INTERNATIONAL IBERIAN NANOTECHNOLOGY LABORATORY

Tackling the Many-Body Problem with Noisy Intermediate-Scale Quantum Computers

Bruno Murta, J. Fernández-Rossier

International Iberian Nanotechnology Laboratory, Braga, **Portugal**

Q Days 2019
Braga, 12 April 2019

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1. Quantum simulation does not scale effectively on NISQCs
2. Adiabatic evolution is universal method to find ground state of many-body systems but requires high-depth quantum circuits
3. Implementation of adiabatic evolution requires more efficient exploration of Hilbert space, which can be accomplished via tensor networks

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0. Quantum simulation is best option to tackle quantum many-body problems

0A. Solving the quantum many-body problem via **classical hardware** is **unfeasible** due to the **exponential wall problem**

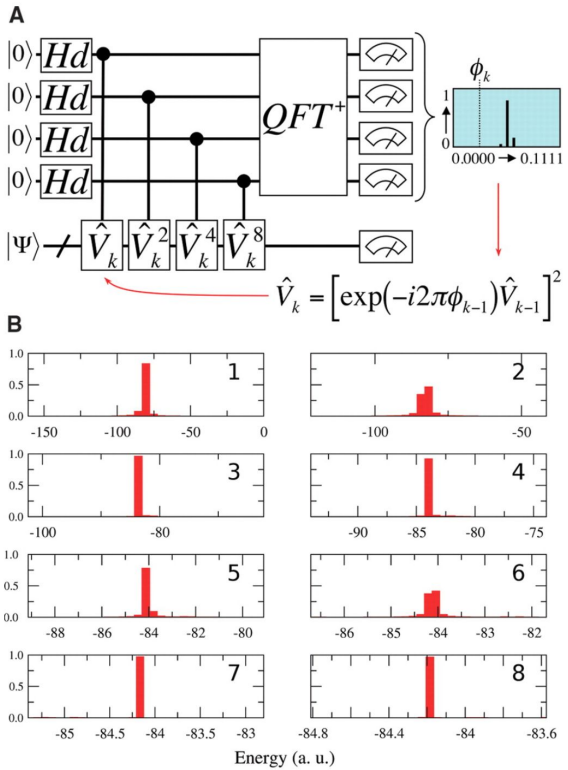
0B. **Exact methods and approximations** only succeed at solving **low-dimensional and weak interactions** problems

0C. **Gate-based quantum computers** are natural candidates to simulate quantum phenomena

A. Aspuru-Guzik et al., Science **309**, 1704 (2005)

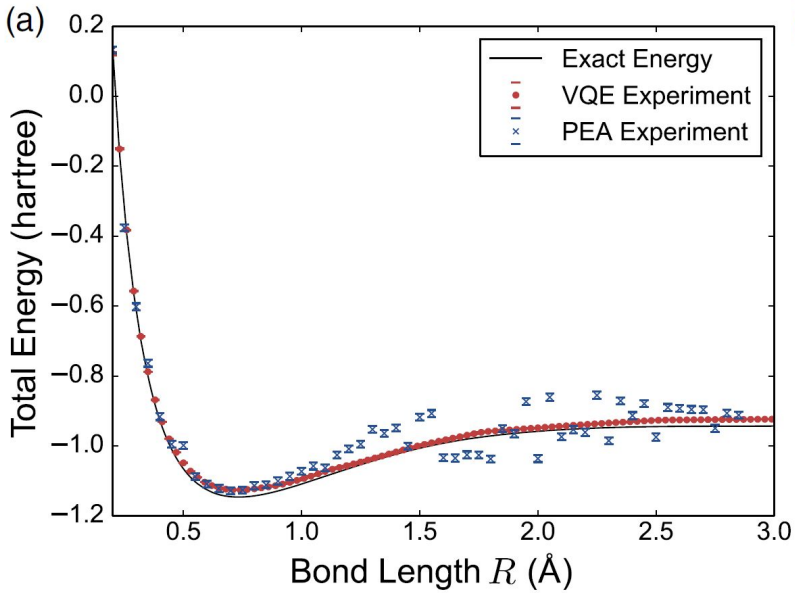
1A. Phase estimation with ground state ansatz was first attempt to find electronic structure, but only for small molecules

