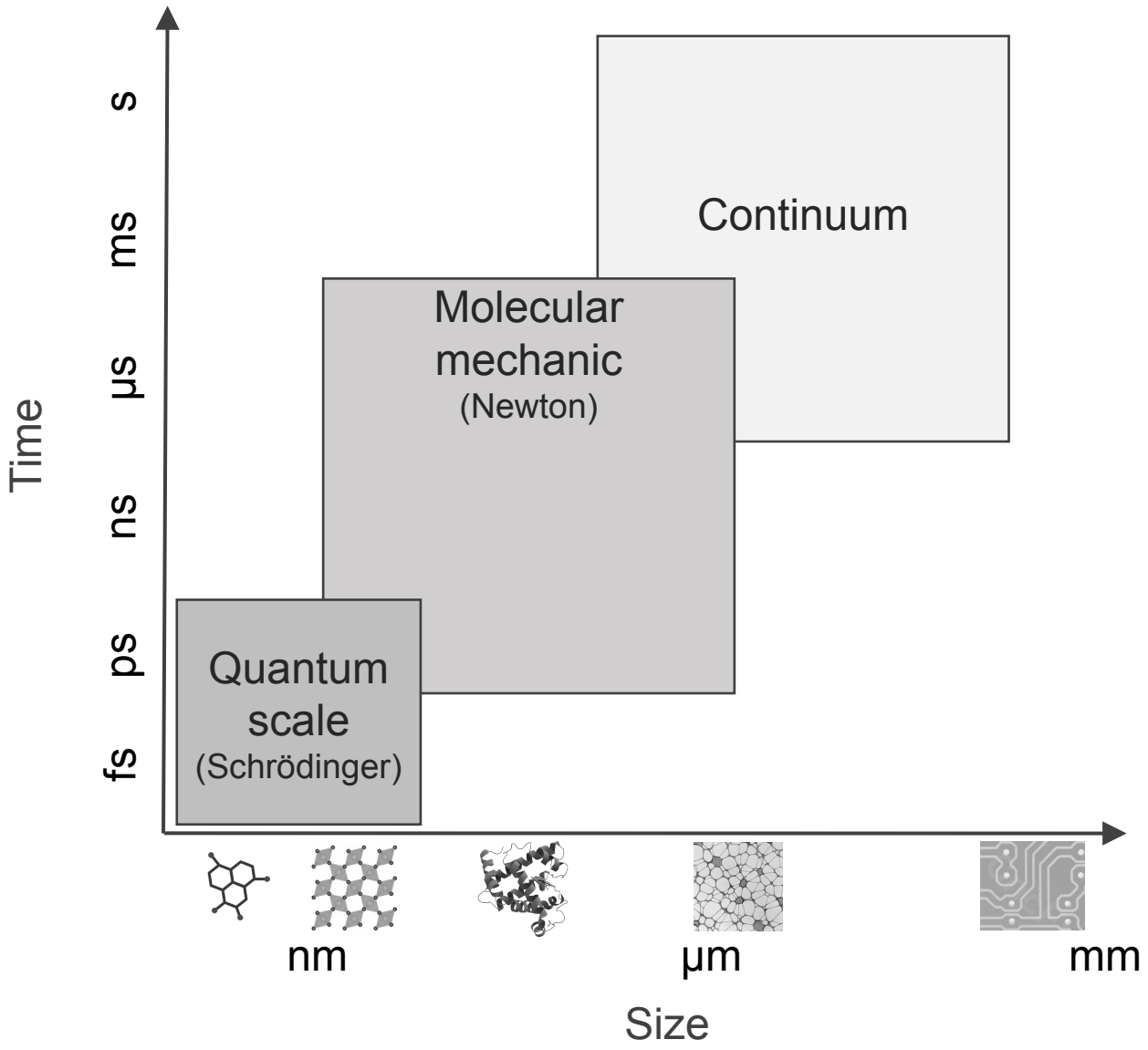
Quantum algorithms for electronic structure

Matthieu Saubanère

Simulate matter today



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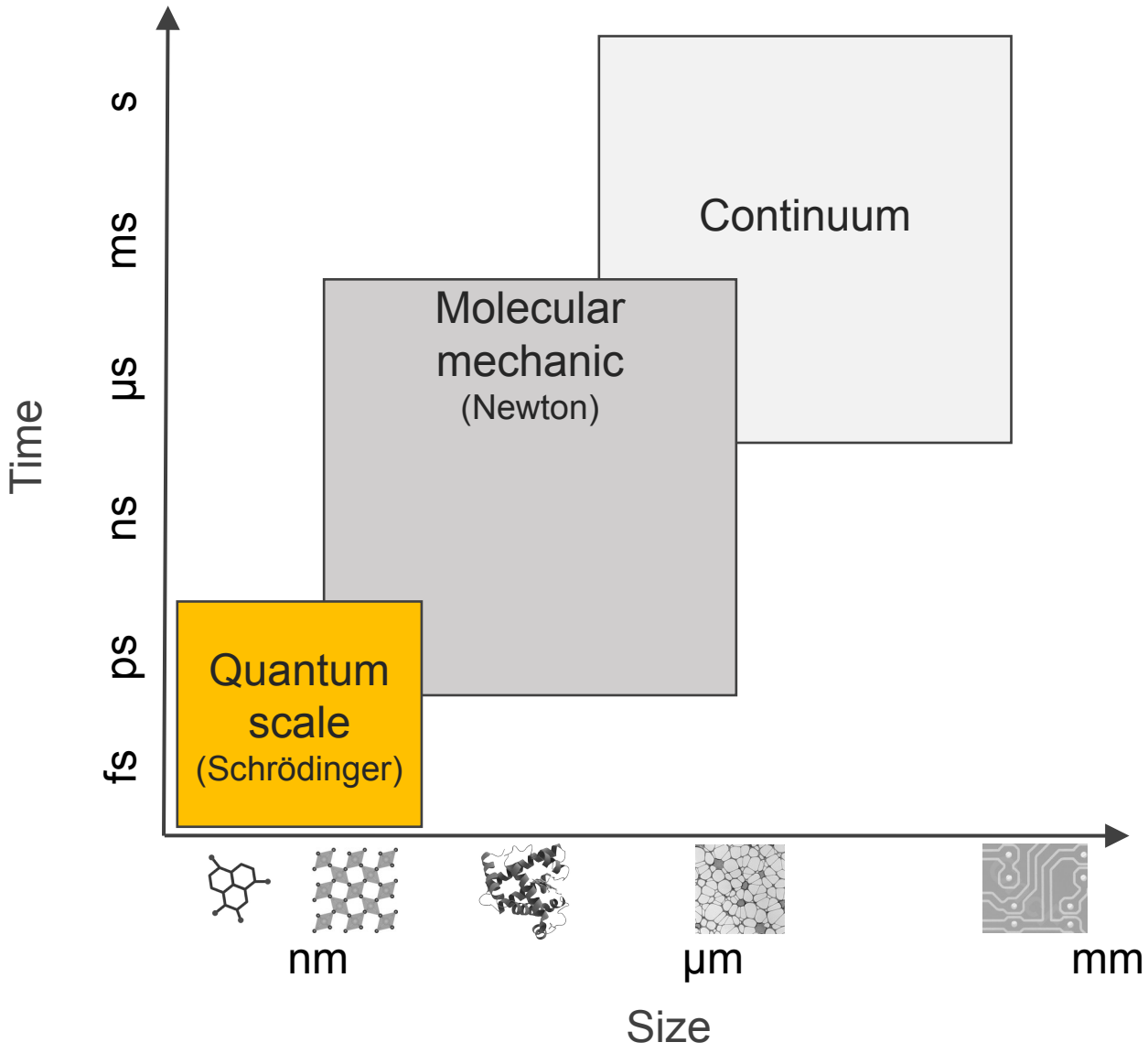
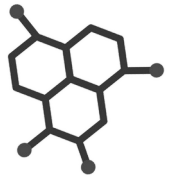
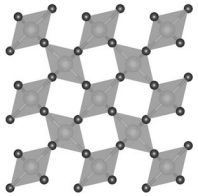
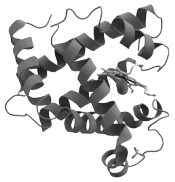


Different systems :

Molecules 

Materials 

Proteins 

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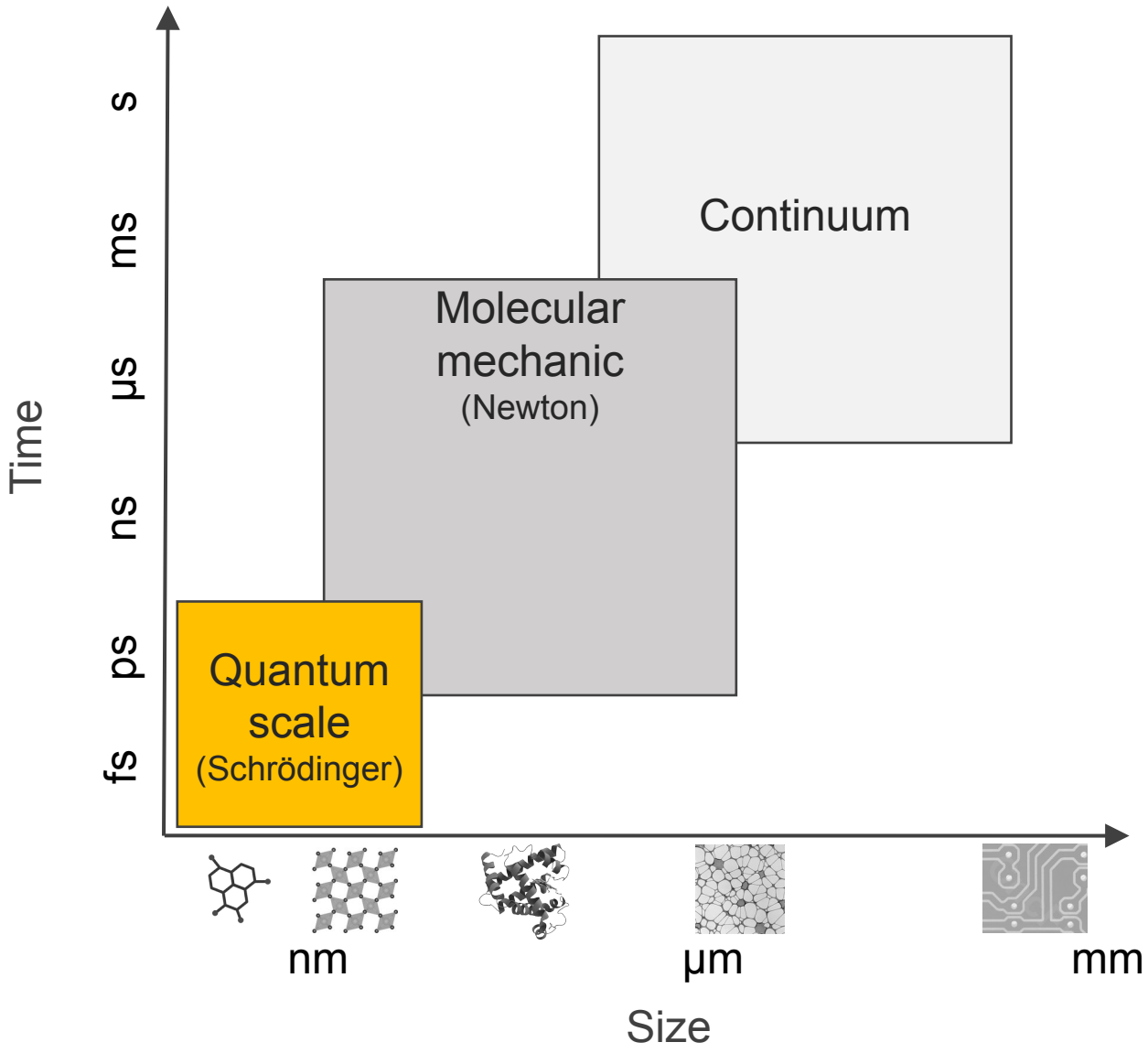


Different applications :

Health (drug design)

