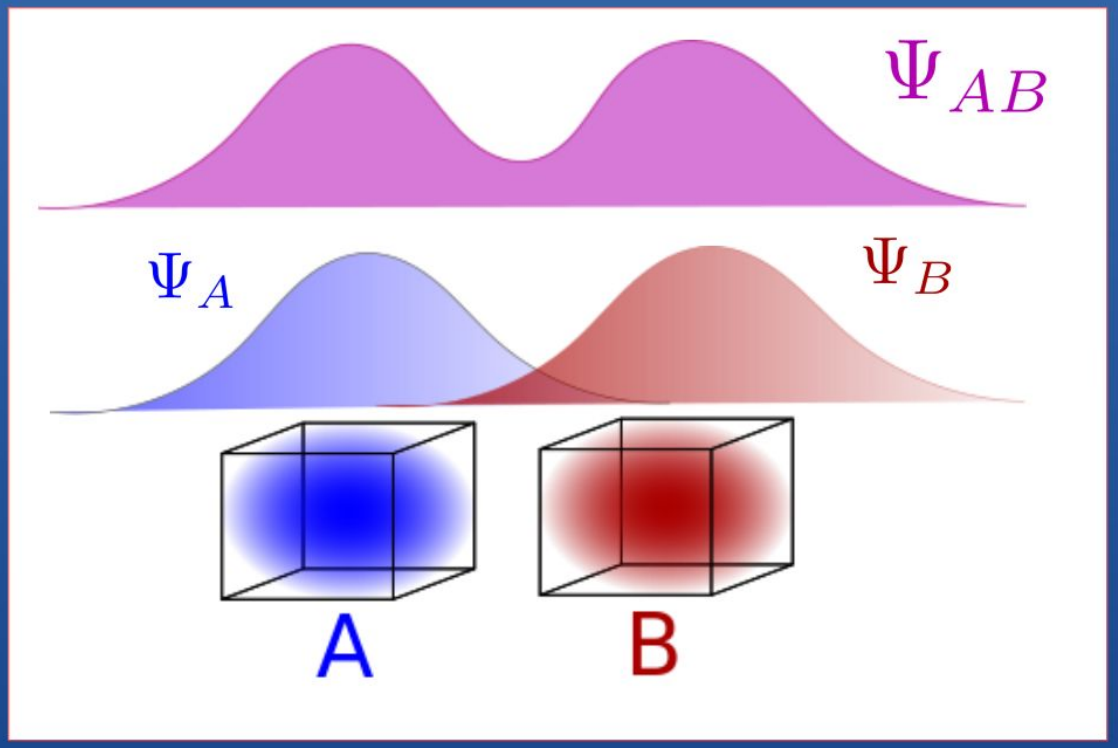
Introduction

- Quantum entanglement:

Non interacting

Separable!

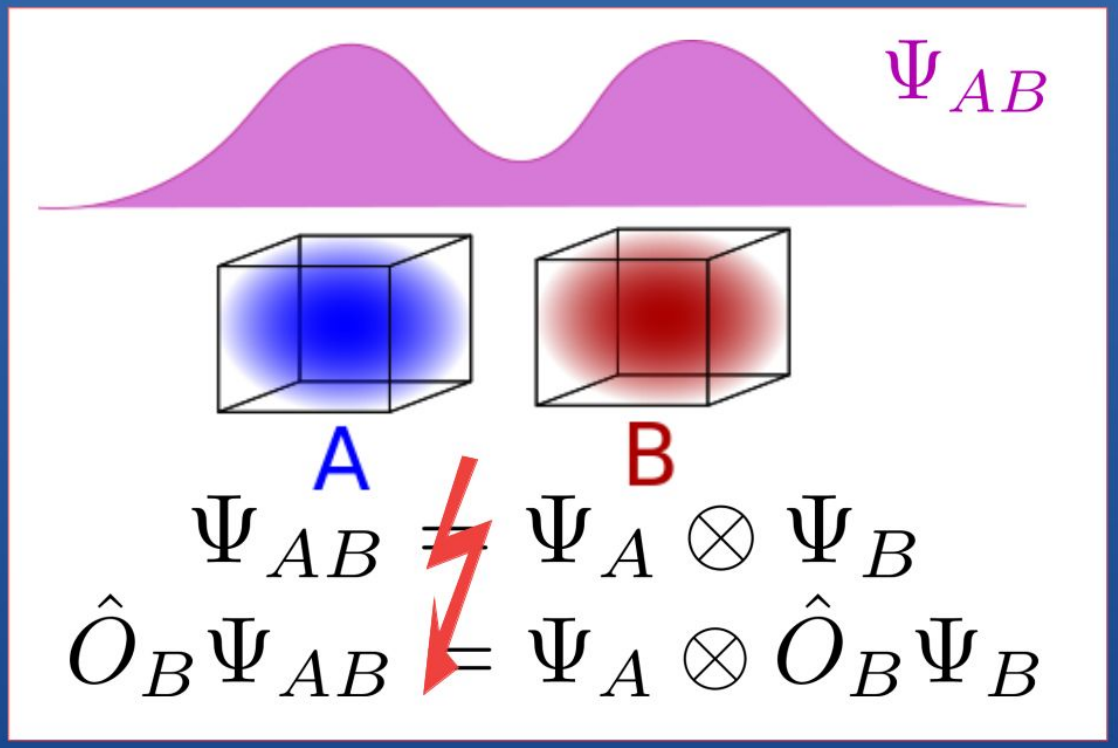


Interacting

Separable?

