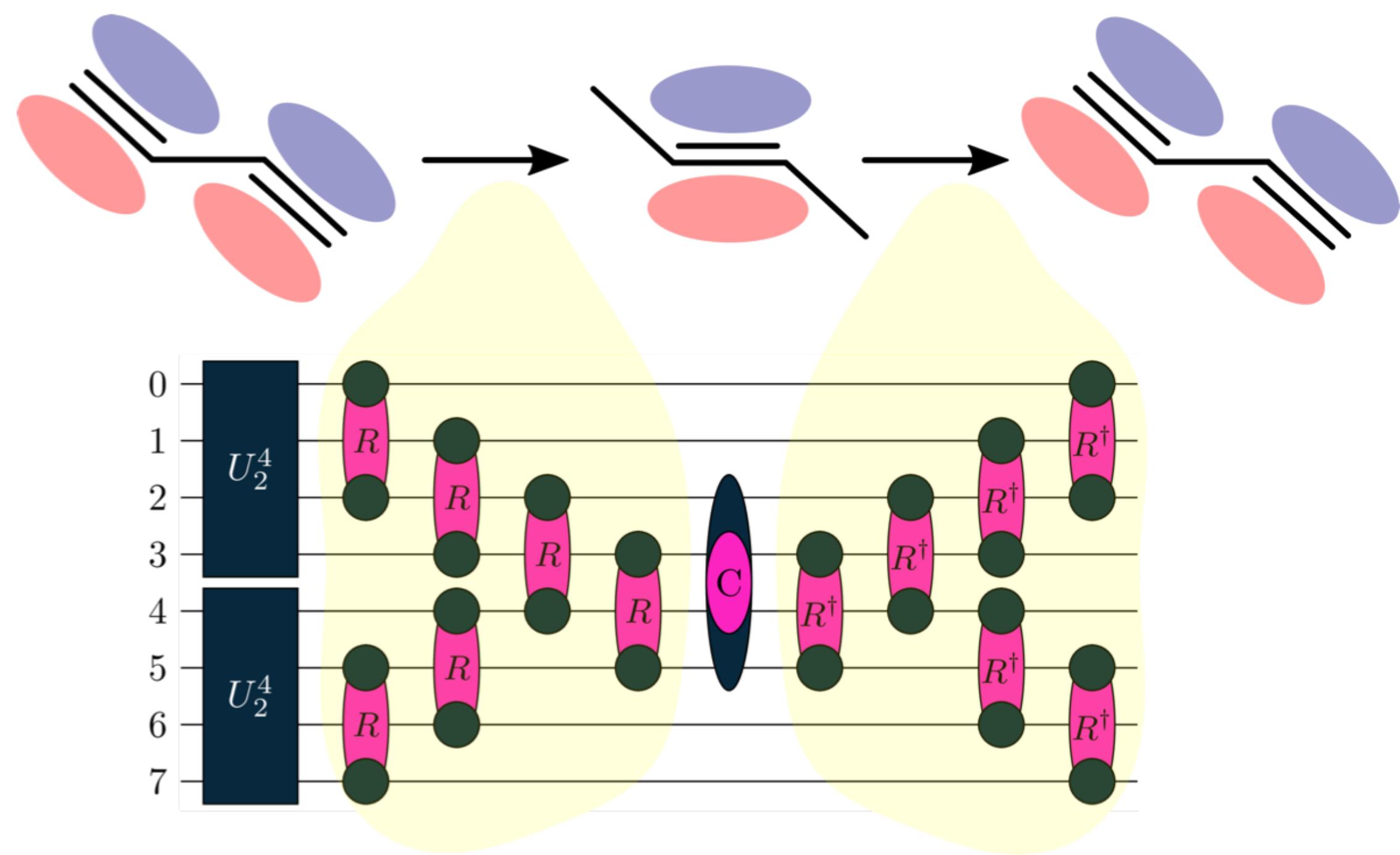
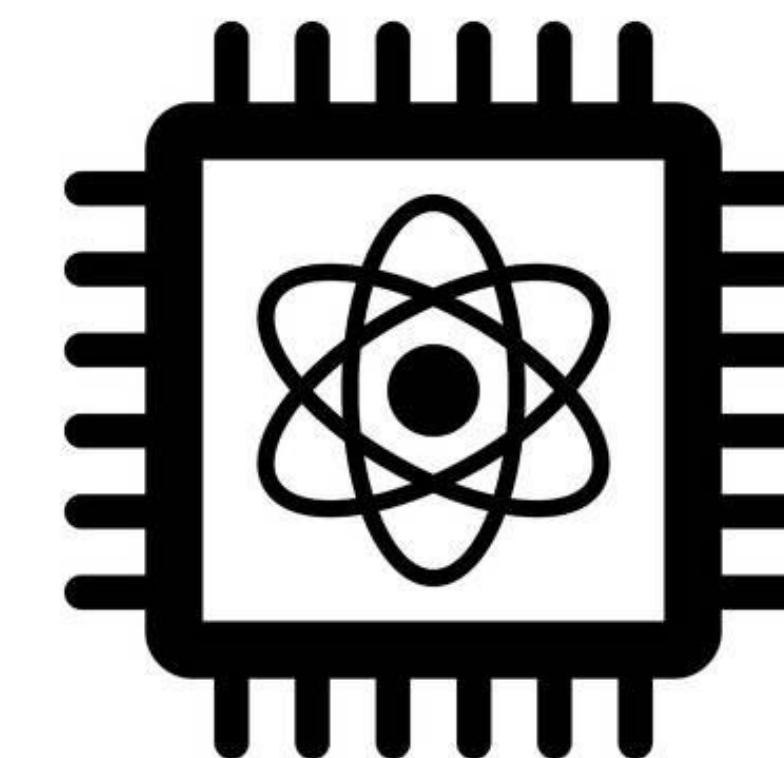
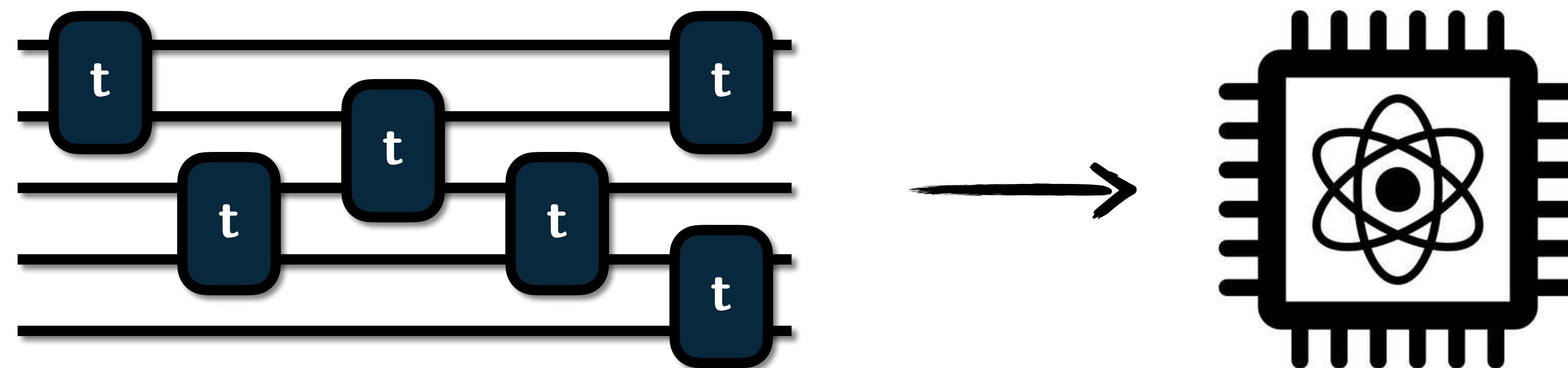


Molecular Quantum Circuit Design

Jakob S. Kottmann
Institute for Computer Science
University of Augsburg





Variational
Quantum
Eigensolvers (VQE)



measure expectation value and
gradient



Perruzzo/McClean, Nat. Comm, 2014

McClean, NJP, 2016

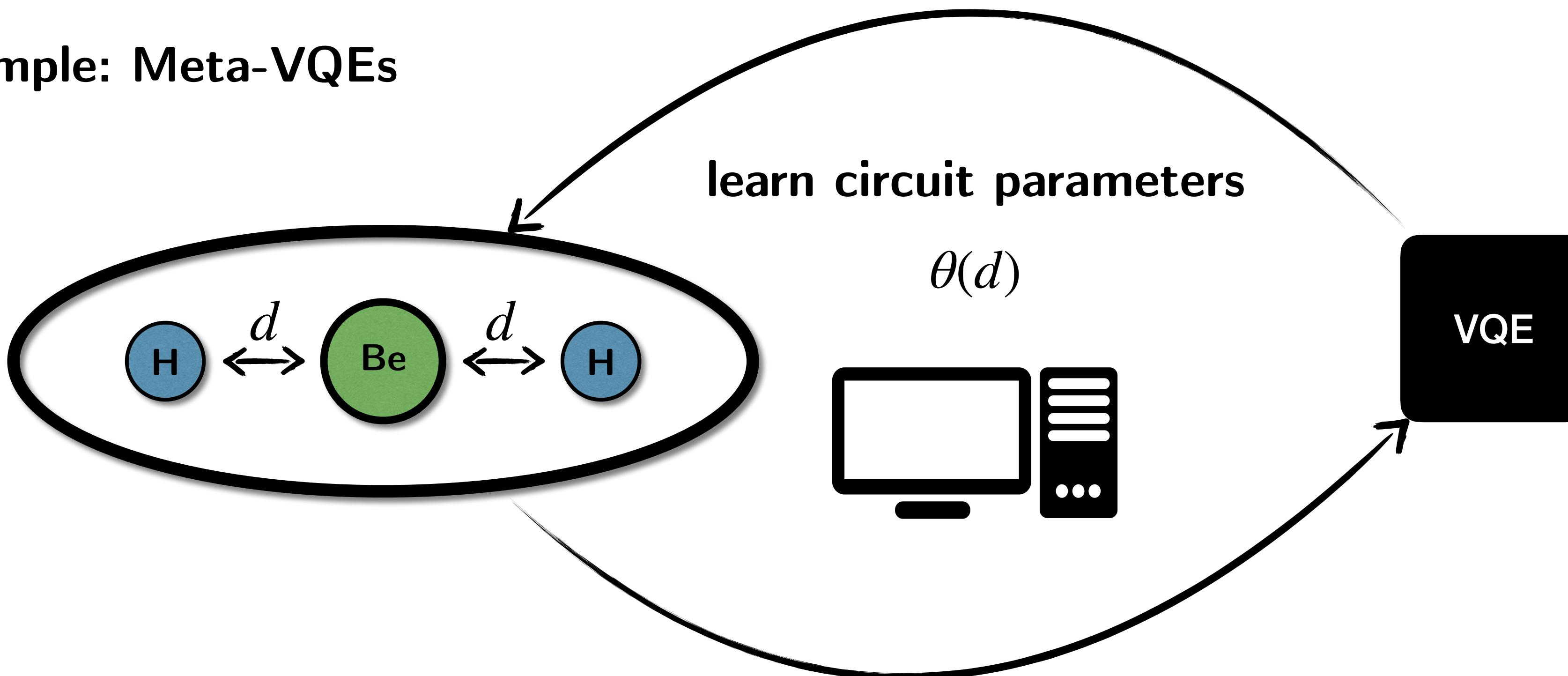
Motivation: VQEs as black-boxes

Many projects need robust VQEs

Motivation: VQEs as black-boxes

Proof of concept 
scalability: challenging!

Example: Meta-VQEs

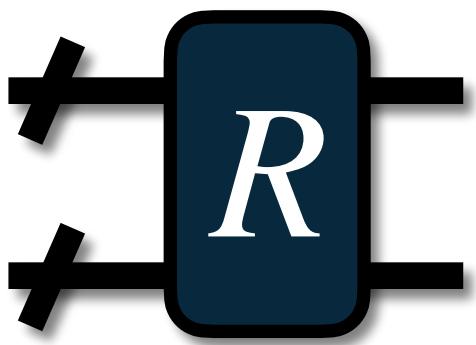


Basic Building Blocks

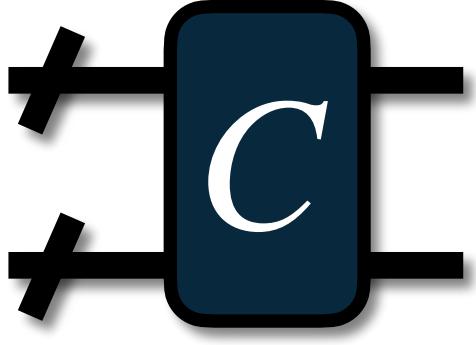
Analogy

basis change

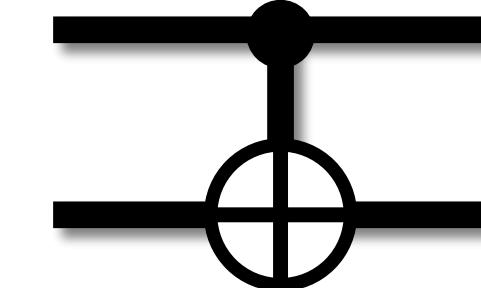
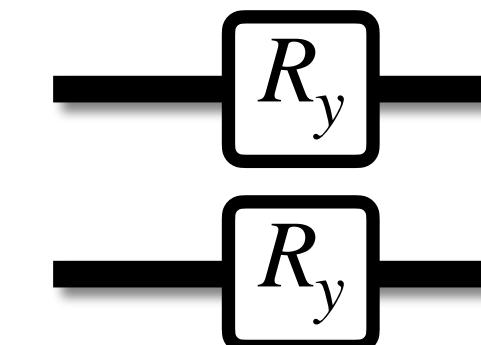
electronic structure