Energy conversion and storage

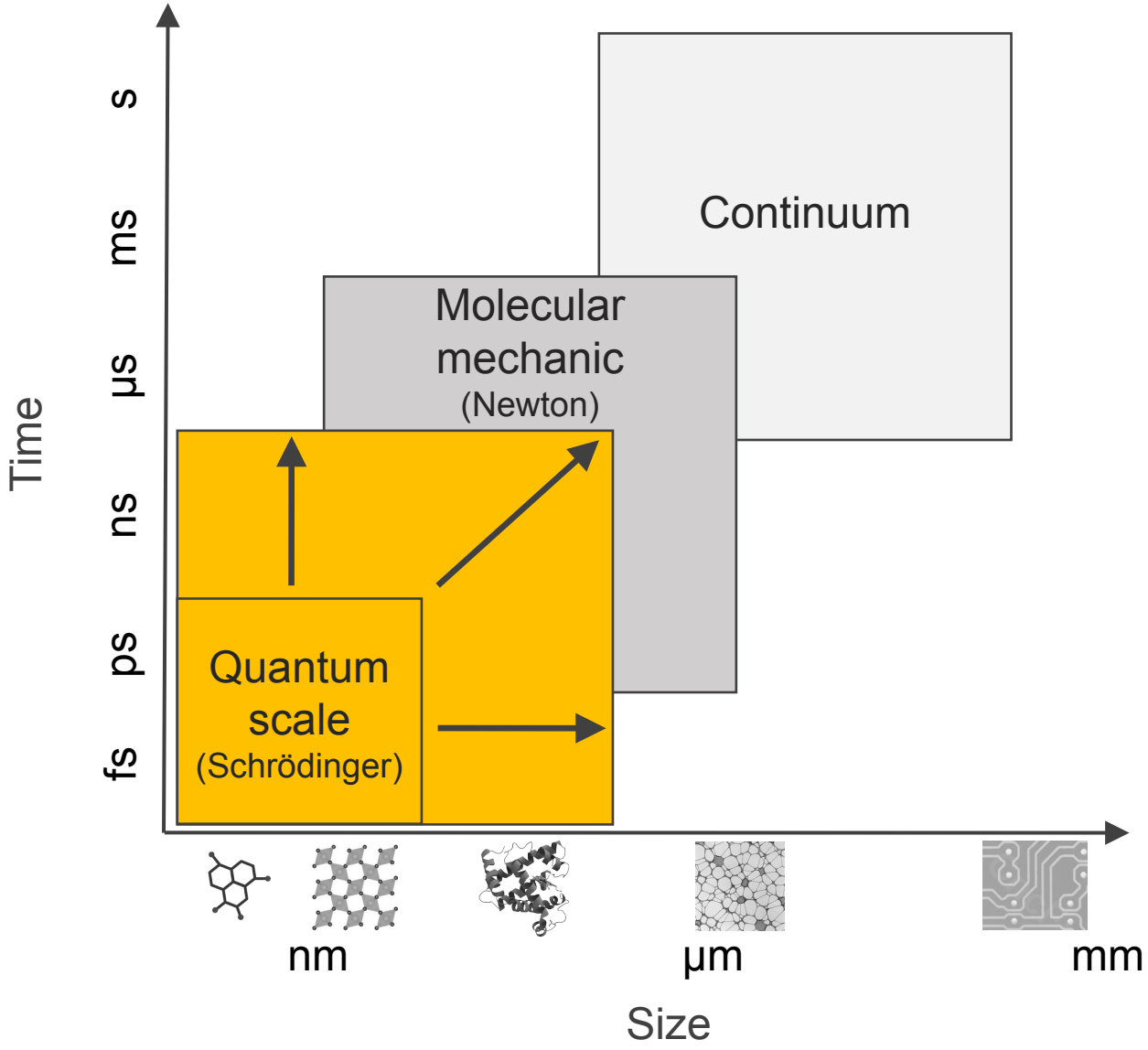
Quantum technologies

Environment

Electronics

…

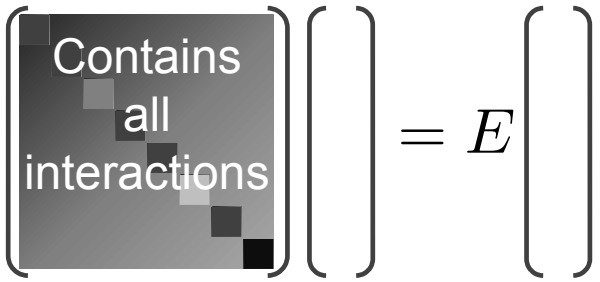
Simulate matter on a quantum computer (QC) ?



Toward more complex systems and phenomena

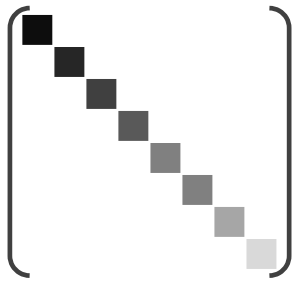
Challenge: solve the Schrodinger Eq.

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$



Diagonalization

$$\tilde{H} = U^{\dagger} H U$$



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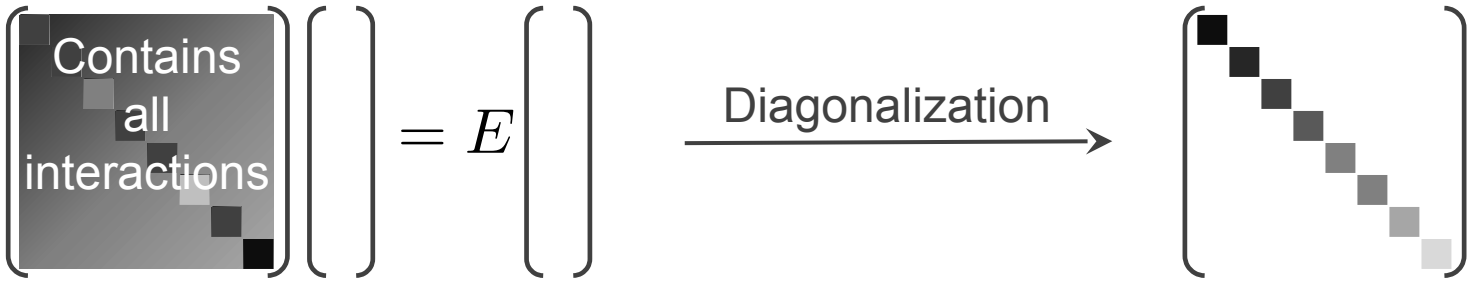

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Given a mono-electronic basis containing N_o spin-orbitals $\rightarrow$

Challenge: solve the Schrodinger Eq.

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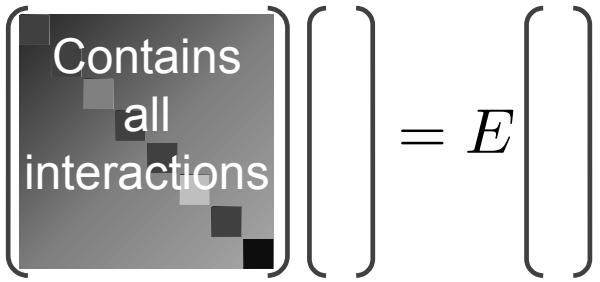

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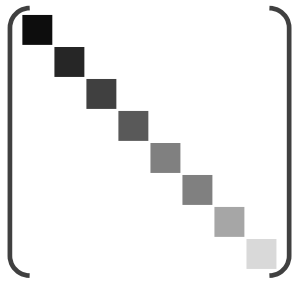

Classical Algorithms :

- Numerical diagonalization –FCI– (Lanczos, QR)

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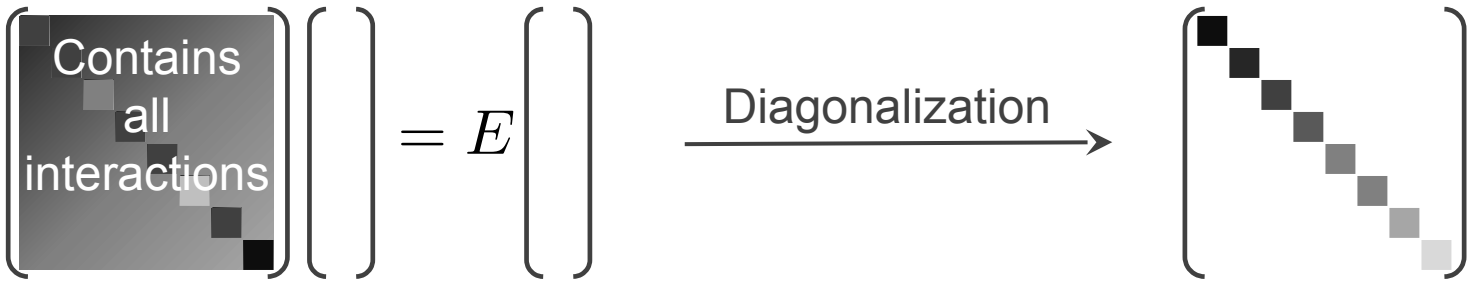

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- Numerical diagonalization –FCI– (Lanczos, QR)
- Basis set truncation / Active space reduction
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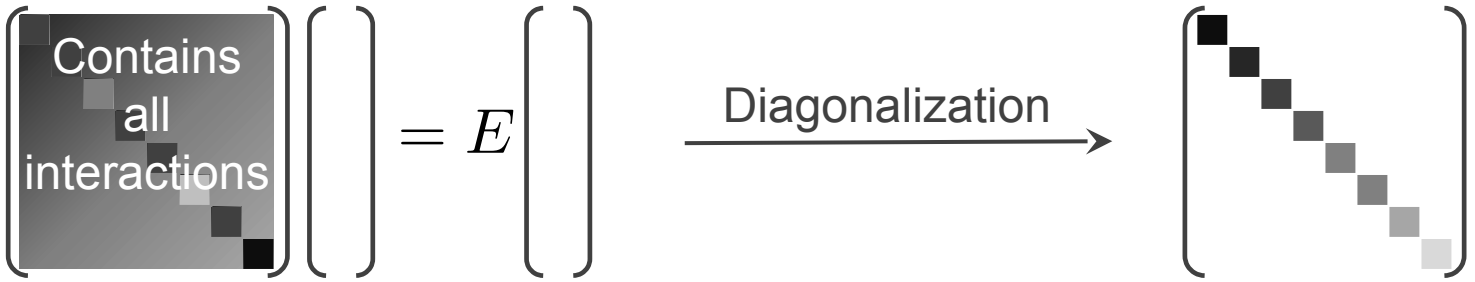

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→ Quantum Algorithms

Variational quantum algorithms: general concept

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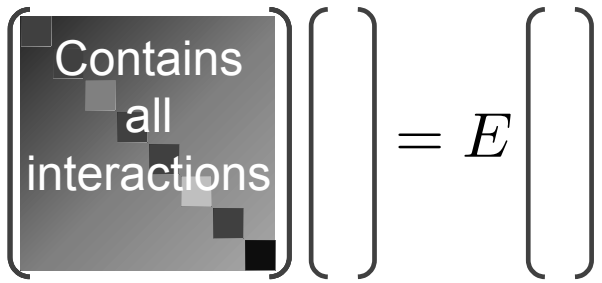

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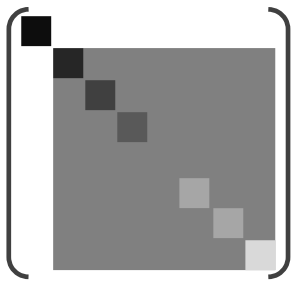

$$U(\theta)$$

$$E = \min_{\theta}\langle\Phi_0|U(\theta)^{\dagger}\hat{H}U(\theta)|\Phi_0\rangle$$

Unitary transformation ~ poly(size) on QC

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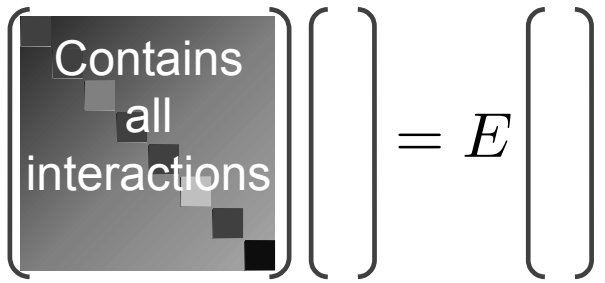

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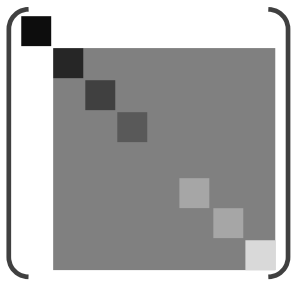

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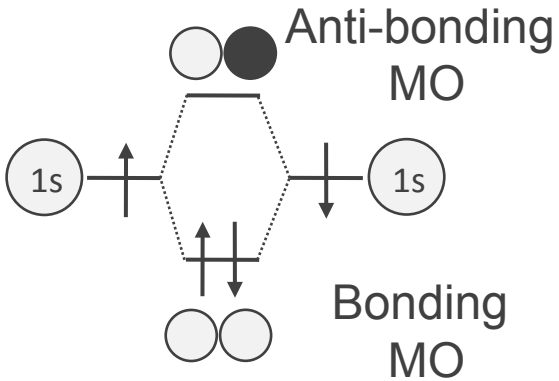
H_2 molecule (sto-3)



Hartree-Fock
$|\Phi_0\rangle$

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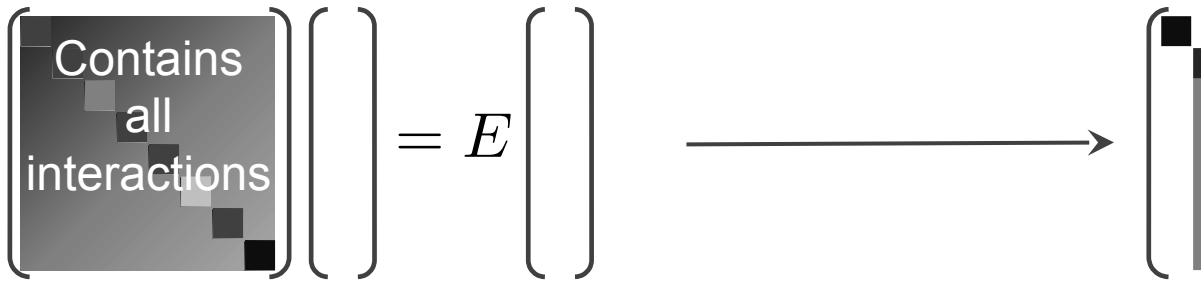

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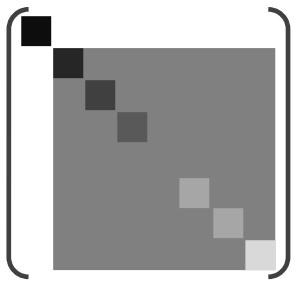

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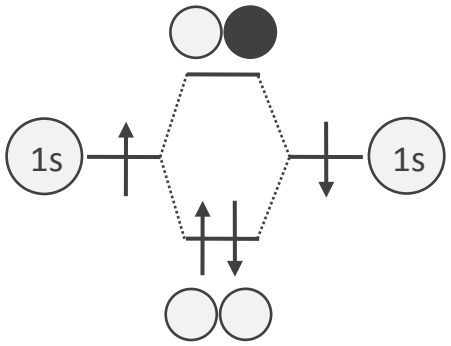

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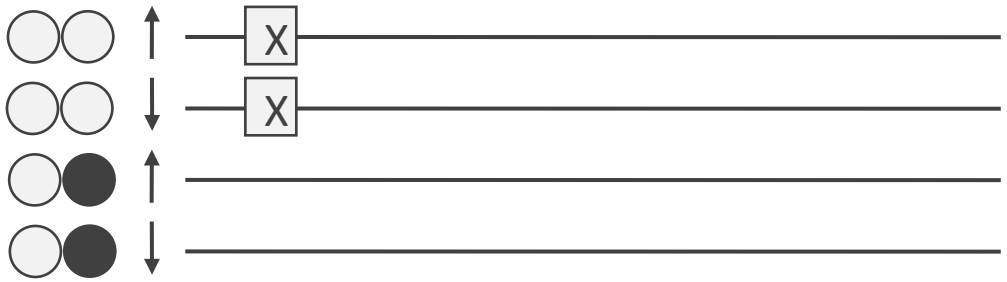
$|\Phi_0\rangle$

