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Institut Charles Gerhardt Montpellier

CHEMISTRY: MOLECULES TO MATERIALS

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Advances and Perspectives in Quantum Computing for Quantum Chemistry and Material Science

Bruno Senjean
ICGM, Université de Montpellier, CNRS

November 12, 2024

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Electronic Structure Problem

Hamiltonian operator for the total electronic energy of the system, $\hat{H} = \hat{T} + \hat{V}_{ne} + \hat{W}_{\mathrm{ee}}$:

$$\hat{H} = -\sum_i \frac{\nabla_i^2}{2} - \sum_{i,I} \frac{Z_I}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r_i} - \mathbf{r_j}|} \qquad \hat{H} |\Psi_n\rangle = E_n |\Psi_n\rangle, \textbf{ To difficult to solve !}$$

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$\hat{H}\,|\Phi_0\rangle = \mathcal{E}_0\,|\Phi_0\rangle$, **Easy to solve !**

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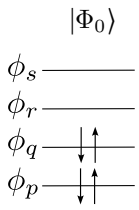
Projected onto a basis of N **spin-orbitals** $\{\phi_p^\alpha(\mathbf{r}), \phi_p^\beta(\mathbf{r})\}$



Non-interacting problem

$$|\Psi_0\rangle \to |\Phi_0\rangle\,, E_0 \to \sum_{i=1}^{\mathrm{occ}} \varepsilon_i$$

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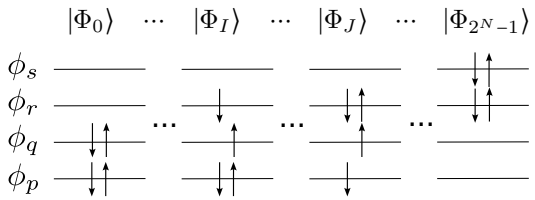

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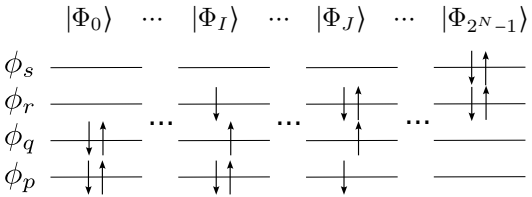
$$|\Psi_0\rangle \to |\Phi_0\rangle, E_0 \to \sum_{i=1}^{\text{occ}} \varepsilon_i$$

Exponential Wall problem

$$|\Psi_0\rangle = \sum_I^{\text{Exponential}} c_I |\Phi_I\rangle$$

Many-body basis

Occupation vector representation of the many-body basis (electronic configuration):



$$\left|\phi^{\beta}_{N/2}, \cdots, \phi^{\beta}_{1}, \phi^{\alpha}_{N/2}, \cdots, \phi^{\alpha}_{1}\right\rangle, \quad \phi_p = \begin{cases} 0 & \text{if empty} \\ 1 & \text{if occupied} \end{cases}$$

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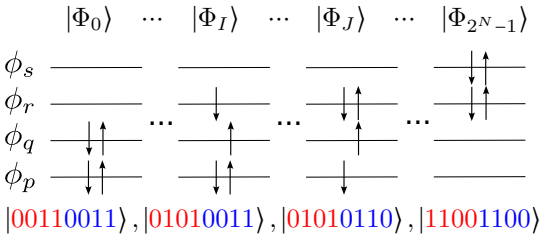

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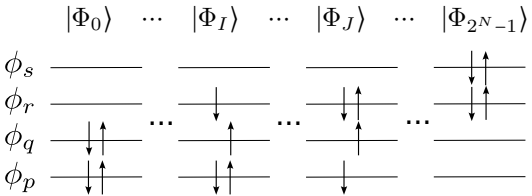

