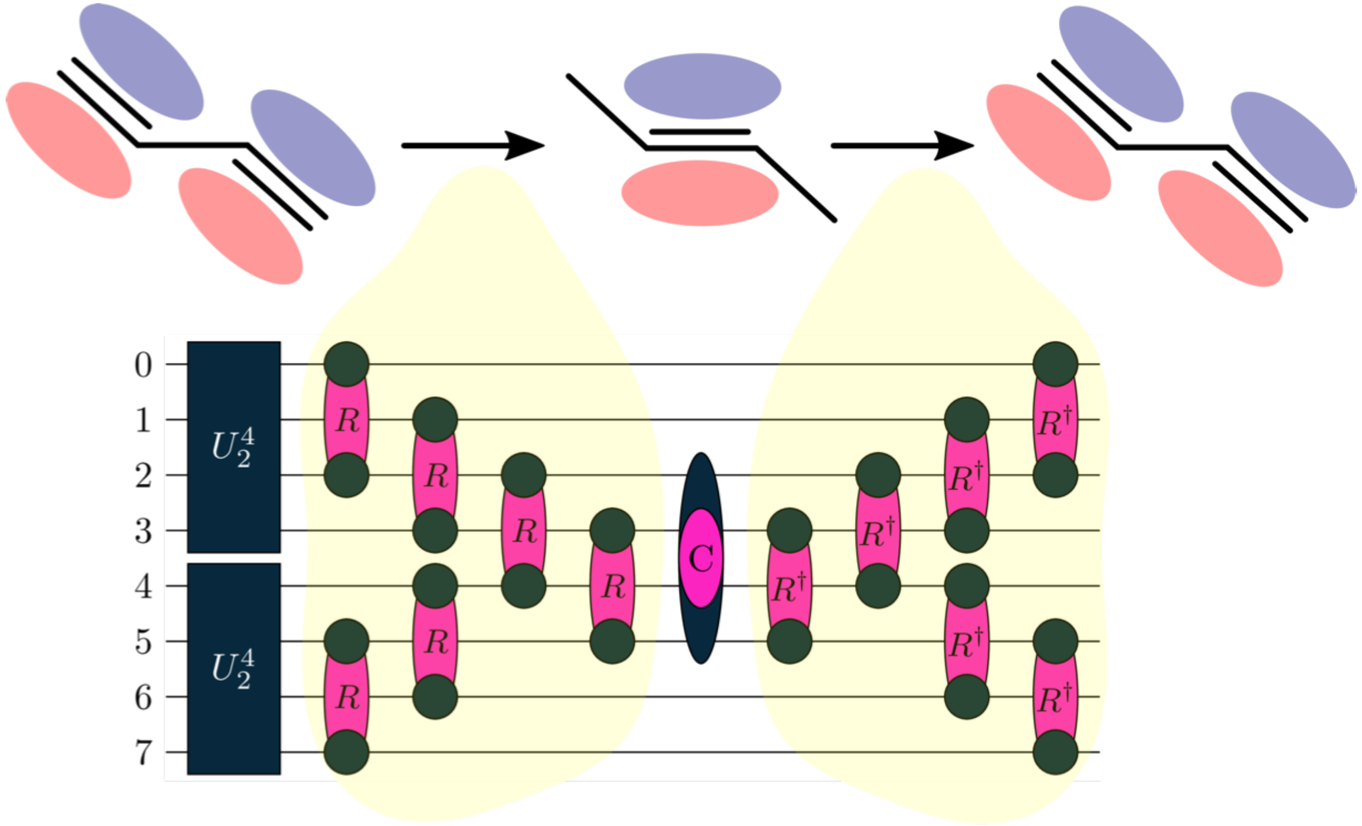
Molecular Quantum Circuit Design

@JakobKottmann

github/tequilahub

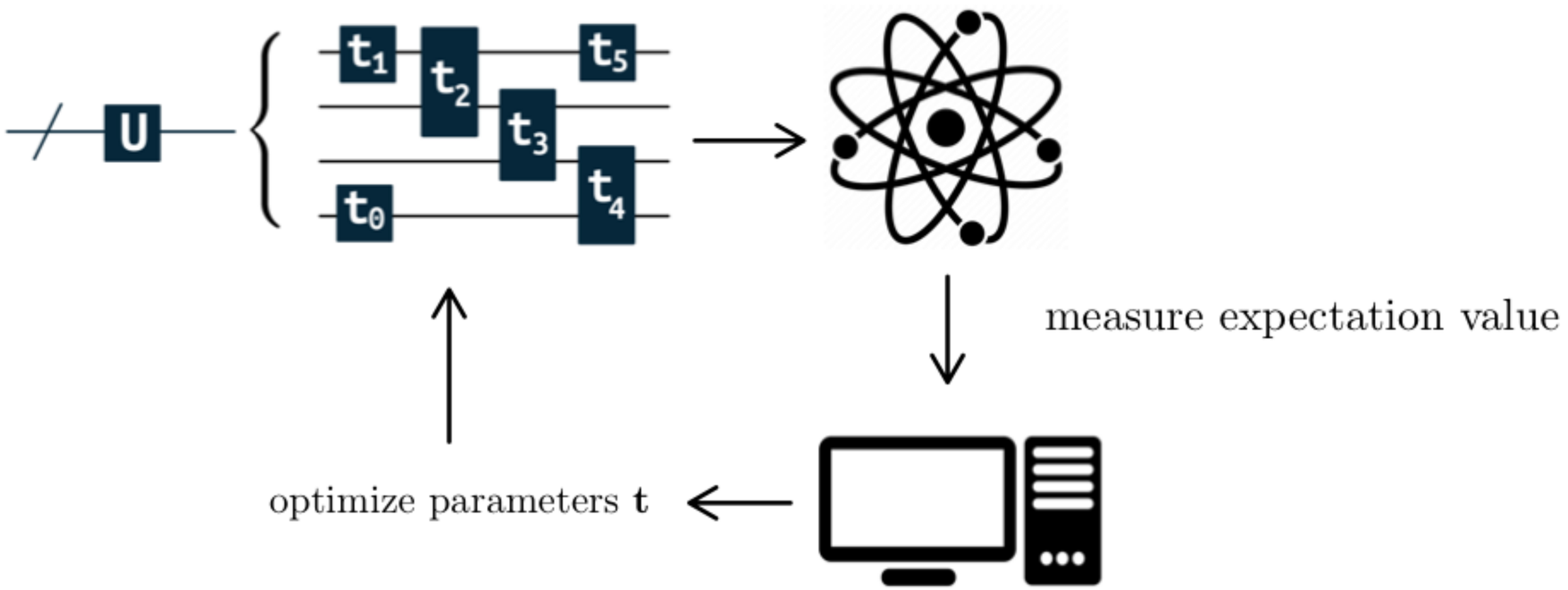


Graph Based Molecular Quantum Circuit Design

Jakob S. Kottmann*
(Dated: July 20, 2022)

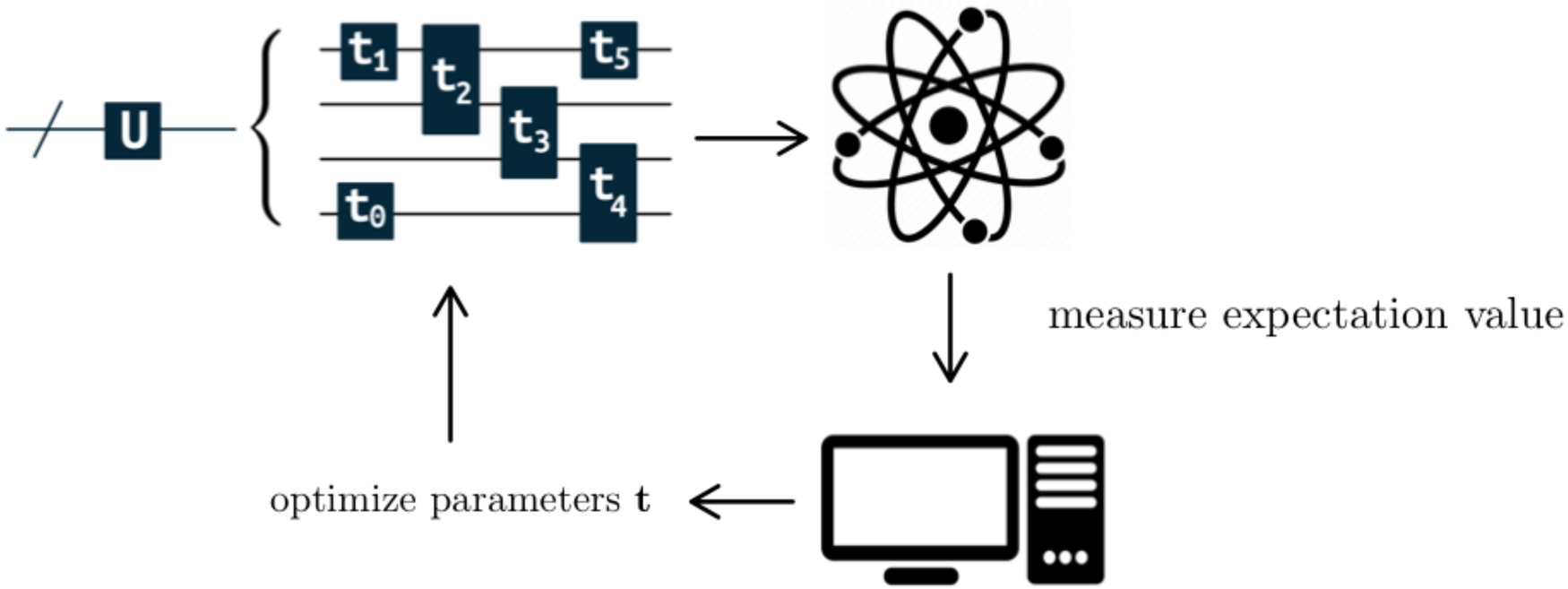
Optimized Low-Depth Quantum Circuits for Molecular Electronic Structure using a Separable Pair Approximation

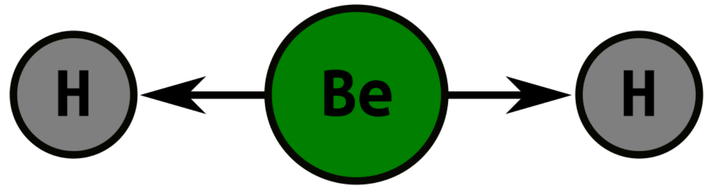
Jakob S. Kottmann[1, 2, *] and Alán Aspuru-Guzik[1, 2, 3, 4, †]

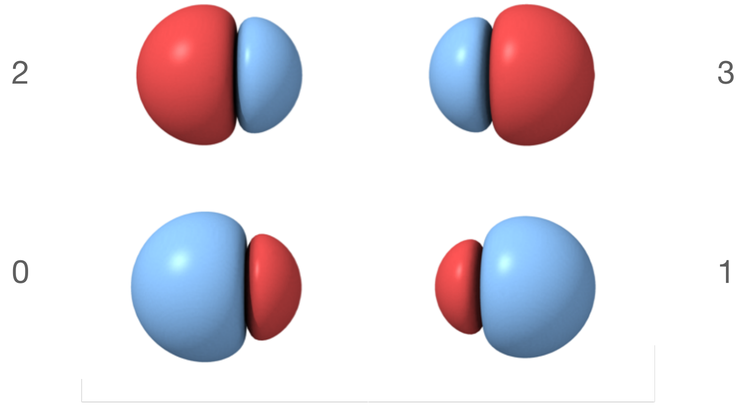

U
t1
t2
t3
t0
t4
t5
measure expectation value
optimize parameters t

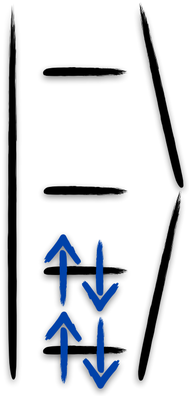
Design principles

- Locality (circuit connections)
- Shallow depth
- Hardware efficient
- Good convergence
- Initialisation heuristics