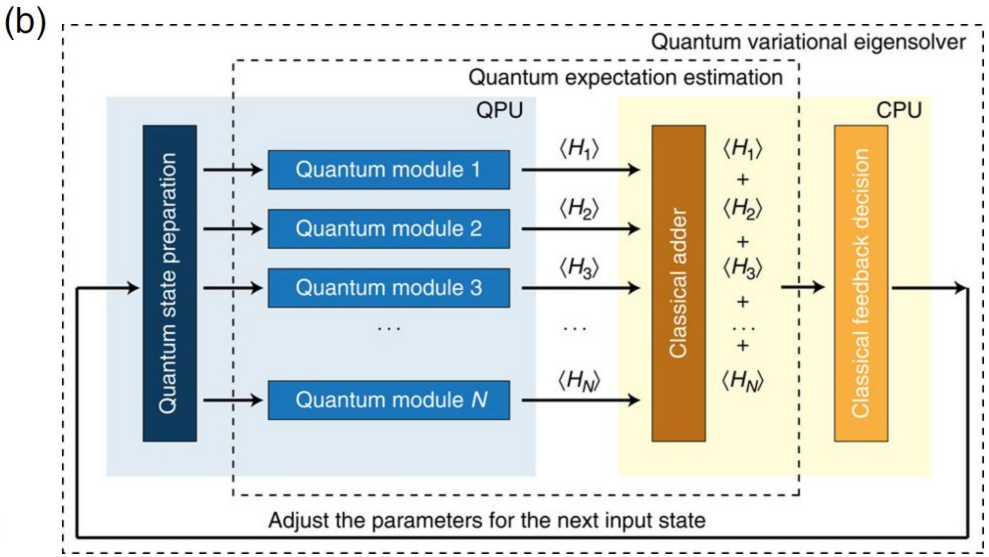
- Aspuru-Guzik et al. (2005) measured the ground state energy of H_2O and LiH
- Method initialized input register in **Hartree-Fock ground state** and carried out **phase estimation** algorithm
- **Success** of procedure depends on **overlap between ansatz and exact ground state**
  - For large systems, as size of Hilbert space increases, this overlap becomes very small
- This algorithm also requires **implementing propagator and high-depth circuits**



A. Aspuru-Guzik et al., Science **309**, 1704 (2005)

1B. VQE improves overlap between trial state and exact ground state, but not enough to address large systems (e.g. in 2D)





(a) Computed H_2 energy curve and errors

(b) Architecture of the quantum-variational eigensolver

Peruzzo et al., Nature Communications **5**, 4213 (2014)
O'Malley et al., Phys. Rev. X **6**, 031007 (2016)

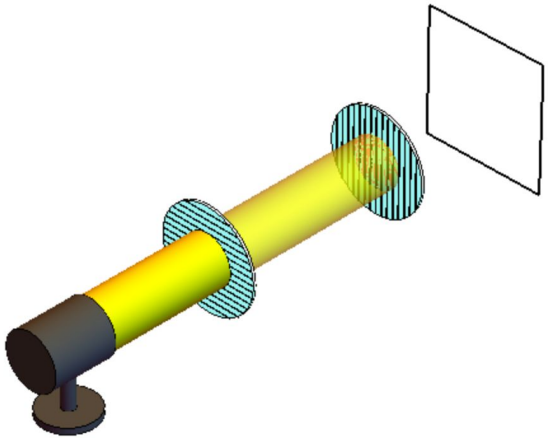
1C. Orthogonality catastrophe suggests variational methods are doomed to fail to simulate large enough systems

- **Orthogonality catastrophe**: the **overlap** between two nearby ground states of fermionic systems **tends to zero in the thermodynamic limit**:
  - Let $|0)$ be the ground state of a fermionic Hamiltonian H. Let us add a small perturbation V, yielding the Hamiltonian $H' = H + V$. Let $|0')$ be the ground state of H'
  - The overlap $(0'|0)$ is vanishingly small in the limit of large number of particles N
- It is therefore likely that, for a large enough system, the **ansatz is orthogonal to the exact ground state**, in which case the **variational procedure will never lead to the ground state energy**
- In the limit of large number of particles, **even a good guess of the ground state may be orthogonal to it** (i.e. the overlap is so small that it is negligible)

