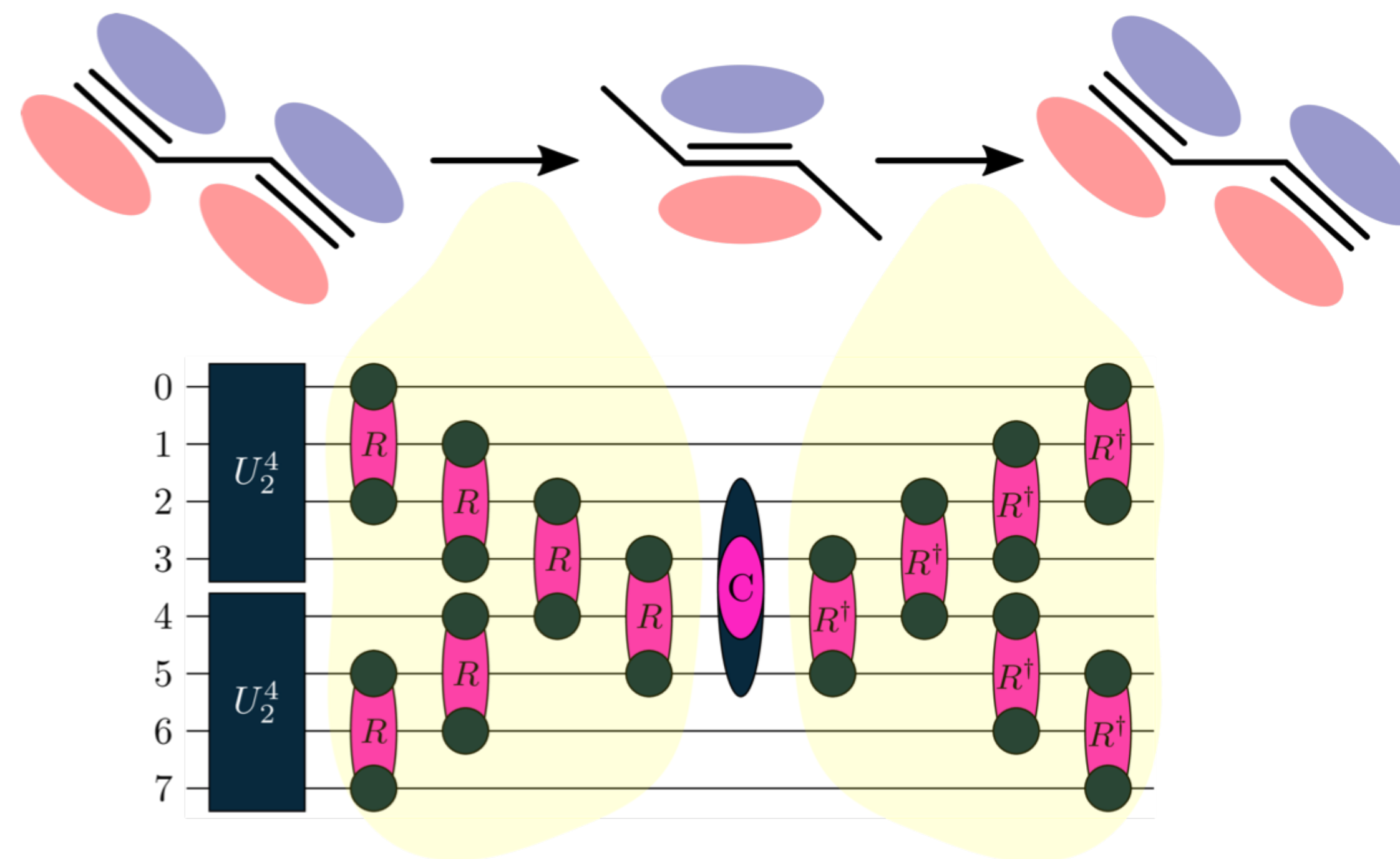
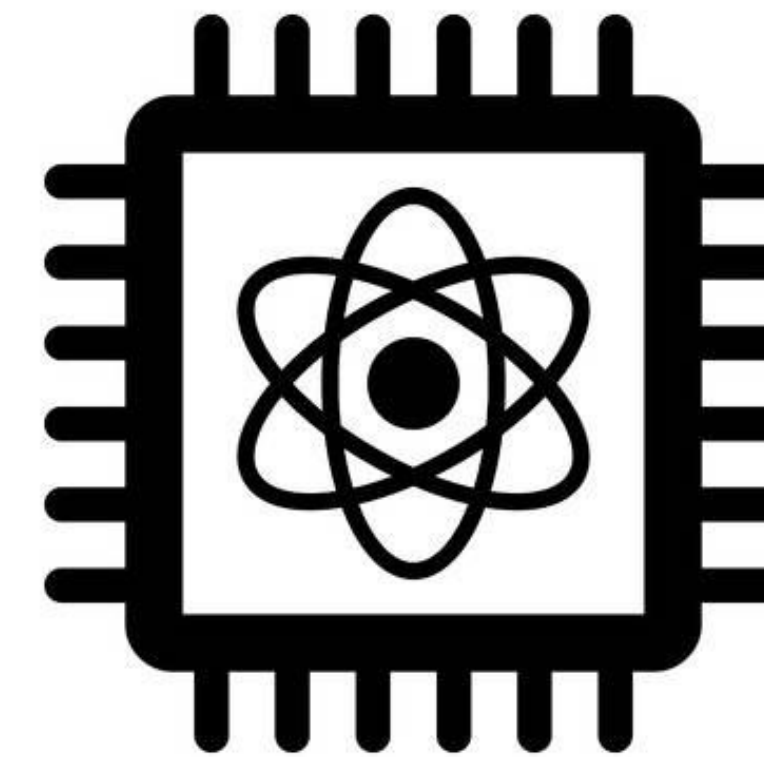
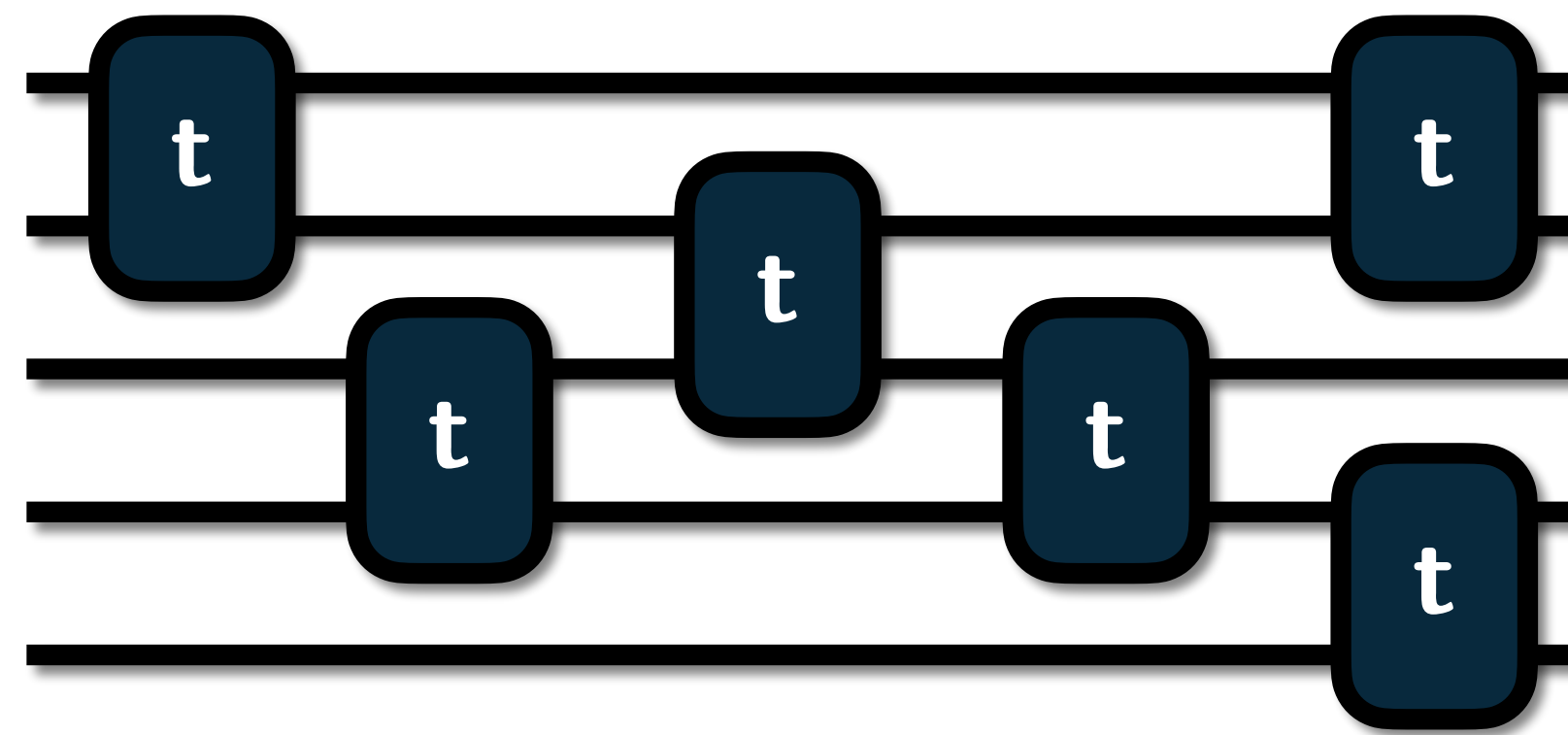


Molecular Quantum Circuit Design

Jakob S. Kottmann
Institute for Computer Science
University of Augsburg





Variational
Quantum
Eigsolvers (VQE)