H
Be
H

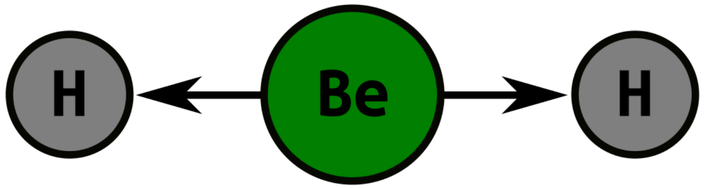

2
3
0
1

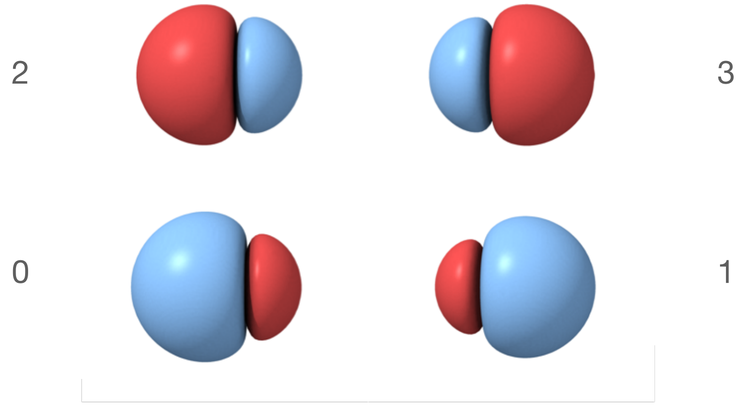


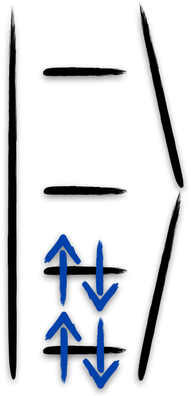
Empty orbitals 2,3

Two electrons in orbital 1

Two electrons in orbital 0



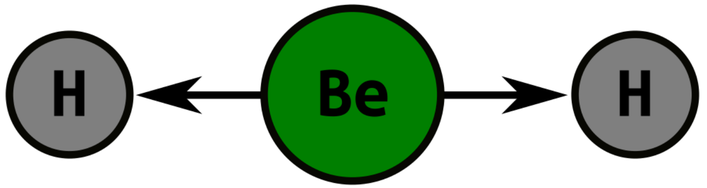


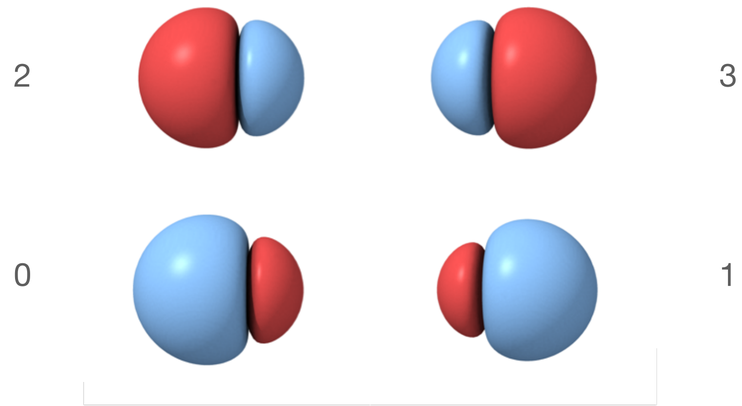


Empty orbitals 2,3

Two electrons in orbital 1

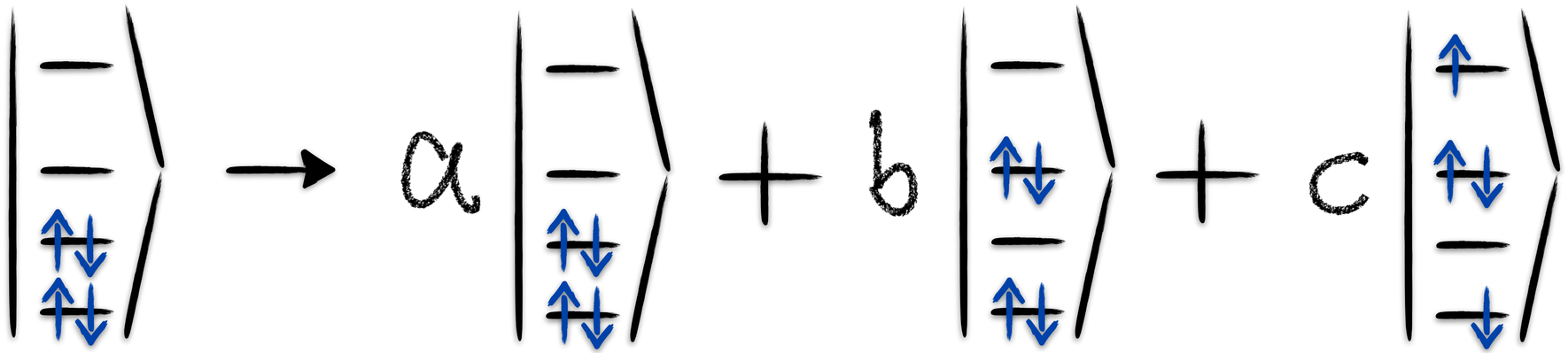
Two electrons in orbital 0



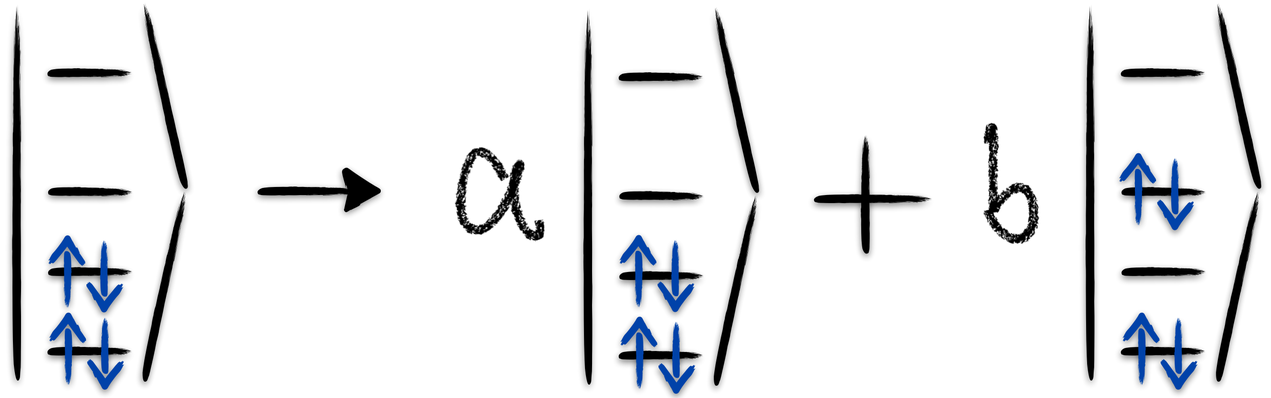


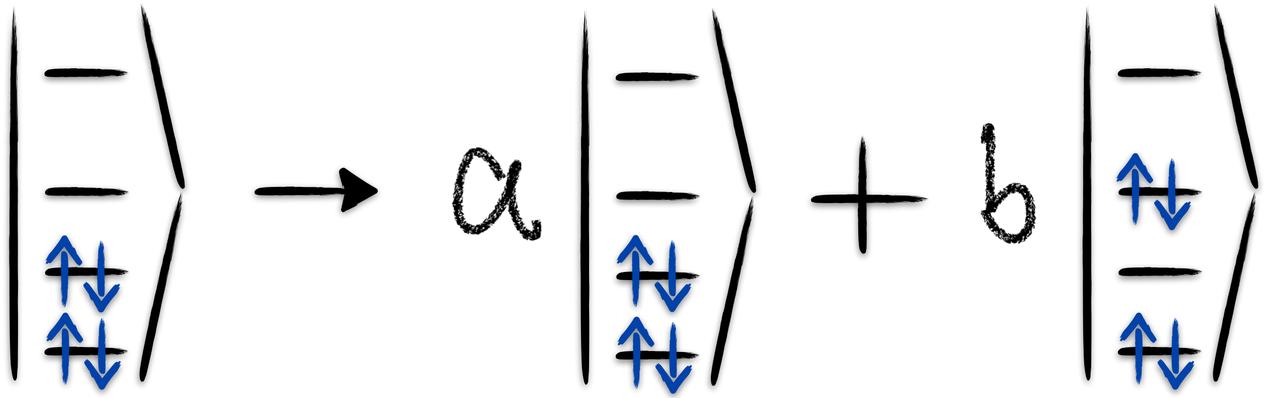
$$|11\ 11\ 00\ 00\rangle$$

Qubit encoding


a
b
c

Building Blocks

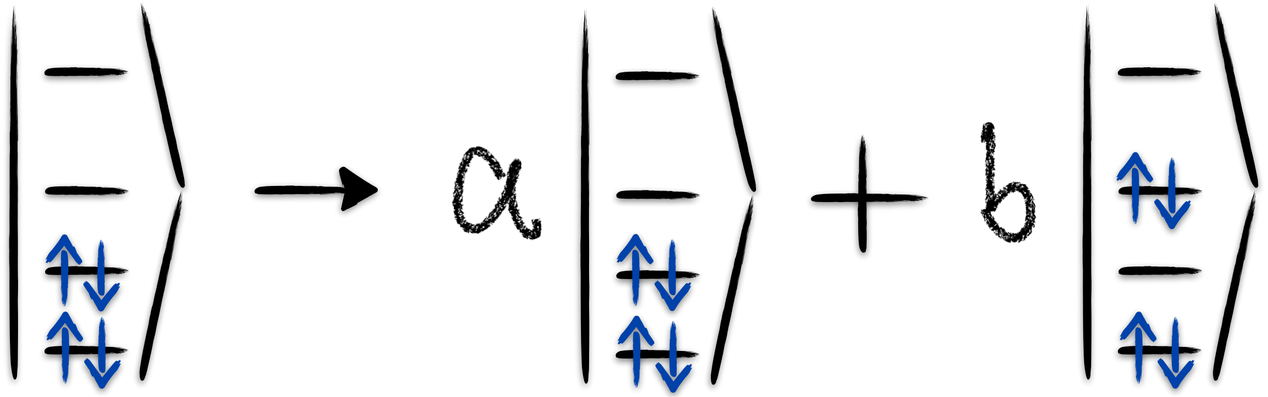




$$U_{\boldsymbol{pq}}(\theta) = e^{-i\frac{\theta}{2}G_{\boldsymbol{pq}}}$$

$$G_{\boldsymbol{pq}} = i\left(\prod_k a^\dagger_{p_k} a_{q_k} - h.c.\right)$$

$$a^\dagger_p \xrightarrow[Wigner]{Jordan} \sigma^+_p \prod_{k<p} \sigma^z_k.$$



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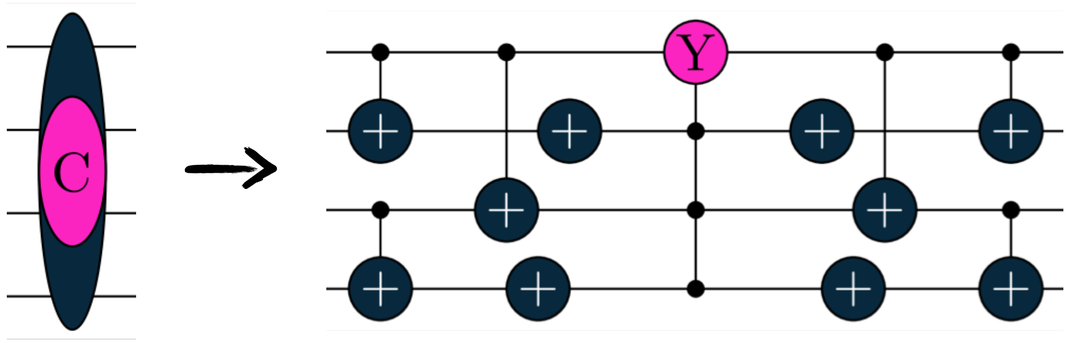
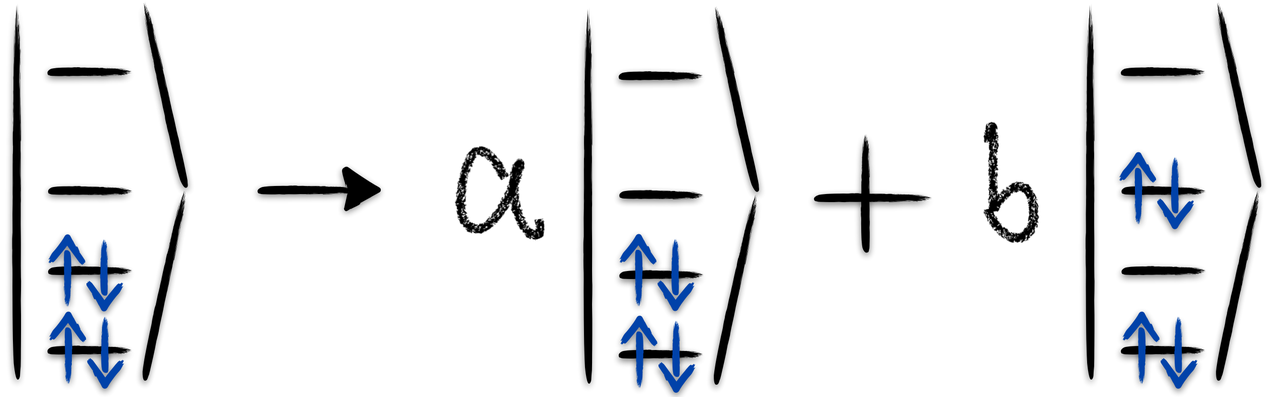
$$a^\dagger_p \xrightarrow[Wigner]{Jordan} \sigma^+_p \prod_{k<p} \sigma^z_k.$$

Example

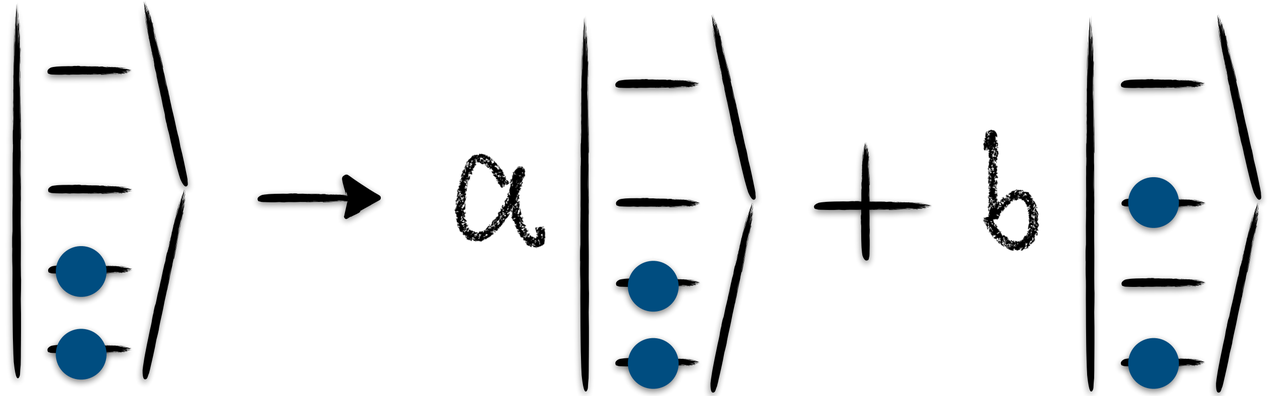
$$G_{p_\uparrow p_\downarrow q_\uparrow q_\downarrow} \equiv \tilde{G}_{pq} = i\left(a^\dagger_{p_\uparrow} a_{q_\uparrow} a^\dagger_{p_\downarrow} a_{q_\downarrow} - h.c\right)$$



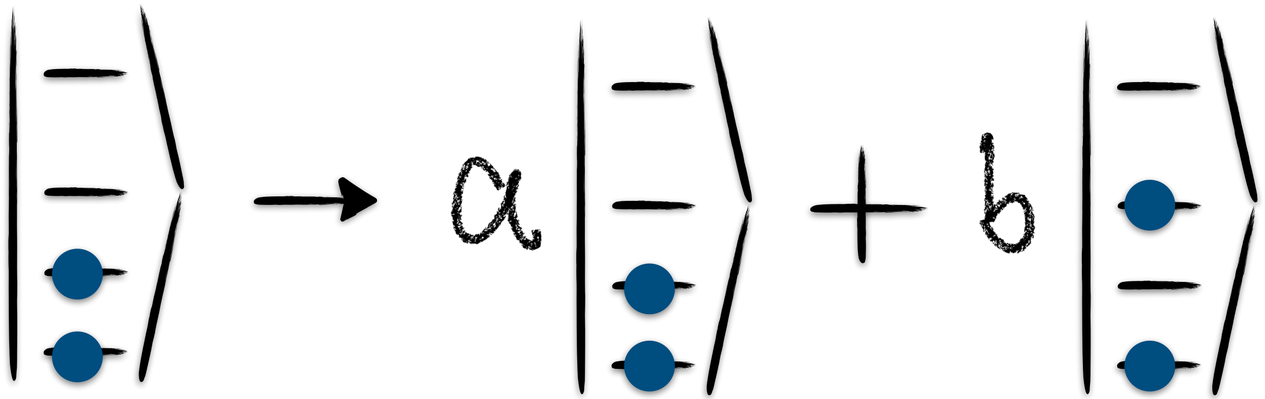


N orbitals → 2N qubits

“Hard-Core Boson”, “seniority zero”, “Doubly Occupied …”

