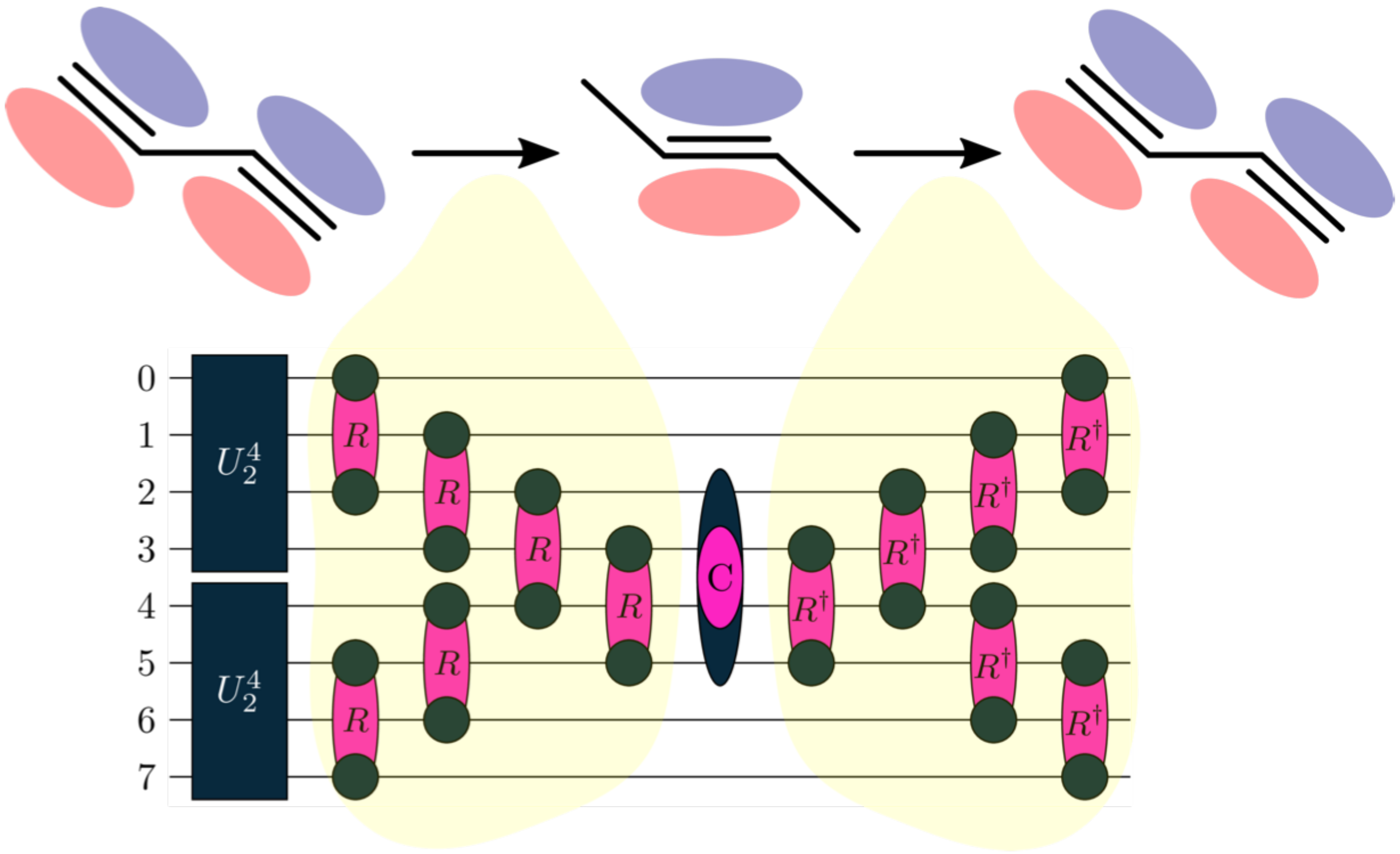
Molecular Quantum Circuit Design

@JakobKottmann

github/tequilahub

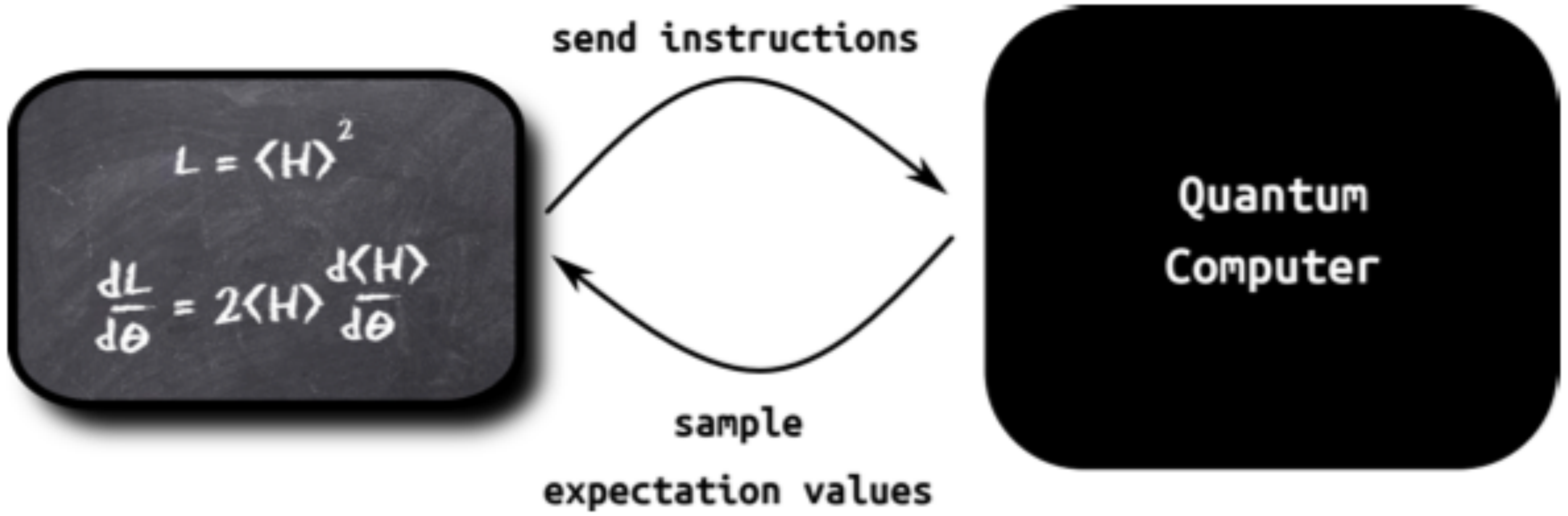


Implementation: Tequila

Sumner
Alperin-Lea
UofT/Chem

Alba
Cervera-Lierta
Barcelona Supercomputing Center

Teresa
Tamayo-Mendoza
Harvard



github.com/tequilahub

API inspired by madness library

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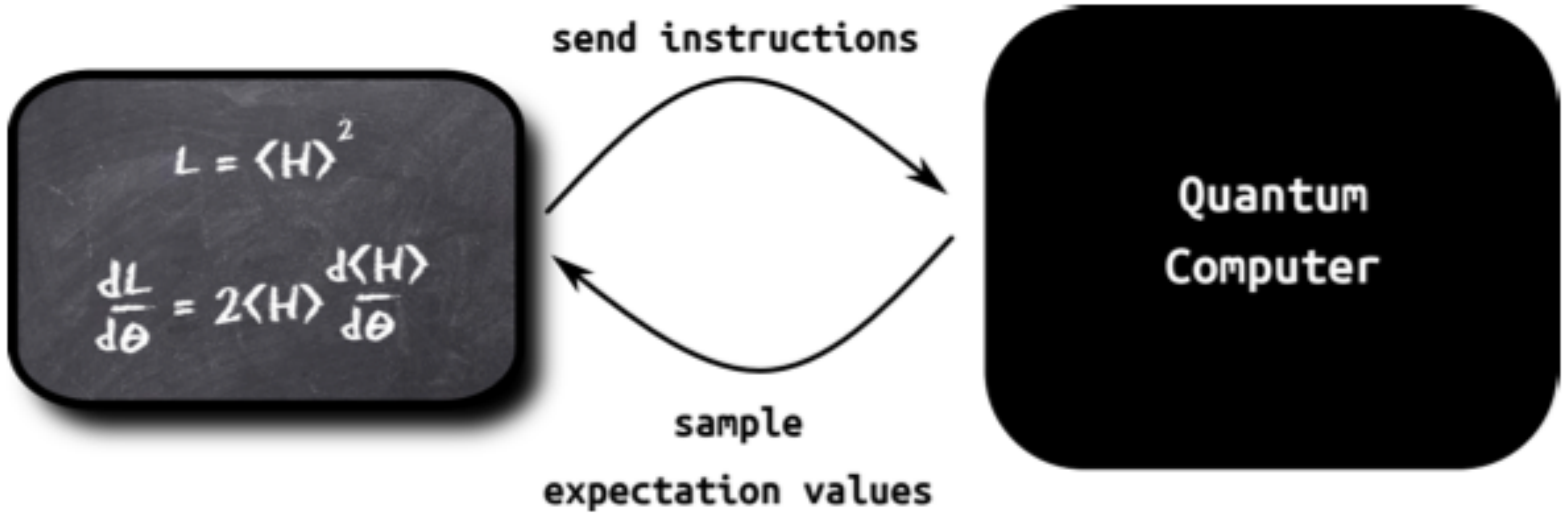


github.com/tequilahub

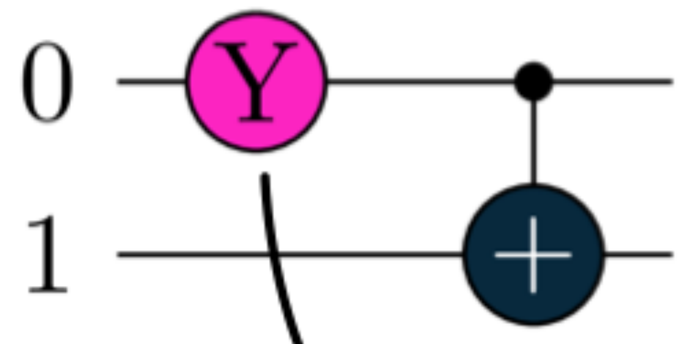
API inspired by madness library

slides and code examples online:
github.com/kottmanj/talks_and_material/barcelona2022

$$L(a) = \langle H \rangle_{U(a)} + e^{-\left(\frac{\partial}{\partial a}\langle H \rangle_{U(a)}\right)^2}$$ $\longleftarrow$ how does this function look?

$$H = X(0)X(1) + \frac{1}{2}Z(0) + Y(1)$$

$U =$

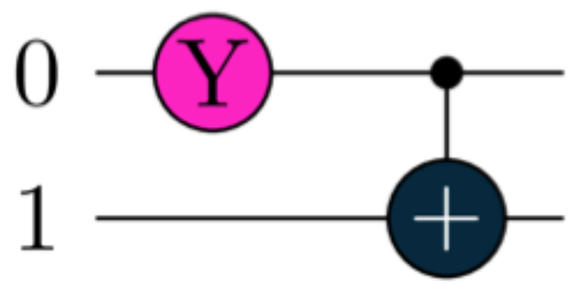


$$e^{-i\frac{f(a)}{2}Y(0)}$$

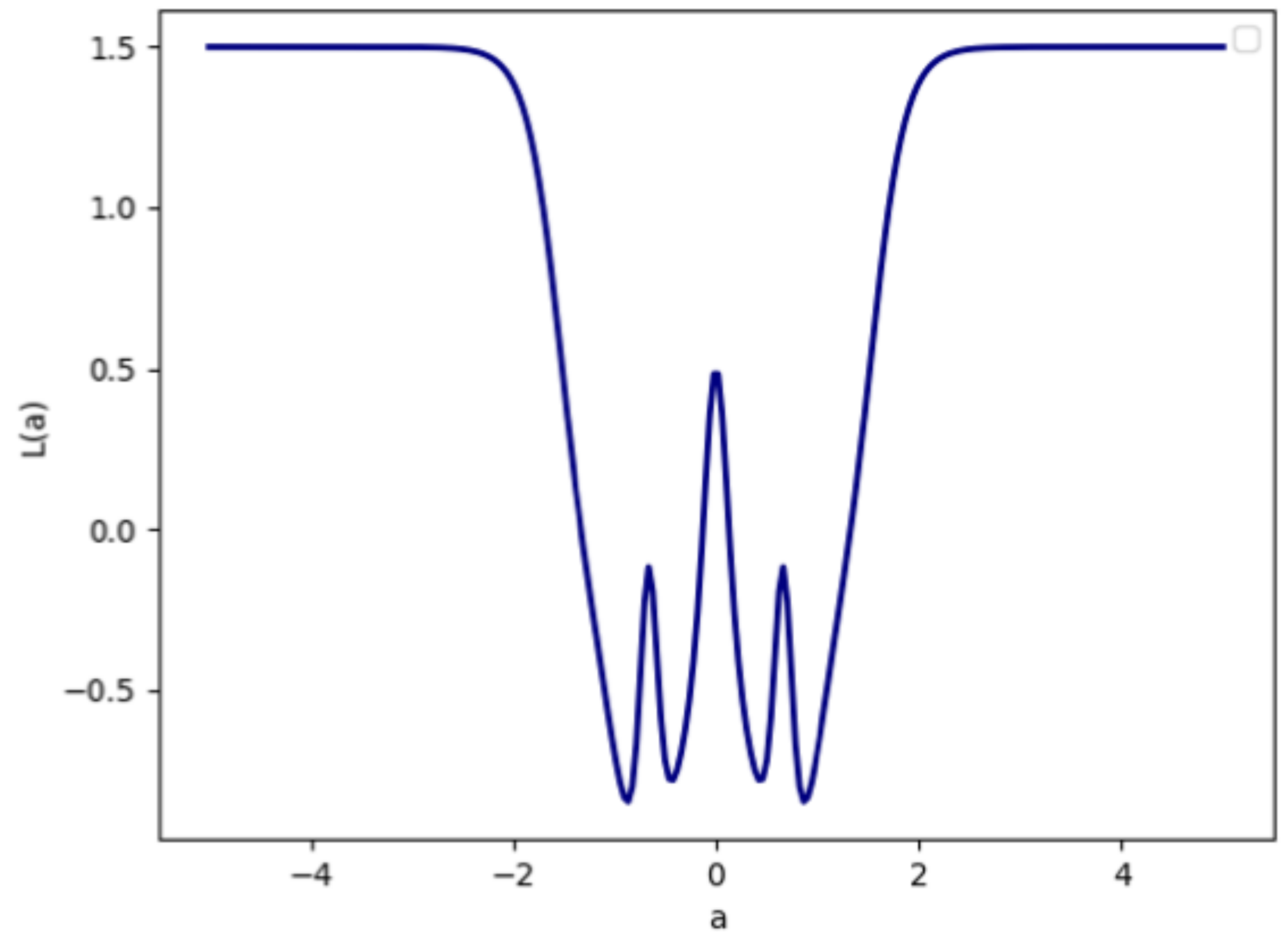
$$f(a) = e^{-a^2}$$

$$L(a) = \langle H \rangle_{U(a)} + e^{-\left(\frac{\partial}{\partial a}\langle H \rangle_{U(a)}\right)^2}$$

$$H = X(0)X(1) + \frac{1}{2}Z(0) + Y(1)$$

$U =$ 


```
tq.compile(L)
```

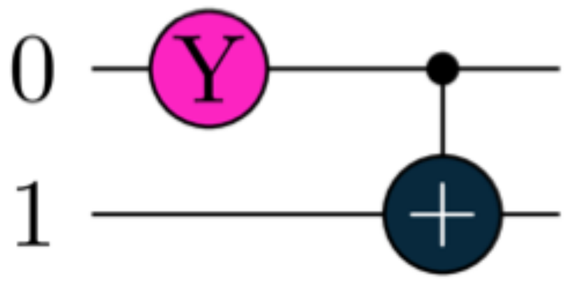



```
a = tq.Variable("a")
f = (-a**2).apply(tq.numpy.exp)

U = tq.gates.Ry(angle=f*numpy.pi, target=0)
U += tq.gates.CNOT(0,1)

H = tq.paulis.from_string("-1.0*X(0)X(1)+0.5*Z(0)+Y(1)")

E = tq.ExpectationValue(H=H, U=U)
dE = tq.grad(E, "a")

L = E + (-dE**2).apply(tq.numpy.exp)
```

example_objective.py

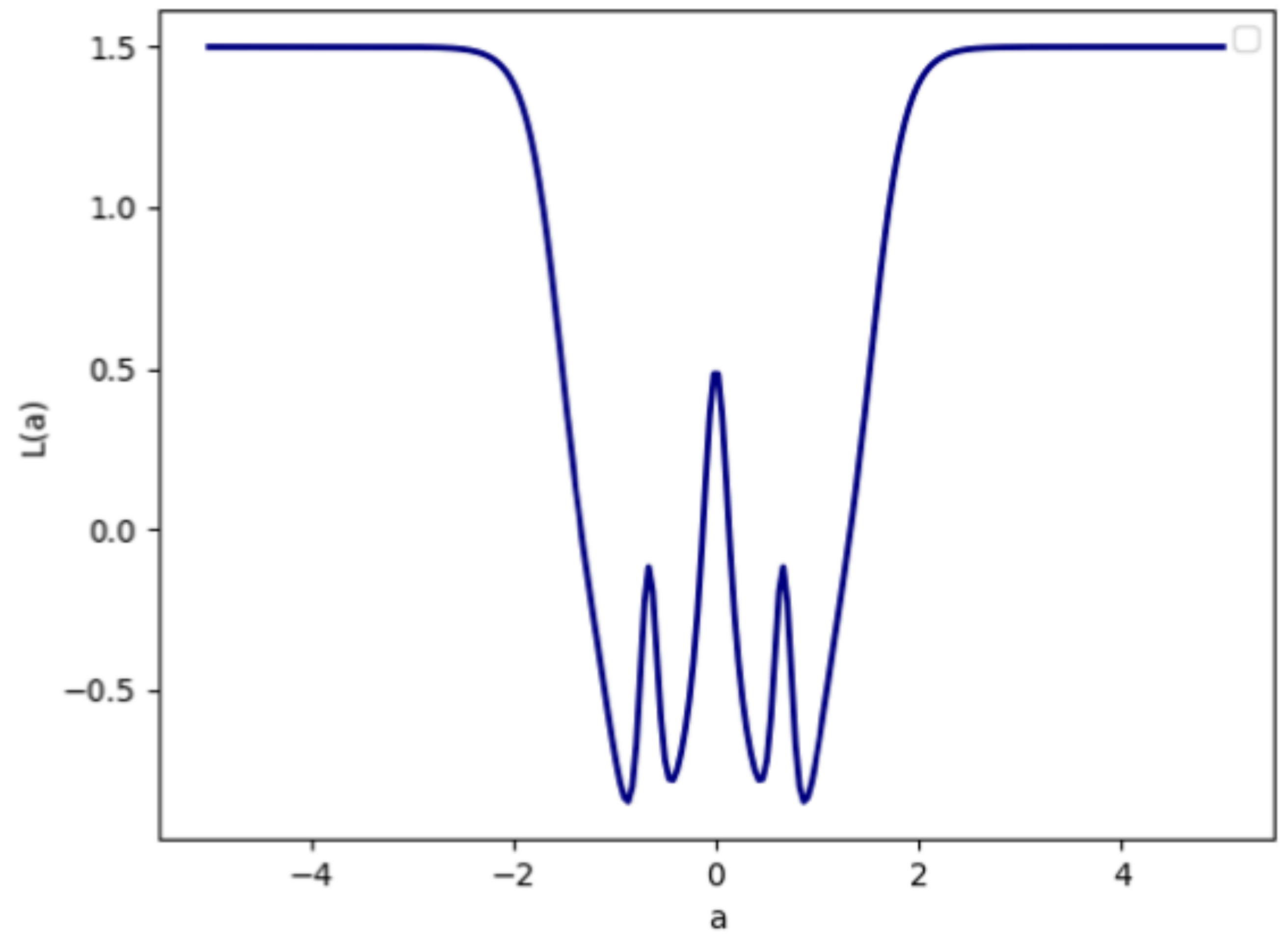
$$L(a) = \langle H \rangle_{U(a)} + e^{-\left(\frac{\partial}{\partial a}\langle H \rangle_{U(a)}\right)^2}$$

$$H = X(0)X(1) + \frac{1}{2}Z(0) + Y(1)$$

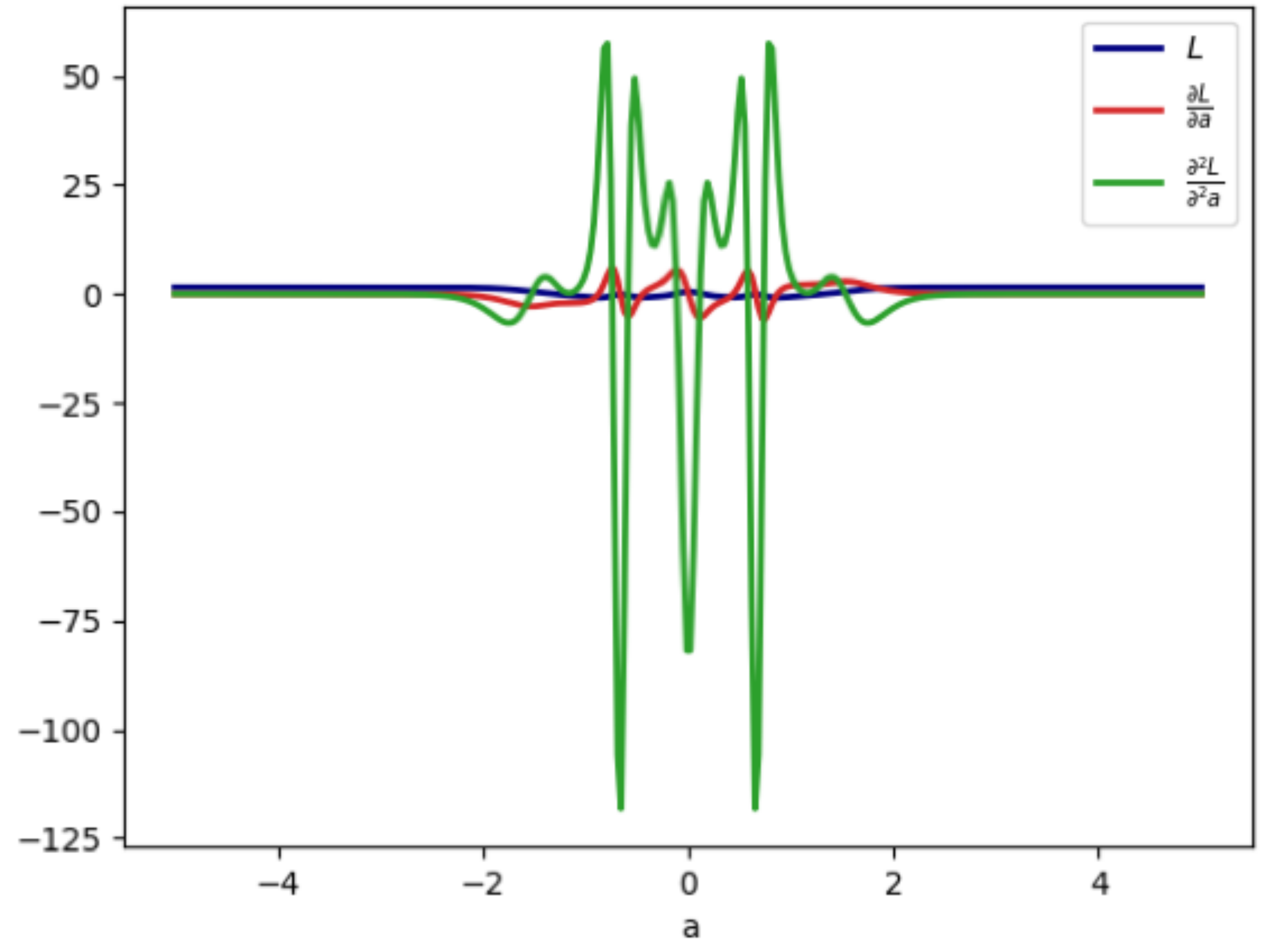
$U =$ 


```
a = tq.Variable("a")
f = (-a**2).apply(tq.numpy.exp)

U = tq.gates.Ry(angle=f*numpy.pi, target=0)
U += tq.gates.CNOT(0,1)

H = tq.paulis.from_string("-1.0*X(0)X(1)+0.5*Z(0)+Y(1)")

E = tq.ExpectationValue(H=H, U=U)
dE = tq.grad(E, "a")

L = E + (-dE**2).apply(tq.numpy.exp)
```

```
tq.compile(L)
```




```
dL = tq.grad(L, "a")
dL2 = tq.grad(dL, "a")
```




```
print(L)
```

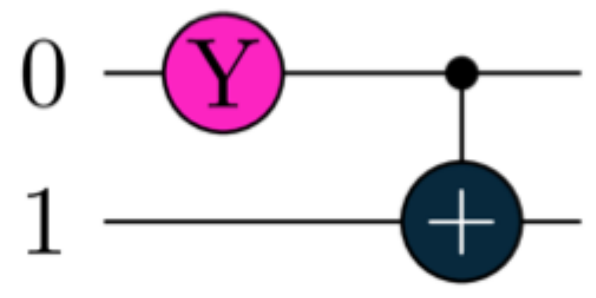
```
>>> Objective with 3 unique expectation values
    total measurements = 9
    variables          = [a]
    types              = not compiled
```

example_objective.py

$$L(a) = \langle H \rangle_{U(a)} + e^{-\left(\frac{\partial}{\partial a}\langle H \rangle_{U(a)}\right)^2}$$

$$H = X(0)X(1) + \frac{1}{2}Z(0) + Y(1)$$

$U =$

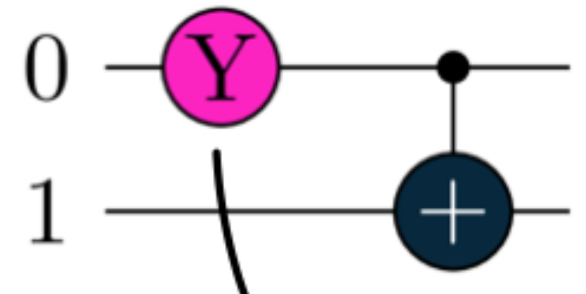



```
L = tq.compile(L)
U2 = tq.gates.Ry(angle=L, target=0)
U2+= tq.gates.CNOT(0,1)
```

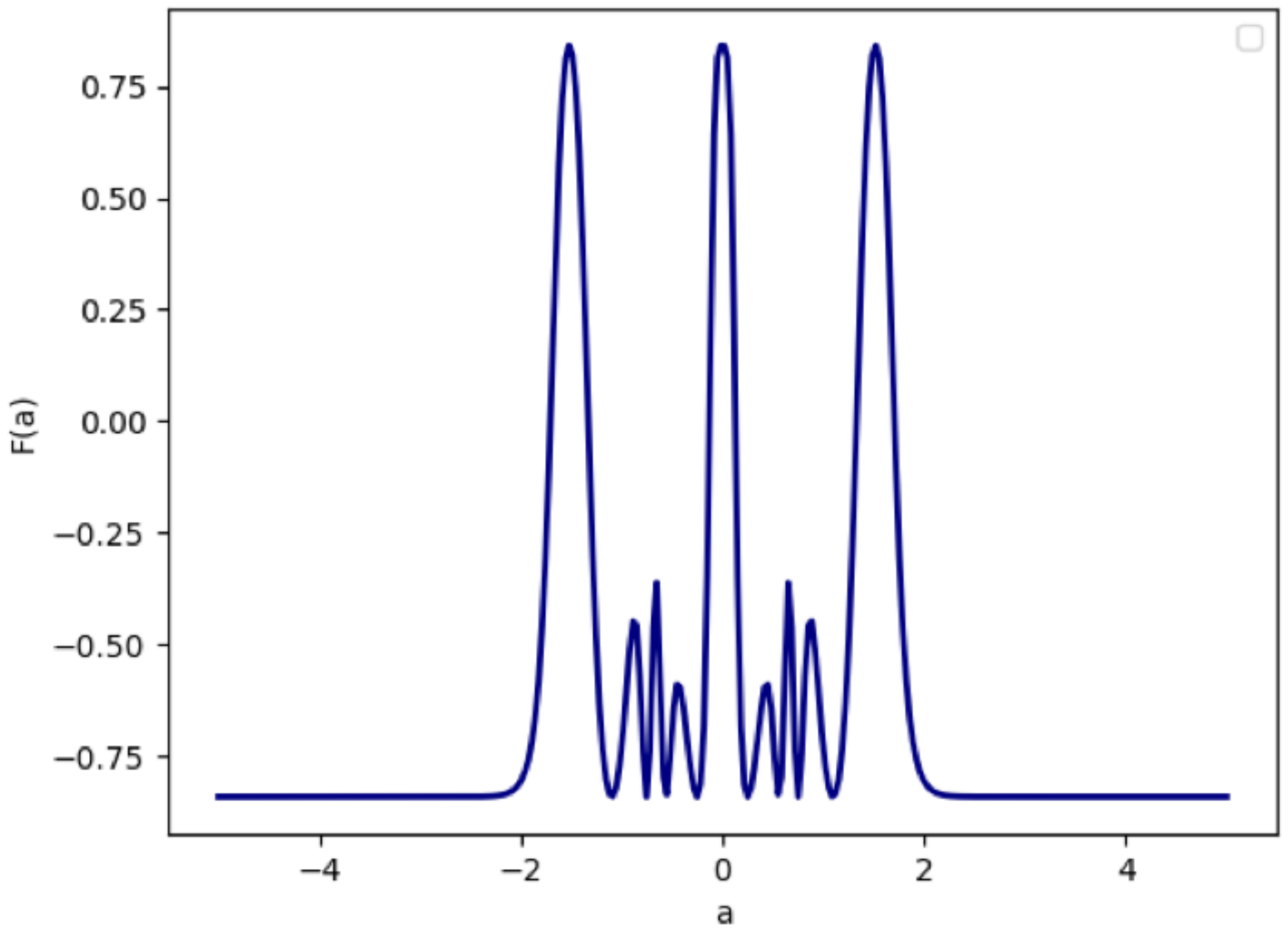
$$F(a) = \sin\left(\langle H_2 \rangle_{U_2}\right)$$

$$H_2 = X(0) + X(1) + X(0)X(1)$$

$U_2 =$



$$e^{-i\frac{L(a)}{2}Y(0)}$$



example_nested_objective.py

Outline

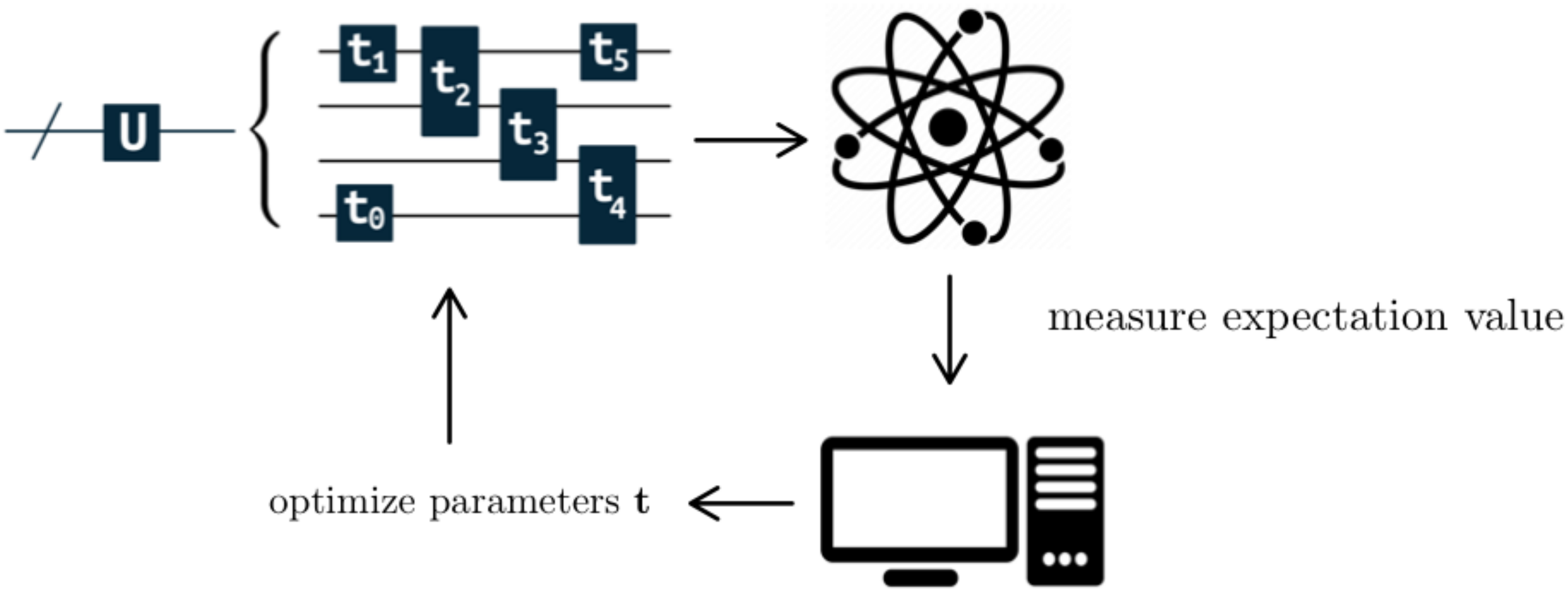
Graph Based Molecular Quantum Circuit Design