measure expectation value and
gradient




Perruzo/McClean, Nat. Comm, 2014

McClean, NJP, 2016

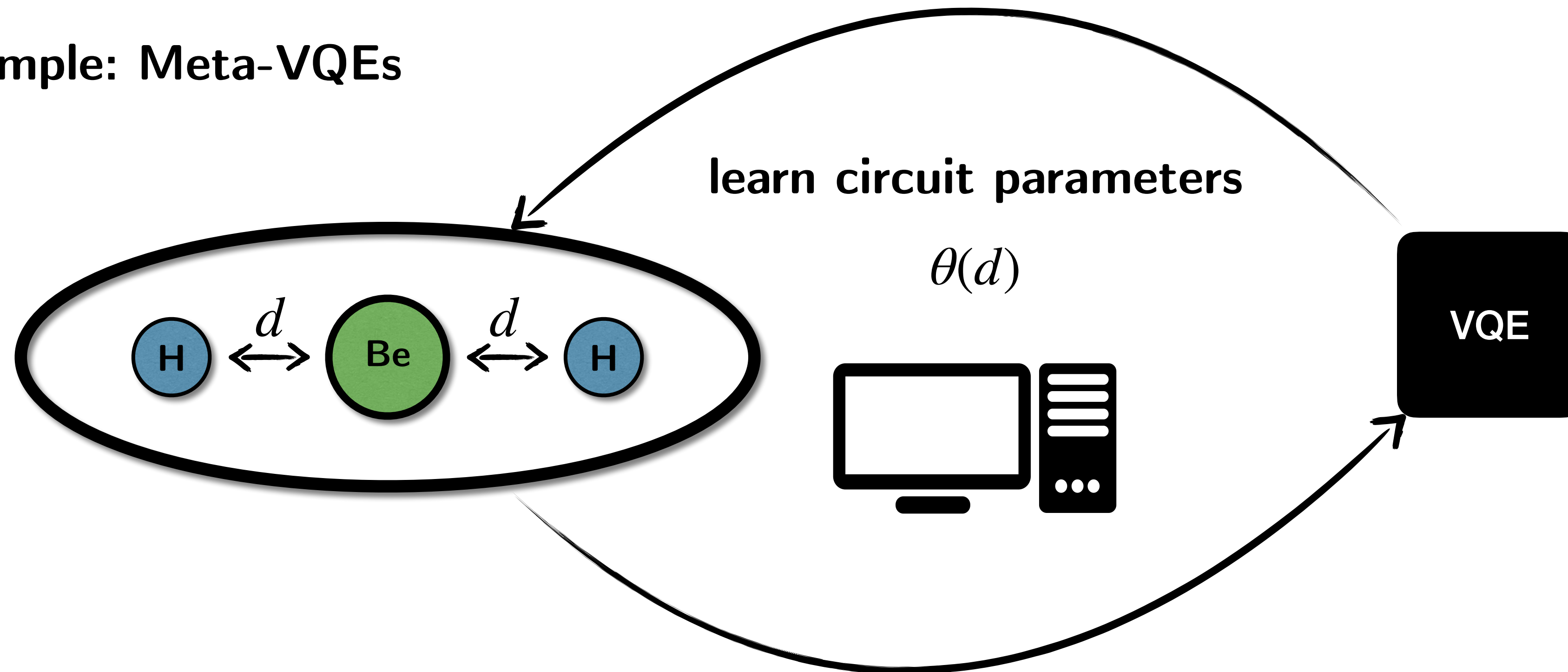
Motivation: VQEs as black-boxes

Many projects need robust VQEs

Motivation: VQEs as black-boxes

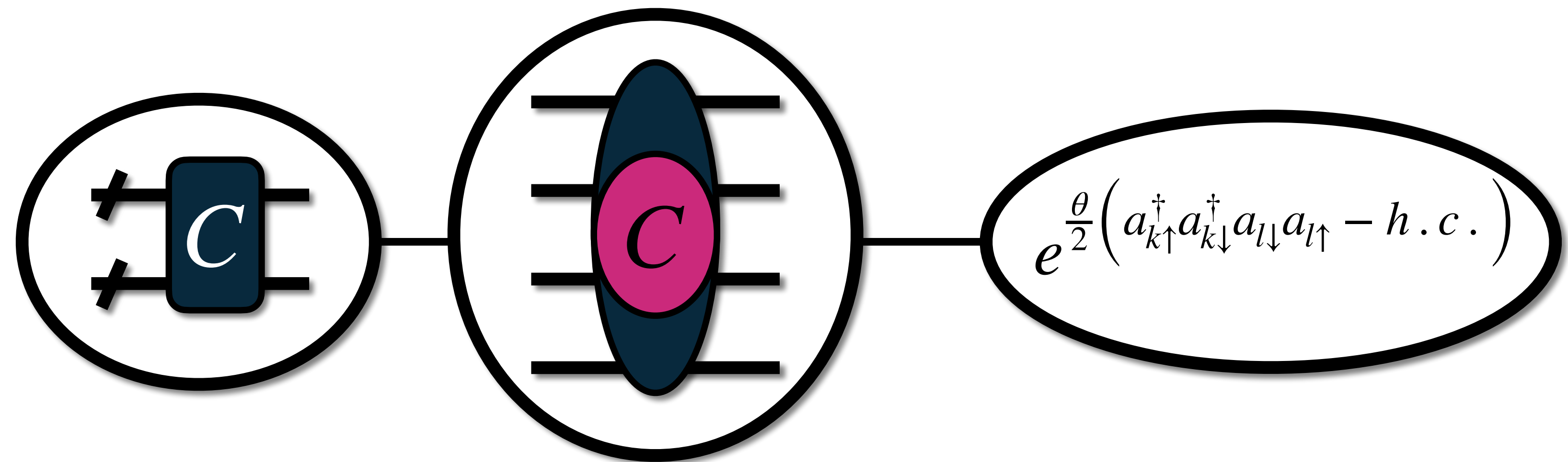
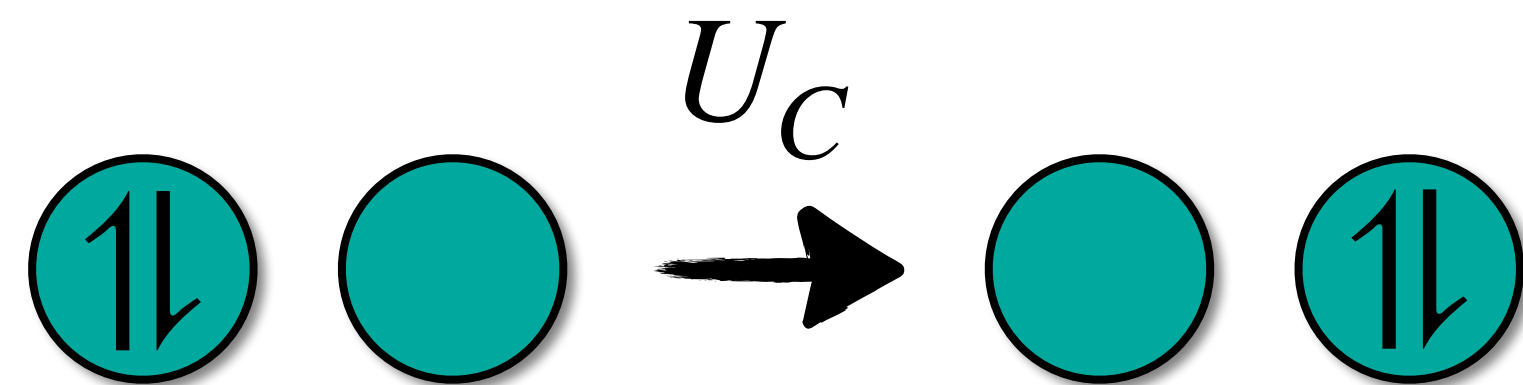
Proof of concept 
scalability: challenging!

Example: Meta-VQEs

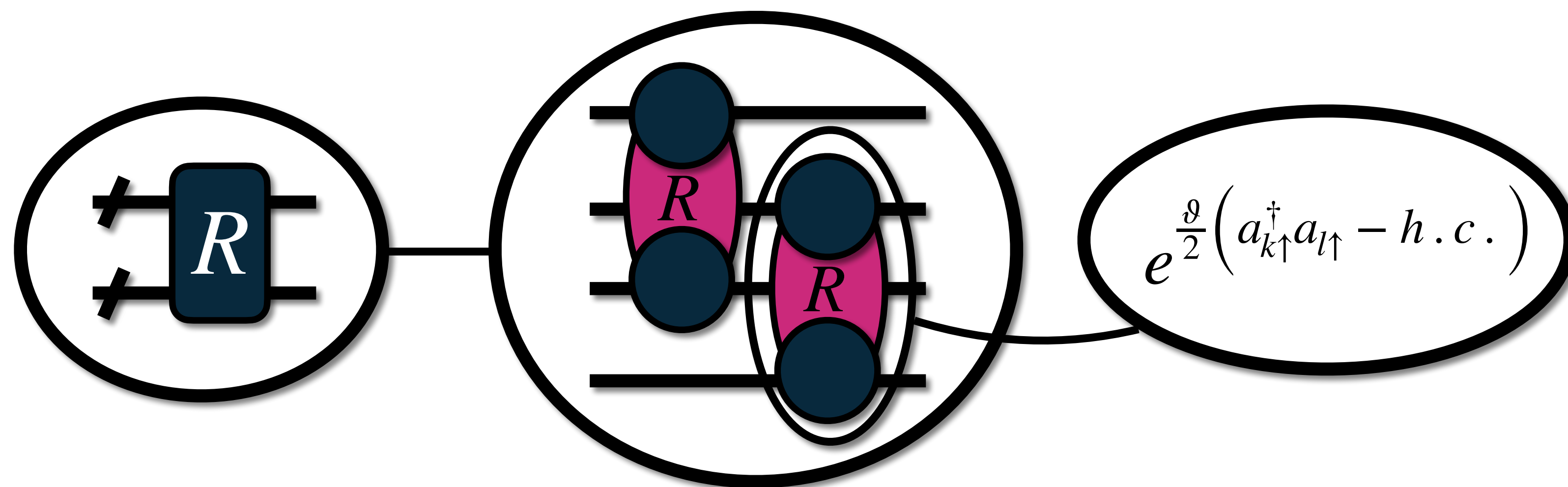
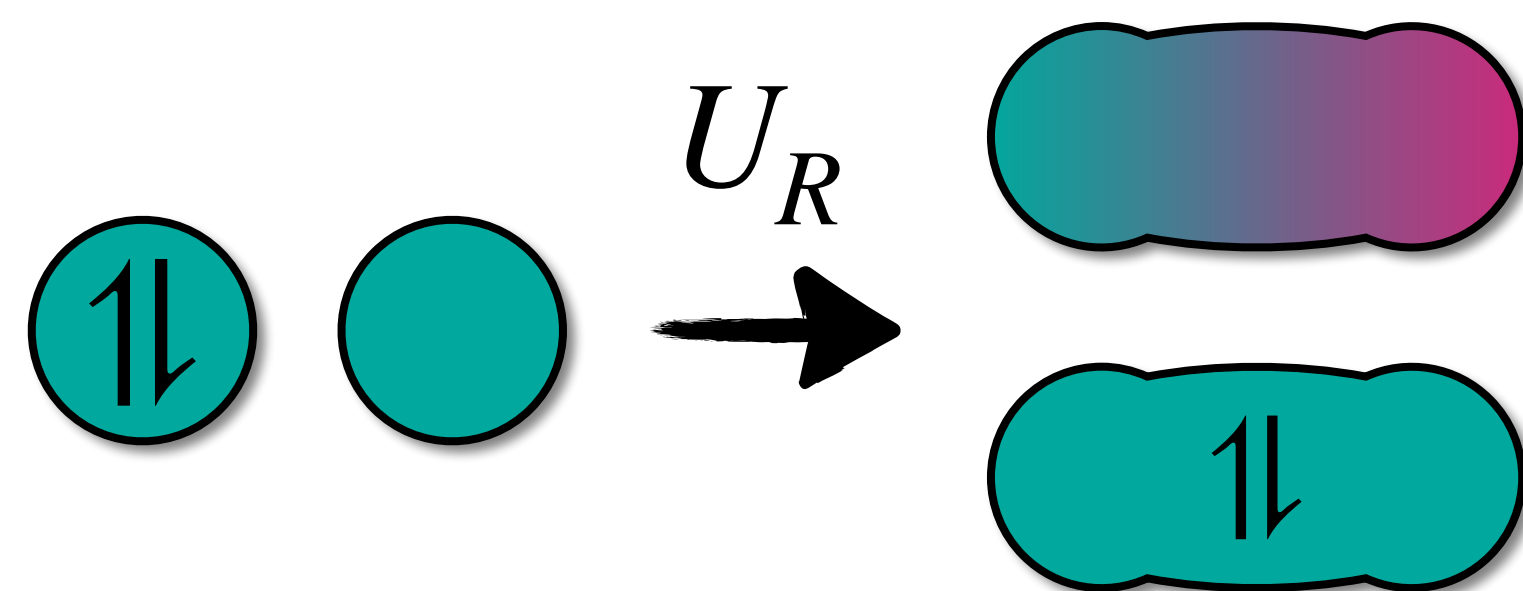


Basic Building Blocks

Pair Correlators



Basis Change

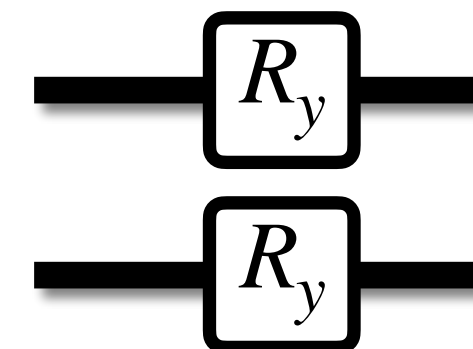
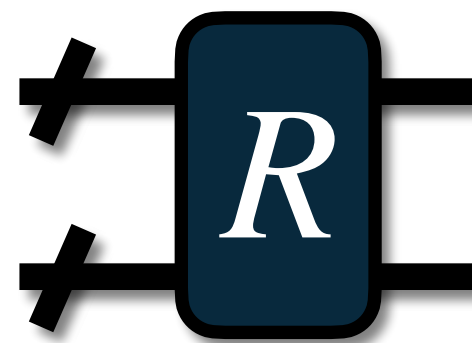