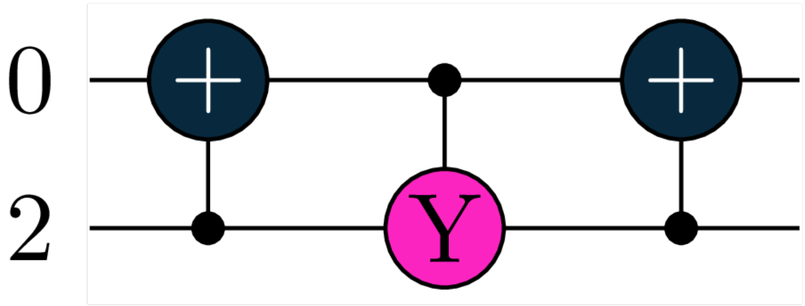


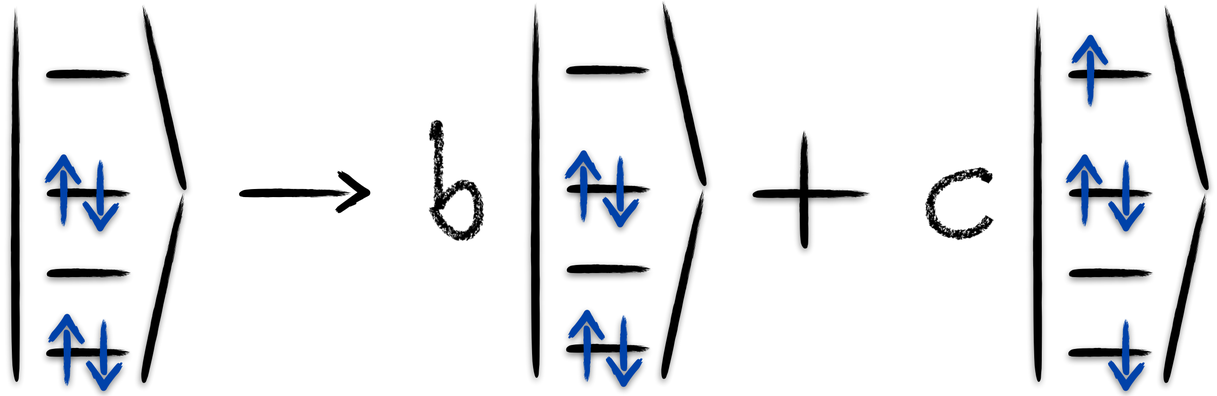
N orbitals → N qubits

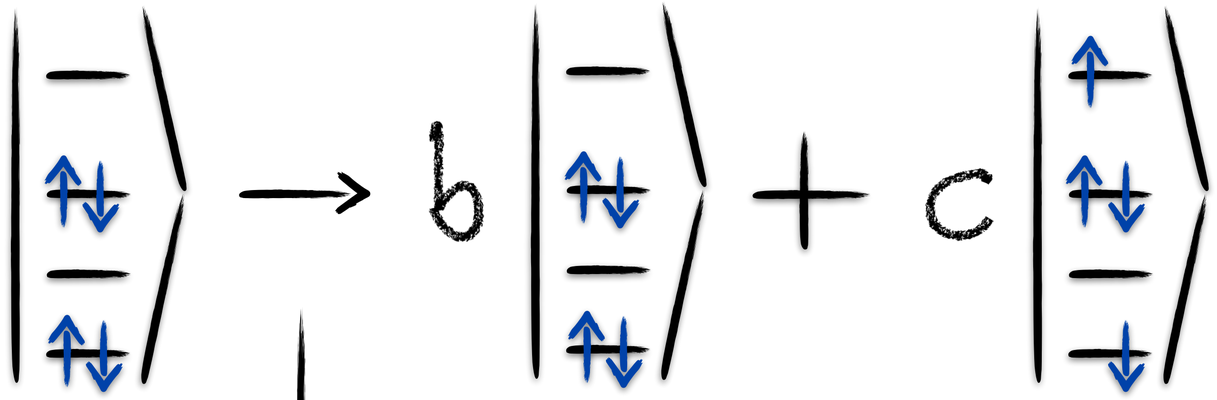


$$\tilde{G}_{pq} \xrightarrow[\text{Wigner}]{\text{Jordan-}} \tilde{G}^{\text{JW}}_{pq} = i\left(\sigma^{+}_{p_\uparrow}\sigma^{-}_{q_\uparrow}\sigma^{+}_{p_\downarrow}\sigma^{-}_{q_\downarrow} - h.c.\right)$$

$$\tilde{G}_{pq} \xrightarrow[\text{Boson}]{\text{hard-core}} \tilde{G}^{\text{HCB}}_{pq} = i\left(\sigma^{+}_{p}\sigma^{-}_{q} - h.c.\right)$$

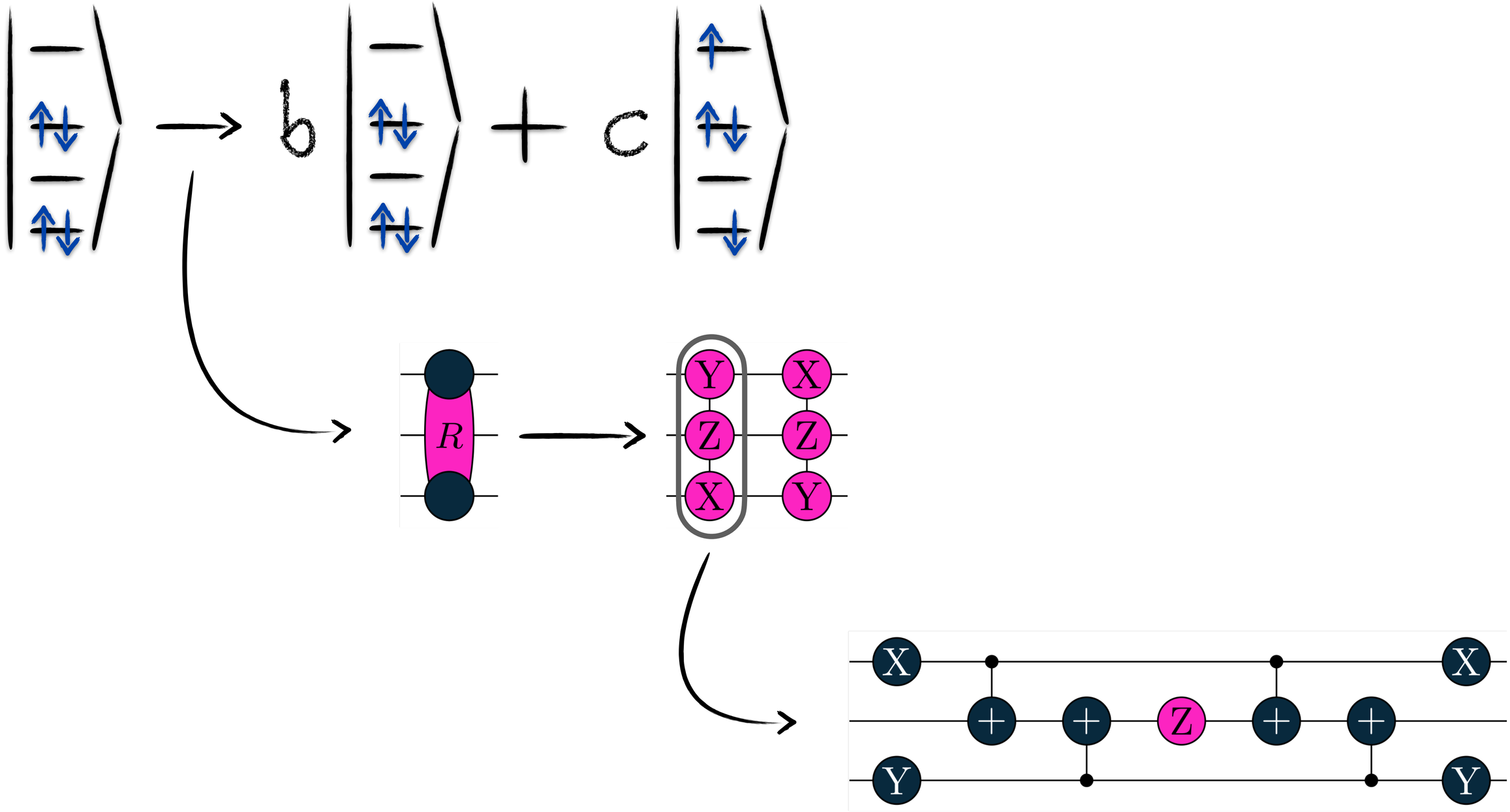




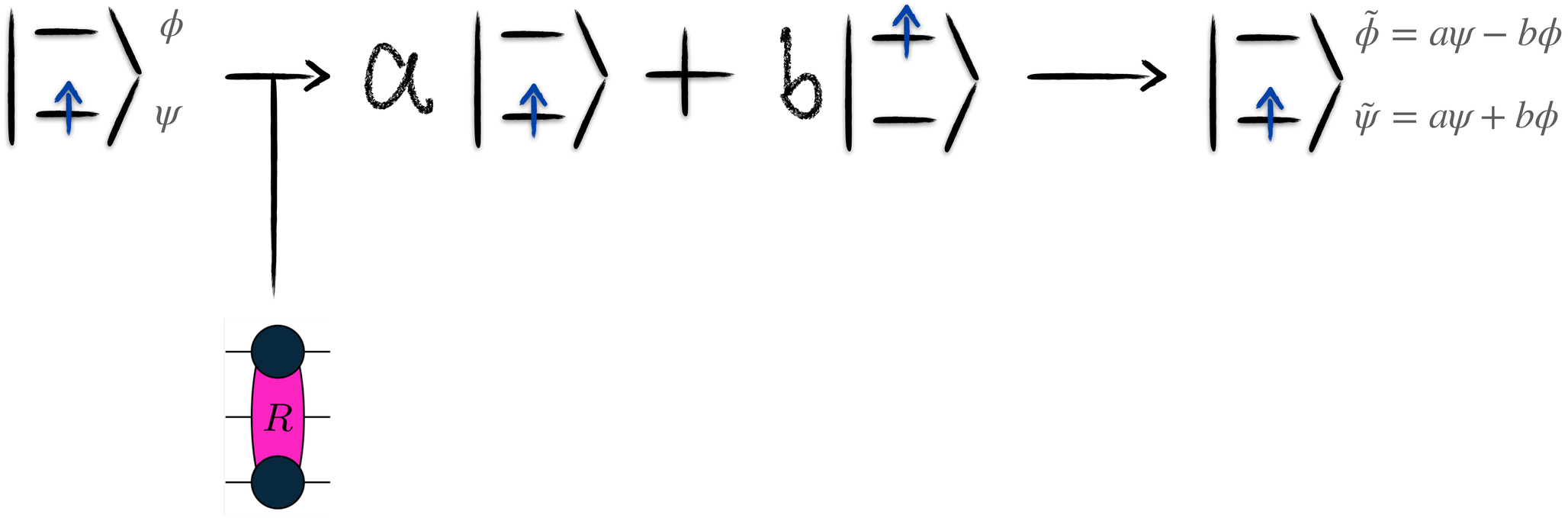


$$U_{i_\uparrow}^{j_\uparrow} = e^{-i\frac{\theta}{2}\left(a_{i_\uparrow}^\dagger a_{j_\uparrow} - a_{j_\uparrow}^\dagger a_{i_\uparrow}\right)}$$

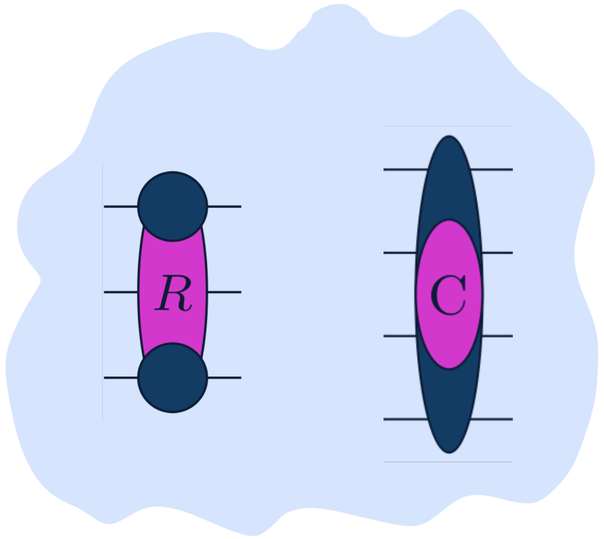
$$e^{-\frac{\theta}{2}\sigma_0^x\sigma_1^z\sigma_2^y}\, e^{-\frac{\theta}{2}\sigma_0^y\sigma_1^z\sigma_2^x}$$


b
c
R
Y
X
Z
Z
X
Y
X
Z
Y
X
Y

orbital rotations



Rotators
and
Correlators



Standard methods
UCCSD
k–UpCCGSD
…

Adaptive Methods
ADAPT–VQE
Qubit–Coupled–Cluster
…

High–Level–Design
Now….

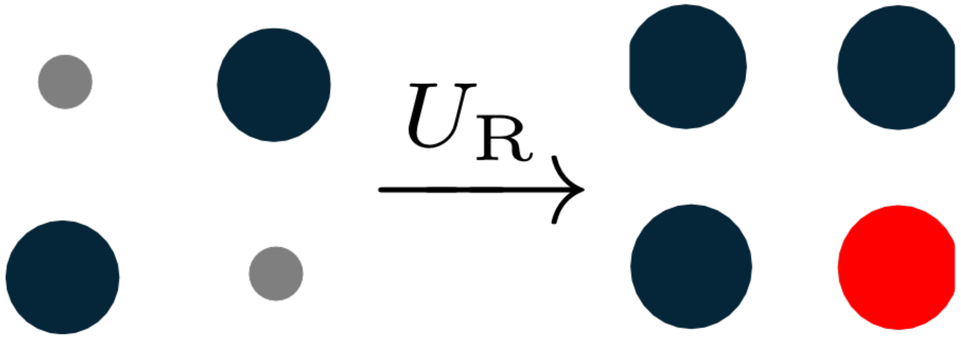
High-Level Design

Example: Hydrogen Molecule

Simple system: 2-Electrons

Atomic orbital basis

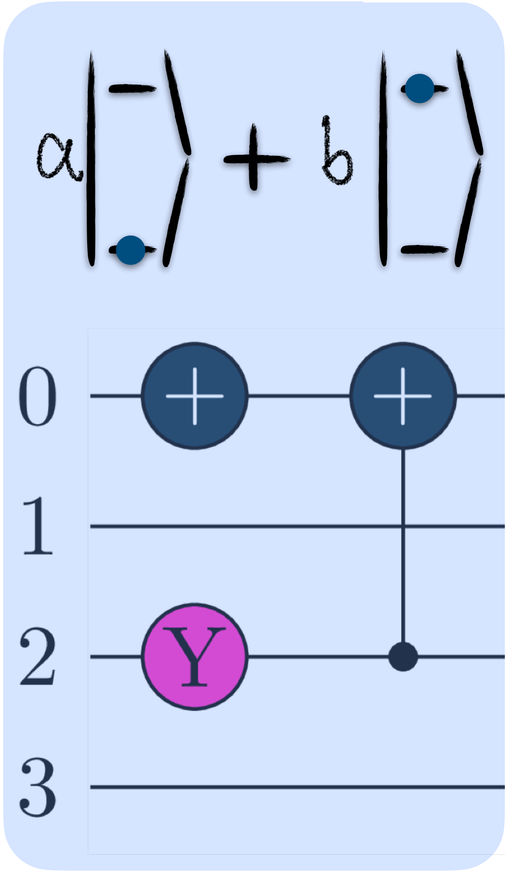
e.g. STO–3G basis set



Molecular orbital basis

Simple system: 2-electrons in 2 orbitals (4 qubits)