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Build and diagonalize the Hamiltonian matrix:

$$\begin{bmatrix} \langle\Phi_0|\hat{H}|\Phi_0\rangle & \cdots & \langle\Phi_0|\hat{H}|\Phi_{2^N-1}\rangle \\ \vdots & \ddots & \vdots \\ \langle\Phi_{2^N-1}|\hat{H}|\Phi_0\rangle & \cdots & \langle\Phi_{2^N-1}|\hat{H}|\Phi_{2^N-1}\rangle \end{bmatrix} \xrightarrow{\text{Diagonalization}} \begin{bmatrix} E_0 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & E_{2^N-1} \end{bmatrix}, |\Psi_0\rangle = \sum_I^{2^N} c_I |\Phi_I\rangle$$

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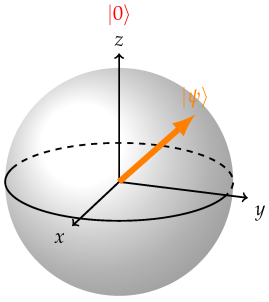
Superposition and Entanglement: Quantum bits

Classical bit to Quantum bit:

Qubit: a (two-)level system

Superposition



$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad |\alpha|^2 + |\beta|^2 = 1$$

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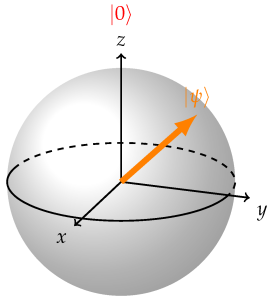


$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad |\alpha|^2 + |\beta|^2 = 1$$

Qubit register:

Superposition and Entanglement

$$|\Psi\rangle = \sum_{q=0}^{2^N-1} c_q\,|q\rangle\,, \quad \sum_q |c_q|^2 = 1$$

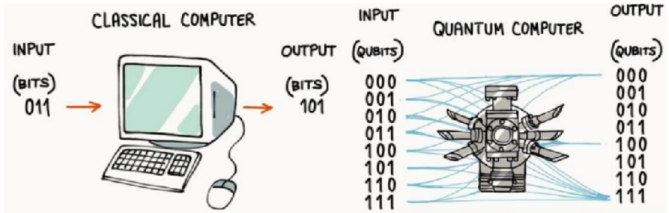
where $q = \{0, \cdots, 2^N - 1\}$ are all possible bit-strings from N qubits

Encoding?

$\mathcal{O}(2^N)$	$\mathcal{O}(N)$
Classical	Quantum

Quantum circuit: model of quantum computation

$$|\Psi\rangle = \frac{1}{\sqrt{8}}\left(|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle + |111\rangle\right)$$



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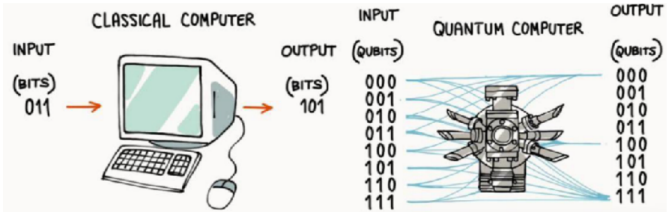

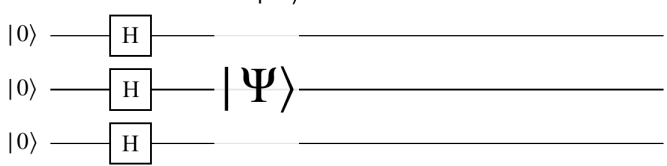

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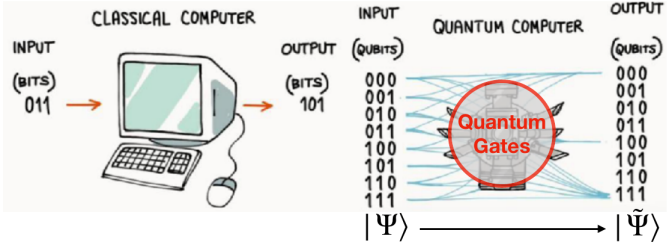