1 qubit = 1 spin-orbital

Jordan-Wigner mapping

Construct
HF state

$|\Phi_0\rangle$



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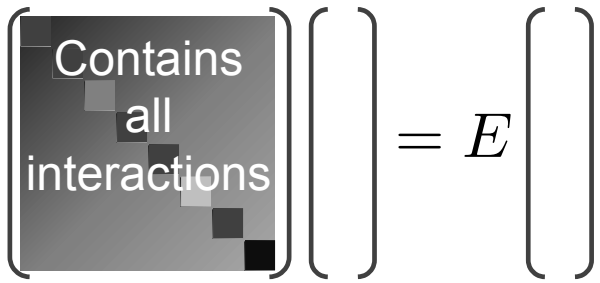

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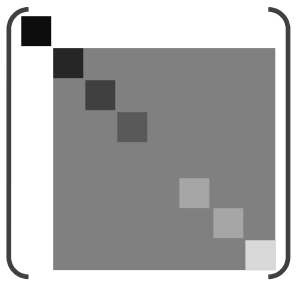

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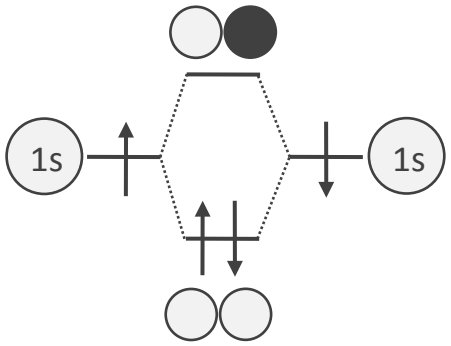

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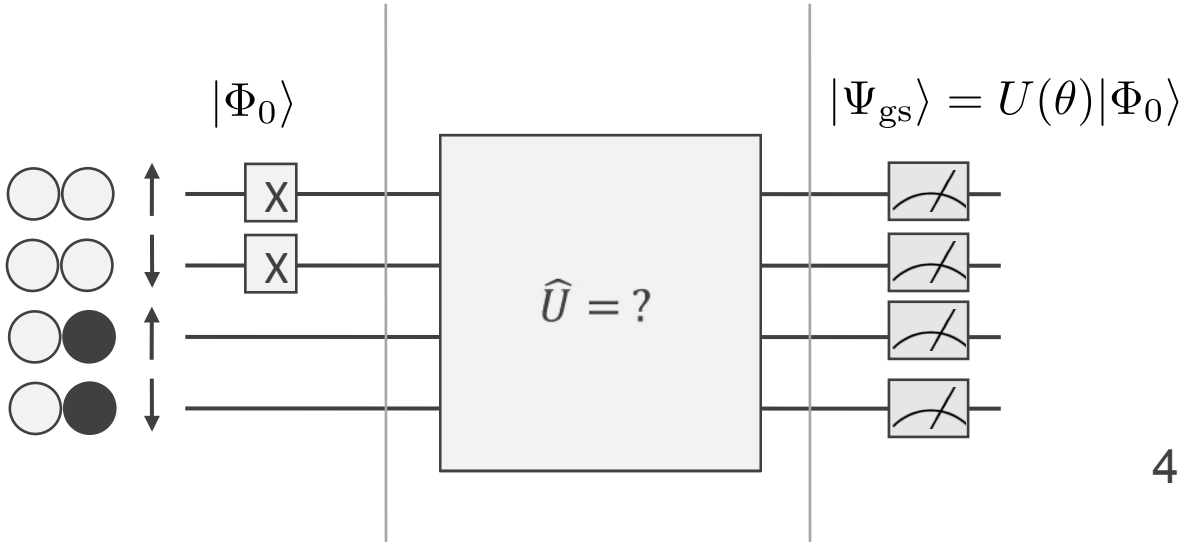
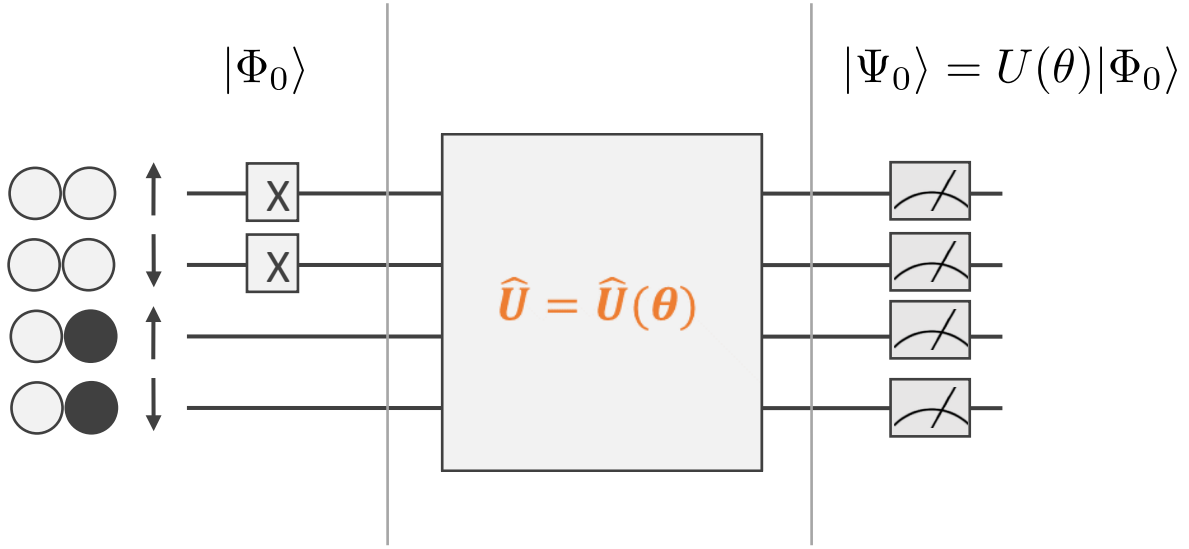
Unitary transform

Measure



Variational quantum algorithms: challenges



Classical Numerical Cost ?

Optimization issues (non convex function / Barren plateau)

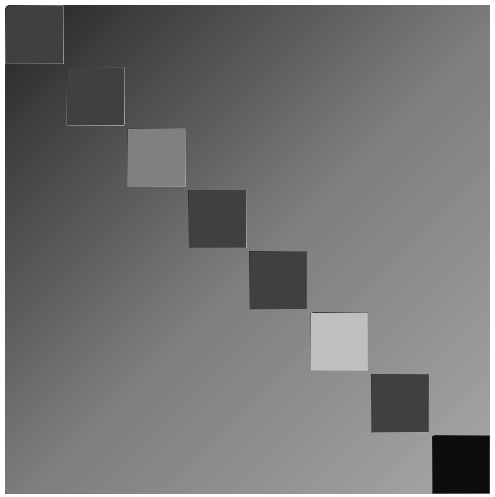
Quantum Numerical Cost:

Physical ansatz : circuit depth ~ size^4

Hardware efficient ansatz : circuit depth ~ size^2

Simplifying the problem:

1– Symmetries : $[\hat{H}, \hat{N}] = [\hat{H}, \hat{S}_z] = [\hat{H}, \hat{S}^2] = \cdots = 0$



Very sparse !

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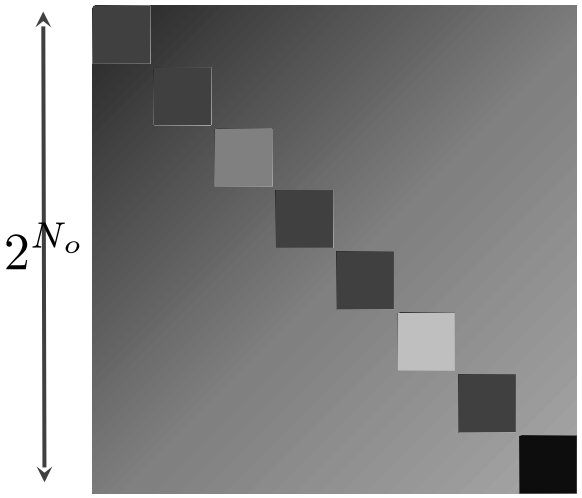

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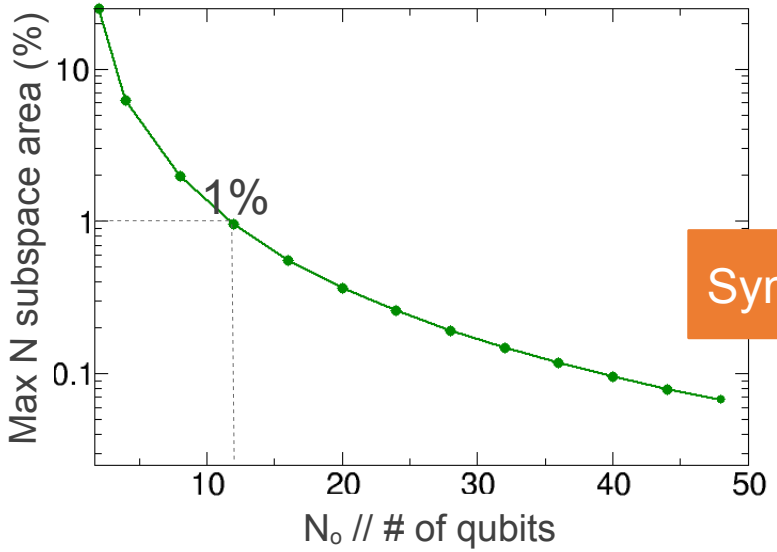

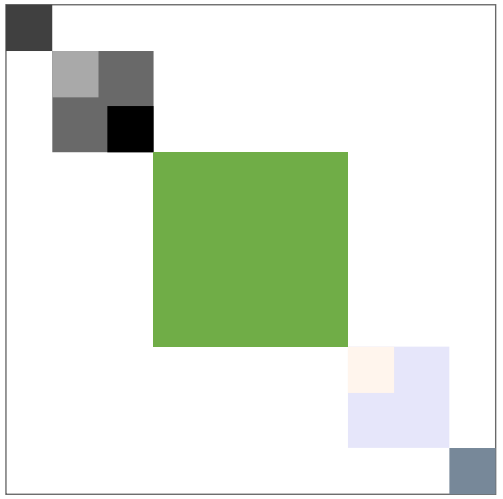

Symmetries consideration mandatory

Simplifying the problem:

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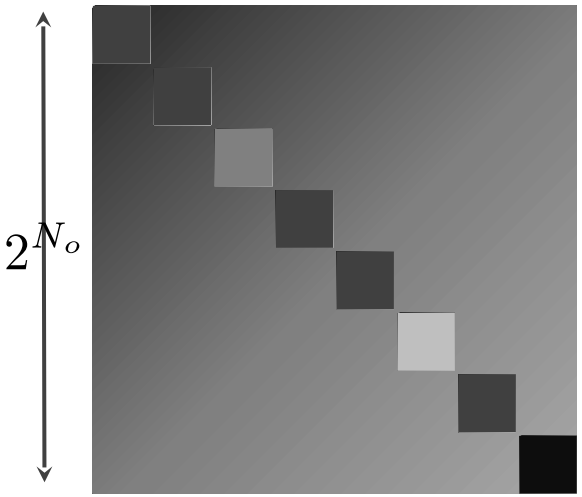
Symmetries consideration mandatory

2– Locality of interaction // Nearsightedness

- Kinetic operator : ∇
- Coulomb operator : $\frac{1}{r} \rightarrow e^{-\kappa r}$ (Thomas-Fermi)



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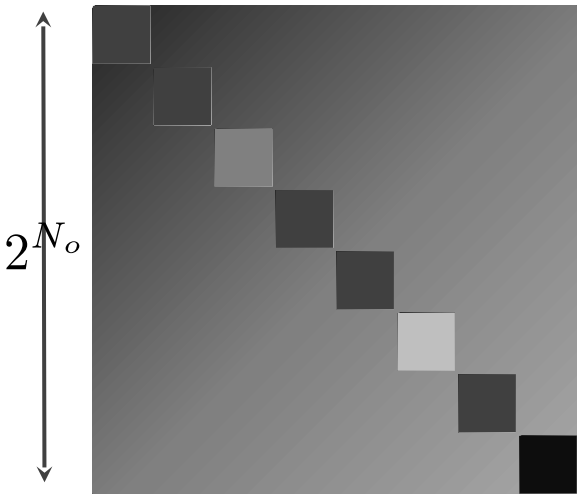

Very sparse !

→ Localized basis-set empty the Hamiltonian !

Pre-optimized (DFT) basis set vs Off-chip optimization

Cheng-Lin Hong et. al. PRX QUANTUM 3, 020360 (2022)

P. Besserve, M. Ferrero, and T. Ayral, arXiv: 2406.14170 (2024)

talk Thomas Ayral !