$$U_2^4 =$$



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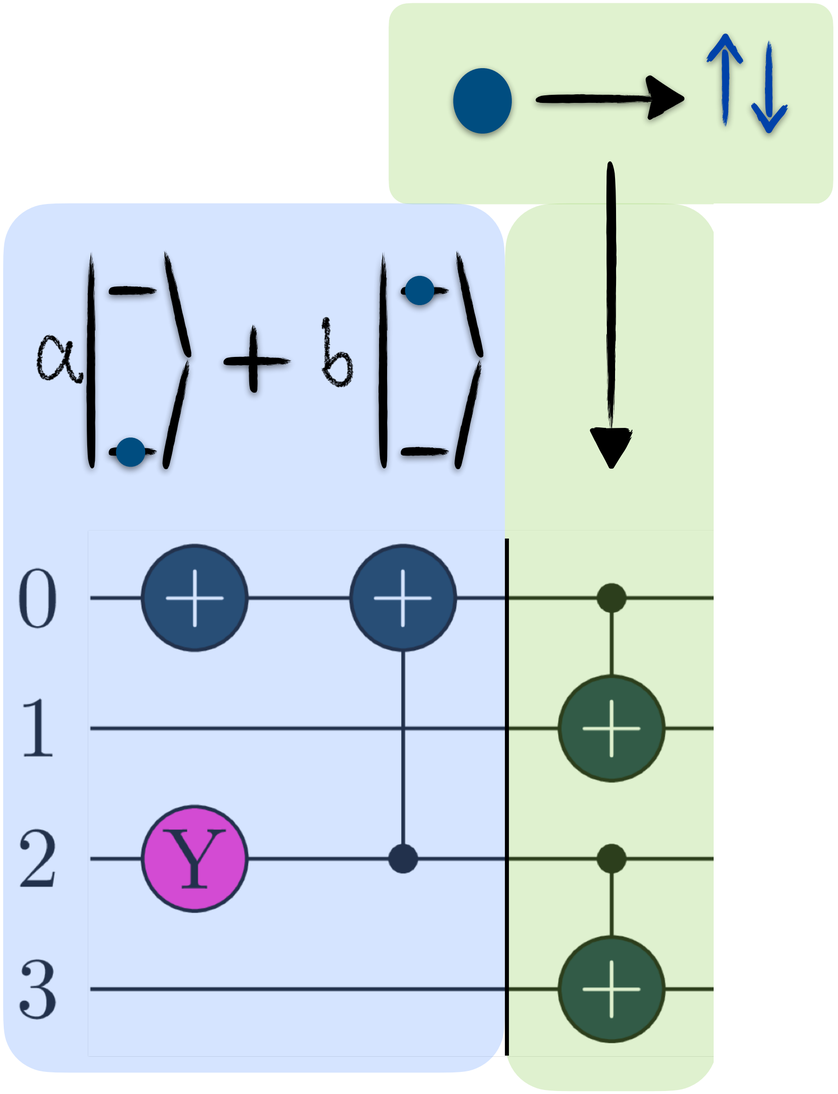
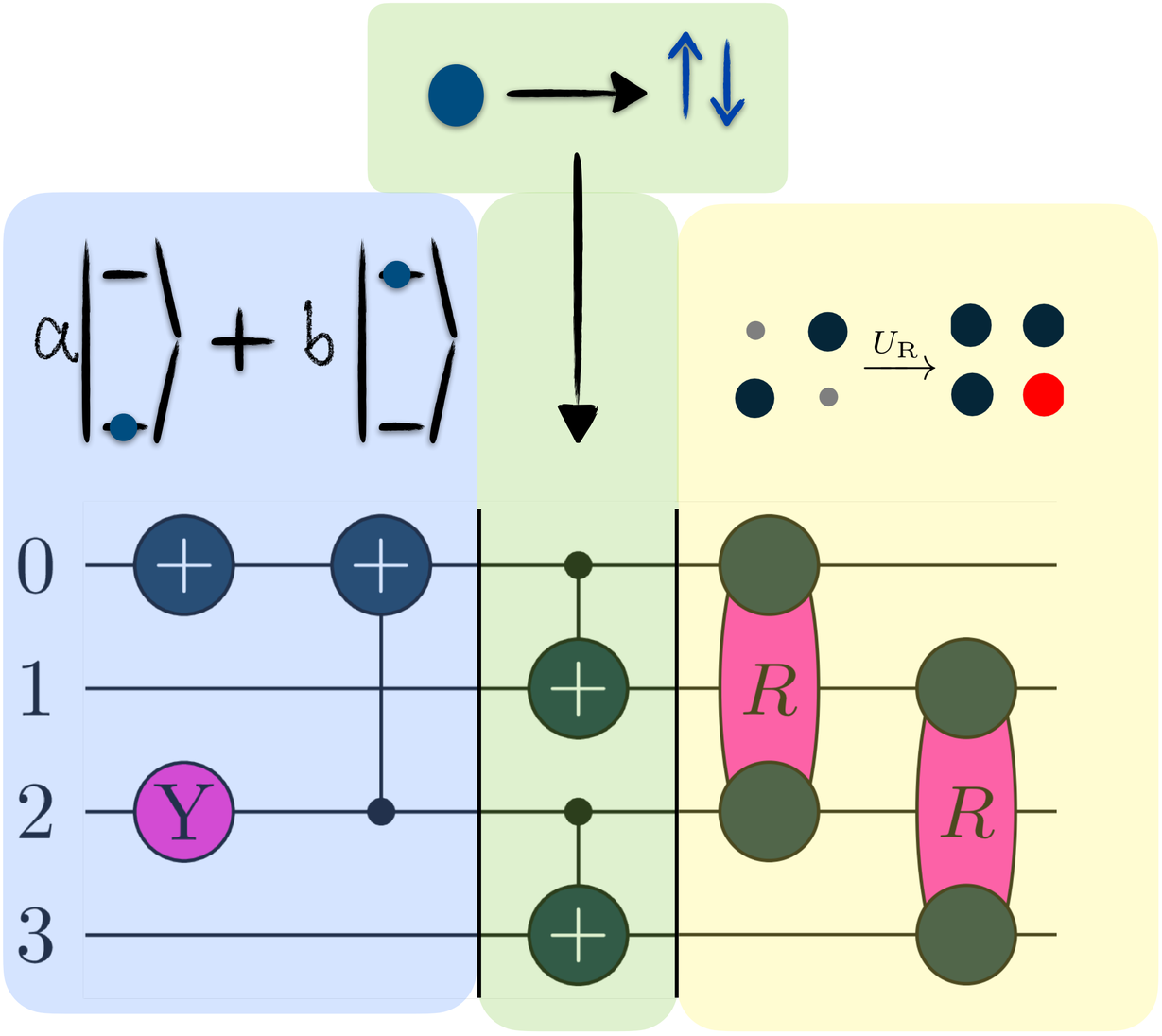
$$U_2^4 =$$



Simple system: 2-electrons in 2 orbitals (4 qubits)

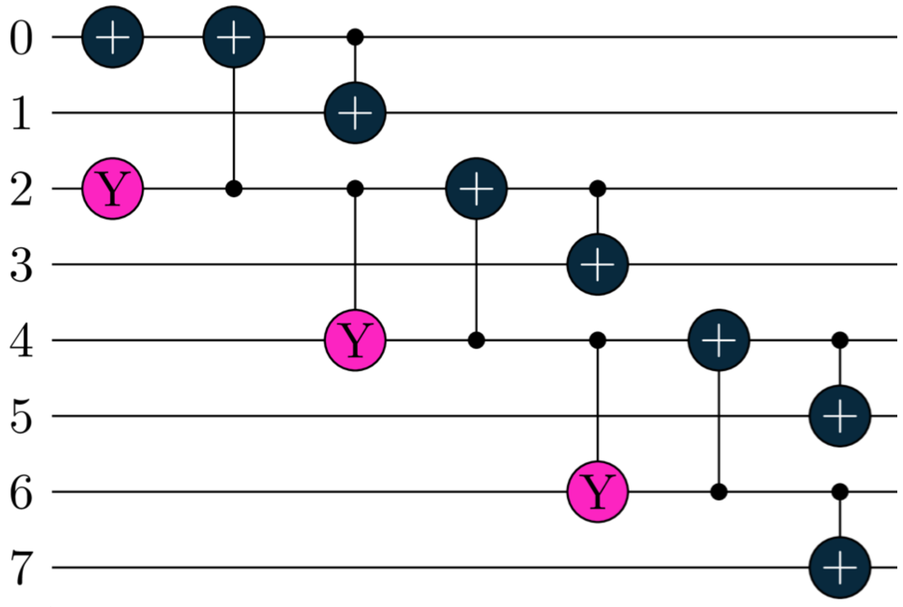
$$U_2^4 =$$



Orbital rotation can be absorbed into the Hamiltonian

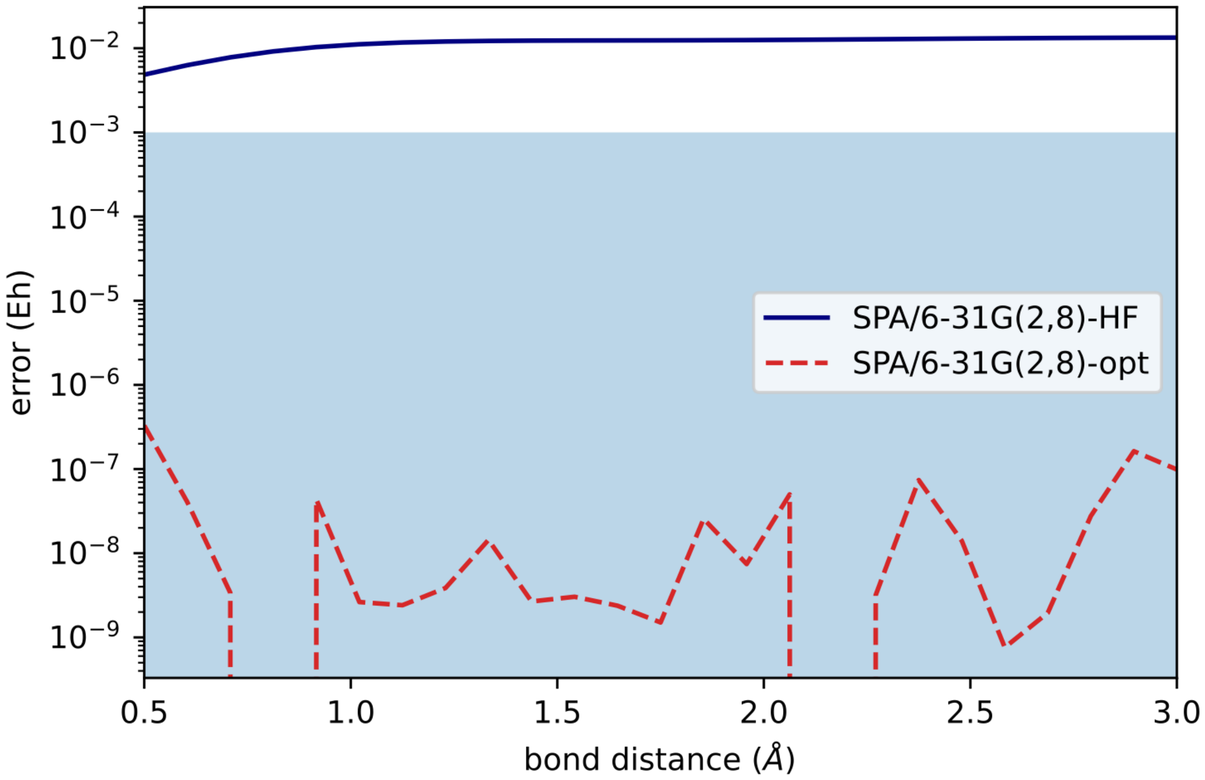
Simple system: 2-electrons in 4 orbitals (8 qubits)

$U_2^8 =$



Larger basis (8 qubits)

Same behaviour
for other (effective) two electron systems
He, LiH, H3+ …

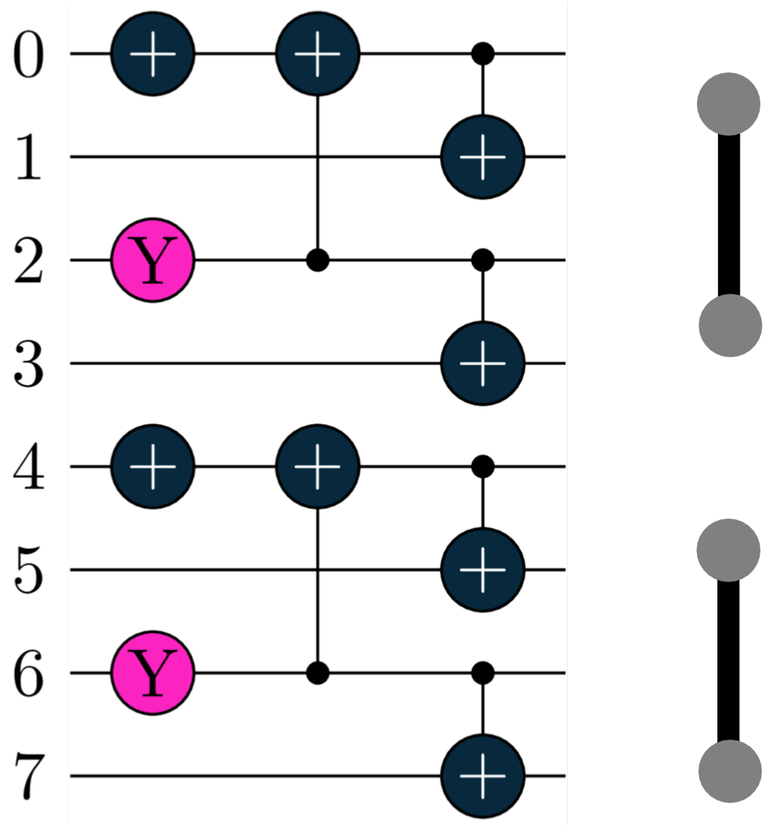


H4 Molecule

As before: Minimal basis STO–3G. One orbital per Hydrogen

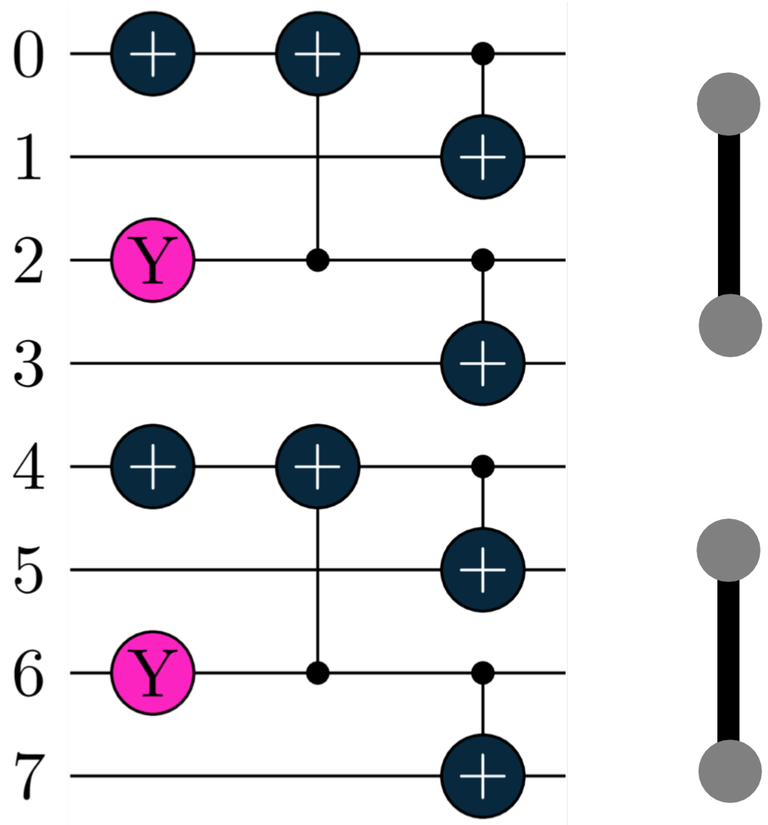
SPA: Separable Pair Ansatz

$$U_{\mathrm{SPA}}^{(4,8)} = U_2^4 \otimes U_2^4 =$$



SPA: Separable Pair Ansatz

$$U_{\mathrm{SPA}}^{(4,8)} = U_2^4 \otimes U_2^4 =$$



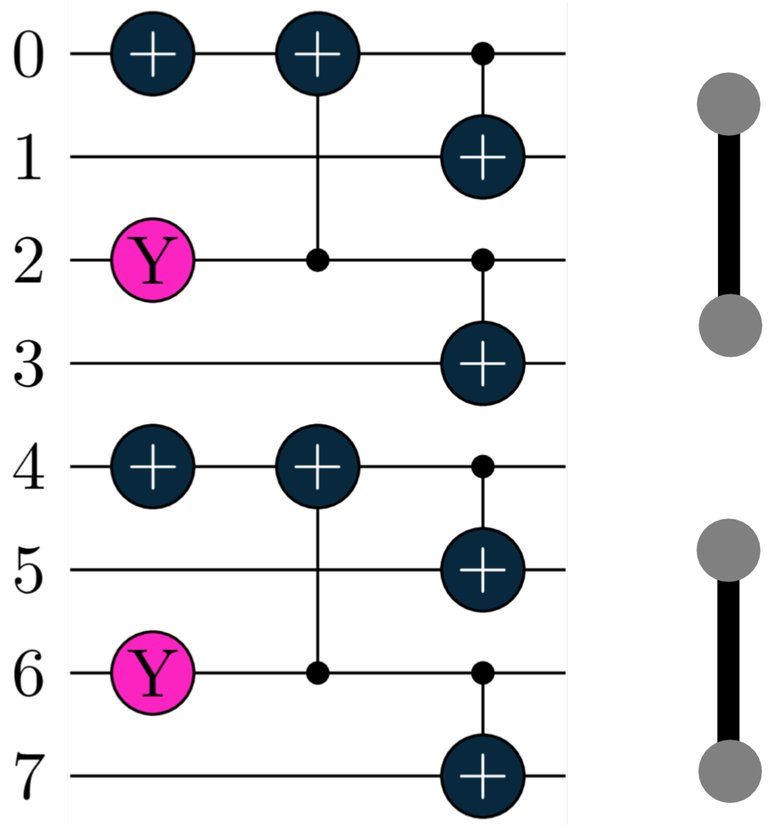
- Locality (circuit connections)
- Shallow depth
- Parallelizable
- Hardware efficient
- Classically tractable wavefunction