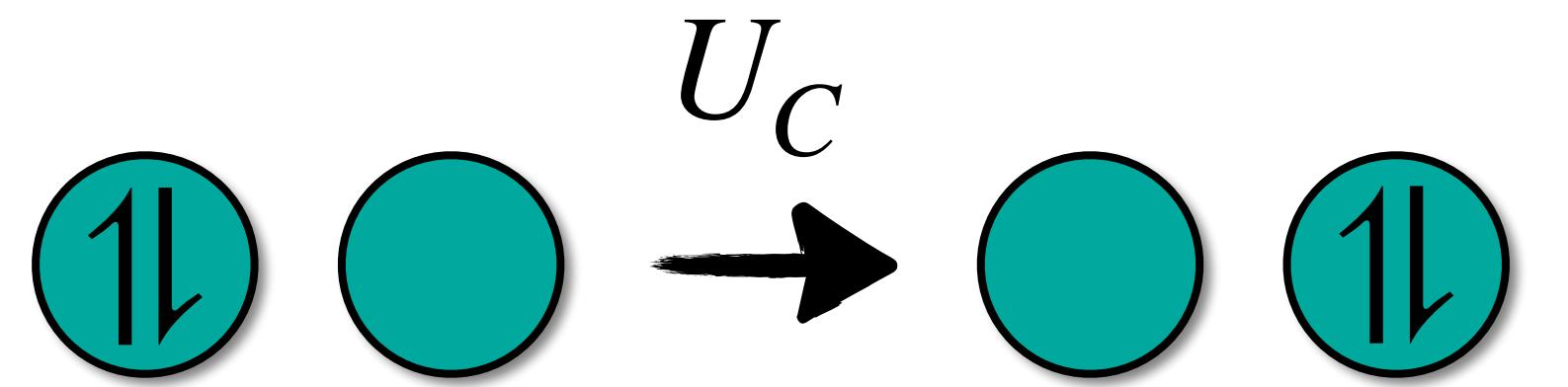
correlate



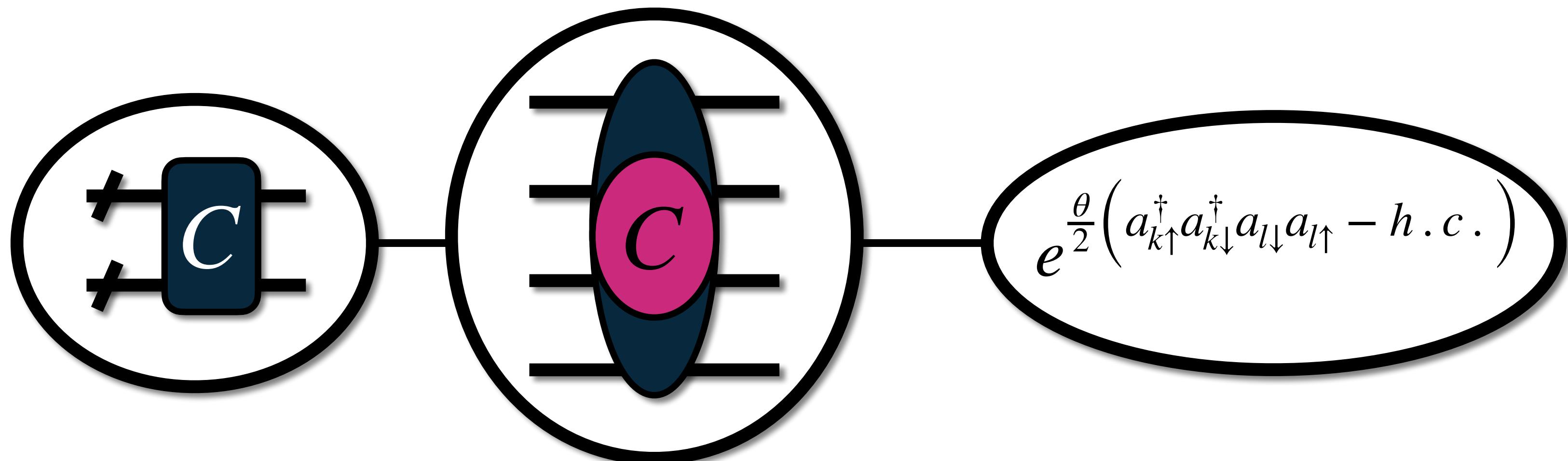
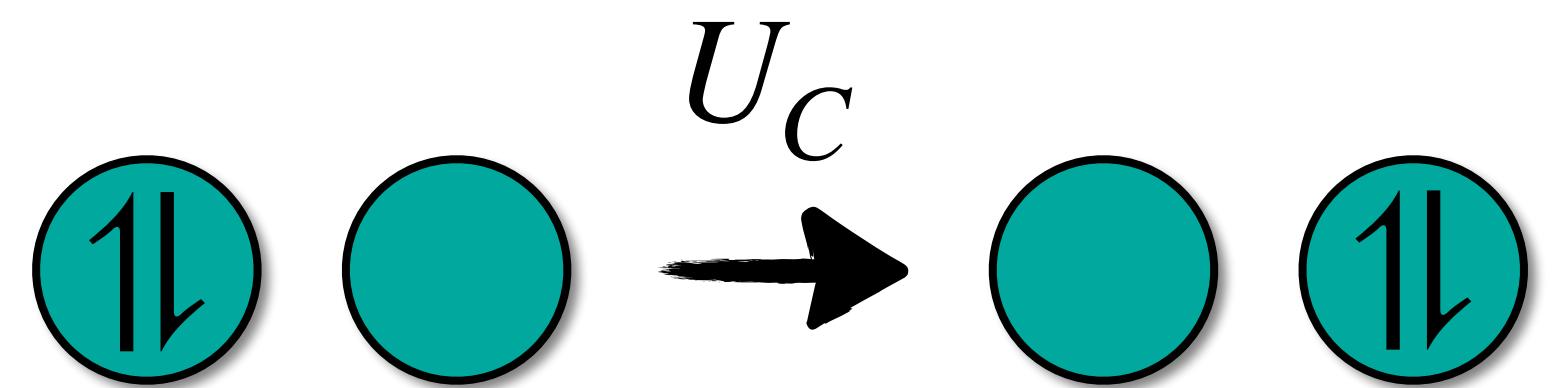
quantum machine learning



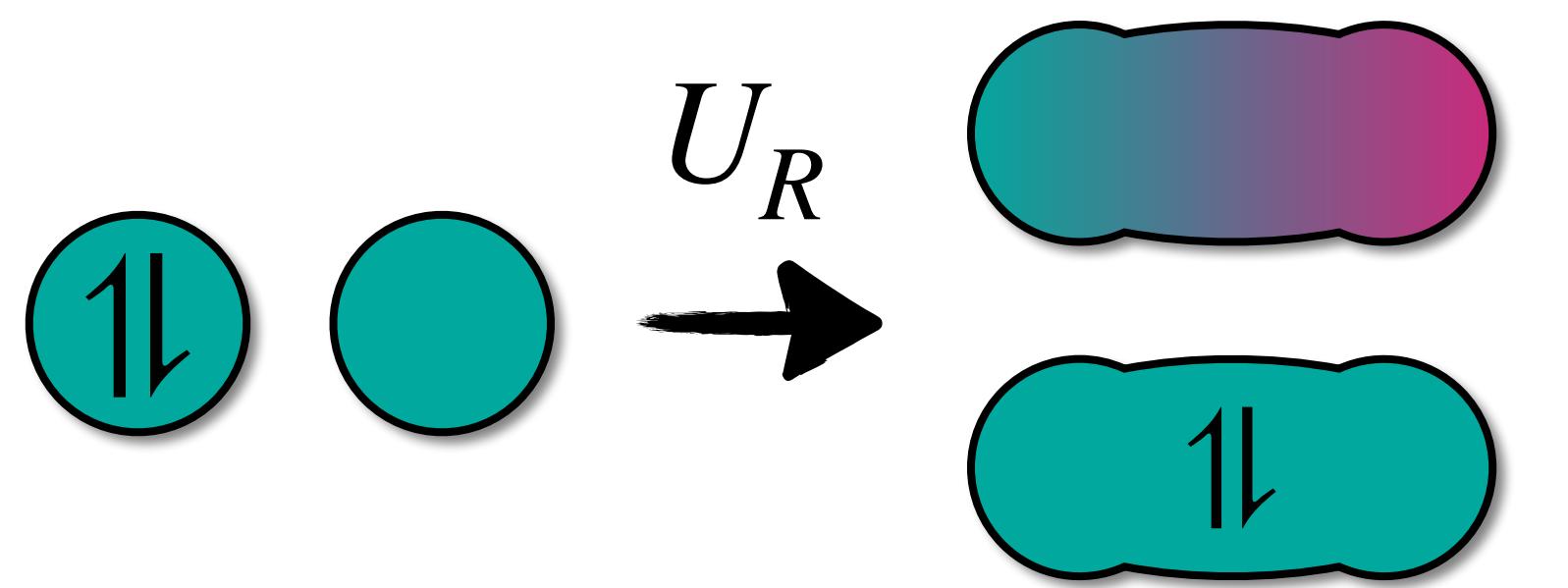
Pair Correlators



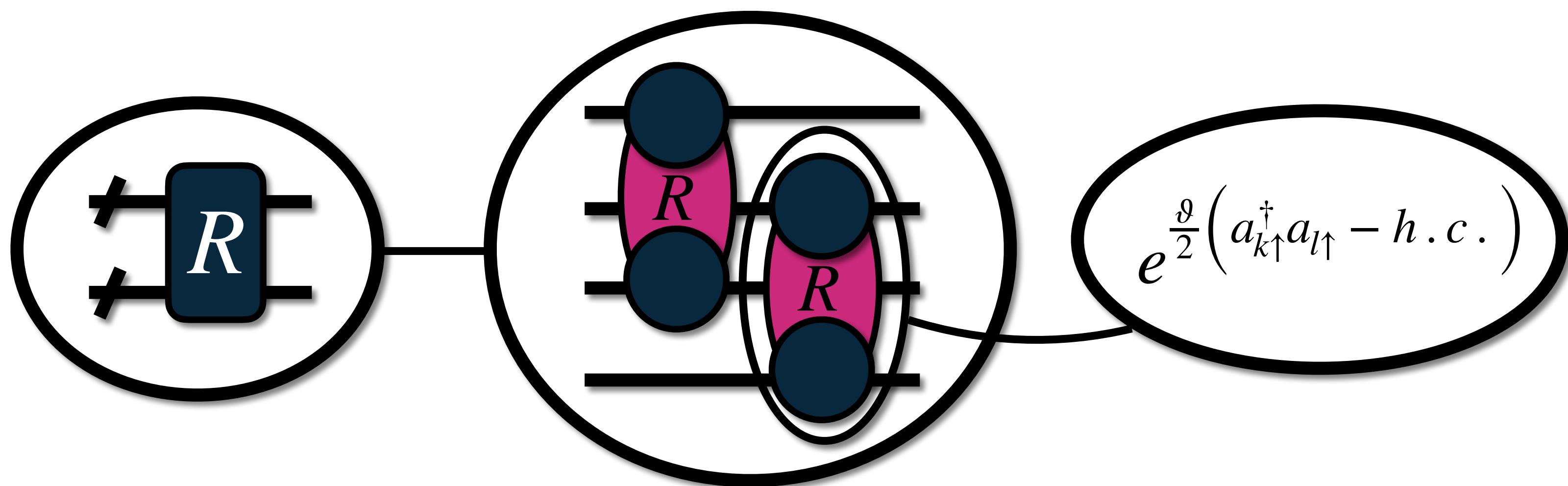
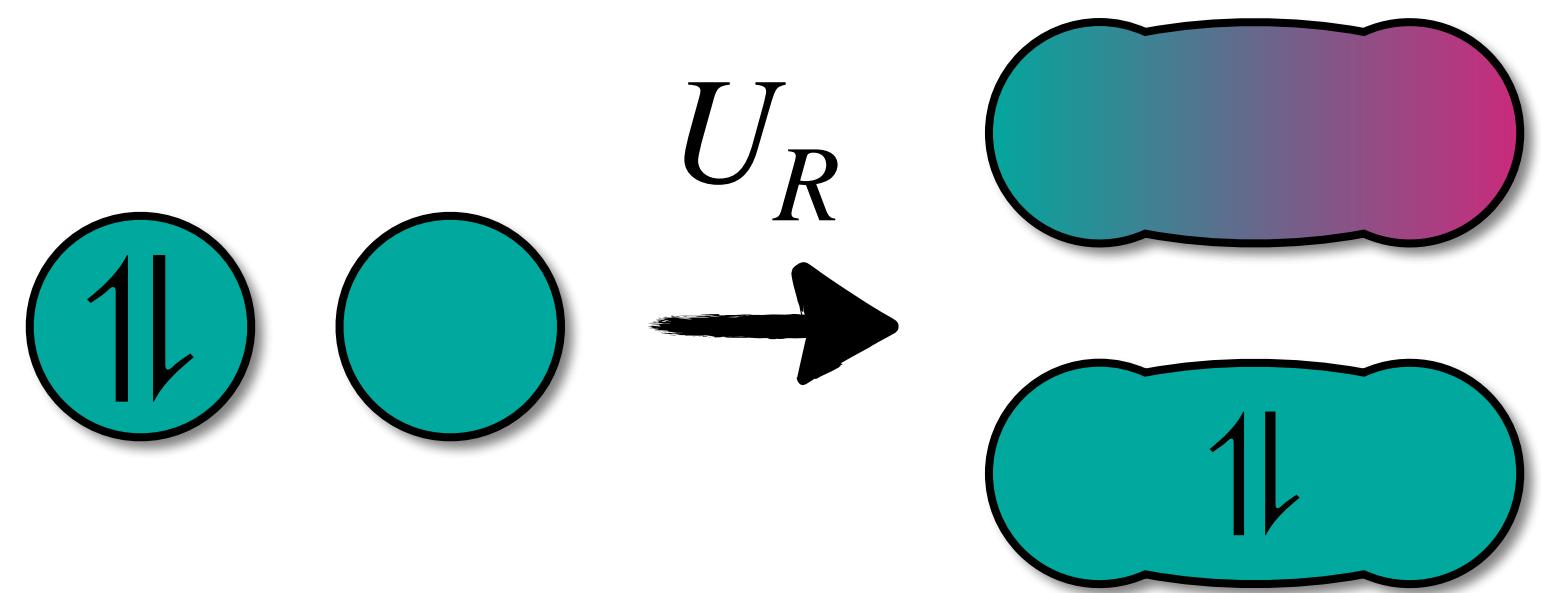
Pair Correlators