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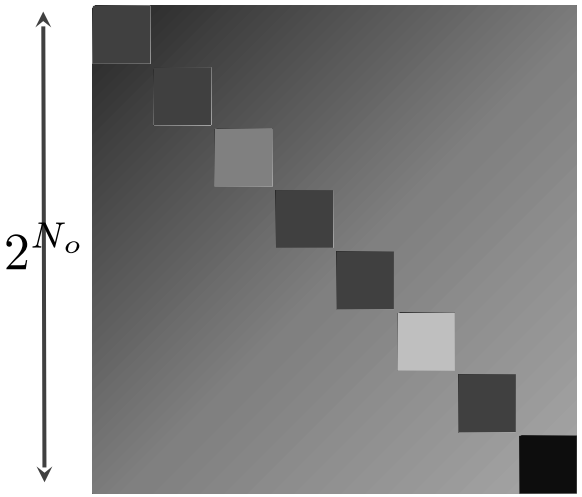

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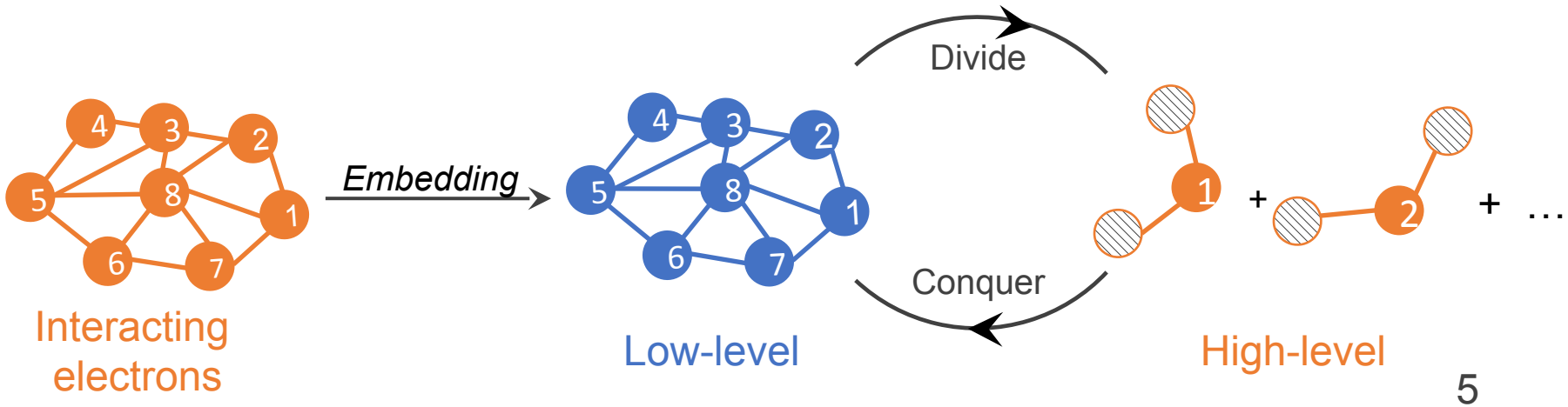
→ Localized basis-set empty the Hamiltonian !

→ Divide-conquer strategy (embedding)



PRR, 3, 033230 (2021)
JPCL, 12, 1104−1109 (2021)
NPJ Comput. Mater., 9, 78 (2023)

Outline:

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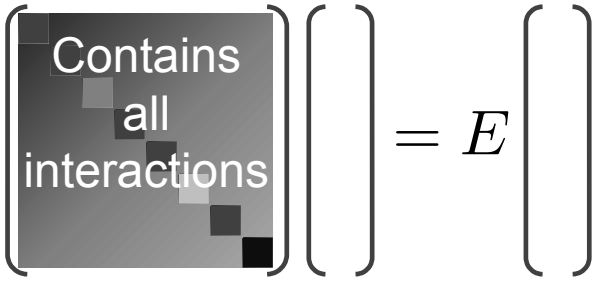
Symmetry preserving cost function

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$



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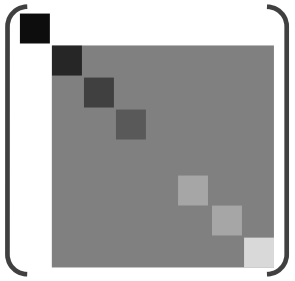

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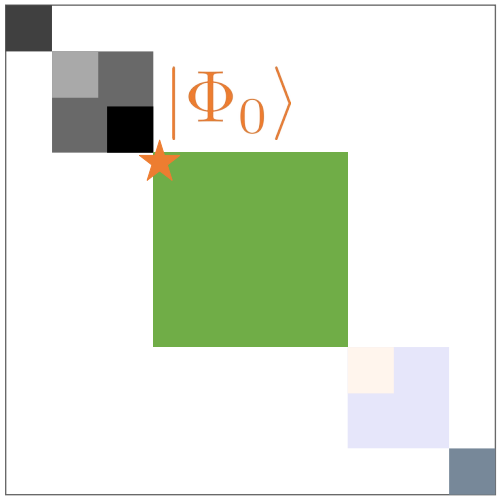

Physically motivated ansatz: preserves symmetry but deep circuit

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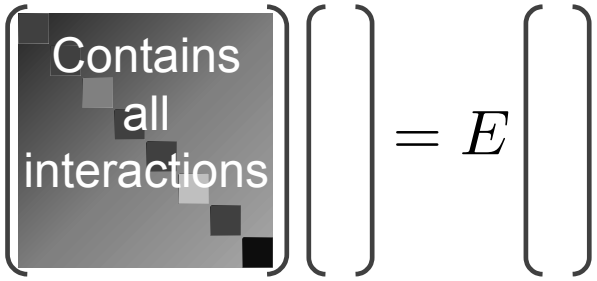

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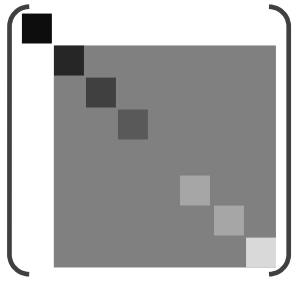

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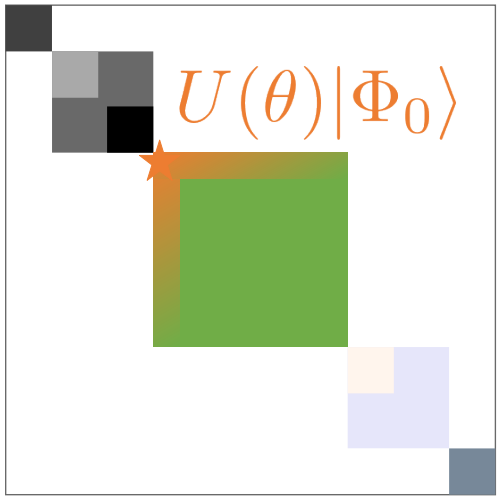

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→ ADAPT-VQE Nat. Commun 10,3007 (2019)

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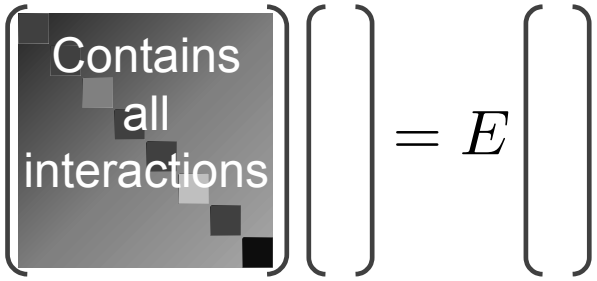

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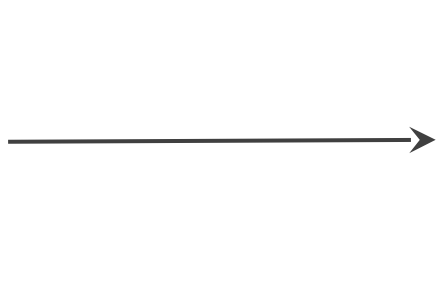

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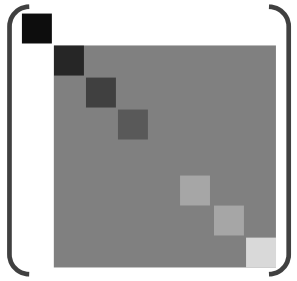

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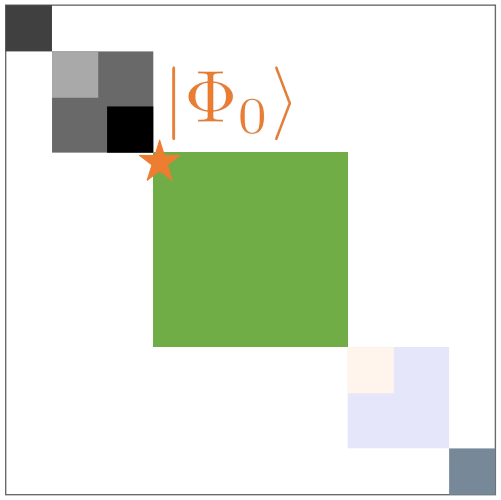
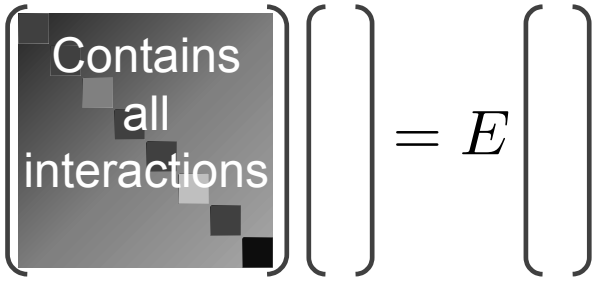


Physically motivated ansatz: preserves symmetry but deep circuit

Hardware efficient ansatz (HEA): do NOT preserve symmetry but shallow circuit

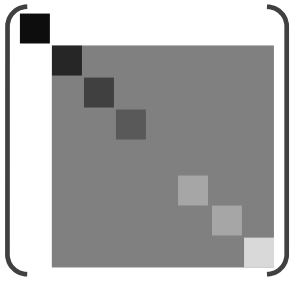
Symmetry preserving cost function

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$



$= E$

$$\widetilde{H} = U^\dagger \hat{H} U$$



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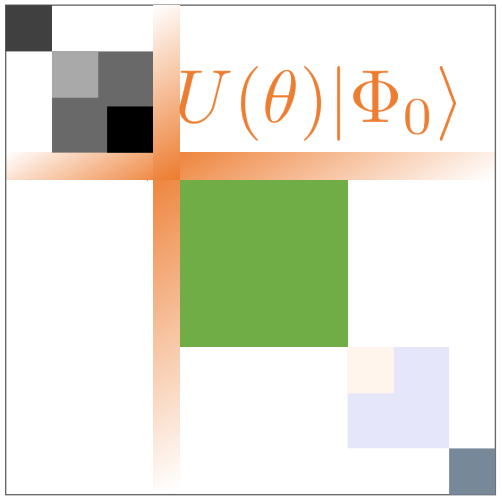

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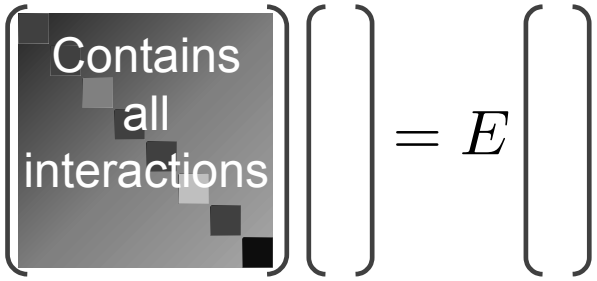

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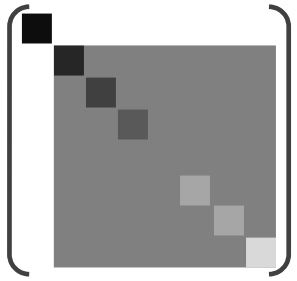

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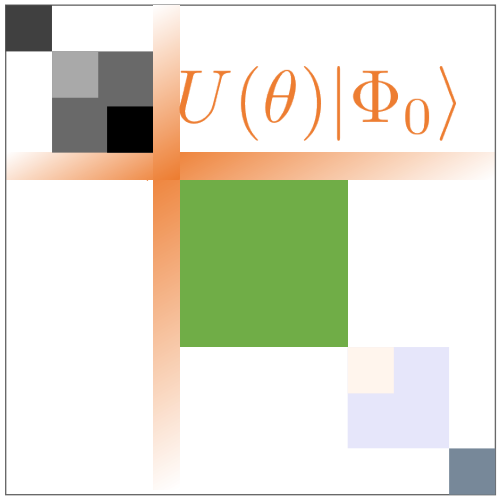
$$E = \min_{\theta}\langle\Phi_0|U(\theta)^{\dagger}\hat{H}U(\theta)|\Phi_0\rangle$$



Physically motivated ansatz: preserves symmetry but deep circuit

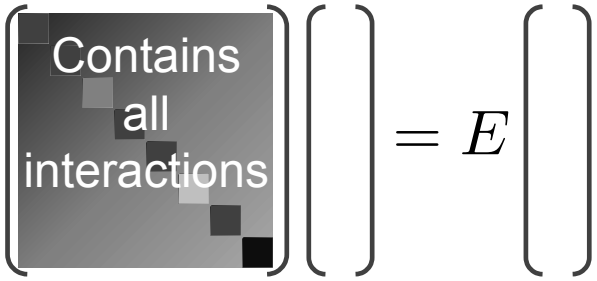
Hardware efficient ansatz (HEA): do NOT preserve symmetry but shallow circuit

→ Sym. Preserving ansätze npj Quantum Inf 6, 1 (2020); New J. Phys. 23, 113010 (2021)

→ Global optimization method (basin hopping) J. Chem. Theory Comput. 19, 1197 (2023)

Symmetry preserving cost function

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$



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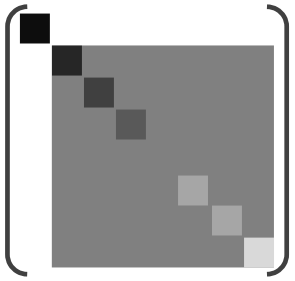

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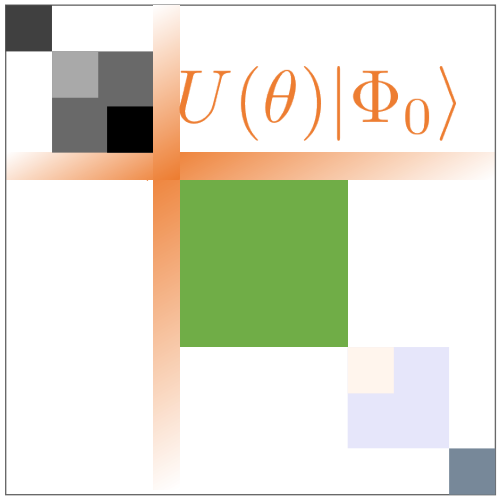


