Molecular Quantum Circuit Design

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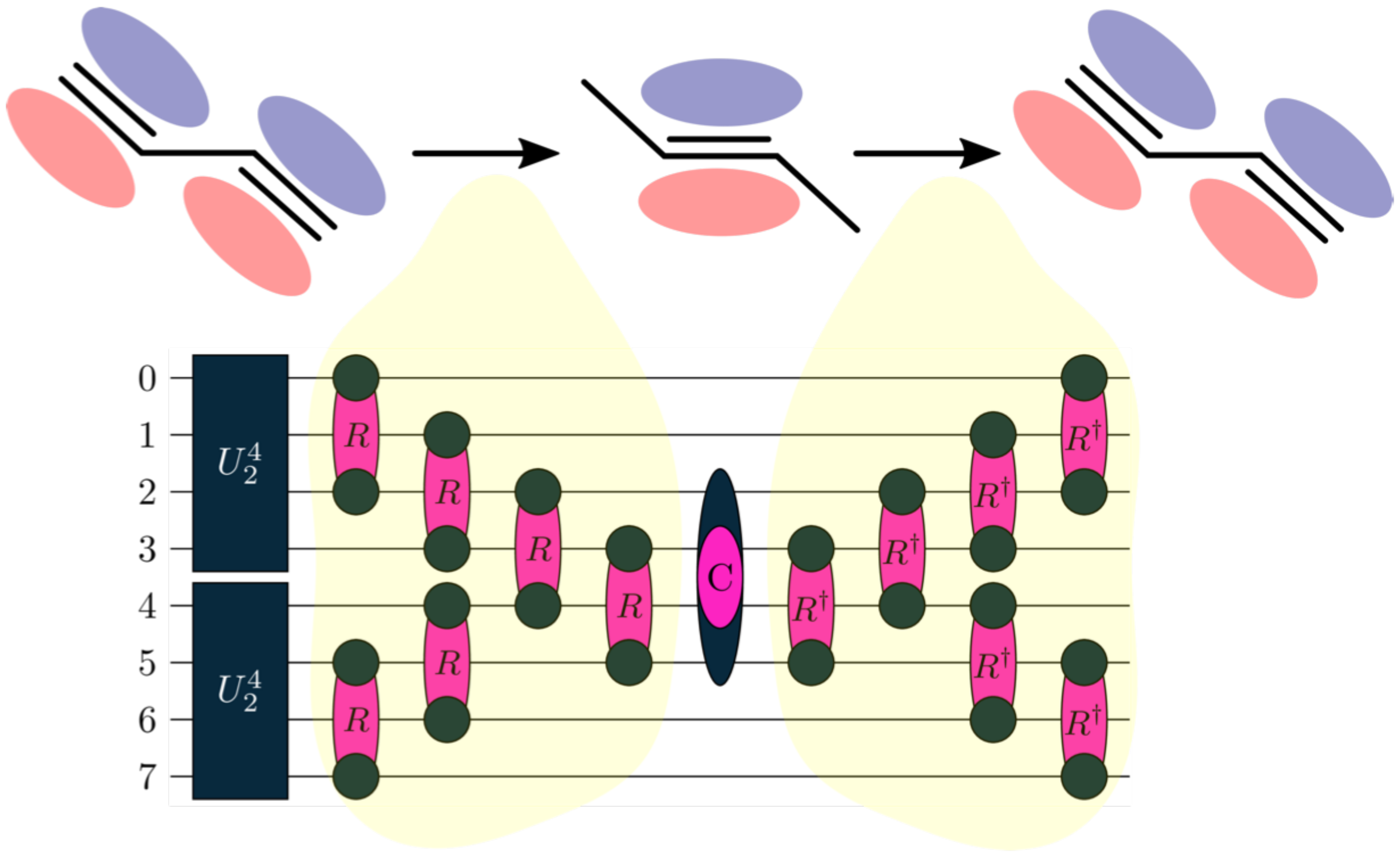
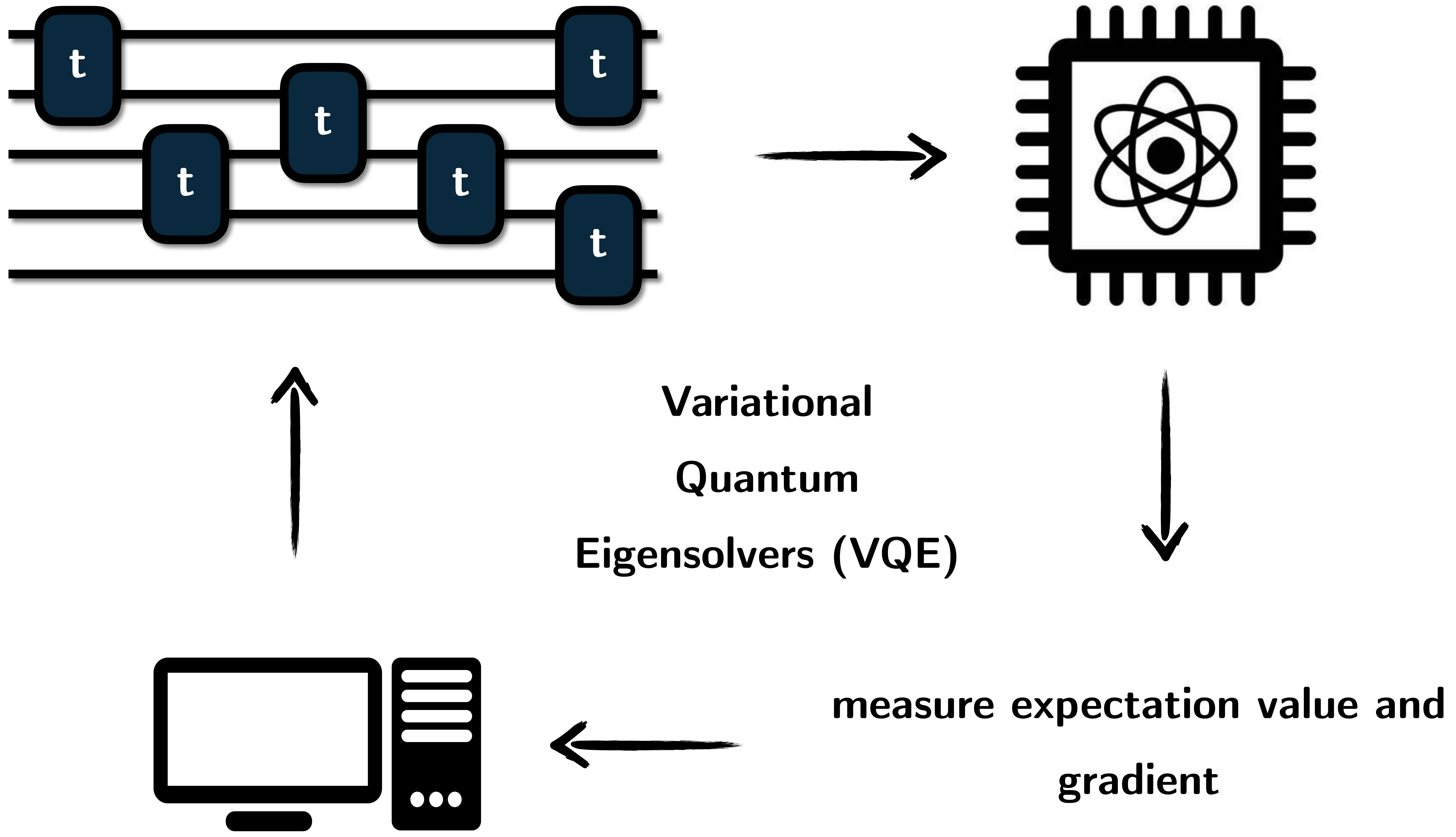




Perruzo/McClean, Nat. Comm, 2014

McClean, NJP, 2016

Motivation: VQEs as black-boxes

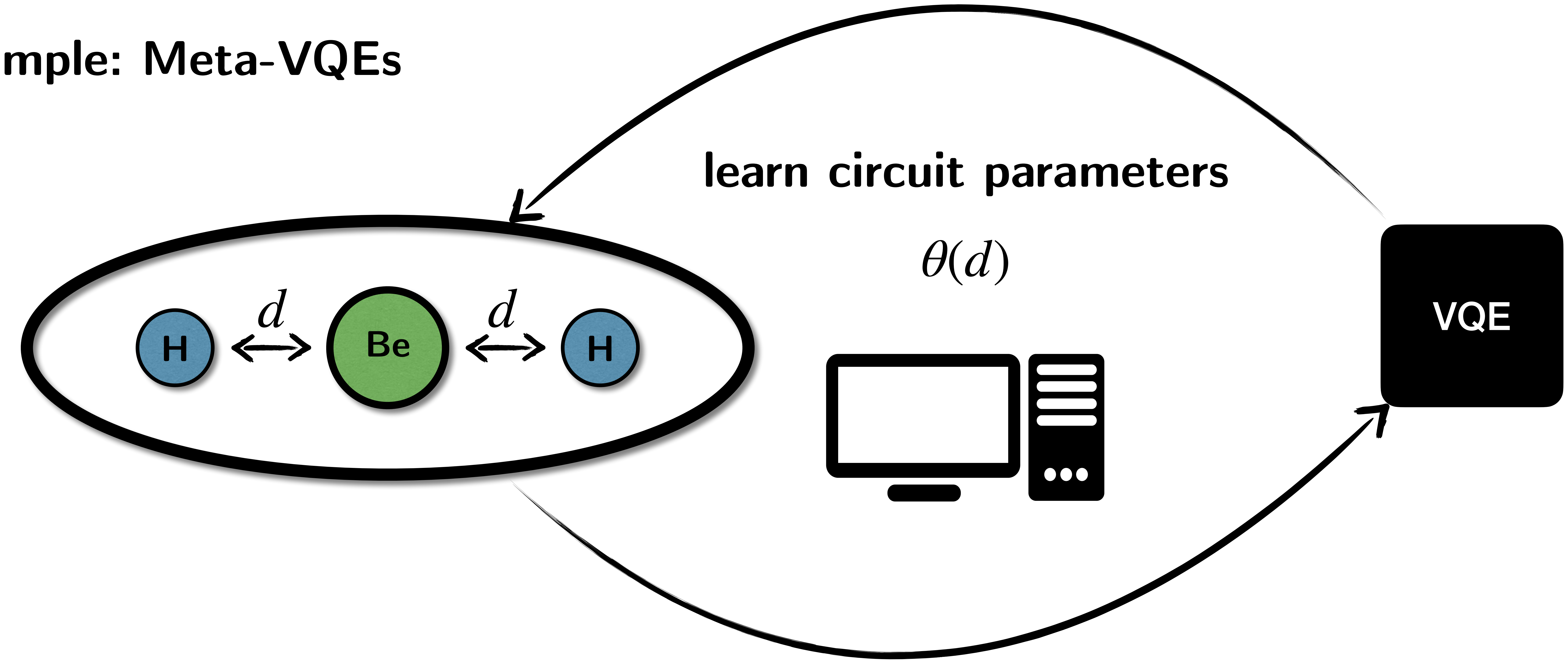
Many projects need robust VQEs

Motivation: VQEs as black-boxes

Proof of concept

scalability: challenging!