becomes a classical pre-compilation step

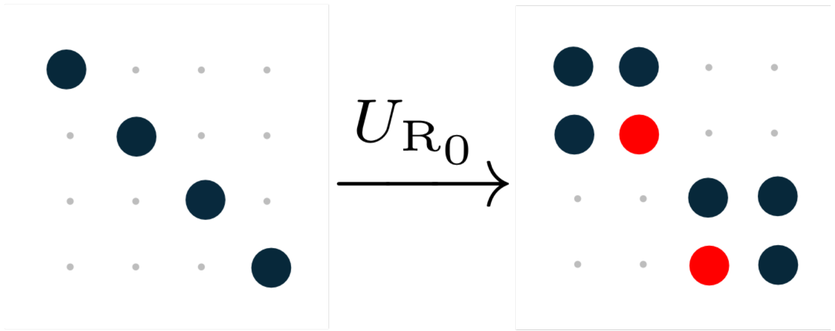
Hartree–Fock error: 167 mEH

SPA: Separable Pair Ansatz

$$U_{\mathrm{SPA}}^{(4,8)} = U_2^4 \otimes U_2^4 =$$



Guess orbitals:
error of 40 mEh



Hartree–Fock error: 167 mEH

SPA: Separable Pair Ansatz

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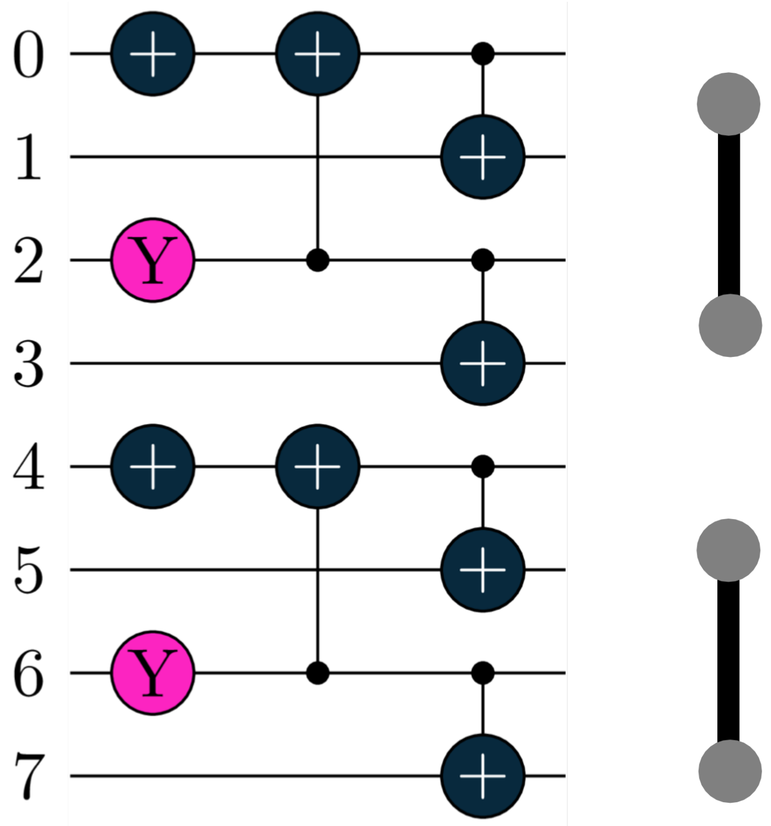
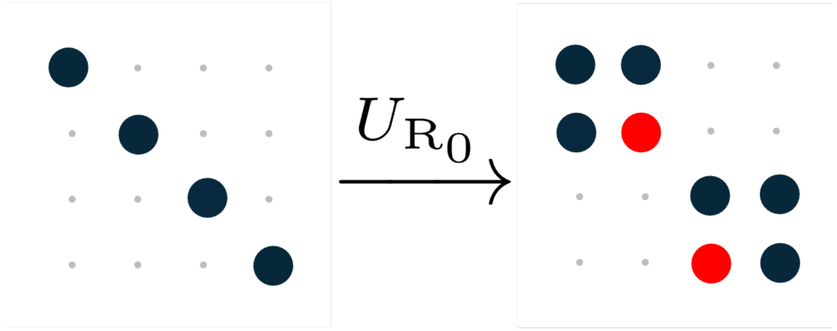
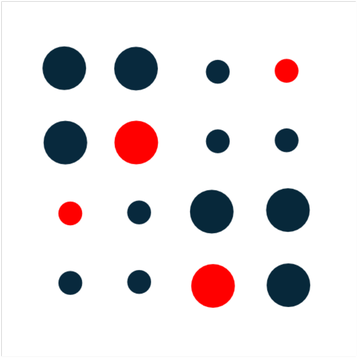


Guess orbitals:
error of 40 mEh



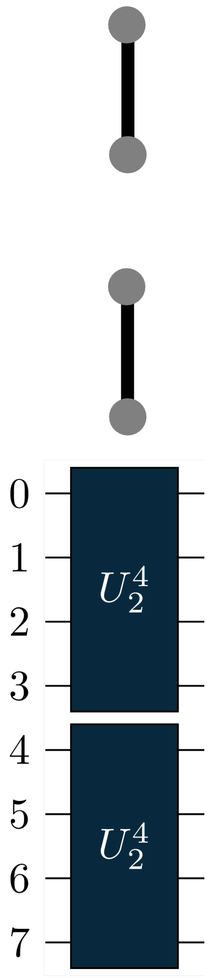
Optimal orbitals:
error of 16 mEh



Alternative Graph

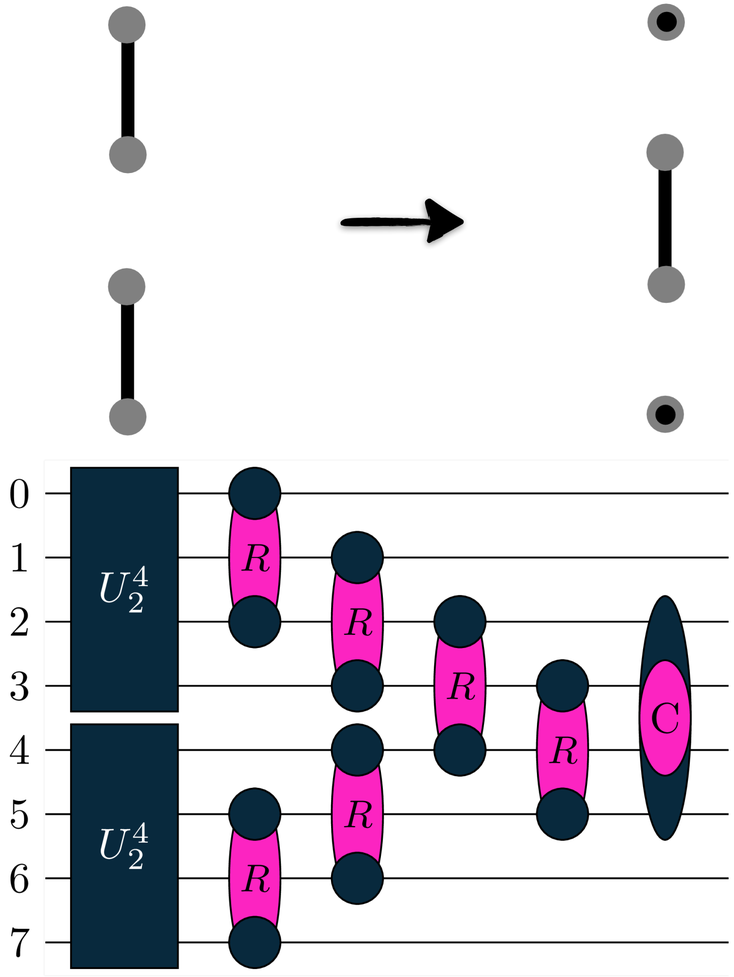
Hartree–Fock error: 167 mEH

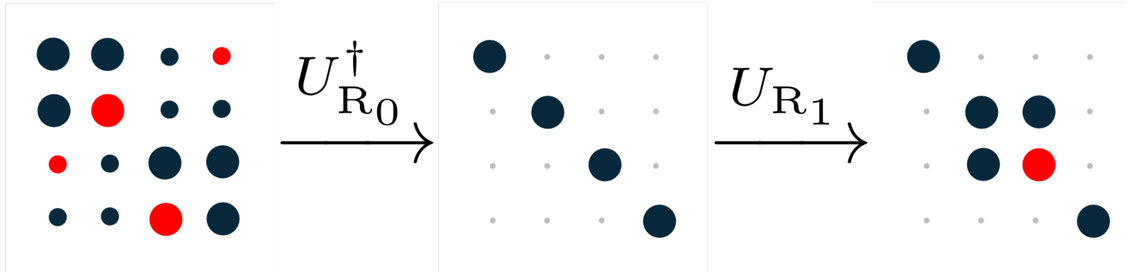
method	error	F	N_v	cnots	depth	iter
SPA	16	94	2	6	3	17*