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

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

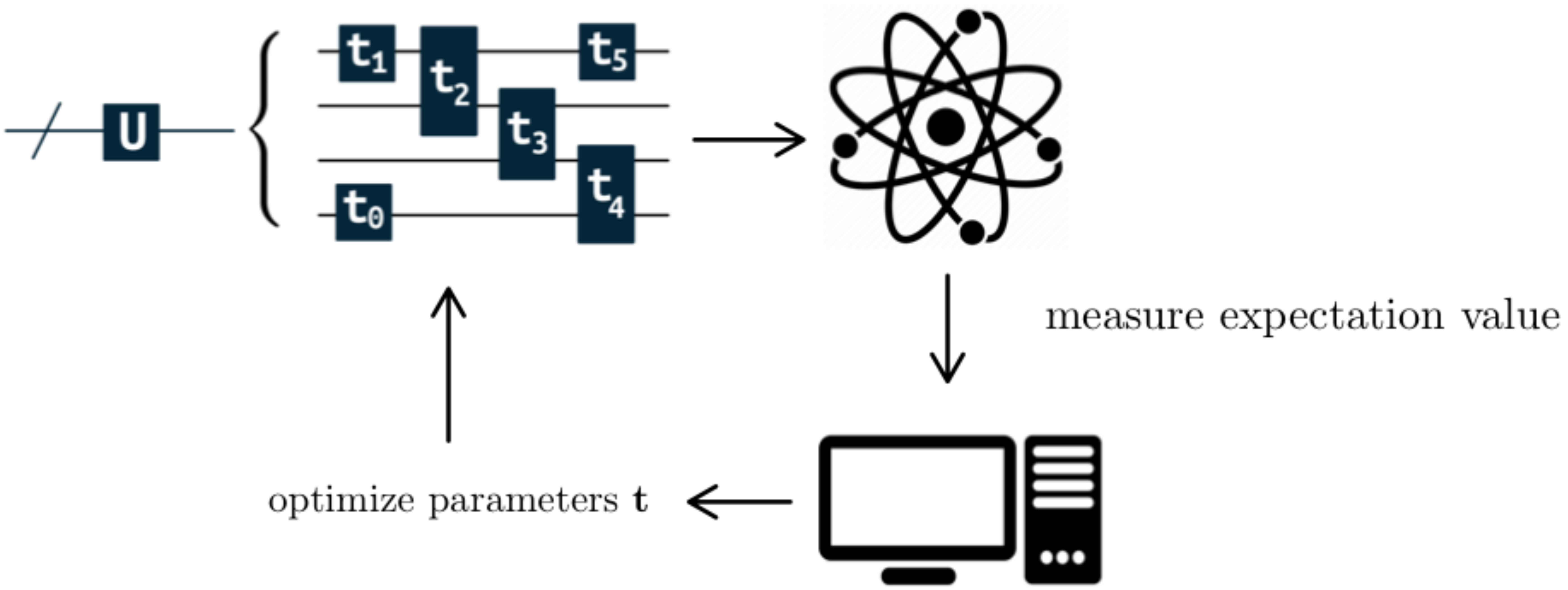
Jakob S. Kottmann[1,2,*] and Alán Aspuru-Guzik[1,2,3,4,†]

Small Recap


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

Design principles

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



Design principles

- Locality (circuit connections)
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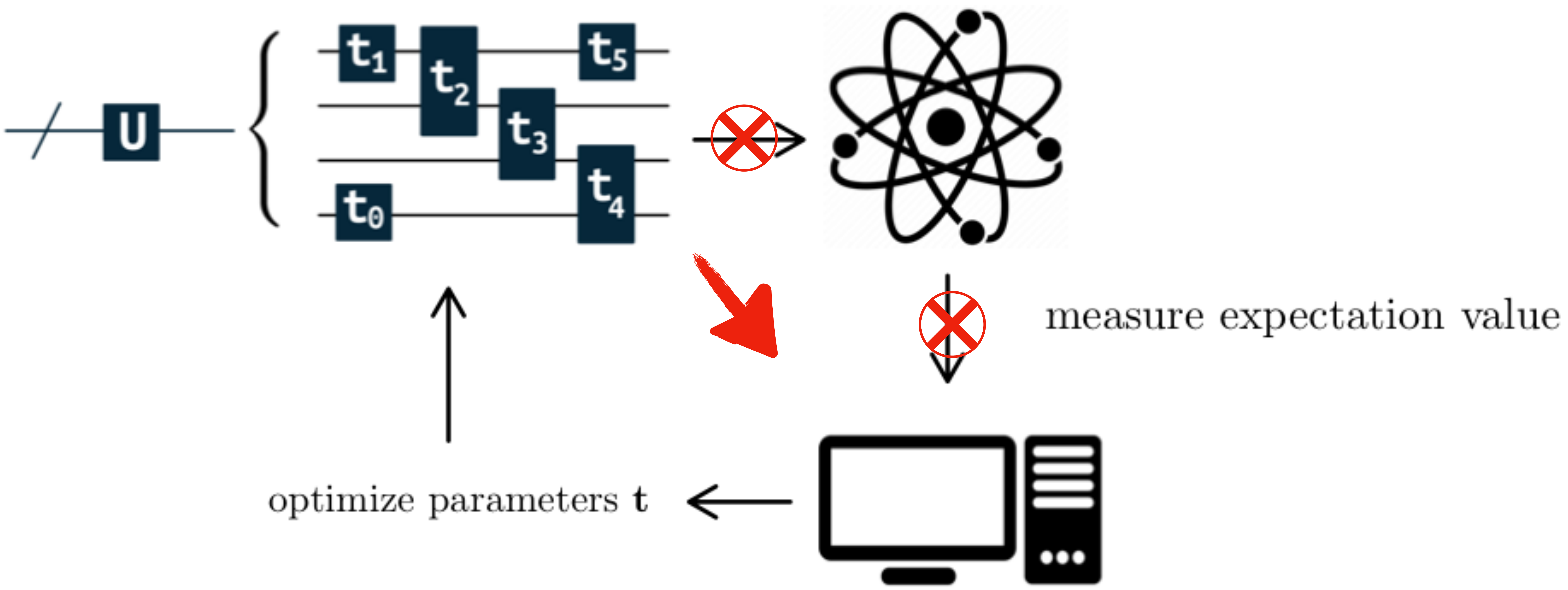
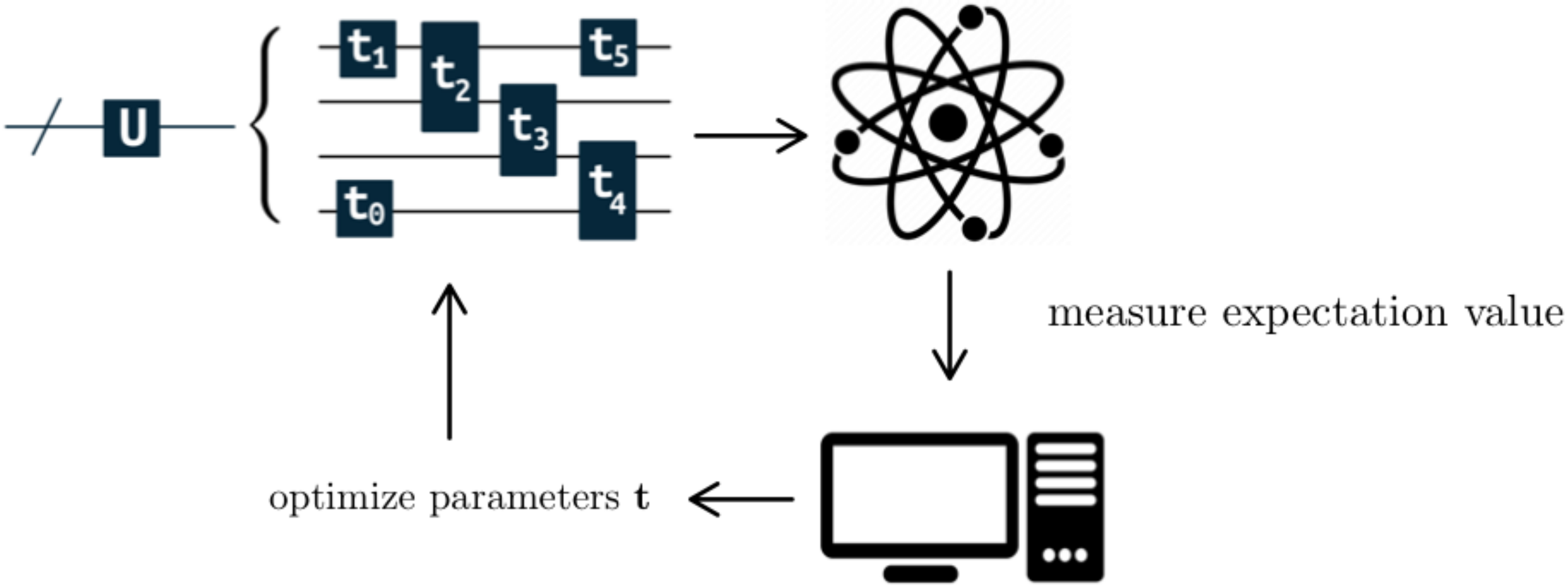
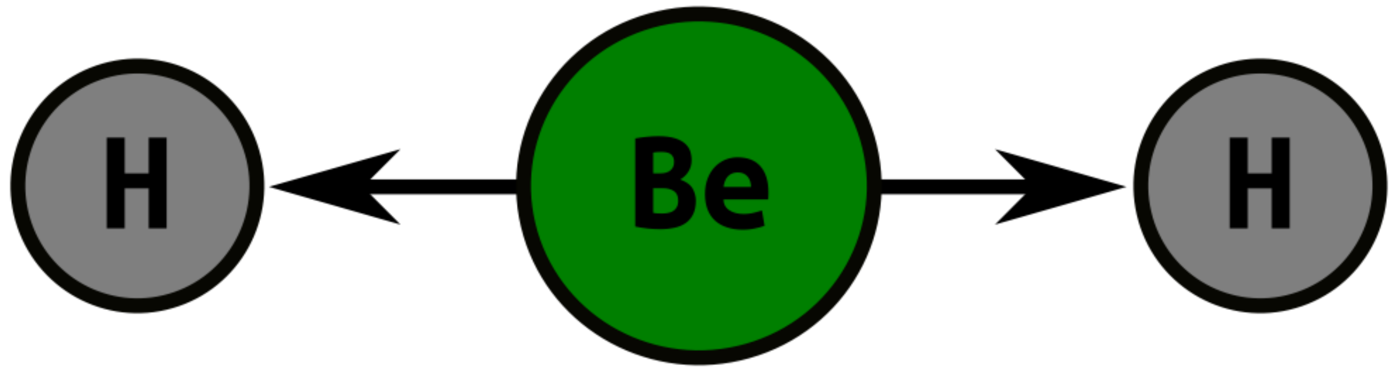
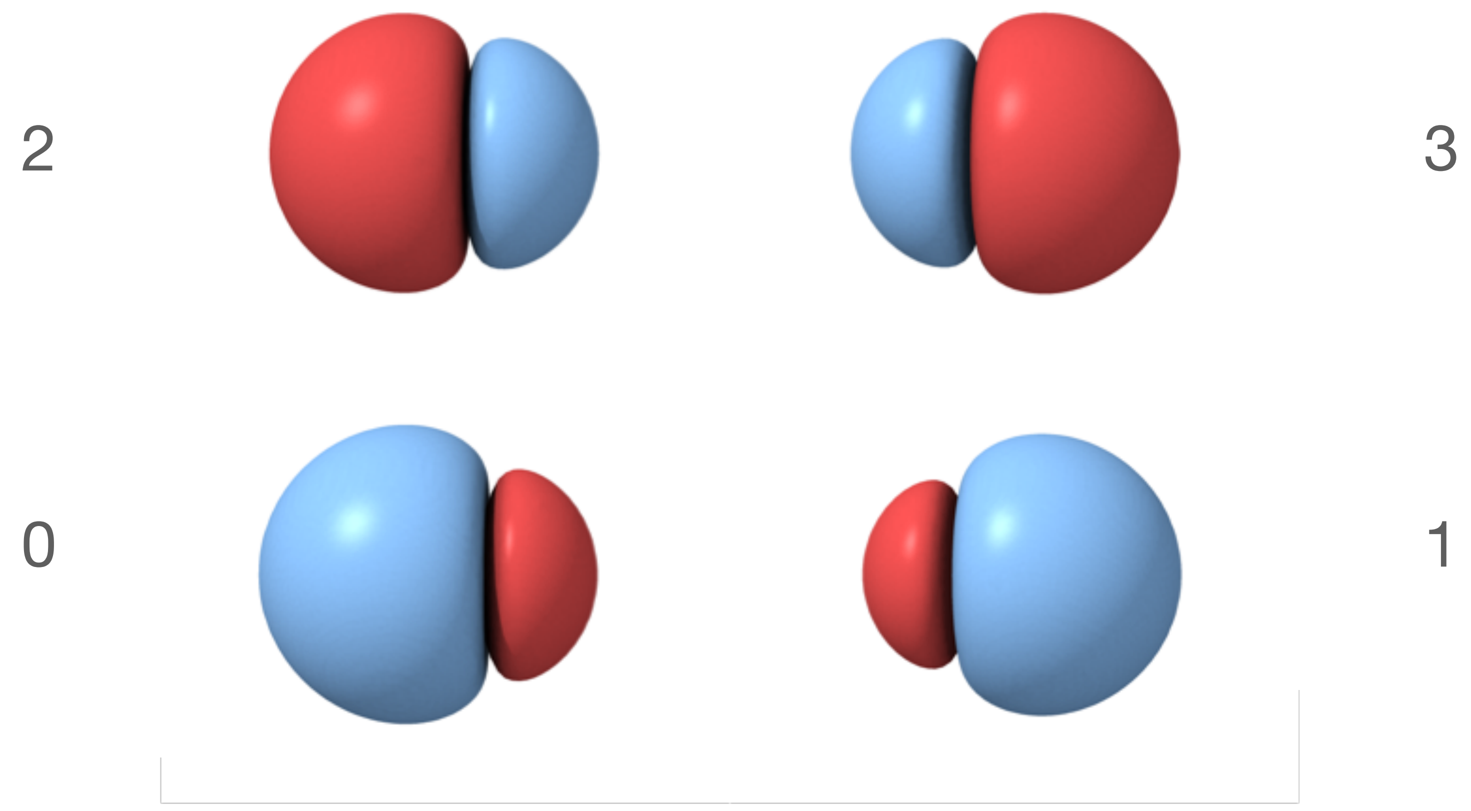