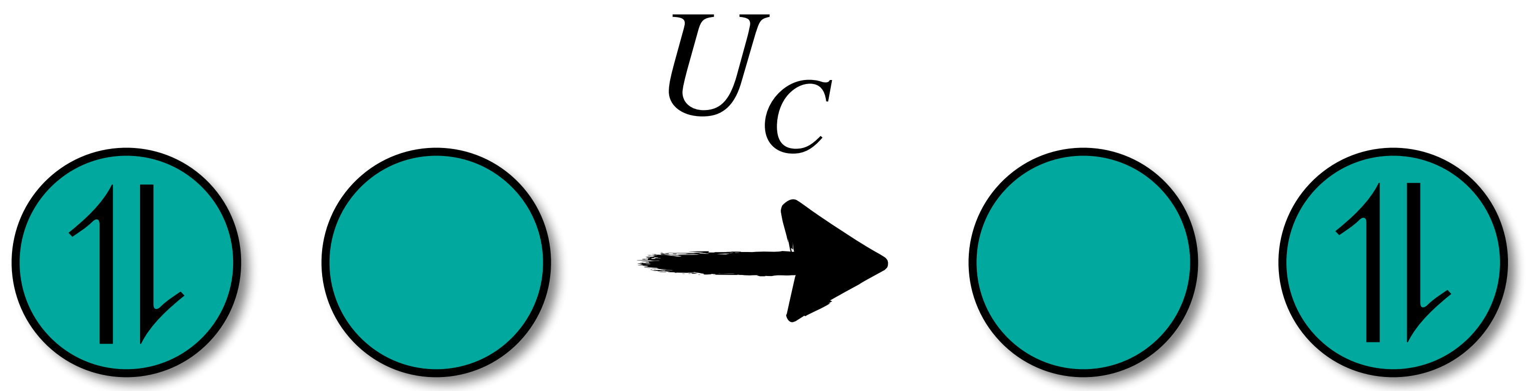
Example: Meta-VQEs

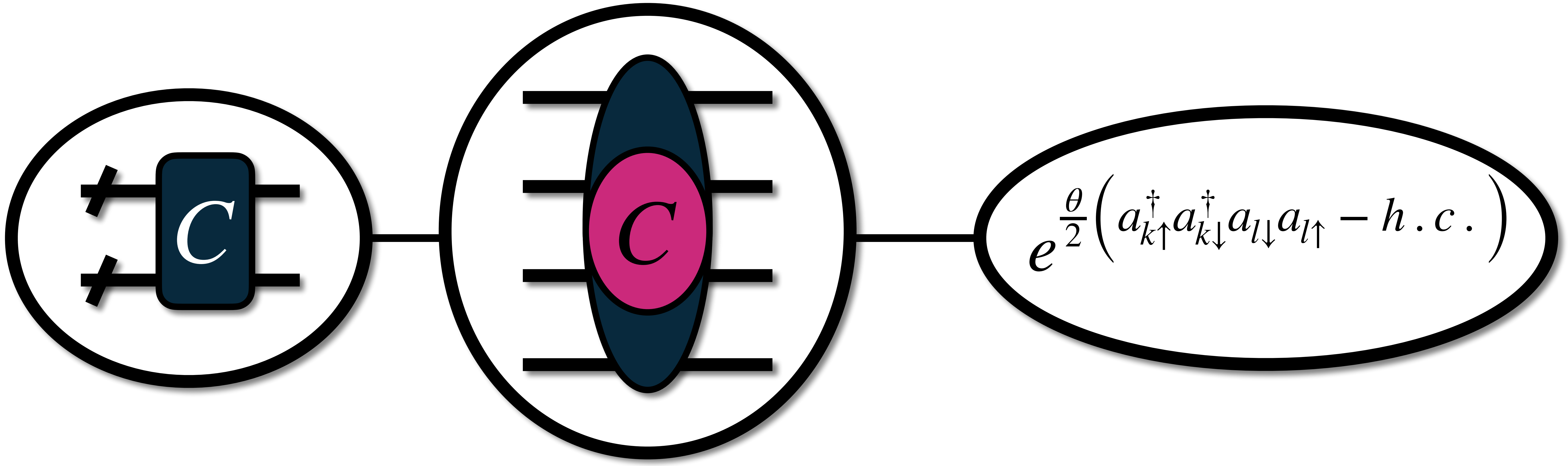


Cervera-Lierta, PRX-Quantum 2021

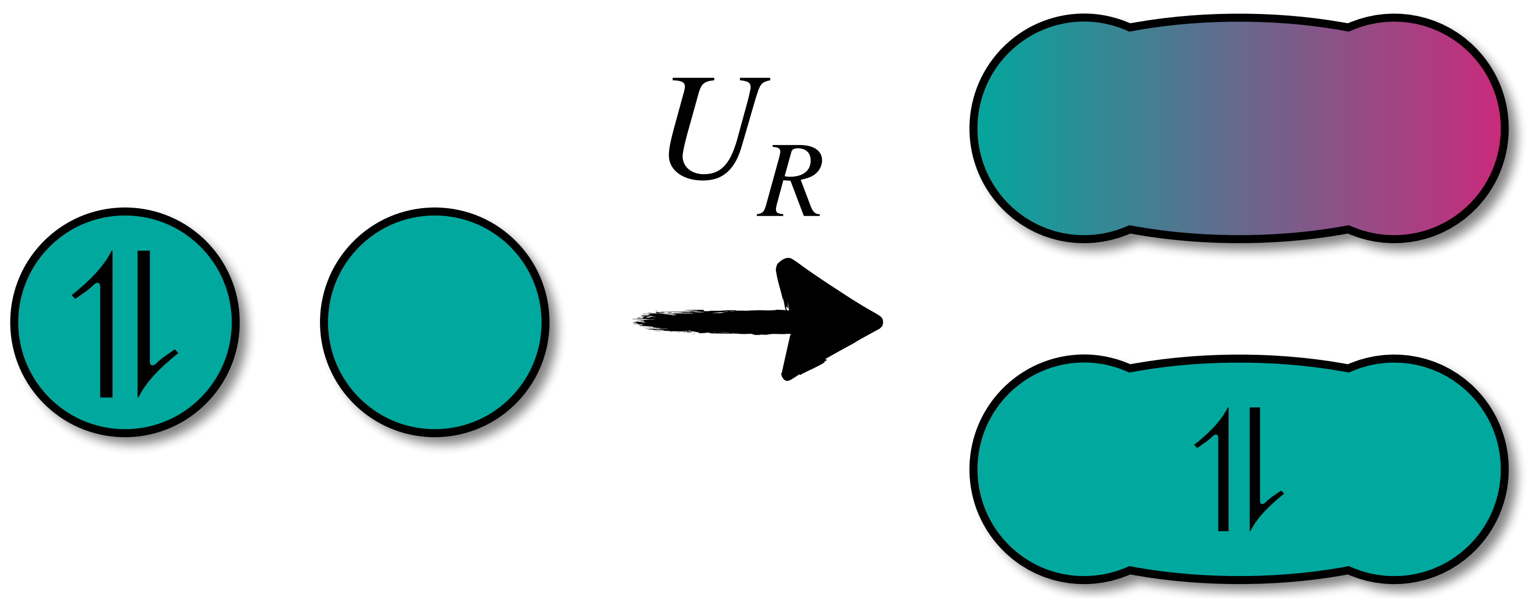
Basic Building Blocks

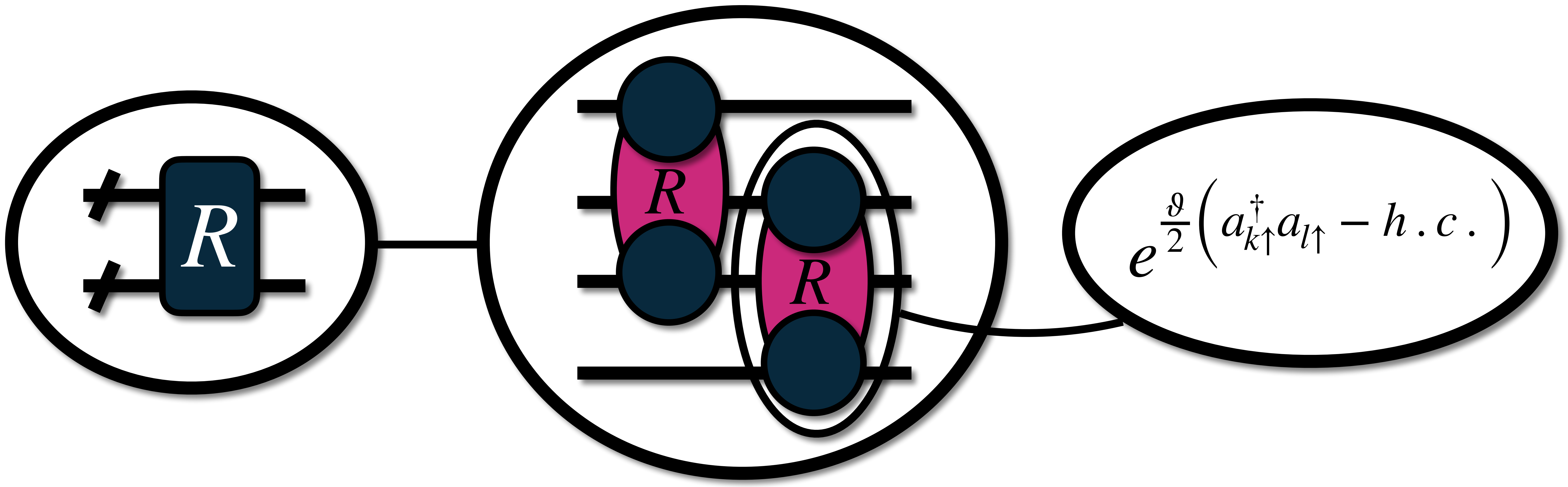
Pair Correlators





Basis Change



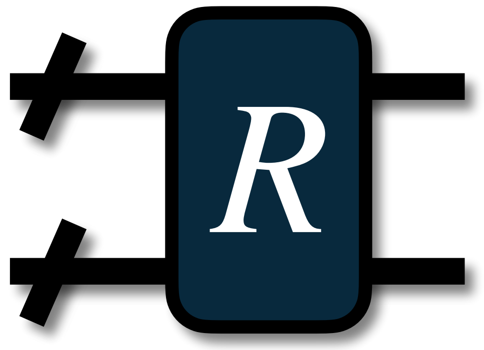


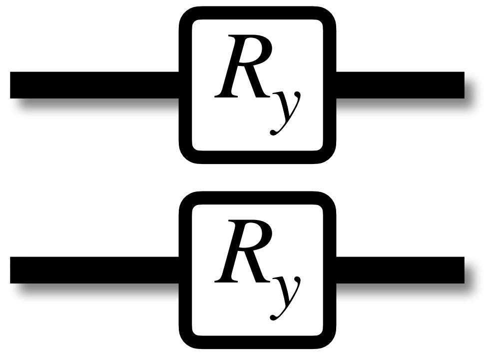
Analogy