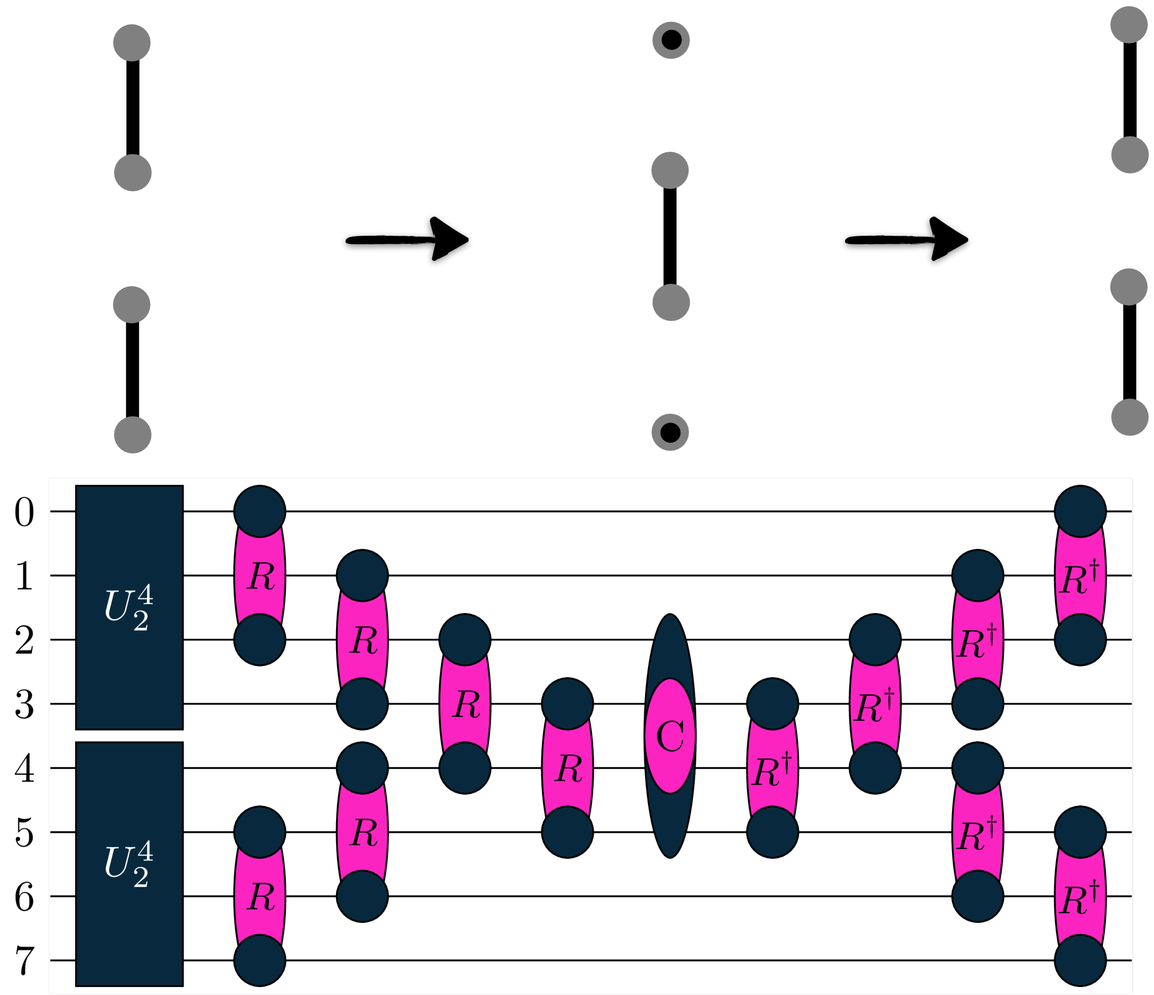
Hartree–Fock error: 167 mEH

method	error	F	N_v	cnots	depth	iter
SPA	16	94	2	6	3	17*



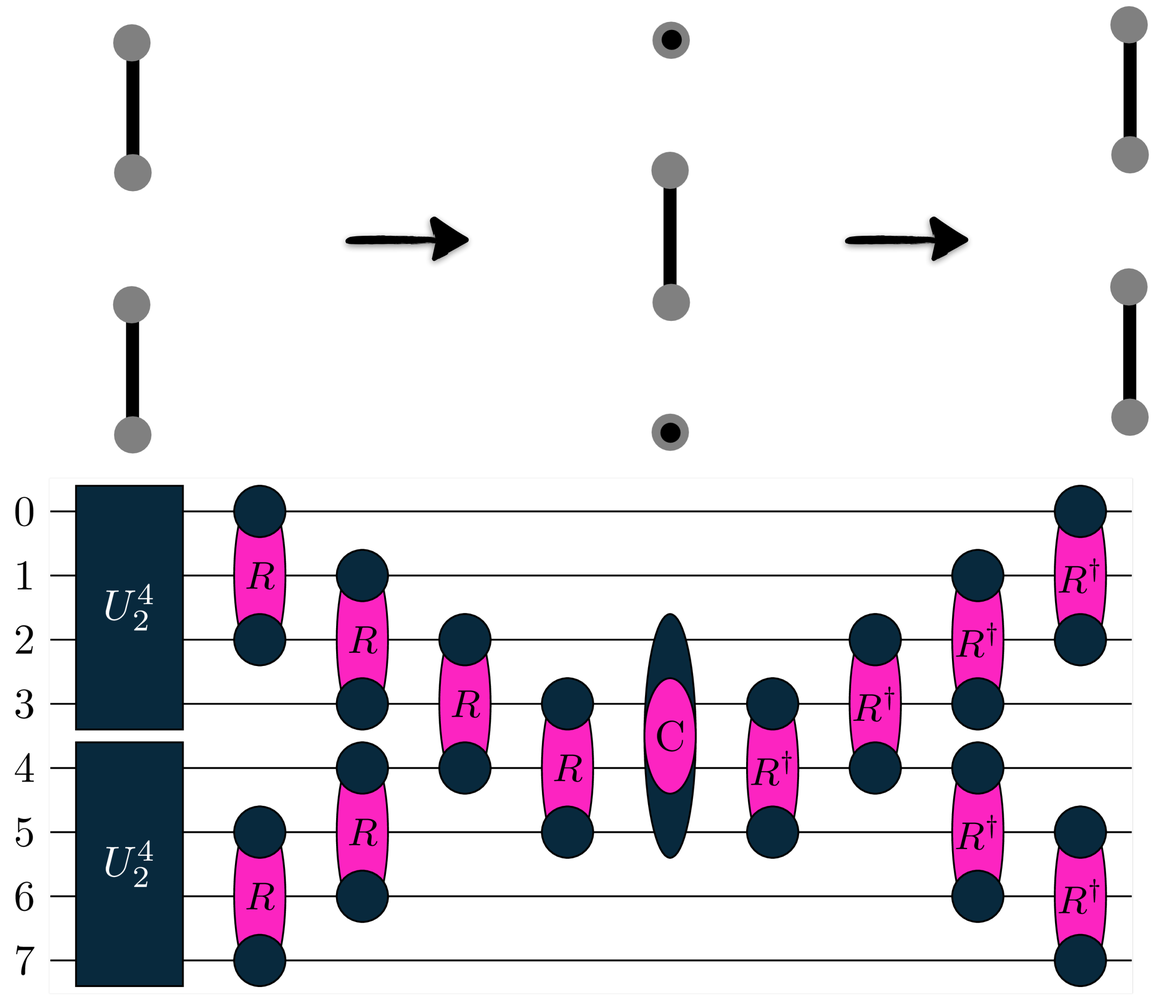


Hartree–Fock error: 167 mEH

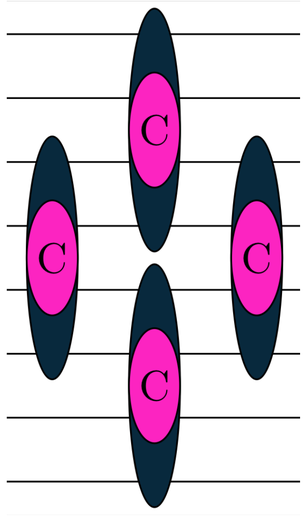


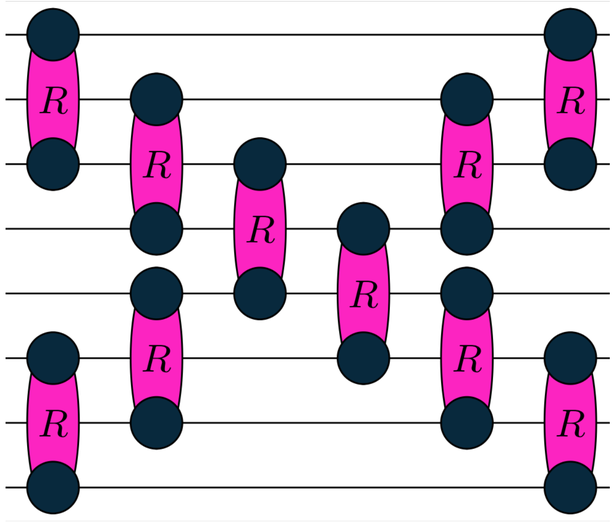
method	error	F	N_v	cnots	depth	iter
SPA	16	94	2	6	3	17*
SPA+	8	96	6	116	131	10

Hartree–Fock error: 167 mEH

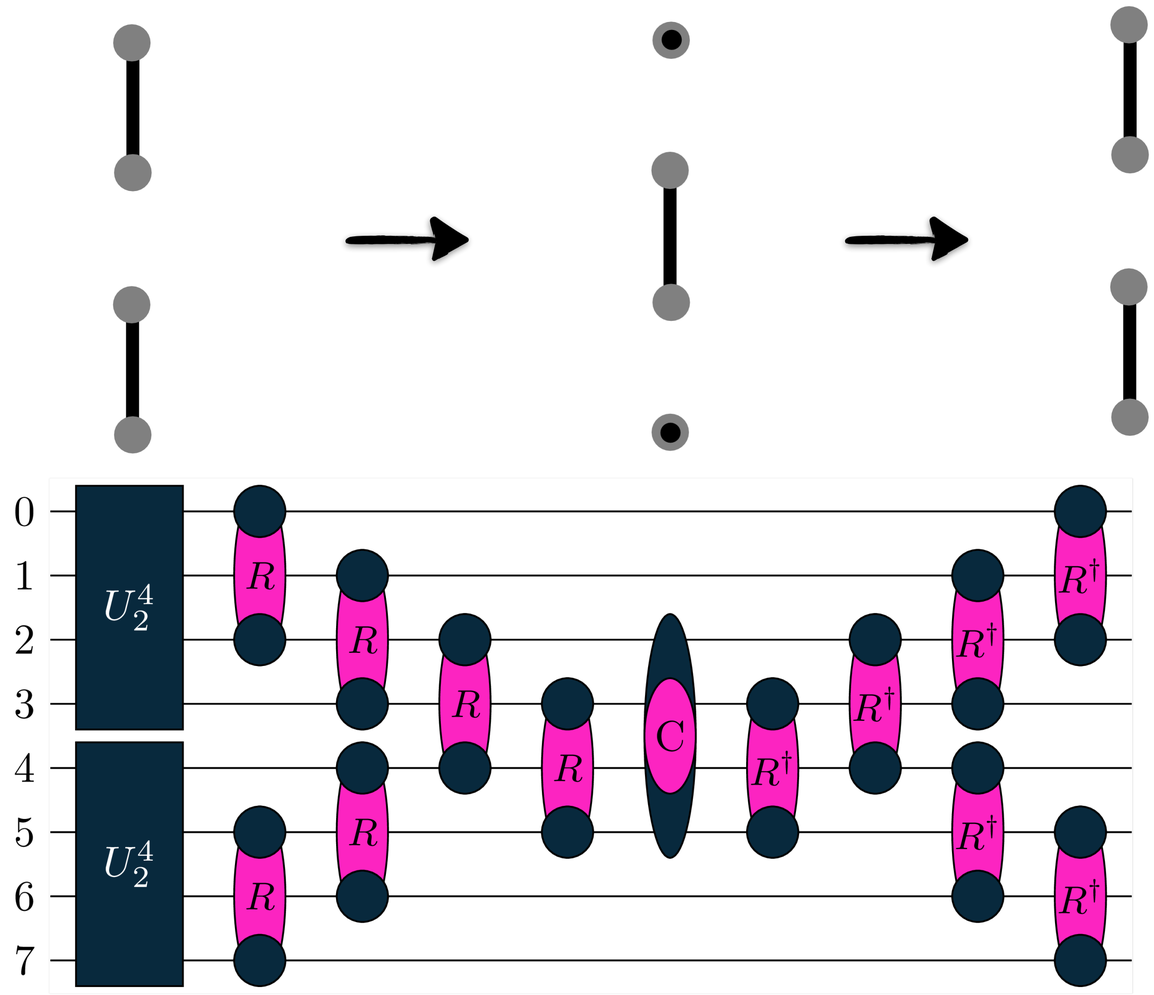


method	error	F	N_v	cnots	depth	iter
SPA	16	94	2	6	3	17*
SPA+	8	96	6	116	131	10
SPA+CRRCRRC	0	100	19	334	367	160





Hartree–Fock error: 167 mEH



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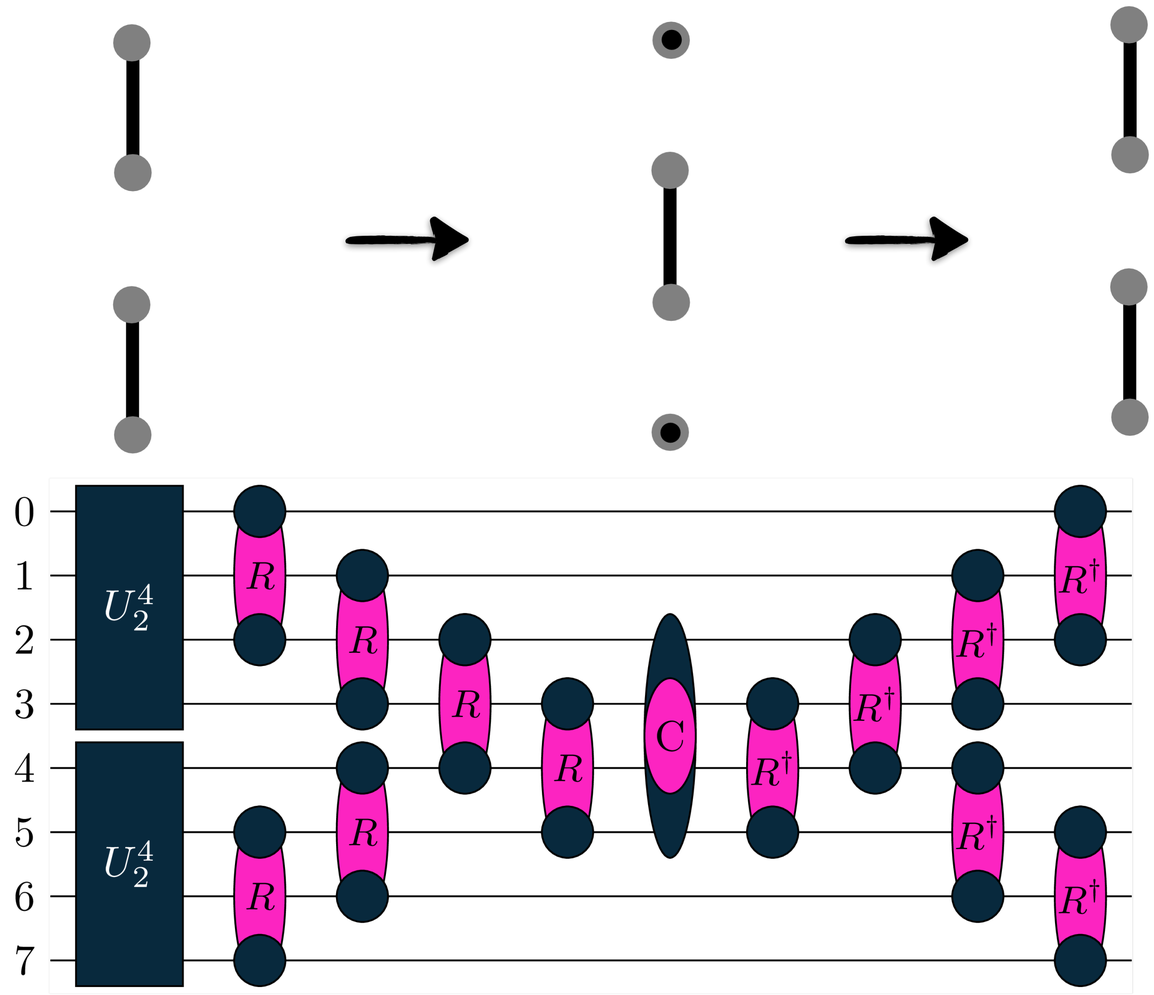
SPA	16	94	2	6	3	17*
SPA+	8	96	6	116	131	10
SPA+CRRCRRC	0	100	19	334	367	160
UpCCD	103	88	4	20	26	8
UpCCSD	86	74	12	148	193	13
UpCCGSD	86	74	18	188	254	13
2-UpCCGSD	32	90	36	432	540	48