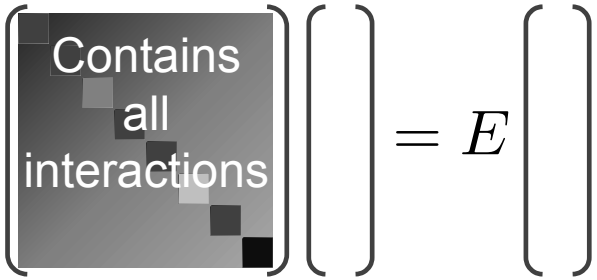
Physically motivated ansatz: preserves symmetry but deep circuit

Hardware efficient ansatz (HEA): do NOT preserve symmetry but shallow circuit

Our strategy: modify the variational principle to preserve symmetry with HEA

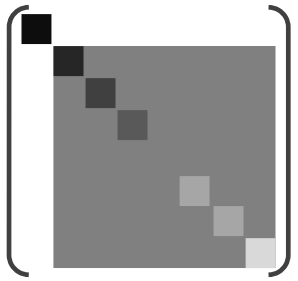
Symmetry preserving cost function

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$



$$= E$$

$$\widetilde{H} = U^\dagger \hat{H} U$$



$$E = \min_\theta \langle \Phi_0 | U(\theta)^\dagger \hat{H} U(\theta) | \Phi_0 \rangle$$

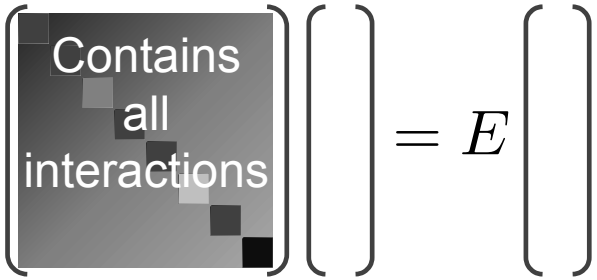
$$E = \min_\theta \left(\text{tr.} \left(\widetilde{\Gamma} U(\theta)^\dagger \hat{H} U(\theta) \right) \right)$$

$$\widetilde{\Gamma}_{ij} = \delta_{0i}\delta_{0j}$$

H. Akande, B. Senjean, M. Saubanère, preprint (2024)

Symmetry preserving cost function

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$



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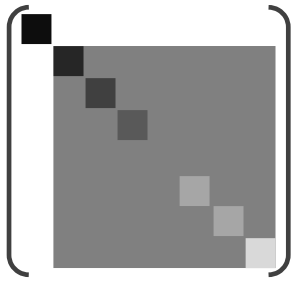

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$$\widetilde{\Gamma}_{ij} = \delta_{0i}\delta_{0j}$$

$$\overline{H} = R^\dagger \hat{H} R$$

$$E = \min_\theta \left(\text{tr.} \left(\overline{\Gamma} R(\theta)^\dagger \hat{H} R(\theta) \right) \right)$$

$$\overline{\Gamma}(\omega) =$$

Counter HF Representation

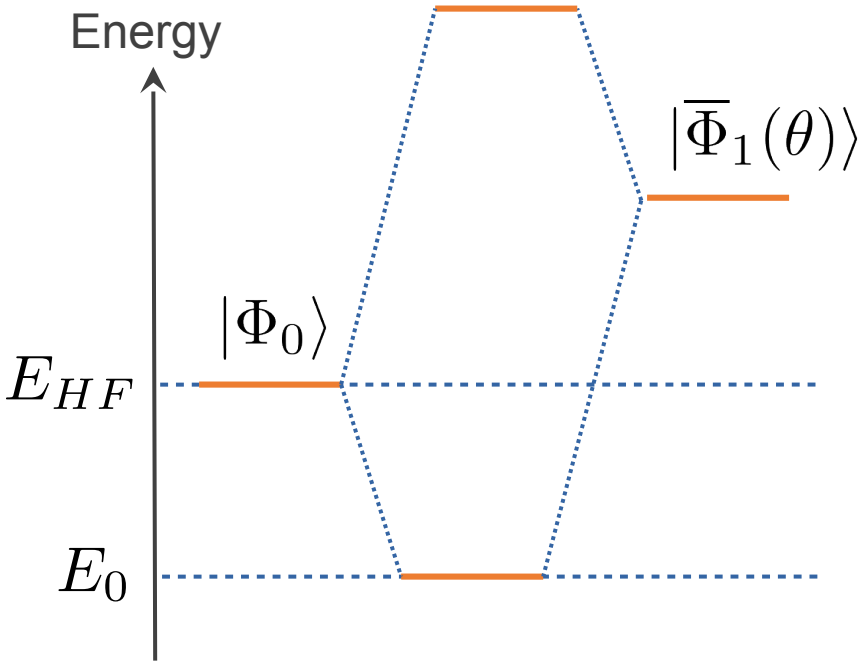
$$R|\Phi_0\rangle = |\Phi_0\rangle \qquad |\overline{\Phi}_1\rangle$$

$$|\Psi_0\rangle = \omega|\Phi_0\rangle \pm \sqrt{1-\omega^2}\, \overbrace{R|\Phi_1\rangle}$$

Decomposition: $U = RP(\omega)$

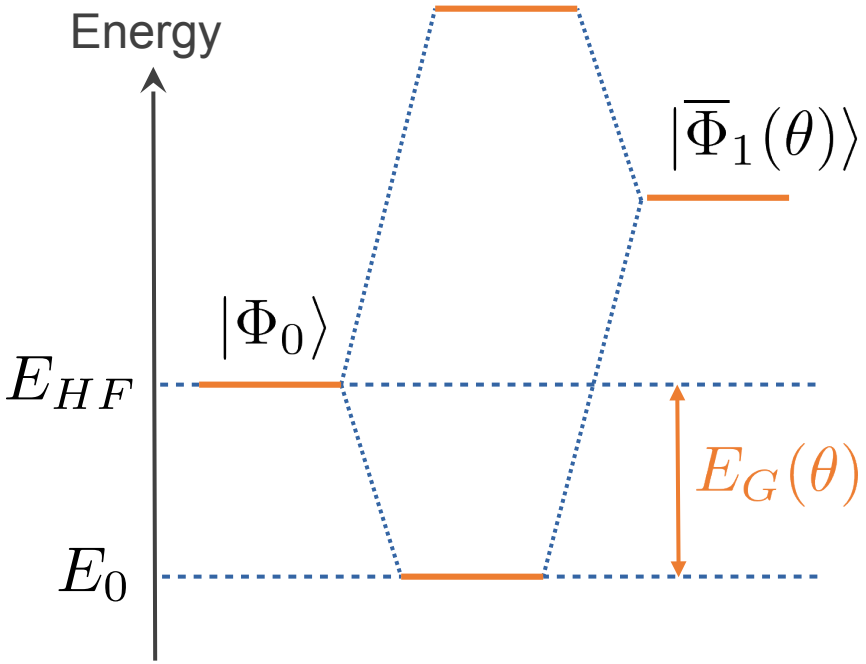
H. Akande, B. Senjean, M. Saubanère, preprint (2024)

Symmetry preserving cost function



H. Akande, B. Senjean, M. Saubanère, preprint (2024)

Symmetry preserving cost function



Instead of minimizing:

$$E = \min_\theta \left(\text{tr.} \left(\overline{\Gamma} R(\theta)^\dagger \hat{H} R(\theta) \right) \right)$$

Good guess hypothesis : $\omega \geq 0.5$

We minimize the Energy gain !

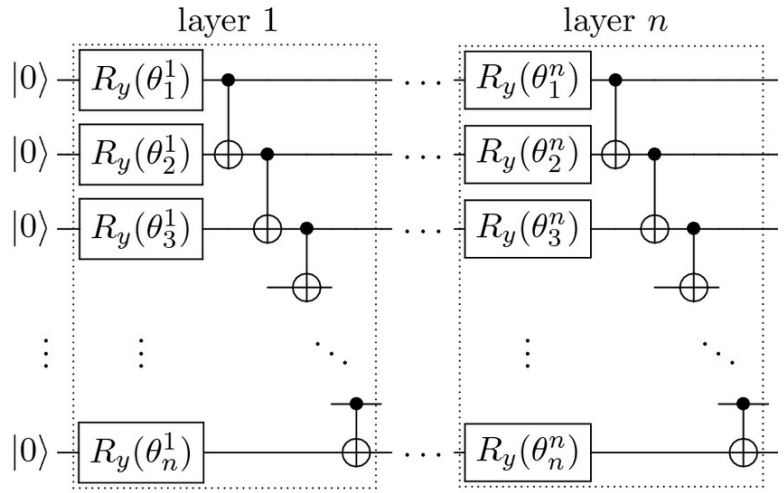
$$E_G(\theta) = 0 \quad \text{if} \quad \langle \Phi_0 | \hat{H} | \overline{\Phi}_1 \rangle$$

Require 3 measurements instead of 1 for standard VQE

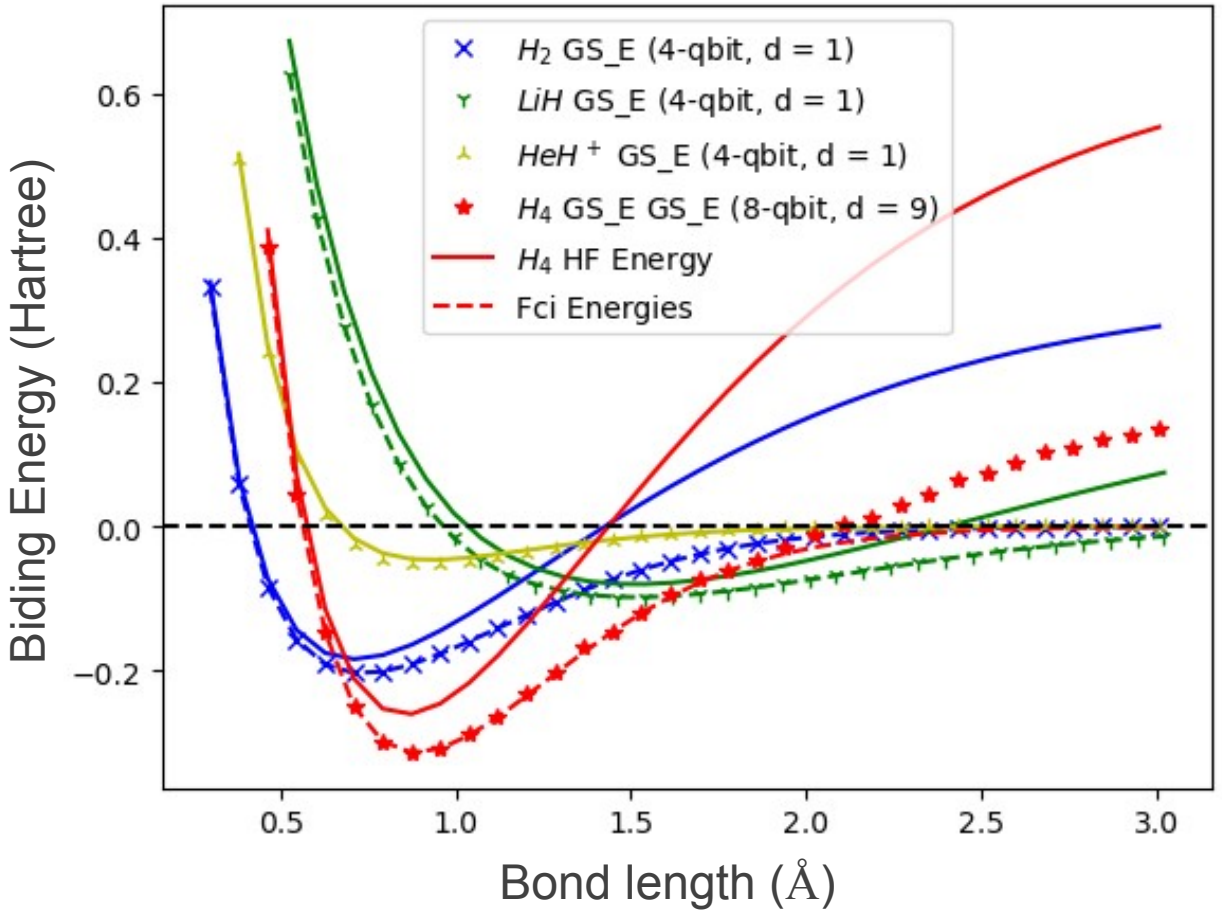
H. Akande, B. Senjean, M. Saubanère, preprint (2024)

Potential energy surface

Basic HEA with d layer // Cobyla optimizer



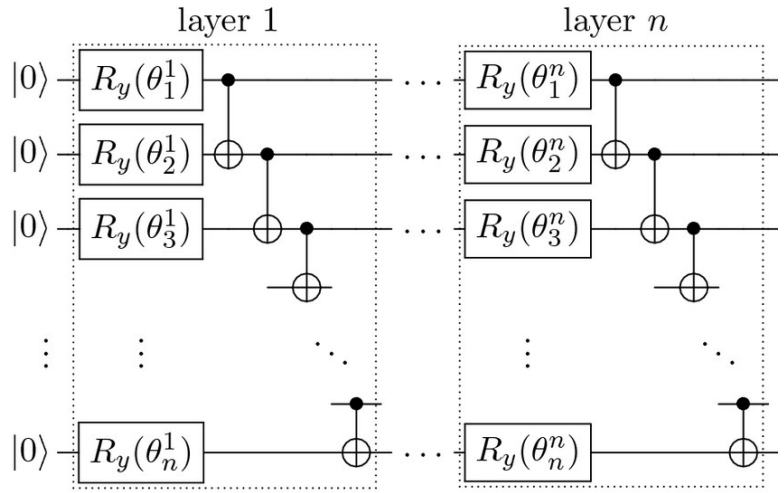
Kandala et. al. Nature 549, 242 (2017).