electronic structure

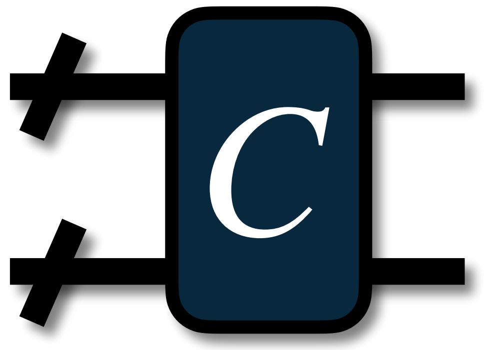
quantum machine learning

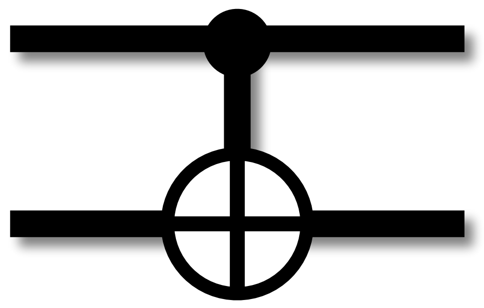
basis change



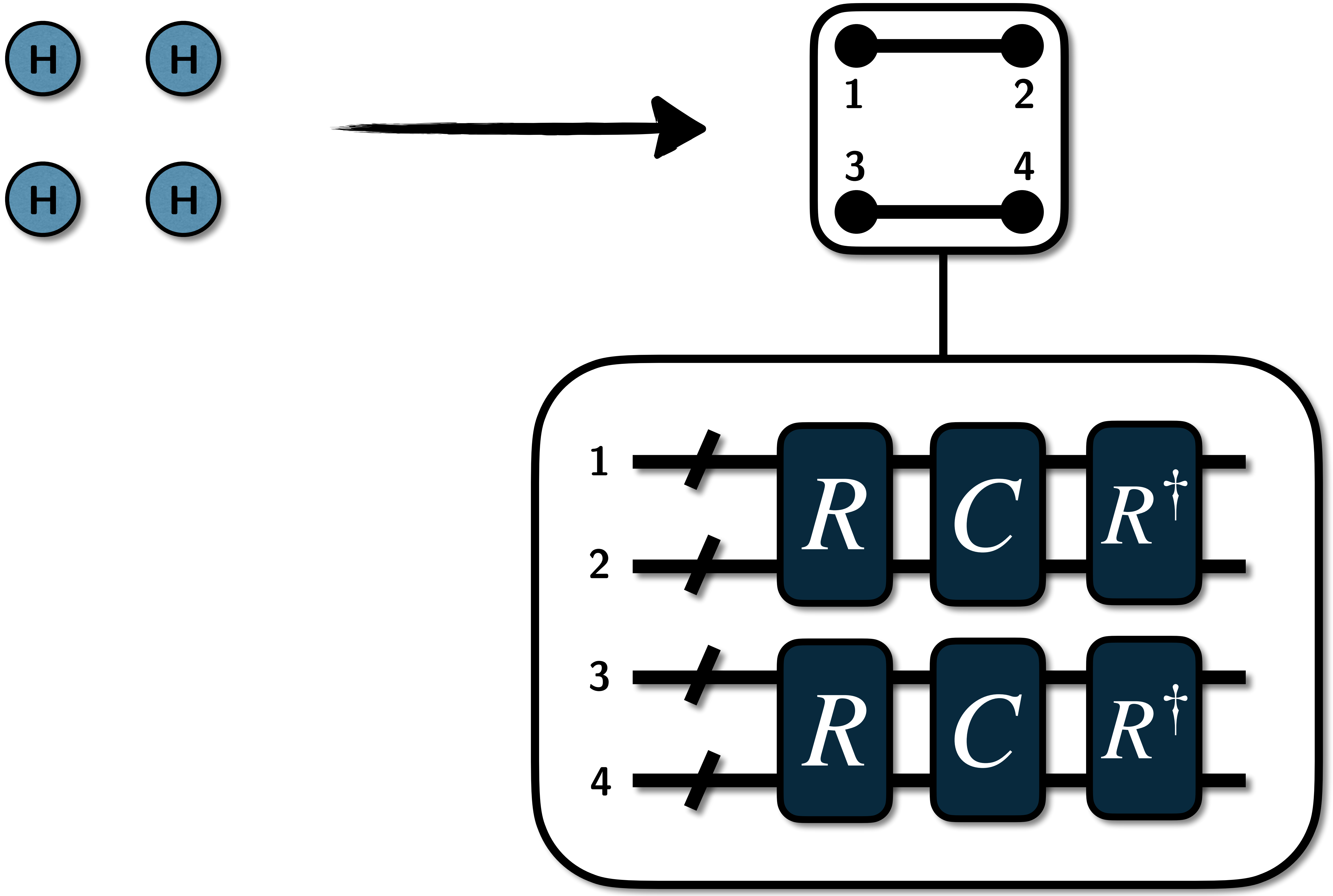


correlate

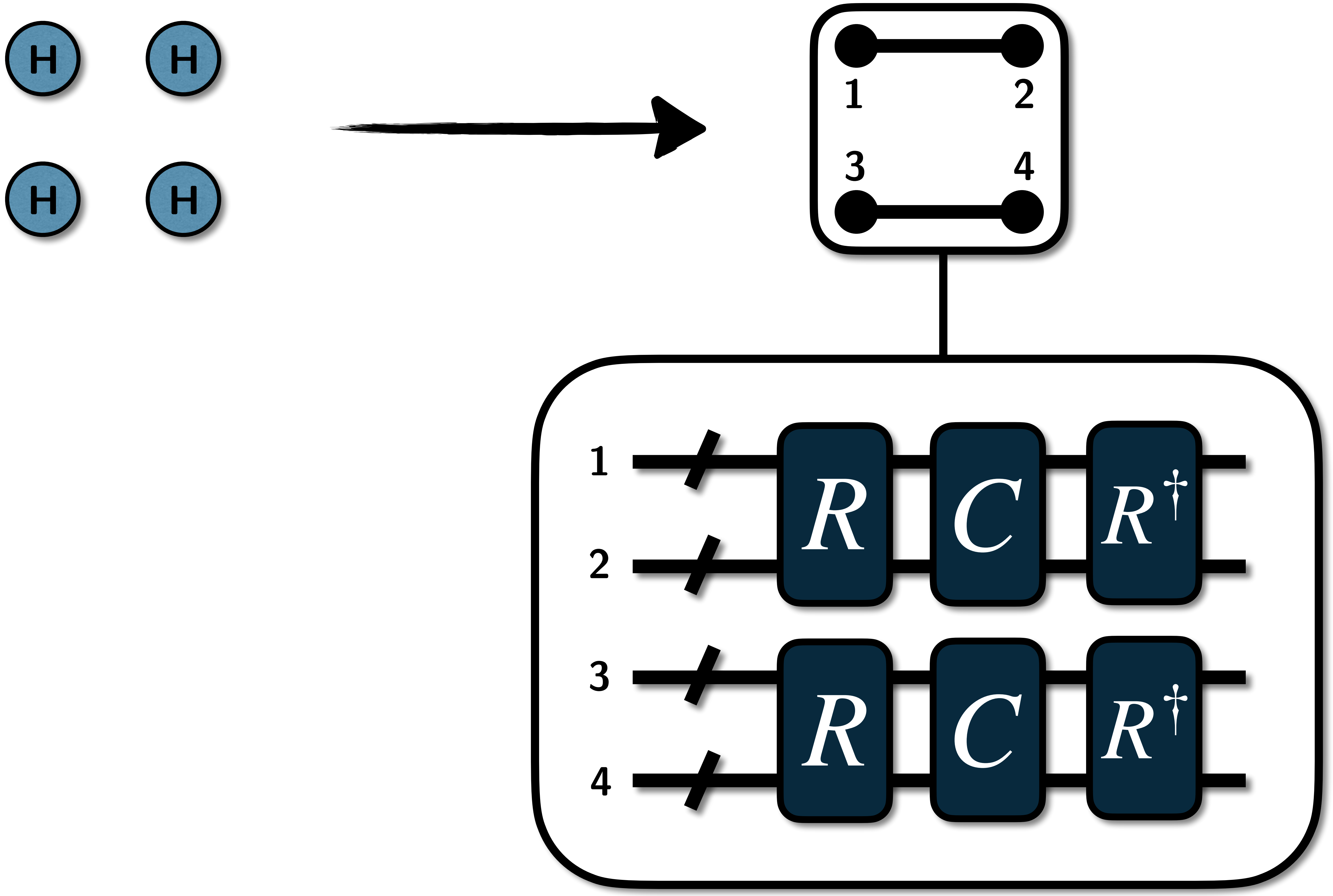


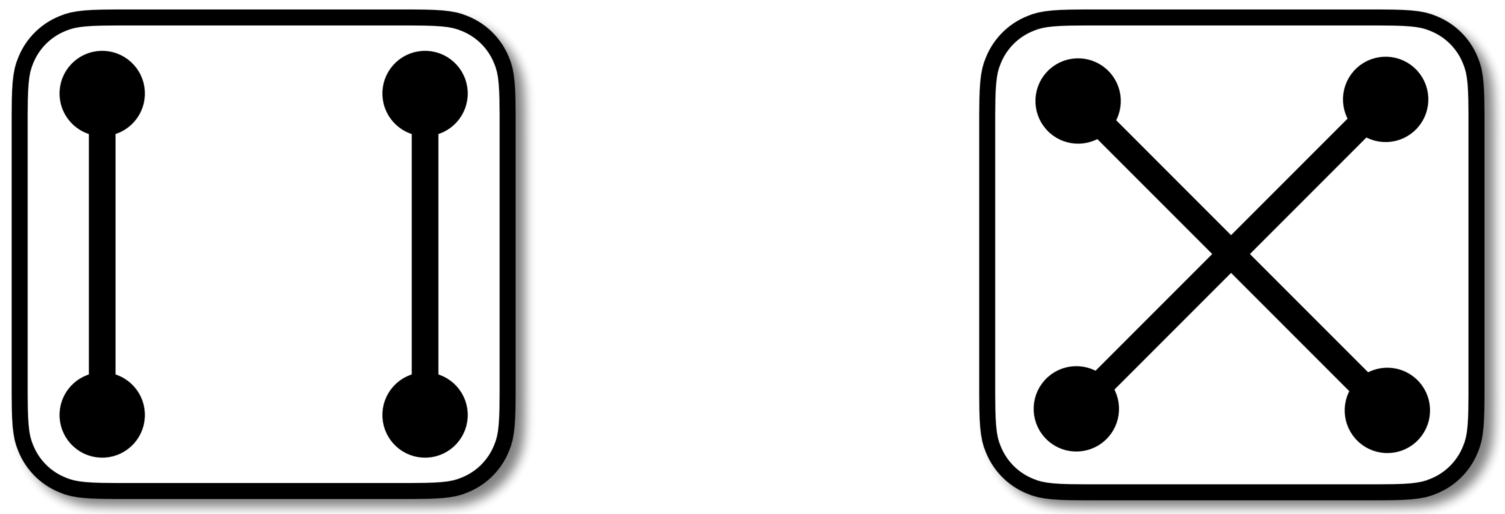


High-Level Design



High-Level Design

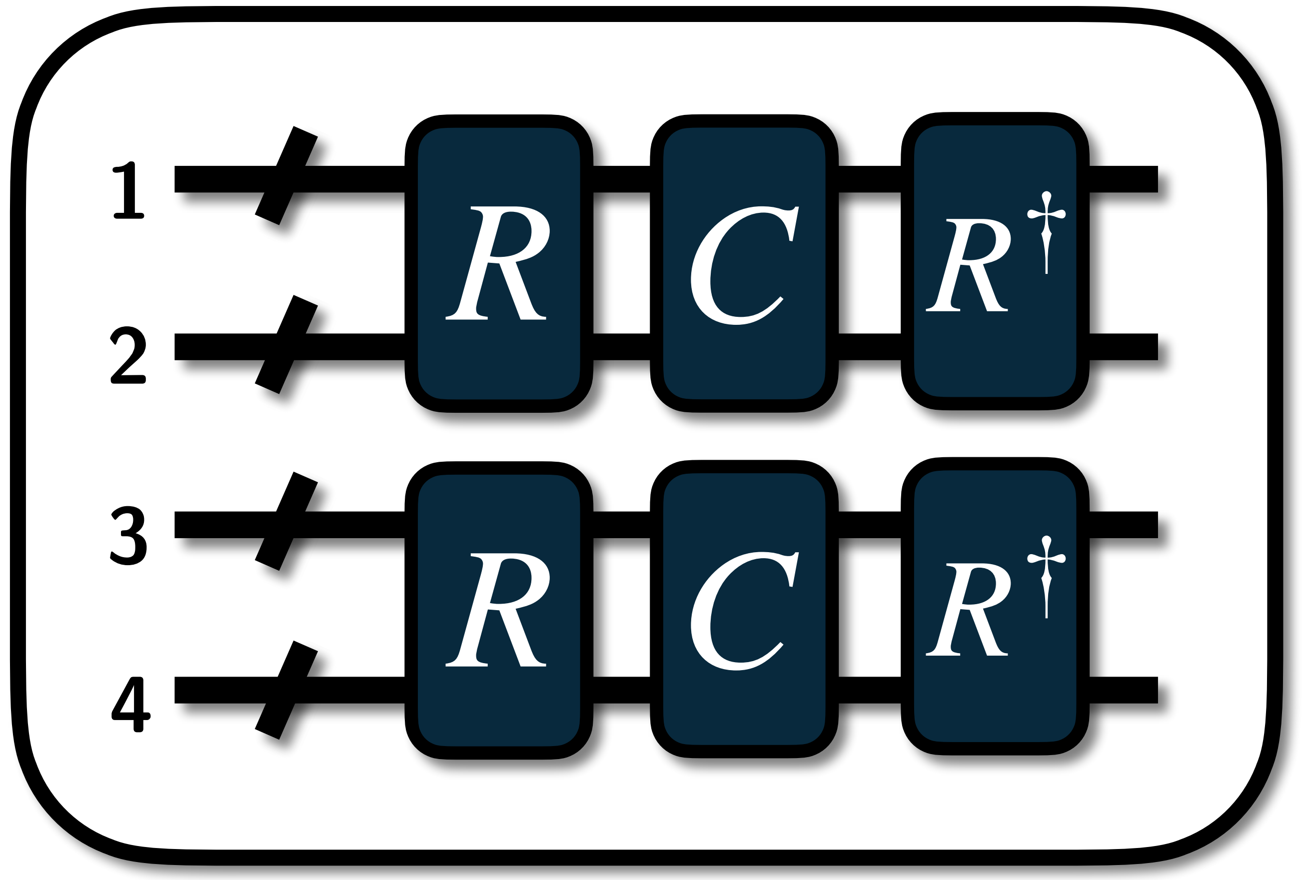