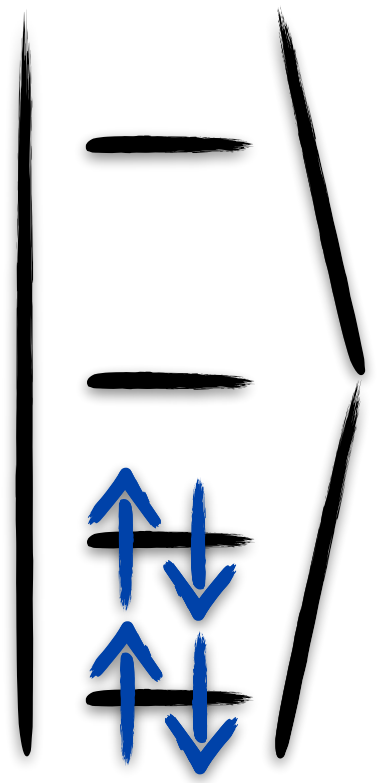
Design principles →

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




H
Be
H

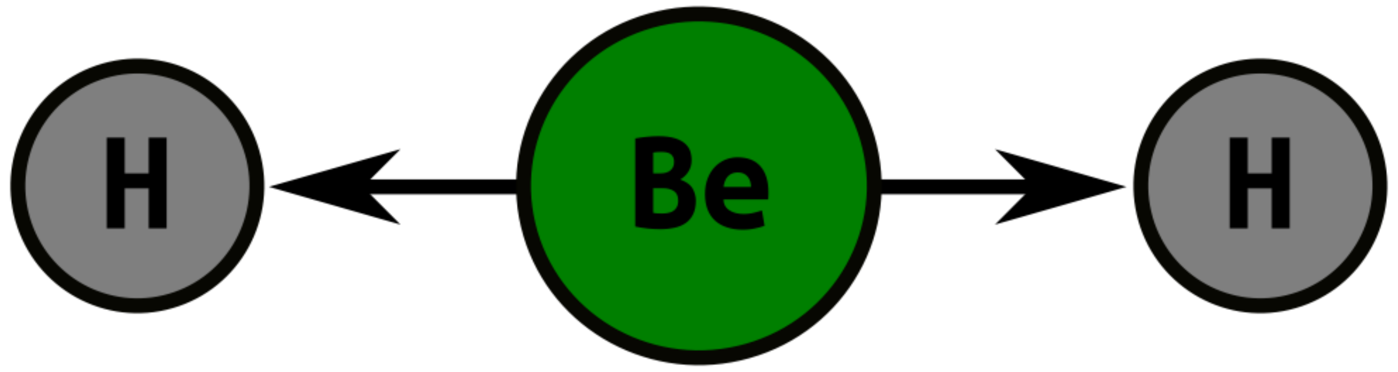

2
3
0
1

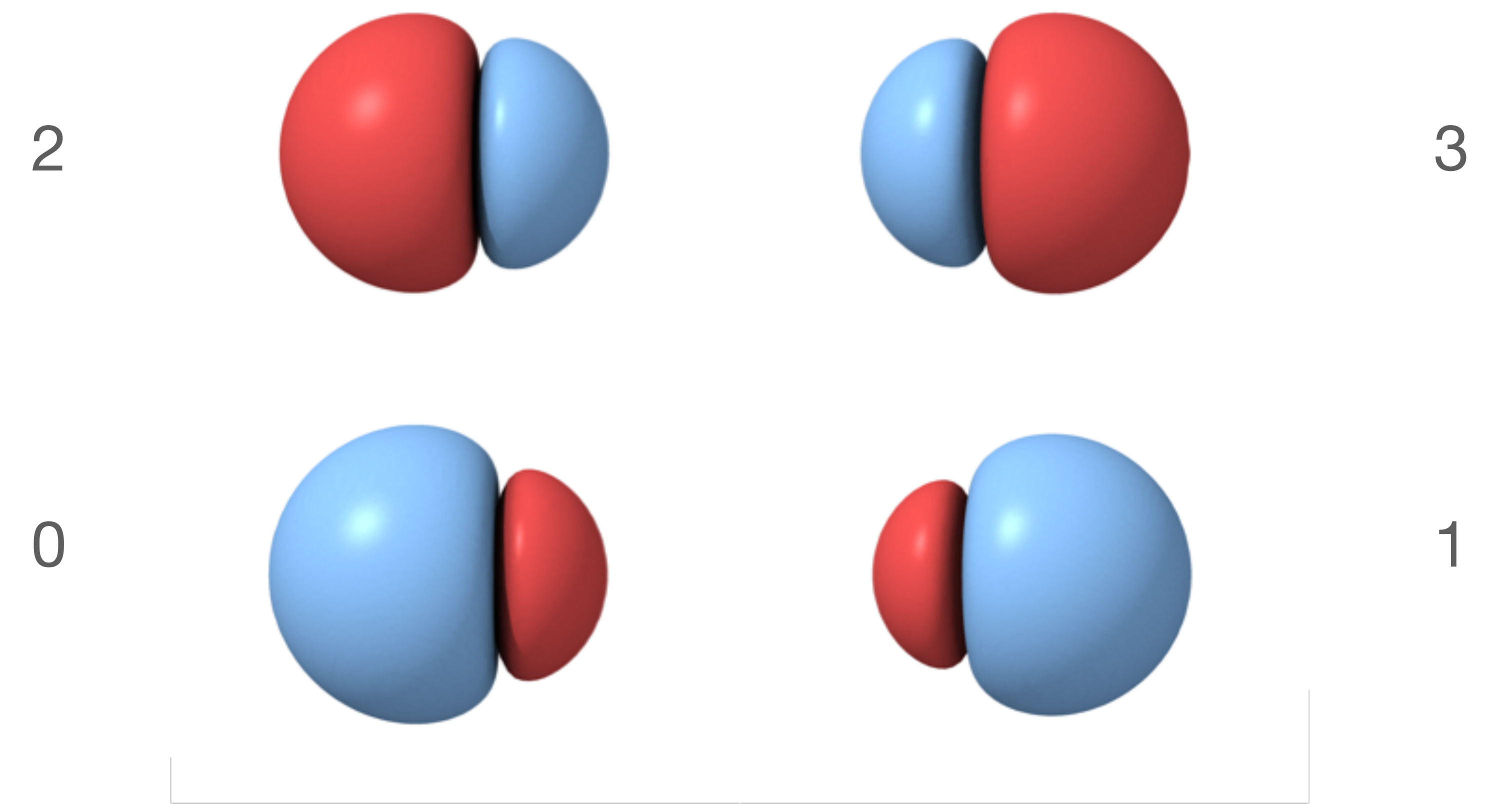


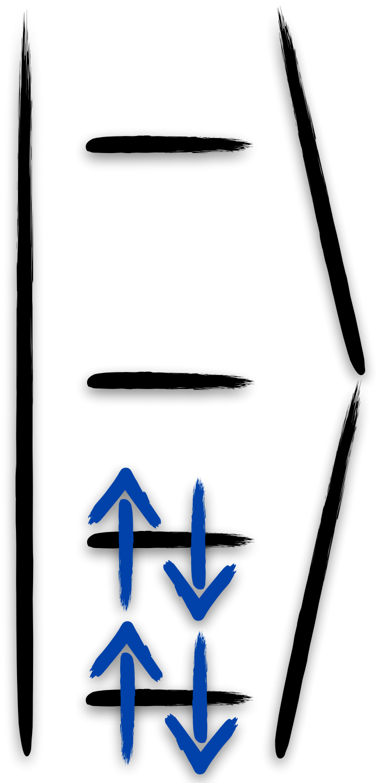
Empty orbitals 2,3

Two electrons in orbital 1

Two electrons in orbital 0



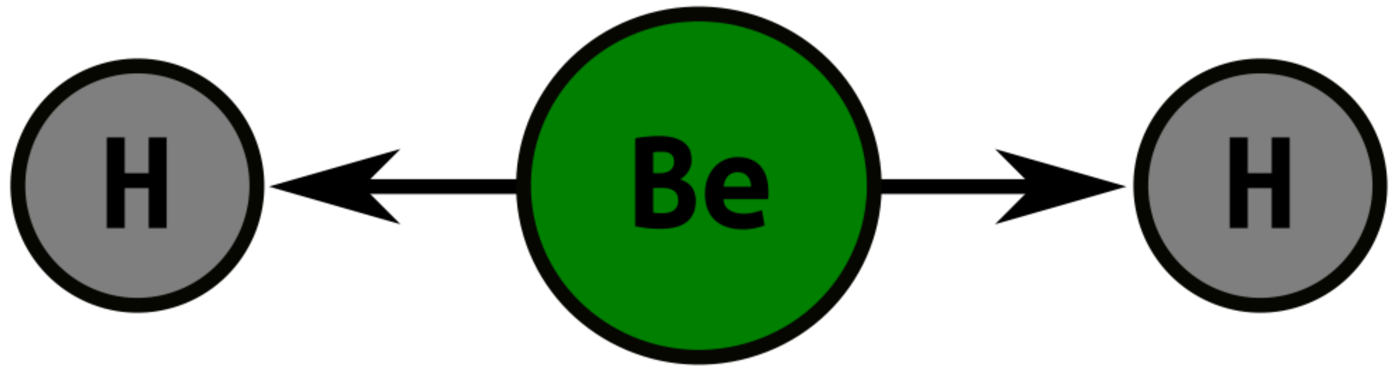




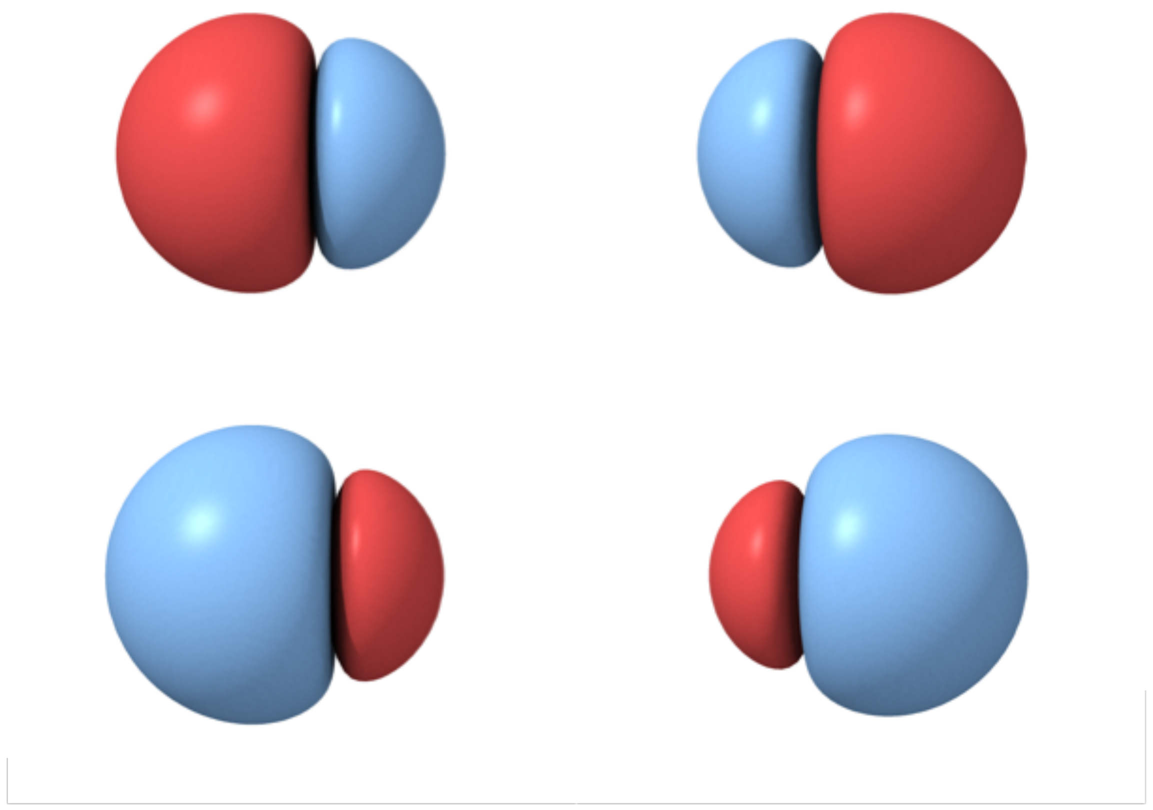
Empty orbitals 2,3

Two electrons in orbital 1

Two electrons in orbital 0



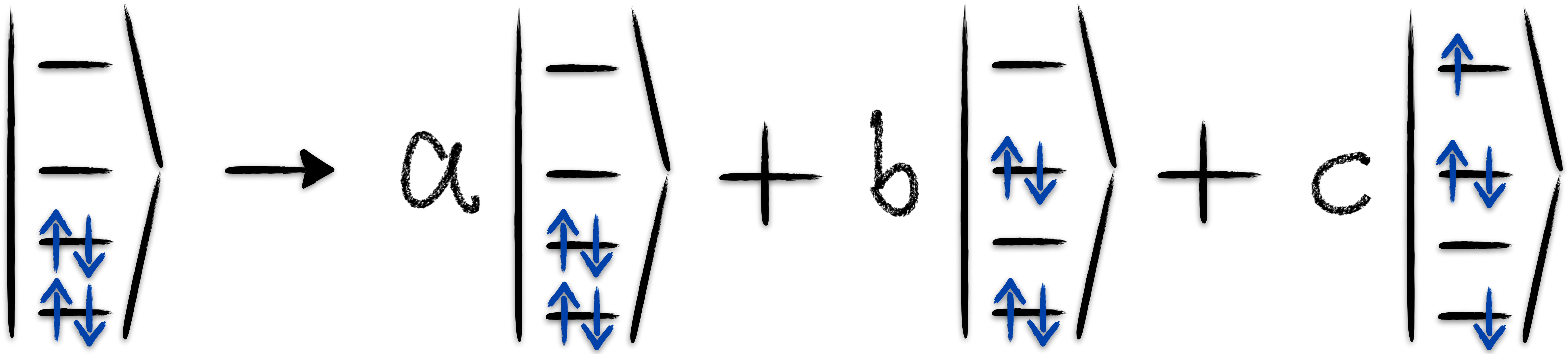
2 3



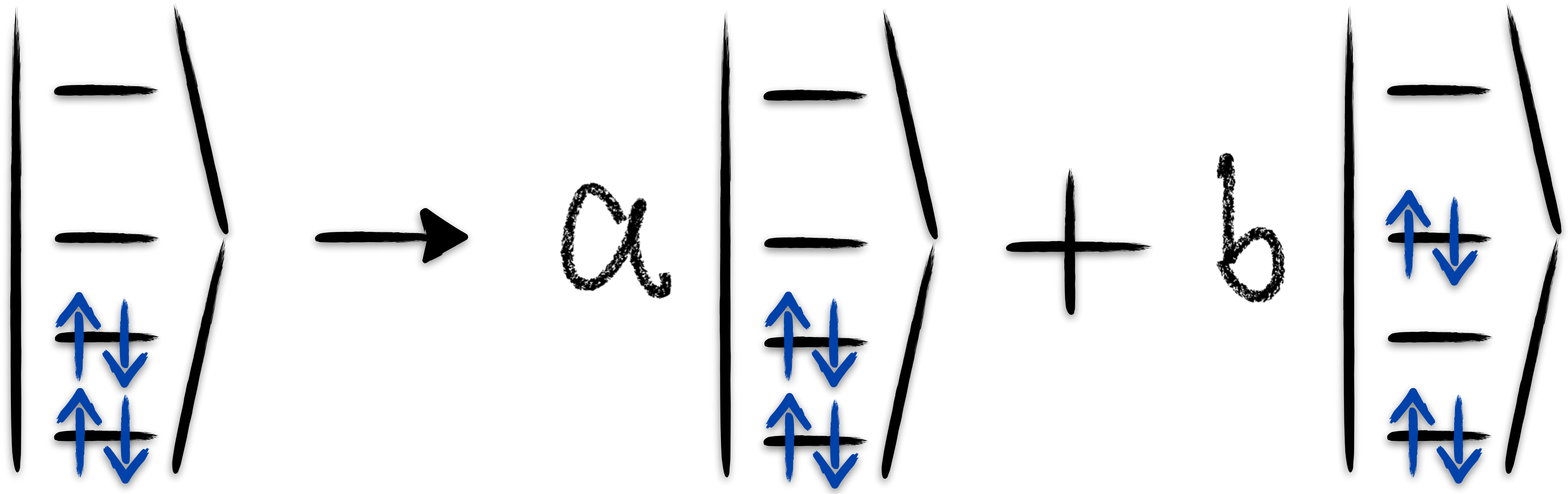
0 1

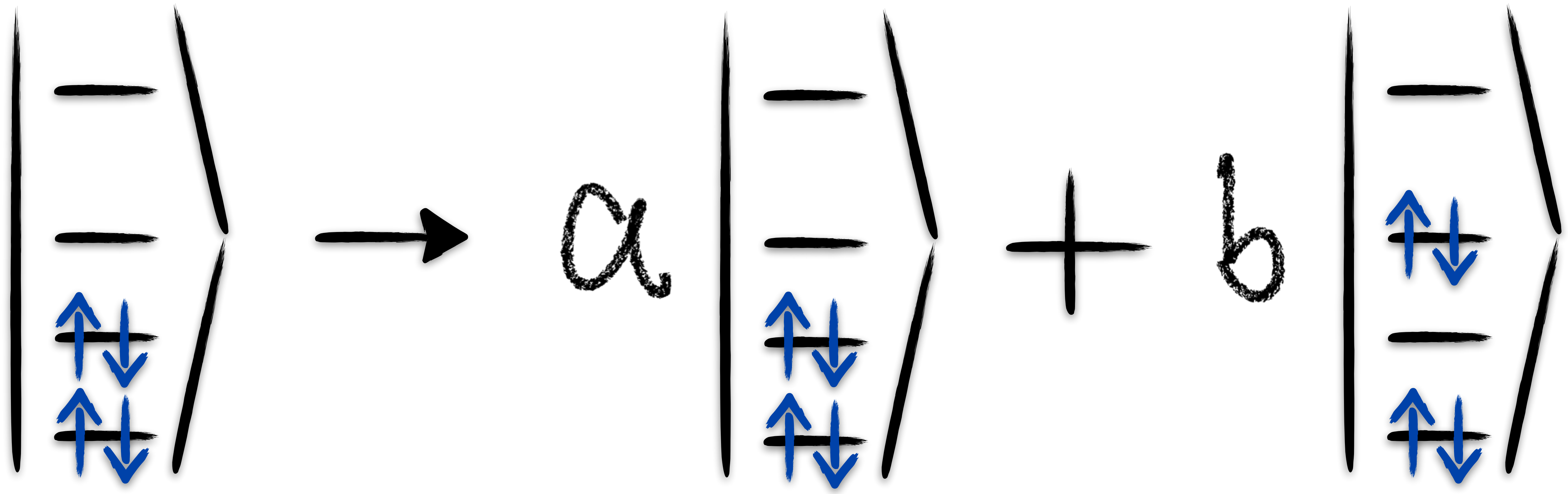
$$|11\ 11\ 00\ 00\rangle$$

Qubit encoding


a
b
c

Building Blocks

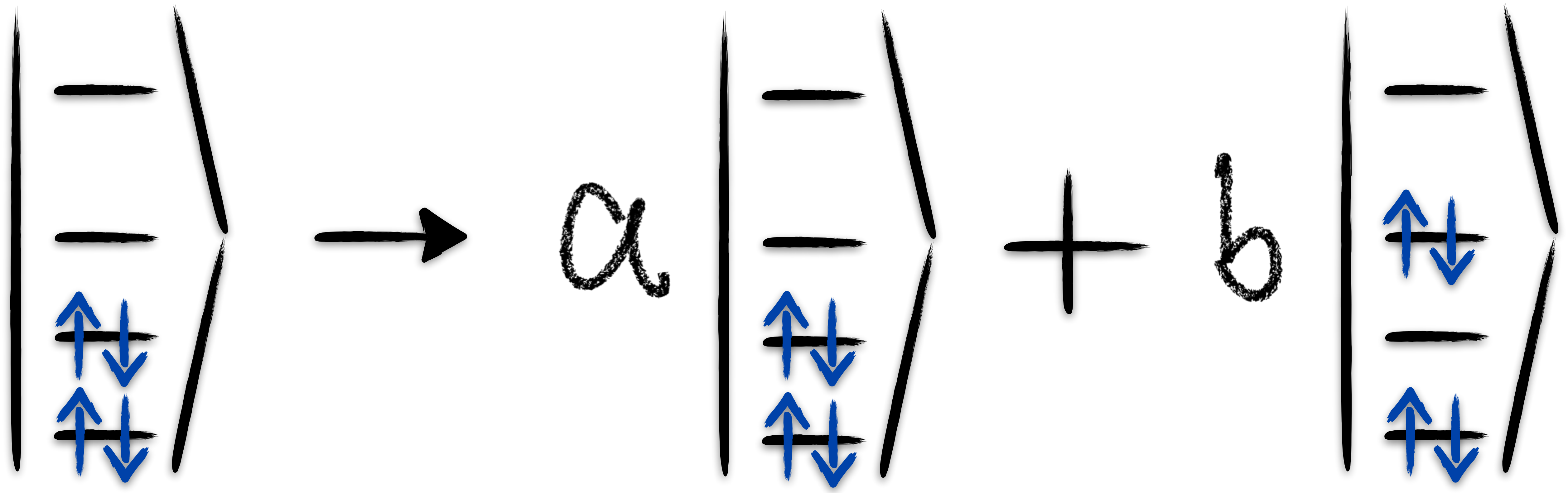

a
+ b



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

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

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



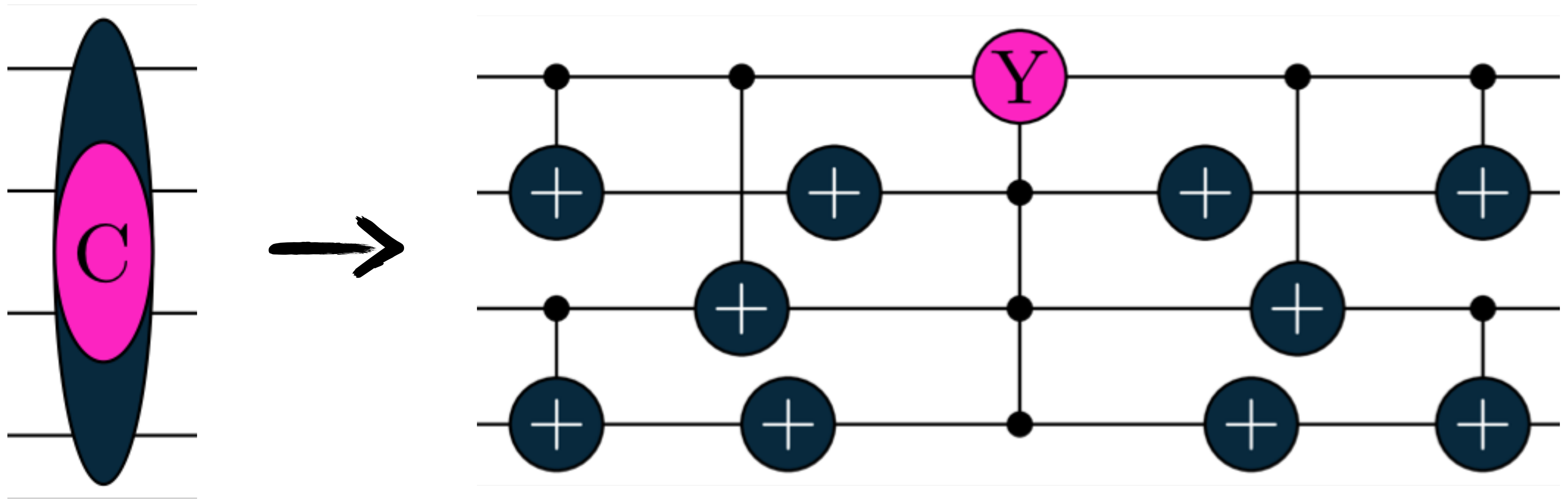
$$U_{\boldsymbol{pq}}\left(\theta\right) = e^{-i\frac{\theta}{2}G_{\boldsymbol{pq}}}$$

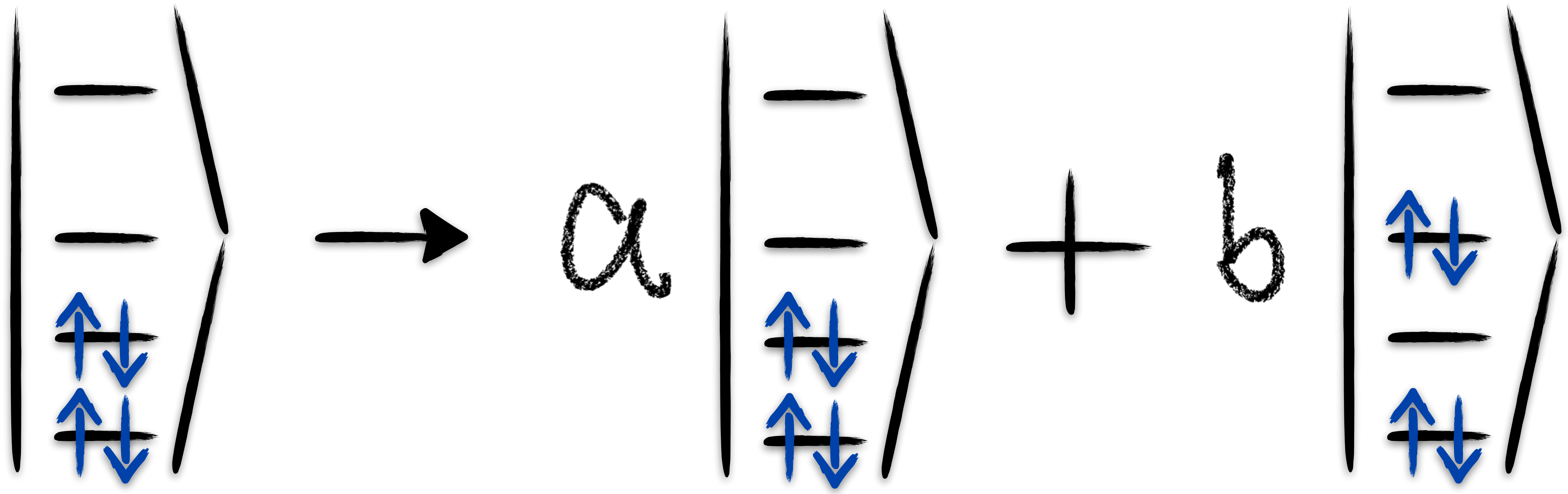
$$G_{\boldsymbol{pq}} = i\left(\prod_k a^\dagger_{p_k} a_{q_k} - h.c.\right)$$

$$a_p^\dagger \xrightarrow[Wigner]{Jordan} \sigma_p^+ \prod_{k<p} \sigma_k^z.$$

Example

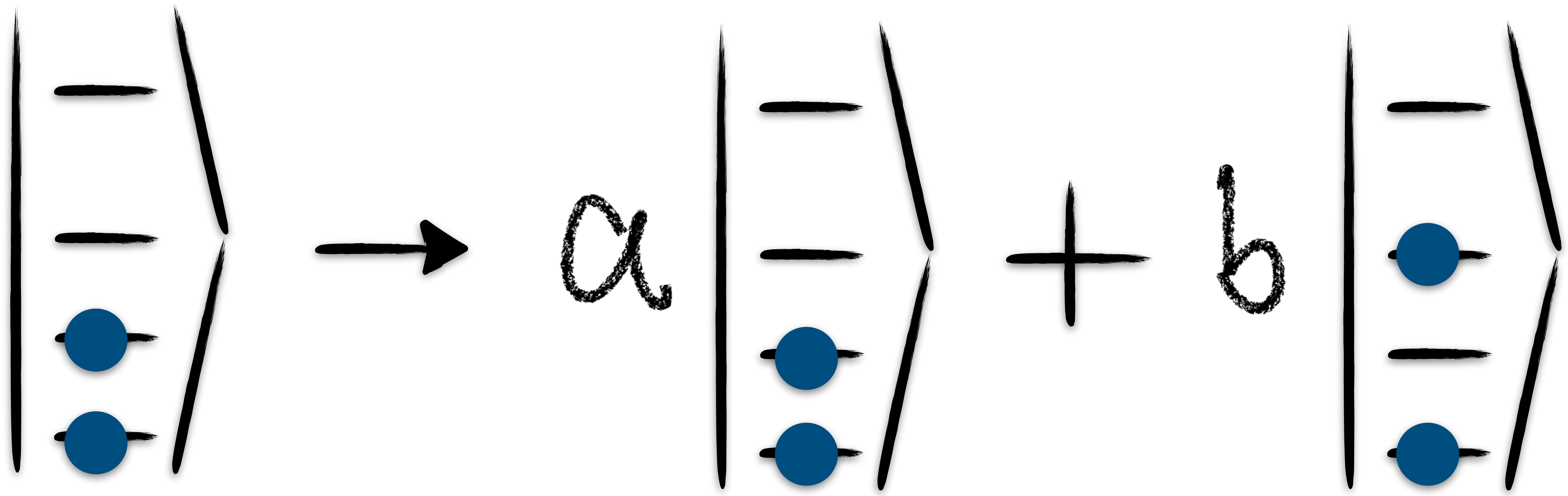
$$G_{p_\uparrow p_\downarrow q_\uparrow q_\downarrow} \equiv \tilde{G}_{pq} = i\left(a^\dagger_{p_\uparrow} a_{q_\uparrow} a^\dagger_{p_\downarrow} a_{q_\downarrow} - h.c\right)$$



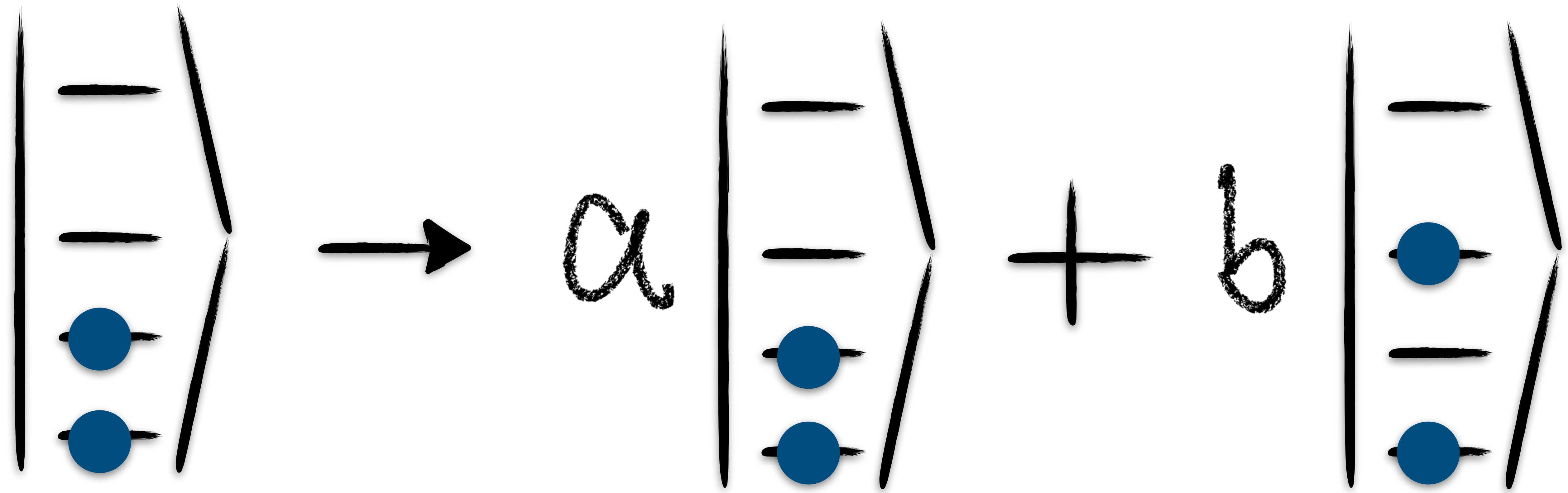


N orbitals ⟶ 2N qubits

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

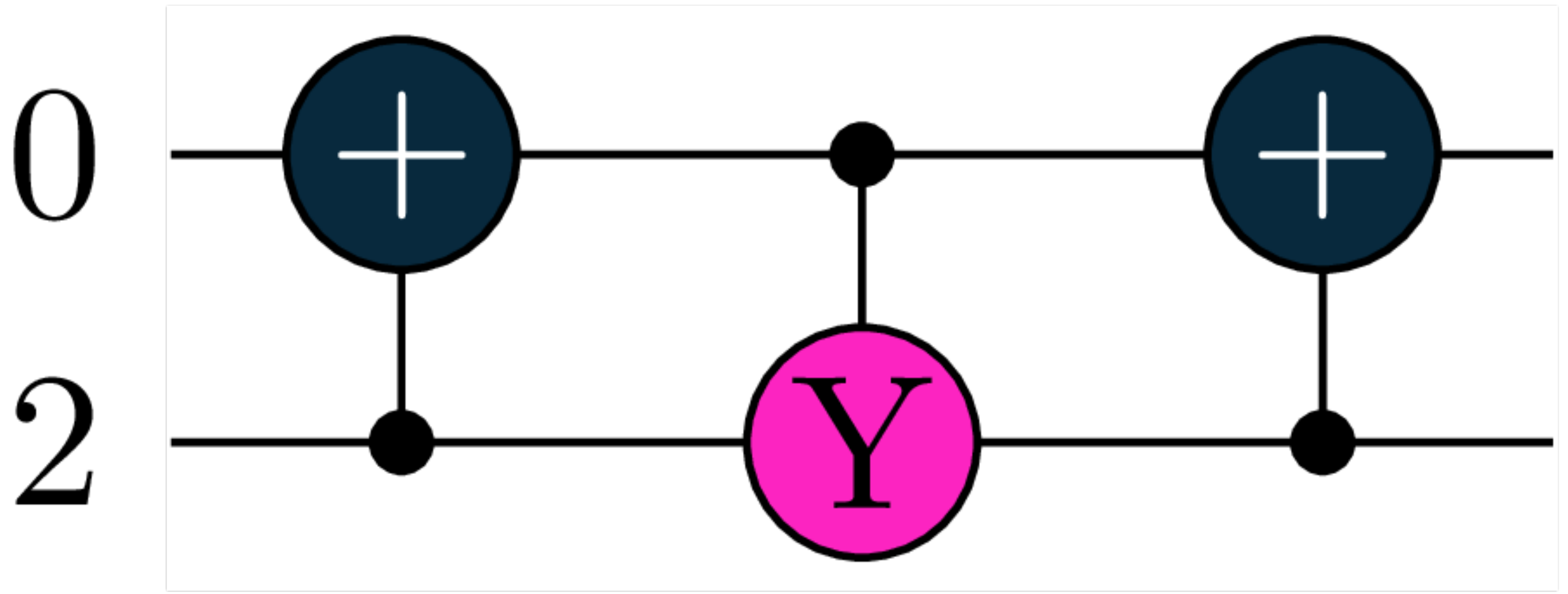


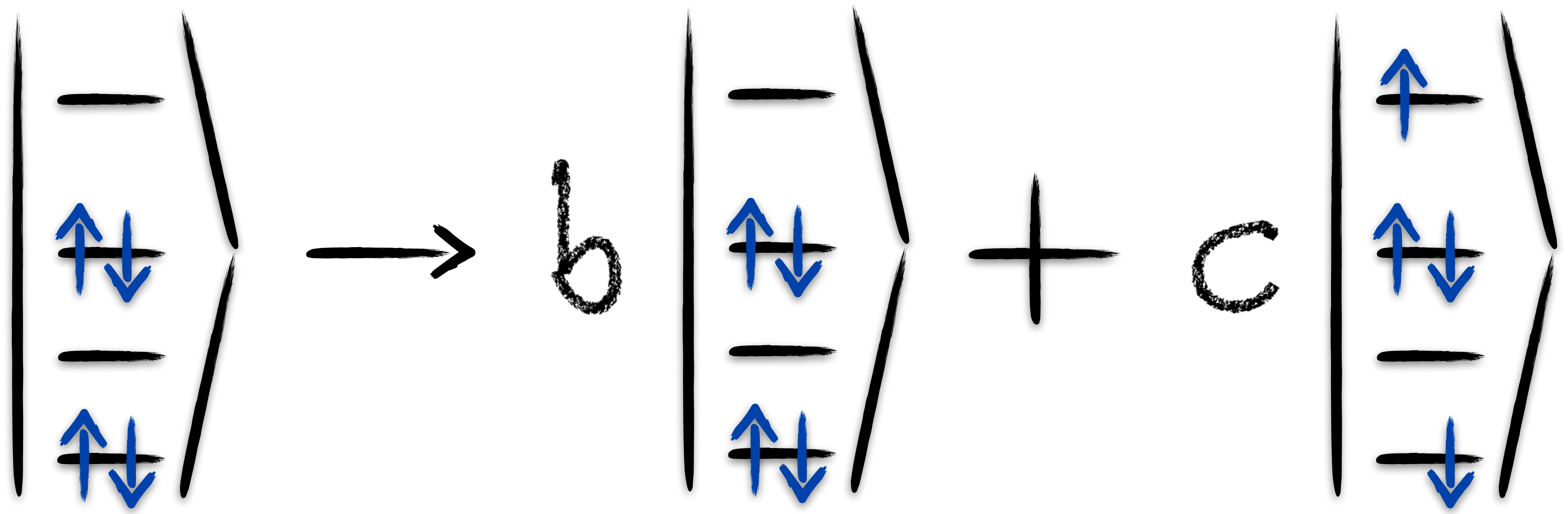
N orbitals ⟶ N qubits

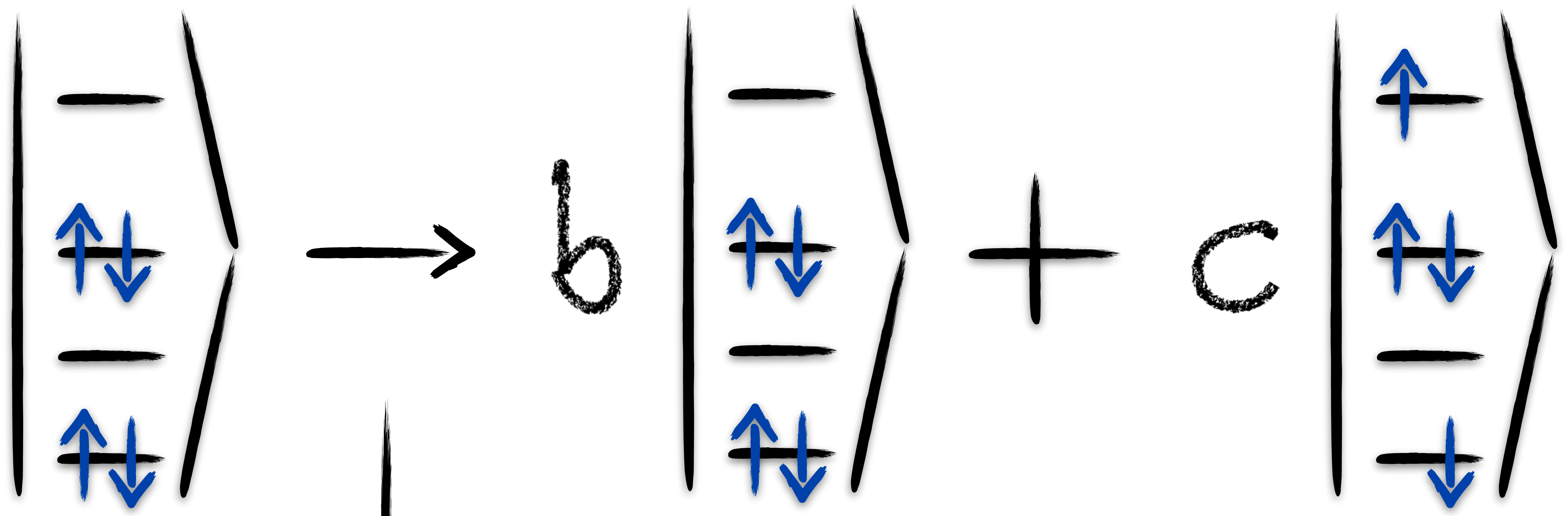


$$\tilde{G}_{pq} \xrightarrow[\text{Wigner}]{\text{Jordan-}} \tilde{G}_{pq}^{\text{JW}} = i\left(\sigma^+_{p\uparrow}\sigma^-_{q\uparrow}\sigma^+_{p\downarrow}\sigma^-_{q\downarrow} - h.c.\right)$$

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

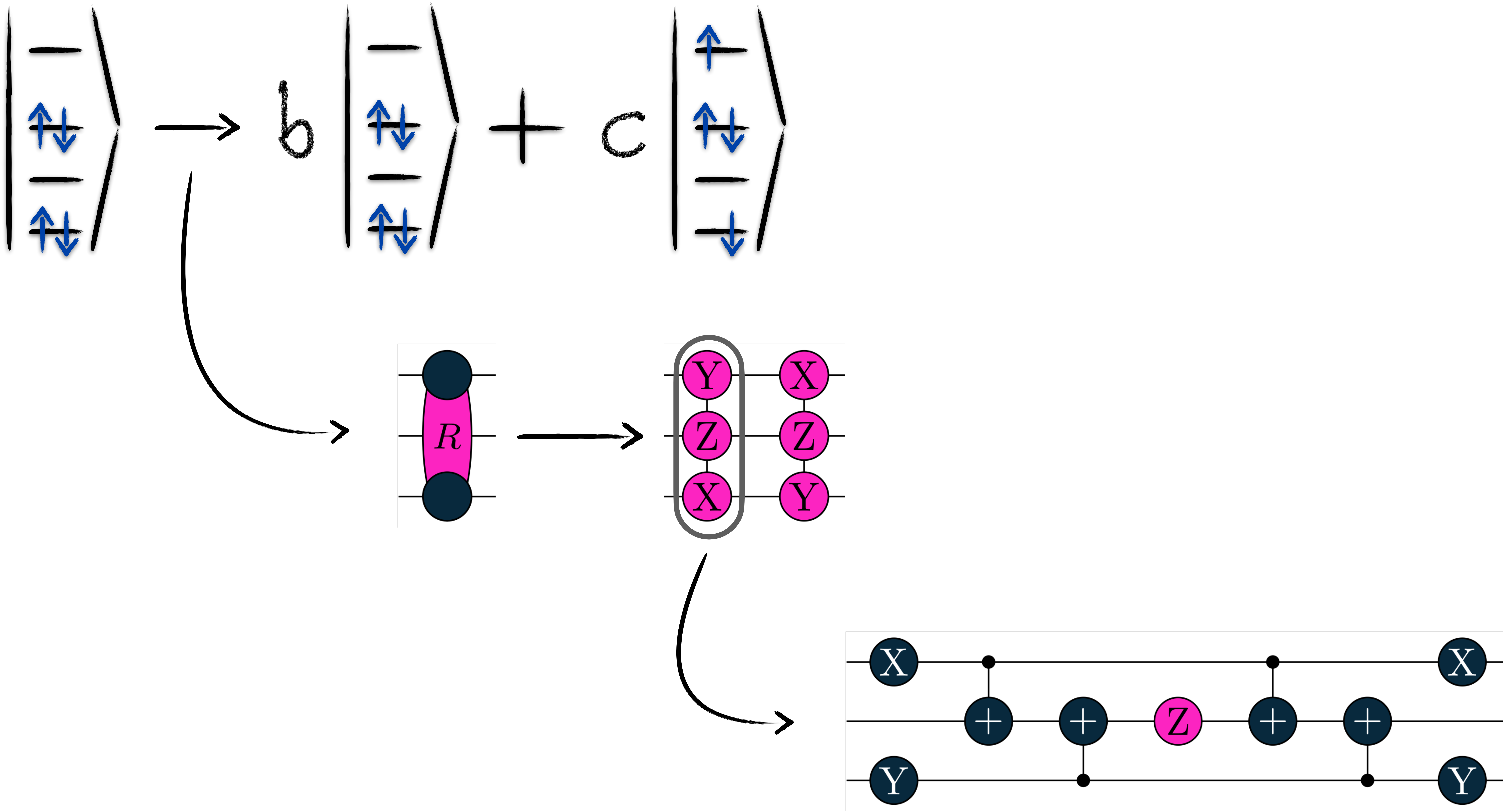



b
c

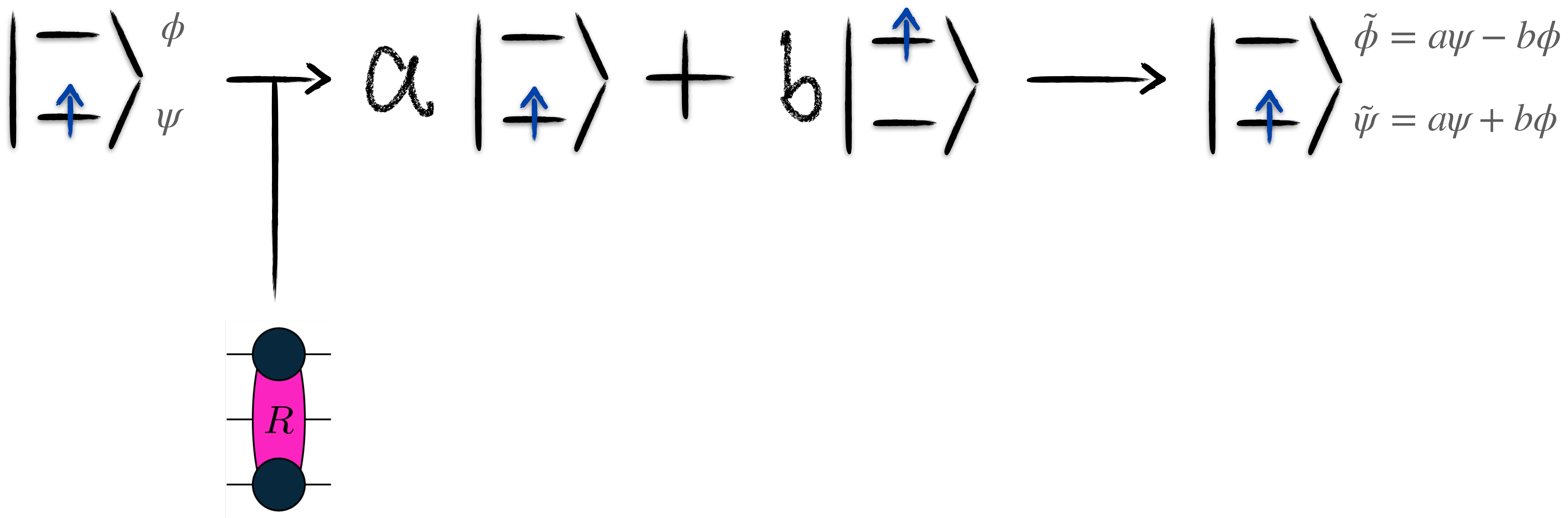


$$U_{i_\uparrow}^{j_\uparrow} = e^{-i\frac{\theta}{2}\left(a^\dagger_{i_\uparrow} a_{j_\uparrow} - a^\dagger_{j_\uparrow} a_{i_\uparrow}\right)}$$