P. W. Anderson, Phys. Rev. Lett. **18**, 1049 (1967)

2A. Adiabatic theorem states that a gapped system remains an instantaneous eigenstate if the perturbation is small

- Let us consider an unpolarized light beam going through a sequence of polarizers:
  - For two orthogonal polarizers no light passes through
  - Adding a polarizer at 45° increases transmissivity to 0.25
  - In general, for a sequence of N polarizers, equally spaced from 0° to 90° the transmissivity is given by $[\cos^2(\pi/2N)]^{2N}$, which tends to 1 as N tends to ∞
- Similarly, **when a quantum system is evolved adiabatically starting from an eigenstate, it follows the instantaneous eigenstate at every step due to an interference phenomenon**



Simulation of Sequence of Polarizers

M. Born and V. Fock, Zeitschrift für Physik **51**, 165-180 (1928)
B. Murta and J. Fernández-Rossier, In preparation

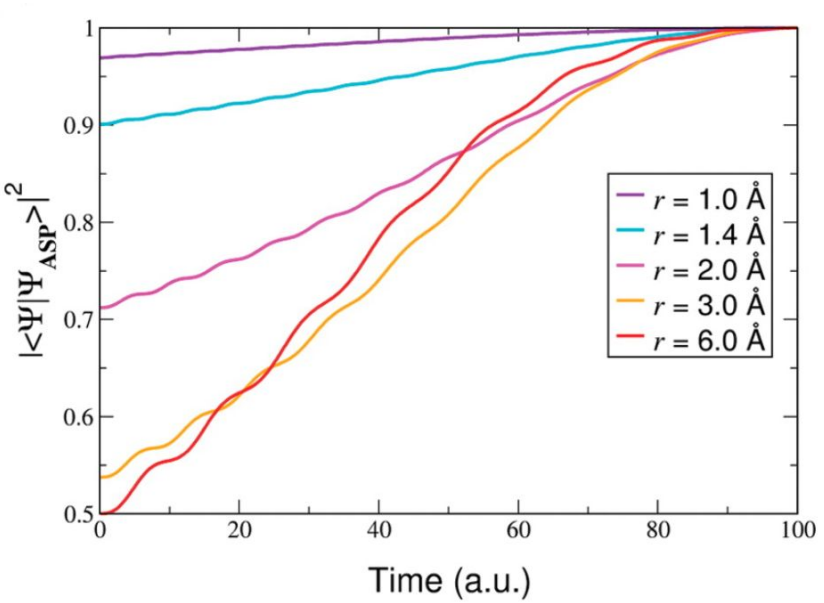
2B. Implementation of adiabatic evolution in quantum computers is conceptually straightforward and universal

(a)

$$\mathcal{H}(t) = \left(1 - \frac{t}{T}\right)\mathcal{H}_0 + \frac{t}{T}\mathcal{H}_I,\ t \in [0, T]$$

(a) Mapping from Hamiltonian whose exact ground state is known, H_0, to H_I, whose ground state is to be found

(b)



(b) Overlap between HF ground state ansatz and exact ground state of H_2 molecule for different separation distances between atoms as a function of time of adiabatic evolution