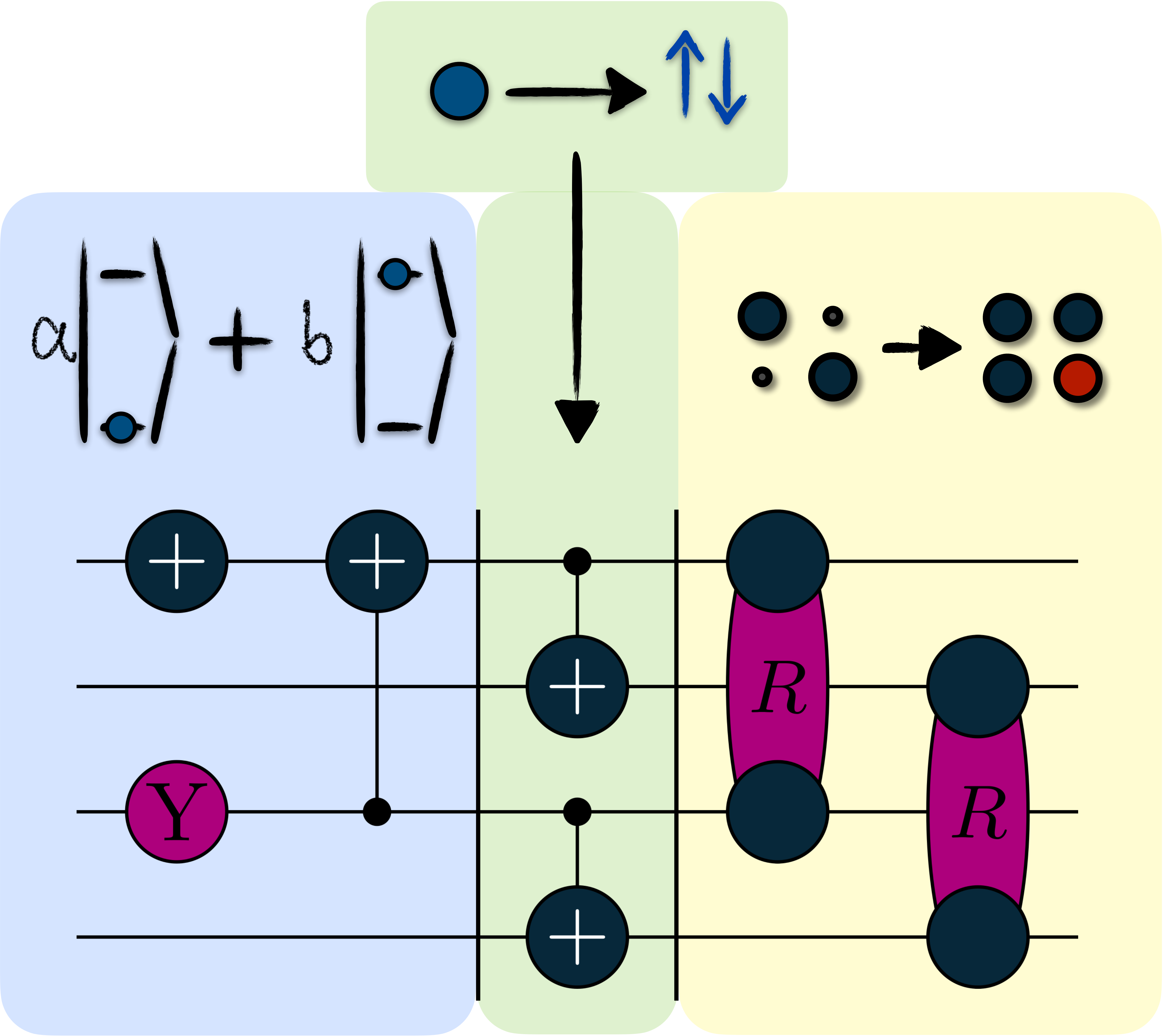


More Graphs
Heuristic Grouping

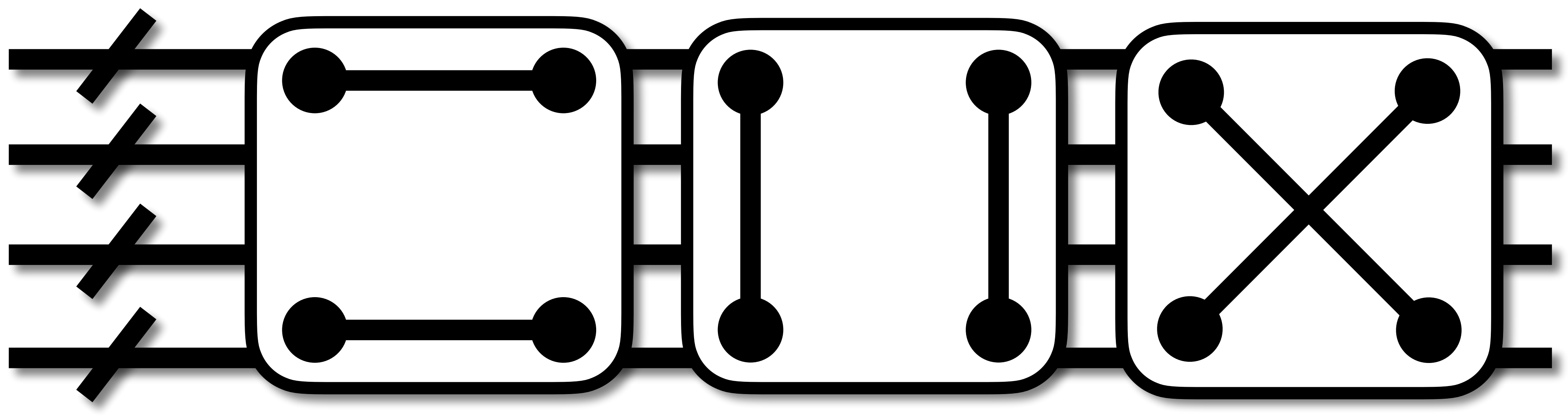
Single graphs are cheap

classically simulable

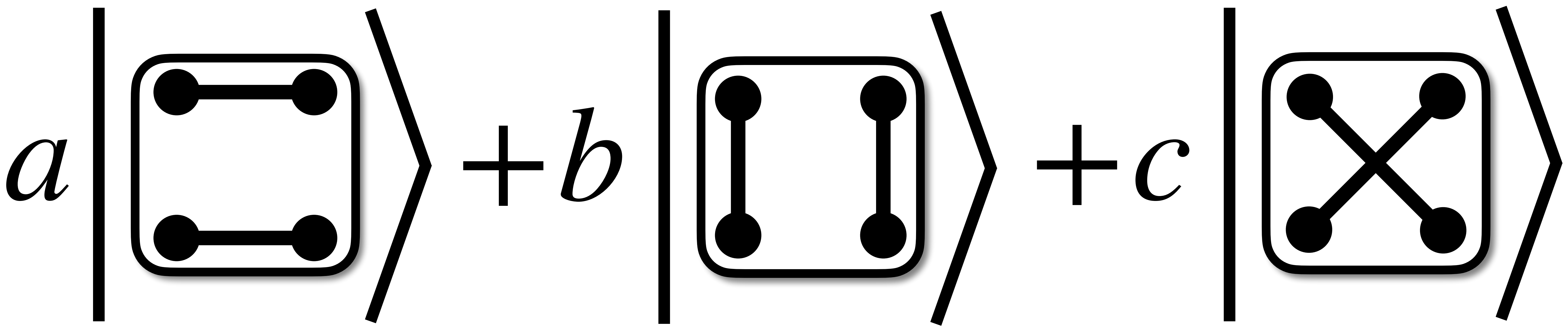




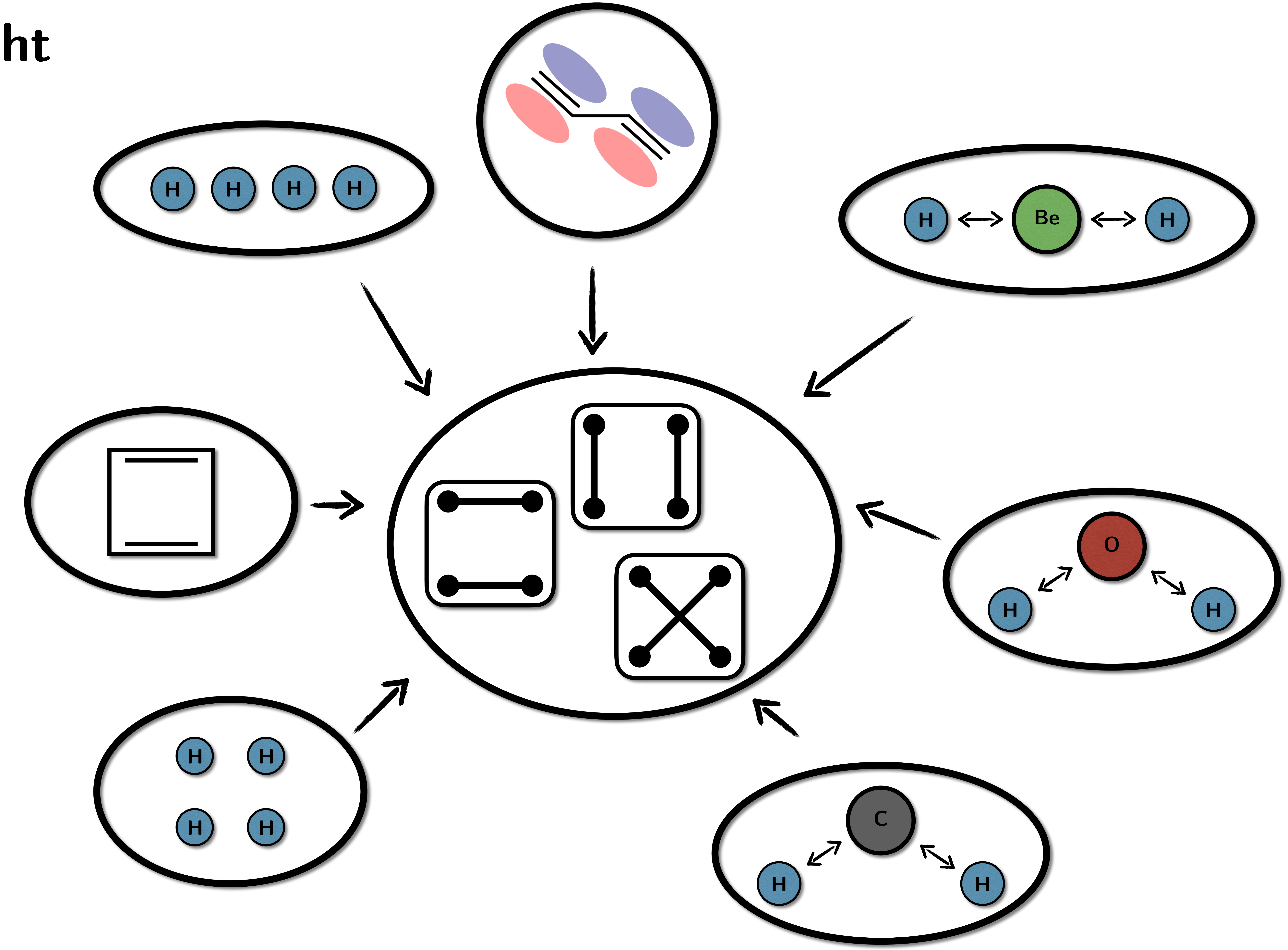
VQE-Style Wavefunction



Krylov-Style Wavefunction

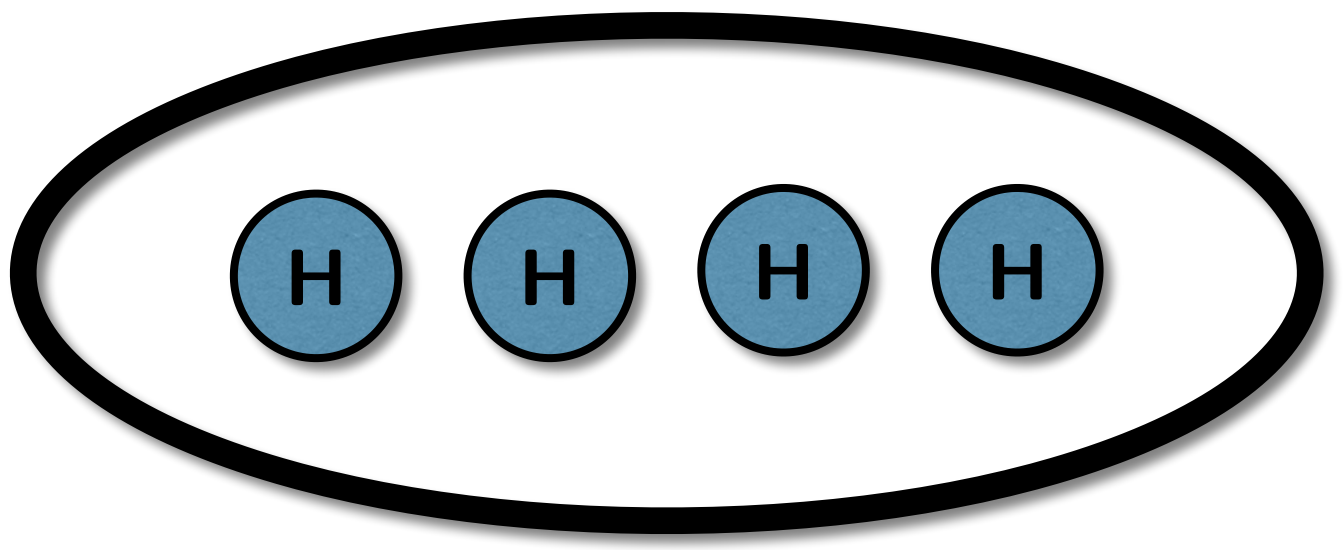


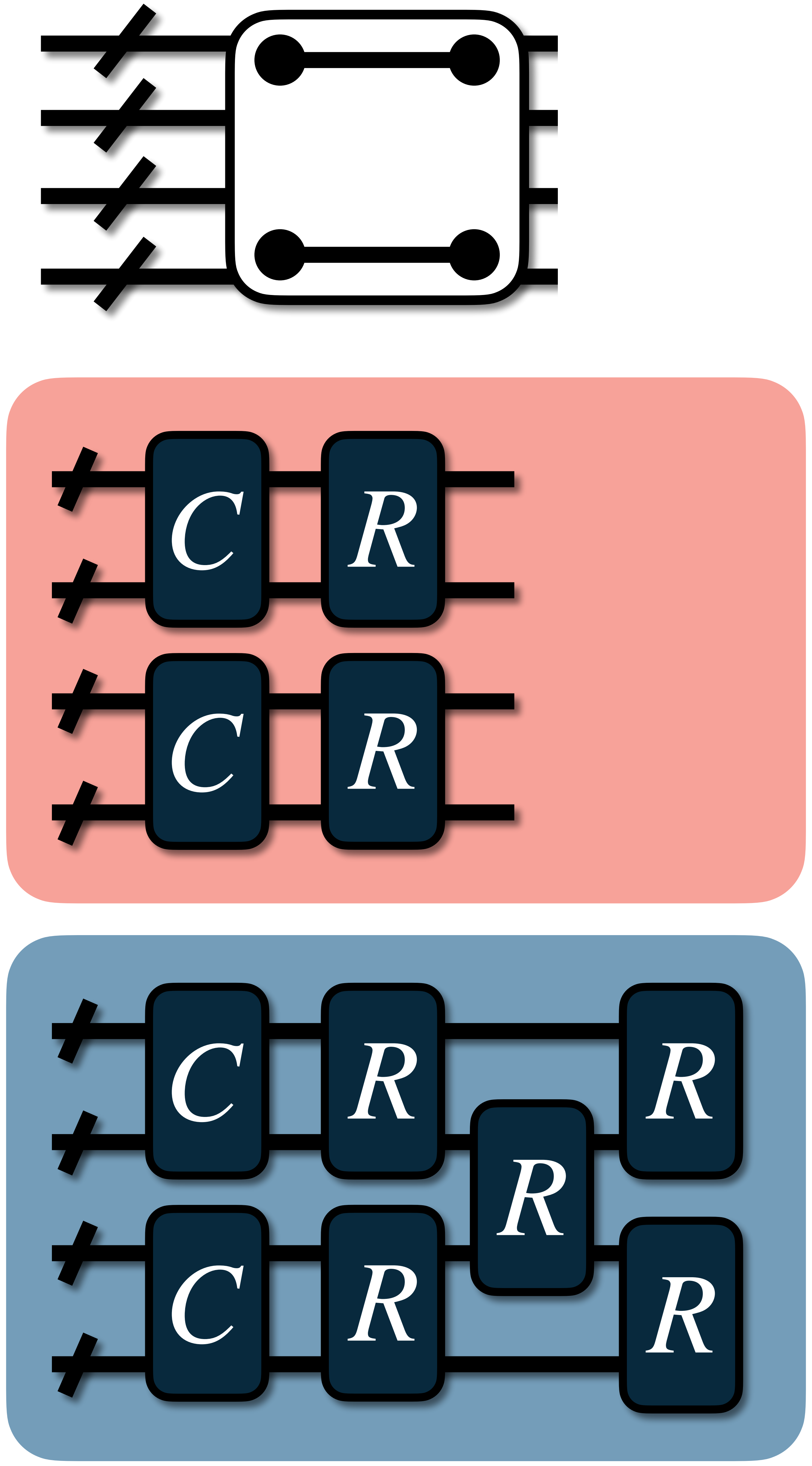