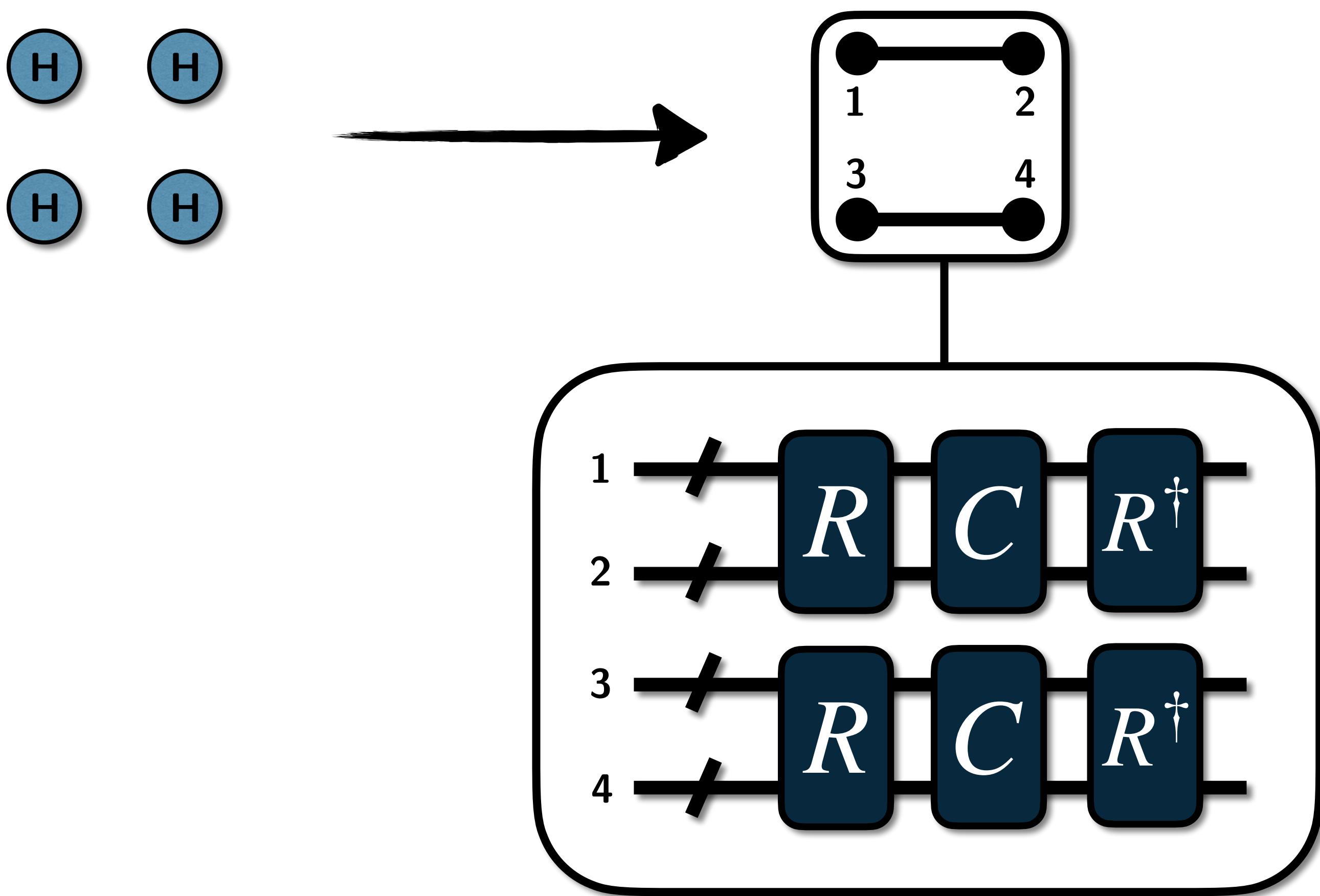
Basis Change



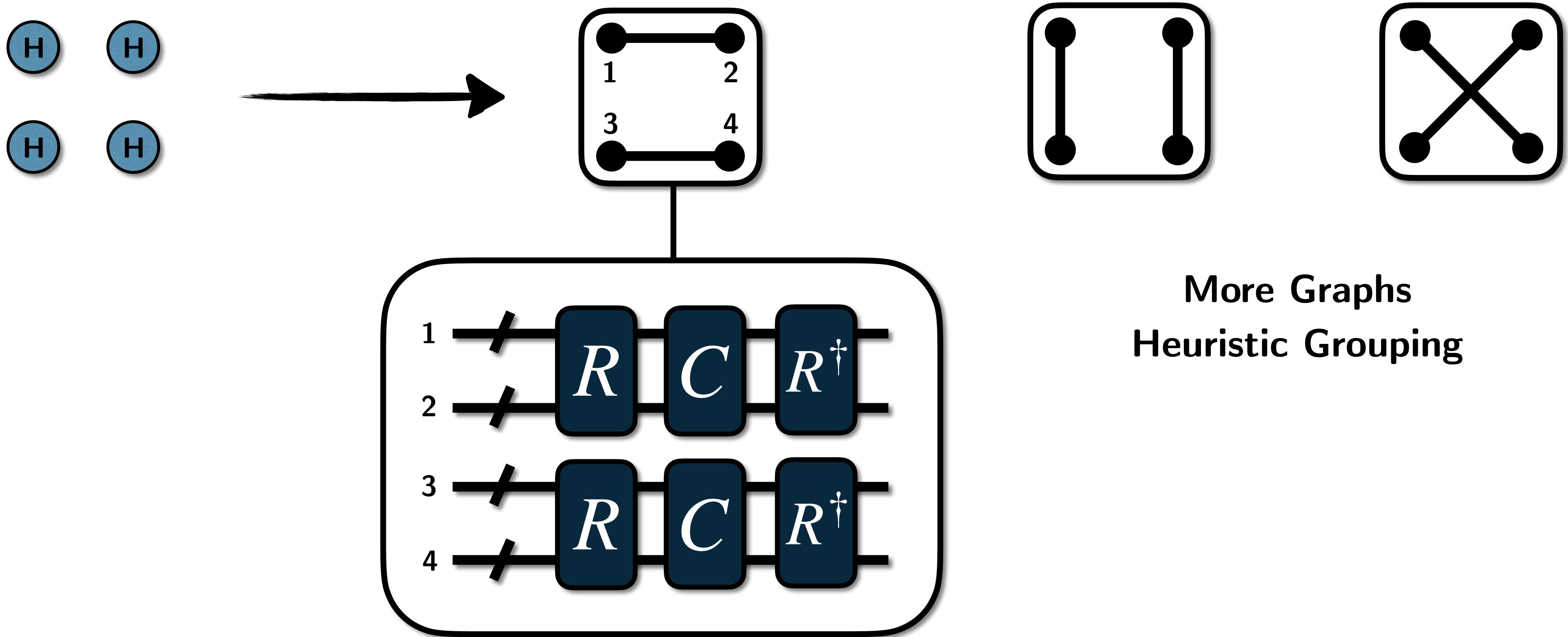
Basis Change



High-Level Design

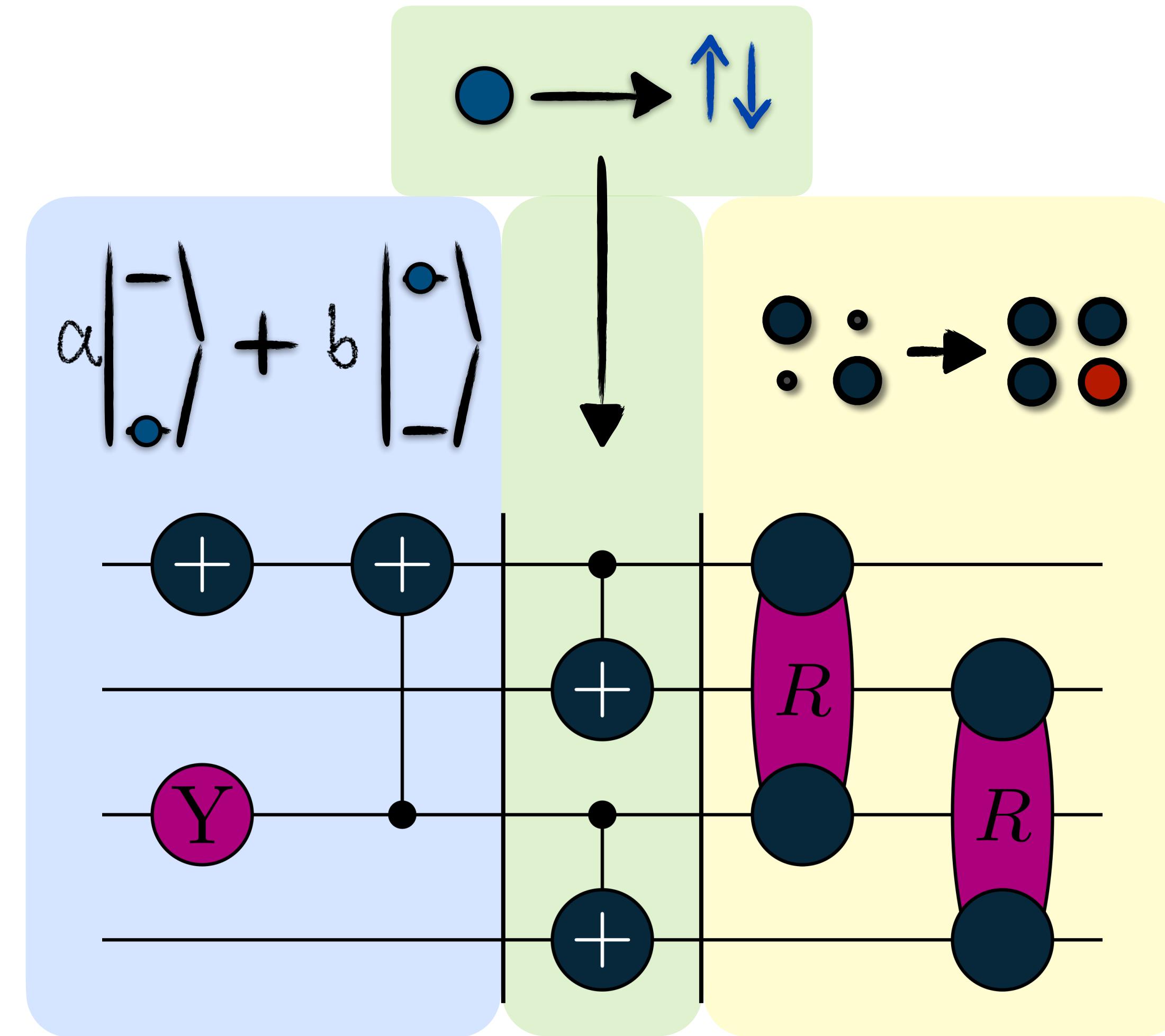
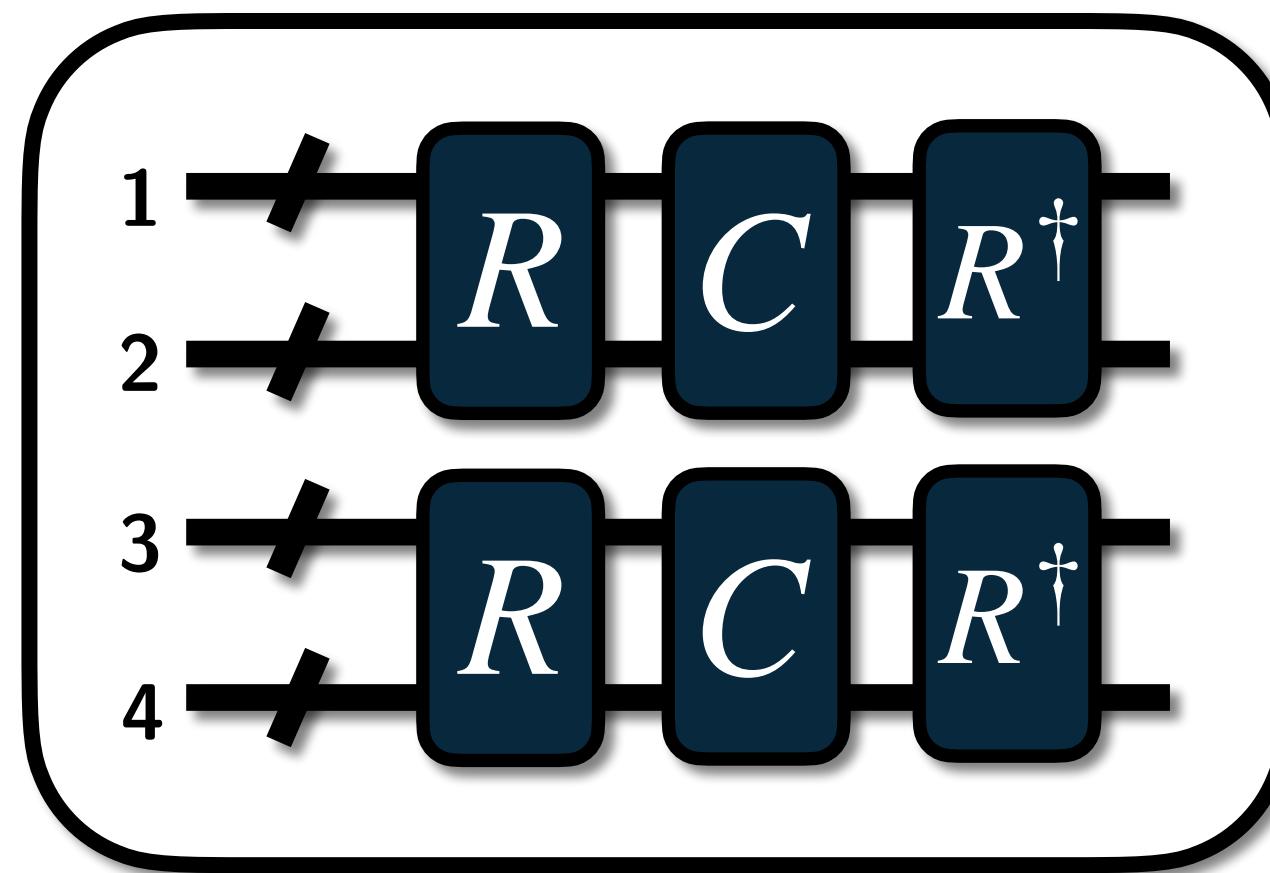


High-Level Design

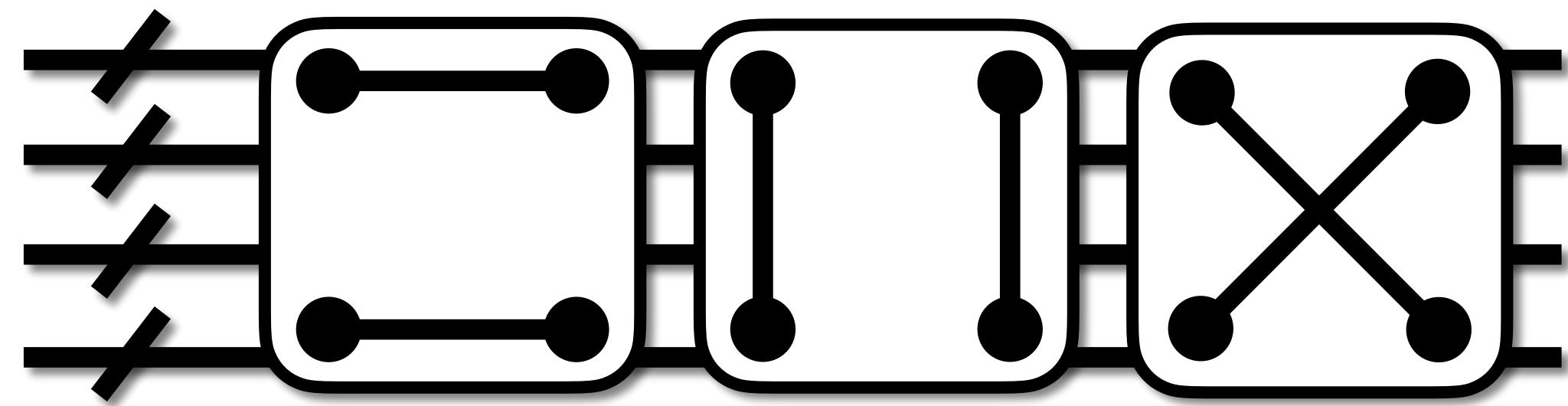


Single graphs are cheap

wavefunctions classically tractable



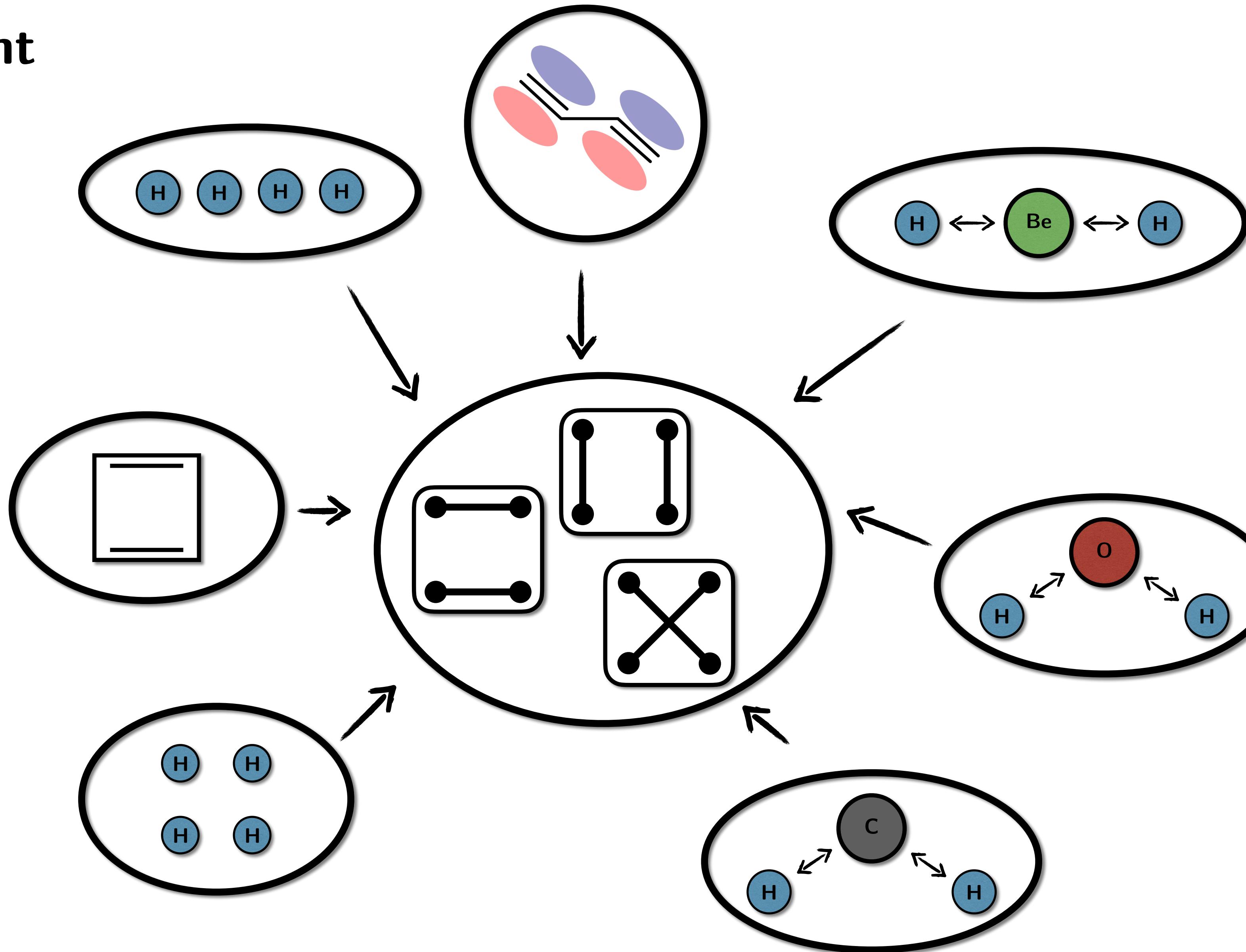
VQE-Style Wavefunction



Subspace Wavefunction

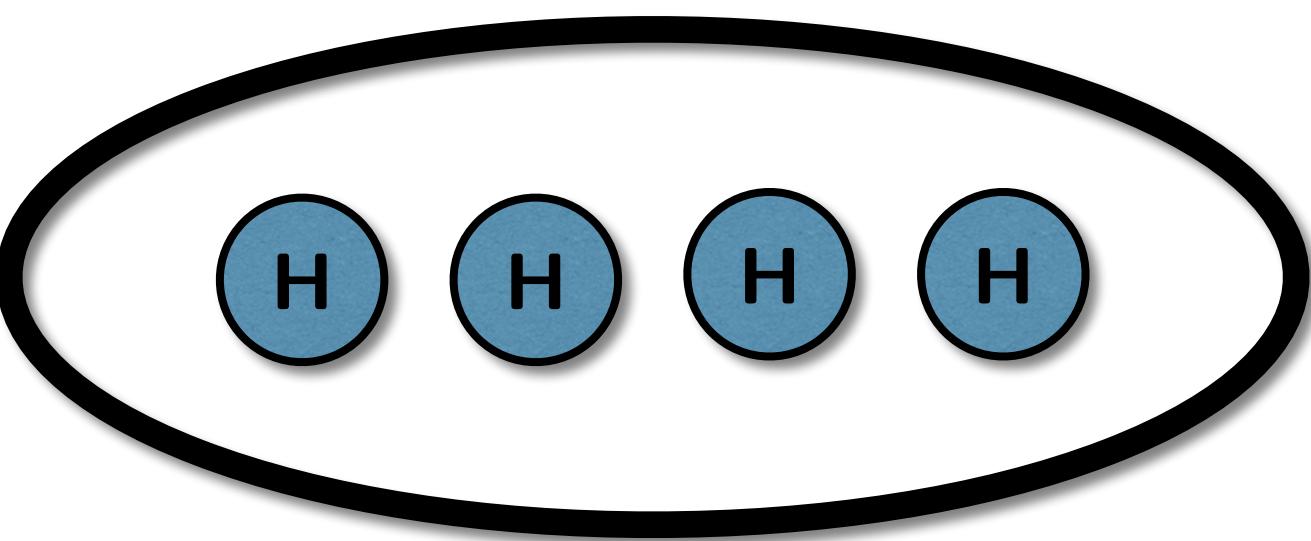
$$a \left| \begin{array}{c} \bullet \\ \square \\ \bullet \end{array} \right\rangle + b \left| \begin{array}{c} \bullet \\ | \\ \bullet \\ | \\ \bullet \end{array} \right\rangle + c \left| \begin{array}{c} \bullet \\ \diagup \\ \diagdown \\ \bullet \end{array} \right\rangle$$