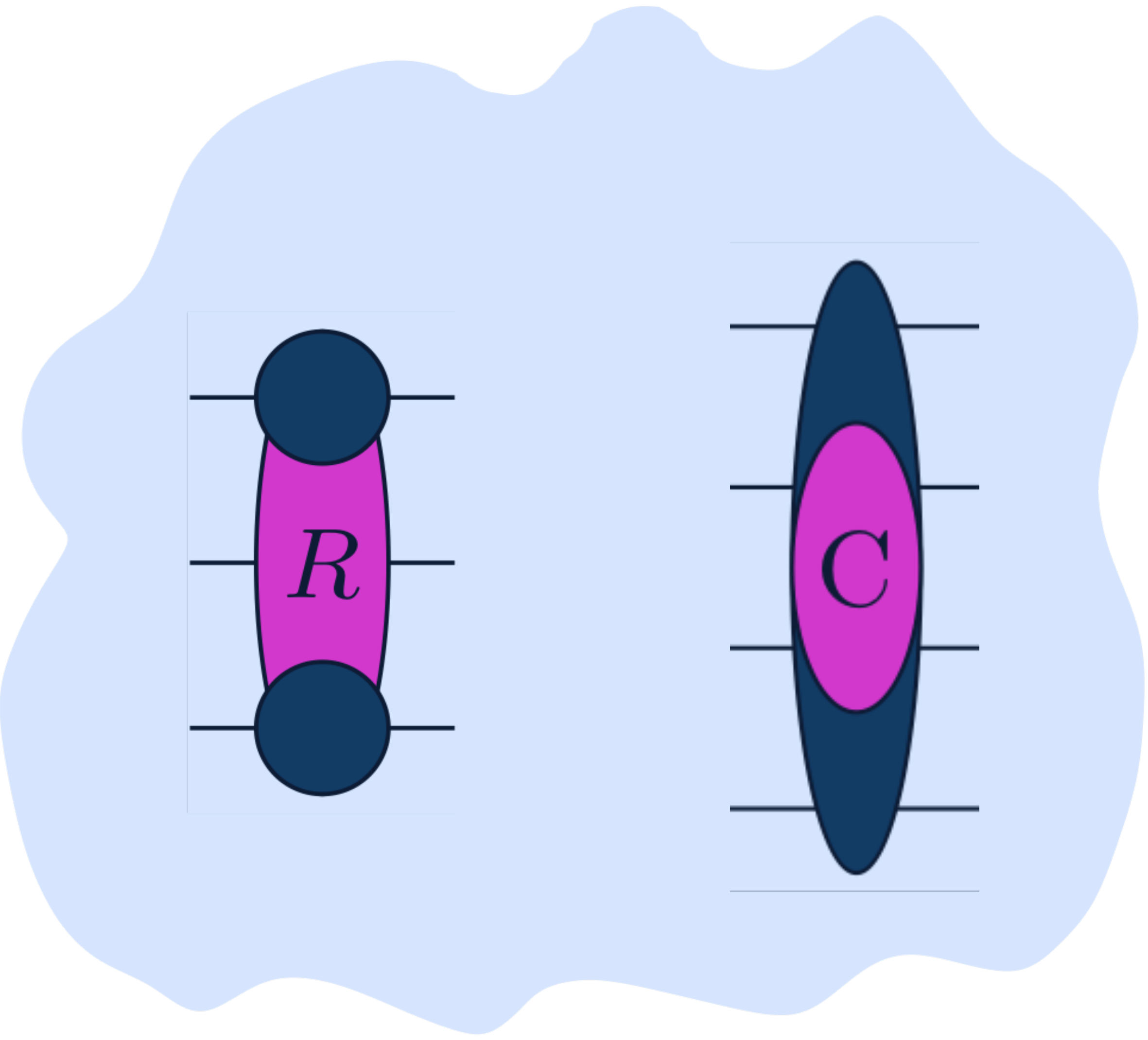
$$e^{-\frac{\theta}{2}\sigma_0^x\sigma_1^z\sigma_2^y}\, e^{-\frac{\theta}{2}\sigma_0^y\sigma_1^z\sigma_2^x}$$


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

orbital rotations



Rotators
and
Correlators

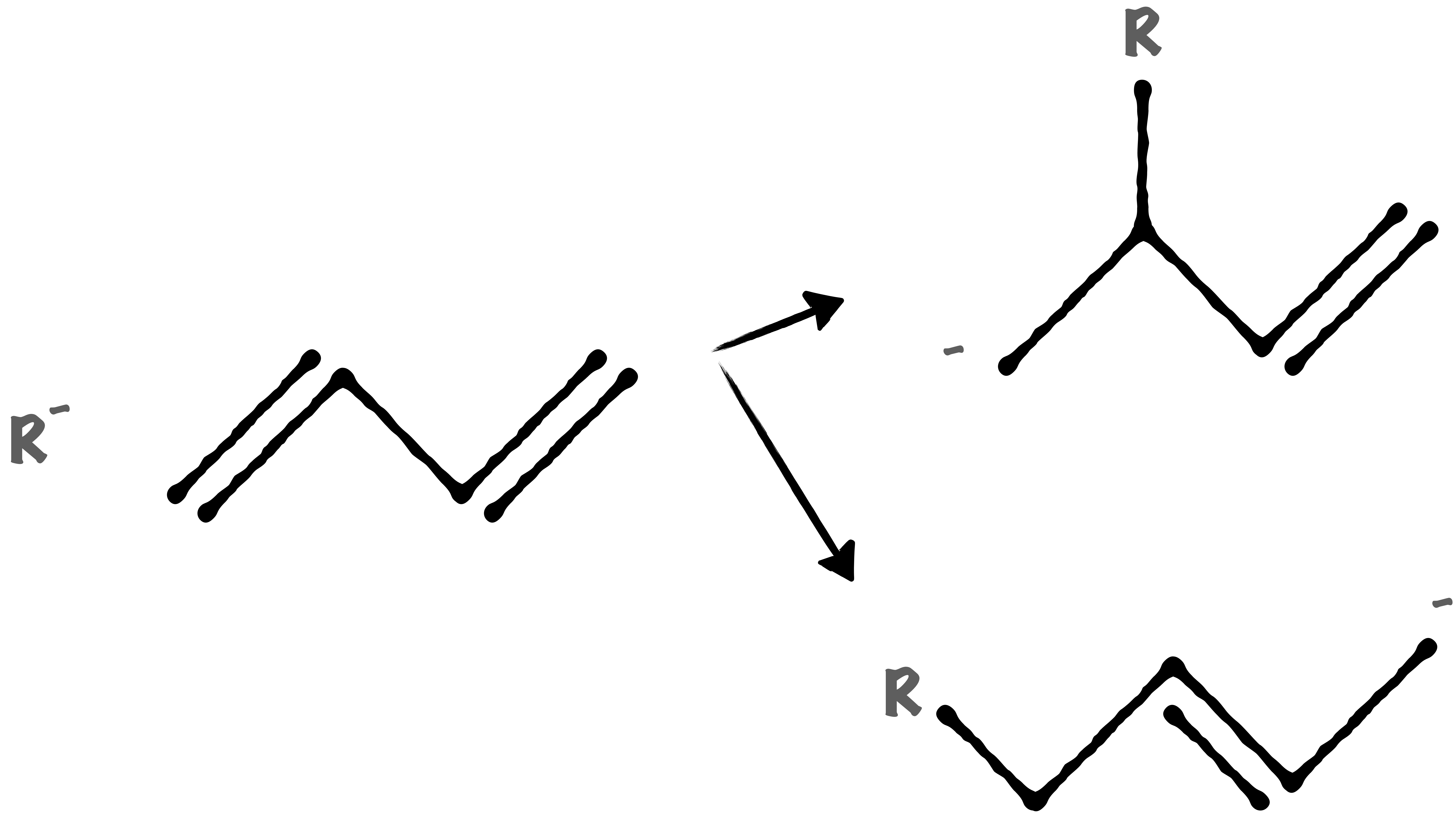


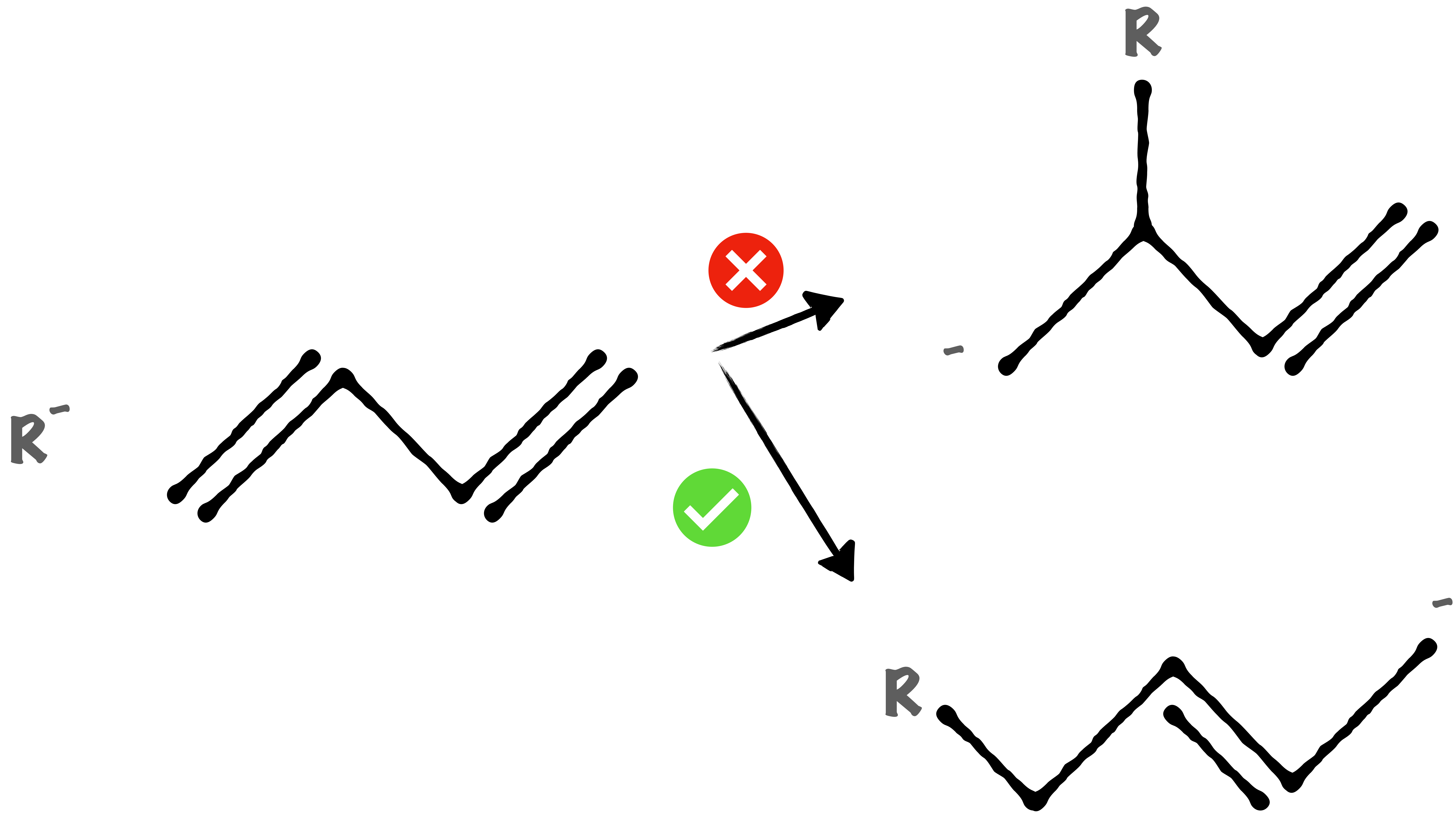
Standard methods
UCCSD
k–UpCCGSD
...

Adaptive Methods
ADAPT–VQE
Qubit–Coupled–Cluster
Imaginary Time Evolution
...

High–Level–Design
Now....

High–Level Design


R⁻
R
R

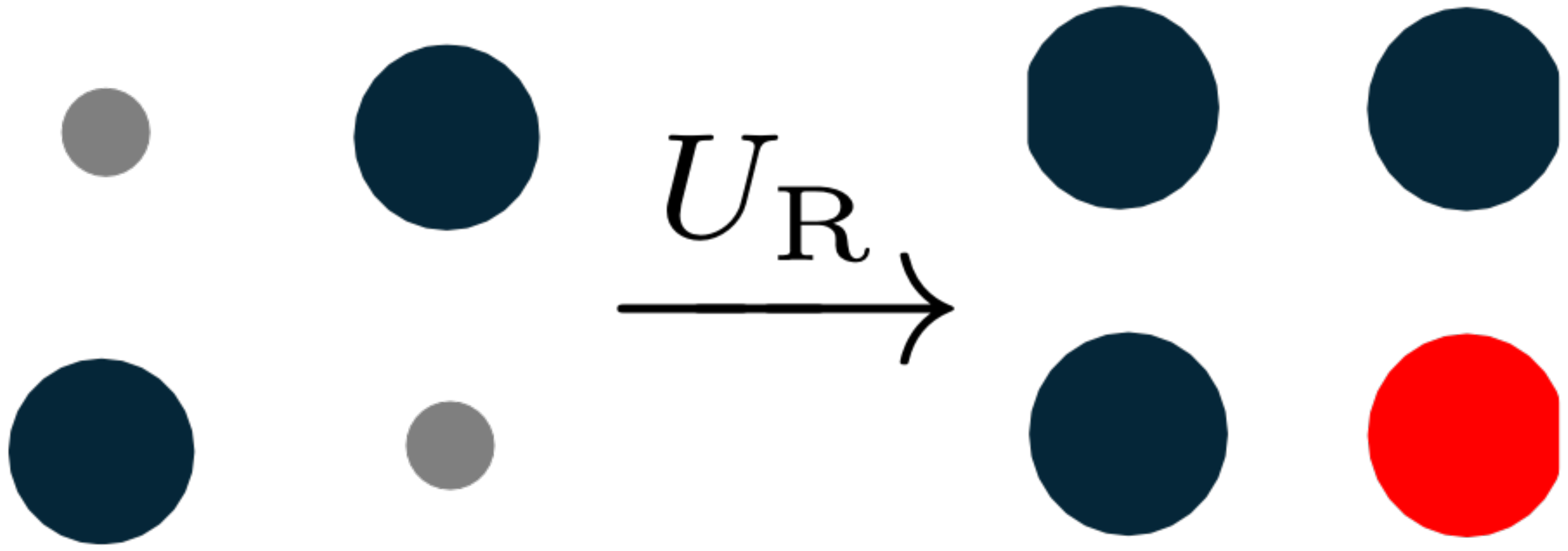


Example: Hydrogen Molecule

Simple system: 2-Electrons

Atomic orbital basis

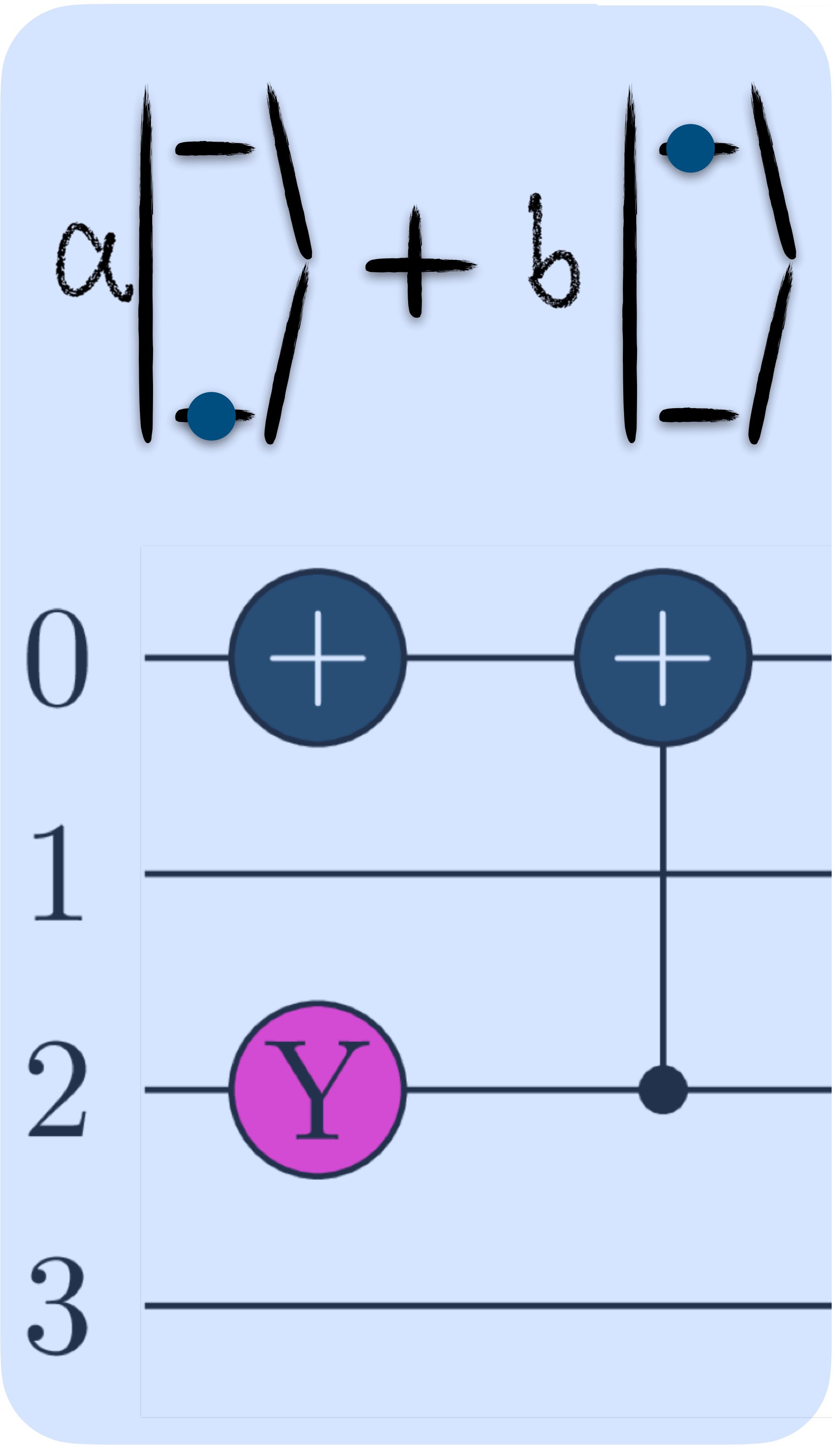
e.g. STO–3G basis set



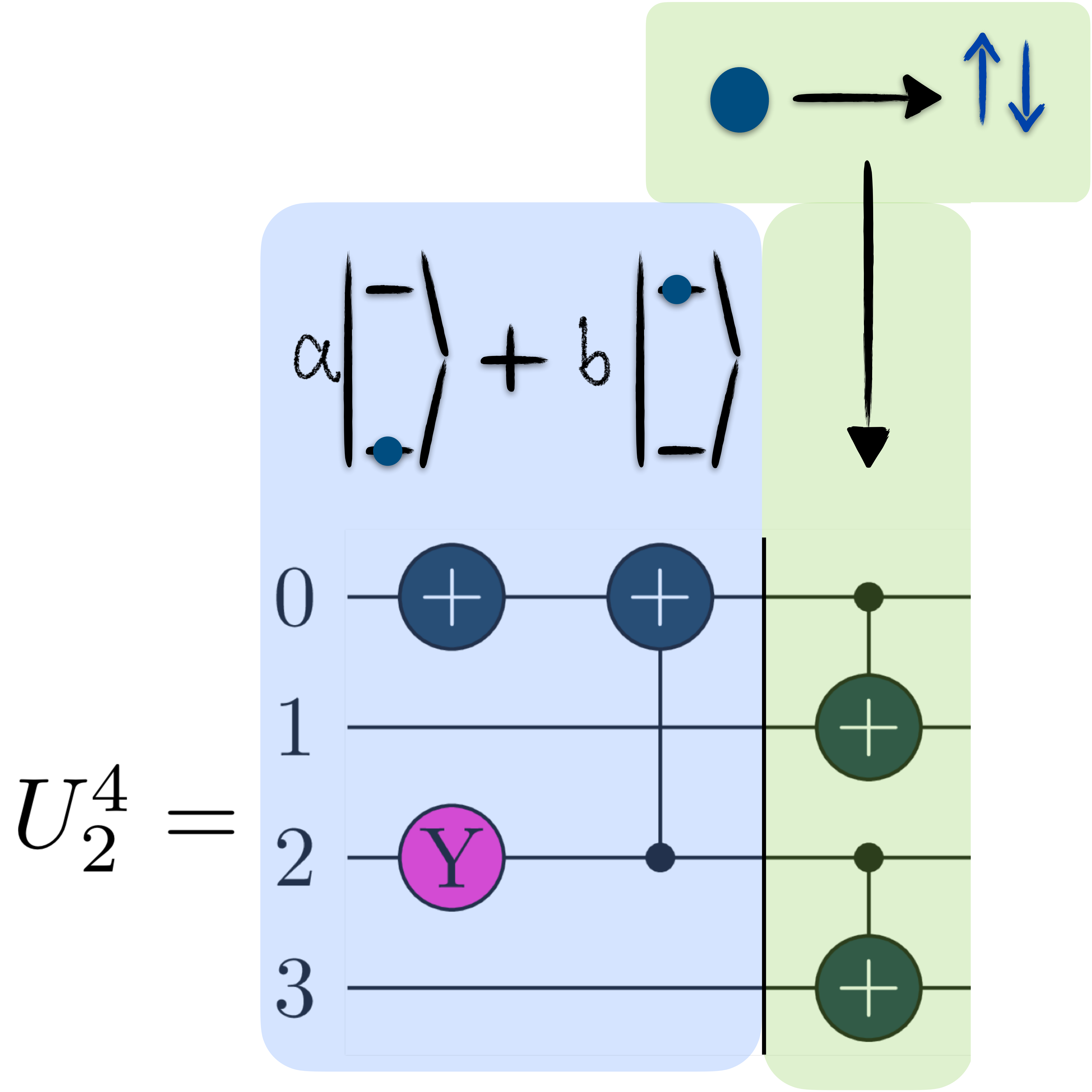
Molecular orbital basis

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

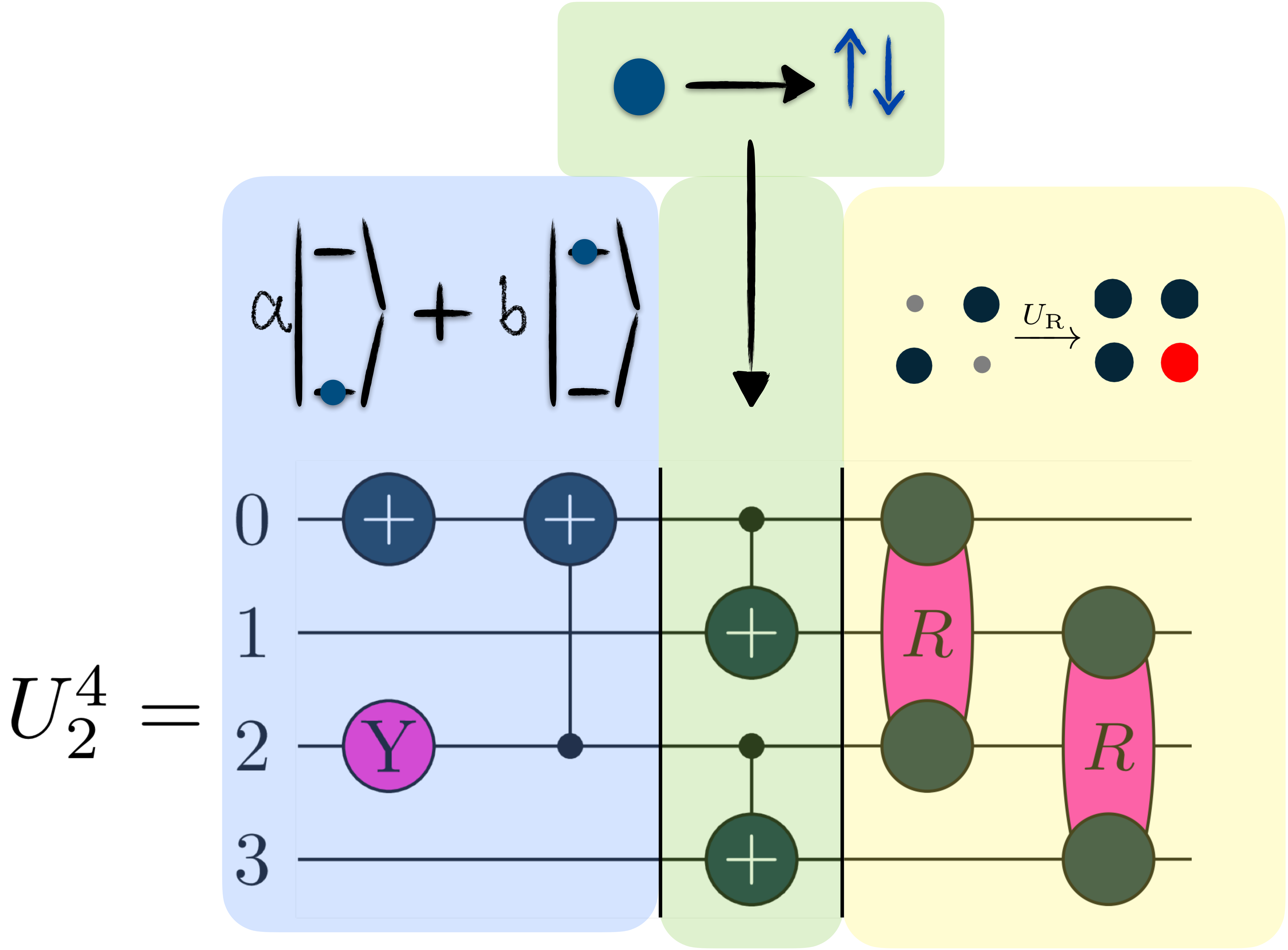
$$U_2^4 =$$



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

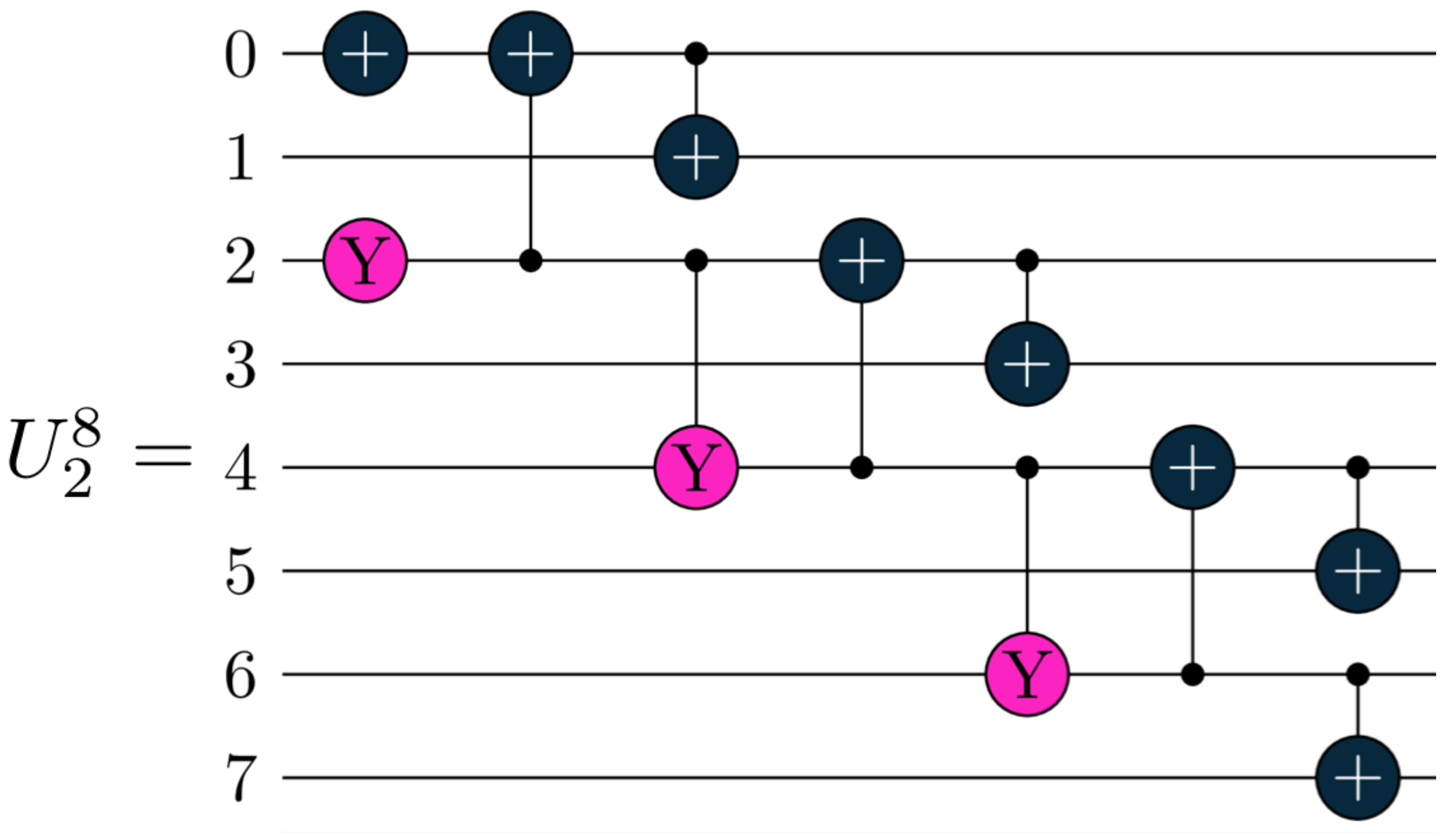


Simple system: 2-electrons in 2 orbitals (4 qubits)