Introduction

- Quantum entanglement:



Interacting

Separable?

Introduction

- Quantum entanglement:

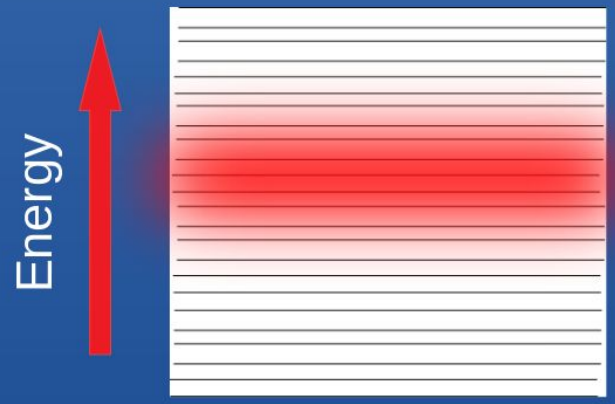
$$\Psi_{AB} \neq \Psi_A \otimes \Psi_B$$
$$\hat{O}_B \Psi_{AB} = \Psi_A \otimes \hat{O}_B \Psi_B$$

$$|S_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \qquad |S_{12}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |01\rangle + |10\rangle + |11\rangle)$$

$$|S_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \qquad |S_{12}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

Introduction

- Pure and mixed states



$$|\Psi_1\rangle$$
$$|\Psi\rangle = \sum c_i |\Psi_i\rangle$$

Pure state representation

$$\rho = \sum P_i |\Psi_i\rangle \langle\Psi_i| = \sum c_{ij} |\phi_i\rangle \langle\phi_j|$$

Mixed state representation

$$Pr = \sum P_i^2$$

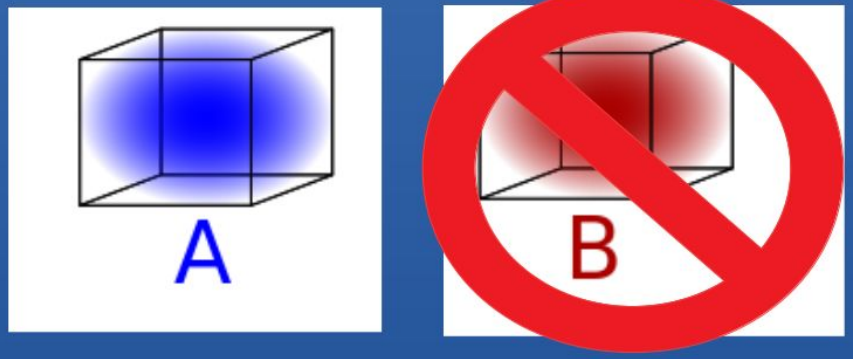
Purity

$$S_{VN} = -tr(\rho \; ln \; \rho) = -\sum P_i \; ln \; P_i \approx 1 - Pr$$

Von Neumann entropy

Introduction

- Entanglement measure



The state is well defined. (Pure)

ρ_{AB}

$$tr_B(\rho_{AB}) = \rho_A$$

$$S(\rho_A) = -tr(\rho_A \, ln \, \rho_A)$$

$$S_L(\rho_A) = 1 - tr(\rho_A^2)$$

Linear entropy

ρ_A Reduced density matrix

Bipartite entanglement

Motivation

- Entanglement properties of systems of interacting particles, in view of their possible use in quantum information technology.
- Atoms, molecules, critical phenomena.
- Many excellent techniques to obtain density matrix for discrete systems (DMRG).
- Few many-particle continuous systems are analytically soluble.
- Hooke’s atom. Moshinsky atom. Crandall atom.

Entanglement in continuous systems

- Two-particle system

$$\hat{\rho}_{12} = \psi(\mathbf{r}_1, \mathbf{r}_2)\psi^*(\mathbf{r}'_1, \mathbf{r}'_2) \left|\mathbf{r}'_1, \mathbf{r}'_2\right\rangle \left\langle \mathbf{r}_1, \mathbf{r}_2\right|$$

$$\hat{\rho}_1 = \int d\mathbf{r}_2 \ \psi(\mathbf{r}_1, \mathbf{r}_2)\psi^*(\mathbf{r}'_1, \mathbf{r}_2) \left|\mathbf{r}_1\right\rangle \left\langle \mathbf{r}'_1\right|$$

$$\rho_1(\mathbf{r}_1, \mathbf{r}'_1) = \int d\mathbf{r}_2 \ \psi(\mathbf{r}_1, \mathbf{r}_2)\psi^*(\mathbf{r}'_1, \mathbf{r}_2)$$

$$Tr[\hat{\rho}_1^2] = \int d\mathbf{r} \ \left\langle \mathbf{r}\right| \hat{\rho}_1\hat{\rho}_1 \left|\mathbf{r}\right\rangle$$

$$Tr[\hat{\rho}_1^2] = \int\int d\mathbf{r}d\mathbf{r}' \ \left\langle \mathbf{r}\right| \hat{\rho}_1 \left|\mathbf{r}'\right\rangle \left\langle \mathbf{r}'\right| \hat{\rho}_1 \left|\mathbf{r}\right\rangle$$

$$Tr[\hat{\rho}_1^2] = \int\int d\mathbf{r}d\mathbf{r}' \ \rho_1(\mathbf{r}, \mathbf{r}')\rho_1(\mathbf{r}', \mathbf{r})$$