E. Farhi et al., Science **292**, 5516 (2001)
A. Aspuru-Guzik et al., Science **309**, 1704 (2005)

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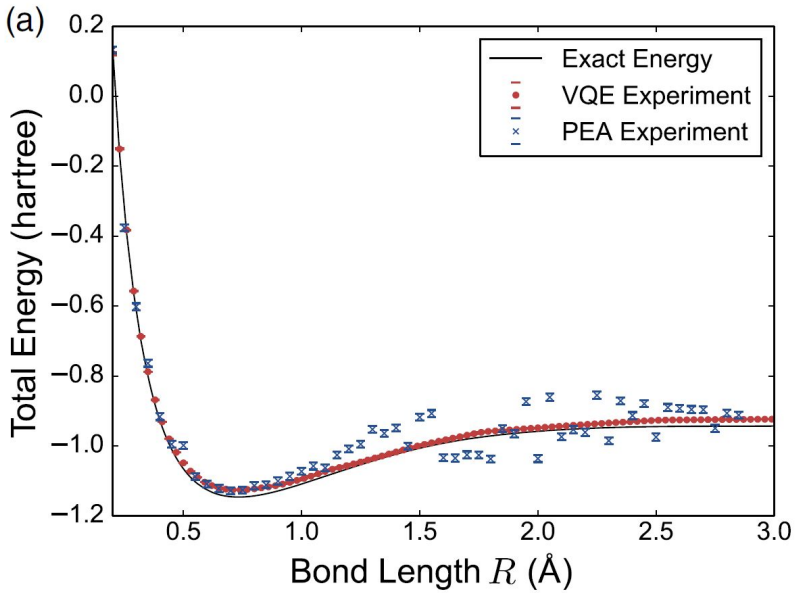
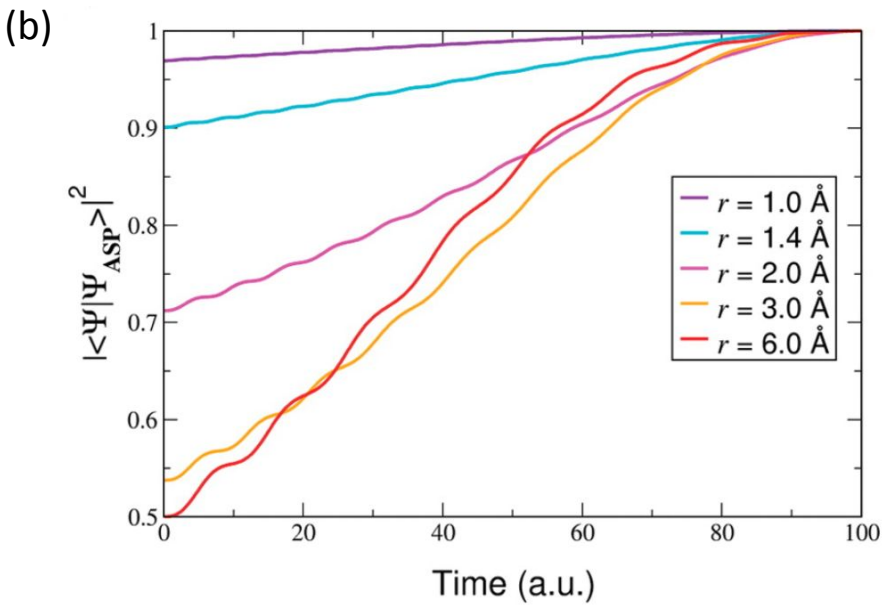