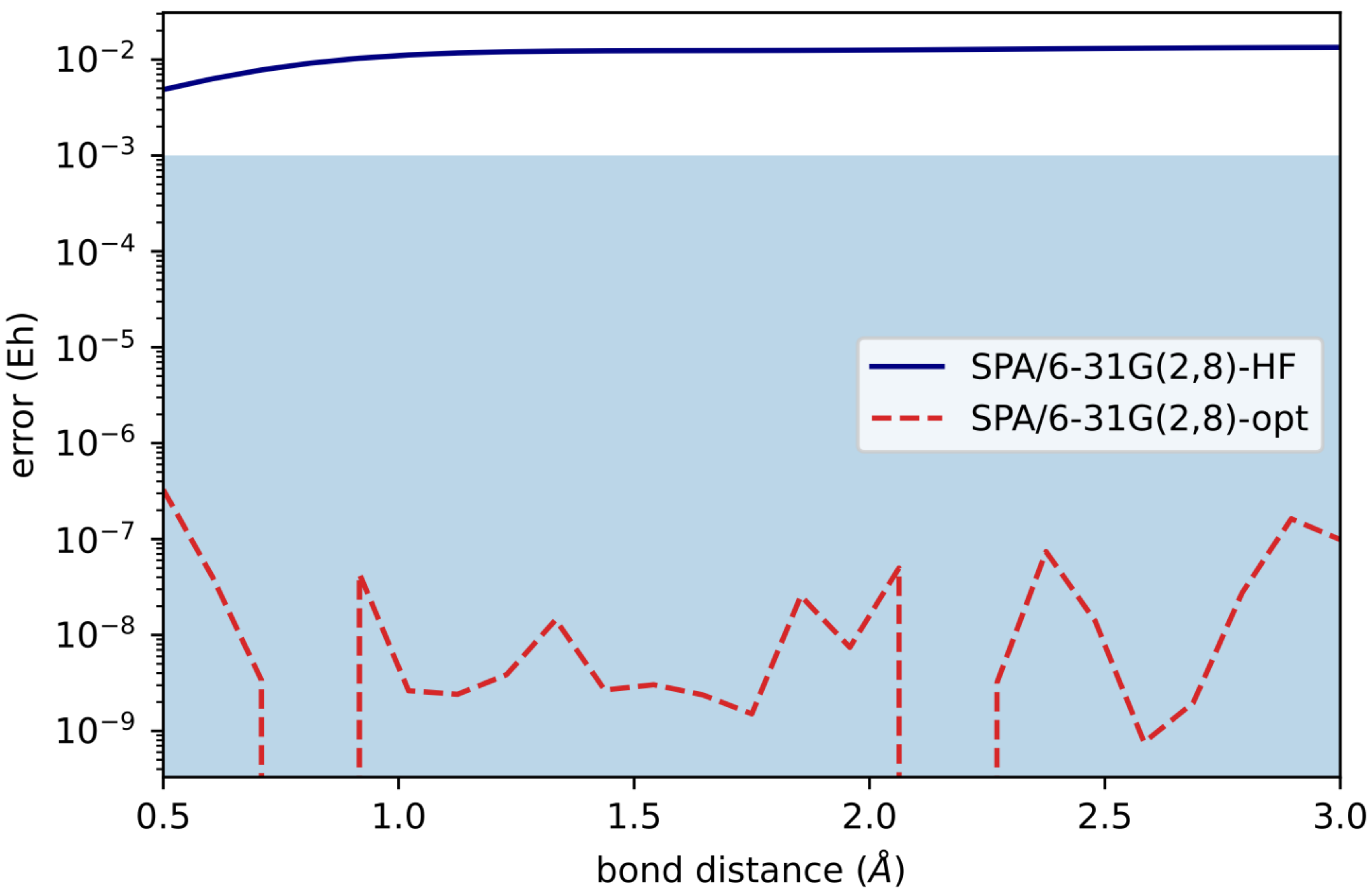
Orbital rotation can be absorbed into the Hamiltonian

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



Larger basis (8 qubits)

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

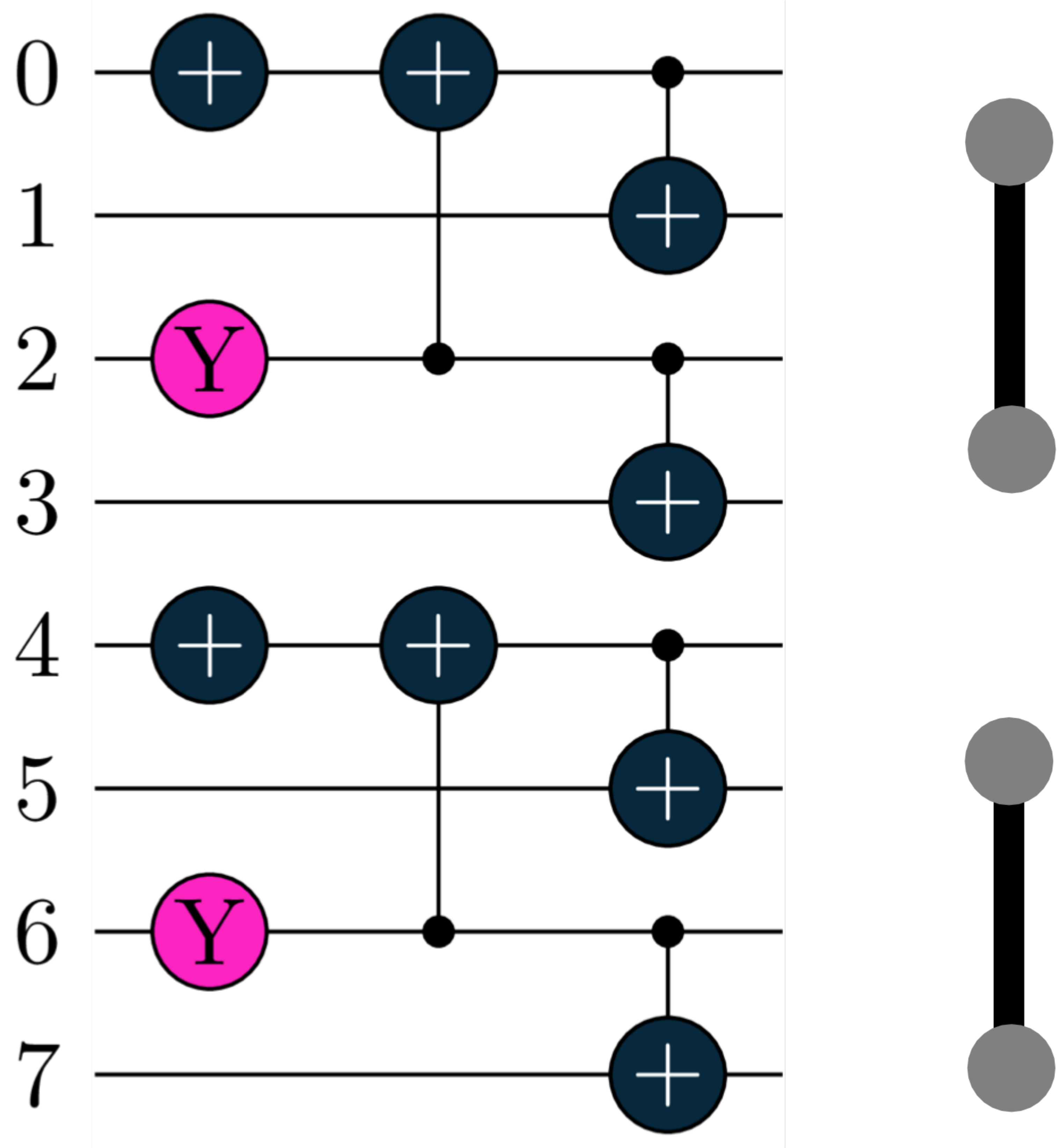


H4 Molecule

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

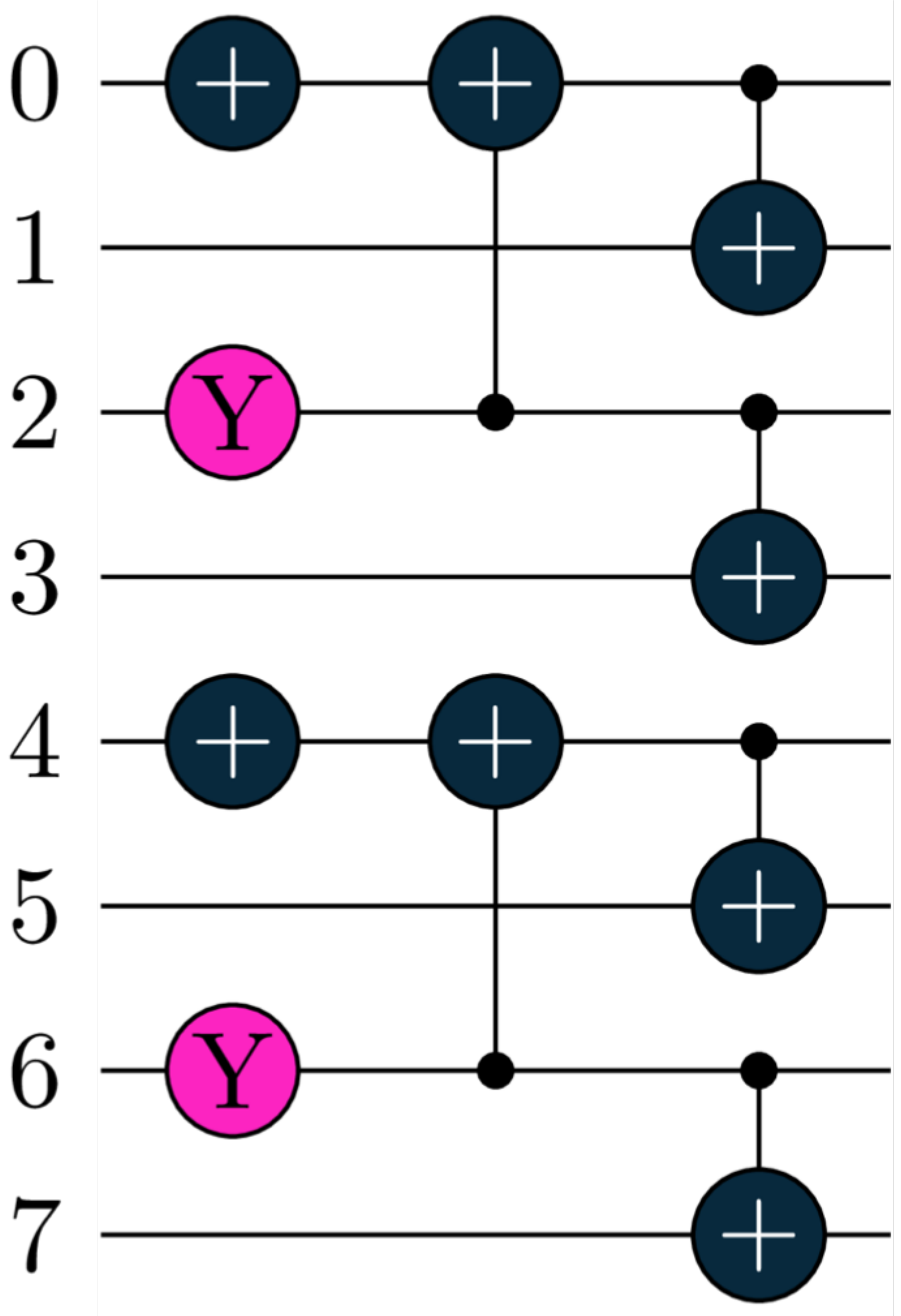
SPA: Separable Pair Ansatz

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



SPA: Separable Pair Ansatz

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



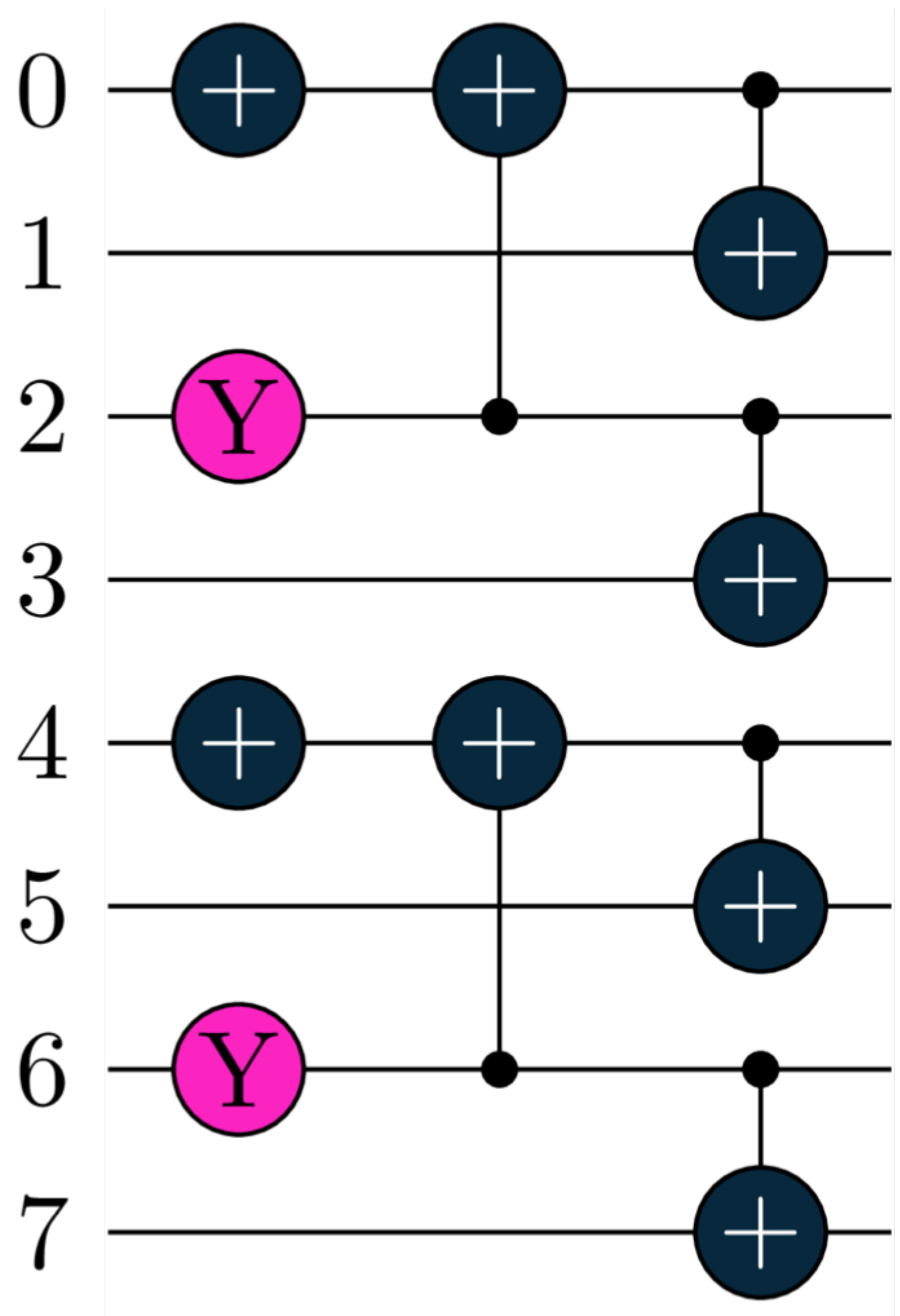
- Locality (circuit connections)
- Shallow depth
- Parallelizable
- Hardware efficient
- Classically tractable wavefunction

becomes a classical pre-compilation step

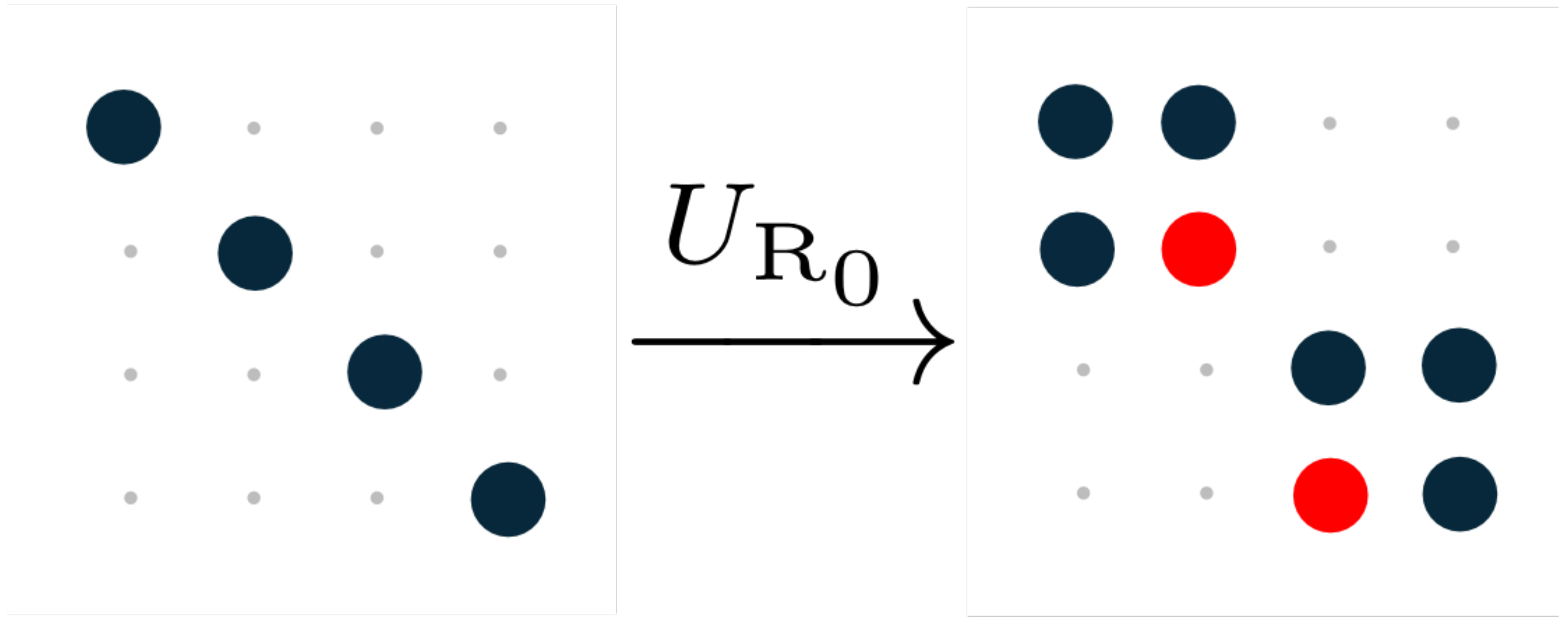
Hartree–Fock error: 167 mEH

SPA: Separable Pair Ansatz

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



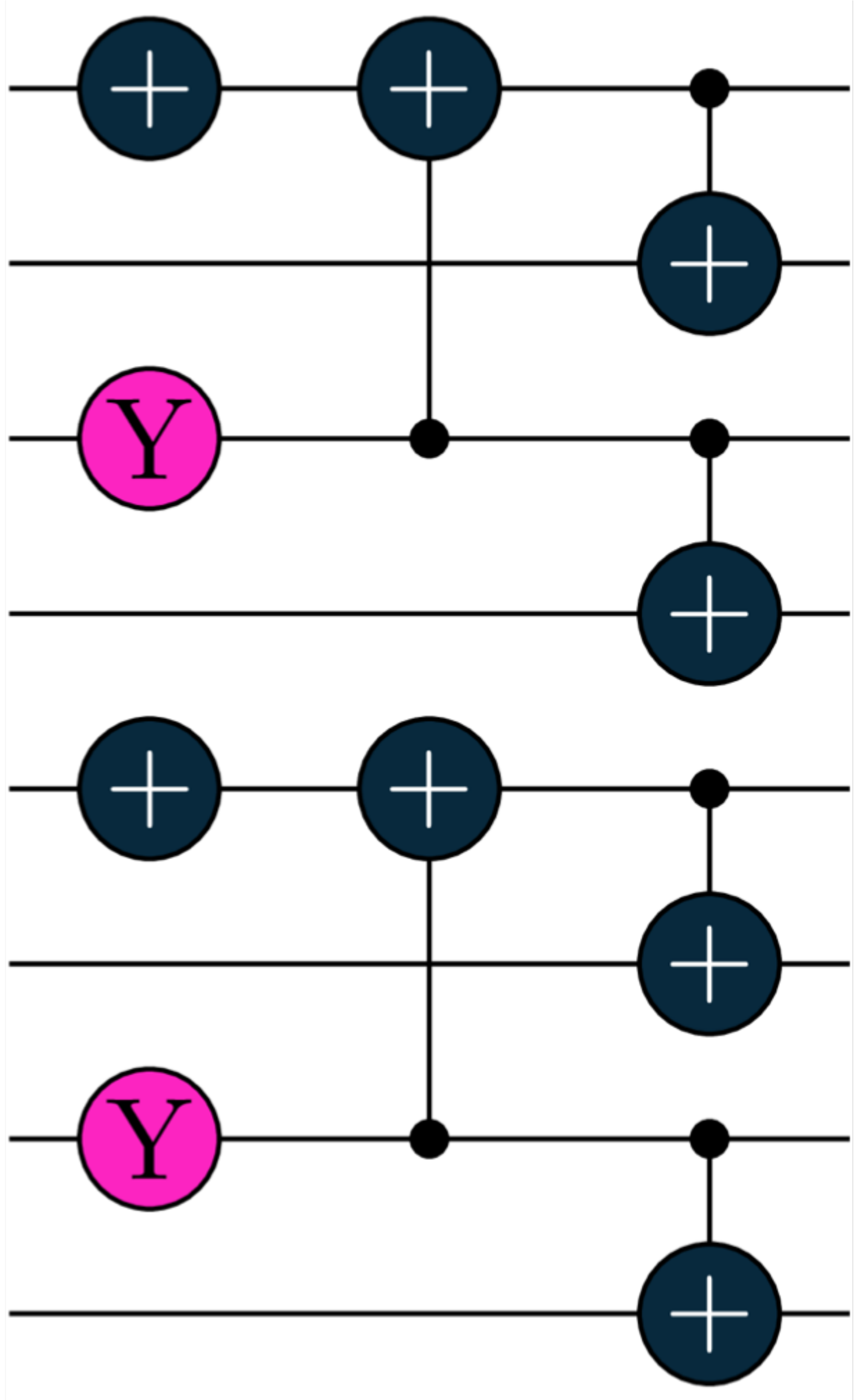
Guess orbitals:
error of 40 mEh



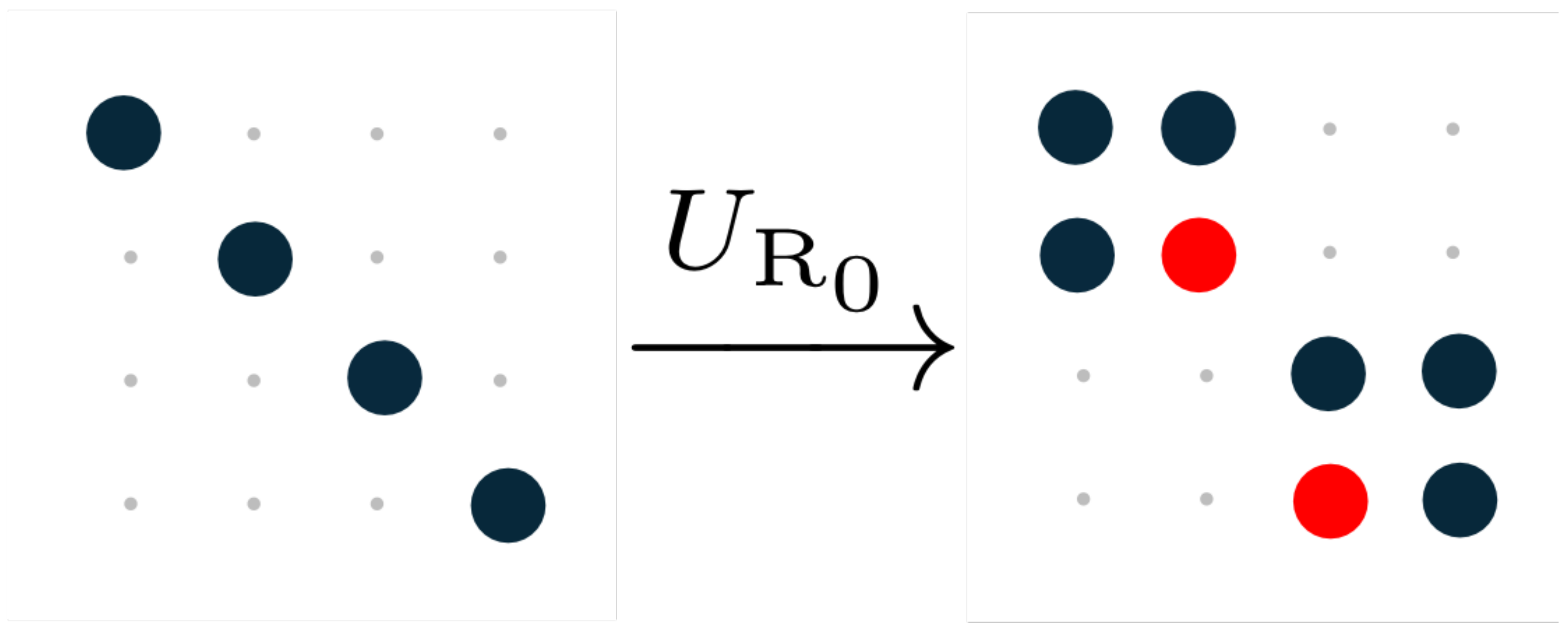
Hartree–Fock error: 167 mEH

SPA: Separable Pair Ansatz

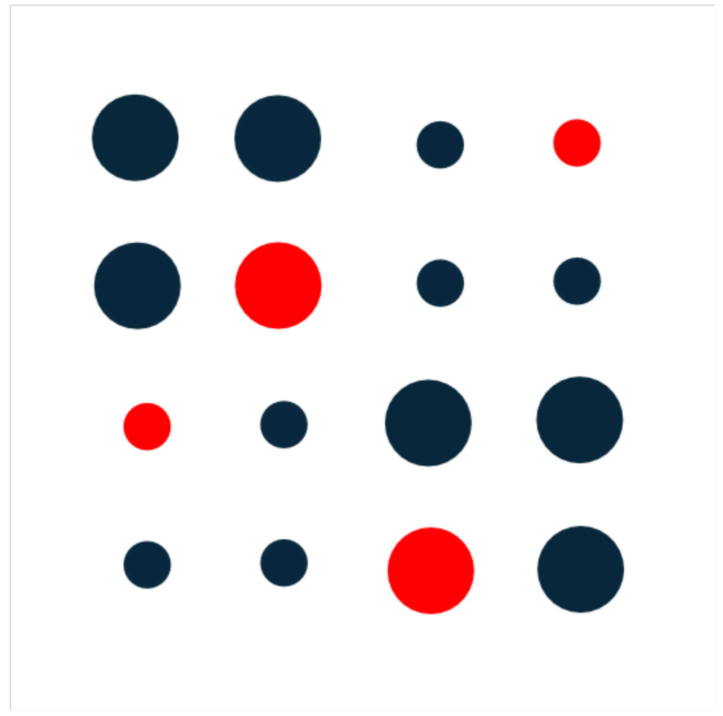
$$U_{\mathrm{SPA}}^{(4,8)} = U_2^4 \otimes U_2^4 =$$



Guess orbitals:
error of 40 mEh



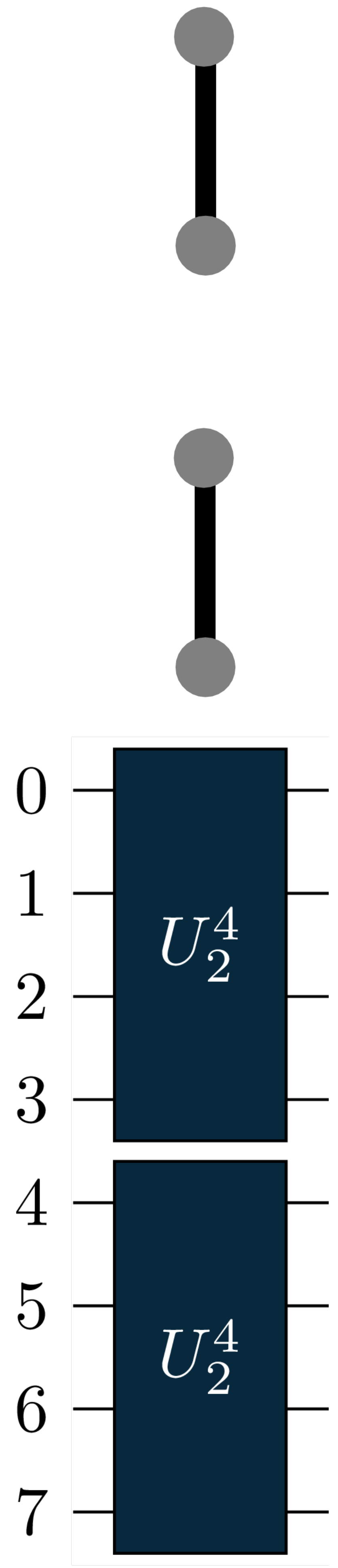
Optimal orbitals:
error of 16 mEh



Alternative Graph

Hartree–Fock error: 167 mEH

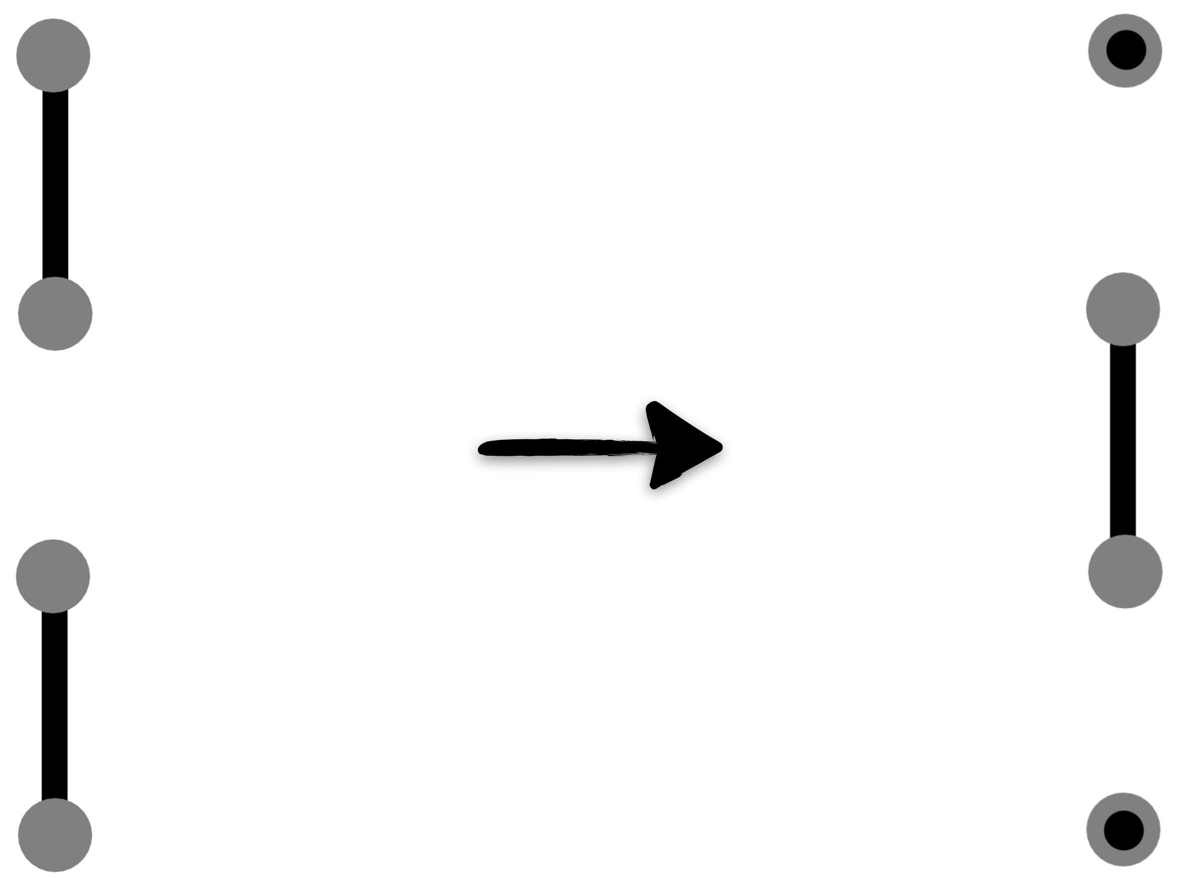
method	error	F	N_{v}	cnots	depth	iter
SPA	16	94	2	6	3	17*