For many indistinguishable particles we have exchange symmetry.

$$\rho_1(\mathbf{r}_1, \mathbf{r}'_1) = \int d\mathbf{r}_2 ... d\mathbf{r}_N \ \psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)\psi^*(\mathbf{r}'_1, \mathbf{r}_2, ..., \mathbf{r}_N)$$

$$S_L(\rho_1) = 1 - tr(\rho_1^2)$$

(N+1)-dimensional integral

Hohenberg Kohn and DFT

$$\mathcal{H} = \mathcal{T} + \mathcal{V}_{ee} + \mathcal{V}_{ext}$$

If the external potential and the electronic density are known, the associated state is unique.

$$n(\mathbf{r}) = \rho_1(\mathbf{r}, \mathbf{r}')|_{\mathbf{r}'=\mathbf{r}}$$

$$n_0(\mathbf{r}) \rightarrow |\Psi_0\rangle$$

If the electronic density minimize the energy, the associated state is the ground state.

DFT is one of the faster techniques for continuous many body systems

Variational Quantum Monte Carlo

$$\left\langle \hat{H} \right\rangle = E_{\mathrm{T}} = \frac{\int \Psi_{\mathrm{T}}(\mathbf{R})^{\star} \hat{H} \Psi_{\mathrm{T}}(\mathbf{R}) \mathbf{dR}}{\int \Psi_{\mathrm{T}}(\mathbf{R})^{\star} \Psi_{\mathrm{T}}(\mathbf{R}) \mathbf{dR}} \geq E_{\mathrm{min}} \, .$$

$$E_{\mathrm{T}} = \int \rho(\mathbf{R}) E_{\mathrm{L}}(\mathbf{R}) \mathrm{d}\mathbf{R},$$

$$\rho(\mathbf{R}) = \frac{\Psi_{\mathrm{T}}^2}{\int \Psi_{\mathrm{T}}^2 \mathrm{d}\mathbf{R}}$$

$$E_{\mathrm{L}} = \frac{\hat{H} \Psi_{\mathrm{T}}}{\Psi_{\mathrm{T}}} \, .$$

1. Propose a trial wave function with variational parameters.
2. Propose an initial value for parameters and for the step size.
3. Calculate the energy integral by using Monte Carlo.
4. Find the step size that gives an acceptance ratio of 50% (Newton-Raphson).
5. Find the parameters that minimizes the trial energy (Steepest Descent).
4. For each new parameters find the optimal step size.

$$E_{\mathrm{T}} = \int \rho(\mathbf{R}) E_{\mathrm{L}}(\mathbf{R}) \mathrm{d}\mathbf{R} \approx \frac{1}{M} \sum_{i=1}^{M} E_{\mathrm{L}}(R_i),$$

$$\text{Acceptance ratio} = \frac{\text{No. of steps accepted}}{\text{Total number of trial steps}} \sim 0.5 \, .$$

Example: Helium atom

$$\mathcal{H}_H = -\frac{\nabla_1^2}{2} - -\frac{\nabla_2^2}{2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}$$

$$\psi_T(\mathbf{r_1}, \mathbf{r_2}, \mathbf{r_{12}}) = exp(-\alpha(r_1 + r_2))exp\left(\frac{r_{12}}{2(1+\beta r_{12})}\right)$$

For more than two particles: Slater determinant, sign problem. For entanglement (MC integral).

$$\mathbf{R}' = \mathbf{R} + \mathbf{r}\delta,$$

$$E_{L2} = E_{L1} + \frac{1}{2(1+\beta r_{12})^2}\left\{\frac{\alpha(r_1+r_2)}{r_{12}}(1 - \frac{\mathbf{r}_1\mathbf{r}_2}{r_1 r_2}) - \frac{1}{2(1+\beta r_{12})^2} - \frac{2}{r_{12}} + \frac{2\beta}{1+\beta r_{12}}\right\},$$

$$E_{L1} = (\alpha - Z)\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{1}{r_{12}} - \alpha^2.$$

Confidence Value after 10^8 steps.
Given alpha beta and delta:
40 threads. (6 min)

Our approach

- Use an analytically soluble model like Hooke's atom.
- Solve by QMC and calculate the linear entropy. Try to speed up by using machine learning:
- 1) ML: Parameters → Step size. For acceptance rate.
- 2) ML: Parameters, step size → Minimum energy.
- Contribute to construct the link:

  Electronic density → Reduced density matrix (linear entropy)

Thank you

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