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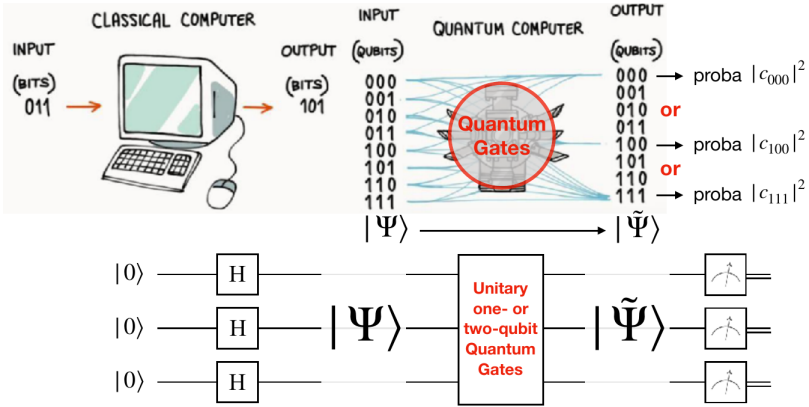

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- Build the Hamiltonian matrix (**exponentially costly to build**)
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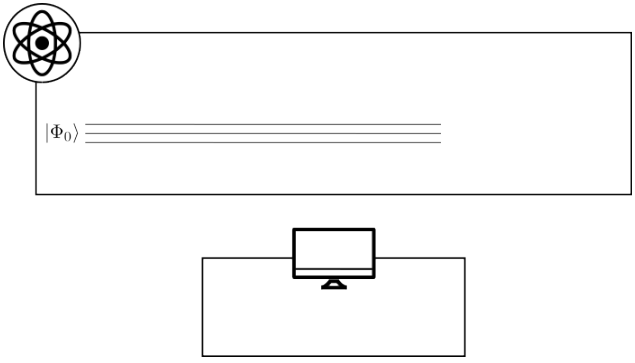
We can:

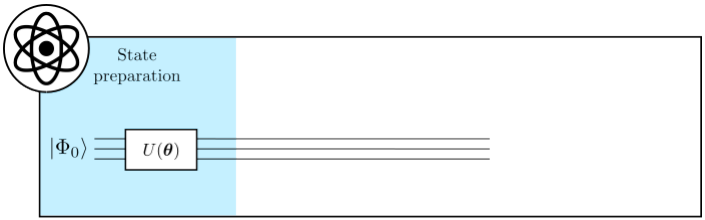
- Generate **exponentially many** electronic configurations with only N **qubits** through **superposition and entanglement**

Variational Quantum Eigensolver



Start with
a very
simple state

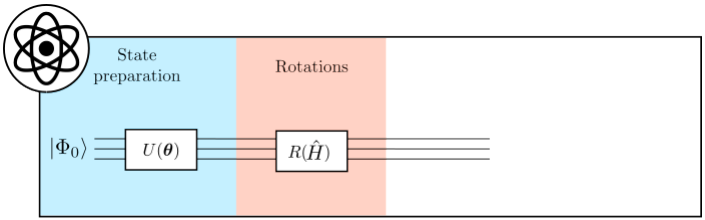
Variational Quantum Eigensolver

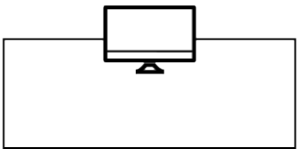


State preparation:

$$|\Psi(\boldsymbol{\theta})\rangle = U(\boldsymbol{\theta})\,|\Phi_0\rangle$$

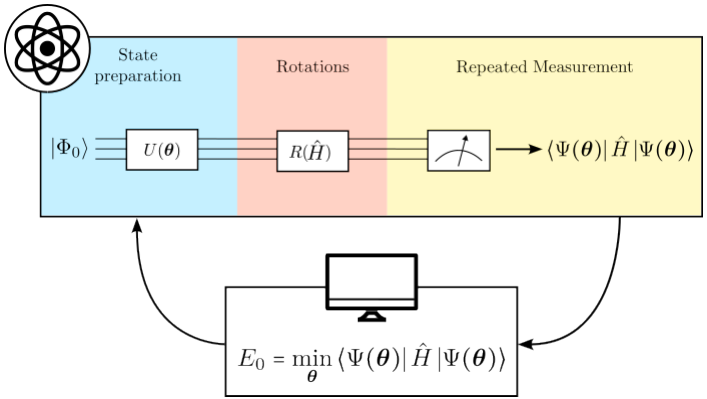
Variational Quantum Eigensolver





Rotations to the computational basis

Variational Quantum Eigensolver



Measurements:
Reconstruction of the energy

Classical optimization following the **variational principle**:
find new $\boldsymbol{\theta}$ parameters