Hartree–Fock error: 167 mEH



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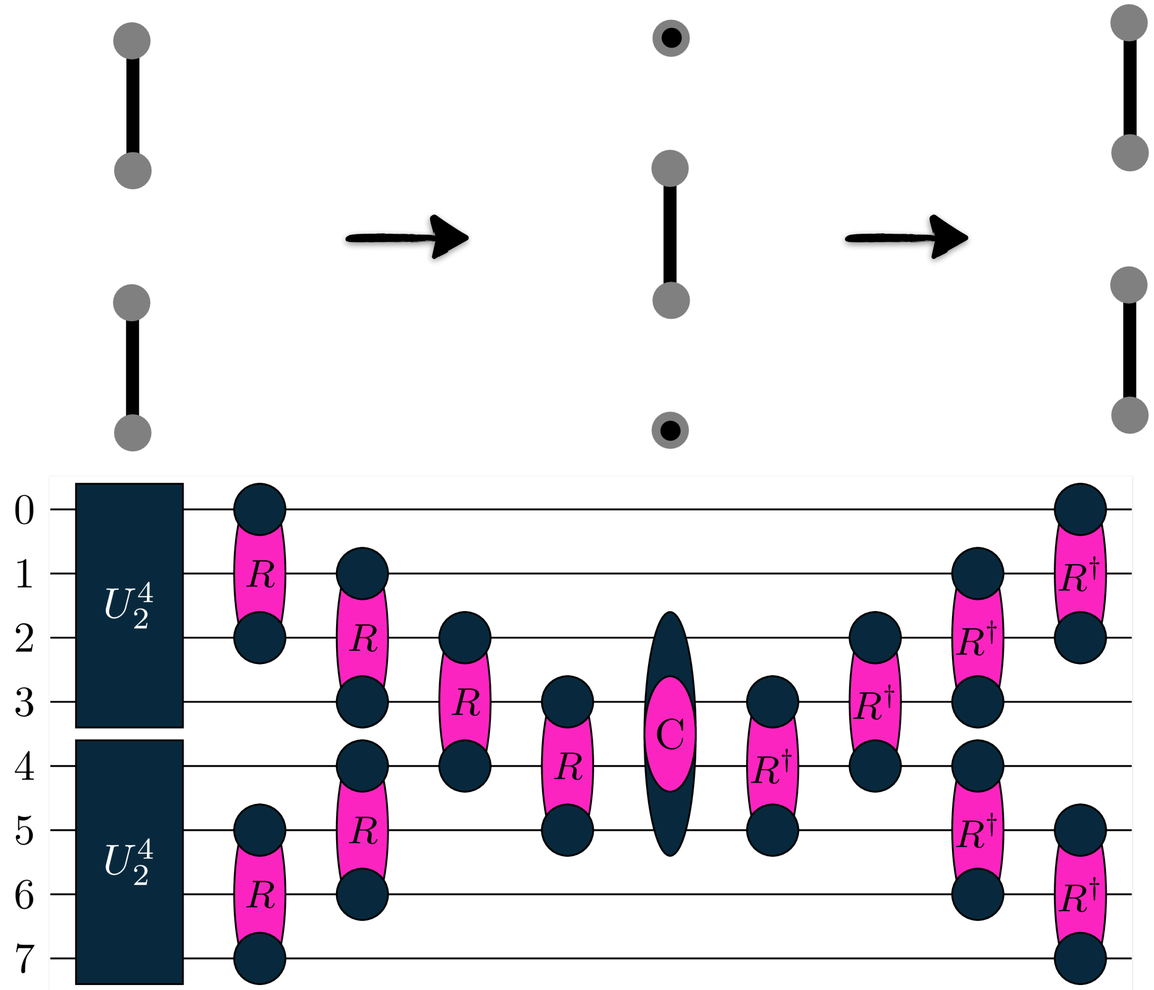
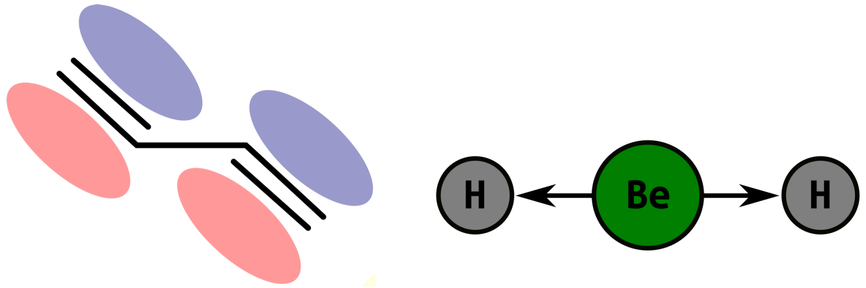
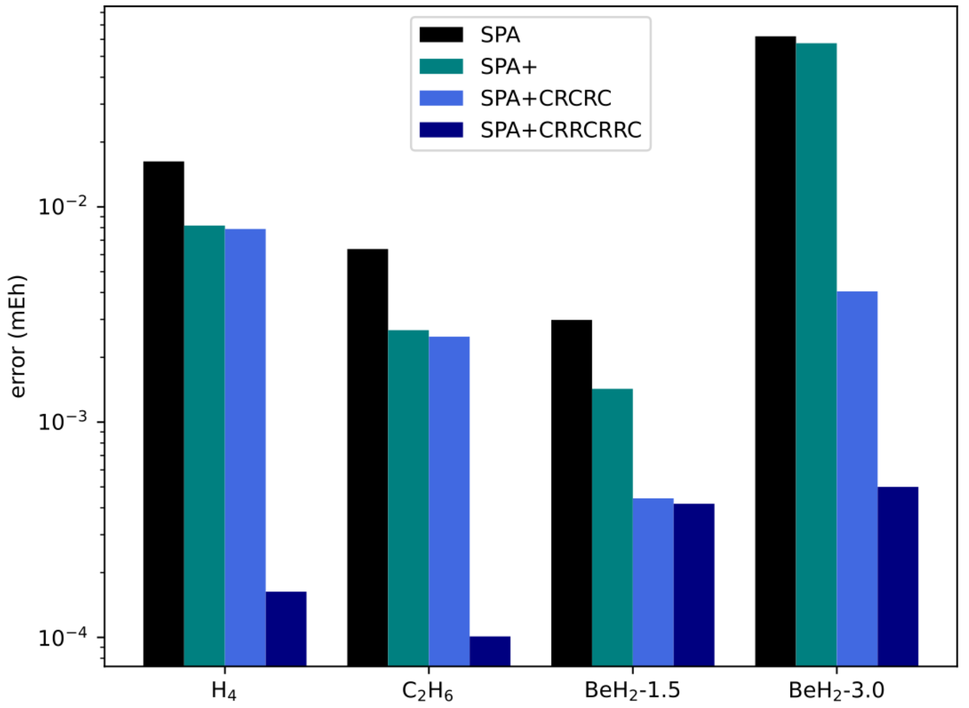
SPA+	8	96	6	116	131	10
SPA+CRRCRRC	0	100	19	334	367	160
UpCCD	103	88	4	20	26	8
UpCCSD	86	74	12	148	193	13
UpCCGSD	86	74	18	188	254	13
2-UpCCGSD	32	90	36	432	540	48
ADAPT(UpCCGSD)	32	90	12	448	442	113
ADAPT(UCCGSD)	0	100	21	1360	1705	58

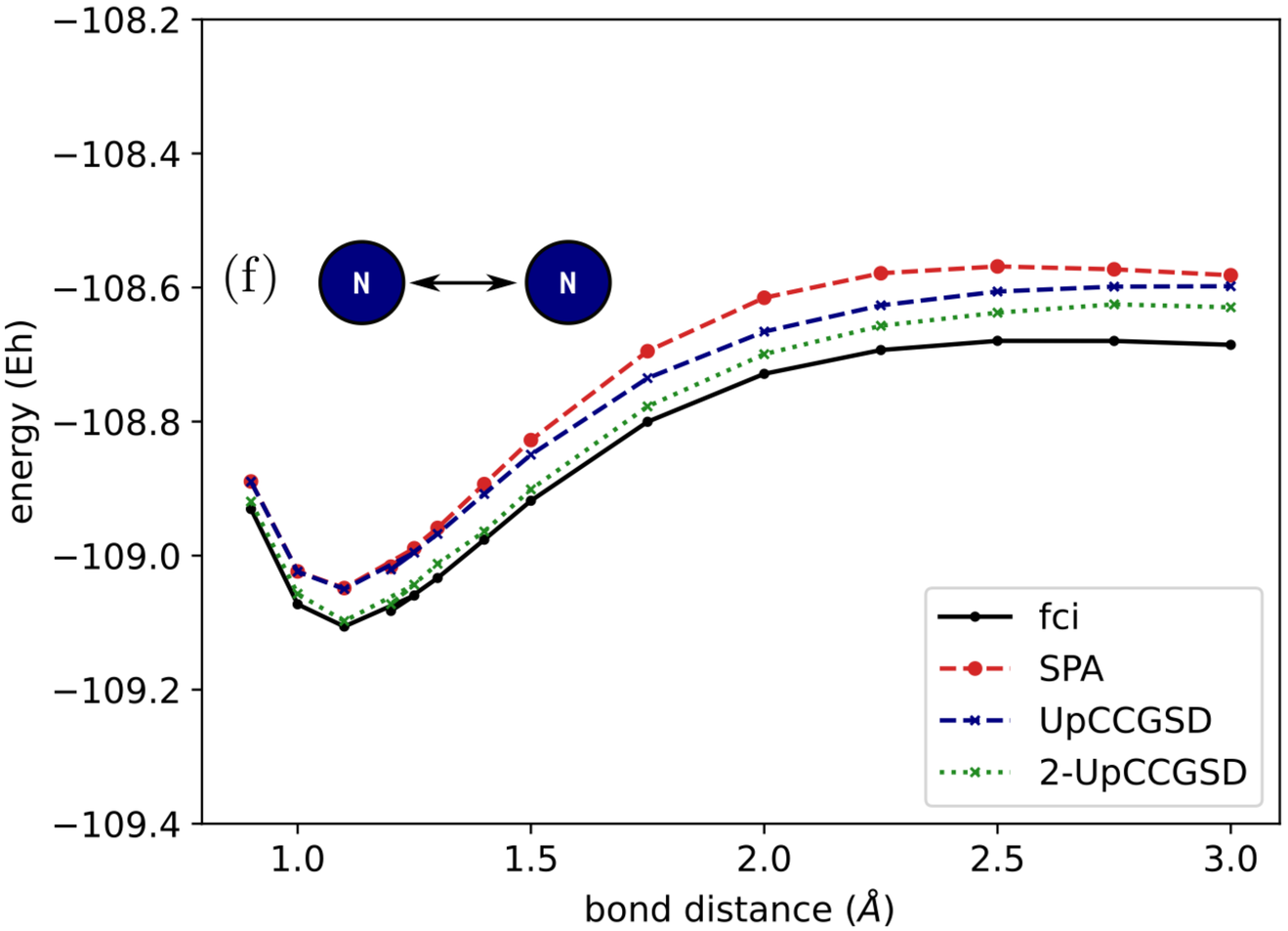
Hartree–Fock error: 167 mEH







Limitations



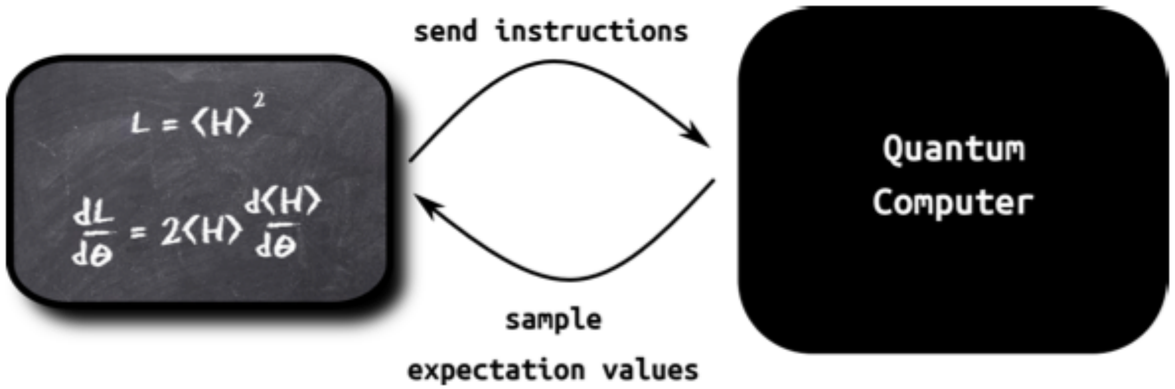
- Well behaved SPA
- Improvement through other graphs not obvious

Implementation: Tequila

Sumner
Alperin-Lea
UofT/Chem

Alba
Cervera-Lierta
Barcelona Supercomputing Center

Teresa
Tamayo-Mendoza
Harvard

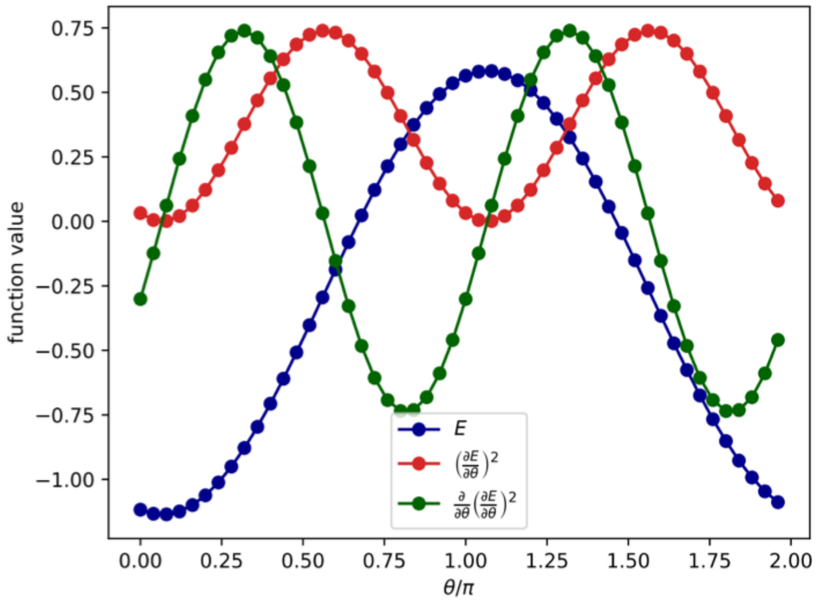


github.com/tequilahub

API inspired by madness library

JSK, Alperin-Lea, Cervera-Lierta, Tamayo-Mendoza, …, Quantum Science & Technology, 2021

```
E    = ExpectationValue(H,U)
dE   = grad(E, "a")
dE2  = dE**2
ddE2 = grad(dE2, "a")
```



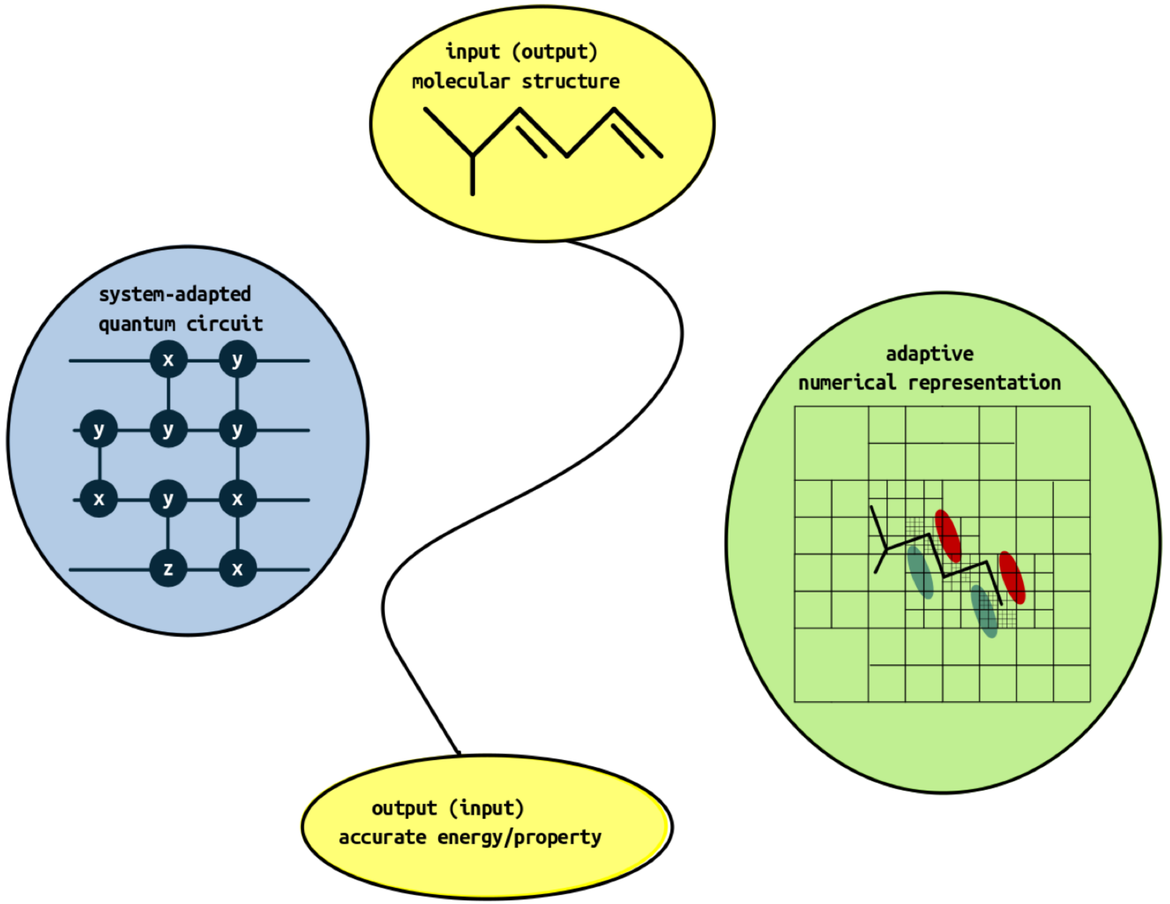
Automatisation

```
import tequila as tq

mol = tq.Molecule(geometry="beh2.xyz")

H = mol.make_hamiltonian()
U = mol.make_ansatz(name="SPA")
E = tq.ExpectationValue(H=H,U=U)

result = tq.minimize(E)
```



Optimized Low-Depth Quantum Circuits for Molecular Electronic Structure using a Separable Pair Approximation

Jakob S. Kottmann[1, 2, *] and Alán Aspuru-Guzik[1, 2, 3, 4, †]