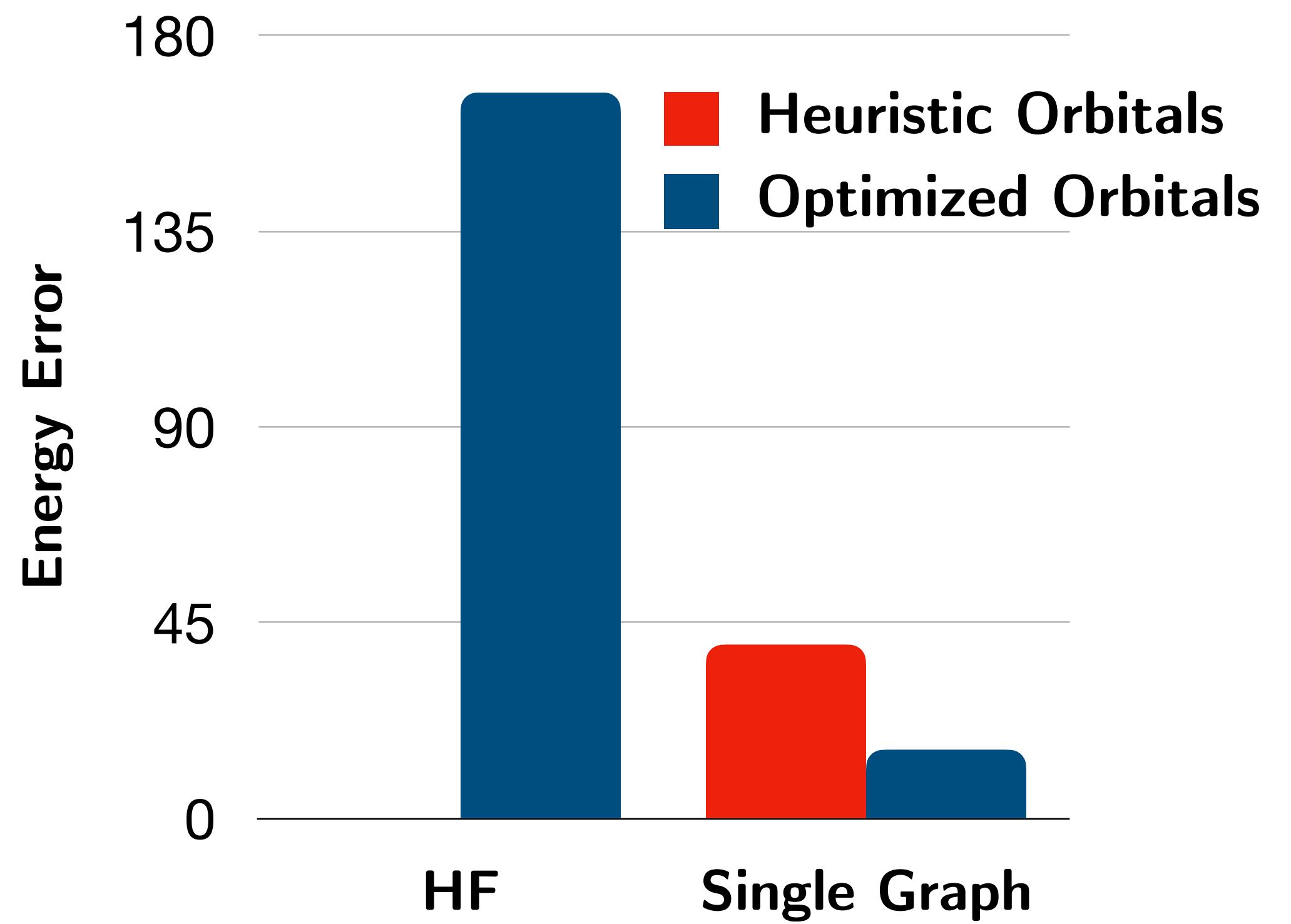
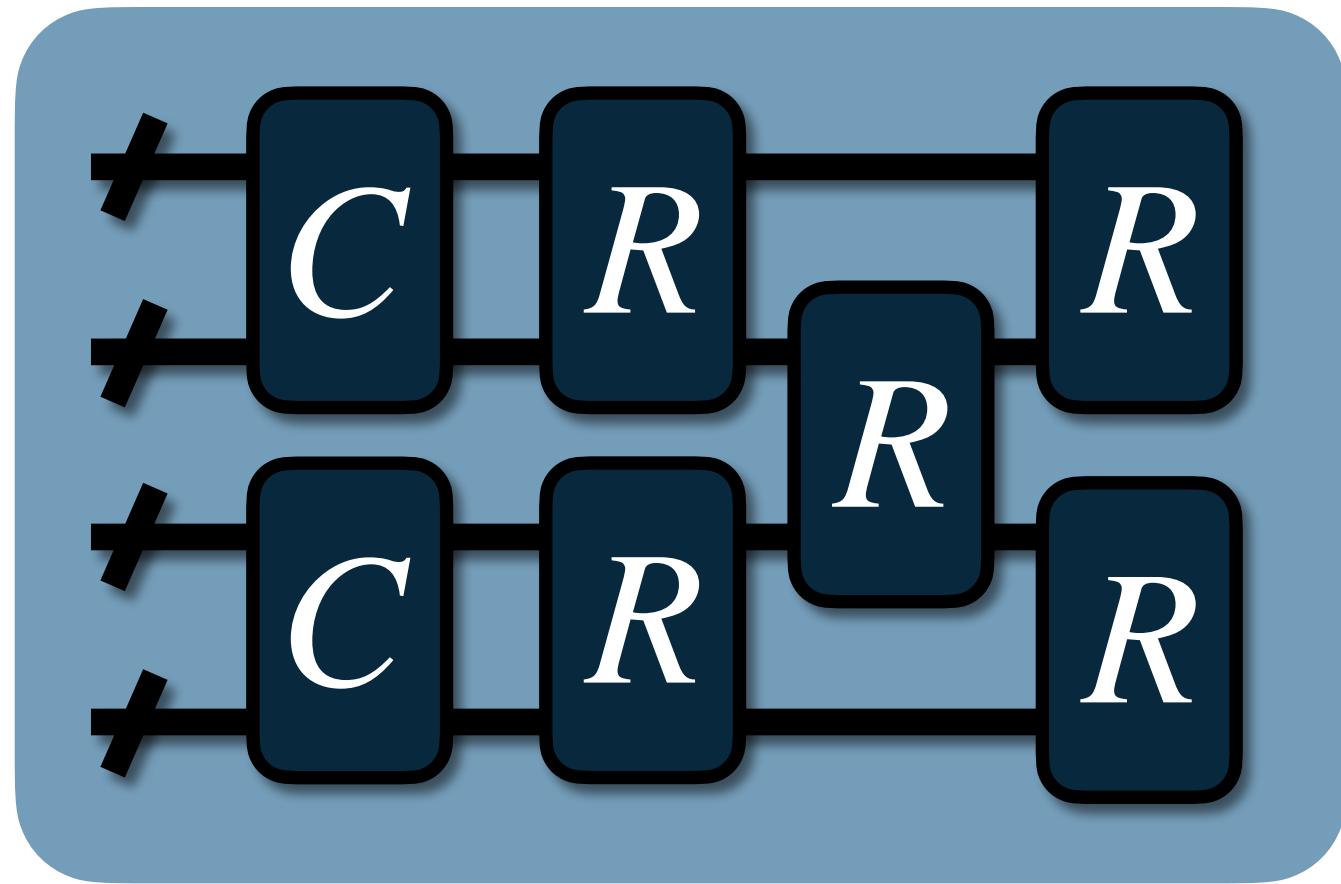
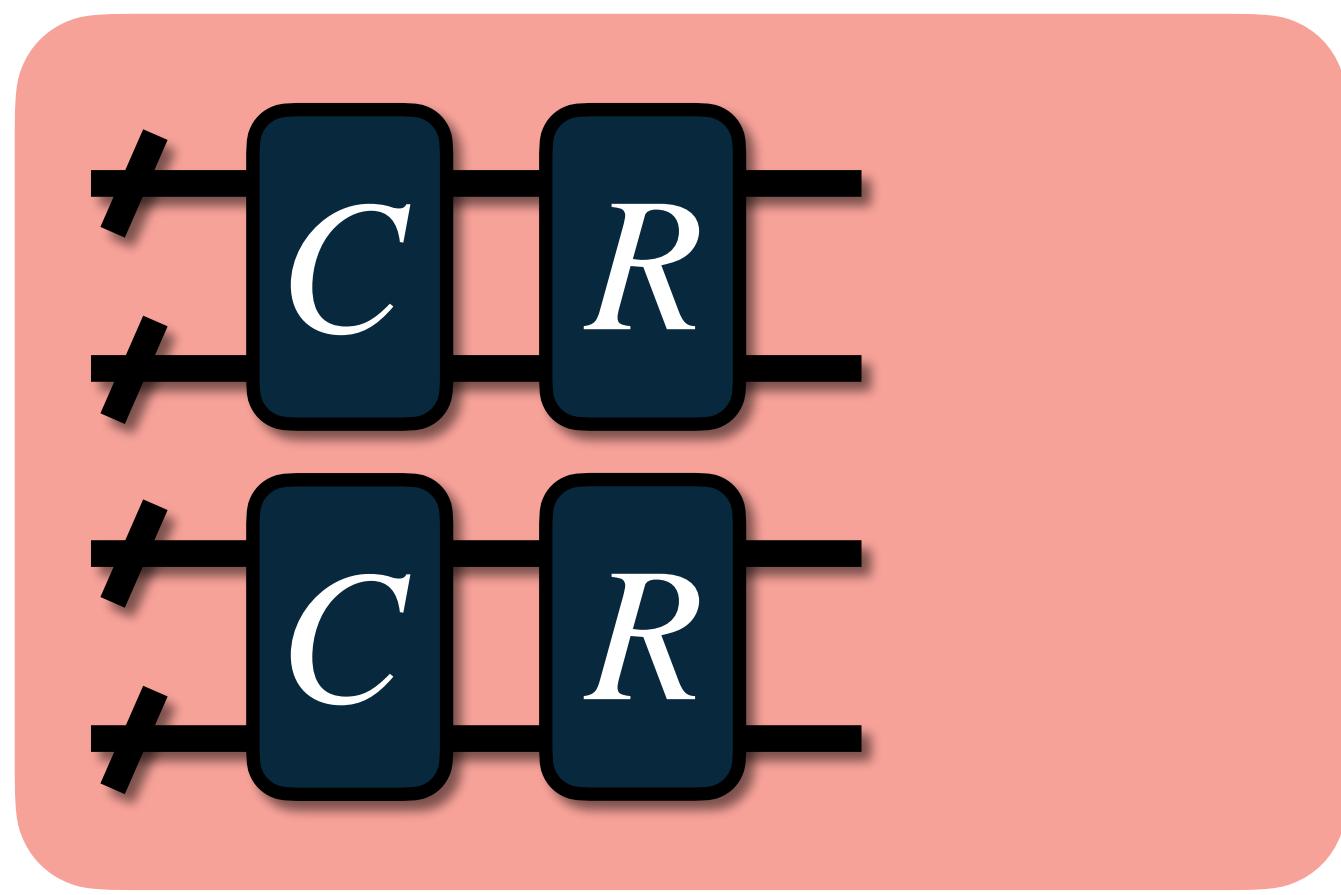
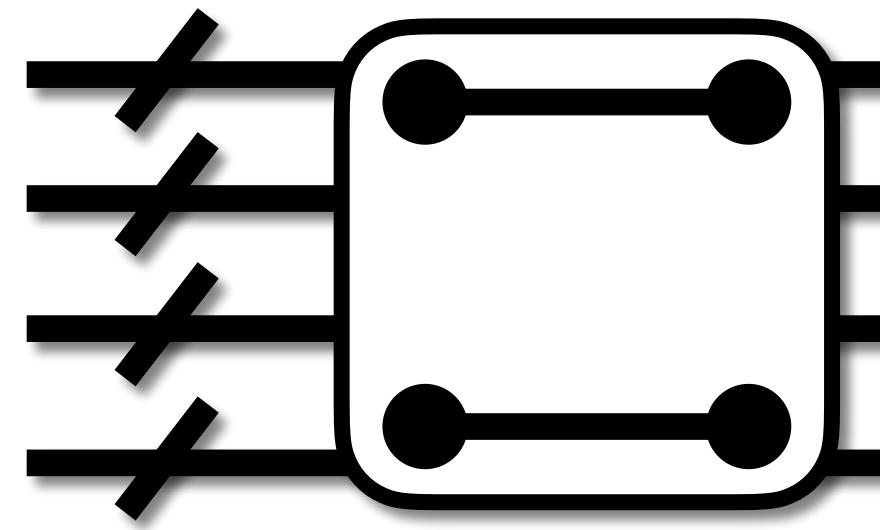
Transfer Insight

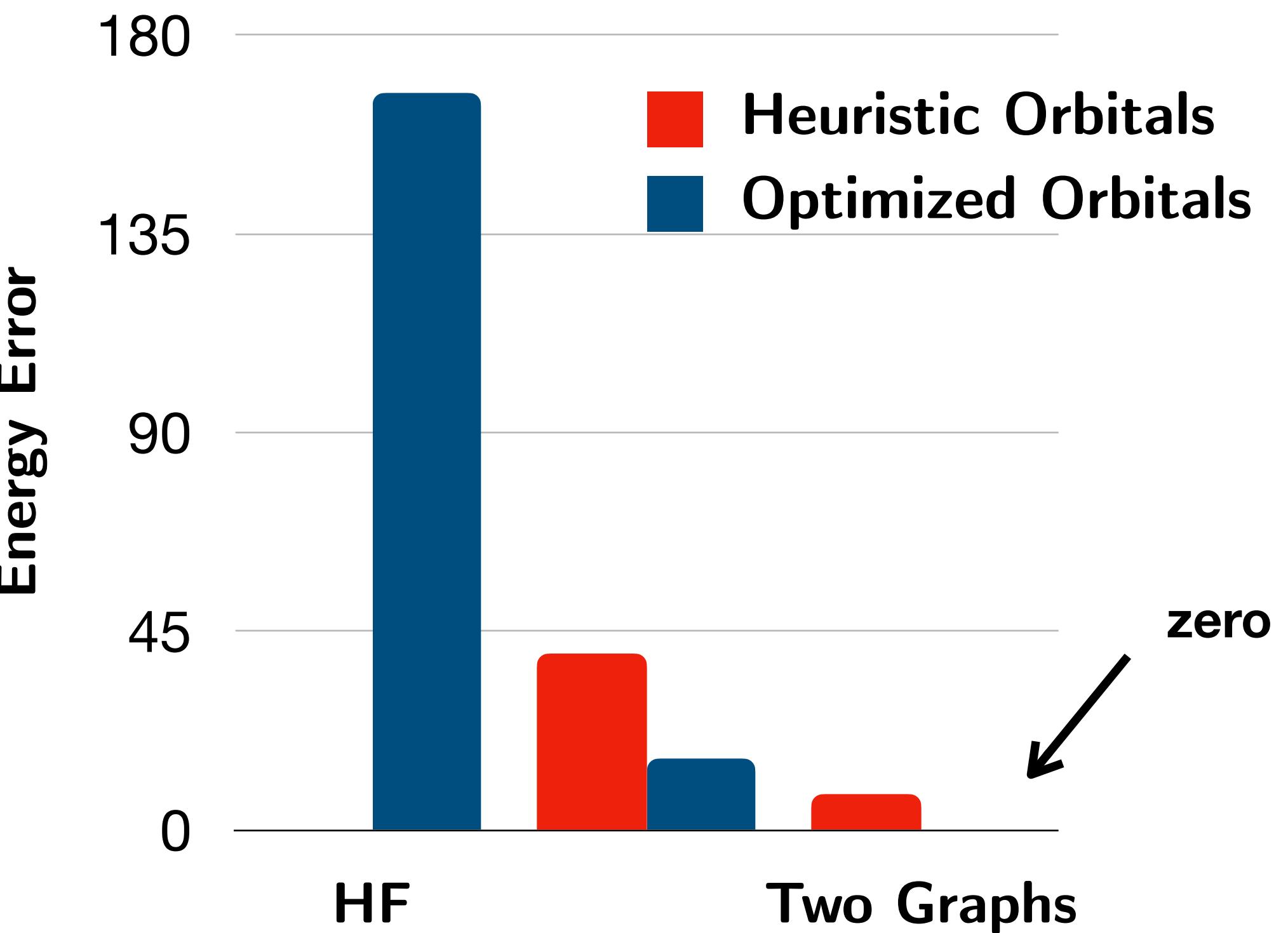
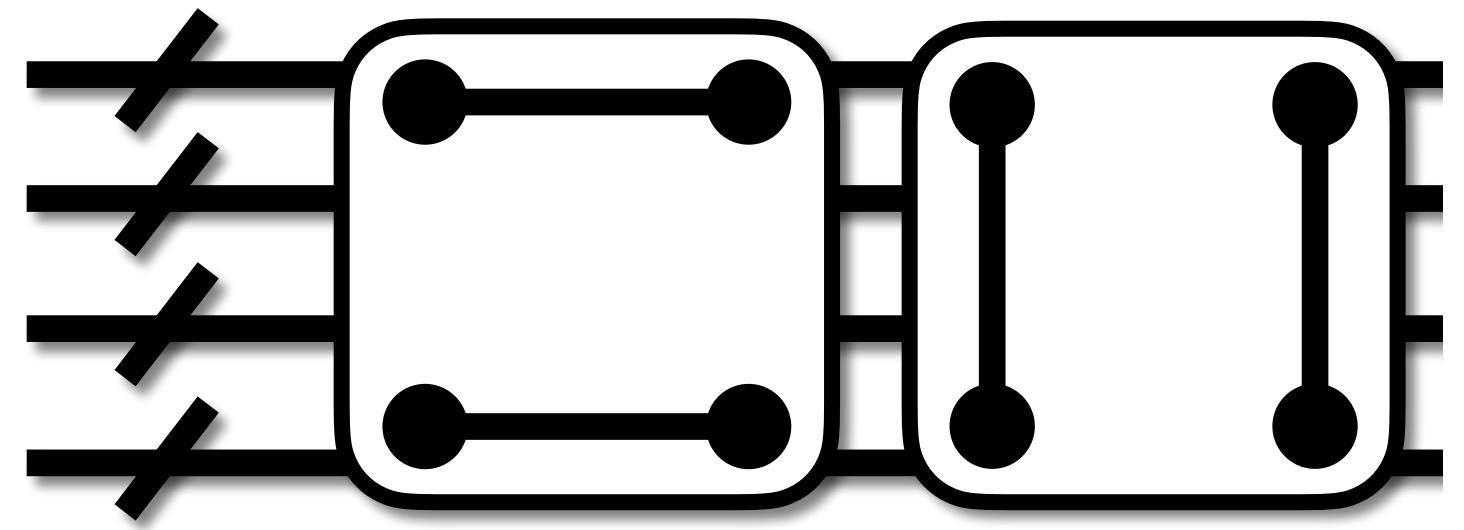