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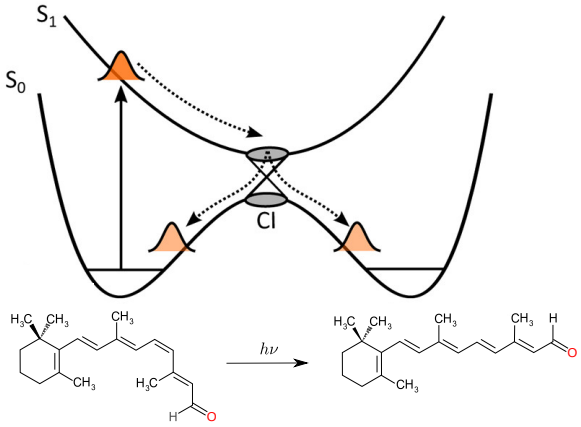
Problematic: avoided-crossings, conical intersections

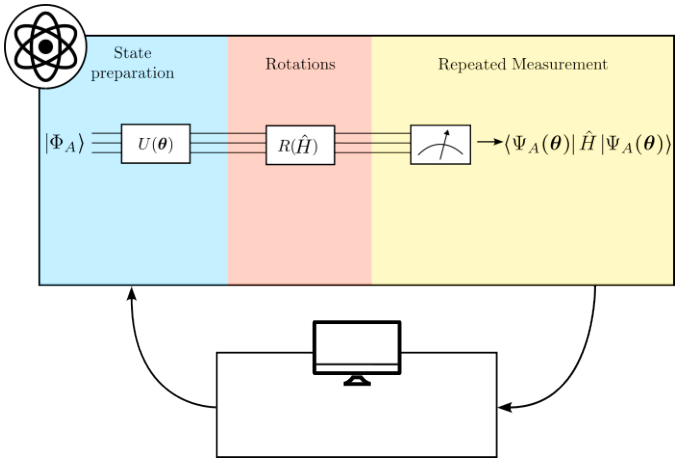
Photoisomerisation of the retinal molecule



Conical intersection → Point of degeneracy between the states

Requires a **DEMOCRATIC** description of the states

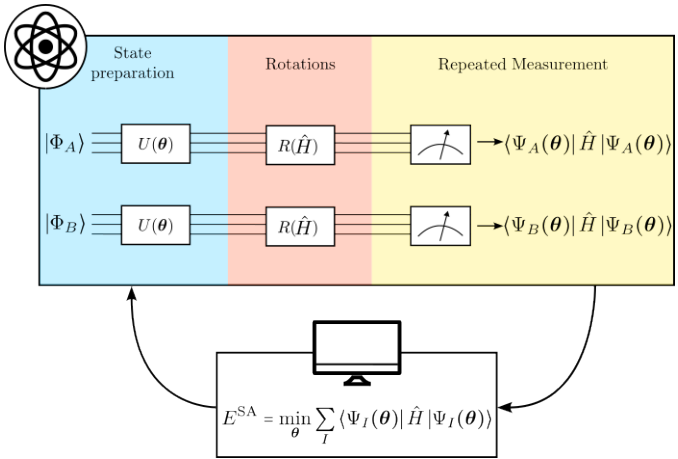
Ensemble VQE[1]



Same approach than VQE

[1] Saad Yalouz *et al.* Quantum Sci. Technol. 6 024004 (2021)

Ensemble VQE[1]