Analogy

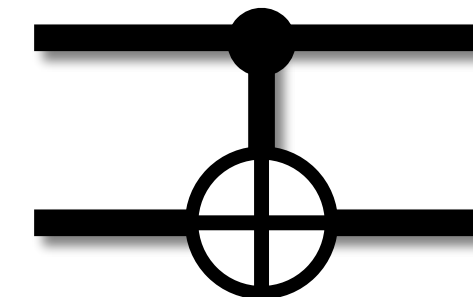
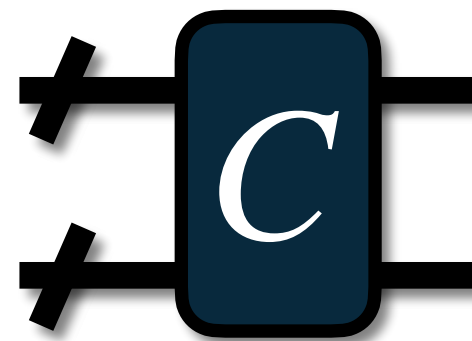
electronic structure

quantum machine learning

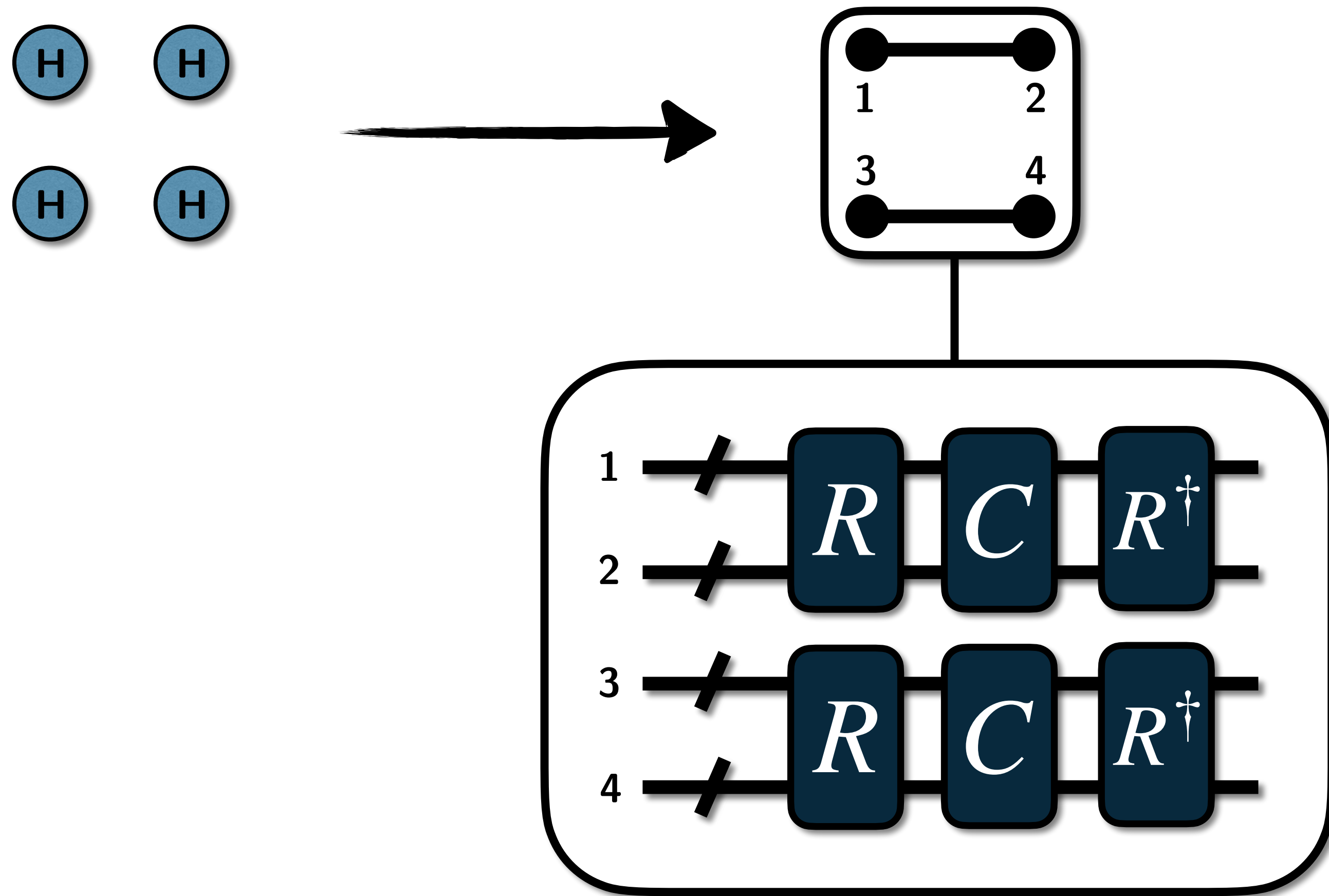
basis change



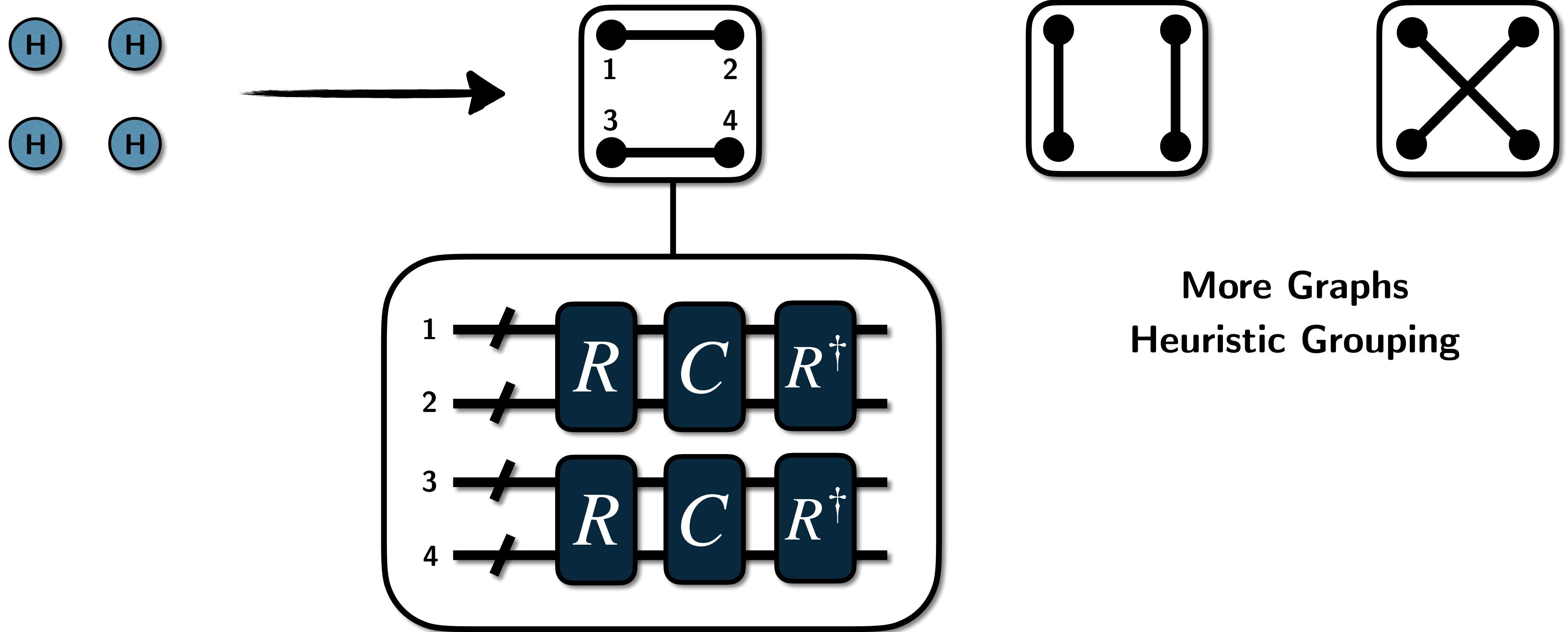
correlate



High-Level Design

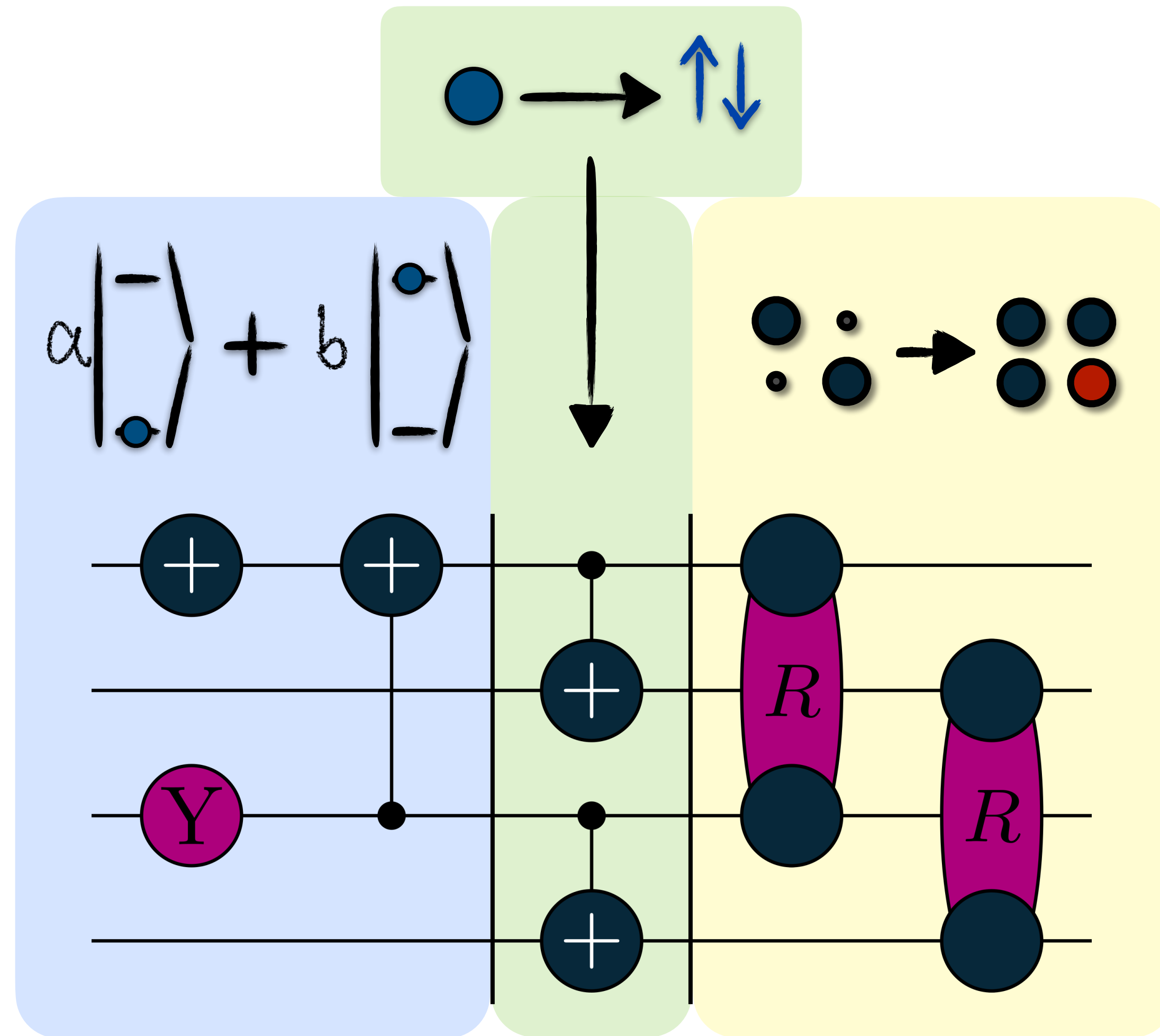
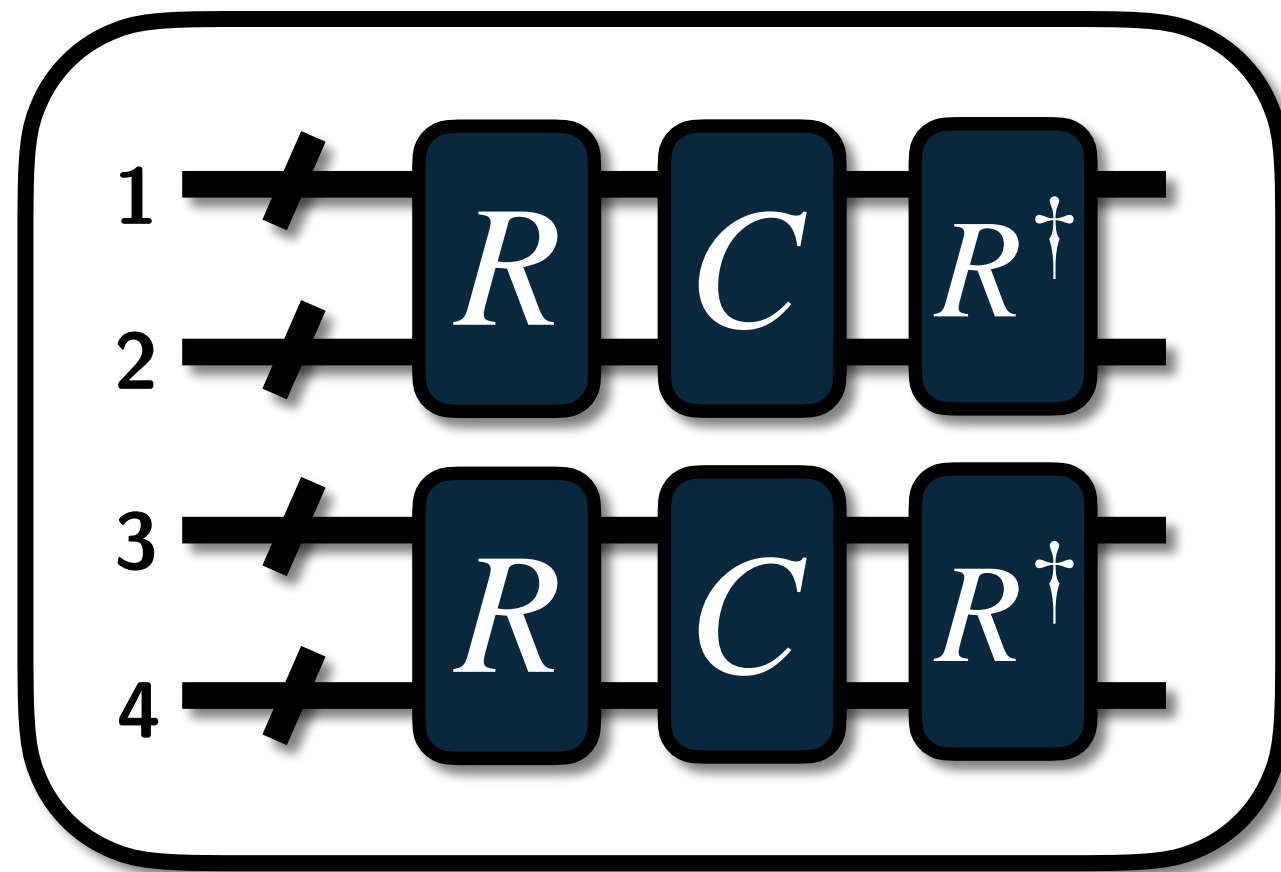


High-Level Design

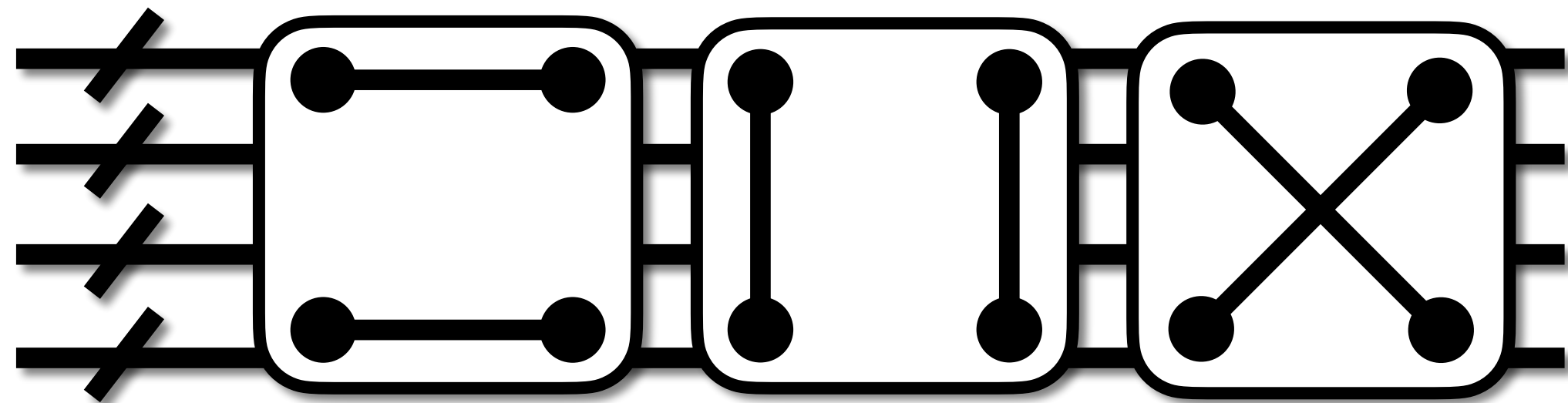


Single graphs are cheap

classically simulable



VQE-Style Wavefunction

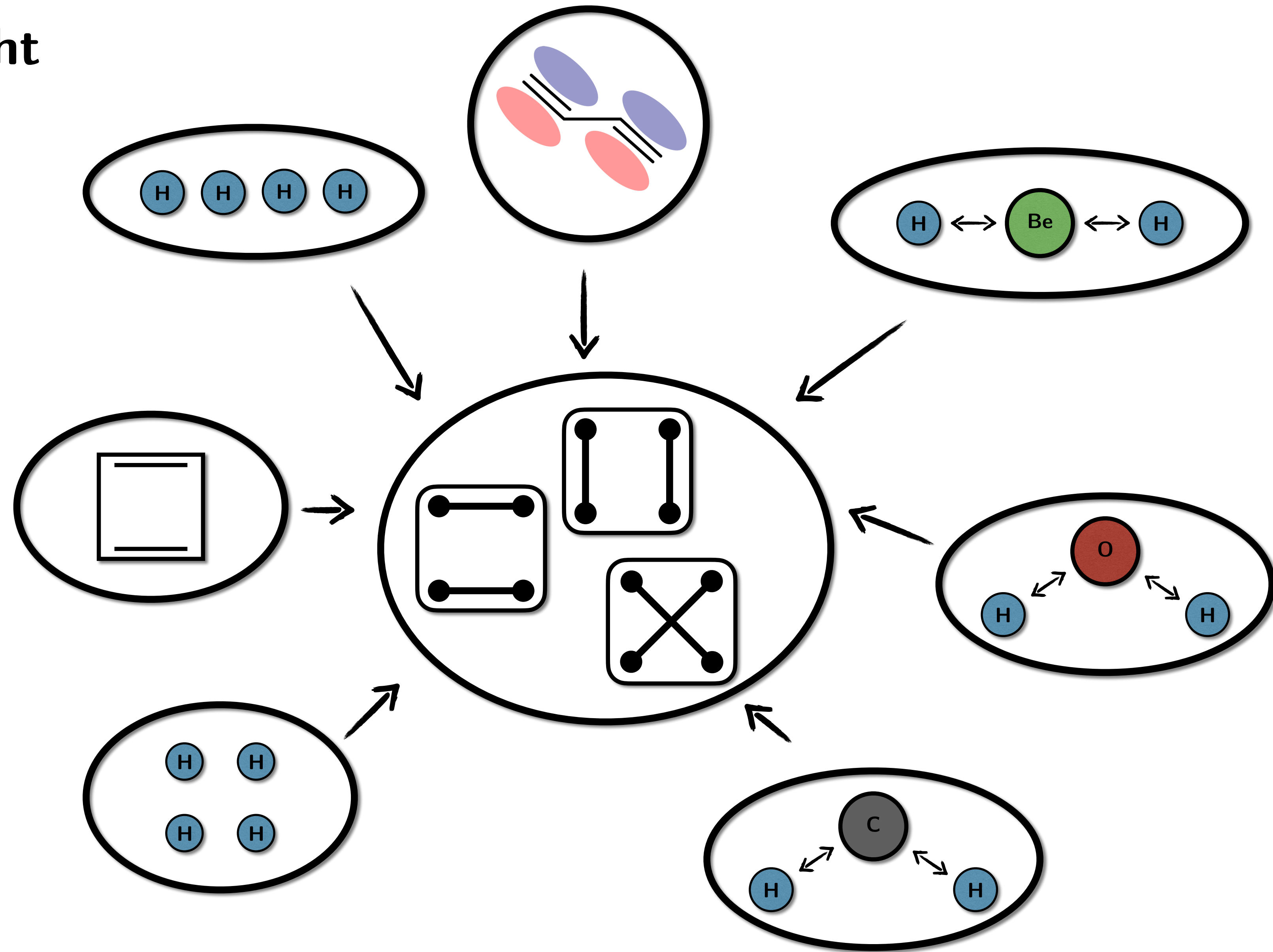


Krylov-Style Wavefunction

$$a \left| \begin{array}{|c|} \hline \text{Gate 1} \\ \hline \end{array} \right\rangle + b \left| \begin{array}{|c|} \hline \text{Gate 2} \\ \hline \end{array} \right\rangle + c \left| \begin{array}{|c|} \hline \text{Gate 3} \\ \hline \end{array} \right\rangle$$