Example

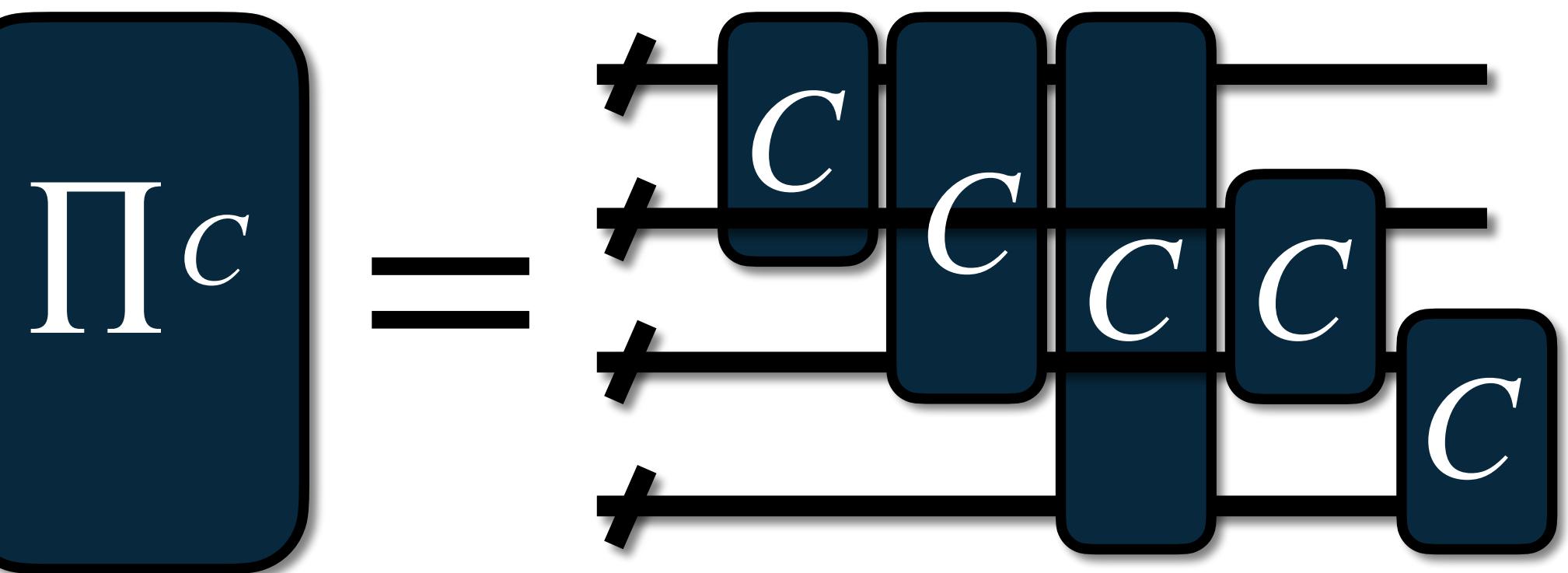
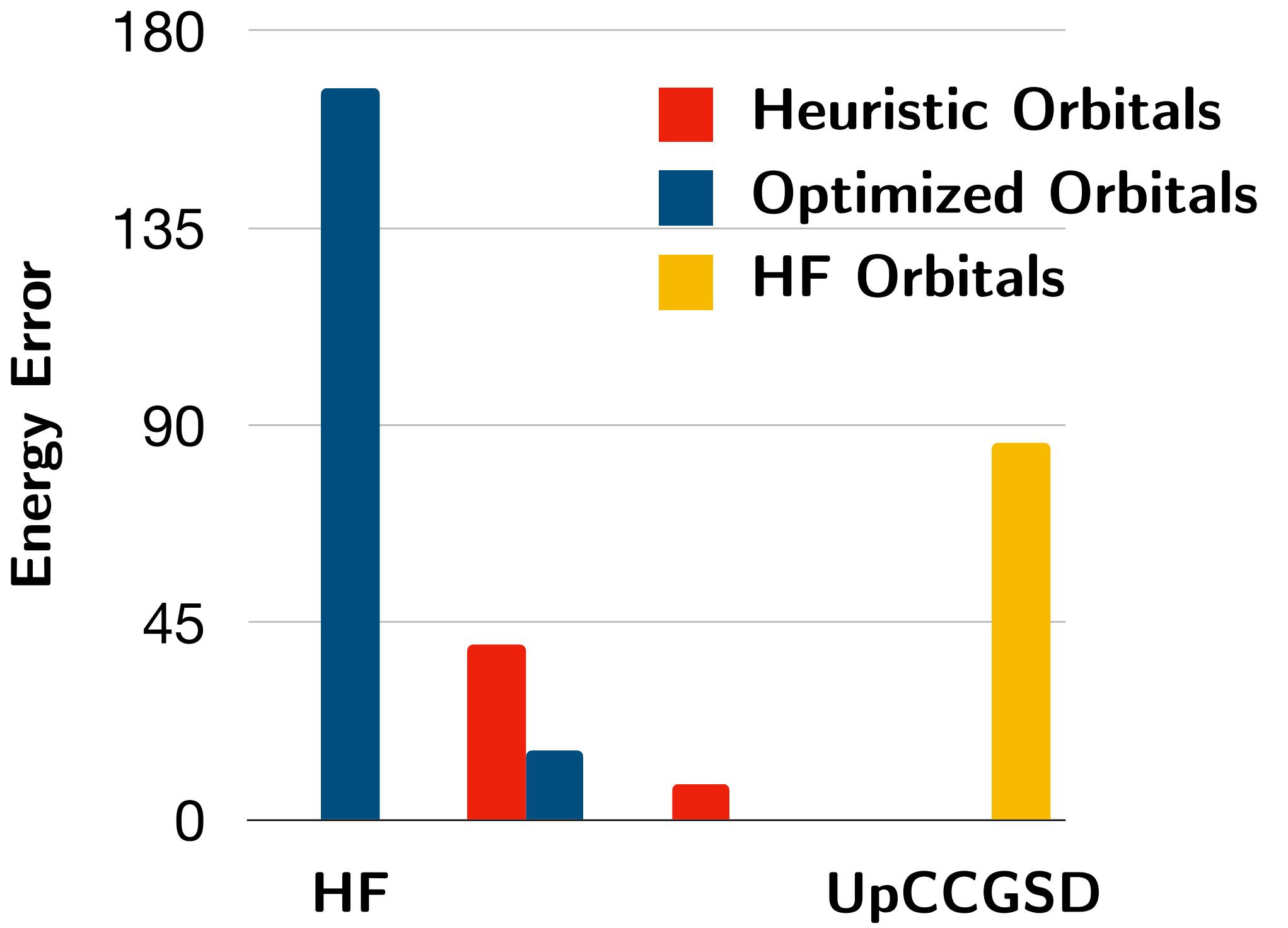
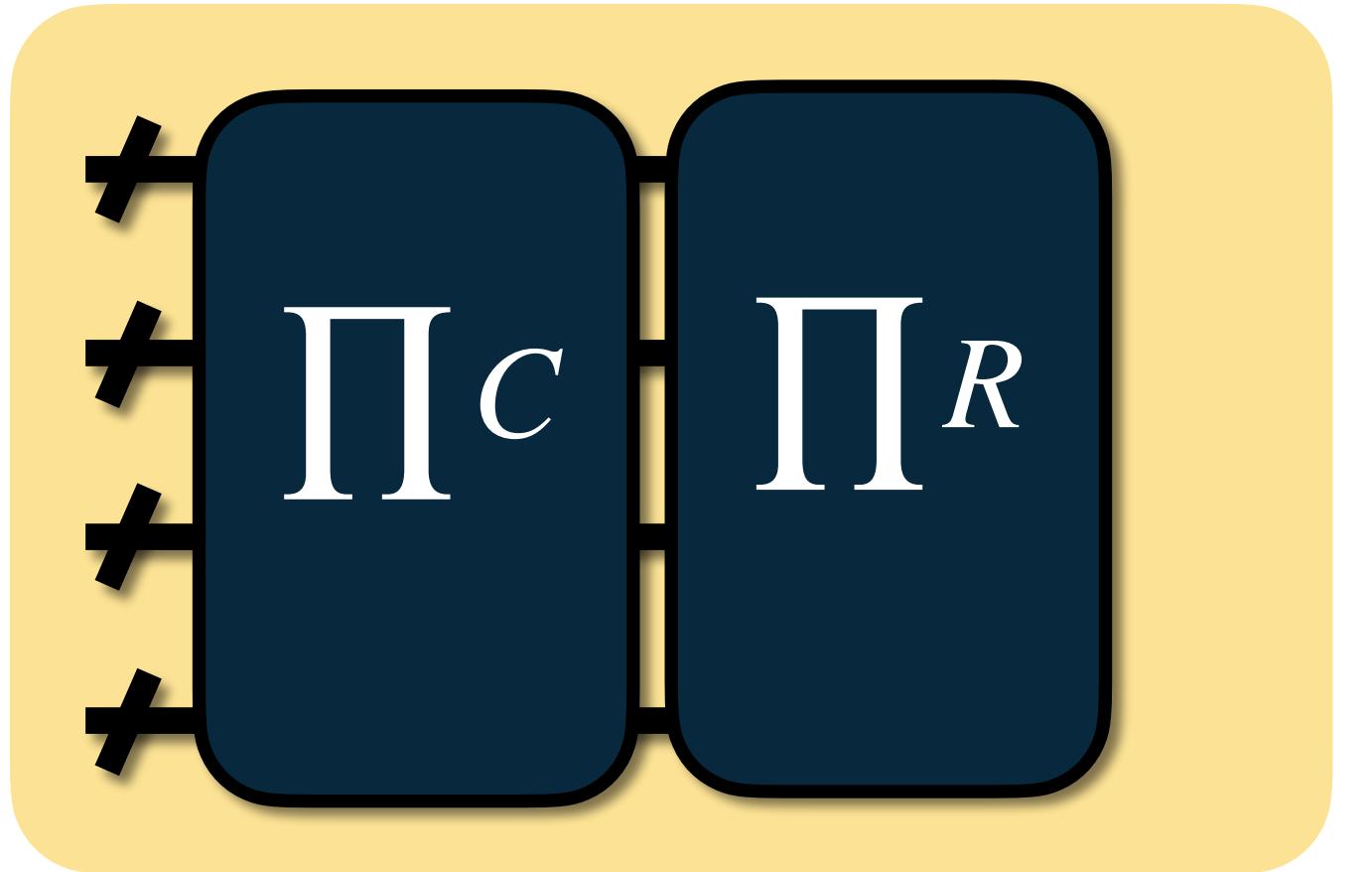
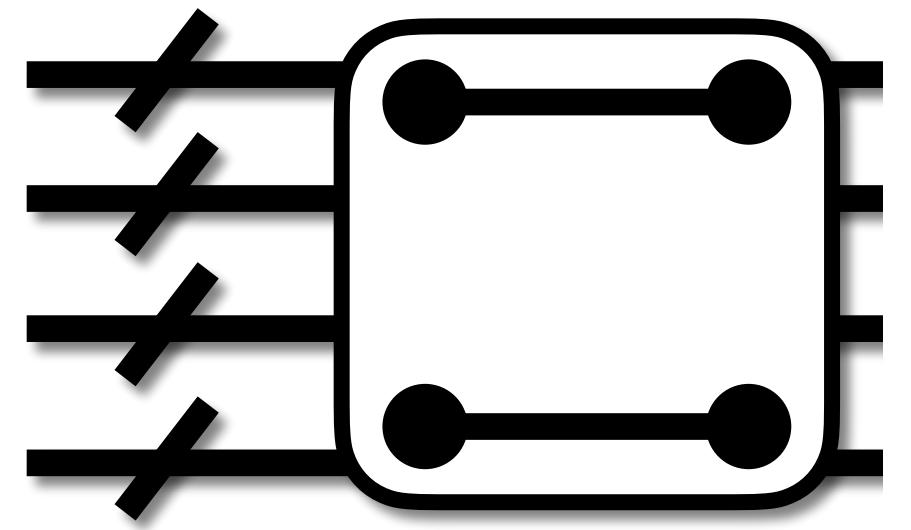
Linear H₄ Molecule