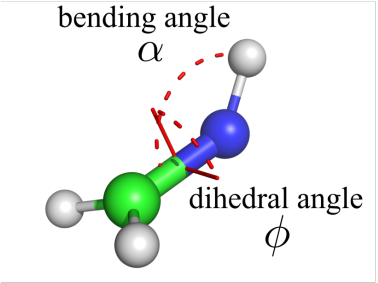
But to a **ensemble** of states

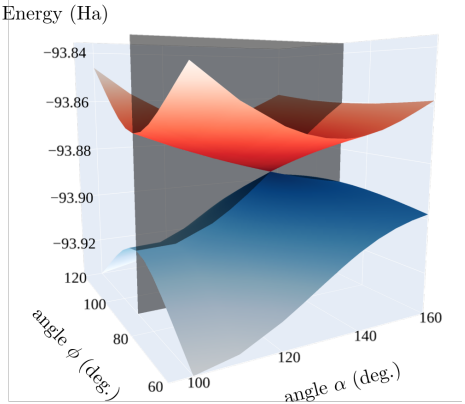
Generalized variational principle

[1] Saad Yalouz *et al.* Quantum Sci. Technol. 6 024004 (2021)

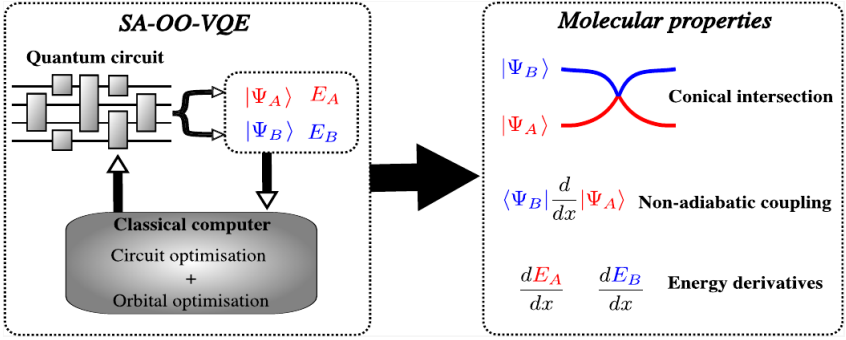
Example on a minimal Schiff base: formaldimine

2D PES obtained by ensemble VQE





Towards excited-state quantum dynamics[3,4]



- We are currently showing the ensemble VQE can lead to **quasi-diabatic states**[2]

[2] S. Illesova, M. Beseda, S. Yalouz, B. Lasorne, **BS**, *to be submitted*
[3] S. Yalouz, **BS** *et al.*, Quantum Sci. Technol. 6, 024004 (2021)
[4] S. Yalouz, E. Koridon, **BS** *et al.* J. Chem. Theory Comput., 18, 776-794 (2022)

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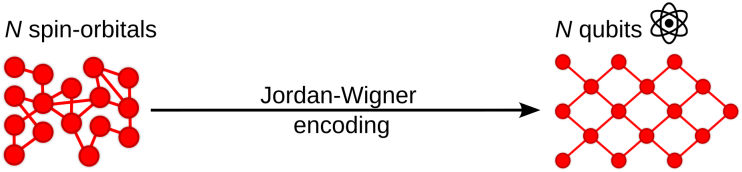
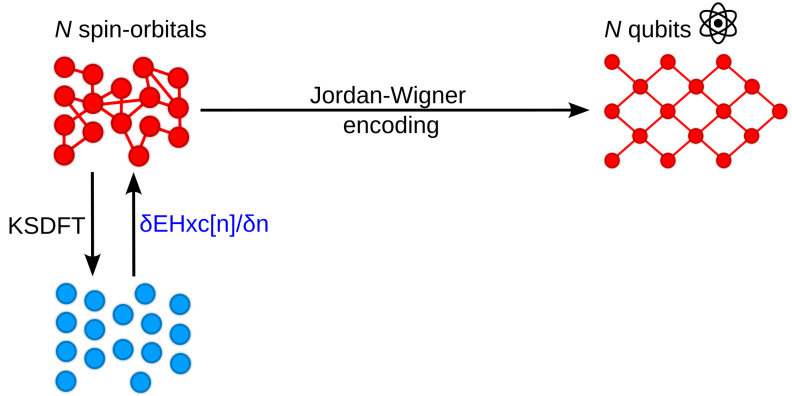
Mappings of the fully interacting problem