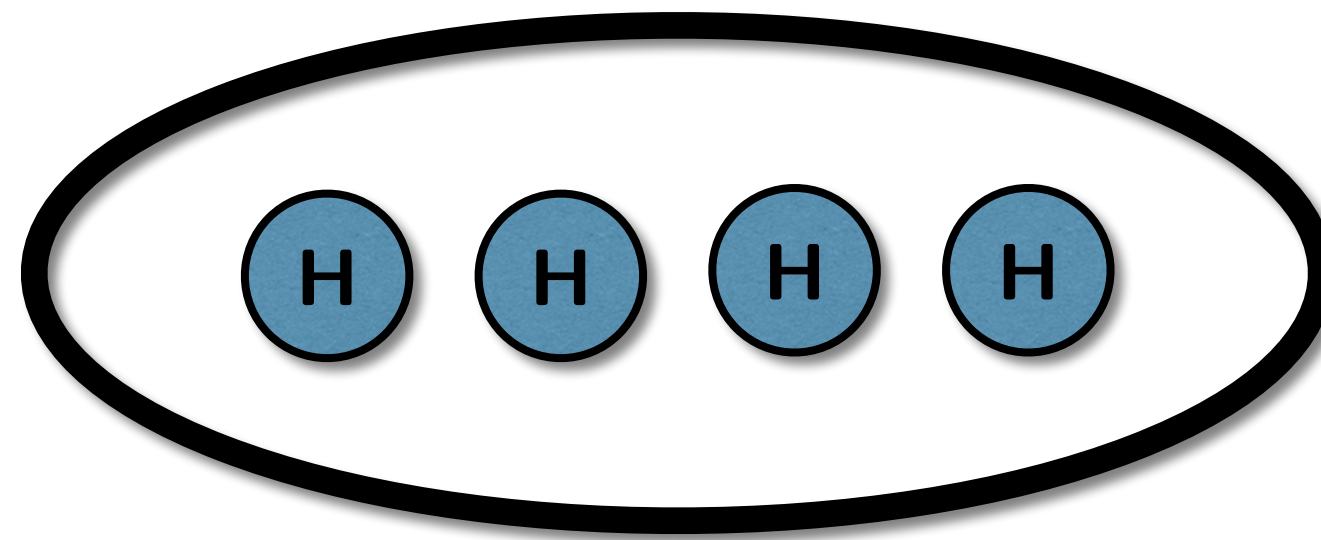
The equation represents a Krylov-style wavefunction as a linear combination of three basis states. Each basis state is represented by a ket symbol $\left| \right\rangle$ containing a diagram of a gate. The first gate (coefficient a) has horizontal lines connecting the top and bottom dots on both the first and second lines. The second gate (coefficient b) has vertical lines connecting the top and bottom dots on both the first and second lines. The third gate (coefficient c) has diagonal lines connecting the top-left dot to the bottom-right dot and the top-right dot to the bottom-left dot.