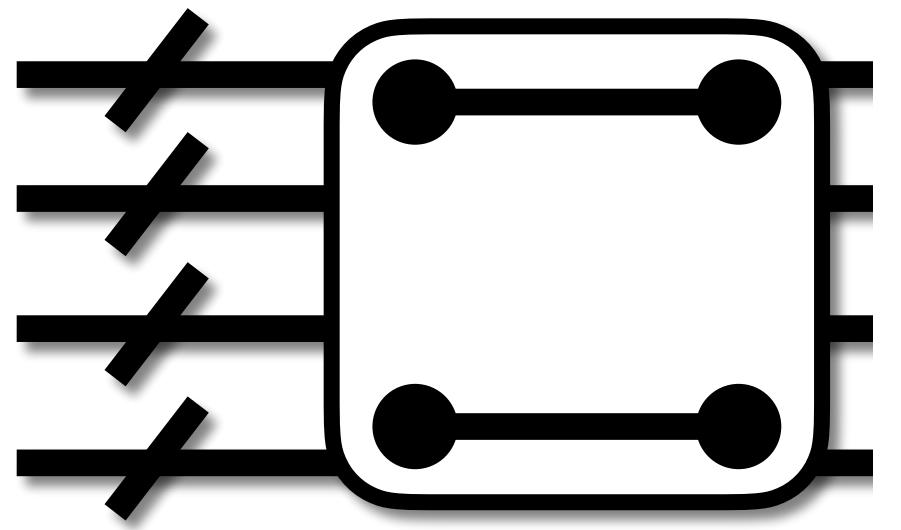




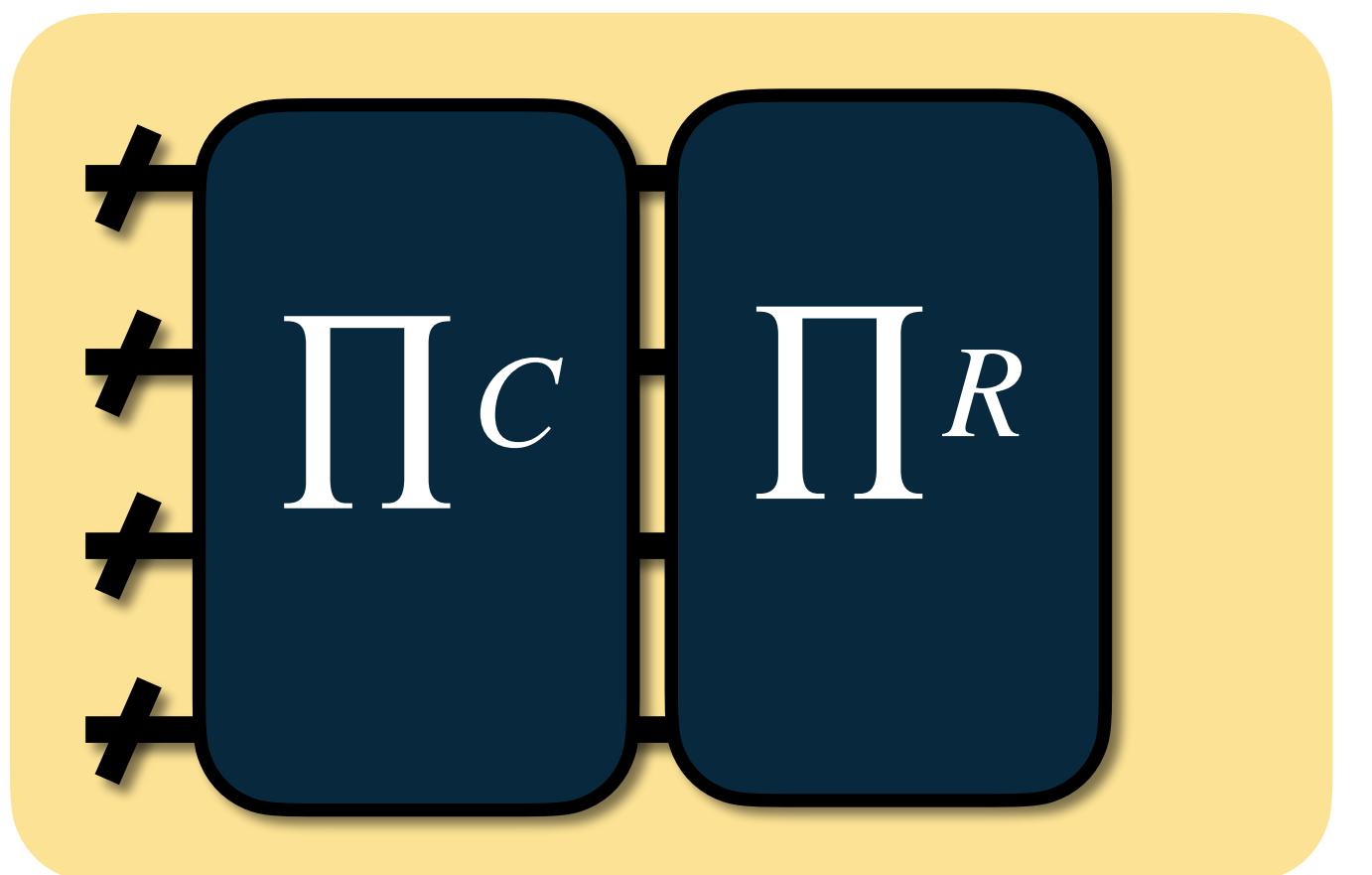


Comparison to Prominent Approaches



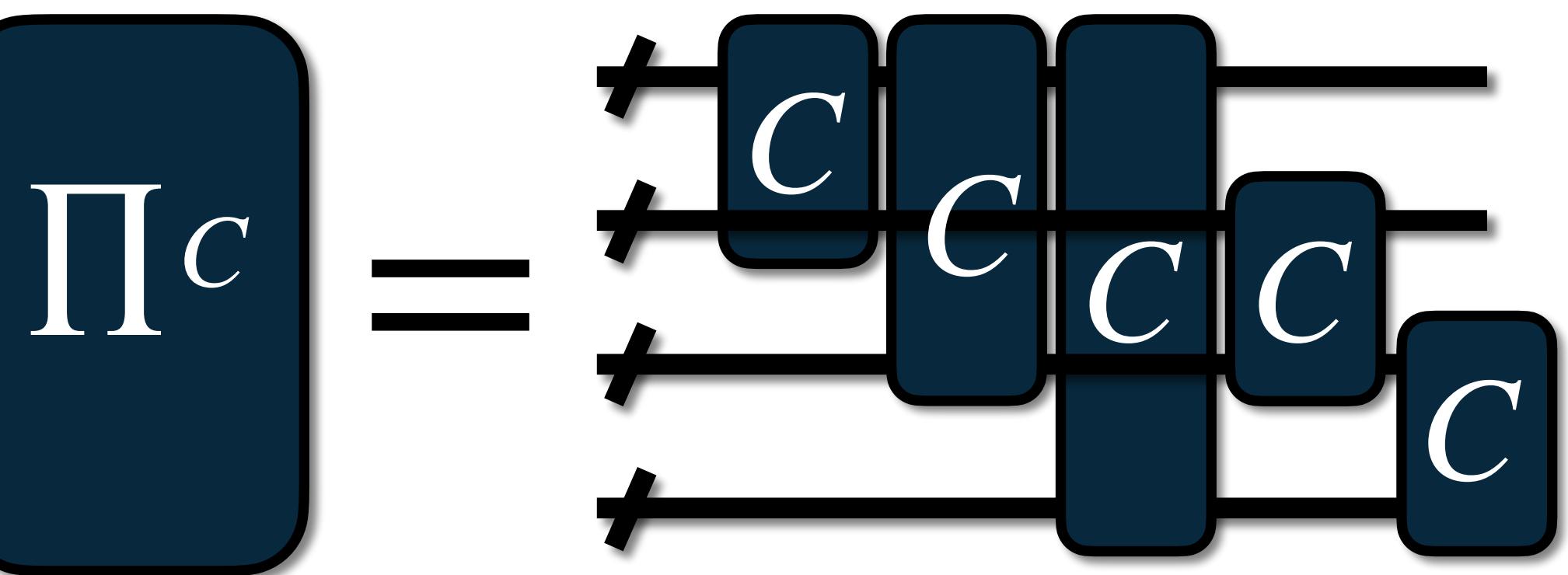
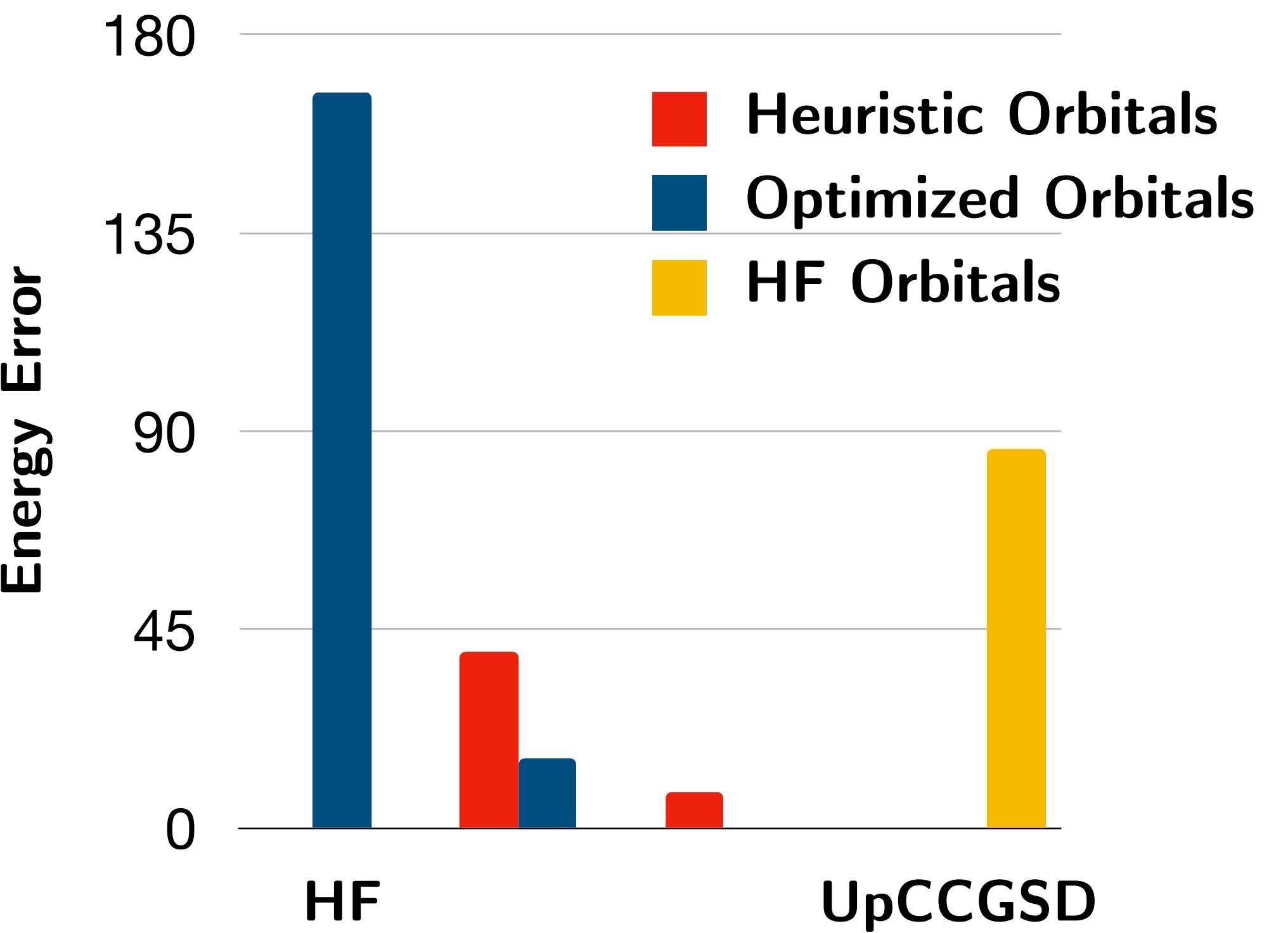