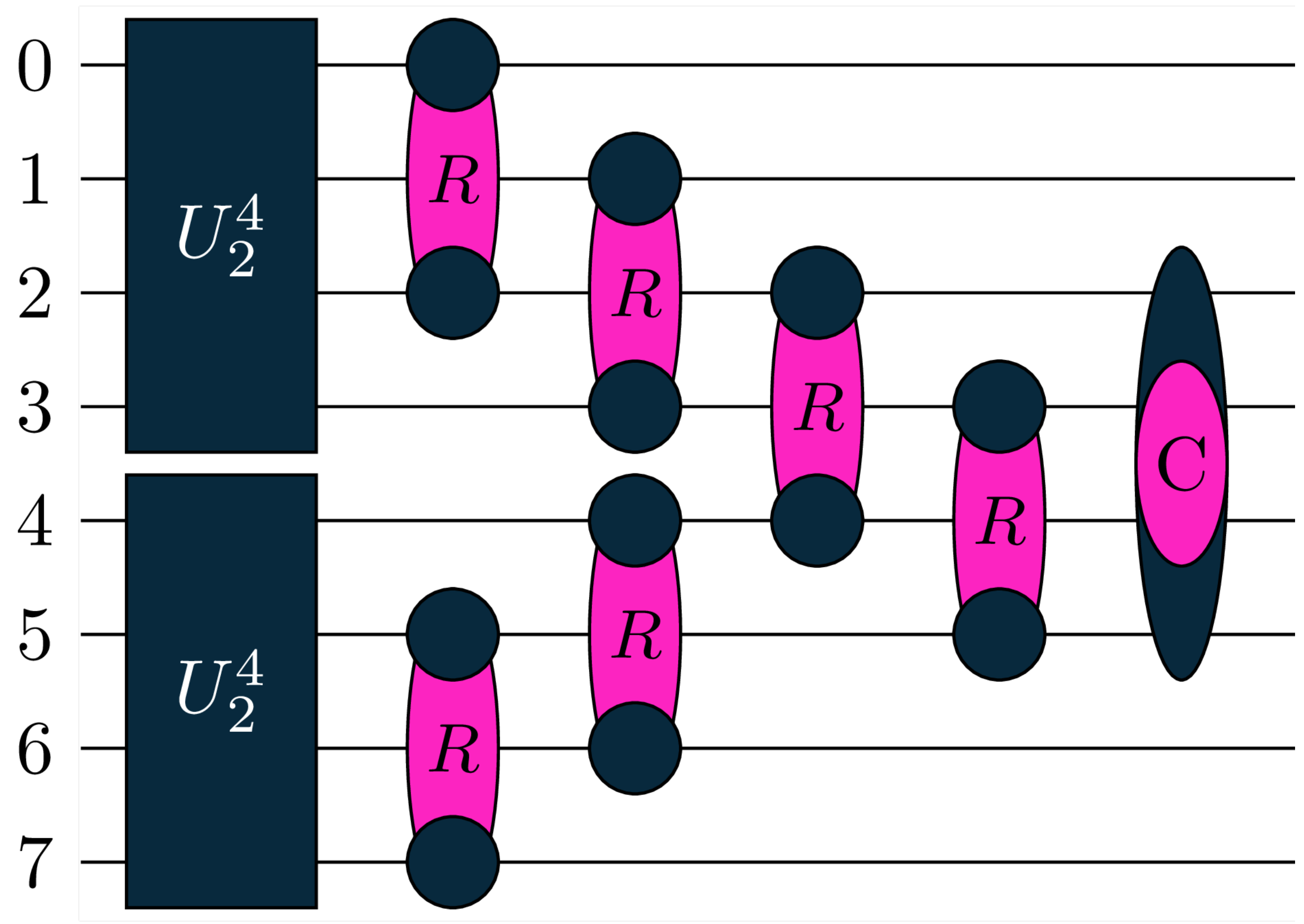


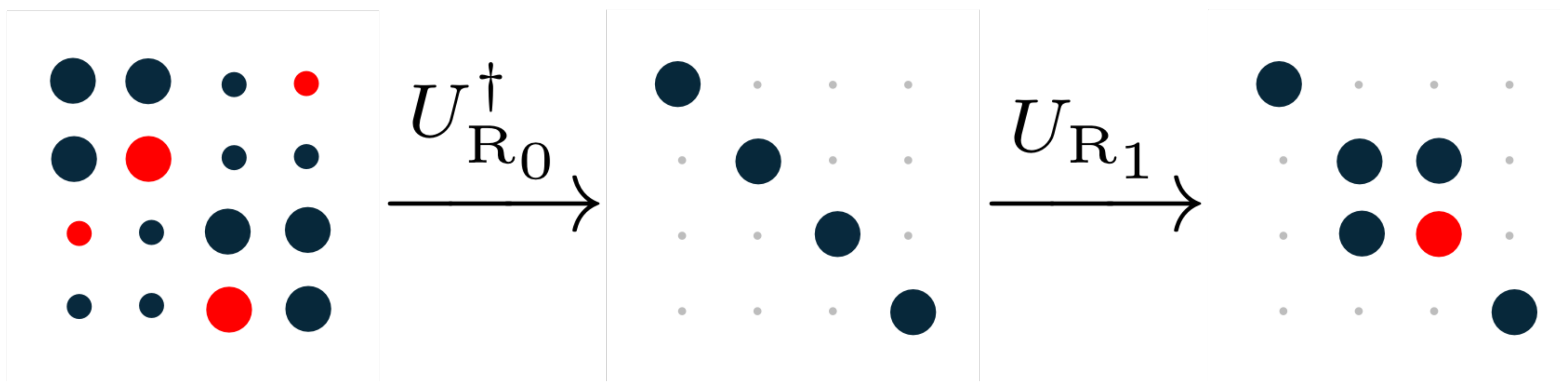
h4.py

Hartree–Fock error: 167 mEH

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

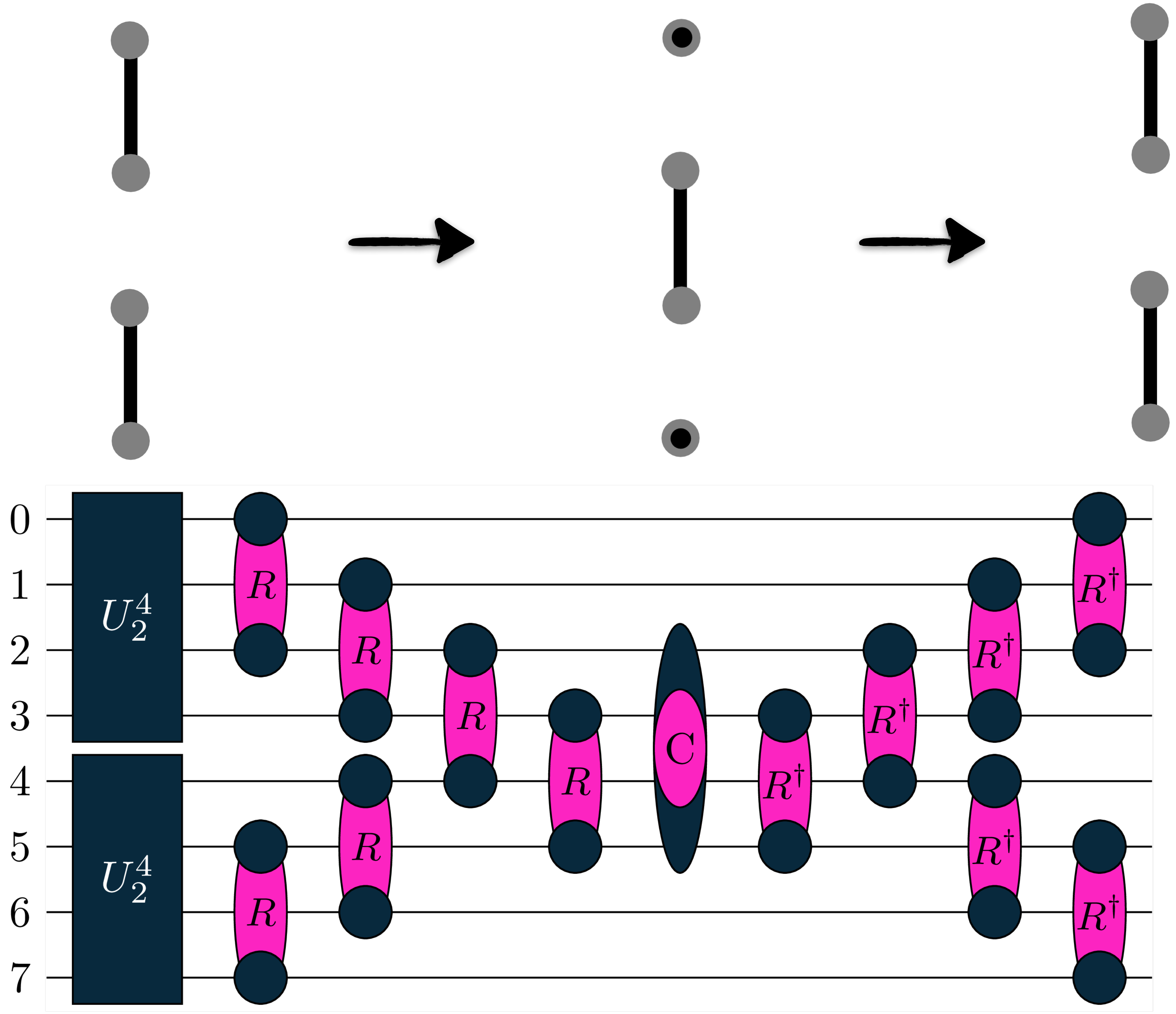






h4.py

Hartree–Fock error: 167 mEH

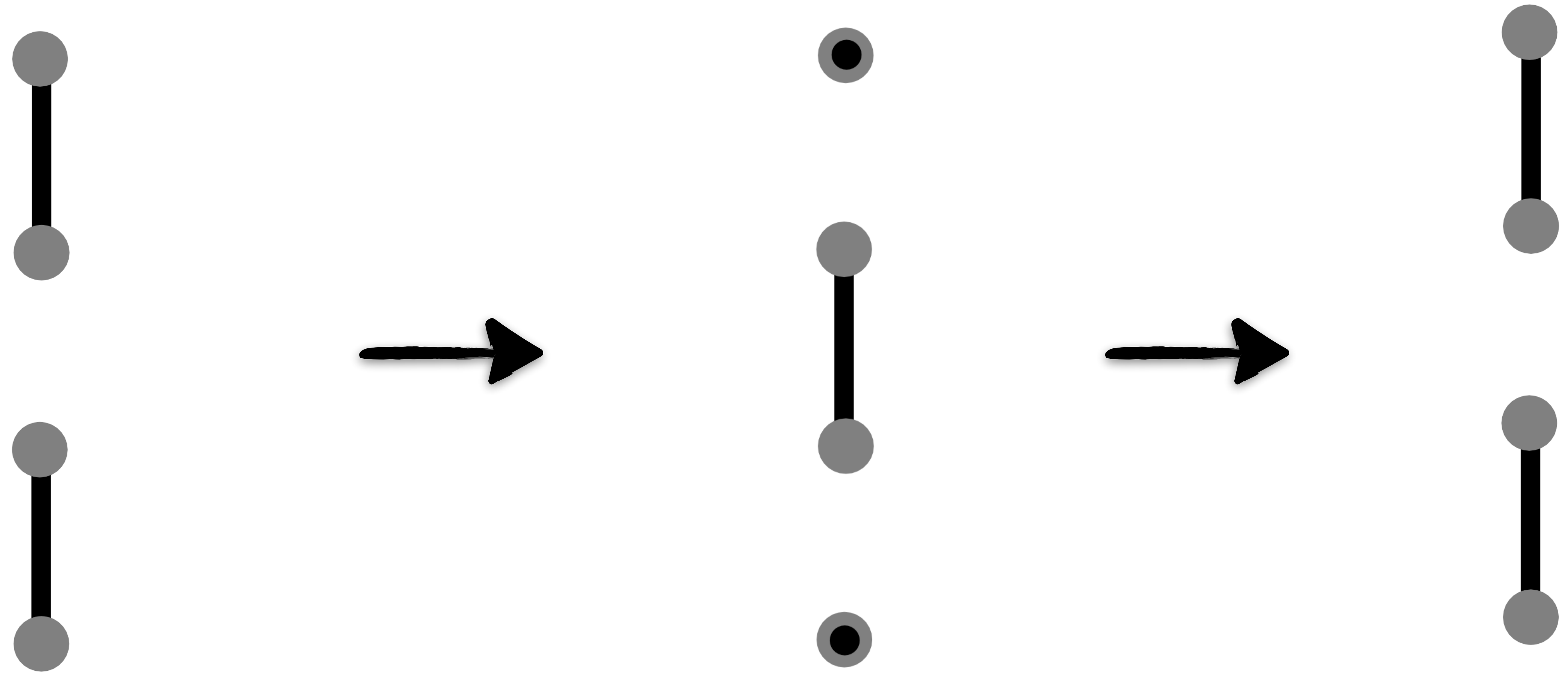


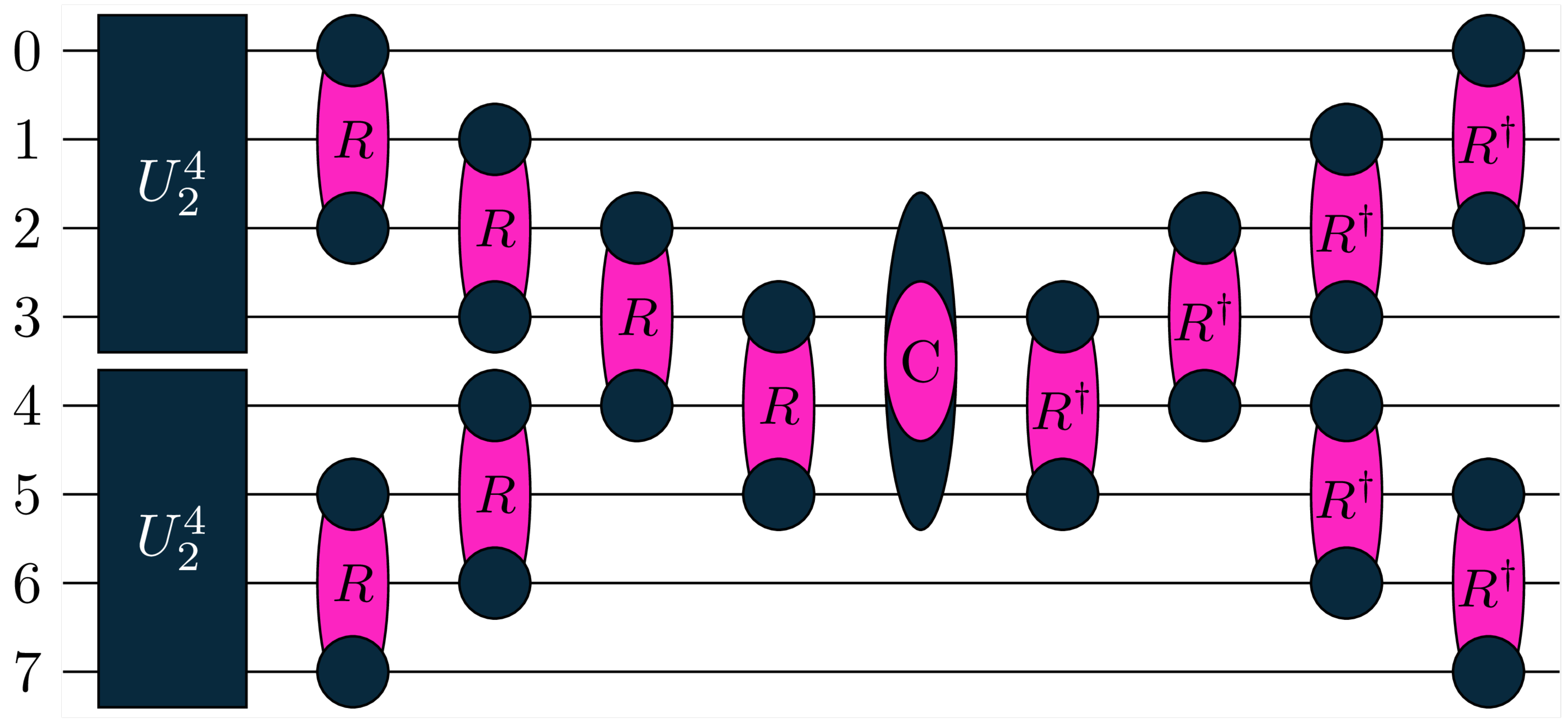
method	error	F	N_{v}	cnots	depth	iter
SPA	16	94	2	6	3	17*
SPA+	8	96	6	116	131	10

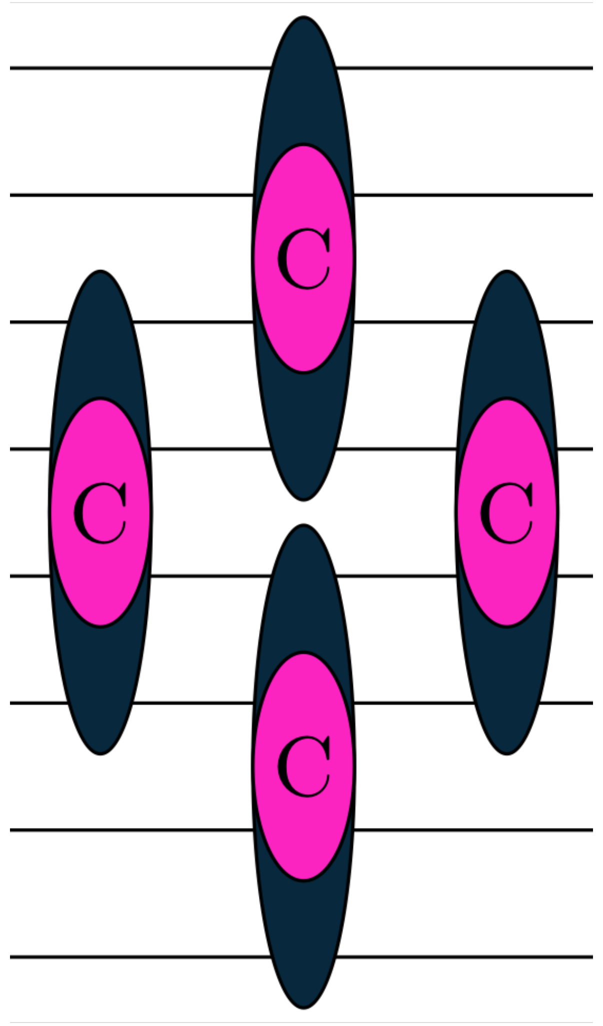
h4.py

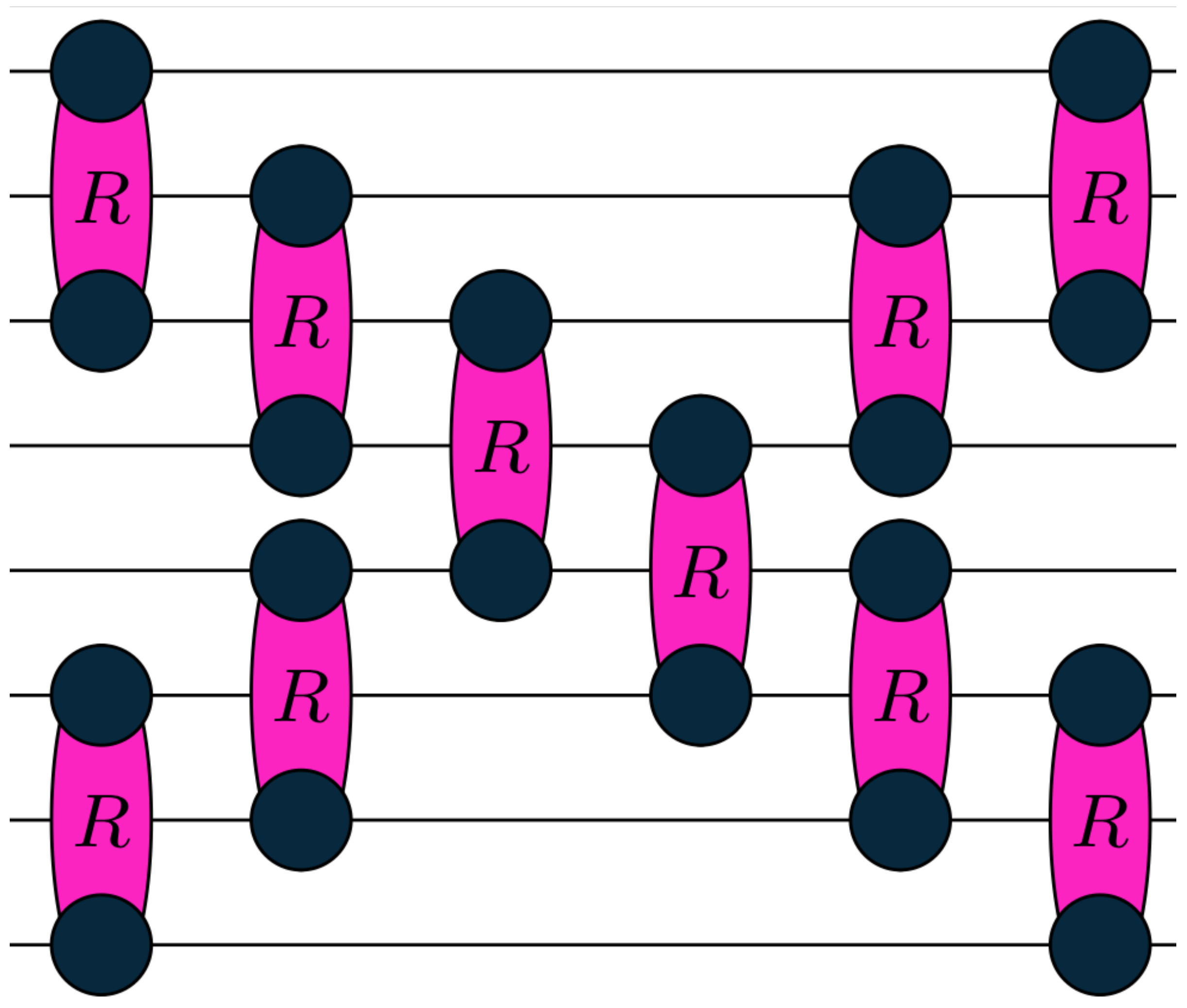
Hartree–Fock error: 167 mEH

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

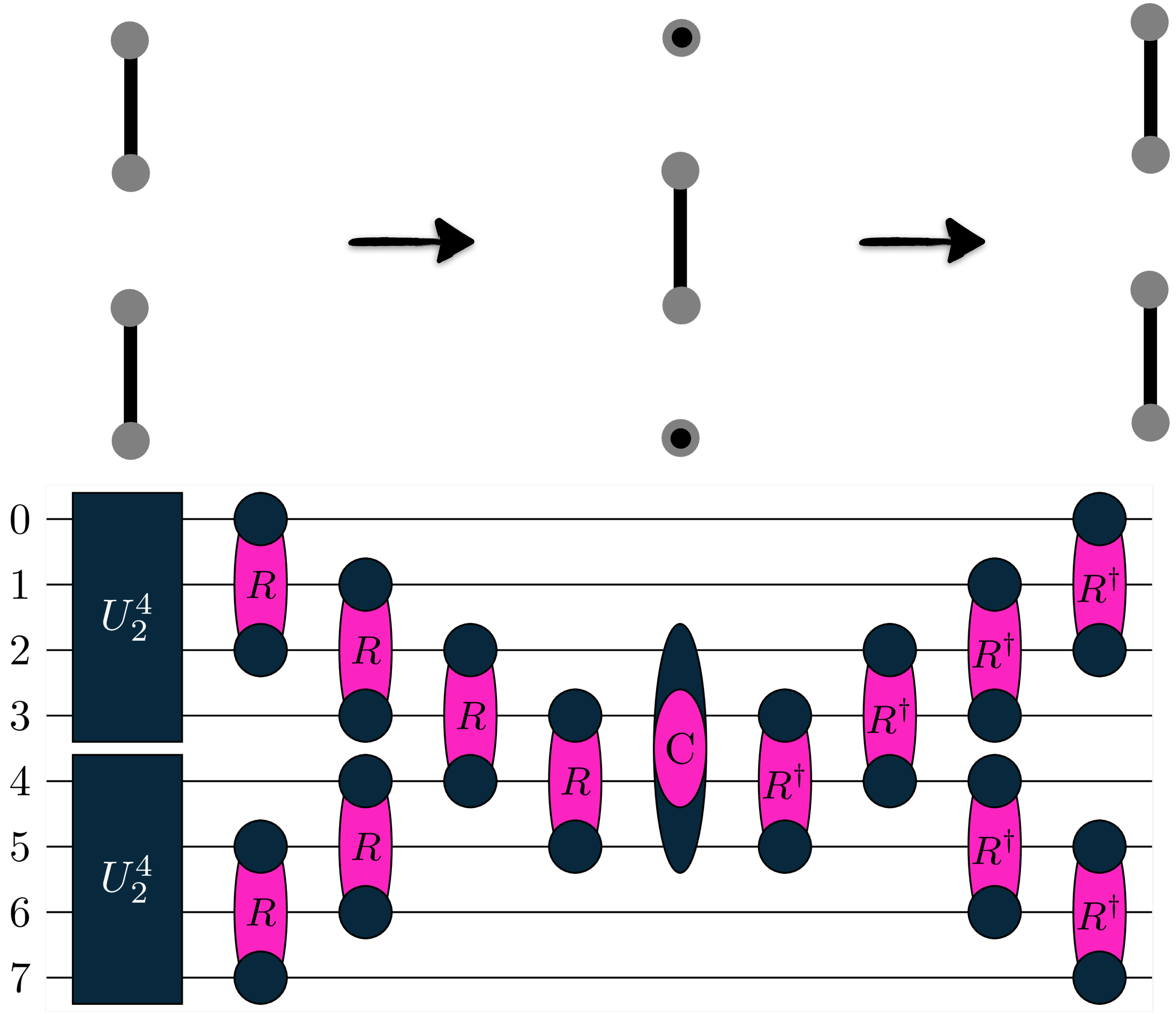








Hartree–Fock error: 167 mEH



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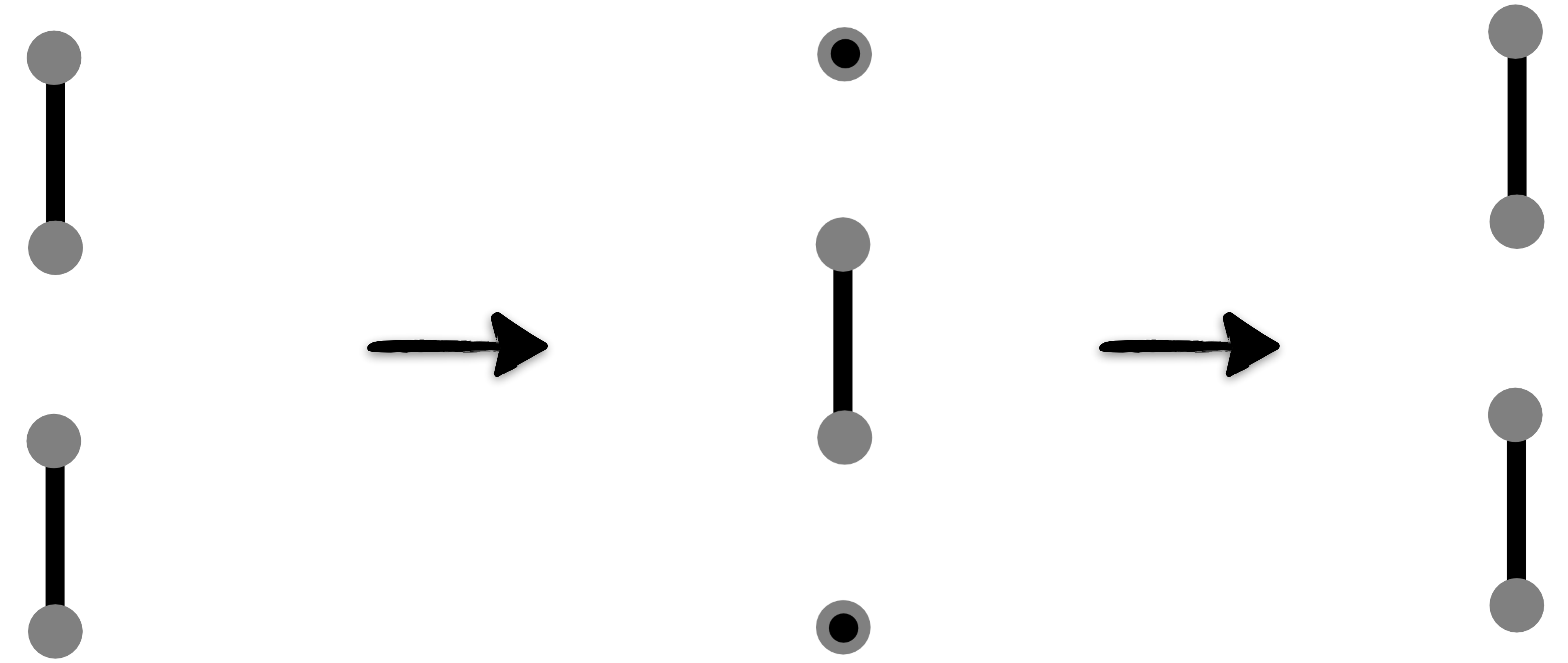
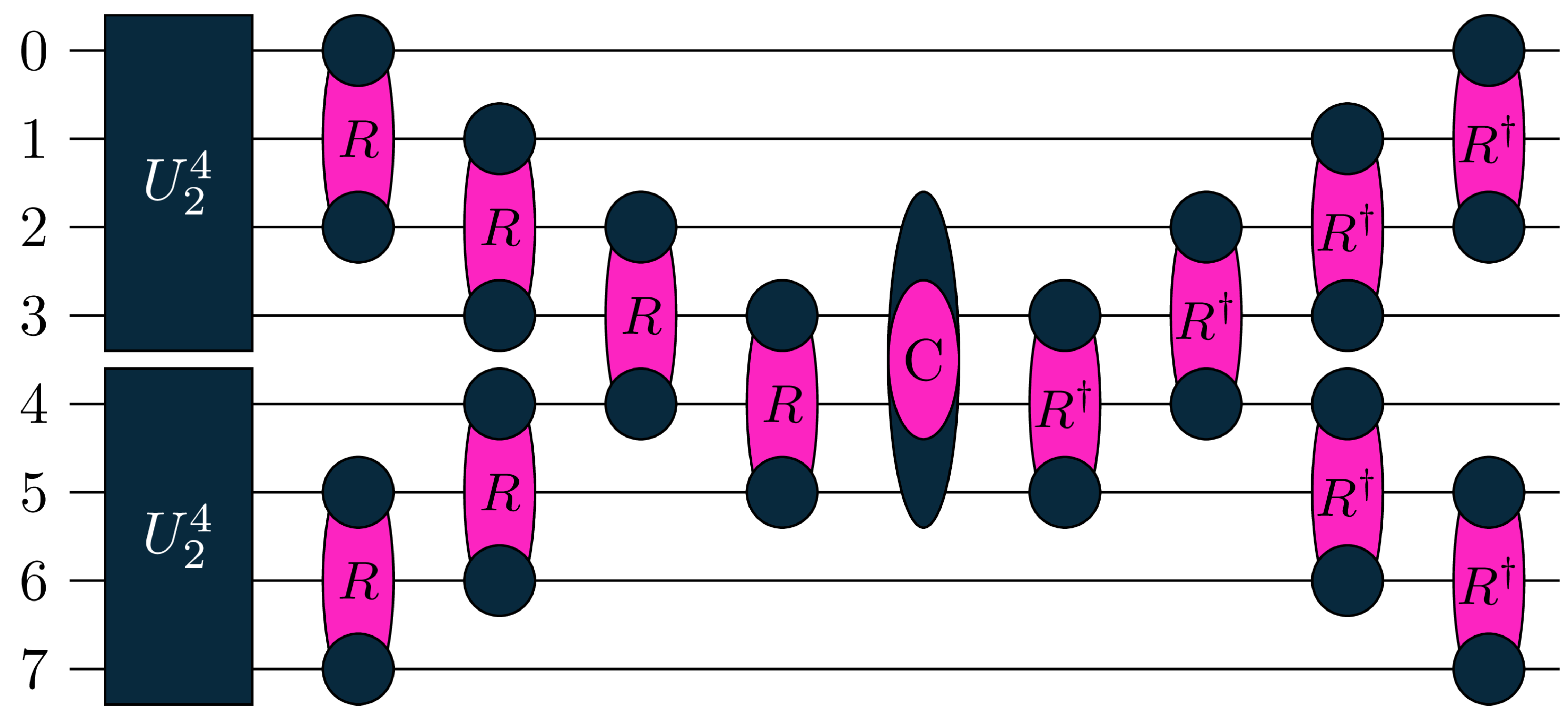
SPA+CRRCRRC	0	100	19	334	367	160
UpCCD	103	88	4	20	26	8
UpCCSD	86	74	12	148	193	13
UpCCGSD	86	74	18	188	254	13
2-UpCCGSD	32	90	36	432	540	48