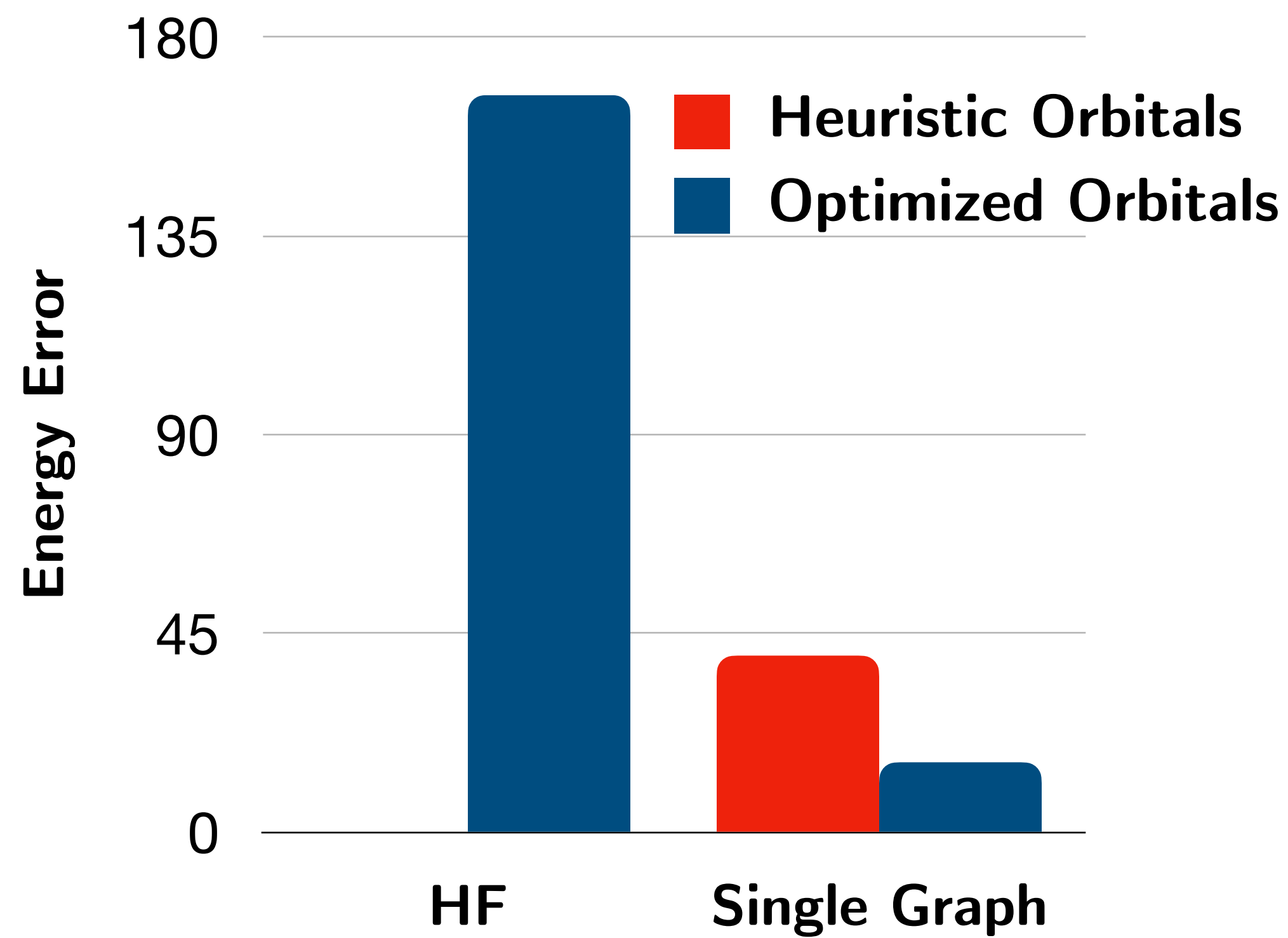
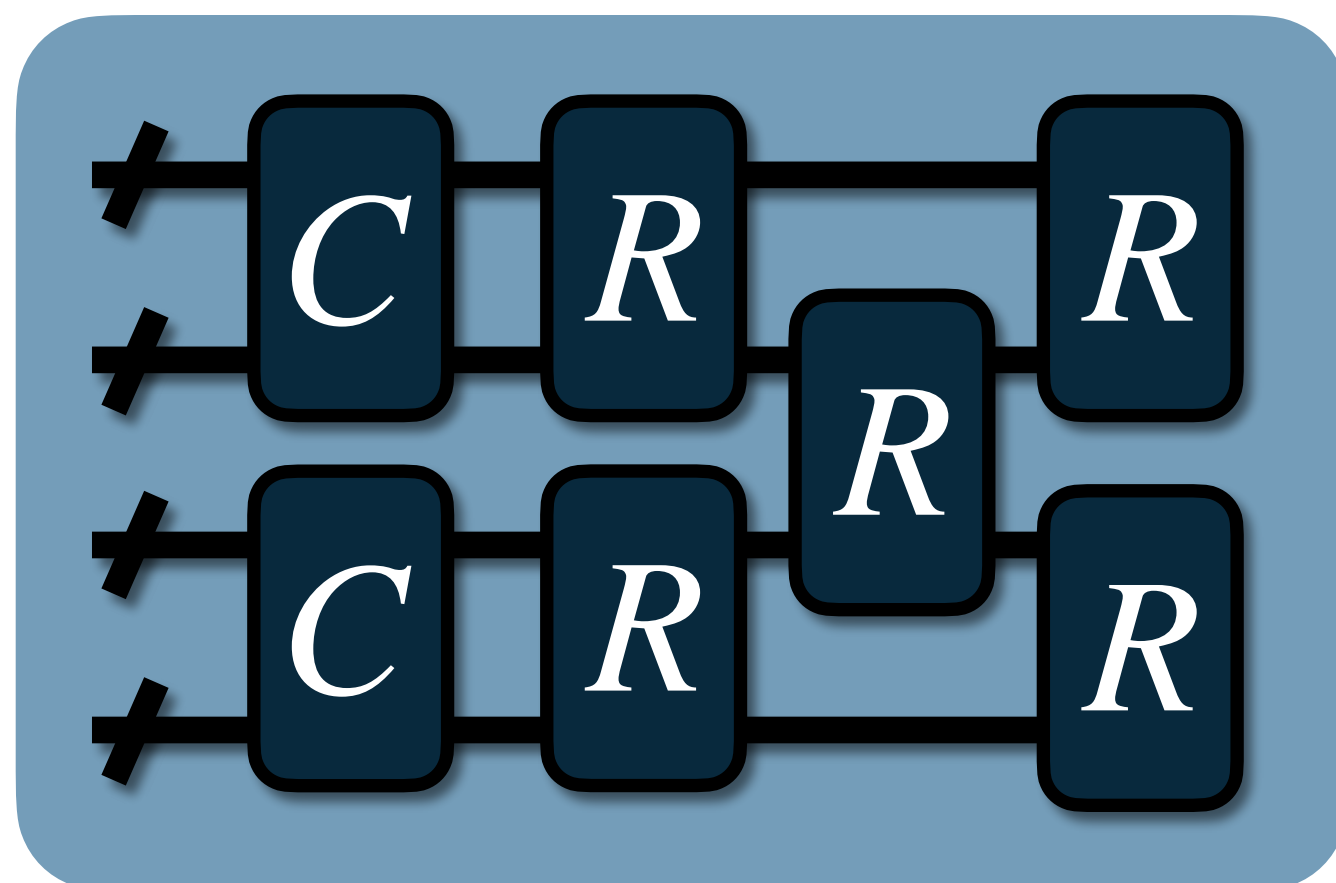
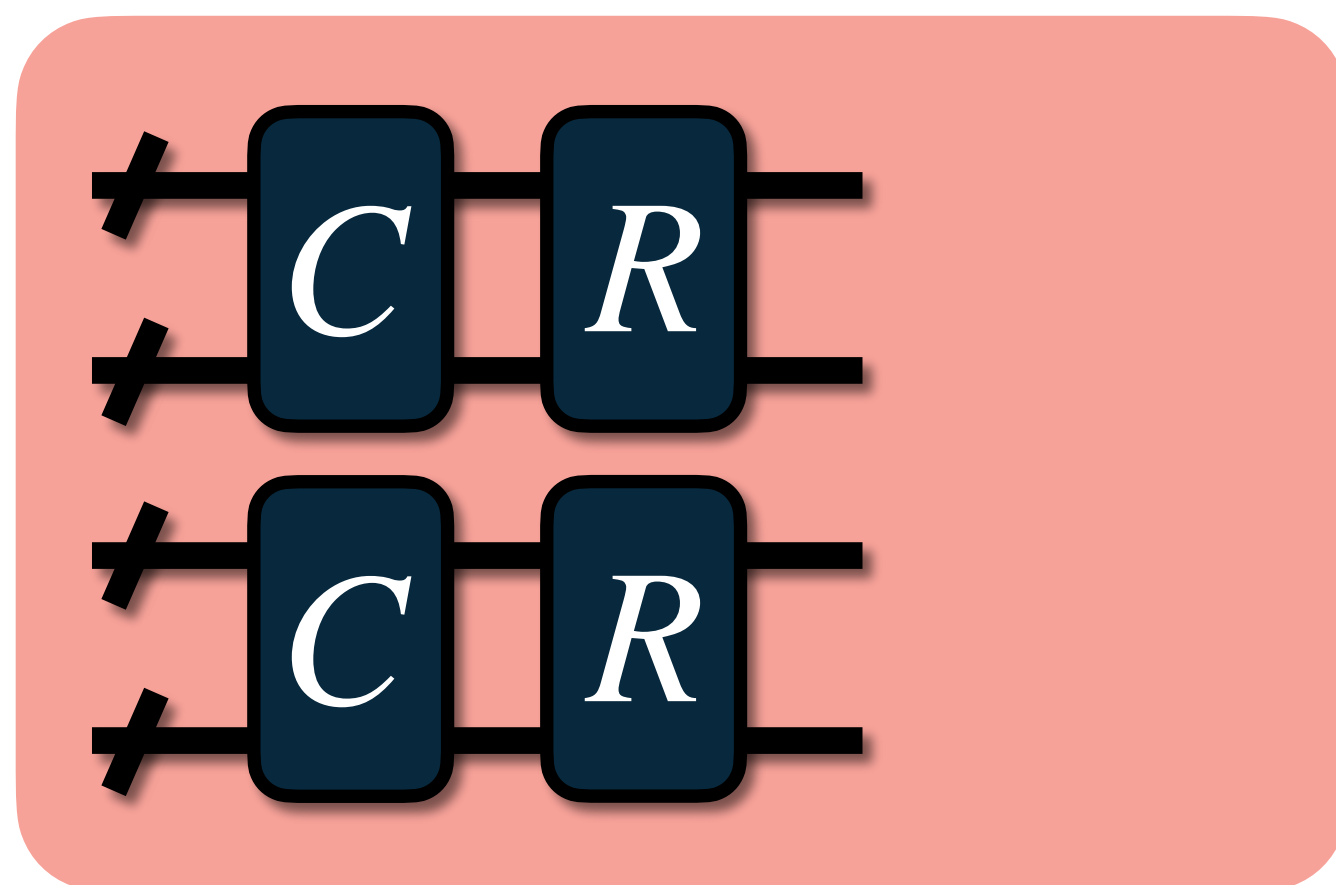
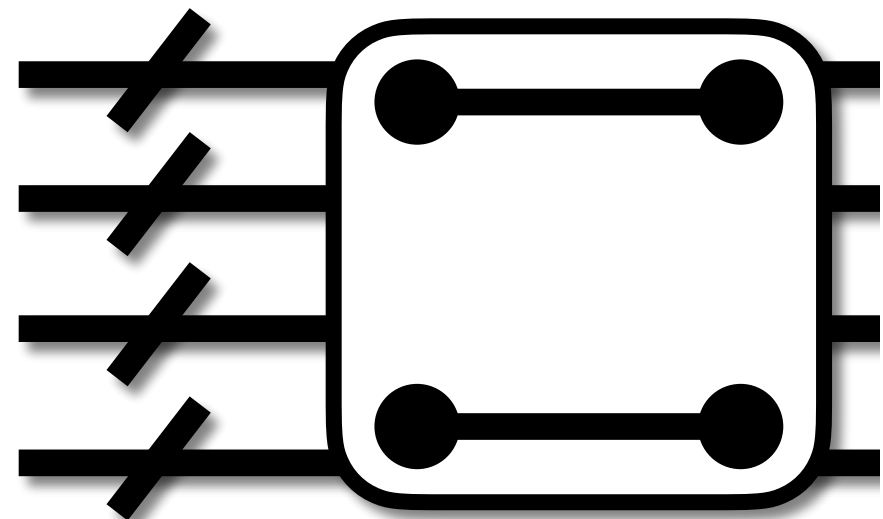
Transfer Insight