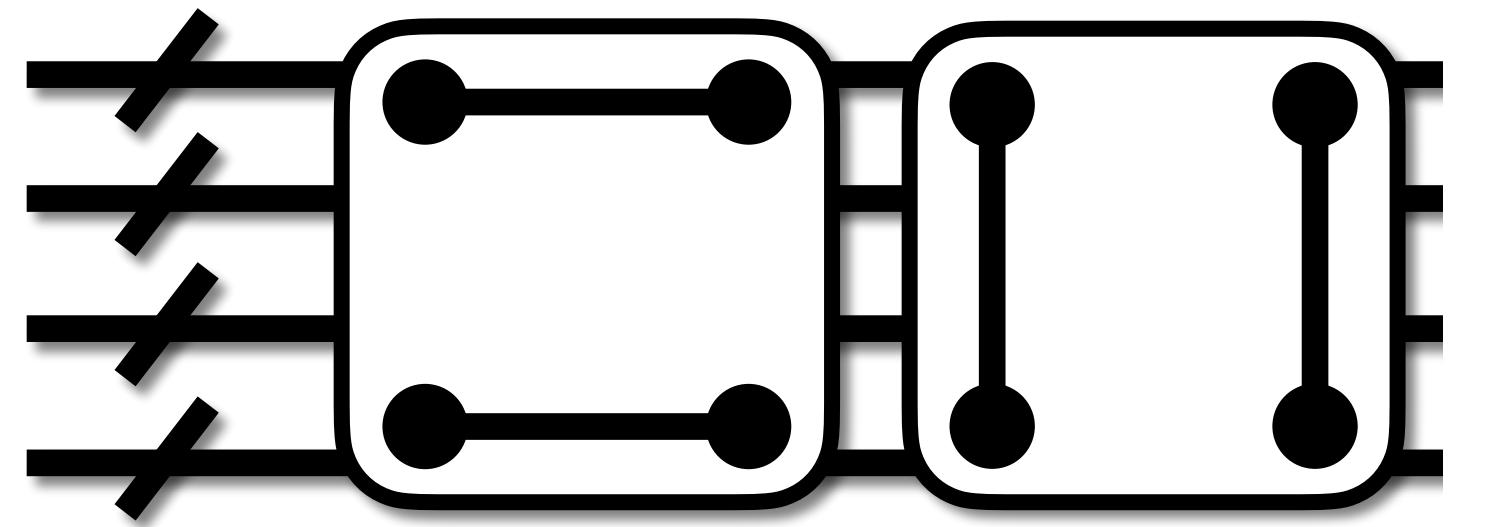
parameters: 4
cnots: 6 – 70



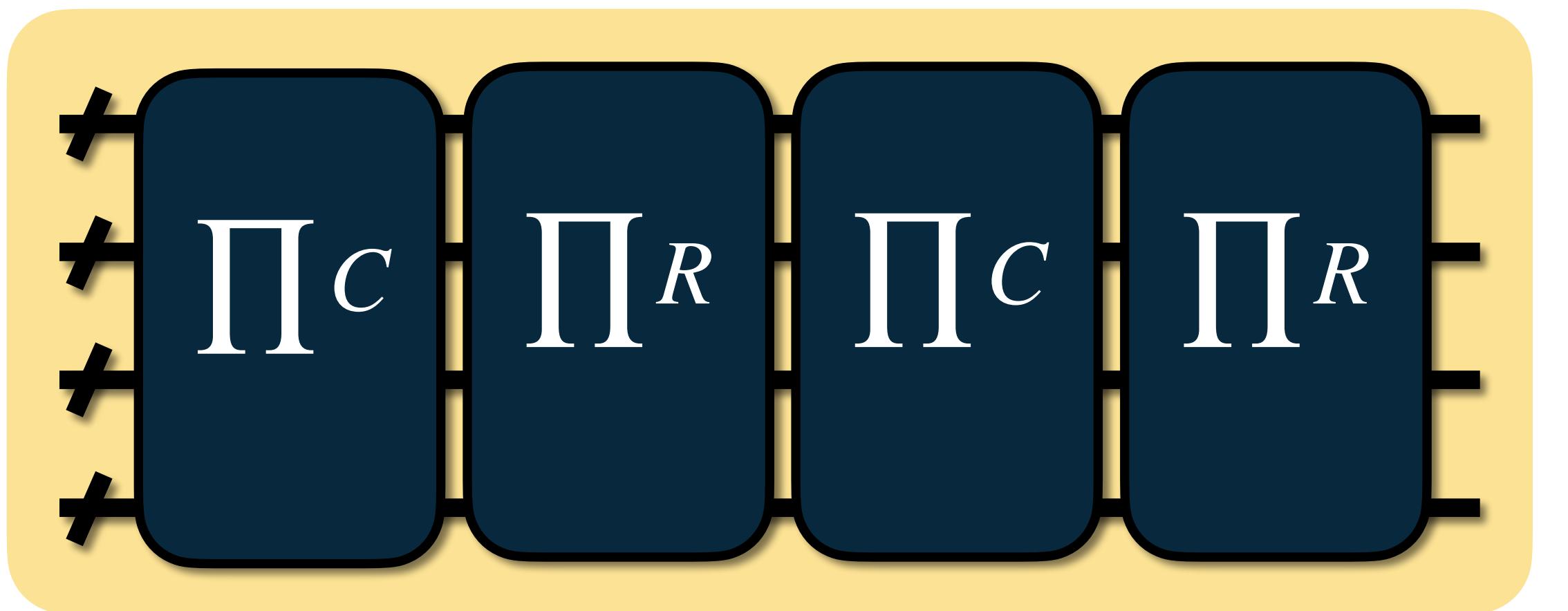
UpCCGSD
parameters: 18
cnots: 66 – 188

k-UpCCGSD: Lee, JCTC, 2018

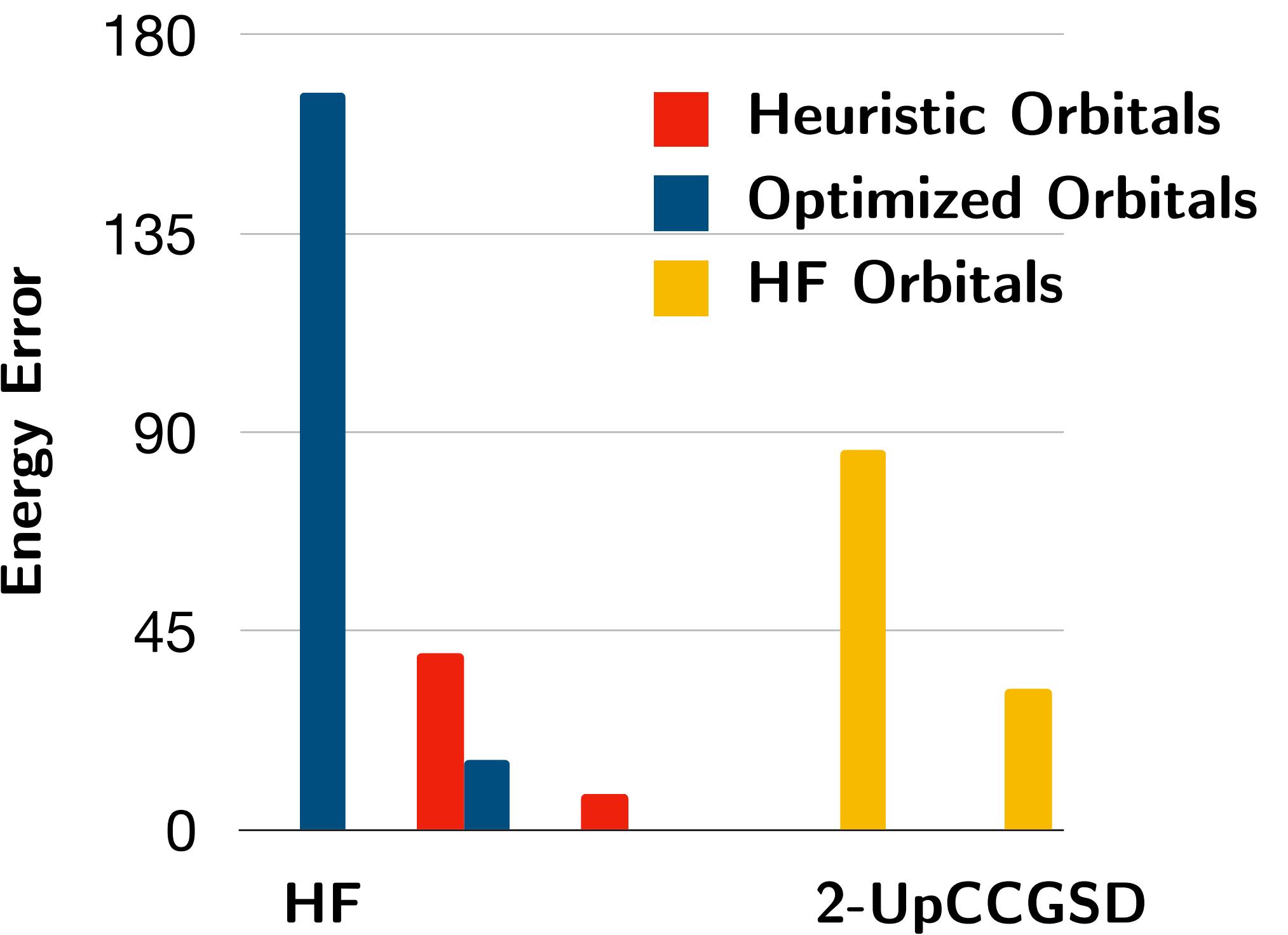


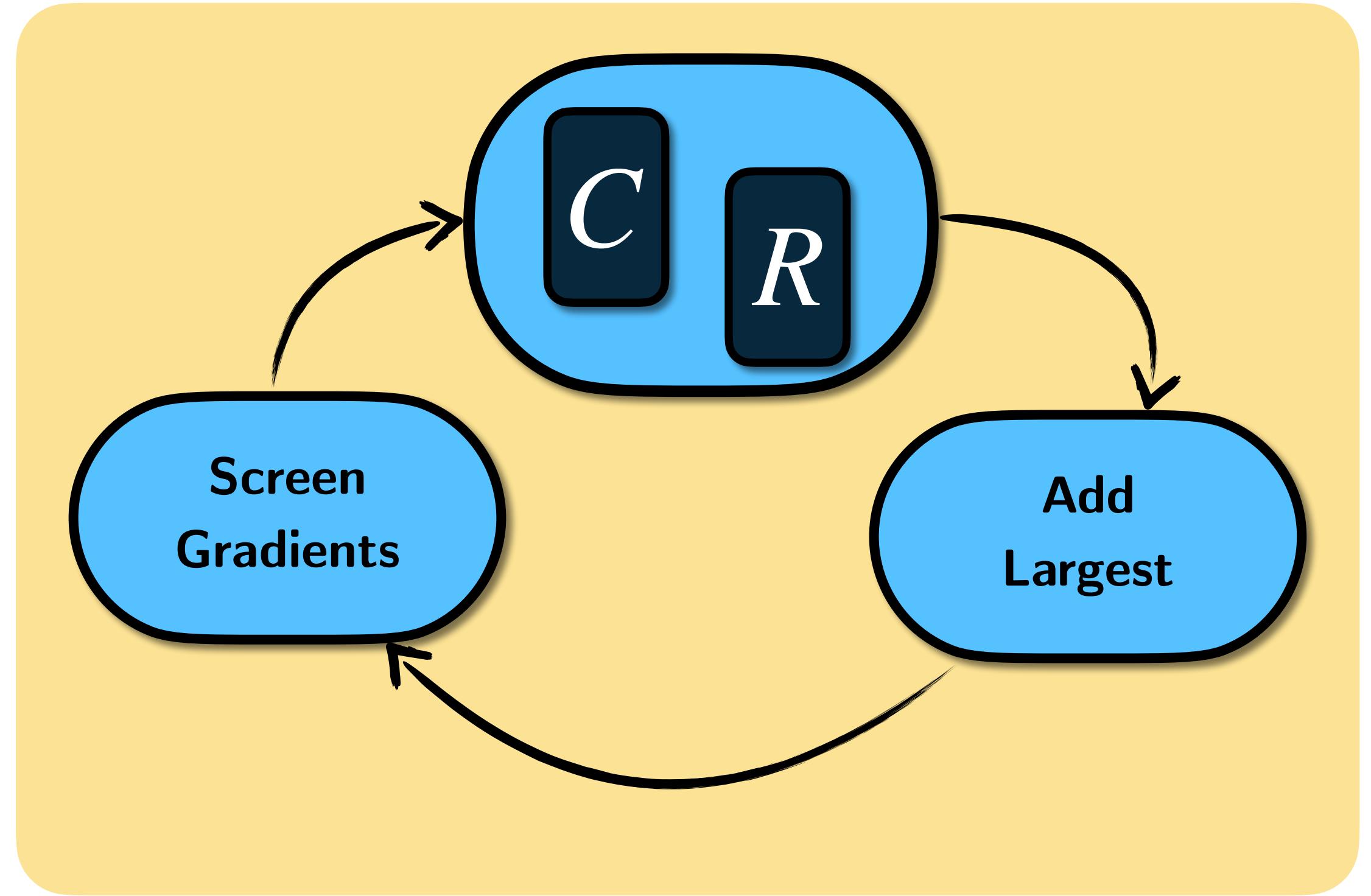


parameters: 6
cnots: 116



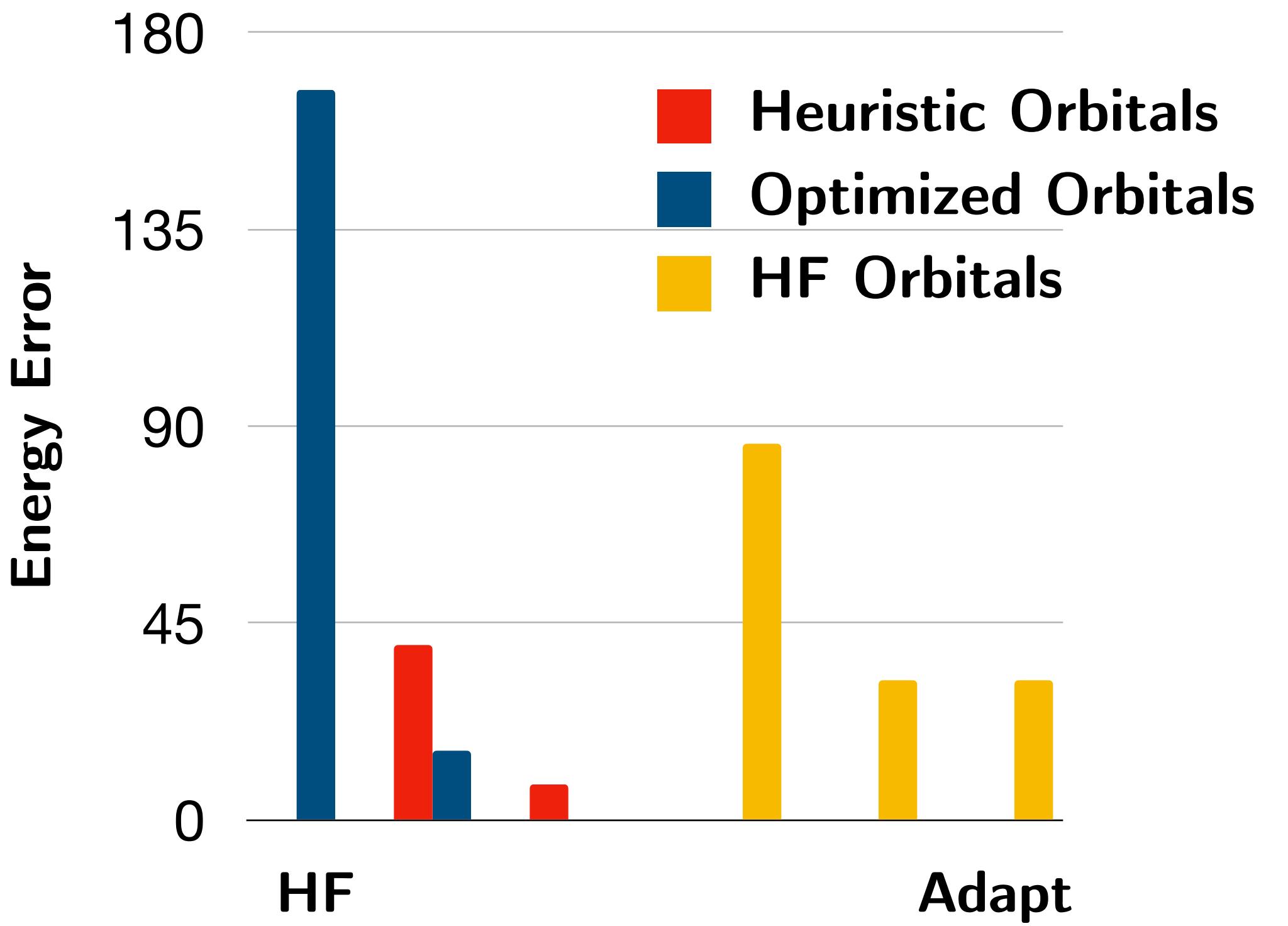
2-UpCCGSD
parameters: 36
cnots: 432



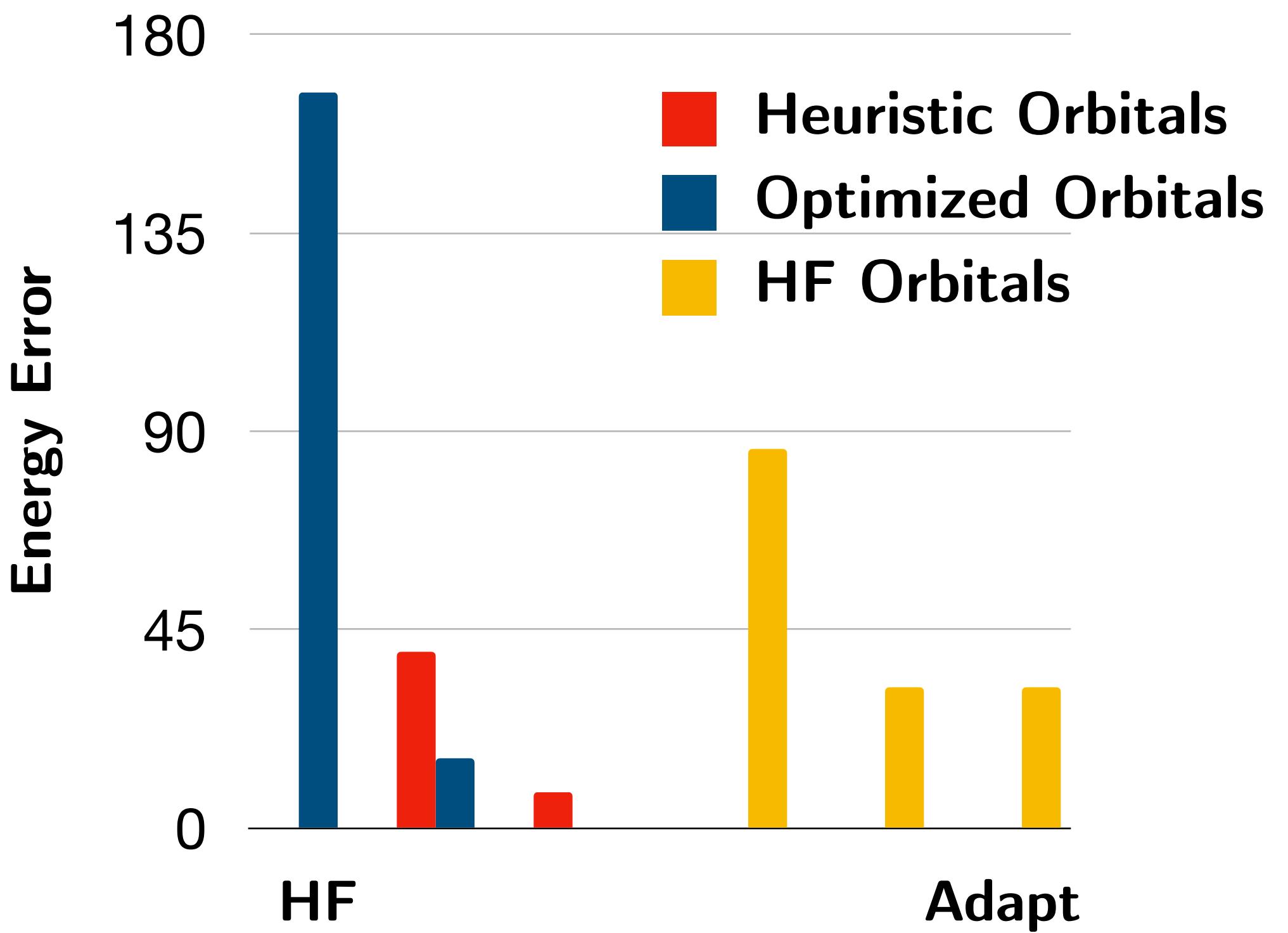
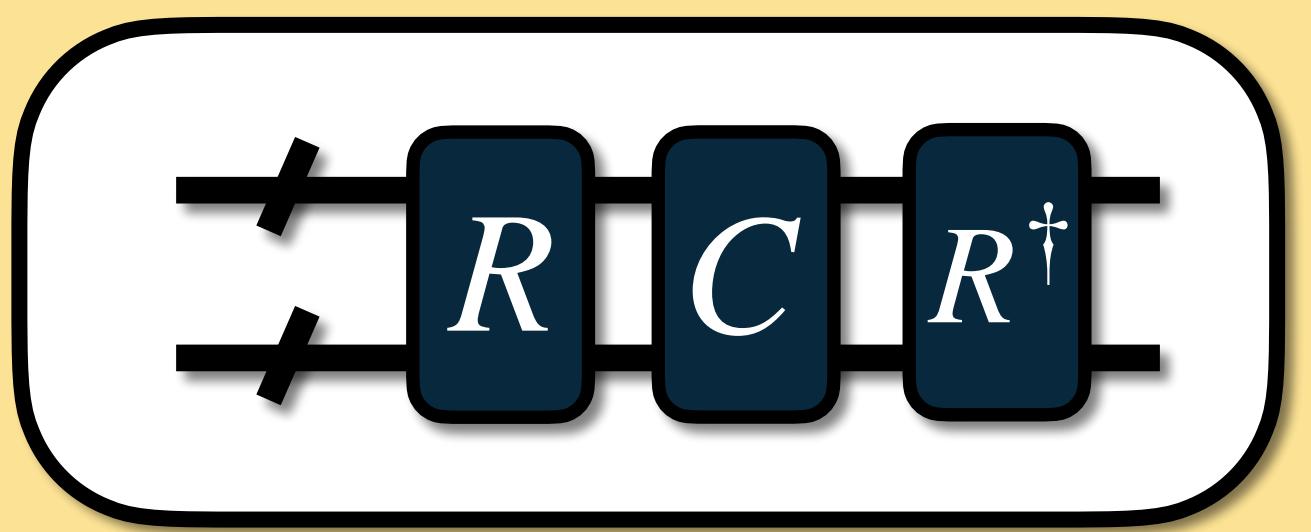