(a) Computed H_2 energy curve and errors



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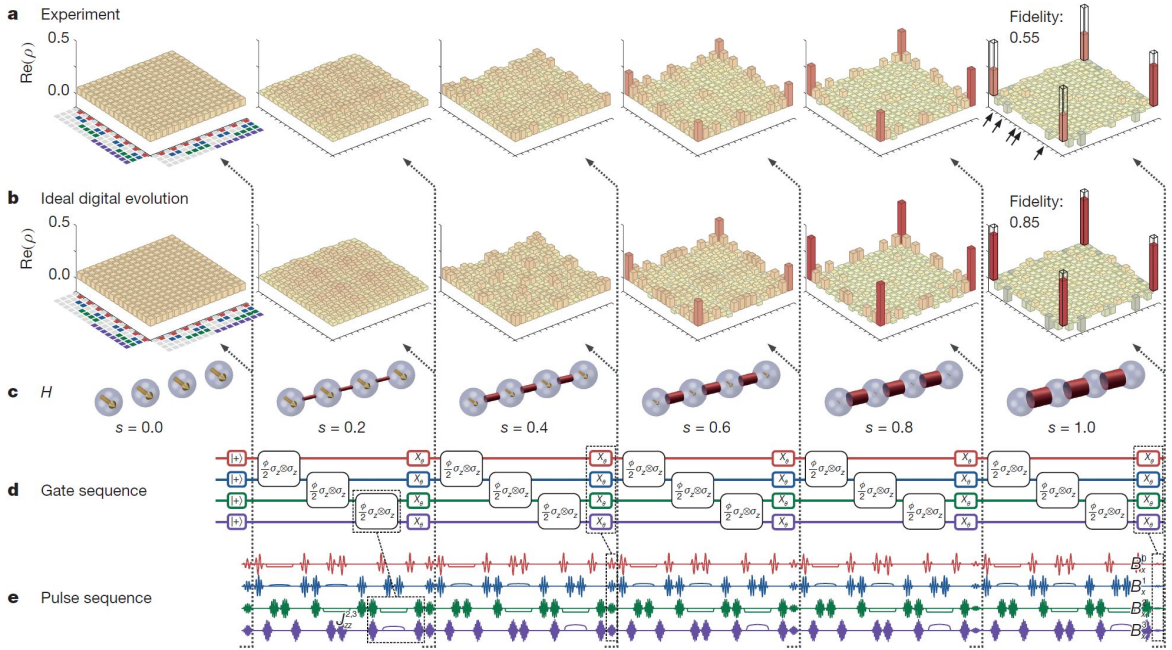
A. Aspuru-Guzik et al., Science **309**, 1704 (2005)
O'Malley et al., Phys. Rev. X **6**, 031007 (2016)

2C. Slow evolution requirement imposed by adiabatic condition makes quantum circuits too deep for current NISQCs

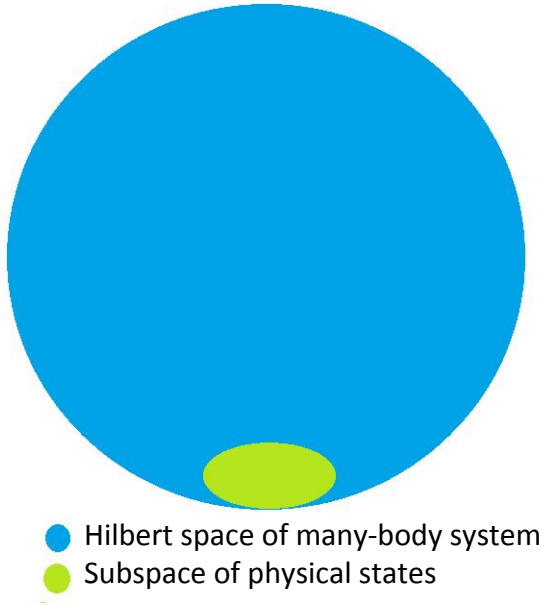


Quantum state tomography of the digital evolution into a GHZ state. A 4-qubit is adiabatically evolved from an initial Hamiltonian in which all spins are aligned to an Ising Hamiltonian with equal ferromagnetic couplings

Barends et al., Nature **534**, 222-226 (2016)

3A. Overwhelming majority of Hilbert space can only be reached after exponentially long time, thus being unphysical

- The property that characterizes the quantum behaviour of a many-body system is **entanglement**:
  - It is because fermions are entangled in the ground state that they can have nontrivial correlations even at zero temperature
  - The entanglement entropy for low-energy states of local Hamiltonians typically scales as the area of the considered region instead of the volume
- The manifold of all quantum many-body states that can be generated by arbitrary time-dependent local Hamiltonians in a time that **scales polynomially with system size** also follows an area law, occupying an **exponentially small volume of the Hilbert space**



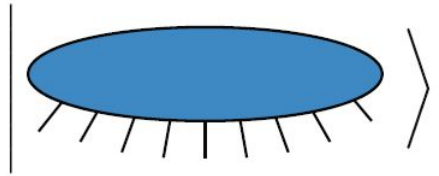
J. Eisert et al., Rev. Mod. Phys. **82**, 277-306 (2010)
D. Poulin et al., Phys. Rev. Lett. **106**, 170501 (2011)