Hartree–Fock error: 167 mEH





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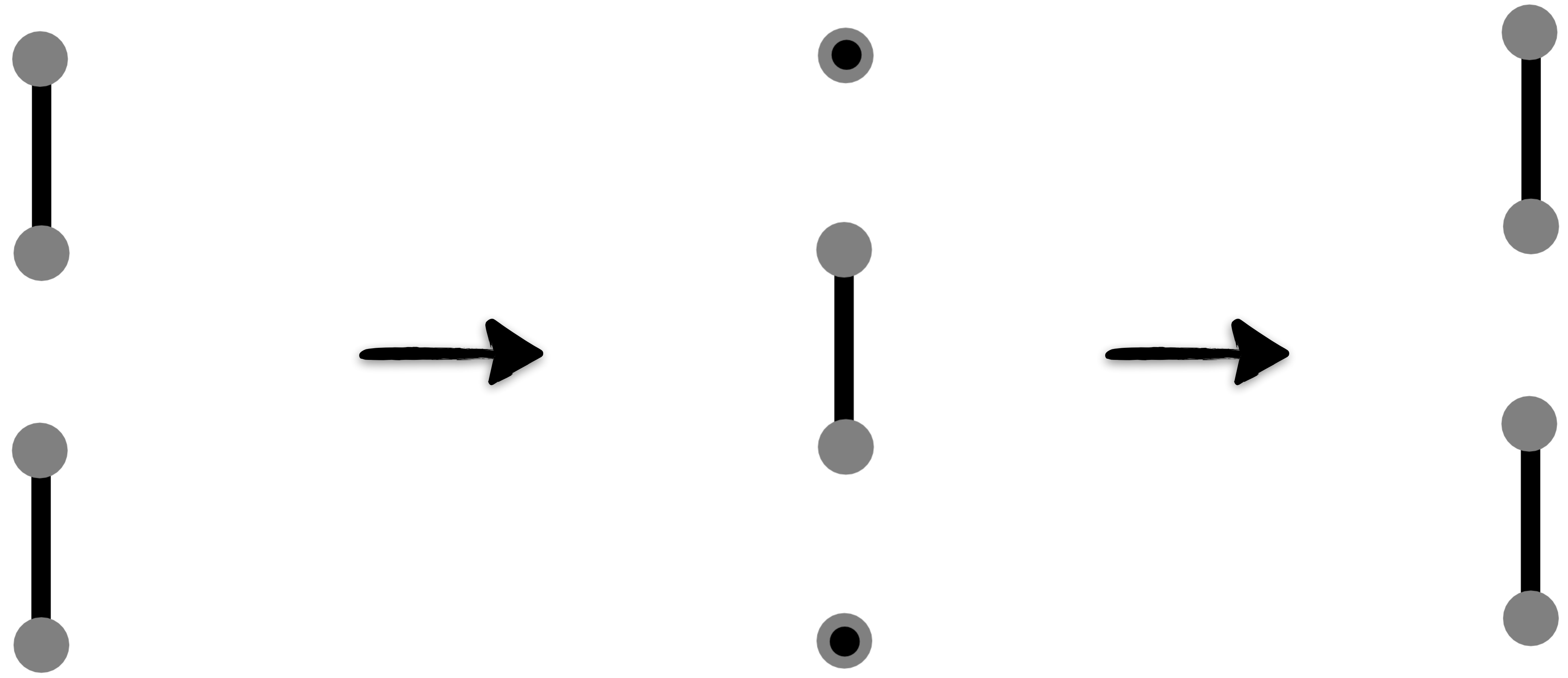
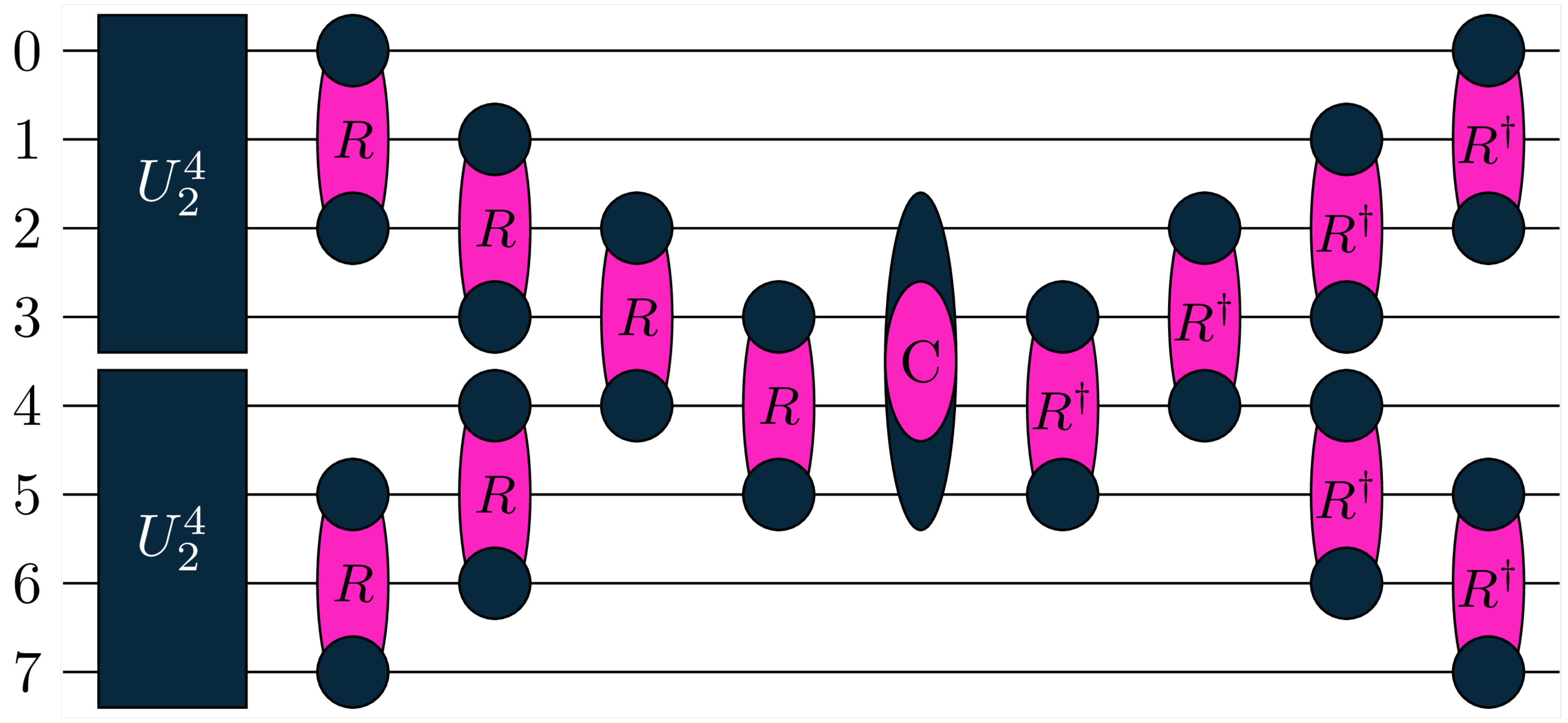
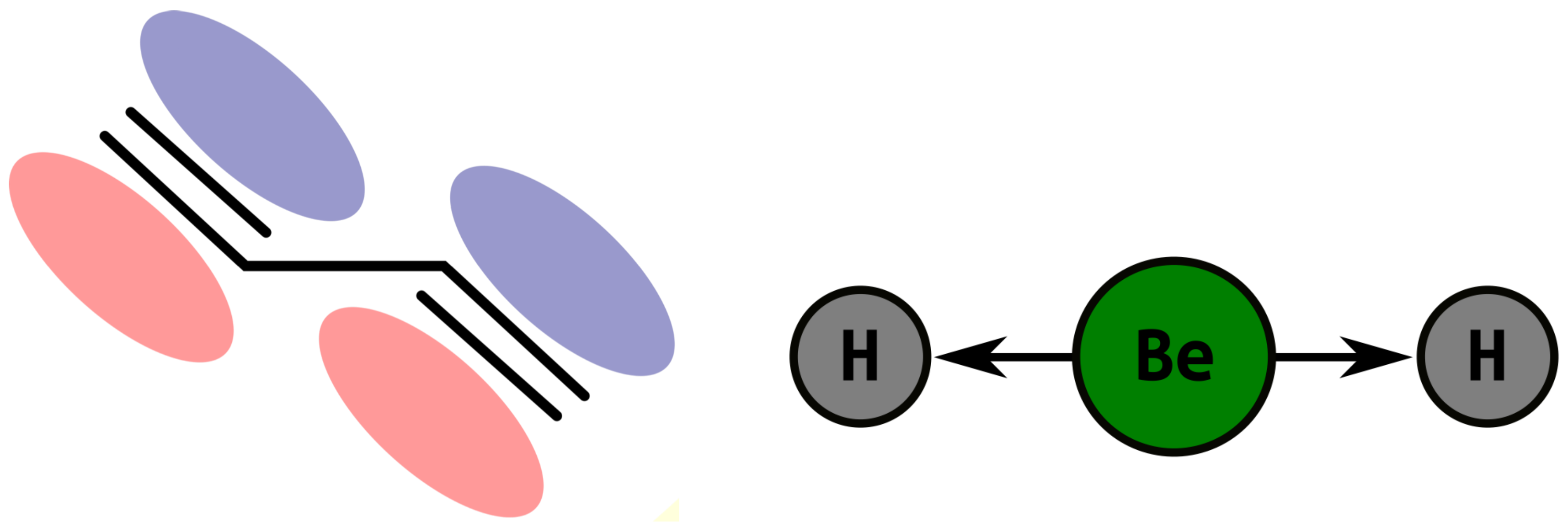
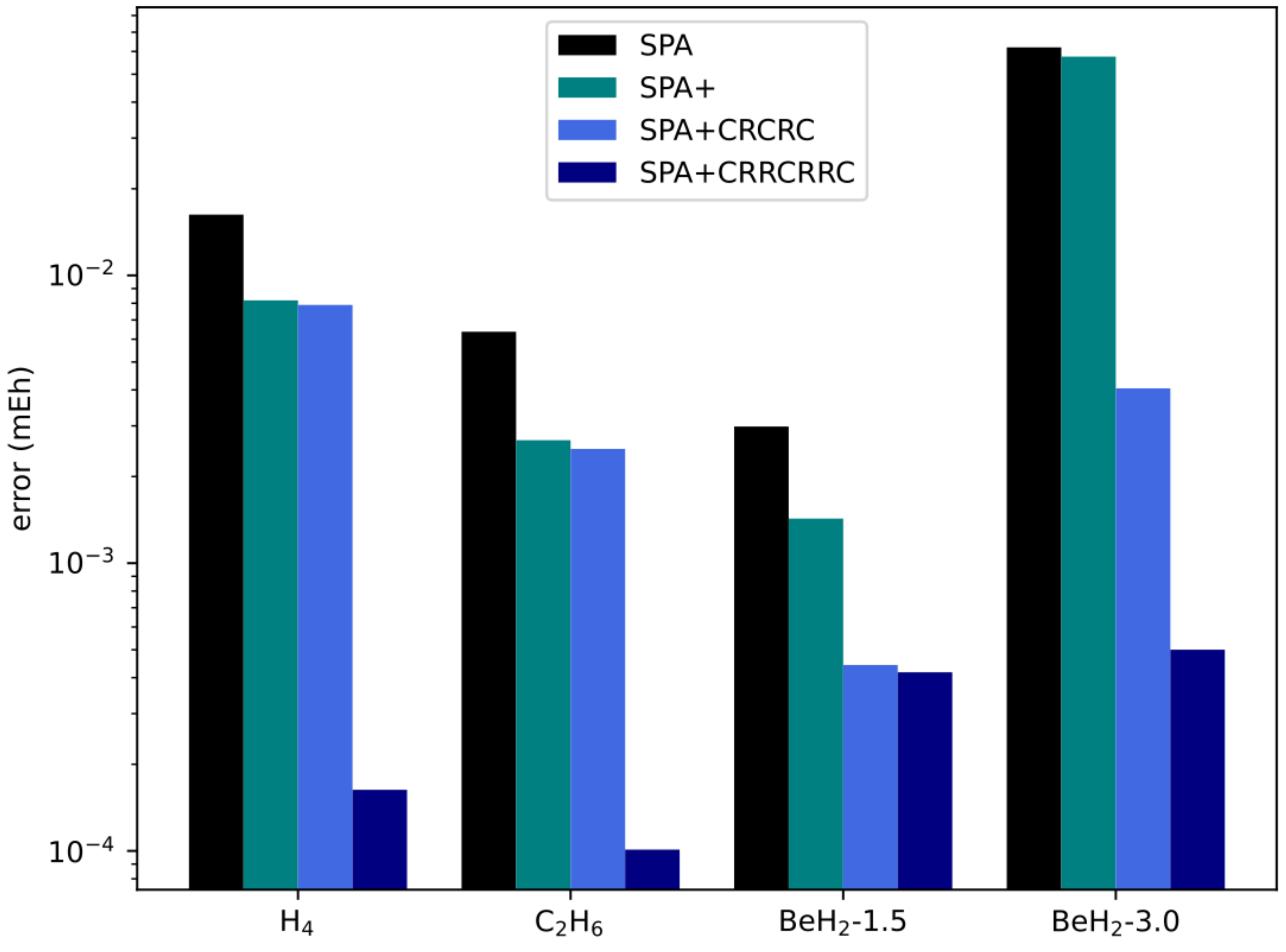
UpCCSD	86	74	12	148	193	13
UpCCGSD	86	74	18	188	254	13
2-UpCCGSD	32	90	36	432	540	48
ADAPT(UpCCGSD)	32	90	12	448	442	113
ADAPT(UCCGSD)	0	100	21	1360	1705	58

Hartree–Fock error: 167 mEH

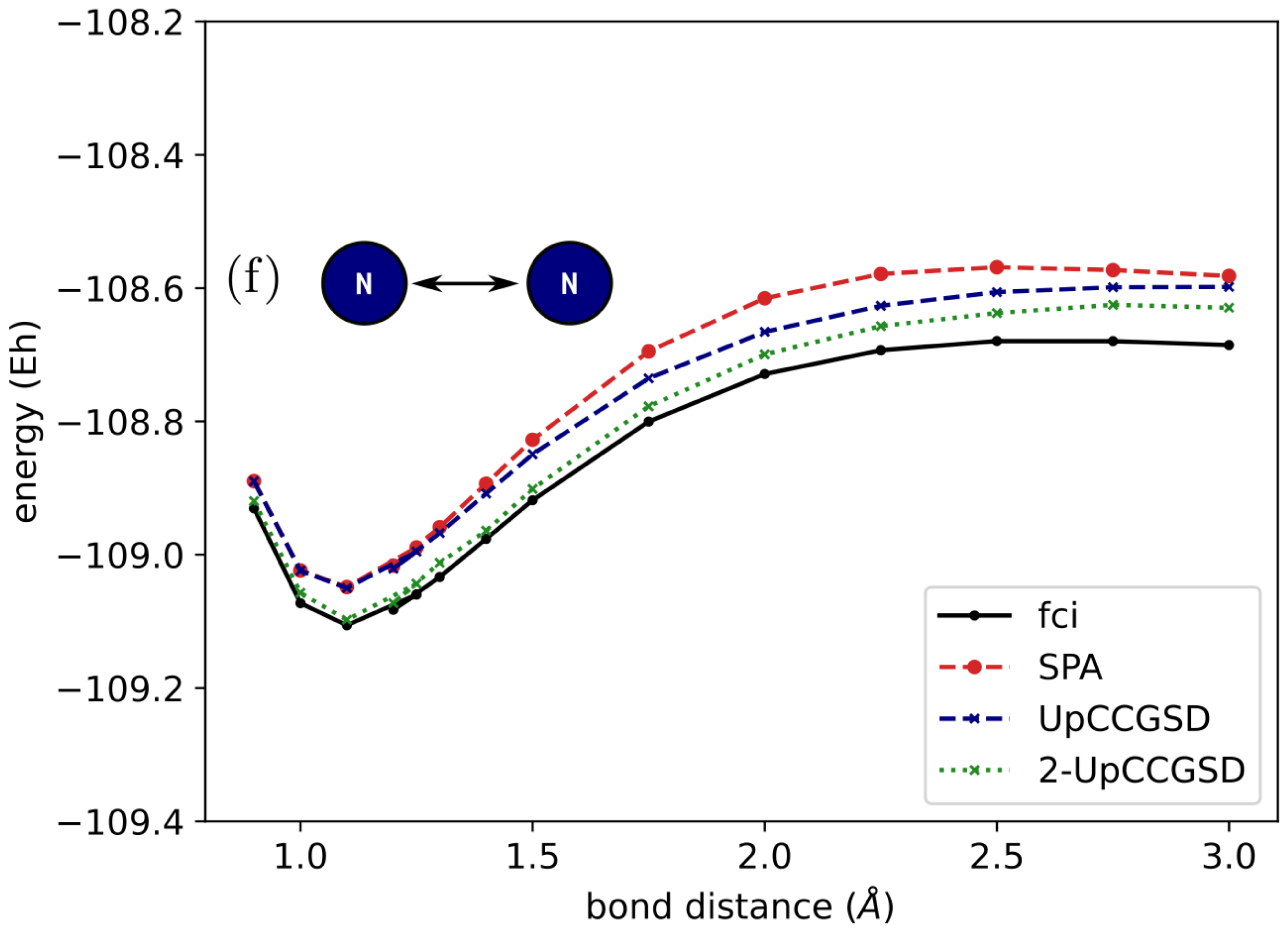








Limitations



- Well behaved SPA
- k-UpCCGSD curve picked from multiple runs with random starting points
- SPA from all-Zero starting point

- Improvement through other graphs not obvious
- Still a better initial state through SPA