Transfer Insight



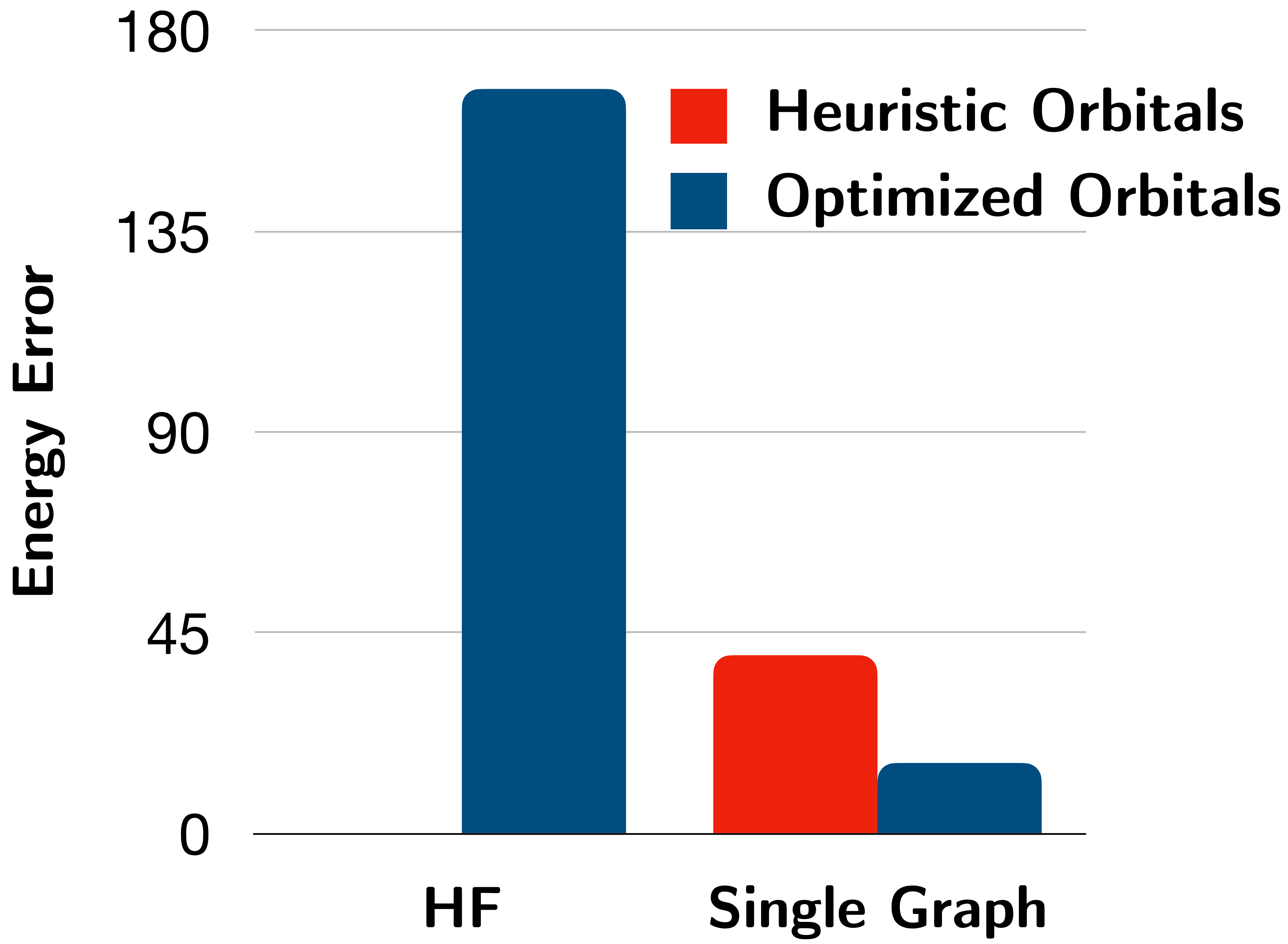
Example

Linear H4 Molecule

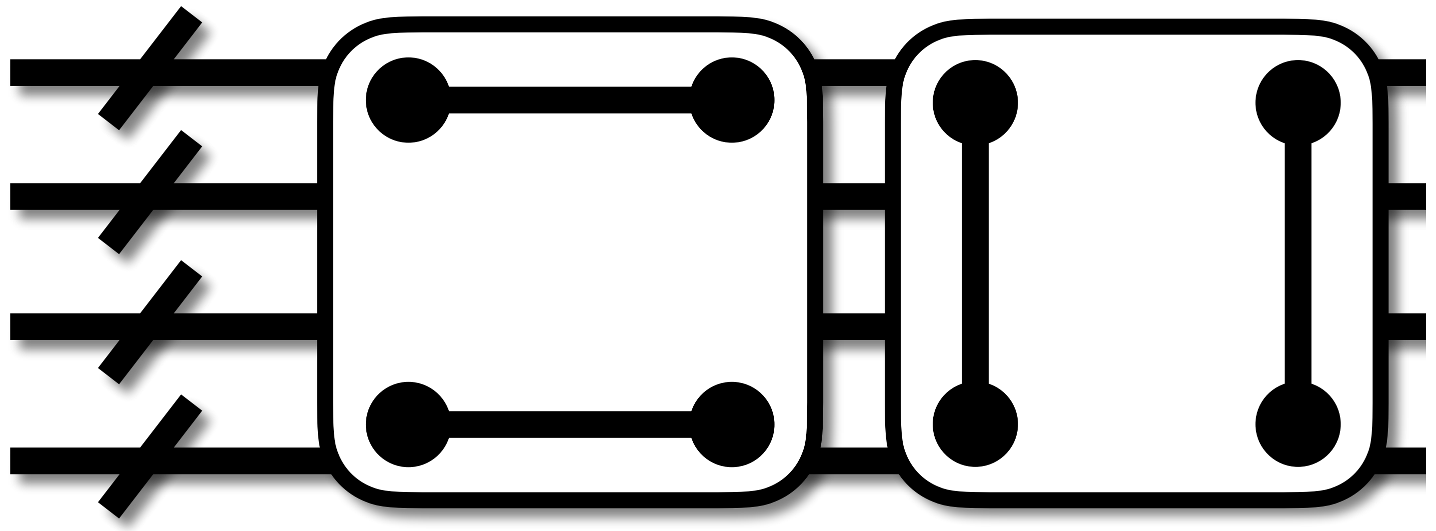


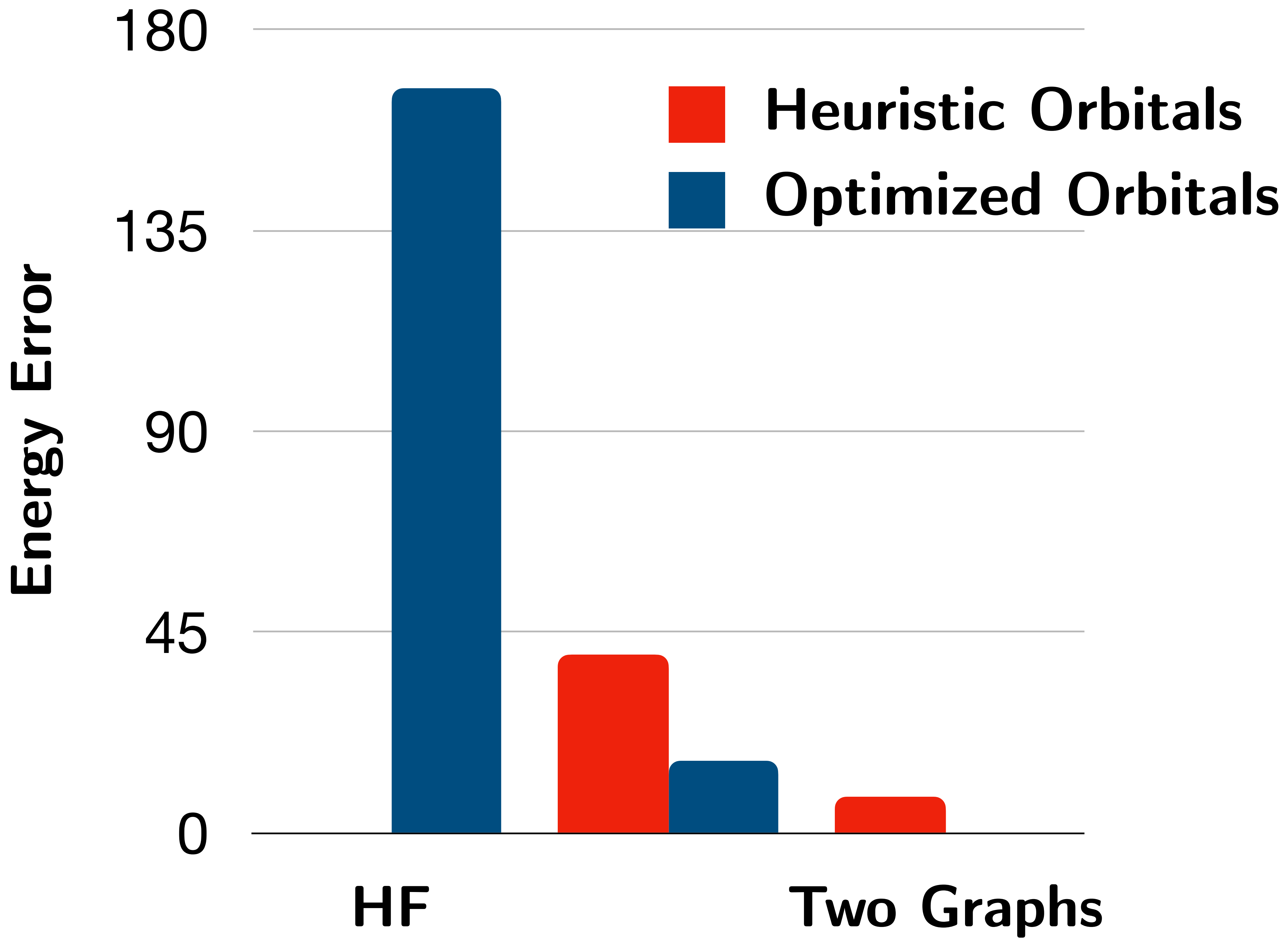


C
R
C
R
C
R
R
R
C
R
R

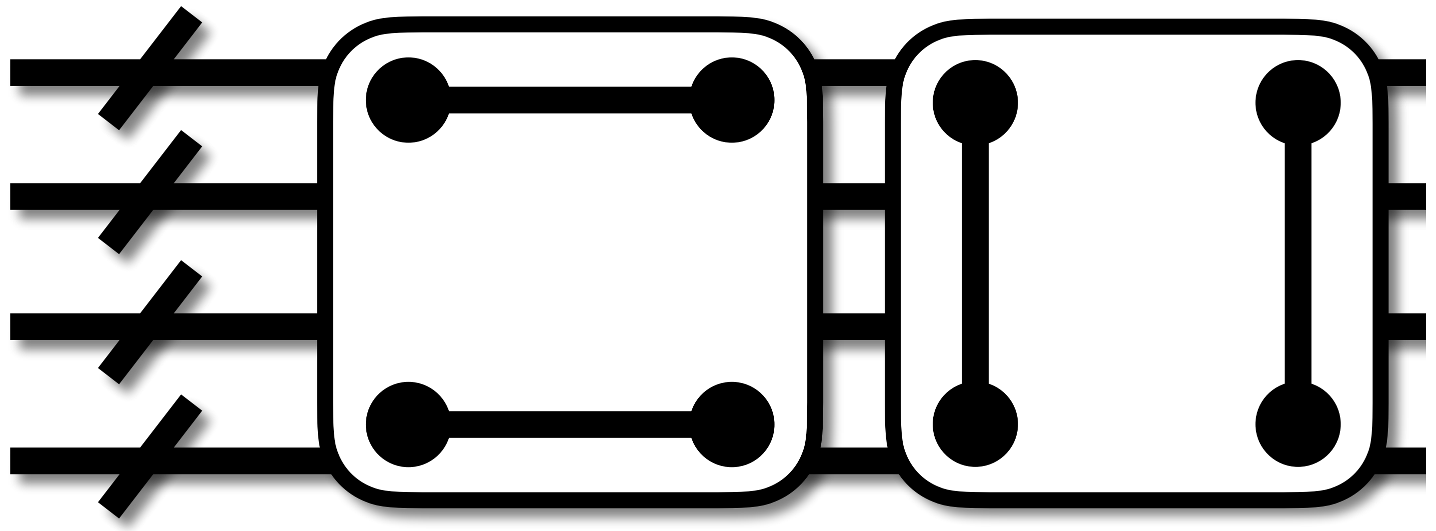


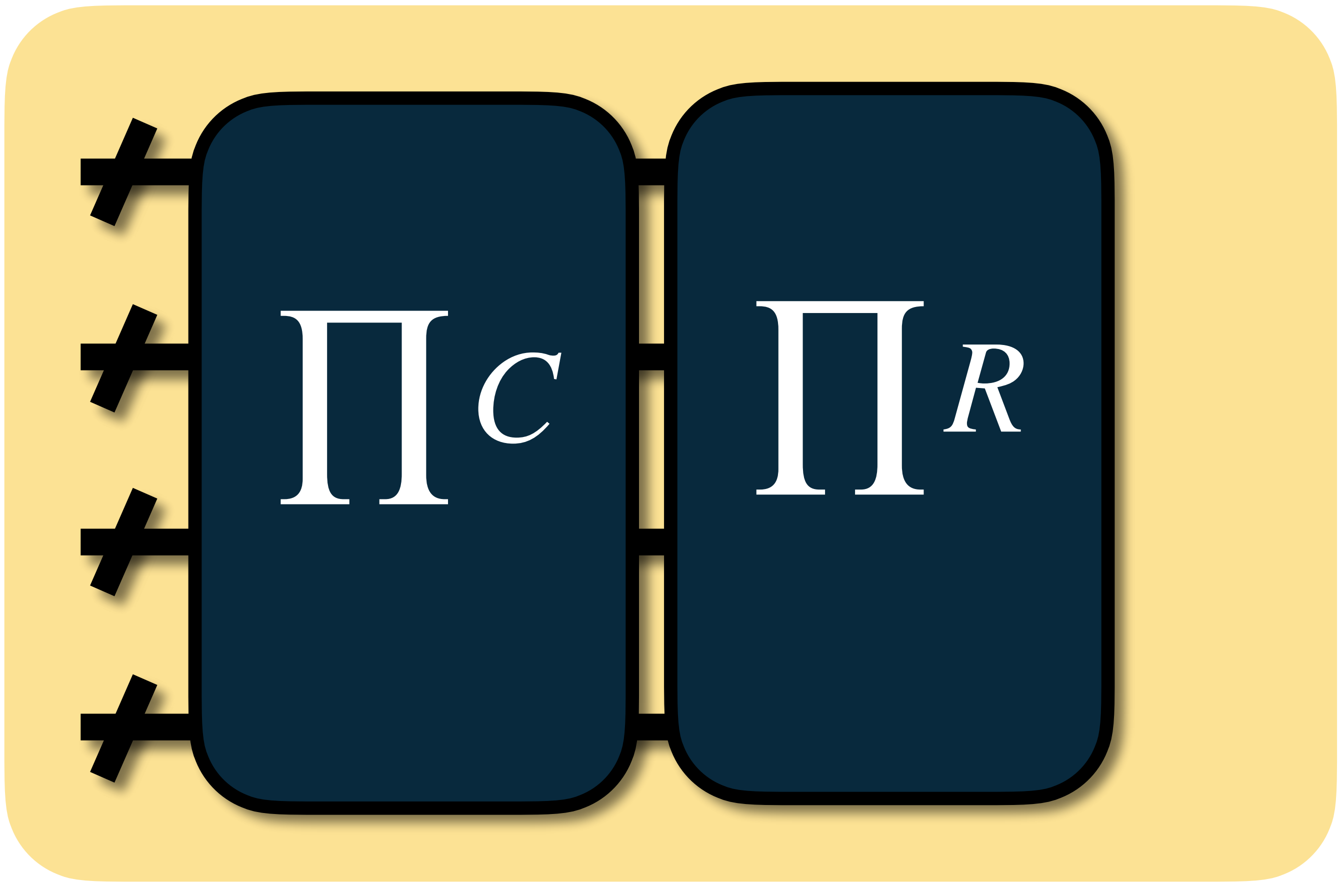
180
135
90
45
0
Energy Error
Heuristic Orbitals
Optimized Orbitals
HF
Single Graph