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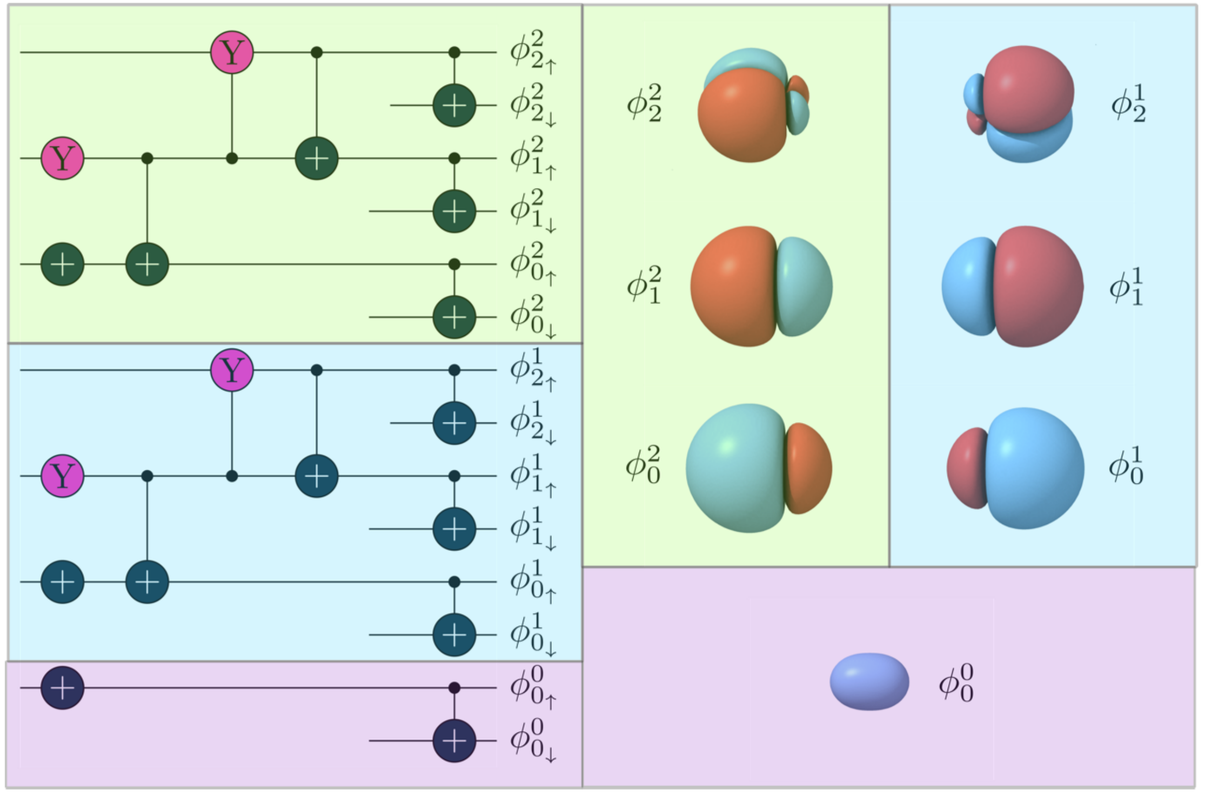

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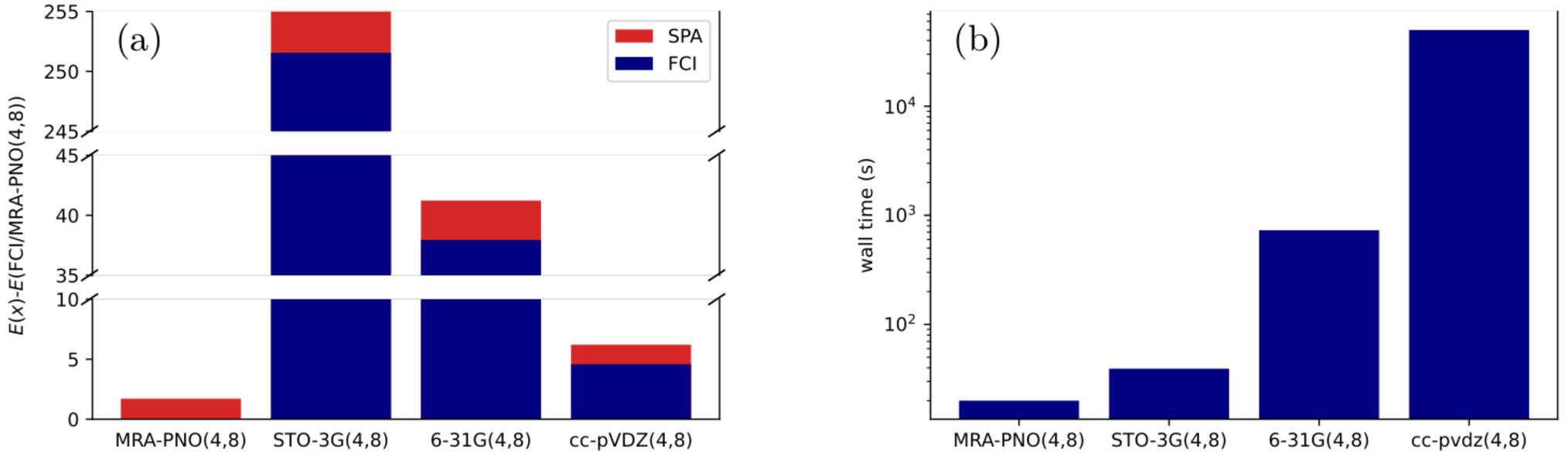
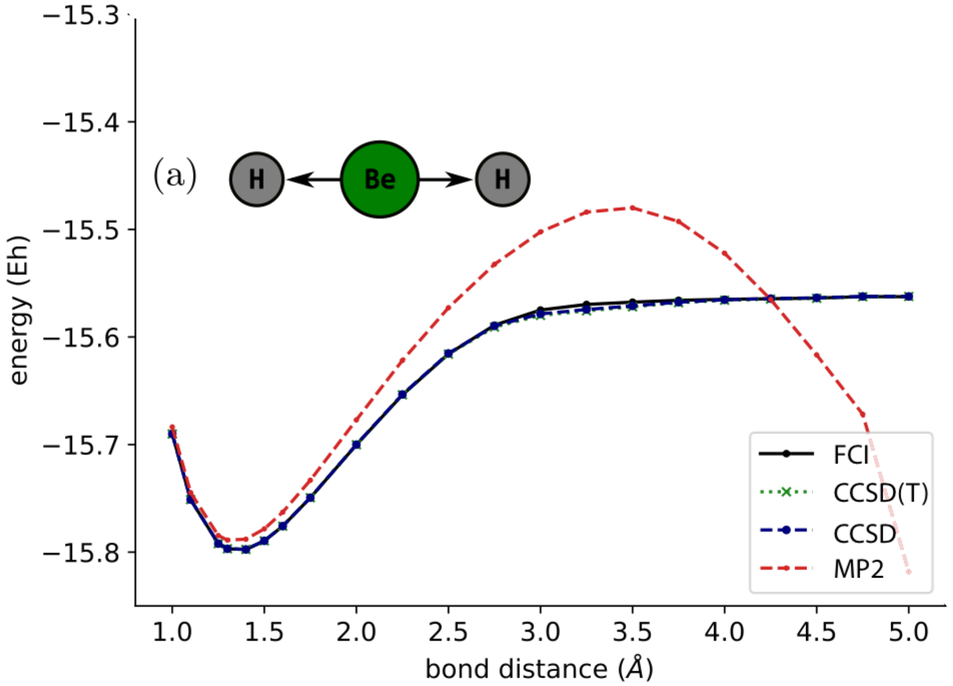
Jakob S. Kottmann[1, 2, *] and Alán Aspuru-Guzik[1, 2, 3, 4, †]

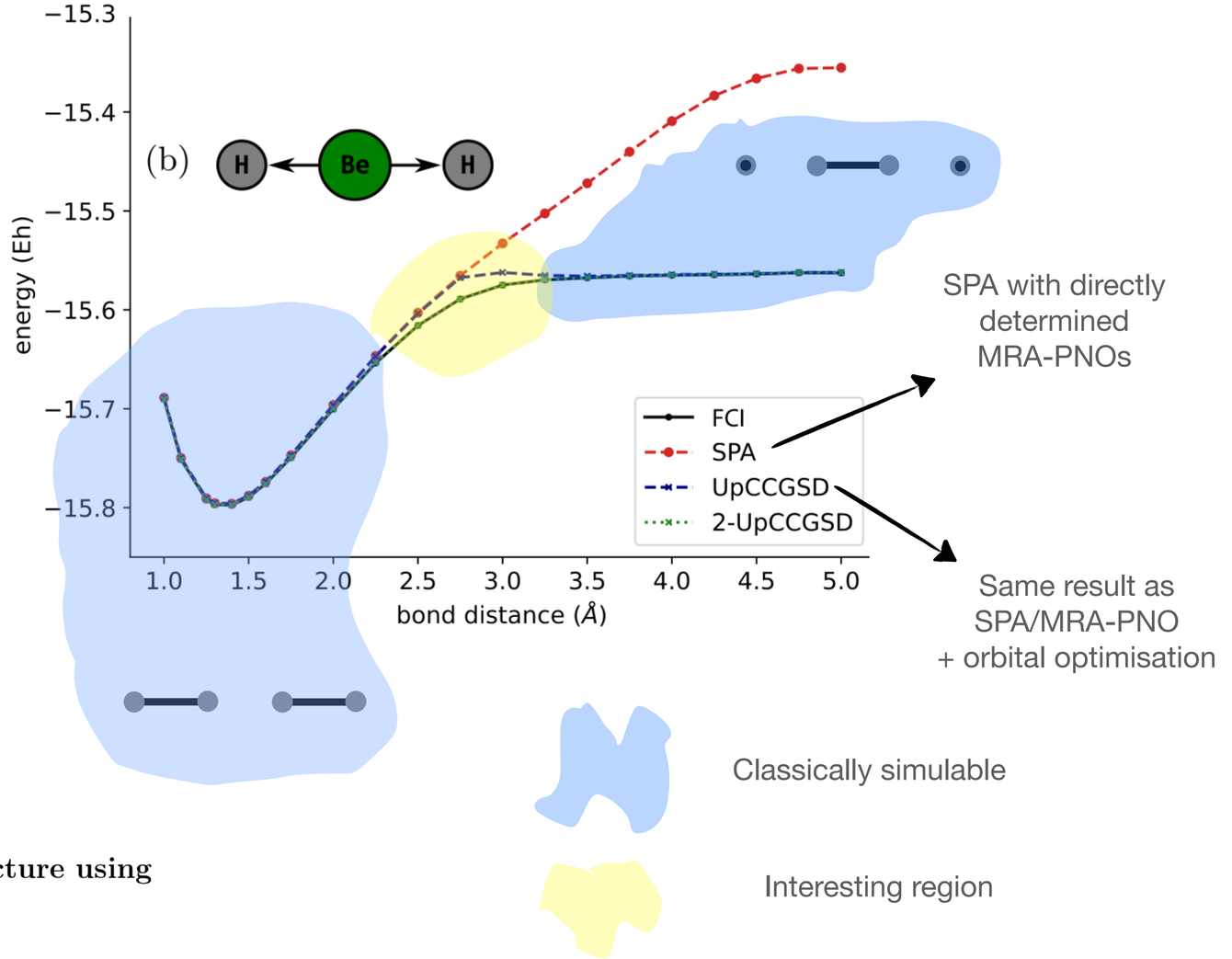
Why Basis–Set–Free?

faster and more accurate



BeH2 with 8 qubits
Standard basis sets: tequila + pyscf
MRA–PNOs: tequila + madness





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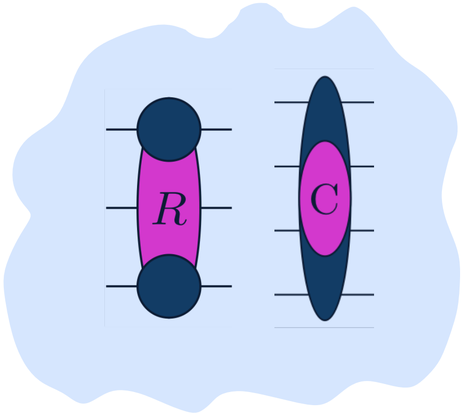
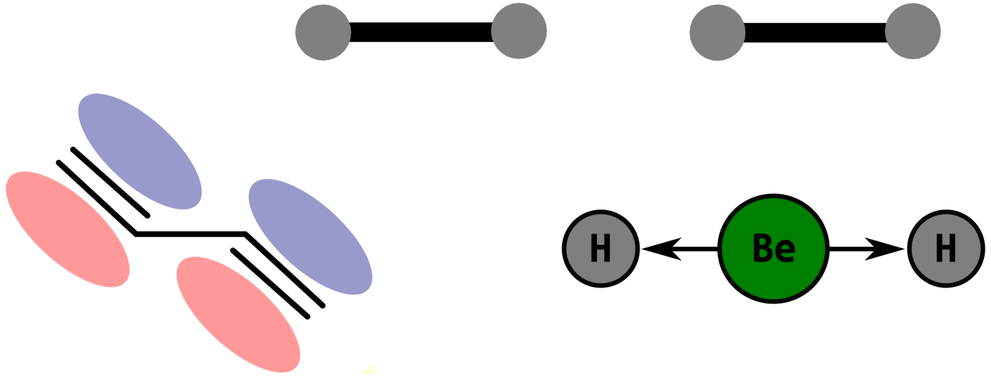
Jakob S. Kottmann[1, 2, *] and Alán Aspuru-Guzik[1, 2, 3, 4, †]

Summary

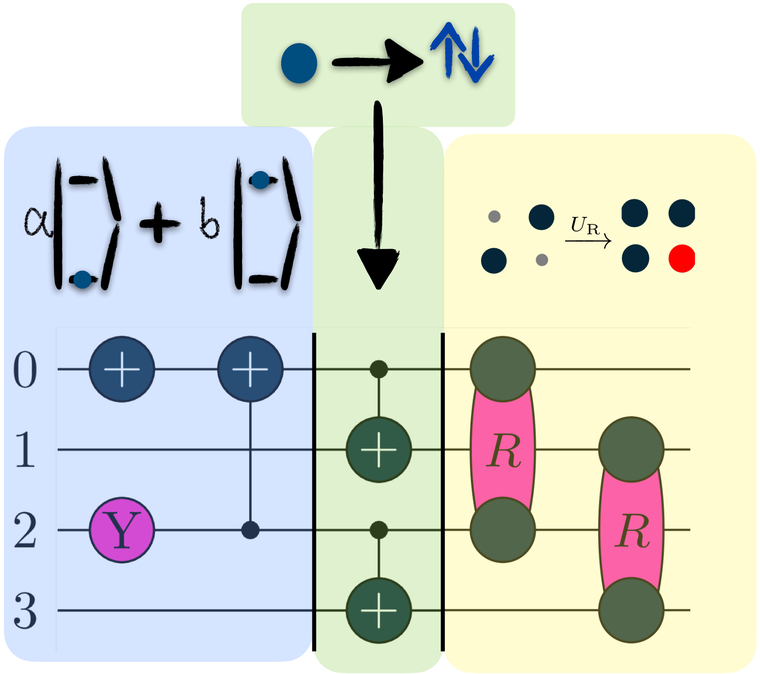
Basic Building Blocks



Abstraction & Transferability



Approximations and Physical Insight



$$U_2^4 =$$

Automatisation