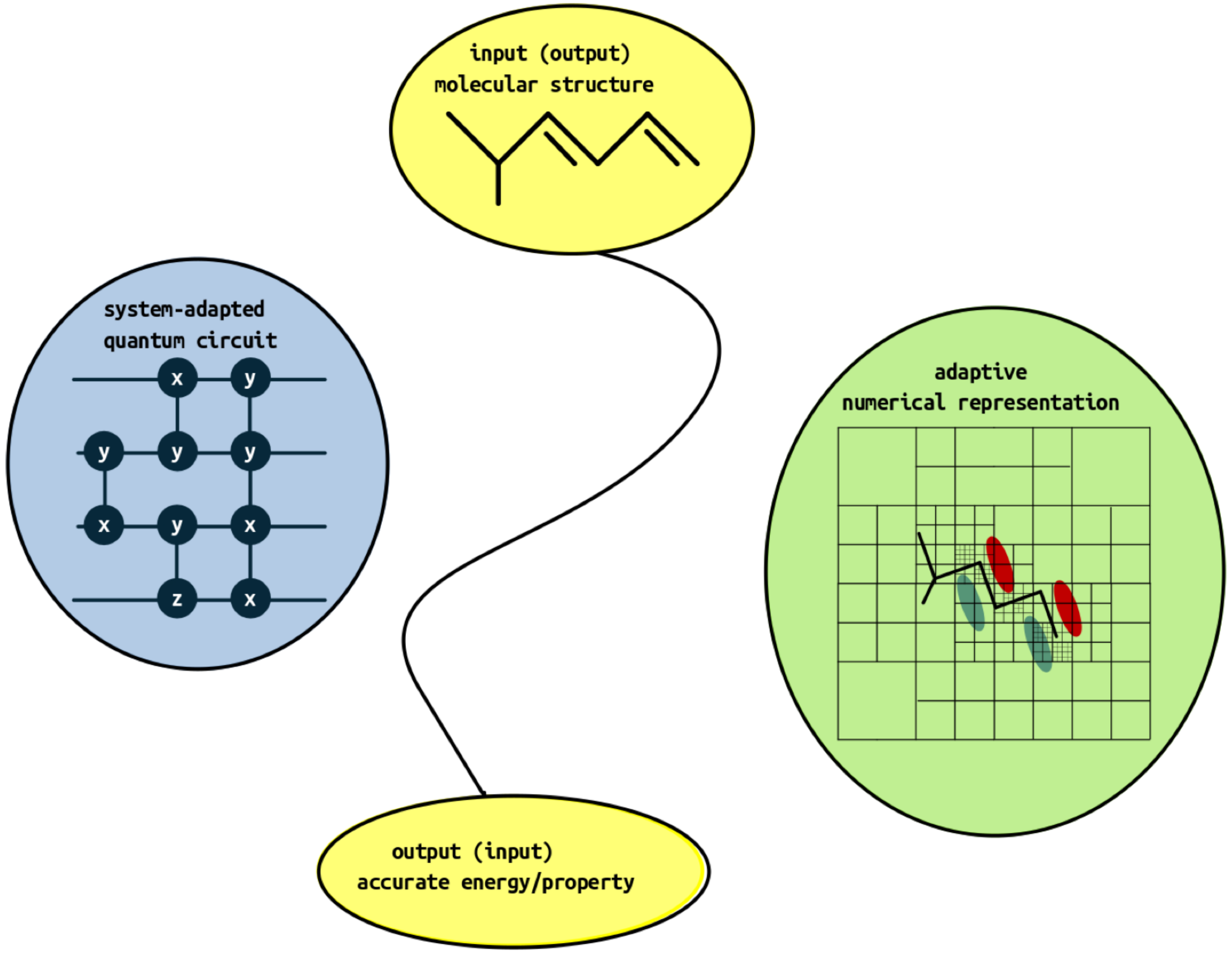
Automatisation

```
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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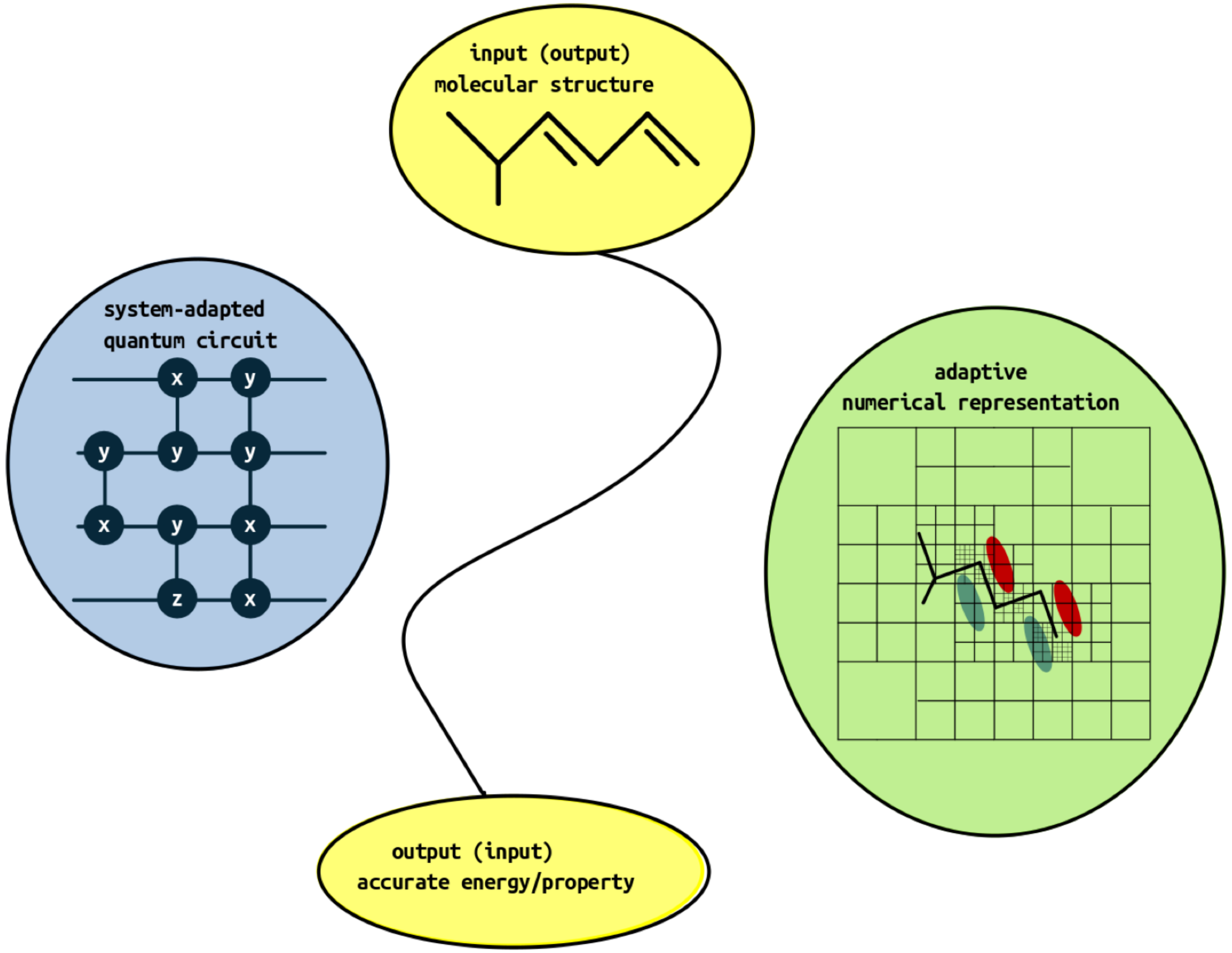

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Direct determination of optimal pair-natural orbitals in a real-space representation: The second-order Moller–Plesset energy

J. Chem. Phys. **152**, 074105 (2020); https://doi.org/10.1063/1.5141880

Jakob S. Kottmann[1,a], Florian A. Bischoff[1,b], and Edward F. Valeev[2,c]

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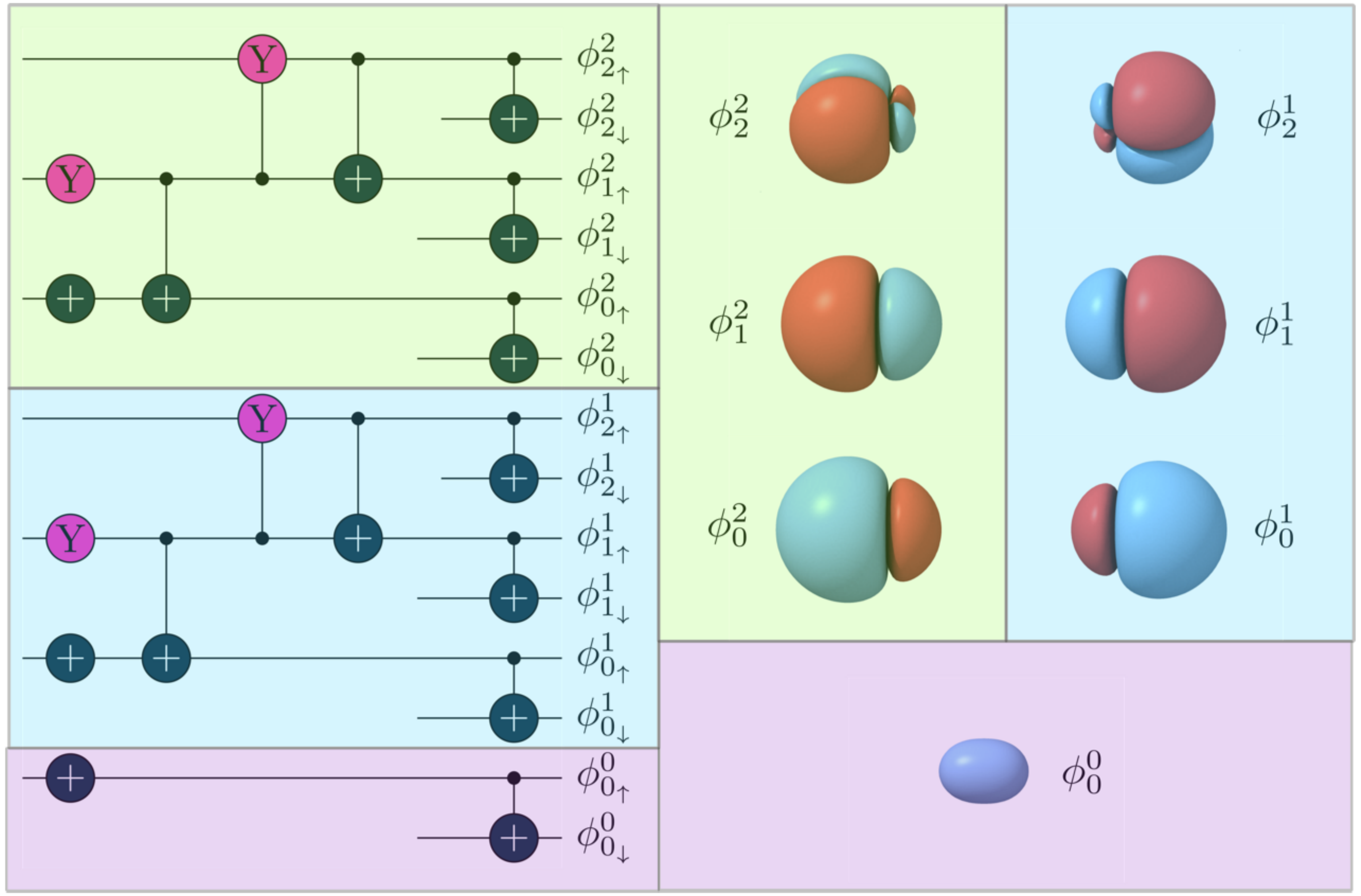

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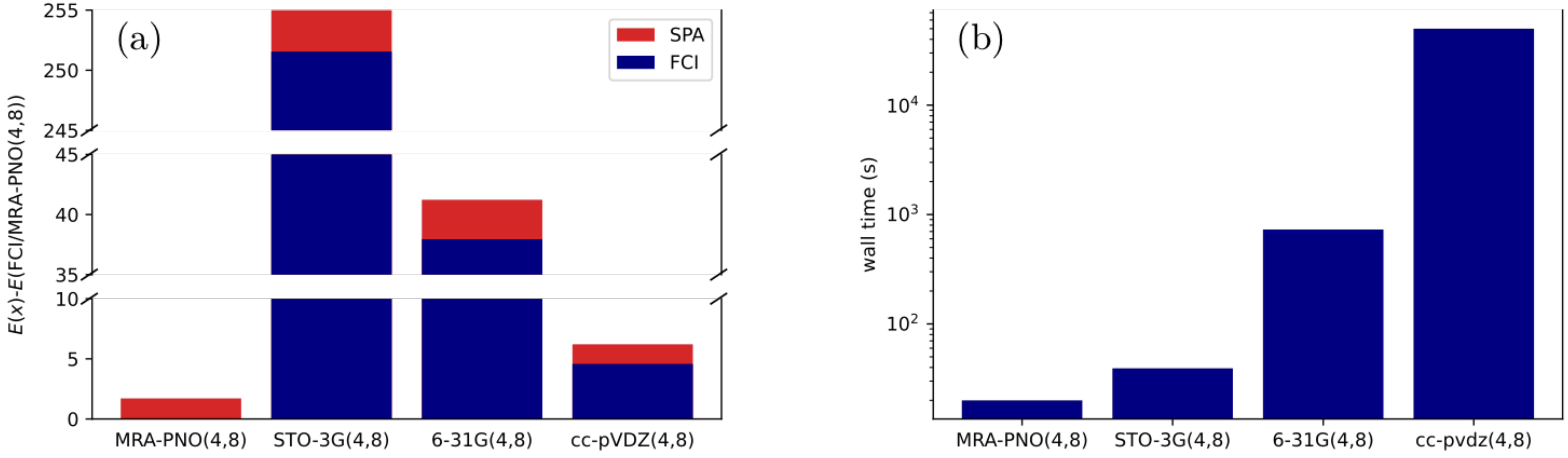
Jakob S. Kottmann[1,2,*] and Alán Aspuru-Guzik[1,2,3,4,†]

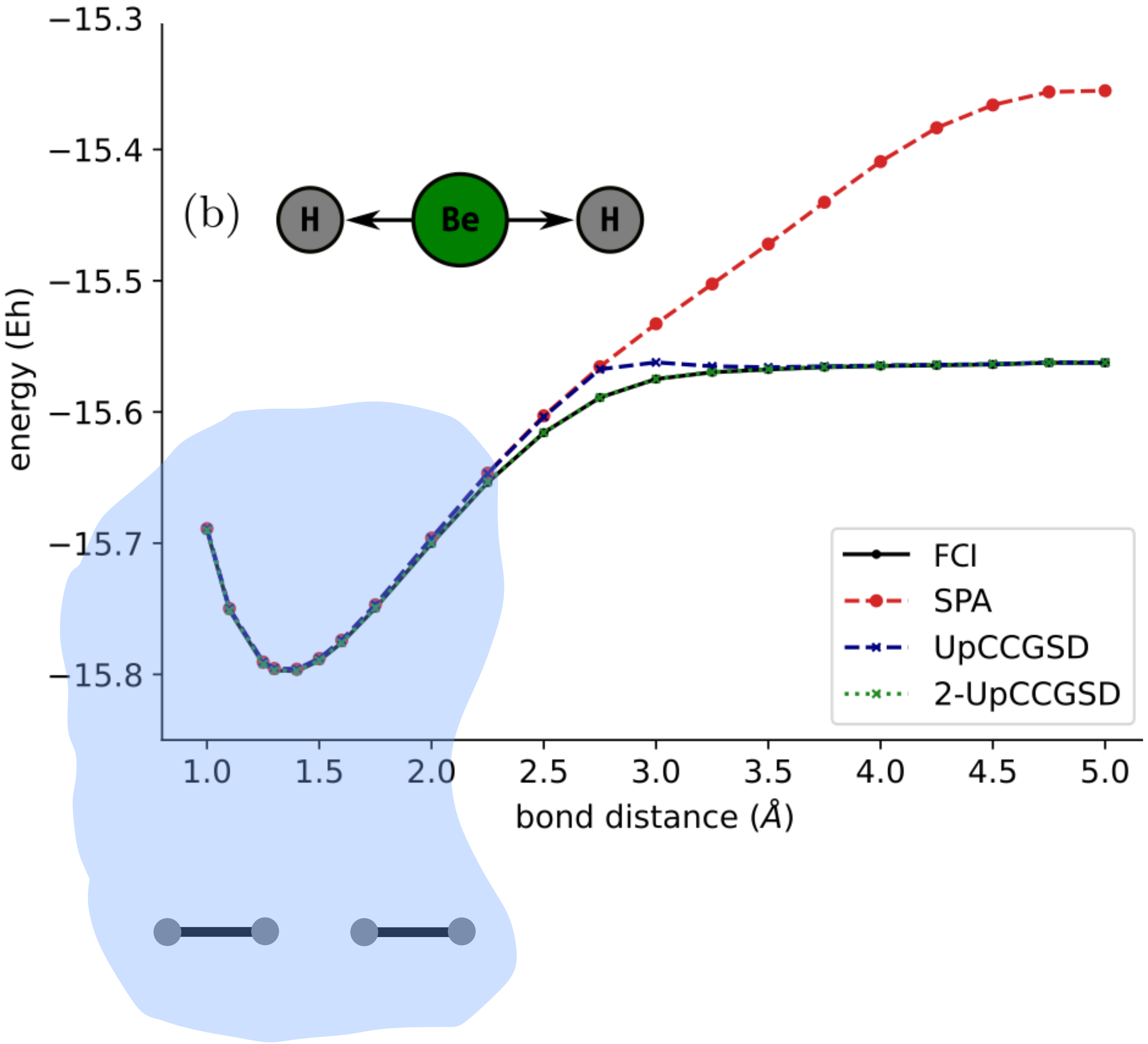
Why Basis–Set–Free?

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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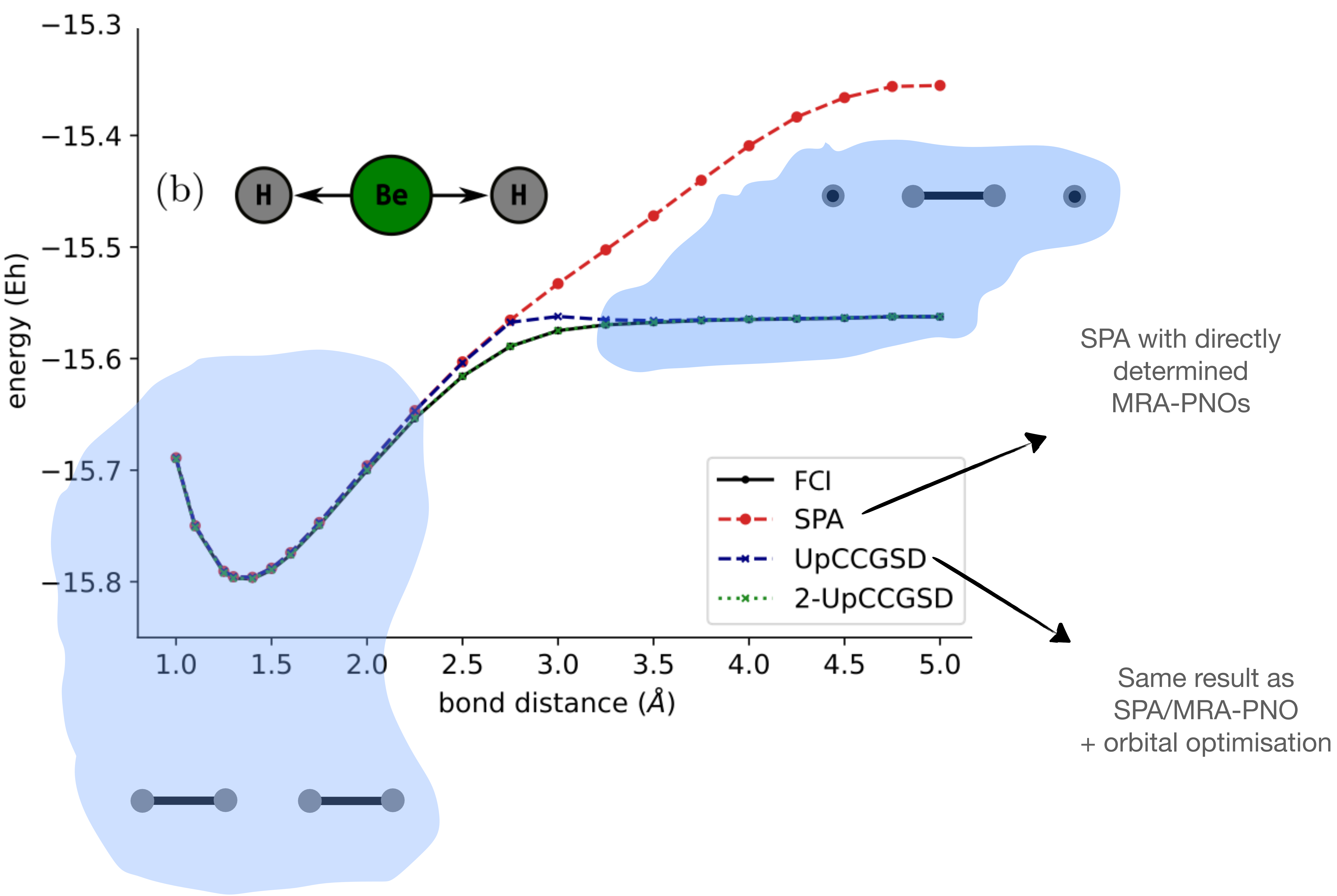
beh2.py



Classically simulable

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

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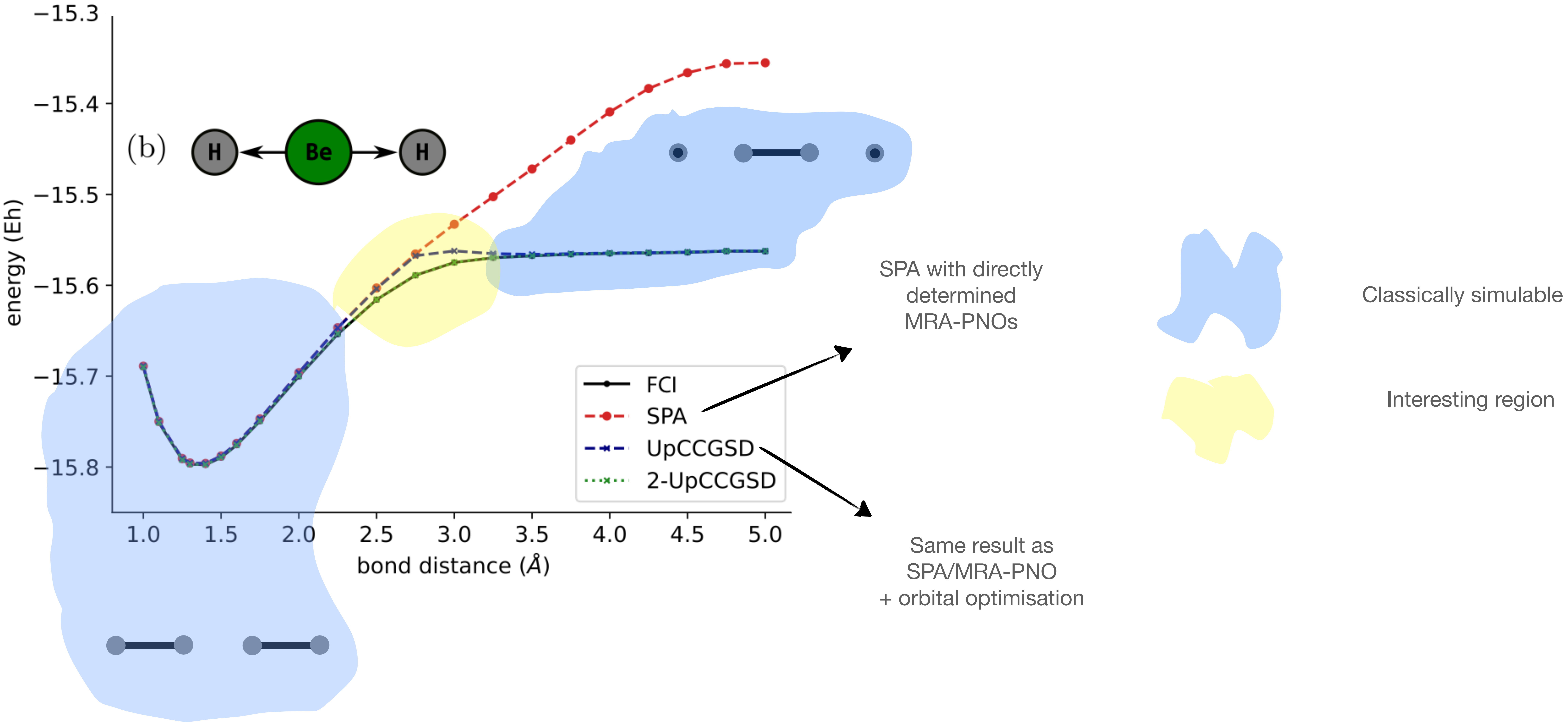
beh2.py



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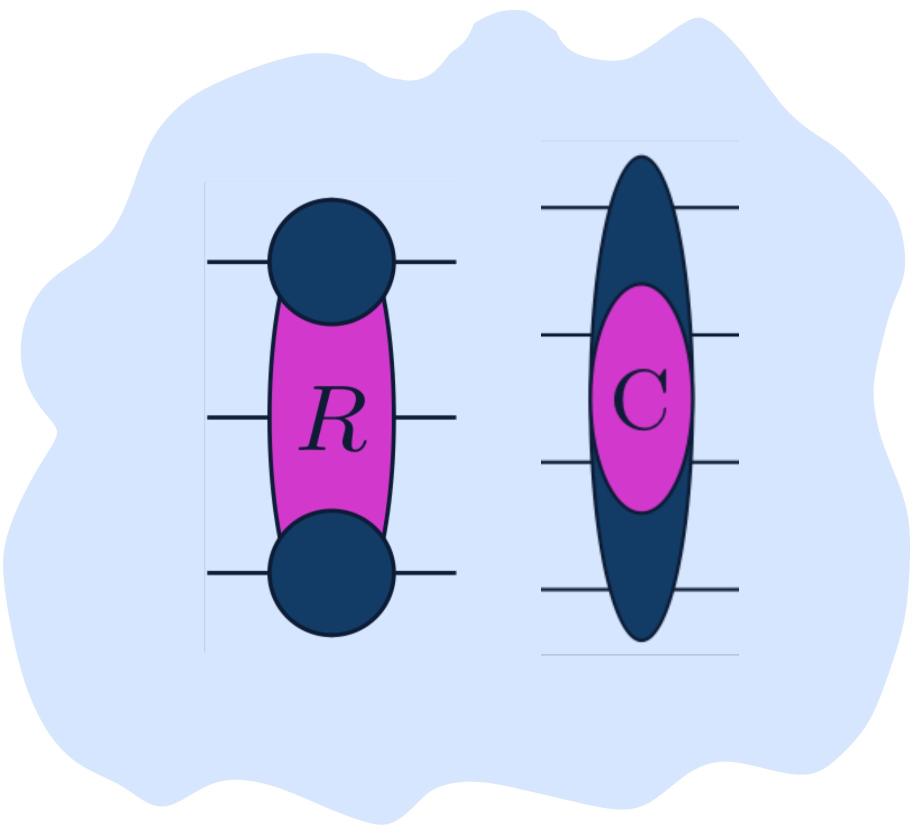
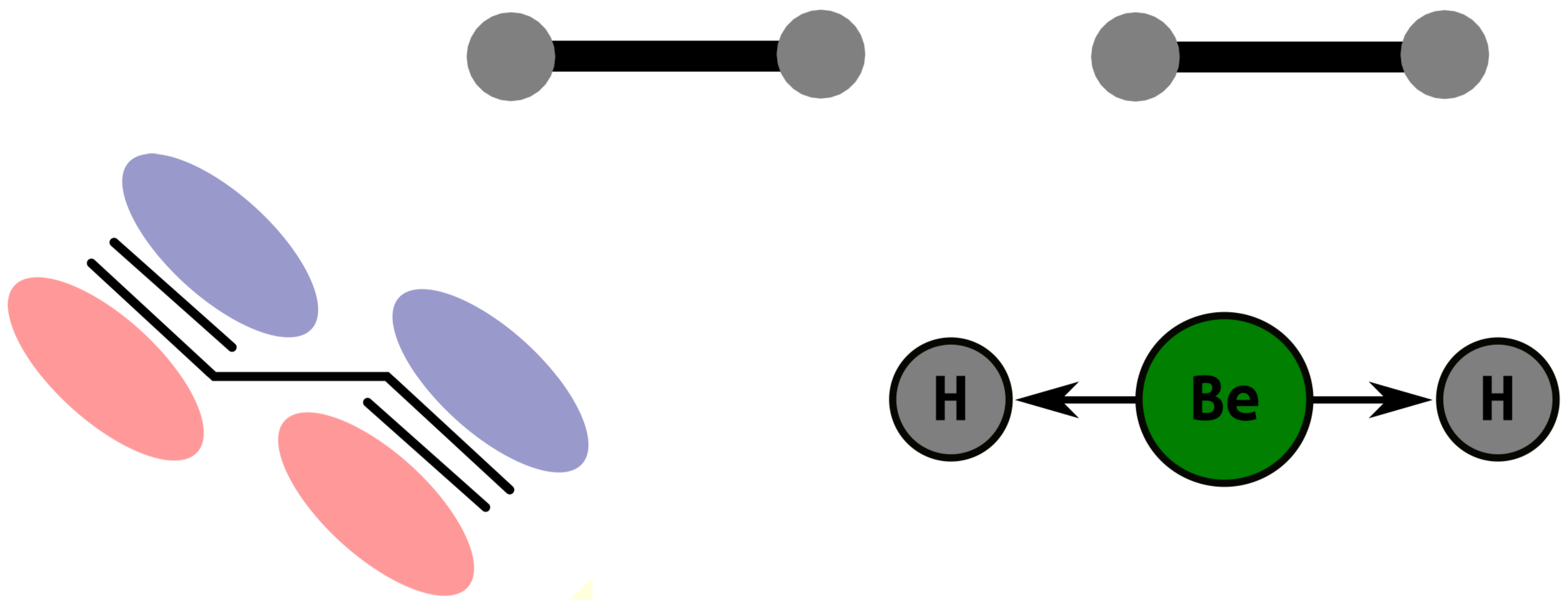
beh2.py

Summary

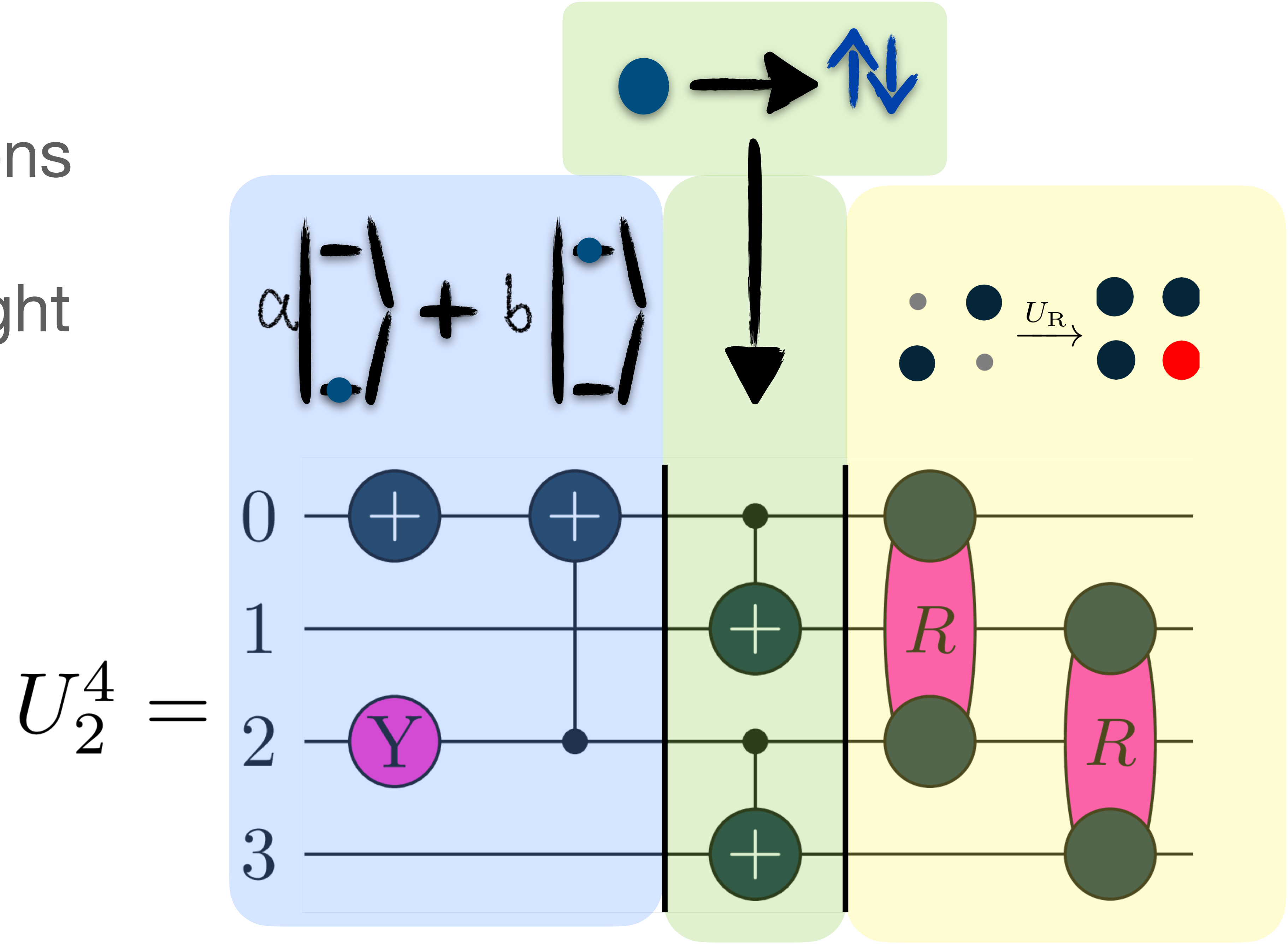
Basic
Building
Blocks



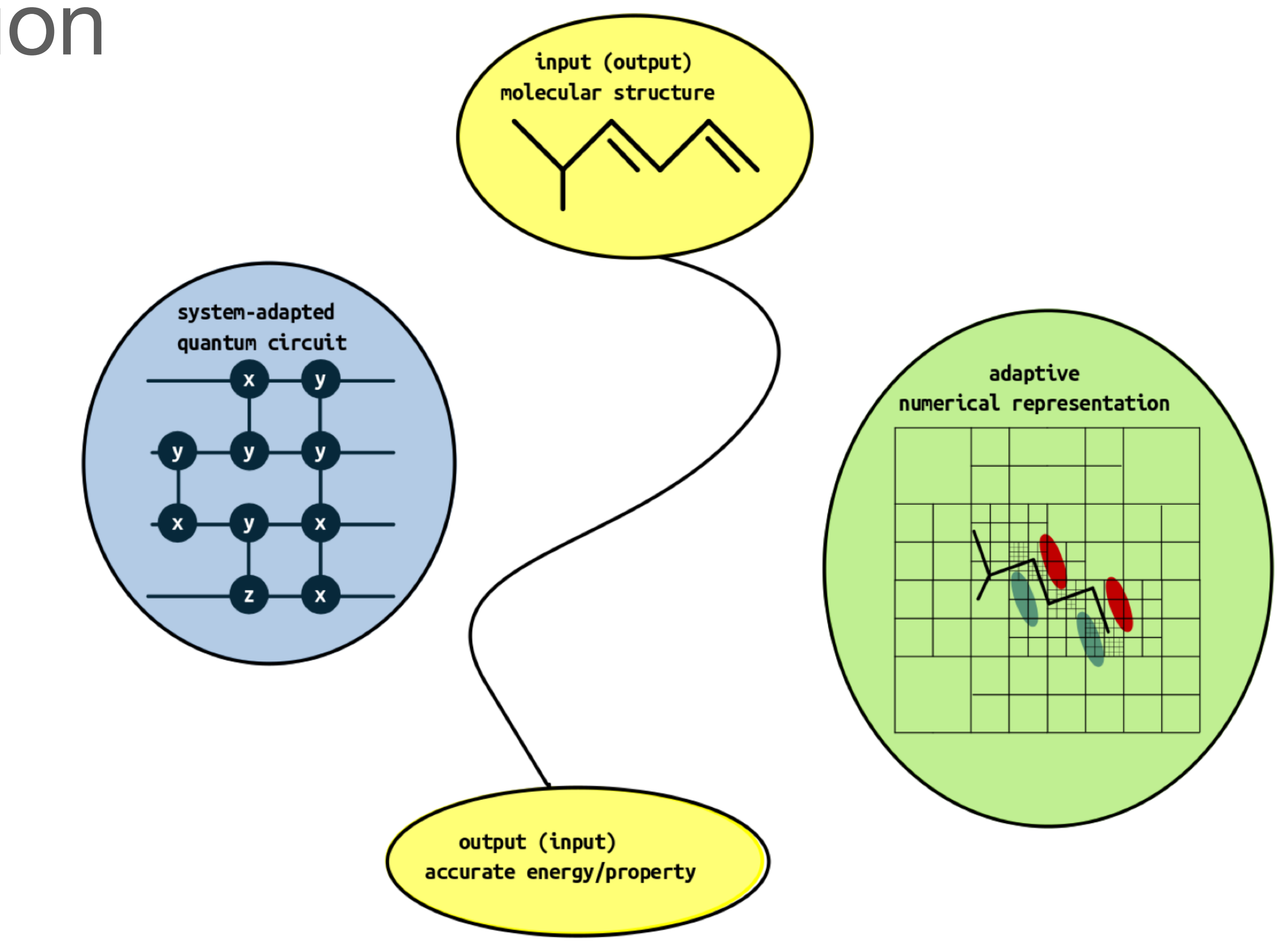
Abstraction & Transferability



Approximations
and
Physical Insight

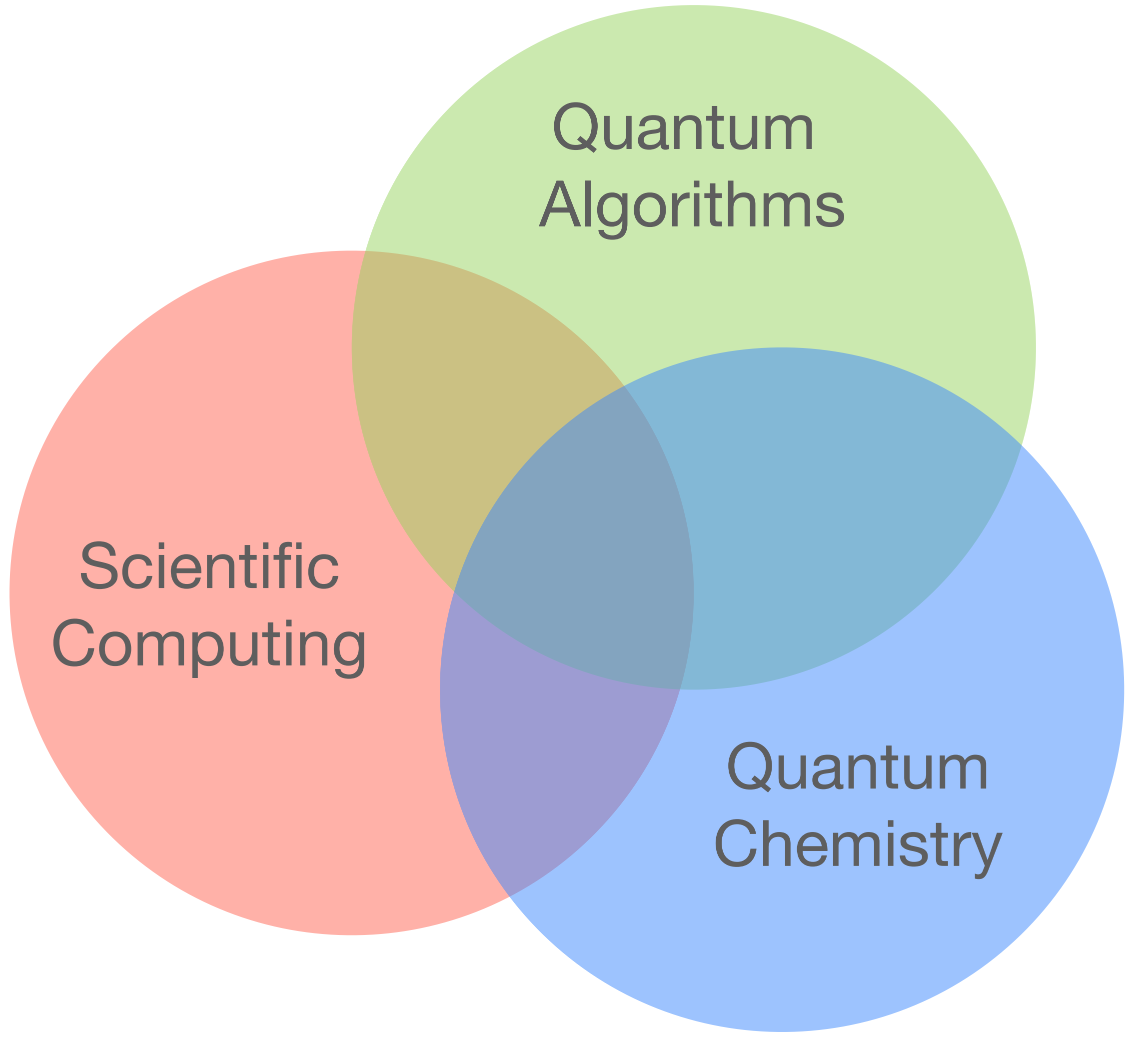


Automatisation



Universität Augsburg University

Positions available (PhD and Postdoc) Starting end of 2022



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