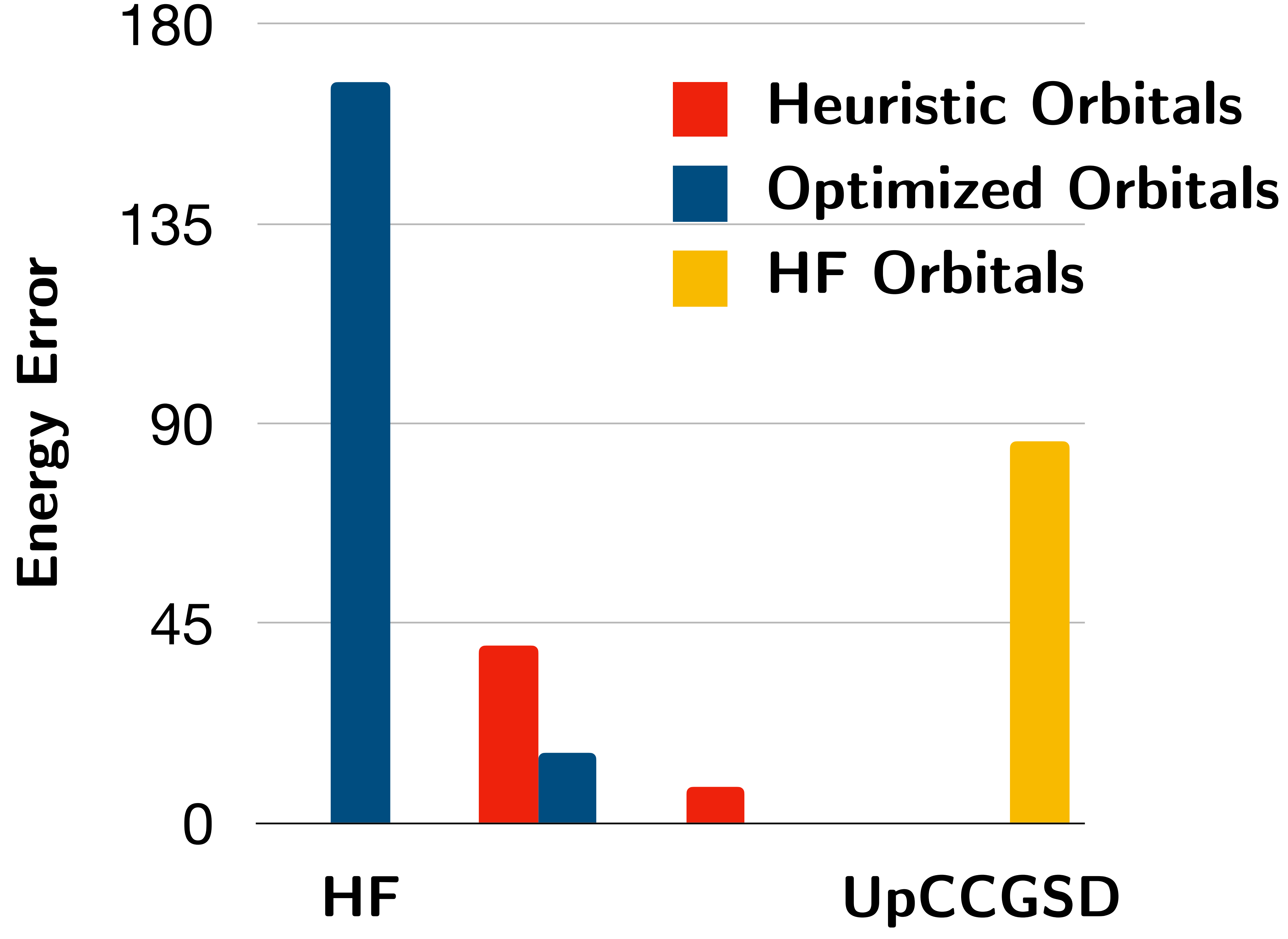


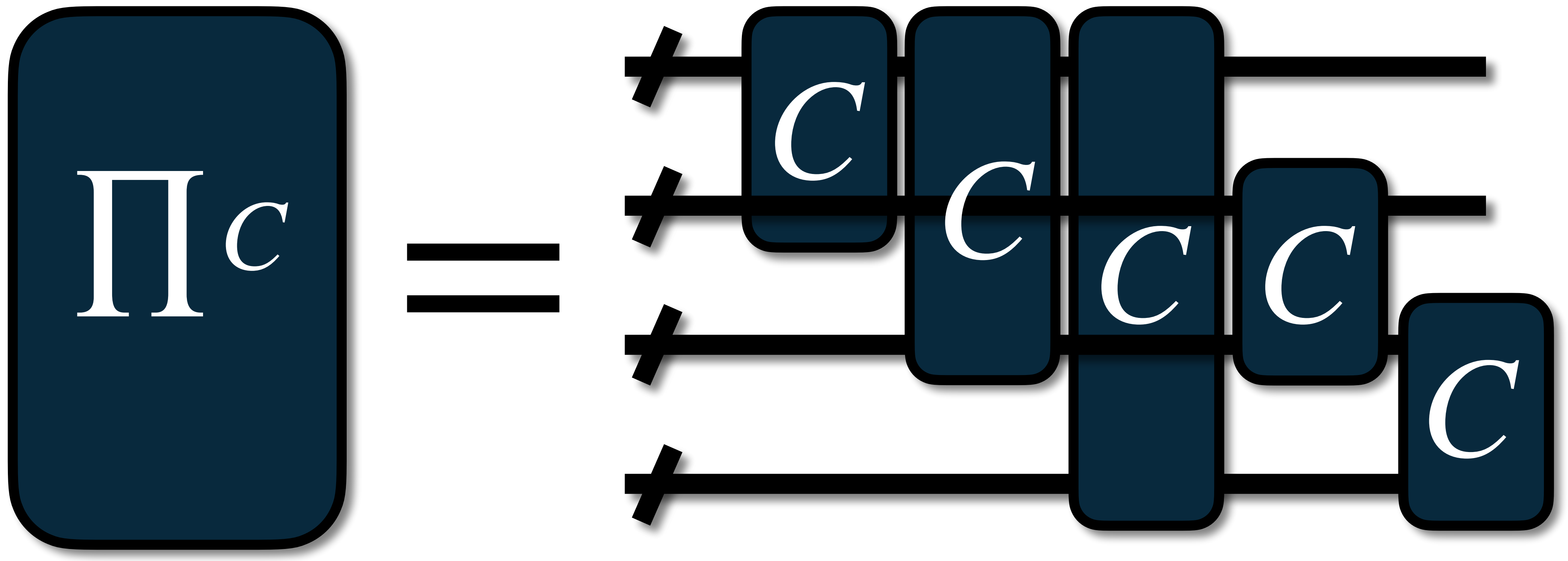


Energy Error
180
135
90
45
0
Heuristic Orbitals
Optimized Orbitals
HF
Two Graphs

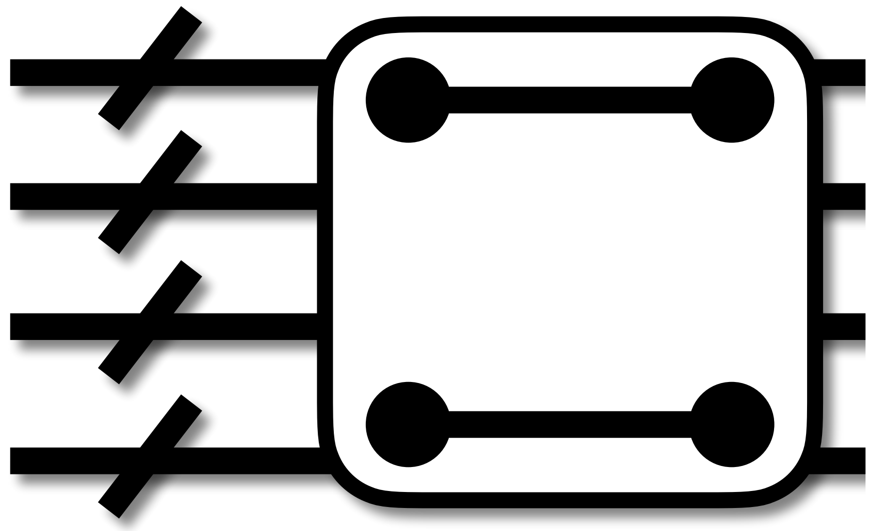




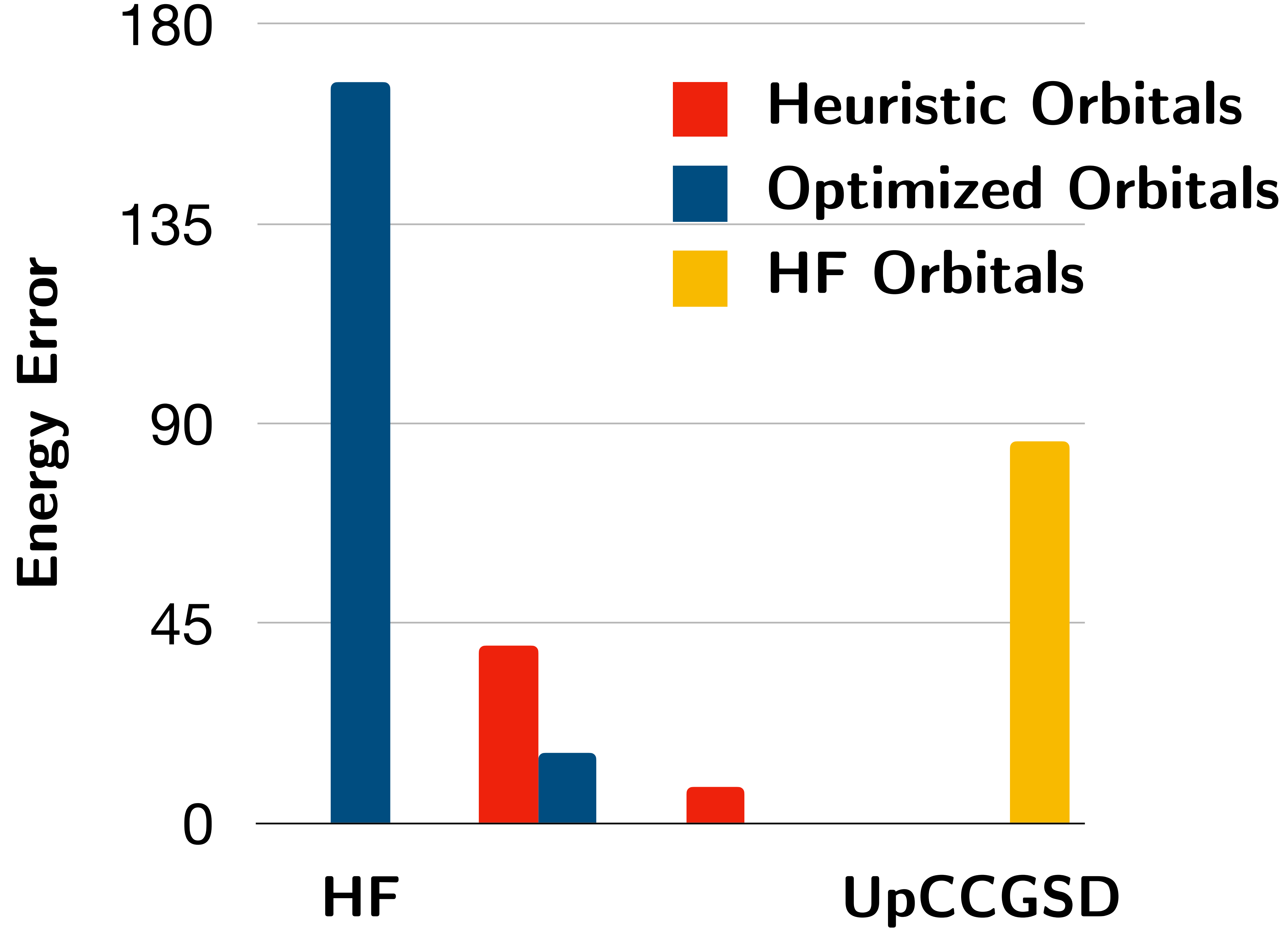


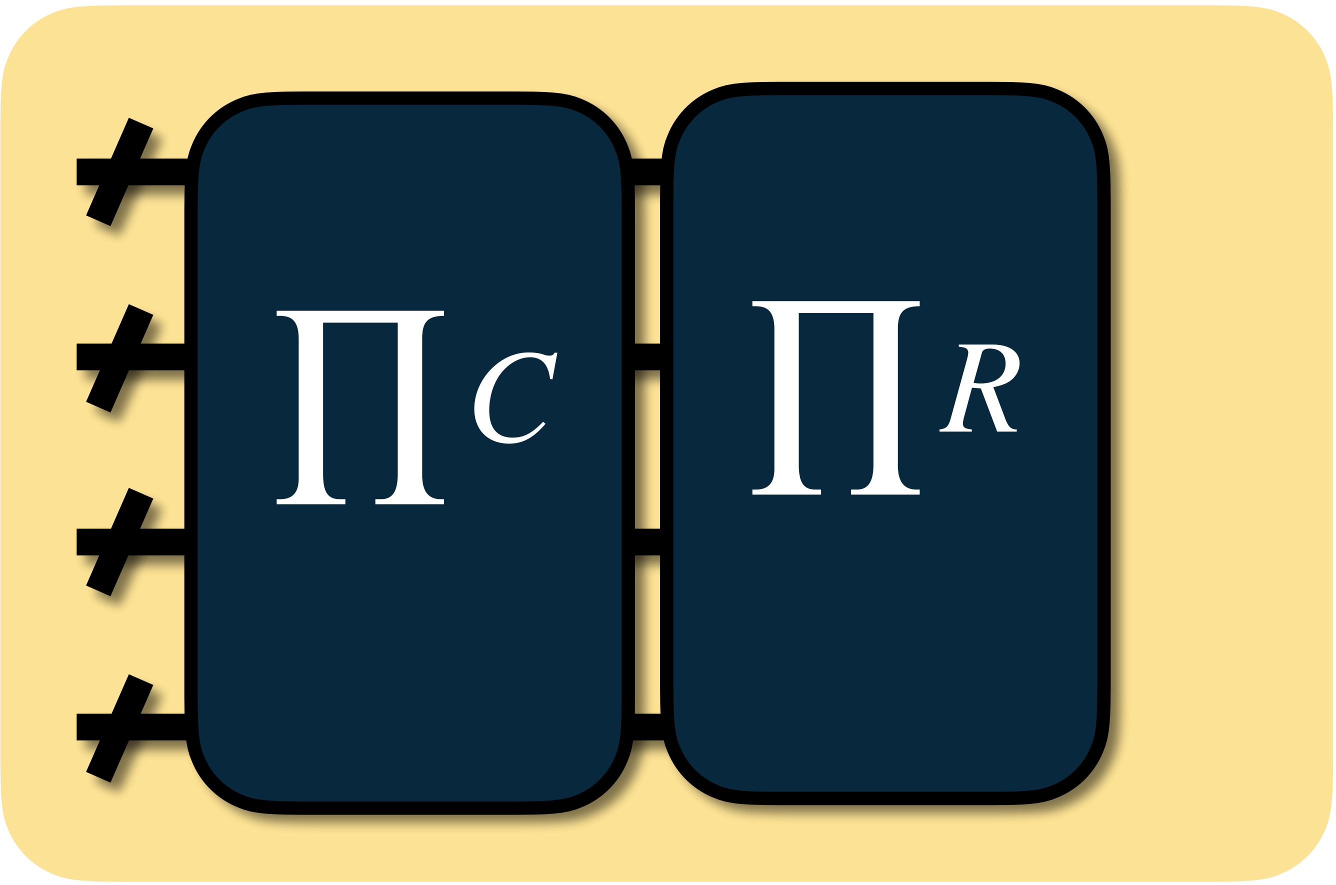


k-UpCCGSD: Lee, JCTC, 2018

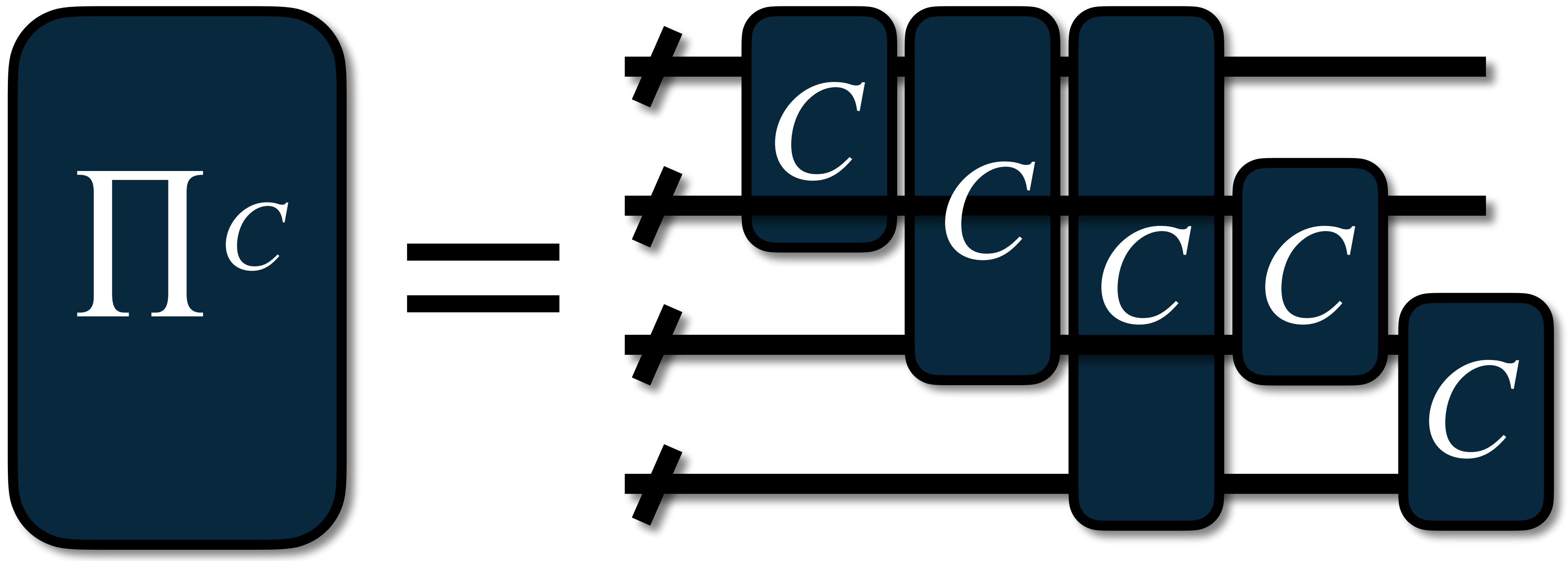


parameters: 4
cnots: 6 — 70

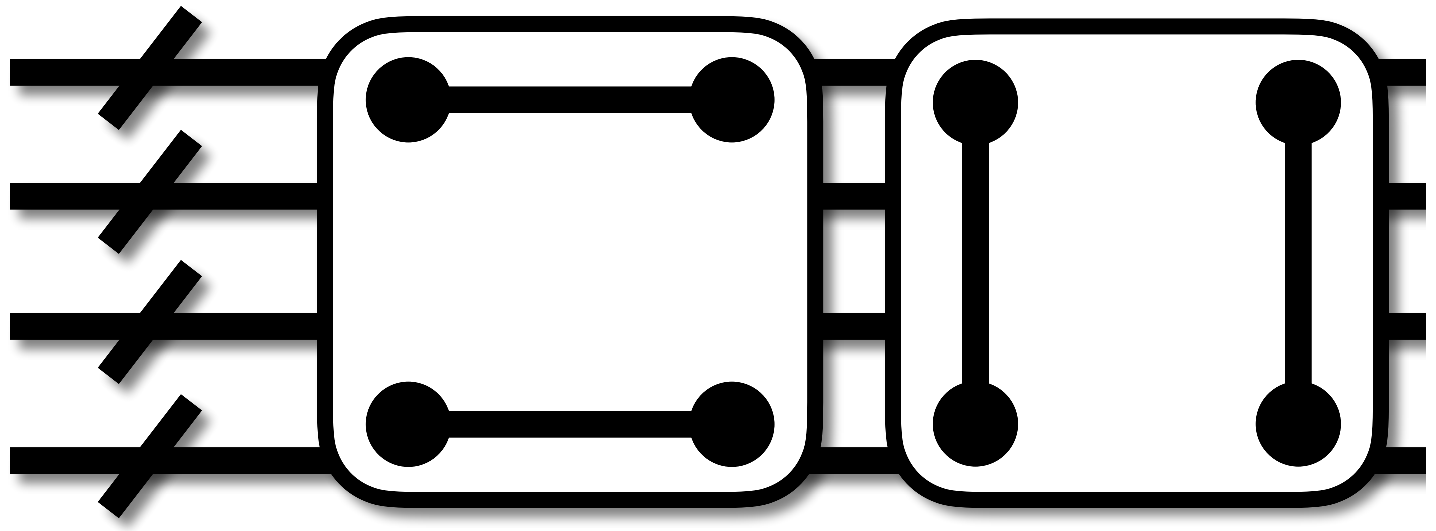




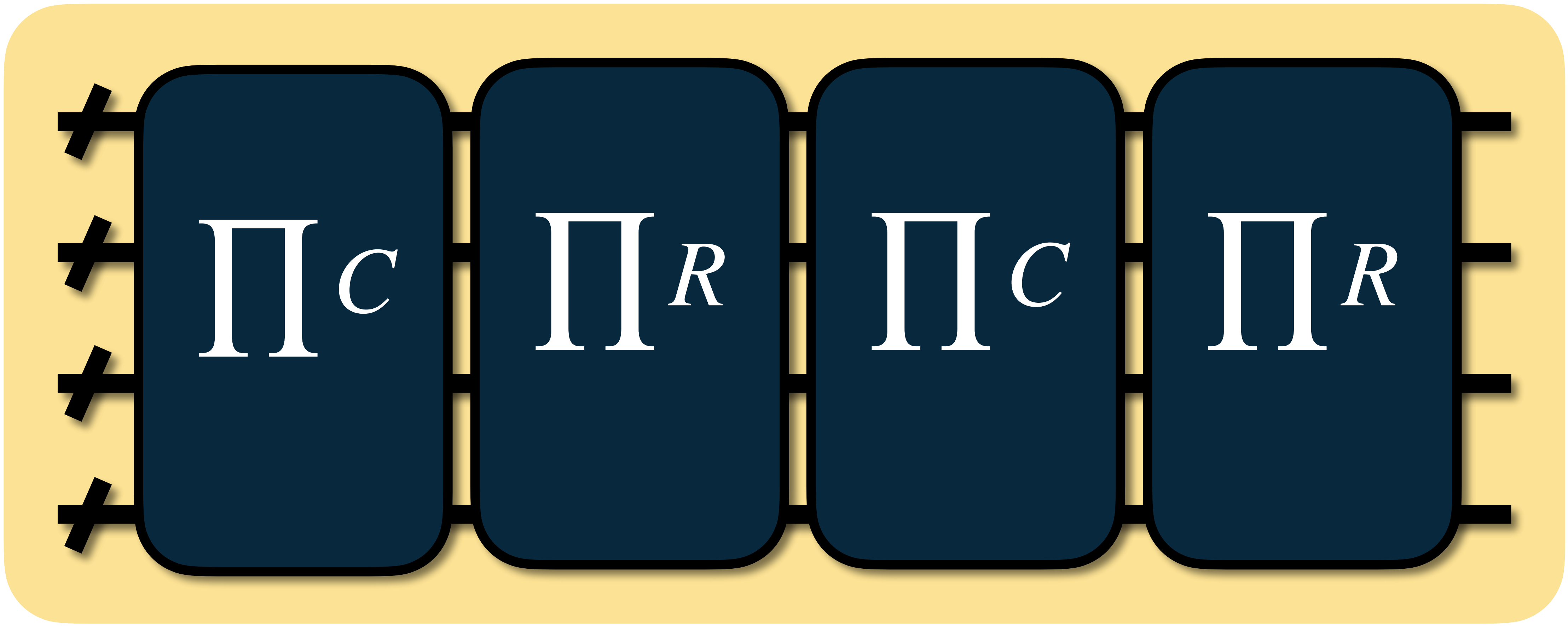
UpCCGSD
parameters: 18
cnots: 66 — 188



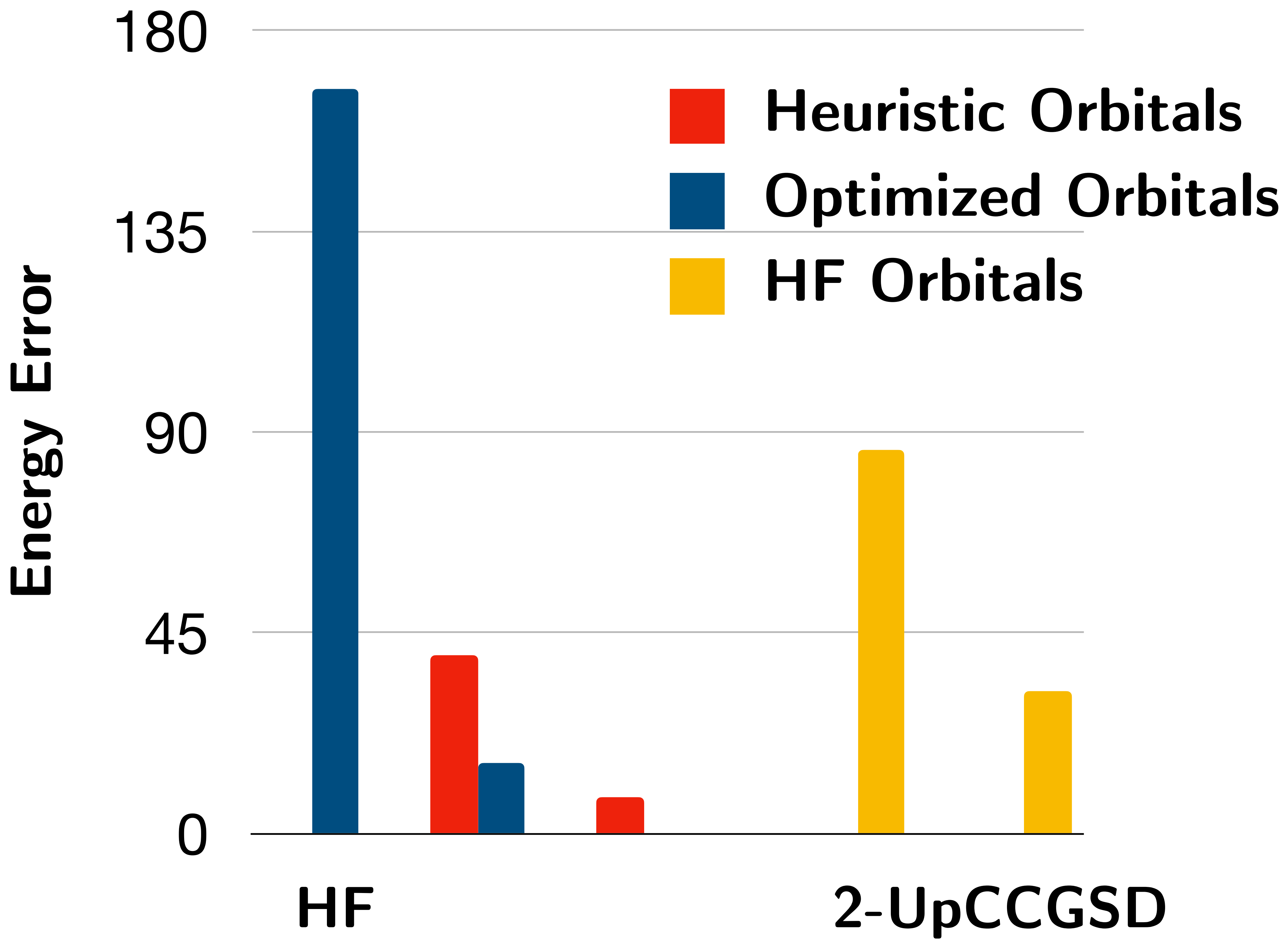
k-UpCCGSD: Lee, JCTC, 2018



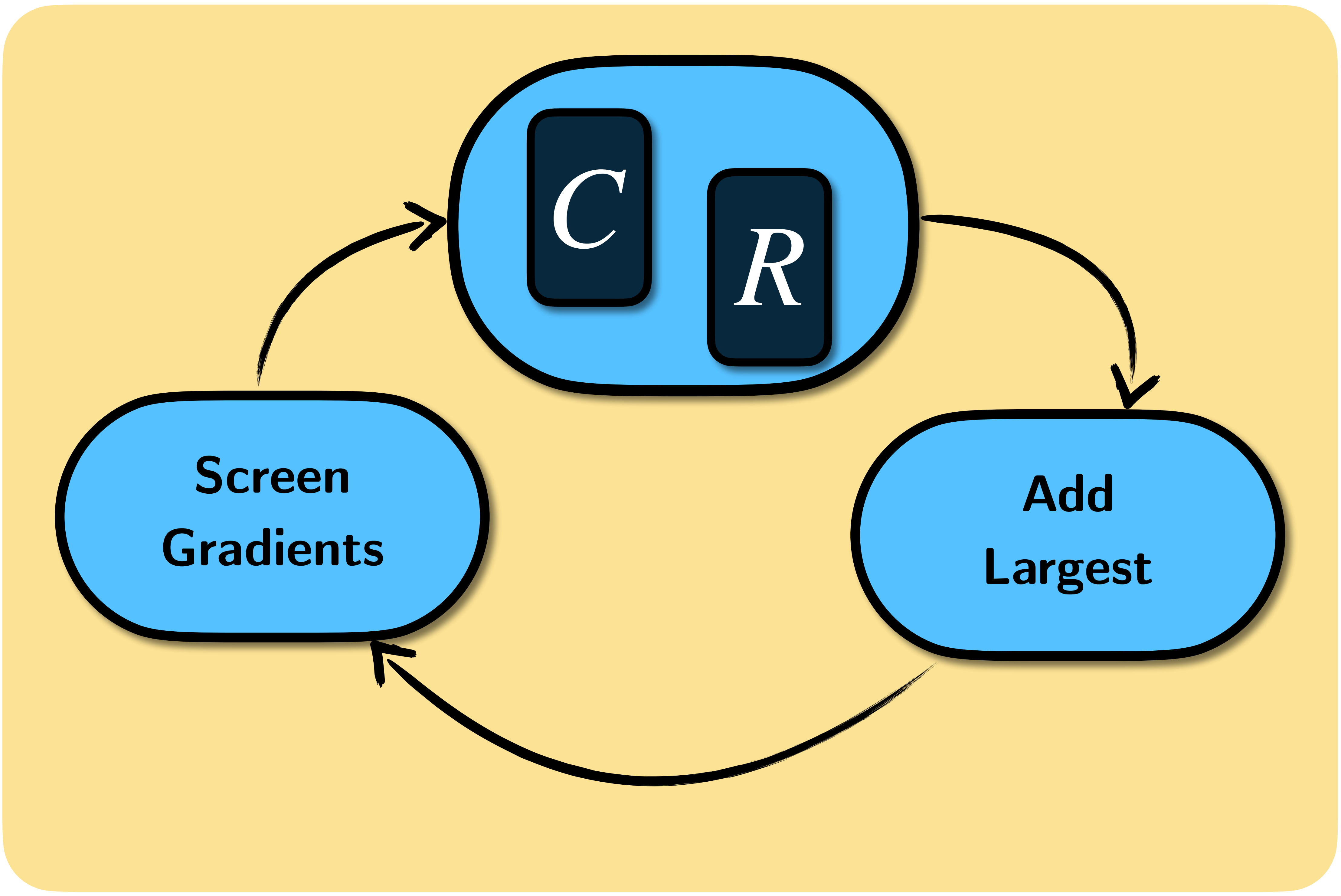
parameters: 6
cnots: 116



2-UpCCGSD
parameters: 36