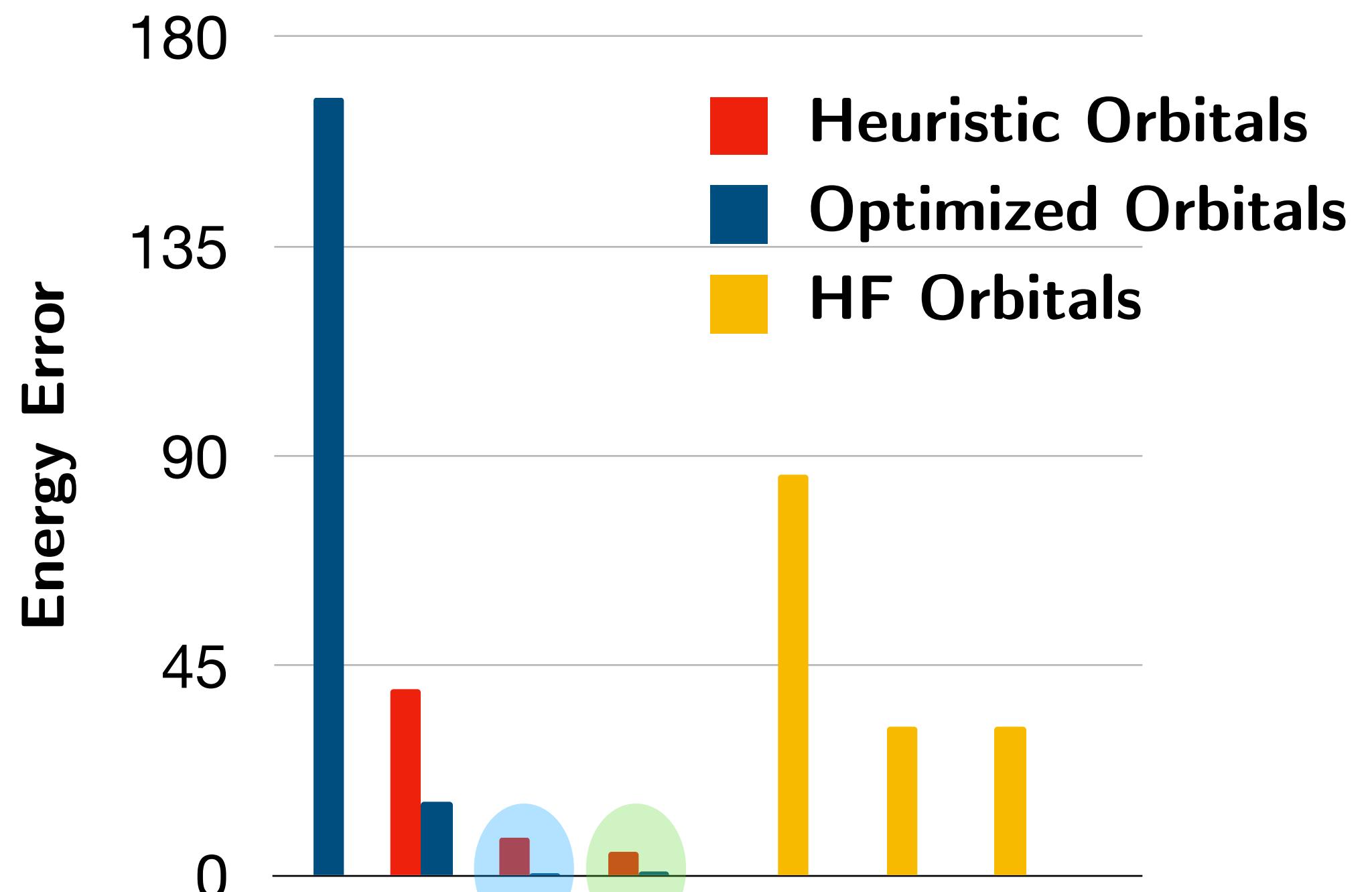
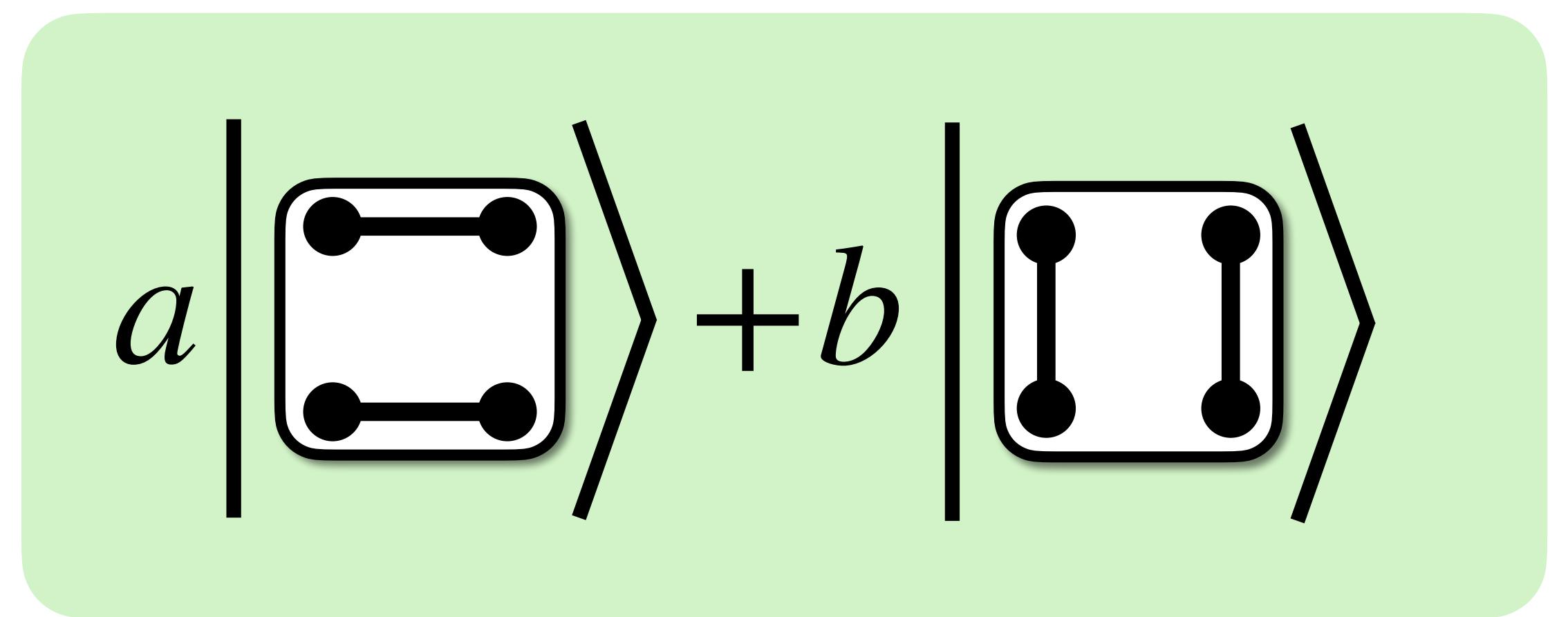
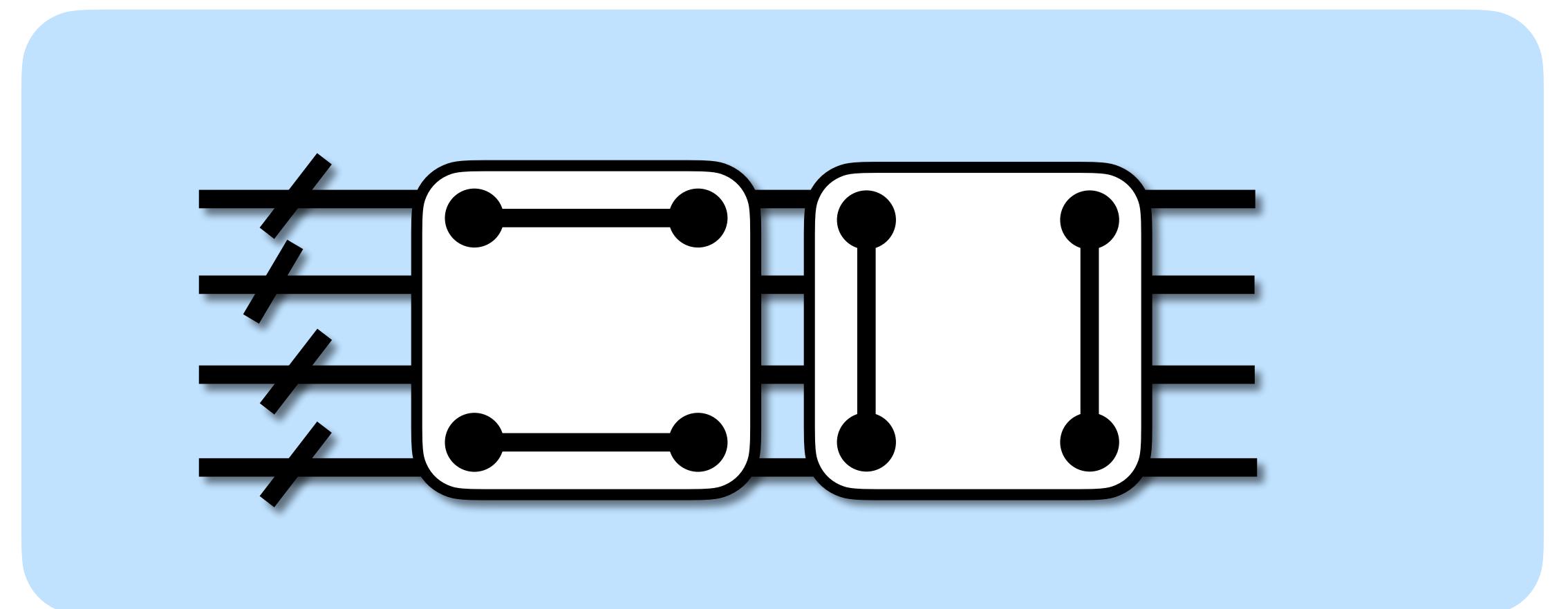
2-UpCCGSD
parameters: 36

Adapt(C,R)
parameters: 12

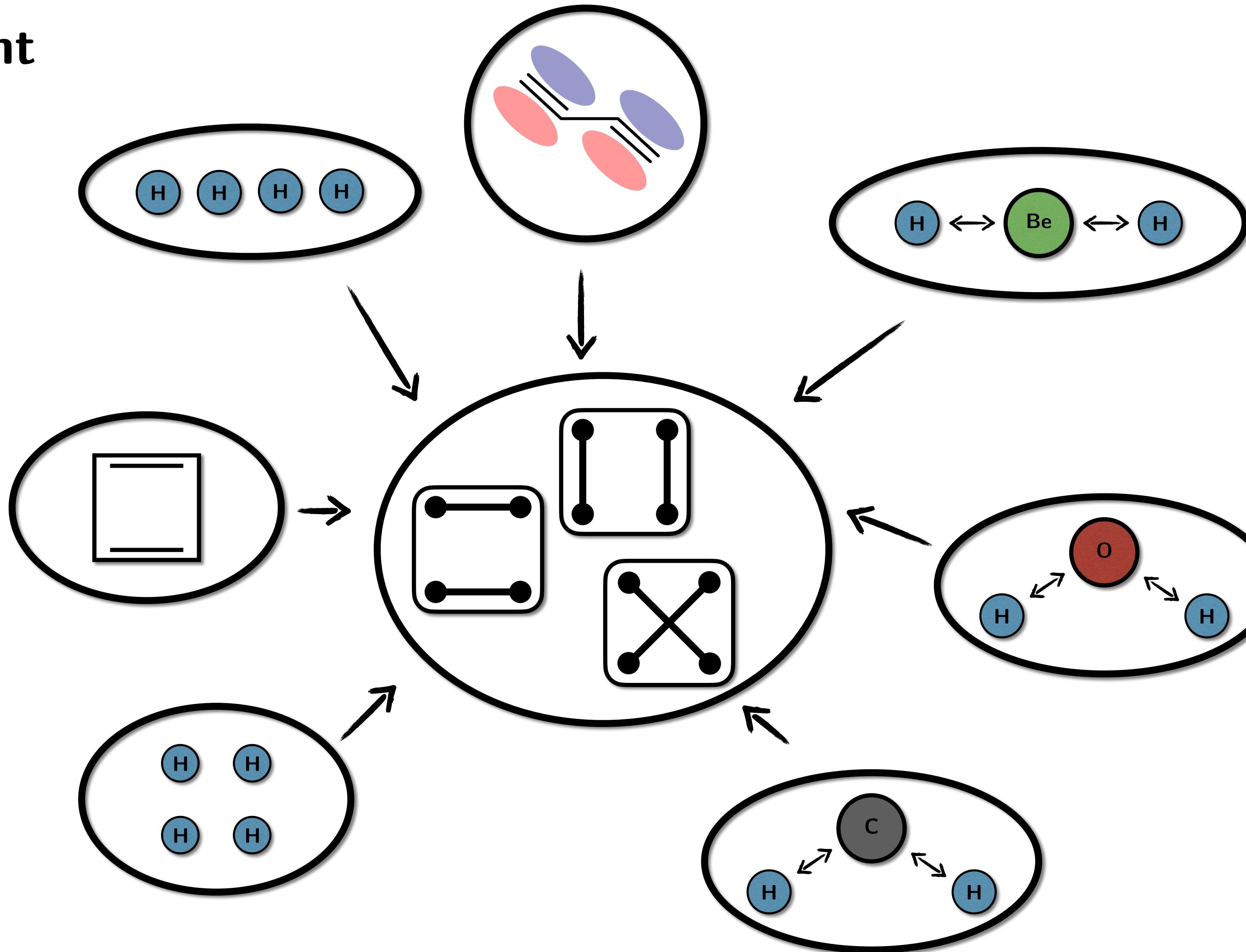


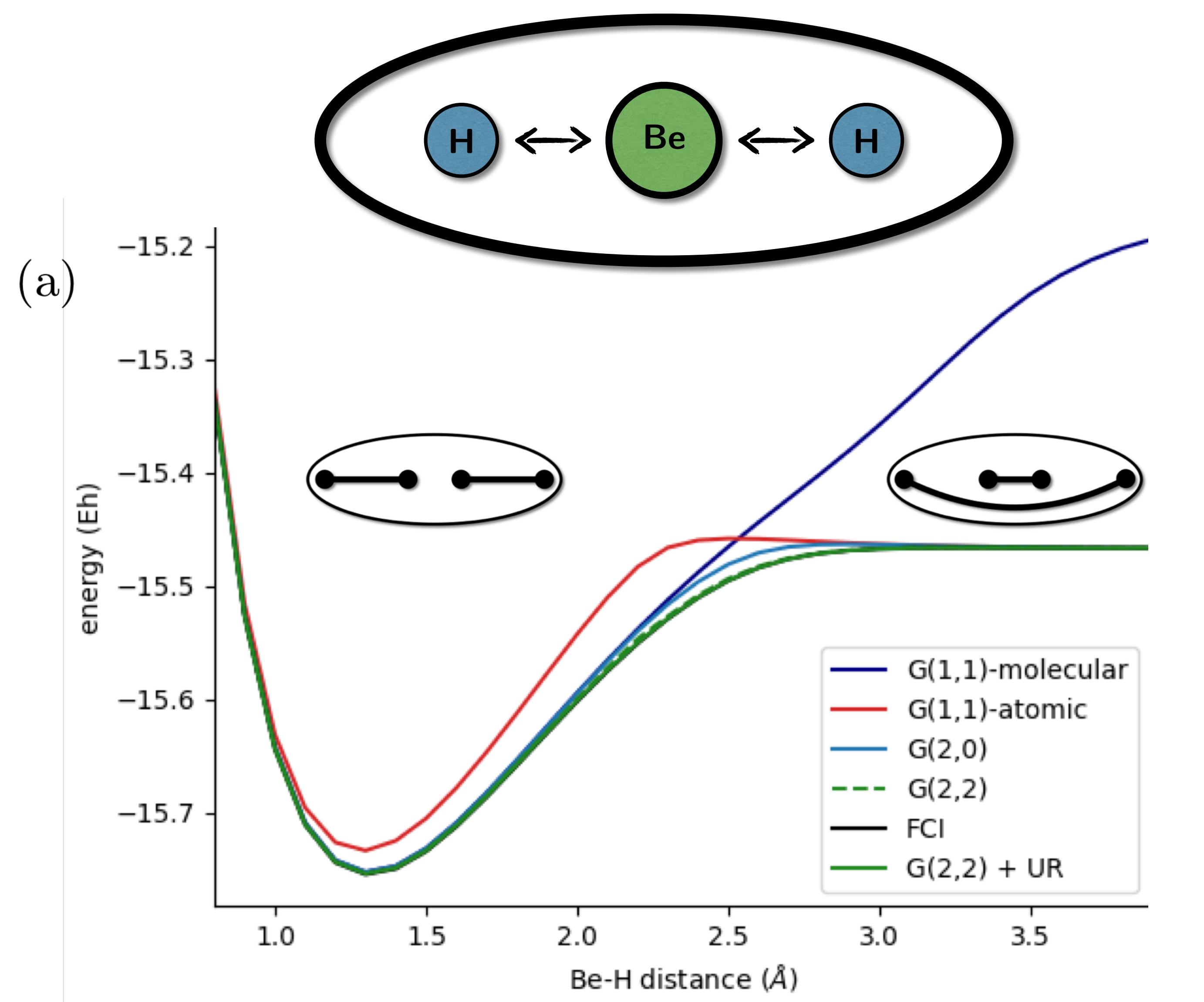
Motif is hard to detect locally





Transfer Insight





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)

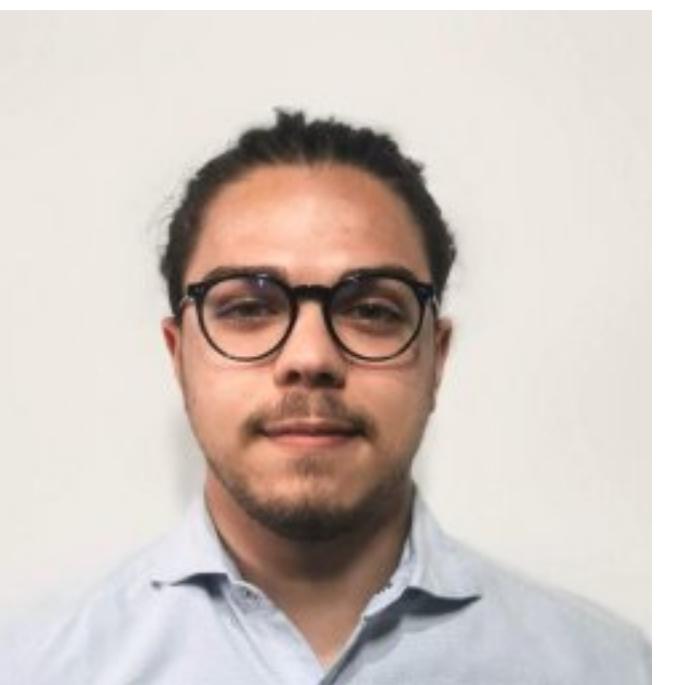
Subspaces of Graph-Wavefunctions

Compact Effective Basis Generation: Insights from Interpretable Circuit Design

Jakob S. Kottmann¹ and Francesco Scala²



quantum
open-source
foundation



PhD Position Opening
this Spring

code examples online



[github/kottmanj/talks_and_material](https://github.com/kottmanj/talks_and_material)



github.com/tequilahub