Mappings of the fully interacting problem



Density Functional Theory (DFT)

- (1964) Hohenberg–Kohn theorem: $n(\mathbf{r}) \longleftrightarrow v(\mathbf{r}) \longleftrightarrow \Psi_0$

$$E_0[v] = \min_n E_v[n], \quad E_v[n] = F[n] + \int \mathrm{d}\mathbf{r}\, v(\mathbf{r}) n(\mathbf{r})$$

The minimizing density is the **ground-state density** $n_0(\mathbf{r})$.

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- **Universal functional**: Levy–Lieb constrained search formalism

$$F[n] = \min_{\Psi \to n} \{ \langle \Psi | \hat{T} + \hat{\mathbf{W}}_{\mathrm{ee}} | \Psi \rangle \}$$

- The problem seems **even more complicated!**

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- The problem seems **even more complicated!** Decomposition:

$$F[n] = \text{unknown} = \text{known} + (\text{unknown} - \text{known})$$

Kohn-Sham DFT

- (1965) Kohn–Sham: noninteracting system with $n_s(\mathbf{r}) = n_0(\mathbf{r})$

$$F[n] = T_s[n] + \mathbf{E}_{\mathrm{Hxc}}[\mathbf{n}], \quad T_s[n] = \min_{\Phi \to n}\{\langle\Phi|\hat{T}|\Phi\rangle\}$$

- Kohn–Sham self-consistent equations:

$$\underbrace{\left(-\frac{\nabla^2}{2} + v(\mathbf{r}) + \frac{\delta \mathbf{E}_{\mathrm{Hxc}}[\mathbf{n}_{\mathbf{\Phi}^{\mathrm{KS}}}]}{\delta \mathbf{n}(\mathbf{r})}\right)}_{\hat{h}^{\mathrm{KS}}[\mathbf{n}_{\mathbf{\Phi}^{\mathrm{KS}}}]} \varphi_{\mathbf{k}}(\mathbf{r}) = \varepsilon_{\mathbf{k}}\varphi_{\mathbf{k}}(\mathbf{r}), \quad \mathbf{n}(\mathbf{r}) = 2\sum_{k=1}^{N_{\mathrm{occ}}} |\varphi_{\mathbf{k}}(\mathbf{r})|^2$$

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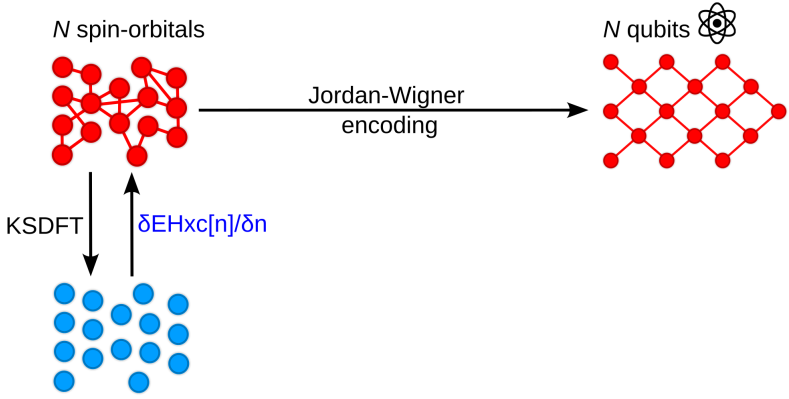
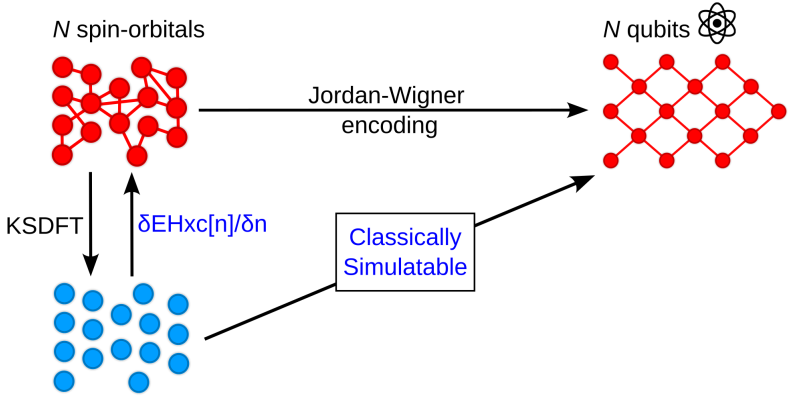
- **(in-principle-exact)** Ground-state energy in $\mathcal{O}(N^3)$:

$$E_0 = 2\sum_{k=1}^{N_{\mathrm{occ}}} \varepsilon_{\mathbf{k}} + E_{\mathrm{Hxc}}[\mathbf{n}^{\mathbf{\Phi}^{\mathrm{KS}}}] - \int \mathrm{d}\mathbf{r}\, v_{\mathrm{Hxc}}[n^{\Phi^{\mathrm{KS}}}](\mathbf{r})\mathbf{n}^{\mathbf{\Phi}^{\mathrm{KS}}}(\mathbf{r})$$

Flowchart


N spin-orbitals
N qubits
Jordan-Wigner
encoding
KSDFT
δEHxc[n]/δn

Flowchart


N spin-orbitals
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Classically
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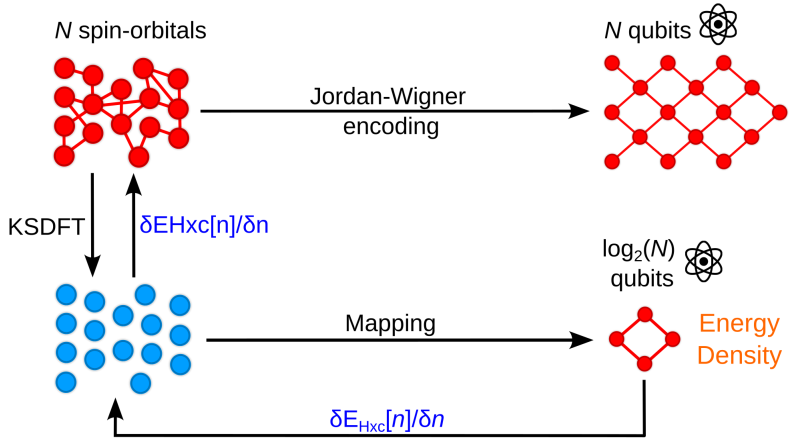
N spin-orbitals
N qubits
Jordan-Wigner encoding
KSDFT
δEHxc[n]/δn
log2(N) qubits
Mapping
Energy Density
δEHxc[n]/δn

DFT encoding

One-body non-int. Hamiltonian with N spin-orbitals $\{|\chi_i\rangle\} \xrightarrow{\text{map}} N$ **qubits**, classically simulatable

Basis set one-body states		**Unary**[5] 8 qubits
$\|\chi_0\rangle$	$\longrightarrow$	$\|00000001\rangle$
$\|\chi_1\rangle$	$\longrightarrow$	$\|00000010\rangle$
$\|\chi_2\rangle$	$\longrightarrow$	$\|00000100\rangle$
$\|\chi_3\rangle$	$\longrightarrow$	$\|00001000\rangle$
$\|\chi_4\rangle$	$\longrightarrow$	$\|00010000\rangle$
$\|\chi_5\rangle$	$\longrightarrow$	$\|00100000\rangle$
$\|\chi_6\rangle$	$\longrightarrow$	$\|01000000\rangle$
$\|\chi_7\rangle$	$\longrightarrow$	$\|10000000\rangle$

[5] N.P.D. Sawaya *et al.*, npj Quantum Inf 6, 49 (2020).