cnots: 432

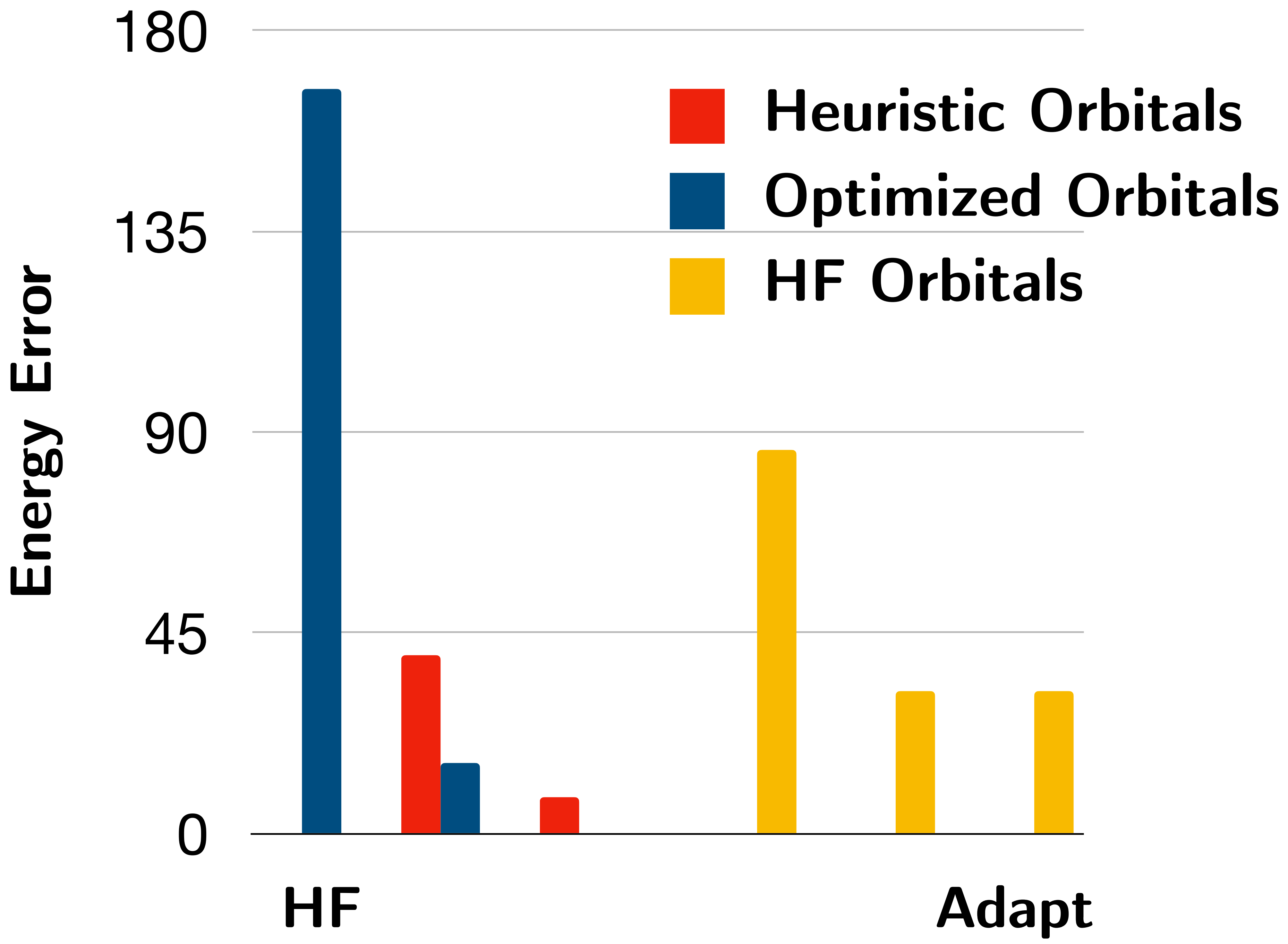


k-UpCCGSD: Lee, JCTC, 2018



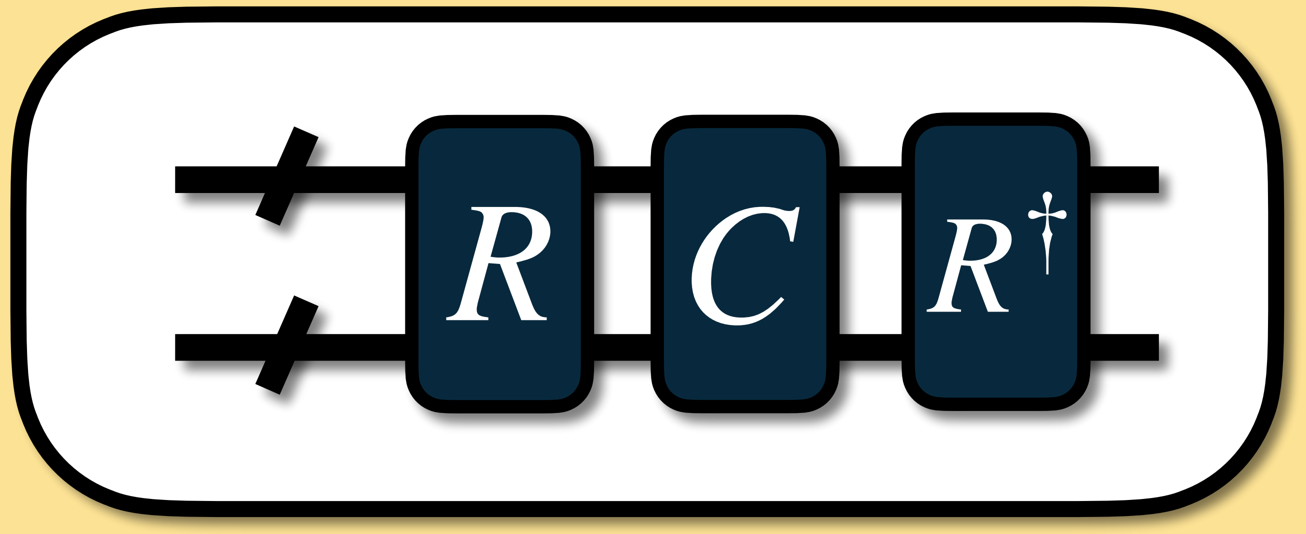
2-UpCCGSD
parameters: 36
cnots: 432

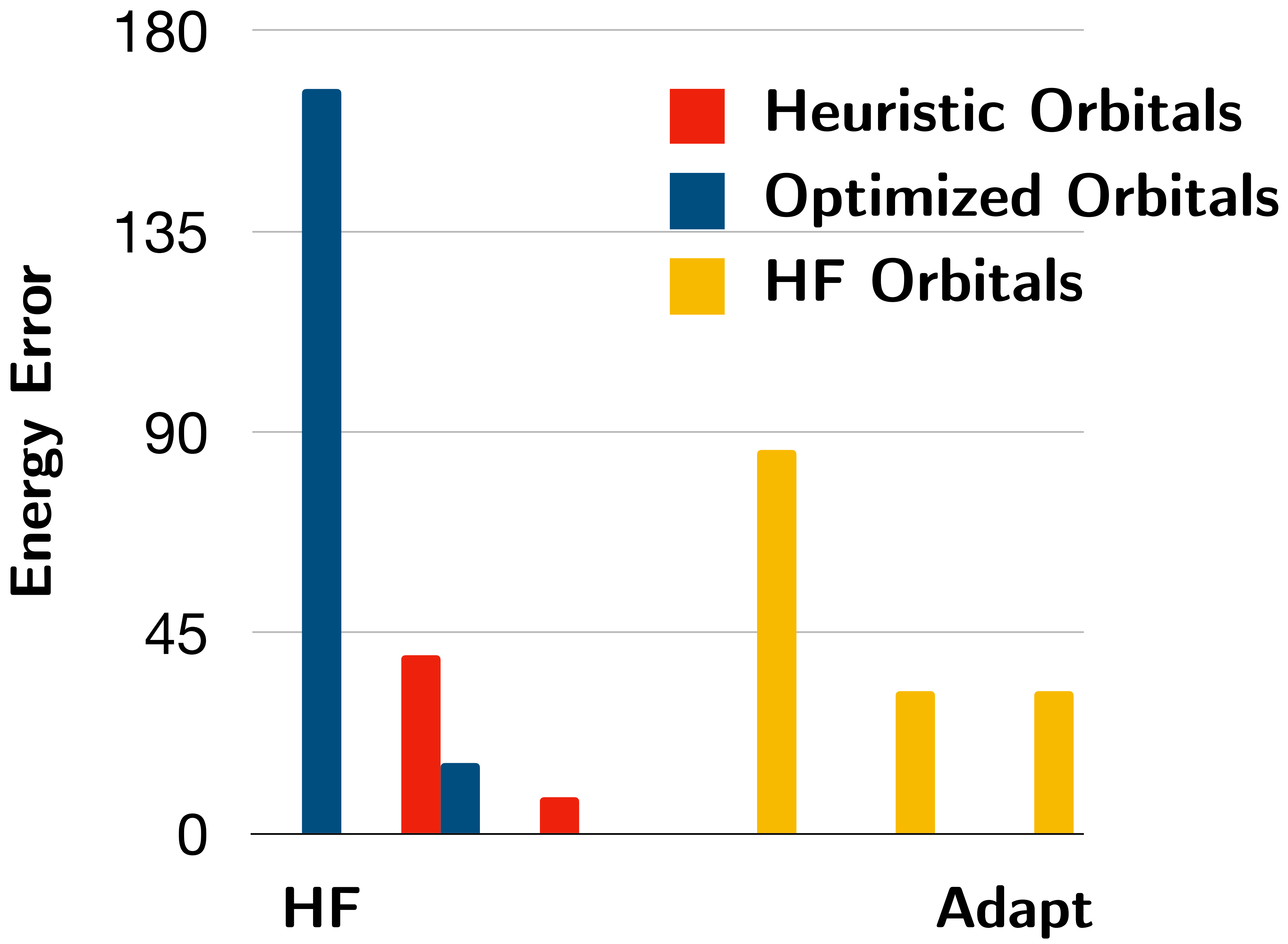
Adapt(C,R)
parameters: 12
cnots: 448



Adapt: Grimsley/Mayhall, Nat. Comm, 2019

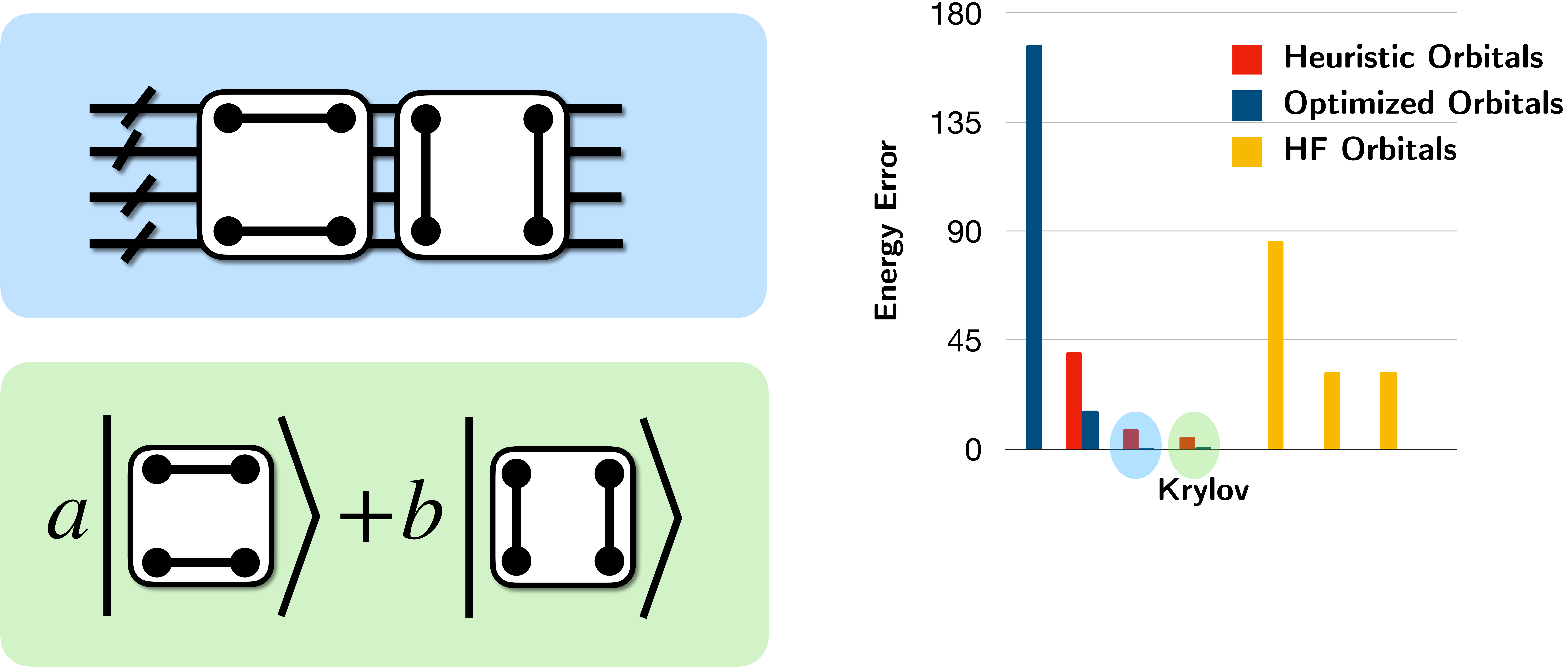
Motif hard to detect locally





2-UpCCGSD
parameters: 36
cnots: 432

Adapt(C,R)
parameters: 12
cnots: 448


180
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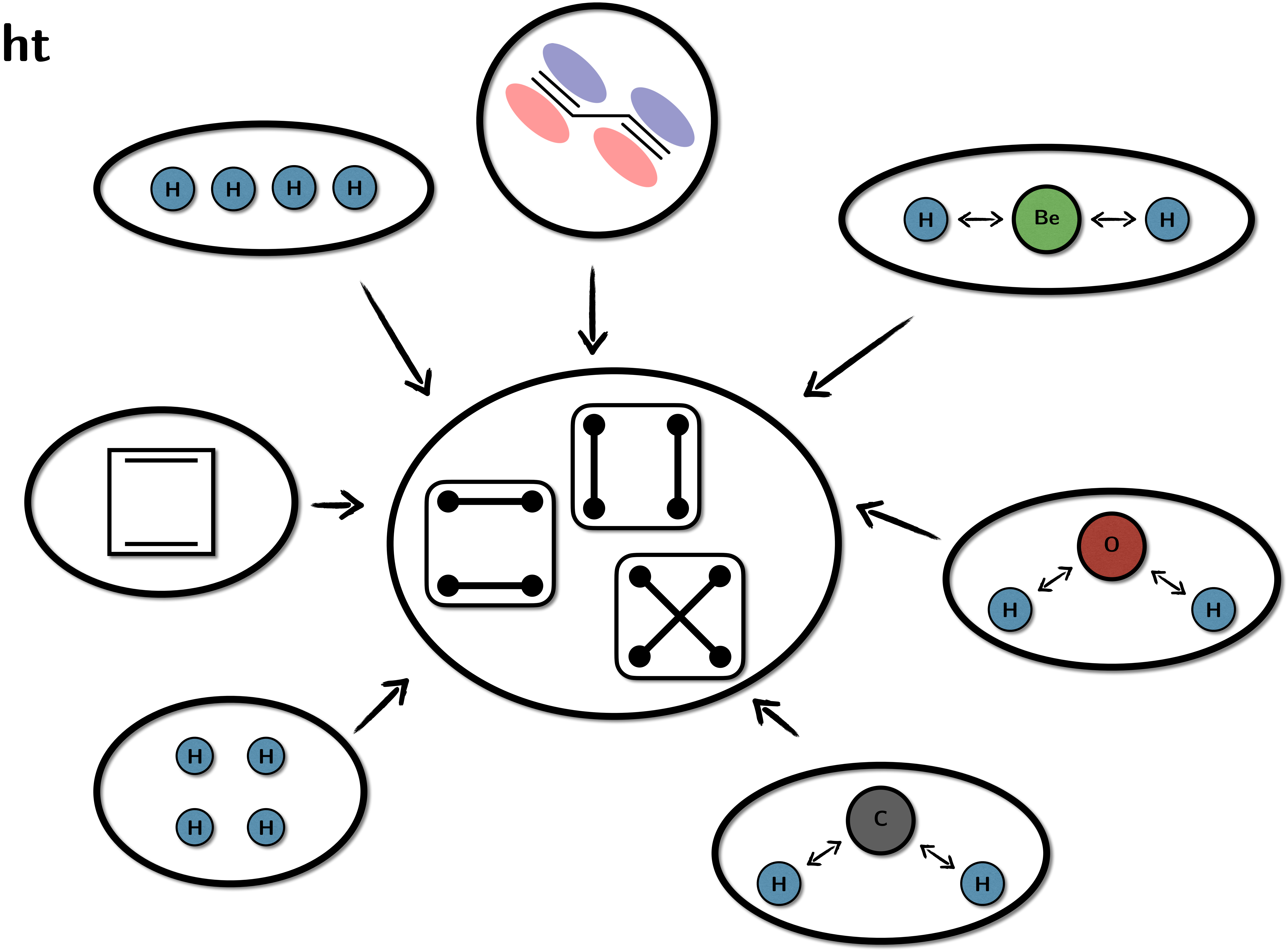
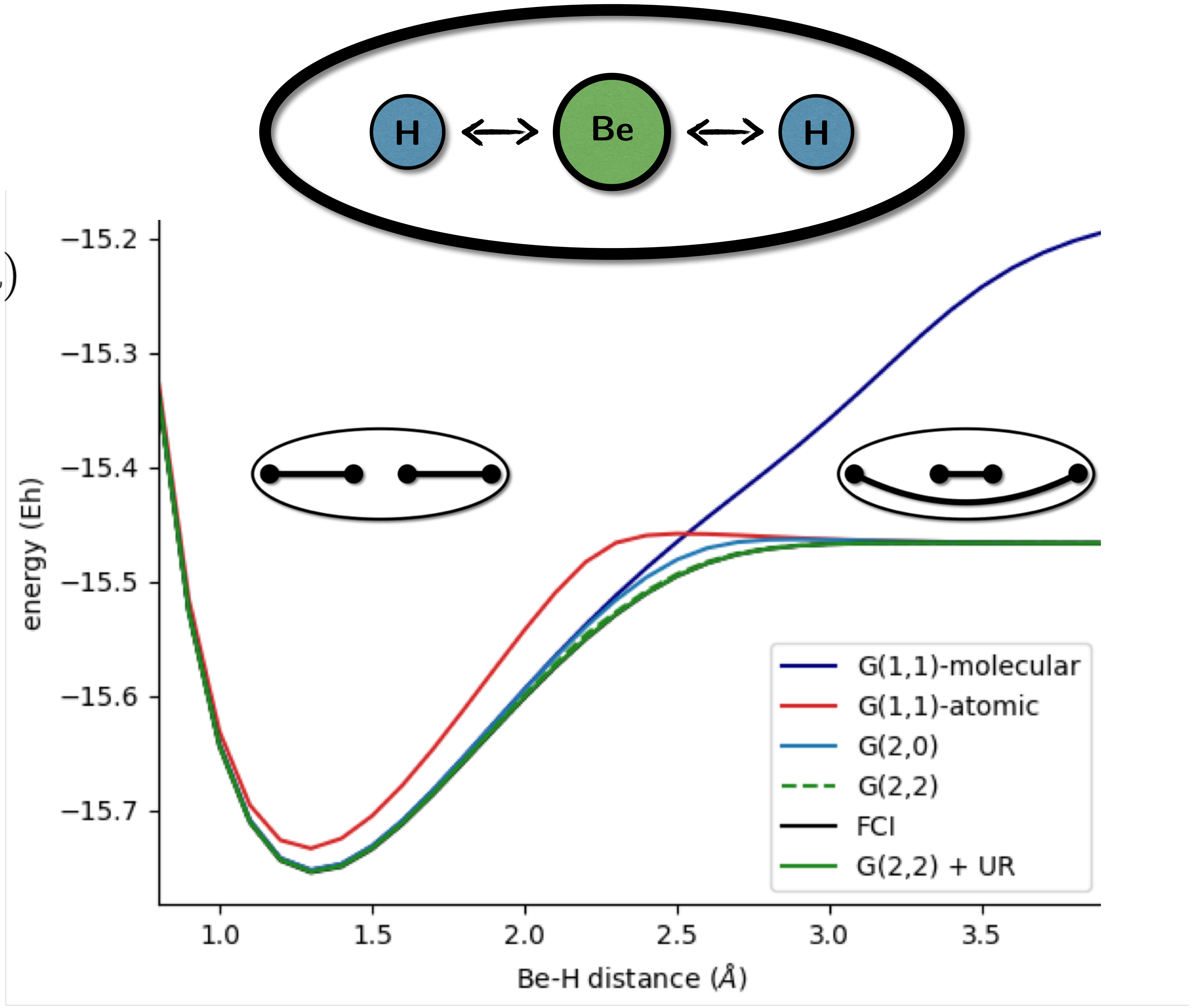
Energy Error
Heuristic Orbitals
Optimized Orbitals
HF Orbitals
Krylov

Transfer Insight



(a)



H
Be
H
−15.2
−15.3
−15.4
−15.5
−15.6
−15.7
energy (Eh)
1.0
1.5
2.0
2.5
3.0
3.5
Be-H distance (Å)
G(1,1)-molecular
G(1,1)-atomic
G(2,0)
G(2,2)
FCI
G(2,2) + UR

Single Graphs (automatized)

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,†]

Multi-Graphs (concept & examples)

Molecular Quantum Circuit Design: A Graph-Based Approach

Jakob S. Kottmann[*]
(Dated: July 27, 2022)

Krylov-Style Multi-Graphs

Compact Effective Basis Generation: Insights from Interpretable Circuit Design

Jakob S. Kottmann[1] and Francesco Scala[2]

quantum
open-source
foundation

Universität
Augsburg
University

PhD Position Available

code examples online

github/kottmanj/talks_and_material

github.com/tequilahub