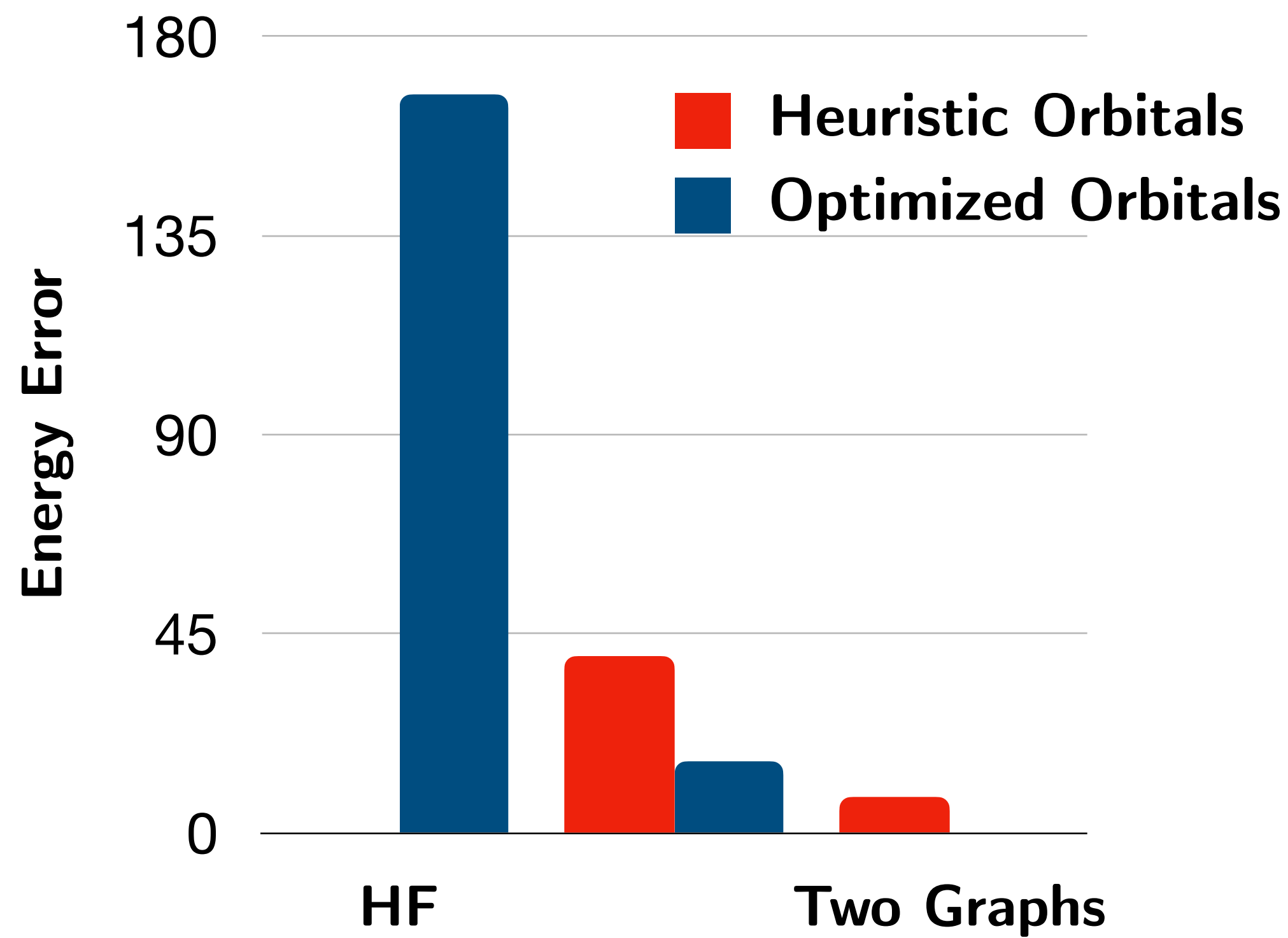
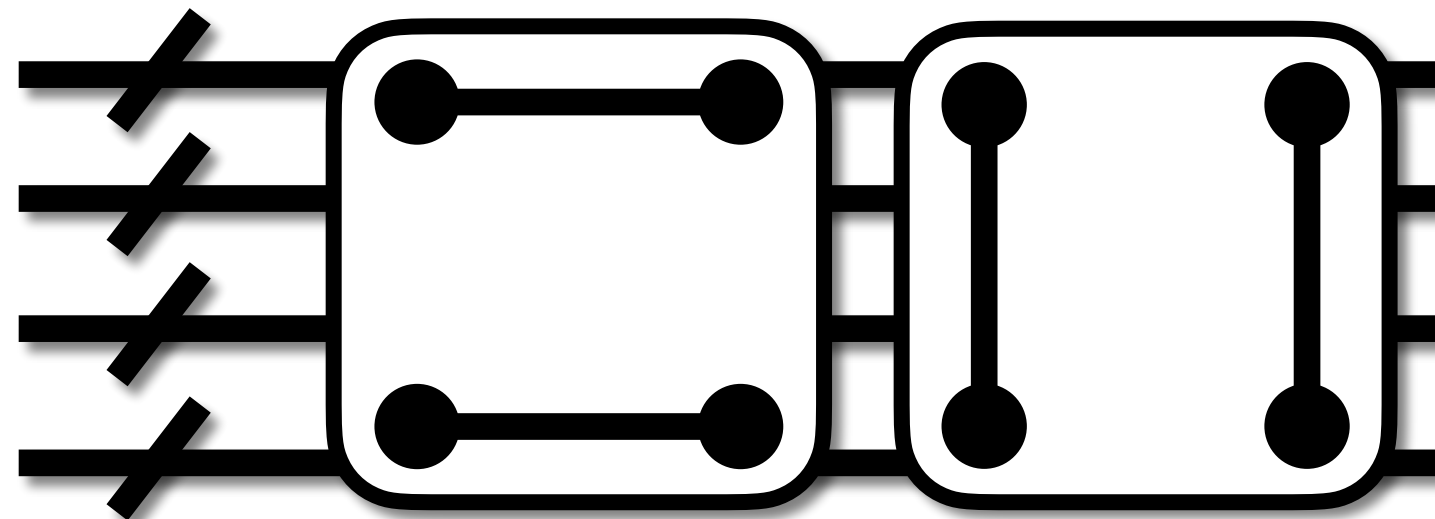