3B. Tensor networks are efficient representation of many-body states (particularly ground states) that satisfies area law

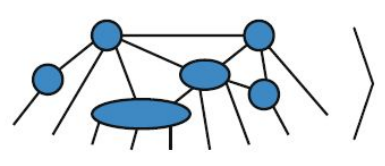
- A tensor network comprises different tensors connected via the contraction of indices
  - Tensors are the bricks building up the quantum state and entanglement plays the role of the glue amongst the different pieces
- **Tensor networks capture the specific entanglement structure of low-energy states:**
  - Tensor networks provide an accurate and efficient parametrization of low-temperature ground states of quantum many-body systems
  - Tensor network states can be thought to parametrize tiny subspace where the relevant physics takes place

$$|\Psi\rangle = \sum_{i_1,\ldots,i_N} c_{i_1,\ldots,i_N} |i_1,\ldots,i_N\rangle$$

$$|\Psi\rangle =$$



$$|\Psi\rangle_{\mathrm{TNS}} =$$



L. Vanderstraeten, *Tensor Network States and Effective Particles for Low-Dimensional Quantum Spin Systems*, Springer (2017)
R. Orús, arXiv preprint, 1812.04011 (2018) [invited contribution to Nature Reviews Physics]

3C. Tensor networks can be simulated with exponentially fewer resources with quantum computers

- Tensor network methods require contracting large tensors efficiently
- A **classical computer** requires **memory and computation time that scales exponentially with D^d**, where D is the number of parameters and d is the number of spatial dimensions
- A **quantum computer**, on the other hand, can **perform such operations in O(D log N) time using $O(D^d)$ qubits**, where N is the system size

I. H. Kim and B. Swingle, arXiv preprint, 1711.07500 (2017)

Conclusions

Quantum simulation via adiabatic evolution starting from tensor network ansatz state is a promising method to solve the quantum many-body problem for strong interactions in 2D and 3D:

- Numerical methods in classical hardware, exact methods and approximations can only tackle low-dimensional and/or weak interactions models
- Hybrid variational methods succeed at finding electronic structure of simple molecules but are doomed to fail to solve large systems due to the orthogonality catastrophe
- Adiabatic evolution requires high-depth circuits, so an efficient representation of the ground states of low-temperature Hamiltonians must be adopted, notably tensor networks

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Thank you!

Questions?

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0A. Solving the quantum many-body problem via classical hardware is unfeasible due to the exponential wall problem

- **Exponential wall problem**: the number of computational resources needed to solve the Schrödinger equation of system with N degrees of freedom scales exponentially with N
- A quantum state describing N spin-½ particles requires **storing 2^N** complex numbers:
  - N ~ 50 reaches memory capacity of state-of-the-art supercomputers
  - N ~ 270 exceeds the number of atoms in the Universe...
- Numerical simulations in classical hardware can thus only address **small systems**

0B. Exact methods and approximations only succeed at solving low-dimensional and weak interactions problems

- **Exact analytical** solutions of quantum many-body models are **mainly restricted to 1D**
- **Perturbation theory is limited** to uninteresting non-perturbative phenomena
- **Quantum Monte Carlo** methods faces the **sign problem** for fermionic systems
- Density Functional Theory (**DFT**) makes use of approximations (e.g. LDA) to find the density functional, which **break down for strong interactions**
- **DMRG and tensor network methods** (e.g. MPSs, PEPSs, MERA) are very successful for 1D systems but **not for 2D and 3D systems**

0C. Gate-based quantum computers are natural candidates to simulate quantum phenomena

- Quantum computers are **exponentially more efficient** than classical computers at **storing the state of quantum systems** thanks to superposition and **exploring quantum phenomena that are not accessible to classical methods** thanks to entanglement
- Analog quantum simulators (e.g. ultracold atoms, quantum annealers) are constrained in terms of the interaction mechanisms that can be implemented; **gate-based quantum computers**, on the other hand, **are universal**
- **Progress in quantum hardware** (number of qubits, coherence times, gate errors) has been **fast over the past years**