[6] **BS**, S. Yalouz, M. Saubanère, SciPost Phys. 14, 055 (2023) ; Y. Shee et al. PRR 4, 023154 (2022)

DFT encoding

One-body non-int. Hamiltonian with N spin-orbitals $\{|\chi_i\rangle\} \xrightarrow{\text{map}} \log_2(N)$ **interacting qubits**

Basis set one-body states		**Unary**[5] 8 qubits		**Standard Binary**[6] 3 qubits[6]
$\|\chi_0\rangle$	$\longrightarrow$	$\|00000001\rangle$	$\longrightarrow$	$\|000\rangle$
$\|\chi_1\rangle$	$\longrightarrow$	$\|00000010\rangle$	$\longrightarrow$	$\|001\rangle$
$\|\chi_2\rangle$	$\longrightarrow$	$\|00000100\rangle$	$\longrightarrow$	$\|010\rangle$
$\|\chi_3\rangle$	$\longrightarrow$	$\|00001000\rangle$	$\longrightarrow$	$\|011\rangle$
$\|\chi_4\rangle$	$\longrightarrow$	$\|00010000\rangle$	$\longrightarrow$	$\|100\rangle$
$\|\chi_5\rangle$	$\longrightarrow$	$\|00100000\rangle$	$\longrightarrow$	$\|101\rangle$
$\|\chi_6\rangle$	$\longrightarrow$	$\|01000000\rangle$	$\longrightarrow$	$\|110\rangle$
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$$\hat{\mathbf{h}}^{\mathrm{KS}}|\varphi_{\mathbf{k}}\rangle = \varepsilon_{\mathbf{k}}|\varphi_{\mathbf{k}}\rangle \longrightarrow \hat{\mathcal{H}}^{\mathrm{aux}}|\varphi_{\mathbf{k}}\rangle = \varepsilon_{\mathbf{k}}|\varphi_{\mathbf{k}}\rangle, \quad k = 1, \ldots, N_{\mathrm{occ}} \longrightarrow \textbf{Ensemble VQE}$$

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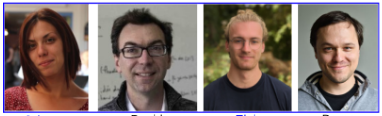
Are we only looking to (asymptotic exponential) quantum advantage?

- Exponential, polynomial or constant factor advantage (G. Chan, arXiv:2407.11235)
- No advantage?... QC is a **new path** to explore the electronic structure problem

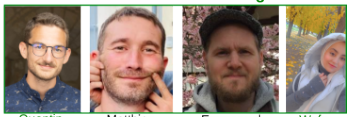
Acknowledgments and Collaborations on Quantum Computing 18 / 18

Q-DFT on Qudits



Johanna Klein — David Guéry-Odelin — Eloi Flament — Bruno Peaudecerf

Schrieffer-Wolf & Embedding & DFT



Quentin Marécat — Matthieu Saubanère — Emmanuel Fromager — Wafa Makhlouf

SA-OO-VQE

Emiel Koridon — Thomas O'Brien — Lucas Visscher

Extensions of SA-OO-VQE — **Vibrational/Vibronic**

Martin Beseda — Silvie Illesova — Benjamin Lasorne — Yohann Scribano — Joachim Knapik

Q-DFT in BigDFT

Thierry Deutsch — Akilan Rajamani — Luigi Genovese

Kind of everything...

Saad Yalouz

Open-access codes:

`https://gitlab.com/MartinBeseda/sa-oo-vqe-qiskit`

`https://github.com/bsenjean/QDFT`

PhD and Postdoc openings in LOMA (Bordeaux), ICGM (Montpellier) and LCQS (Strasbourg)

ICGM
Institut Charles Gerhardt Montpellier

Thank you for your attention

CHEMISTRY: MOLECULES TO MATERIALS

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ENS Chimie Montpellier
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