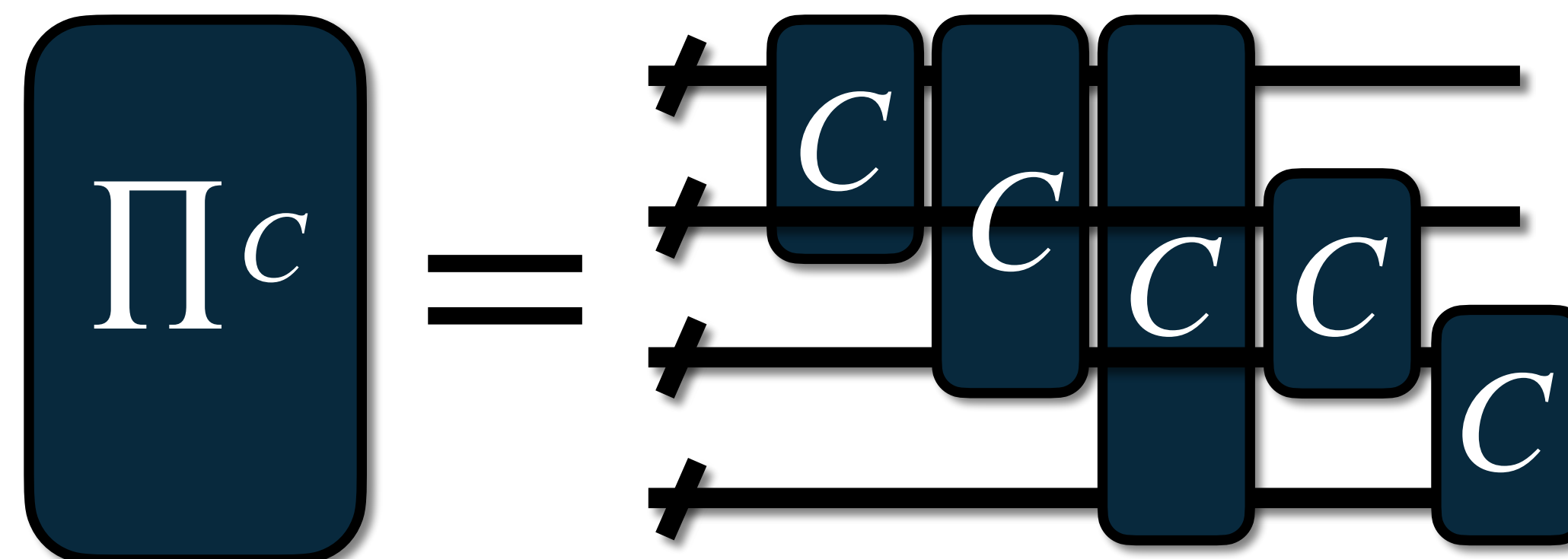
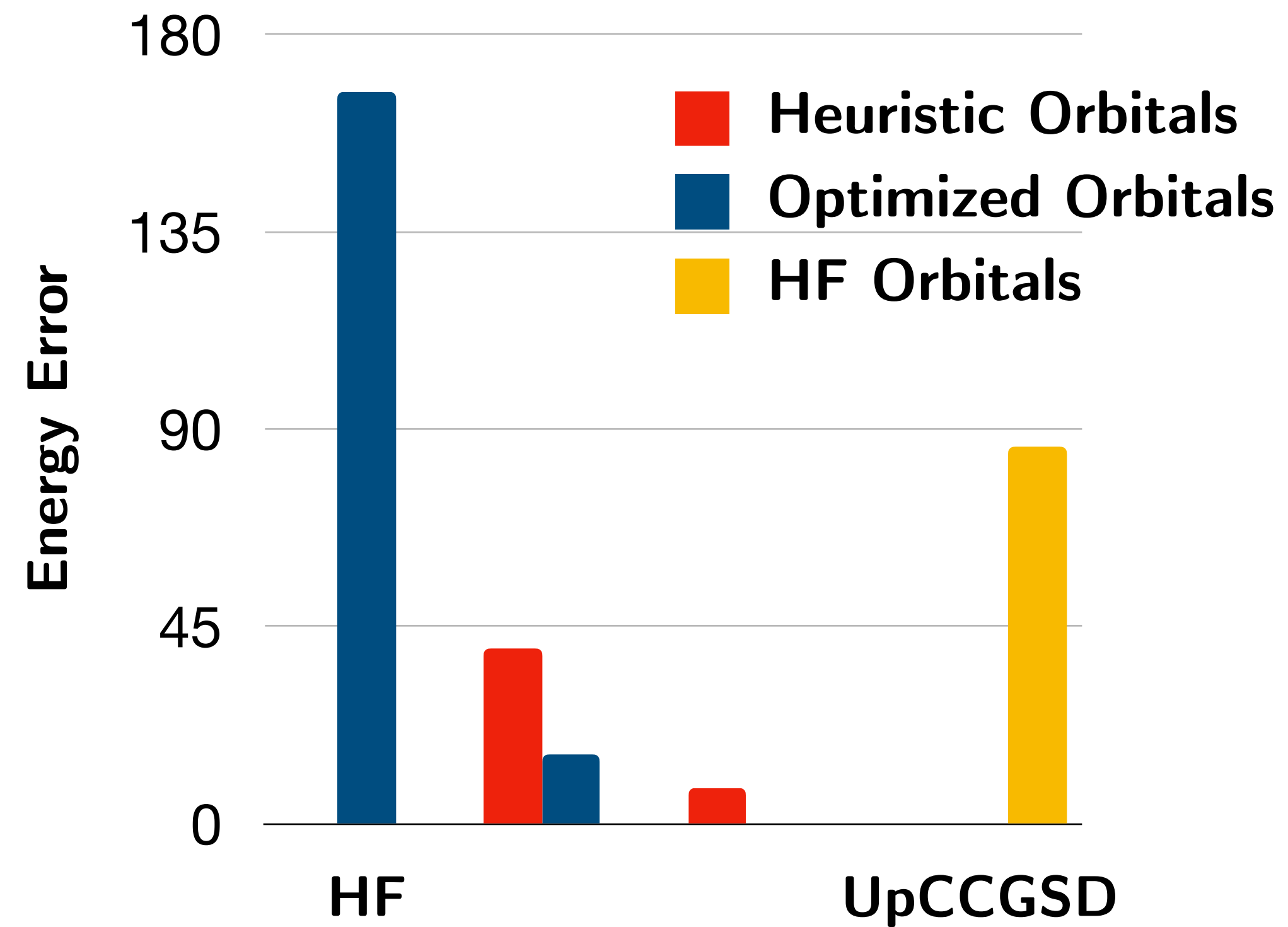
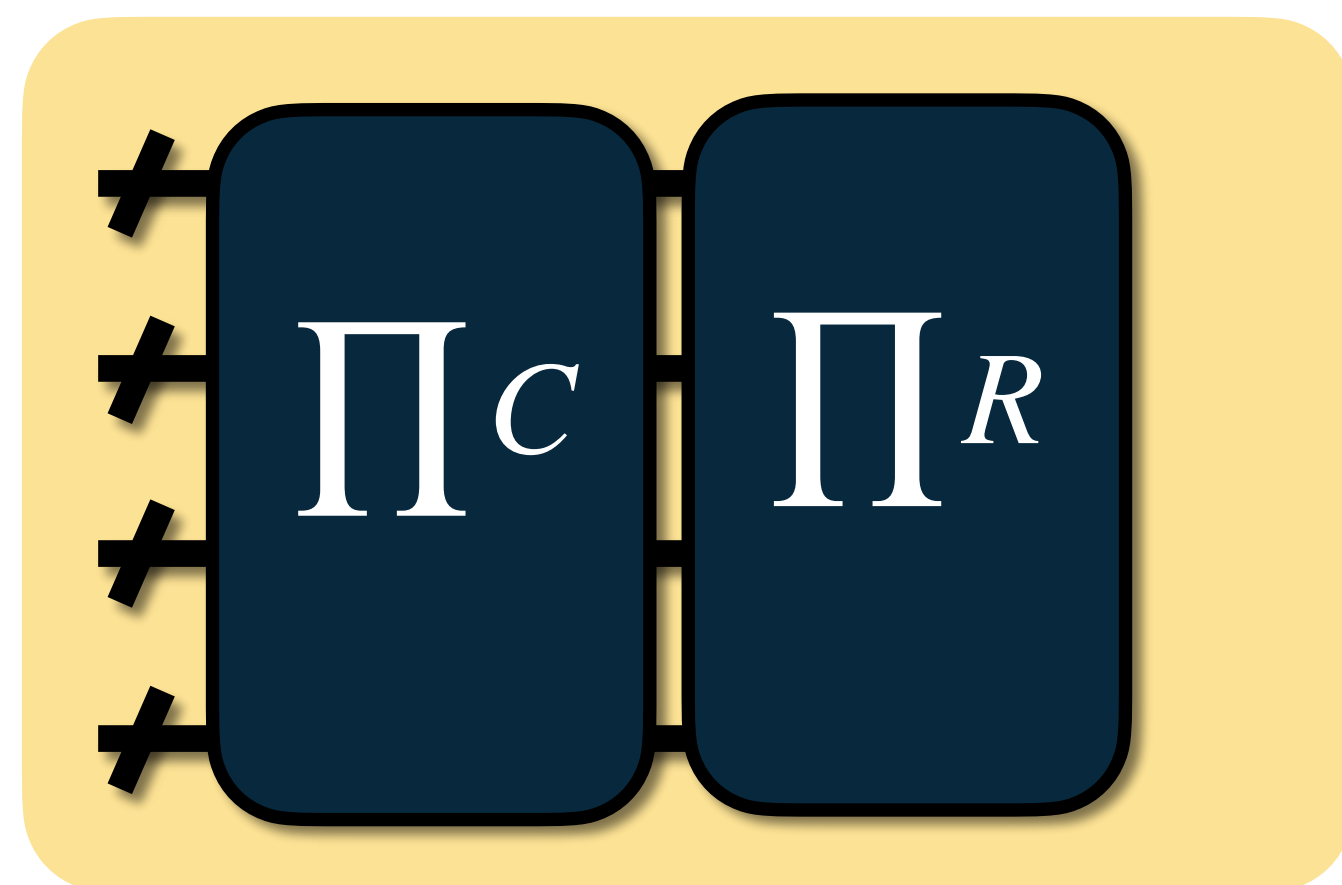
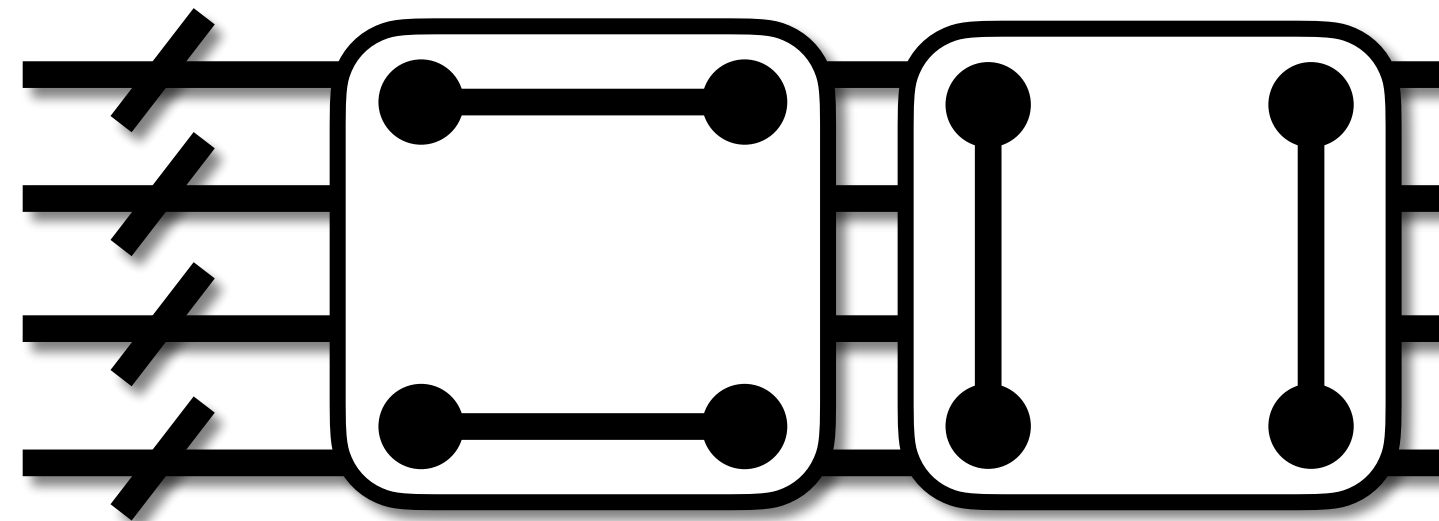
Example