H. Akande, B. Senjean, M. Saubanère, preprint (2024)

Charge gap

Basic HEA with d layer // Cobyla minimizer



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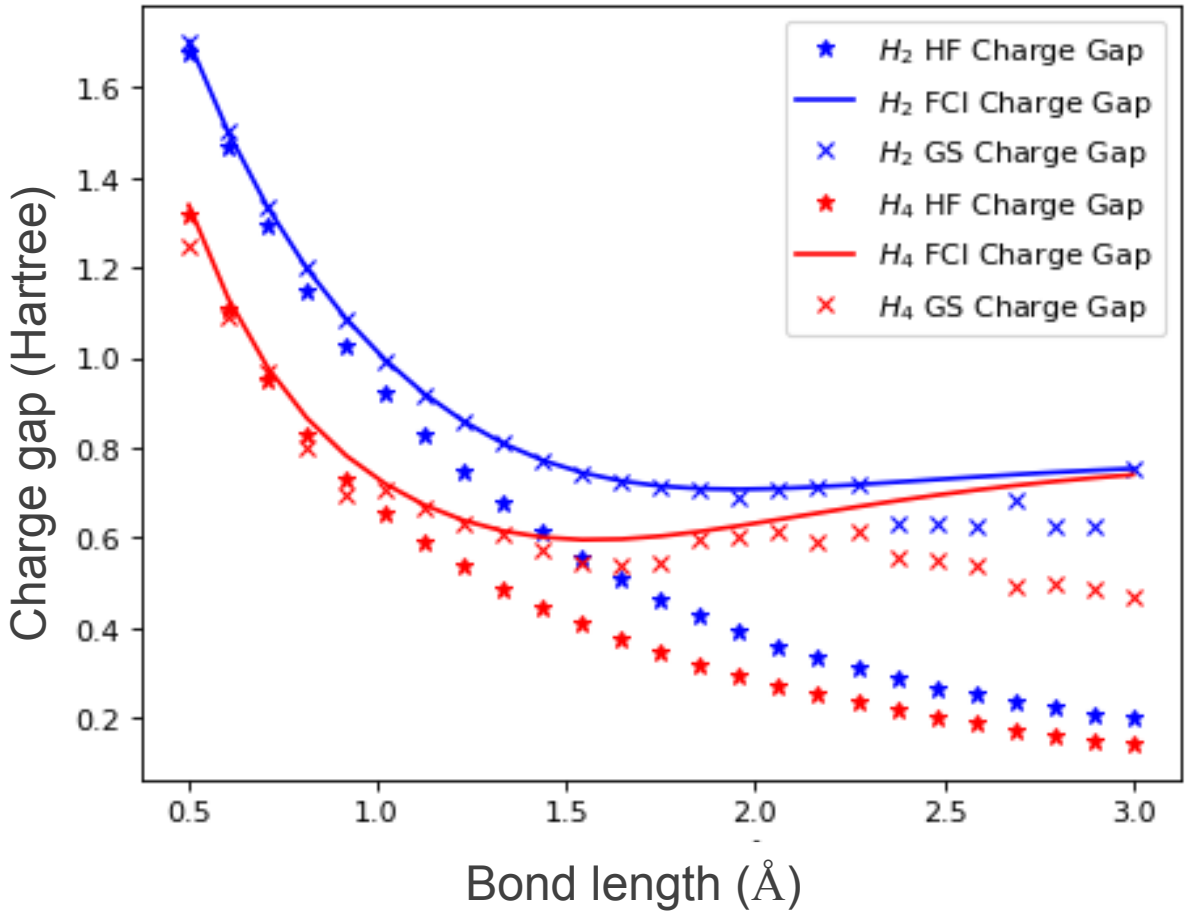
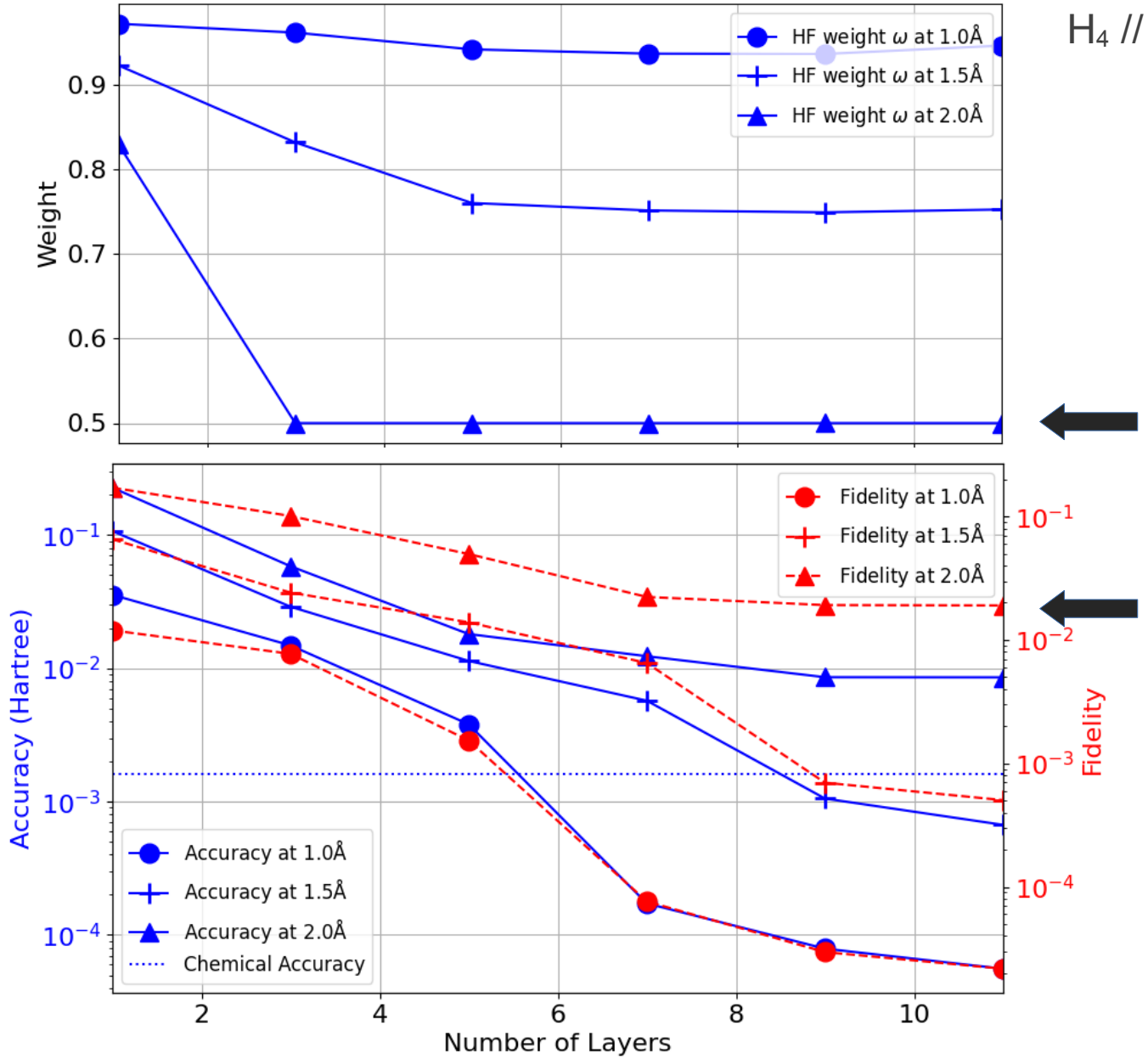


H. Akande, B. Senjean, M. Saubanère, preprint (2024)

Convergency

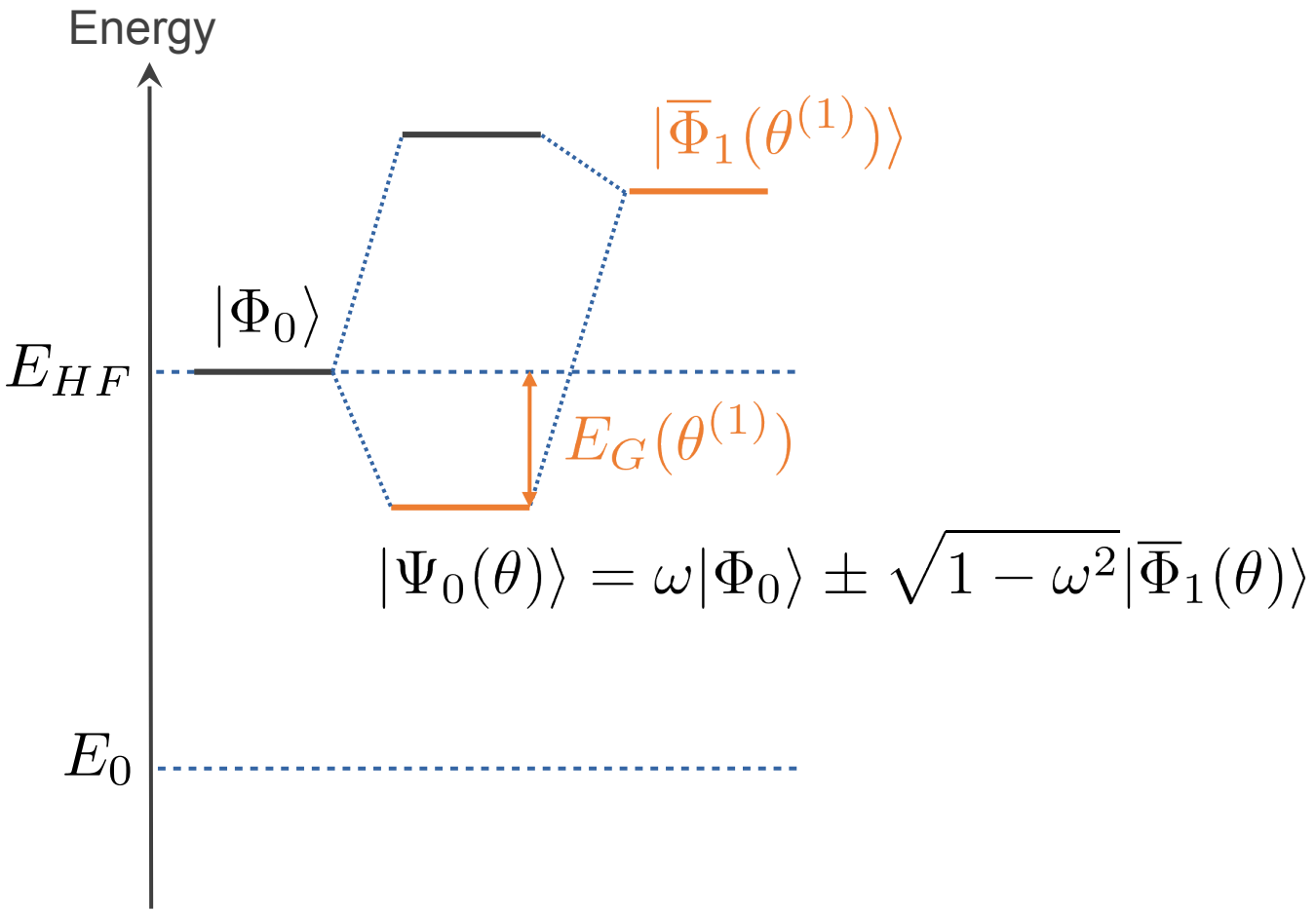


H_4 // 8 qubits

Good guess hypothesis non valid !

Iterative process:

$$|\Psi_0(\theta)\rangle = \omega|\Phi_0\rangle \pm \sqrt{1-\omega^2}|\overline{\Phi}_1(\theta)\rangle \rightarrow |\Phi_0\rangle$$



H. Akande, B. Senjean, M. Saubanère, preprint (2024)

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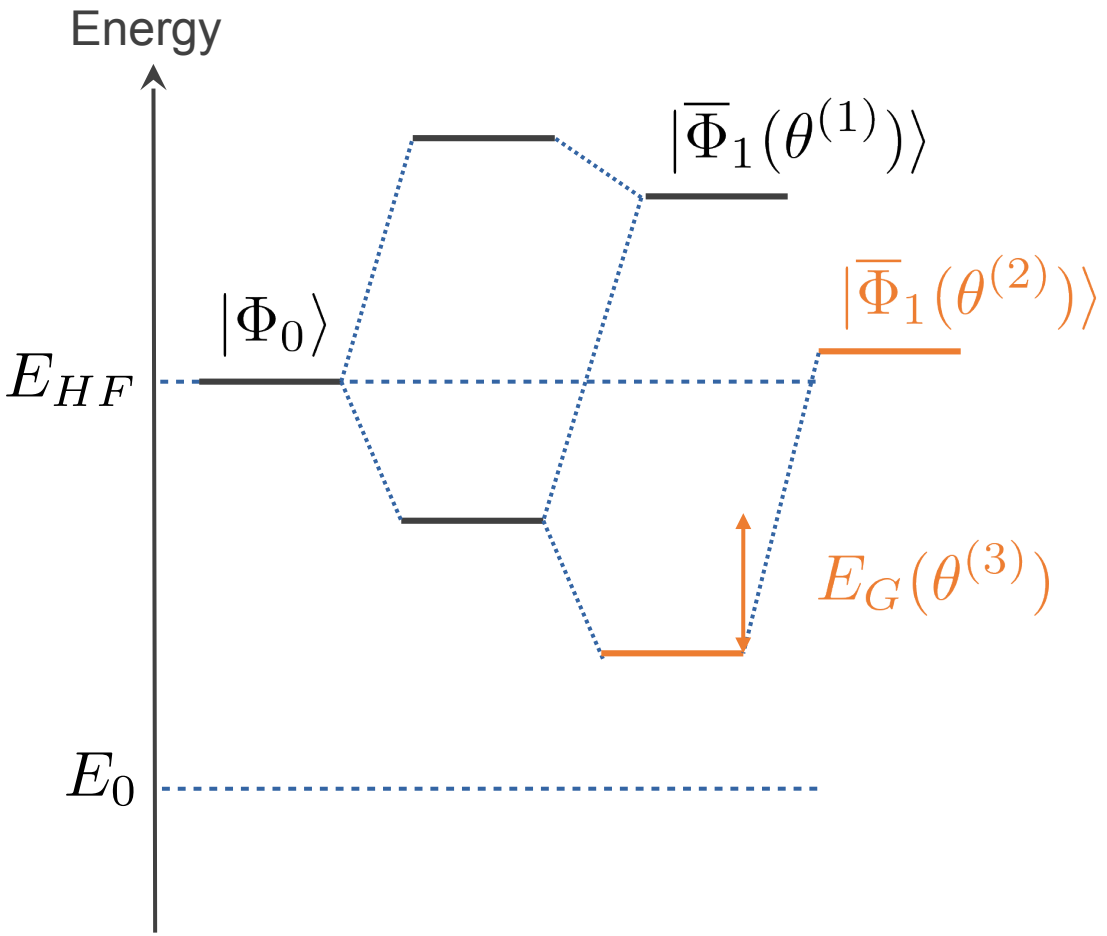

H. Akande, B. Senjean, M. Saubanère, preprint (2024)

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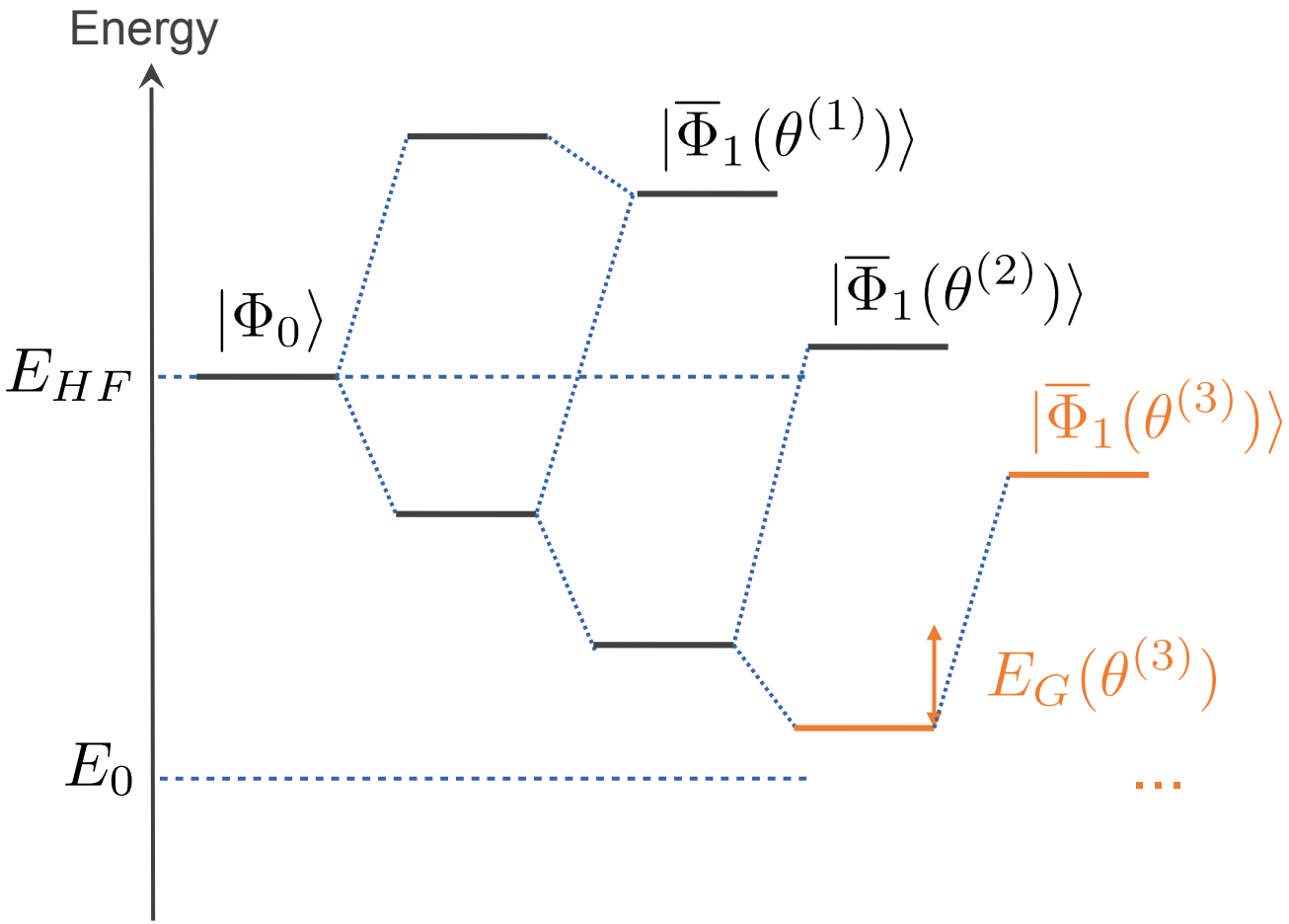

H. Akande, B. Senjean, M. Saubanère, preprint (2024)

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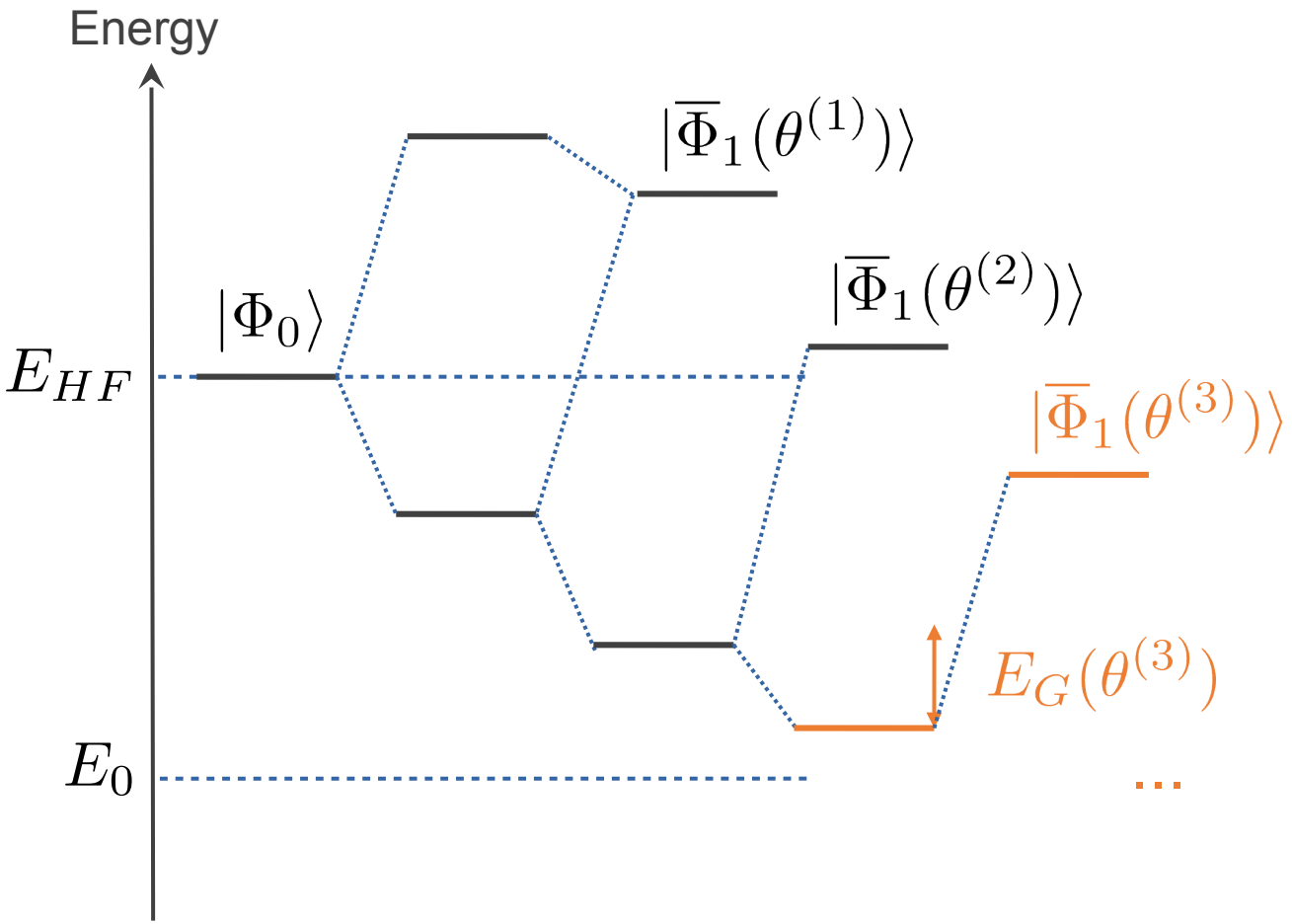
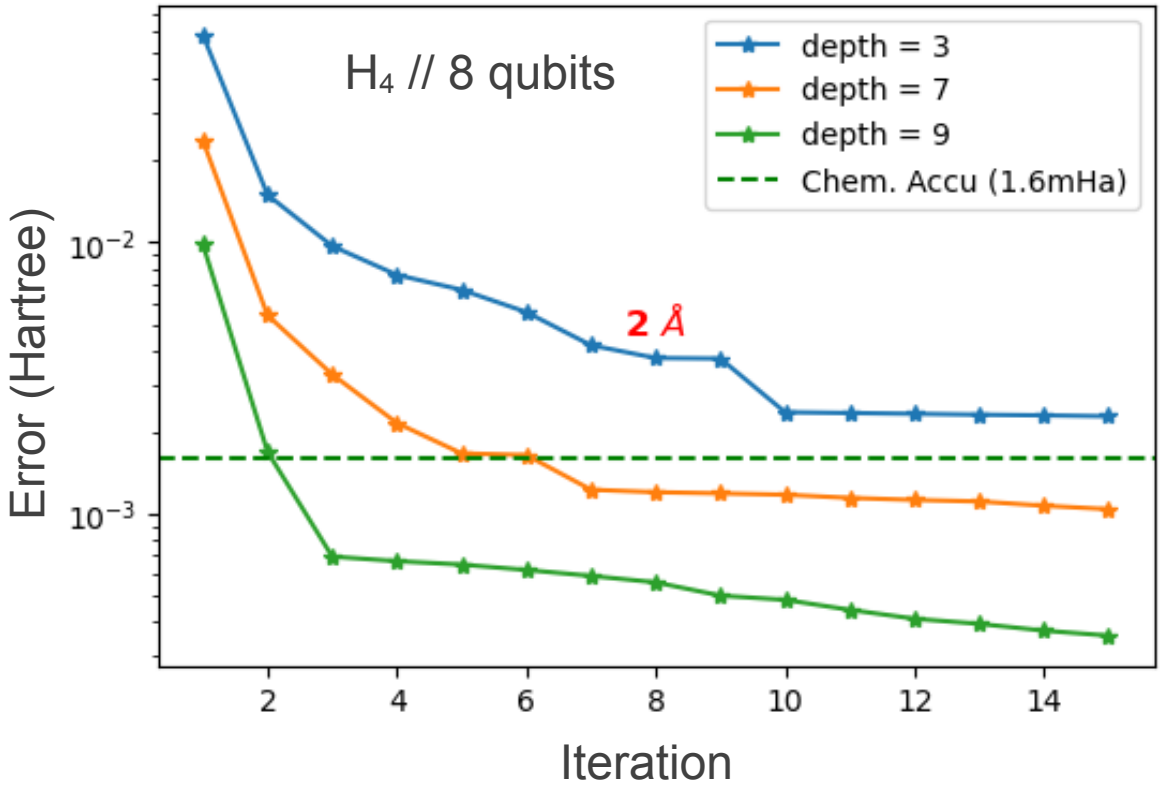




Iterative process converge rapidly !
But more measurement to pay

H. Akande, B. Senjean, M. Saubanère, preprint (2024)

Outline:

1– Symmetries : $[\hat{H}, \hat{N}] = [\hat{H}, \hat{S}_z] = [\hat{H}, \hat{S}^2] = \cdots = 0$

Symmetries consideration mandatory

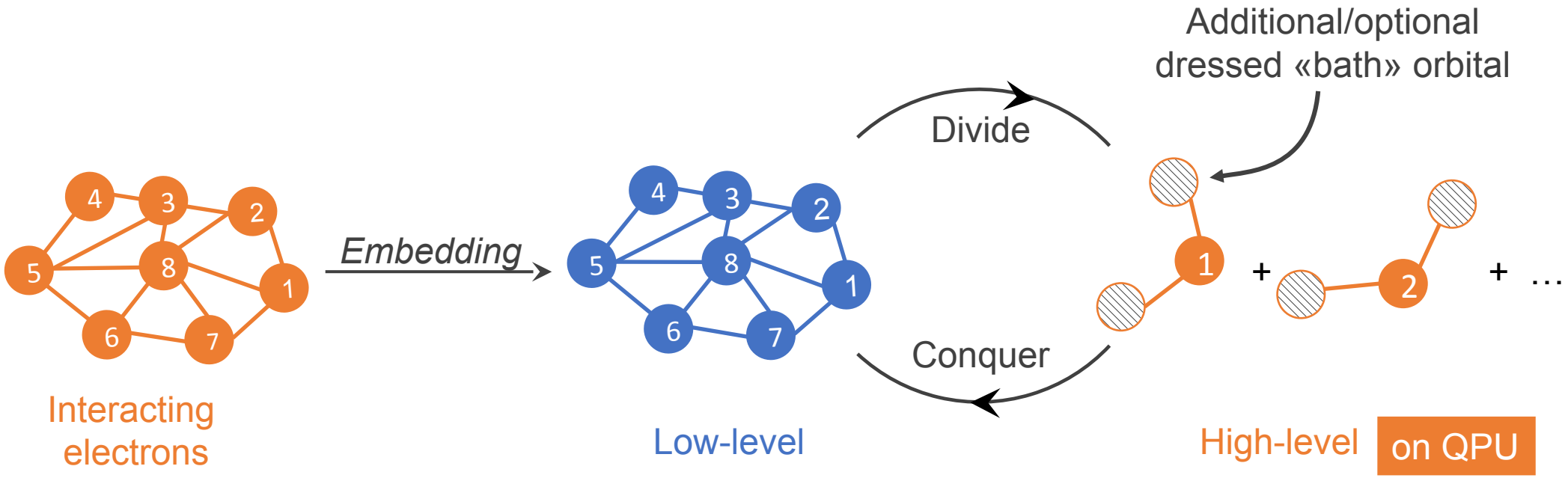
2– Locality of interaction // Nearsightedness

- Kinetic operator : ∇
- Coulomb operator : $\frac{1}{r} \rightarrow e^{-\kappa r}$

→ Localized basis-set empty the Hamiltonian !

Divide-conquer strategy (embedding)

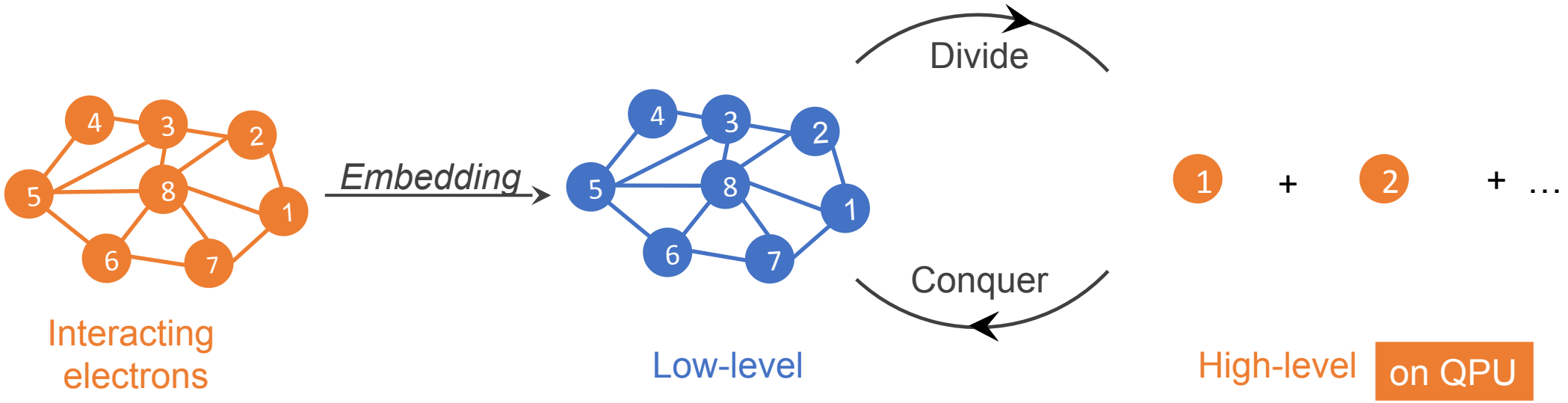
Divide and conquer strategies



Wave Function : Single-Determinant
Reduced quantities : Density //1RDM
Green's function : 1GF // 2GF

JCTC, 13, 4063-4078 (2017)
JCTC, 16, 119-219 (2020)
PRR, 3, 033230 (2021)
JPCL, 12, 1104−1109 (2021)
JCTC, 17, 2116−2125 (2021)
PRX, 12, 011046 (2022)
JCP, 157,214112 (2022)
PRX Quantum, 3, 010339 (2022)
NPJ Comput. Mater., 9, 78 (2023)
JCTC, 19, 1487-1498 (2023)

Divide and conquer strategies for quantum state preparation



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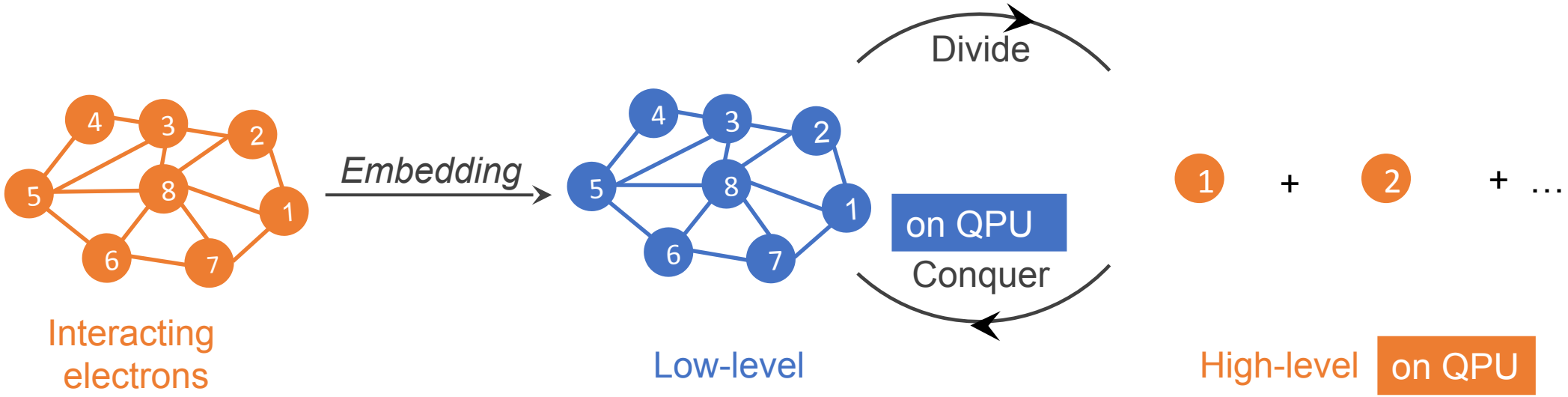


The most simple case : $|\Phi_0\rangle = \prod$

Conquest on QC → $|\Psi_0\rangle = U|\Phi_0\rangle$

Divide and conquer strategies for quantum state preparation

The most simple case :  $|\Phi_0\rangle = \prod$ 

Conquest on QC → $|\Psi_0\rangle = U|\Phi_0\rangle$

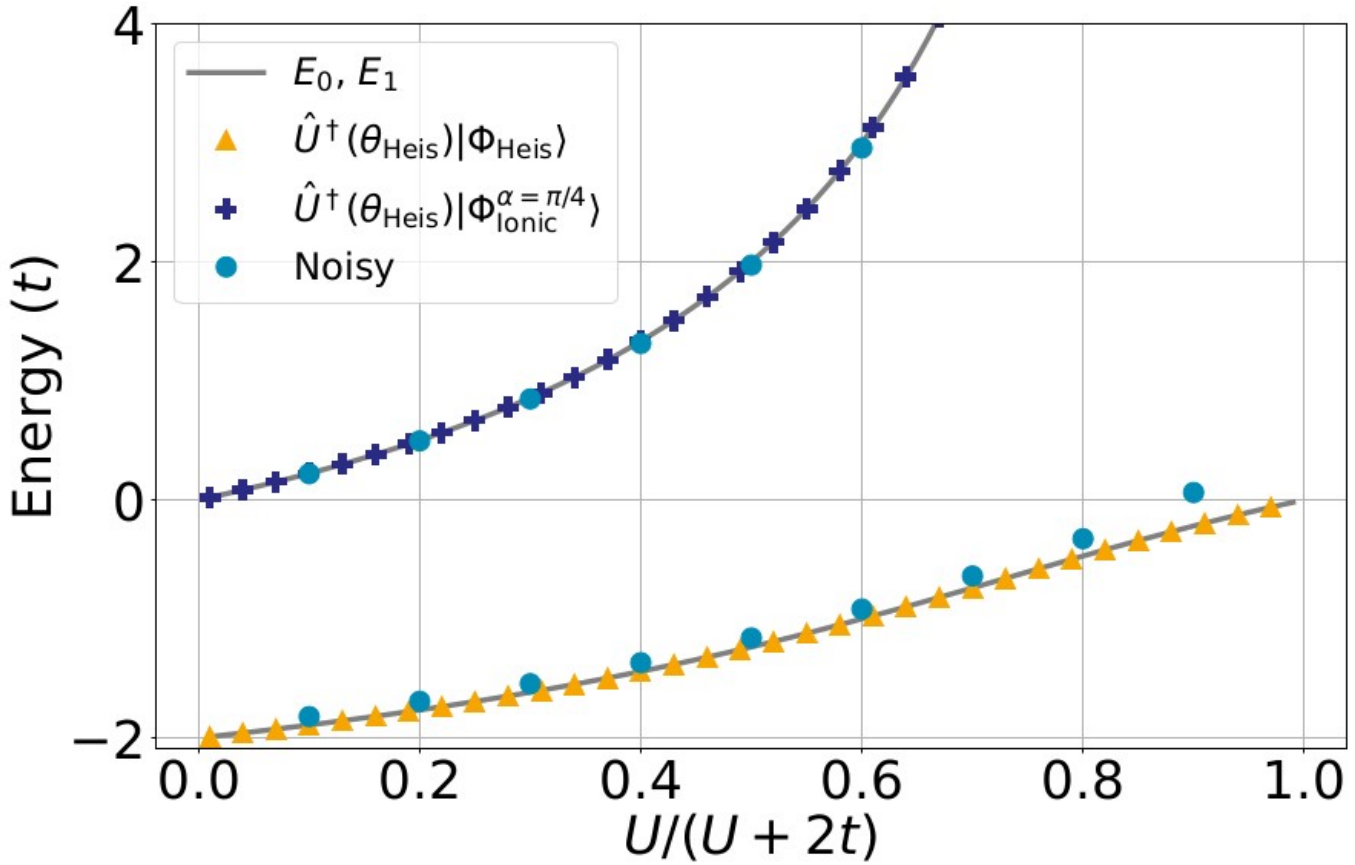
$U = e^S$

$U \rightarrow U(\theta)$

J. R. Schrieffer, P. A. Wolff, Phys. Rev. 149, 491 (1966)Phys. Rev. 149, 491 (1966)

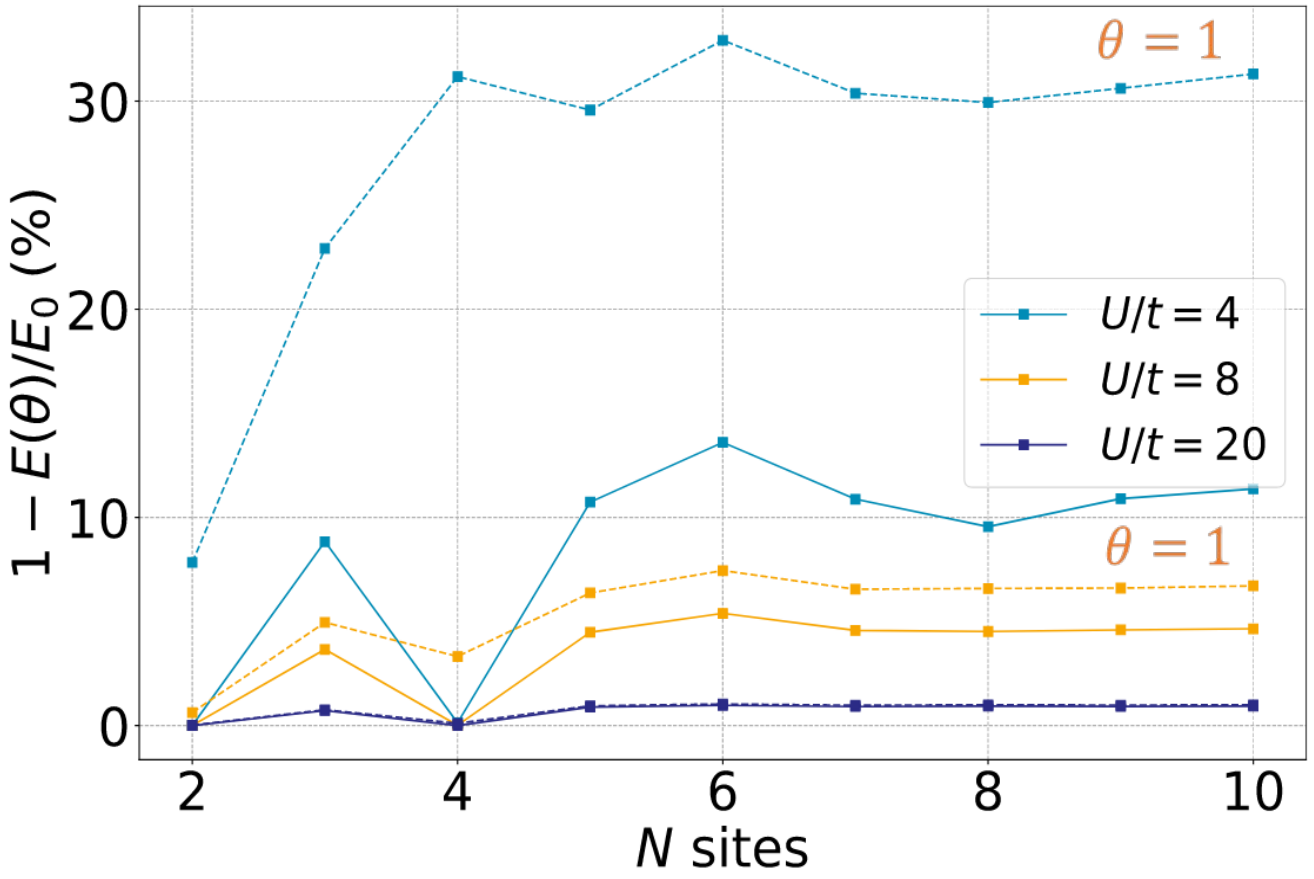
Hubbard dimer

Exact with one single variational parameter ! $U = e^{\theta S}$



Q. Marécat, B. Senjean, M. Saubanère, Phys. Rev. B, 107, 155110 (2023).

Larger Hubbard rings



Collaboration B. Murta, International Iberian Nanotechnology Laboratory
Heisenberg state preparation : Phys. Rev. B 109, 035128 (2024)

Q. Marécat, B. Senjean, M. Saubanère, Phys. Rev. B, 107, 155110 (2023).

UMR5798

Laboratoire Ondes et Matière d'Aquitaine

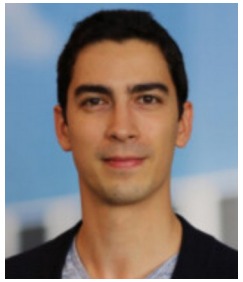
Students/post docs:

Quentin Marécat (graduated)
Schrieffer-Wolff/Embedding

Matteo de Santis
Embedding on QC

Hazat Akande
Symmetry preserving cost-function

Collaborations:



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Non-convex energy landscape