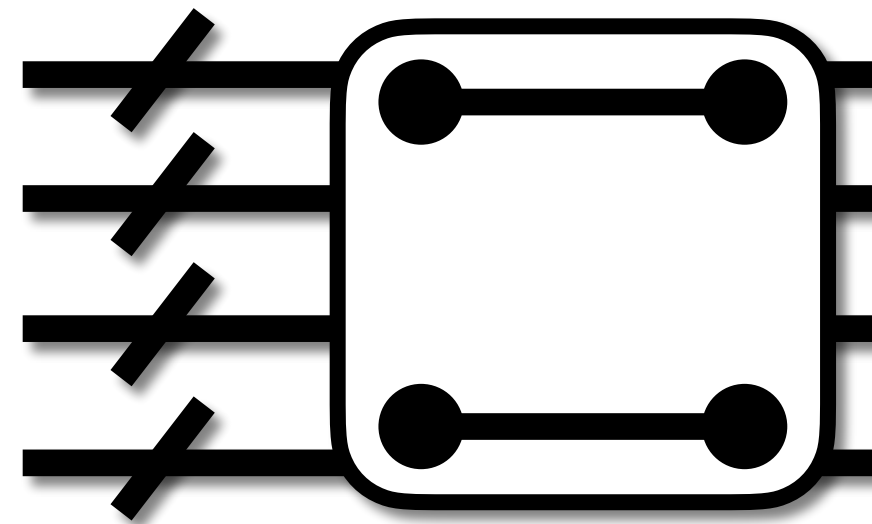
Linear H₄ Molecule



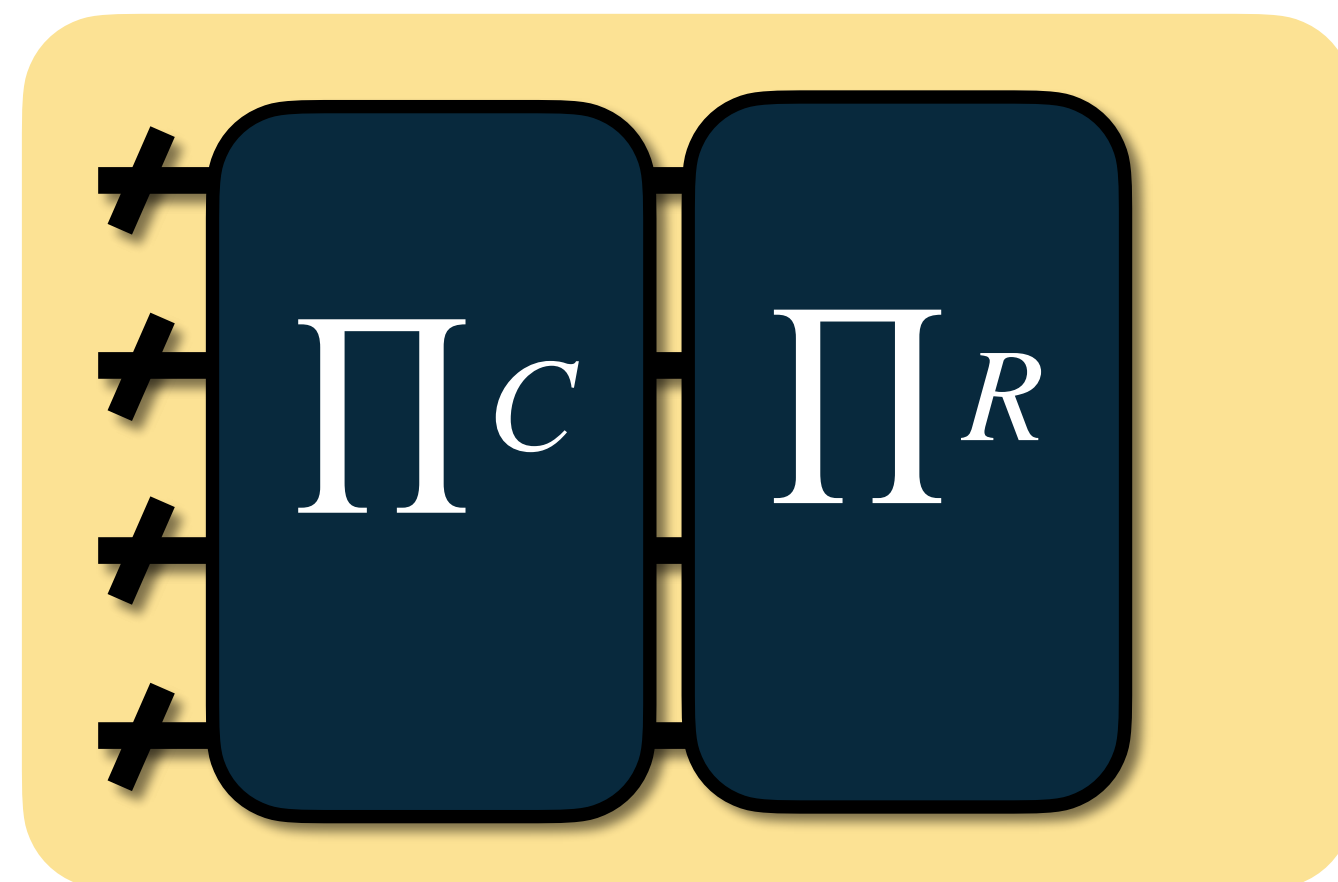






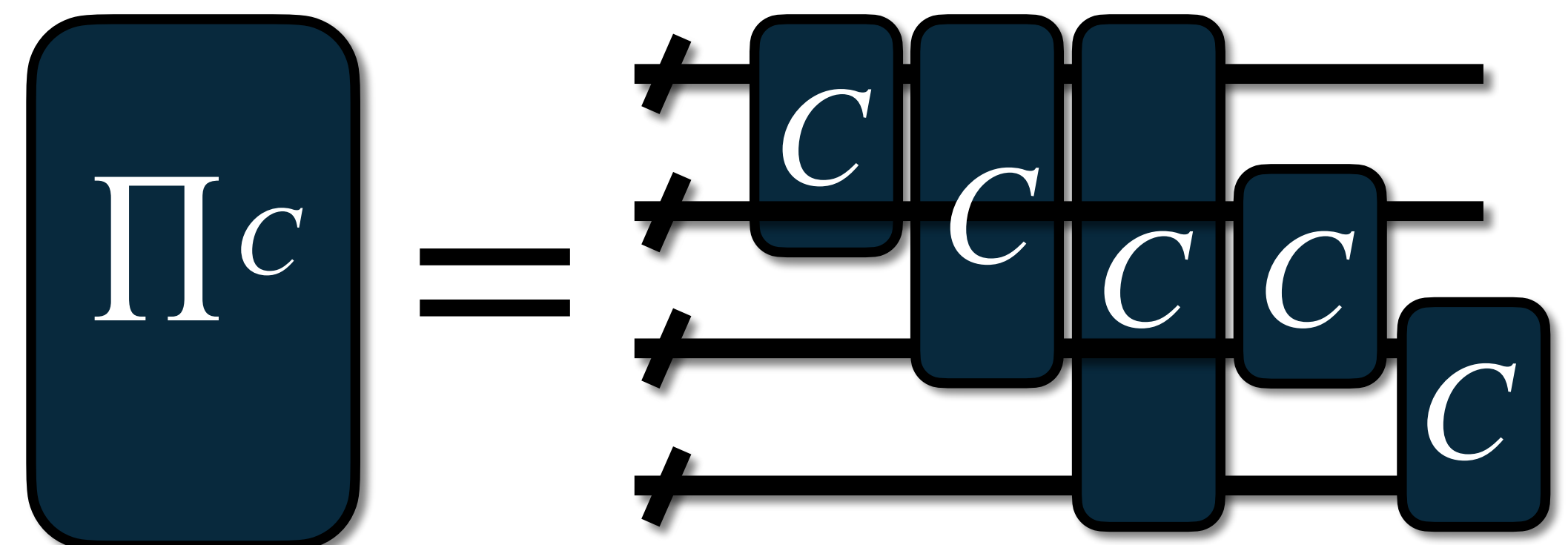
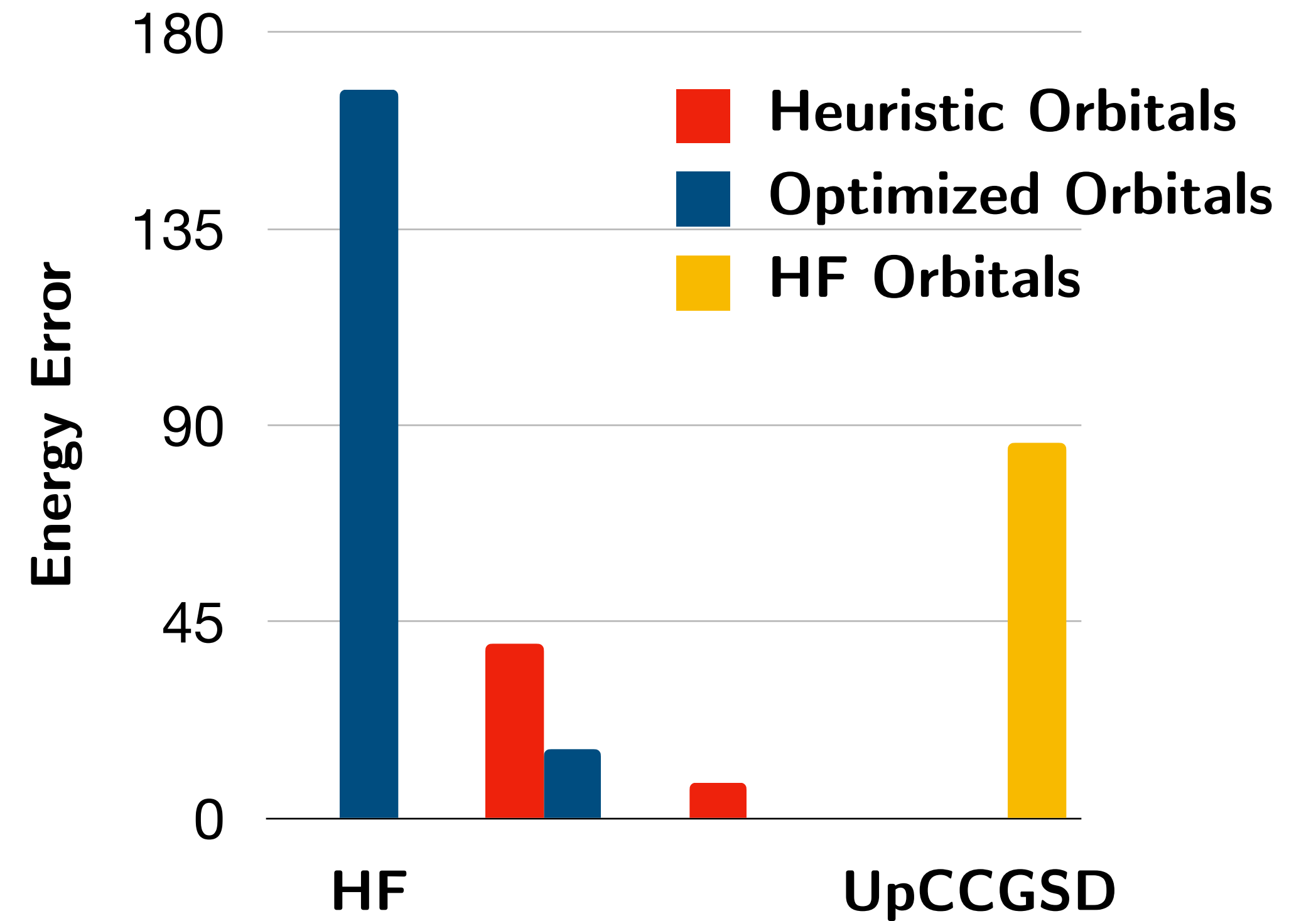


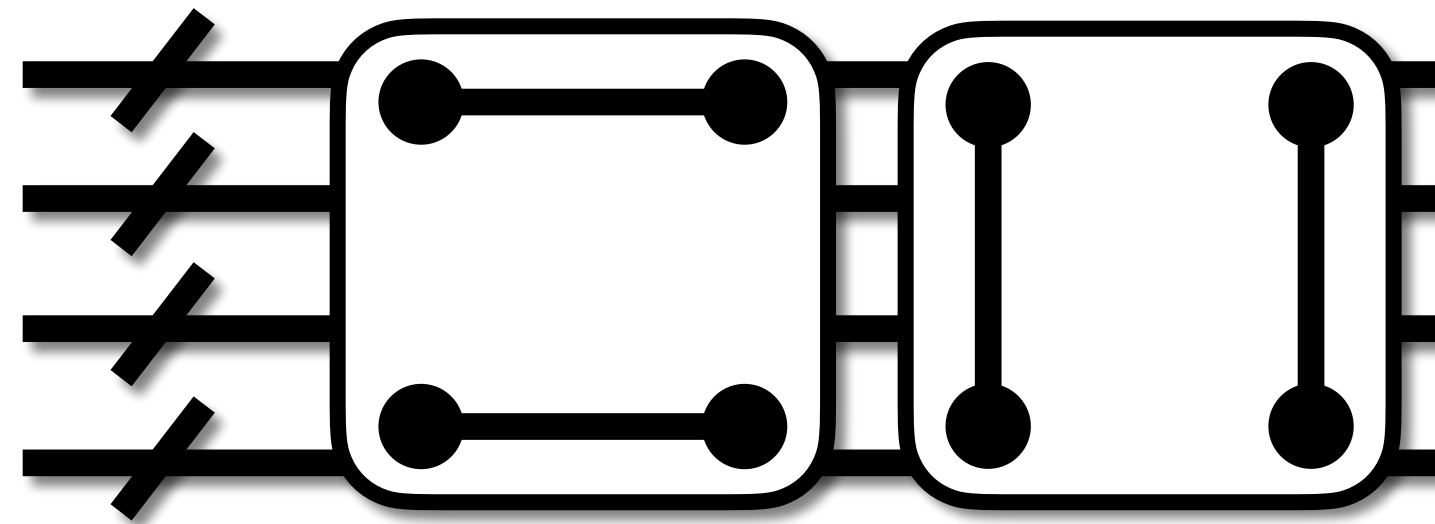
parameters: 4
cnots: 6 — 70



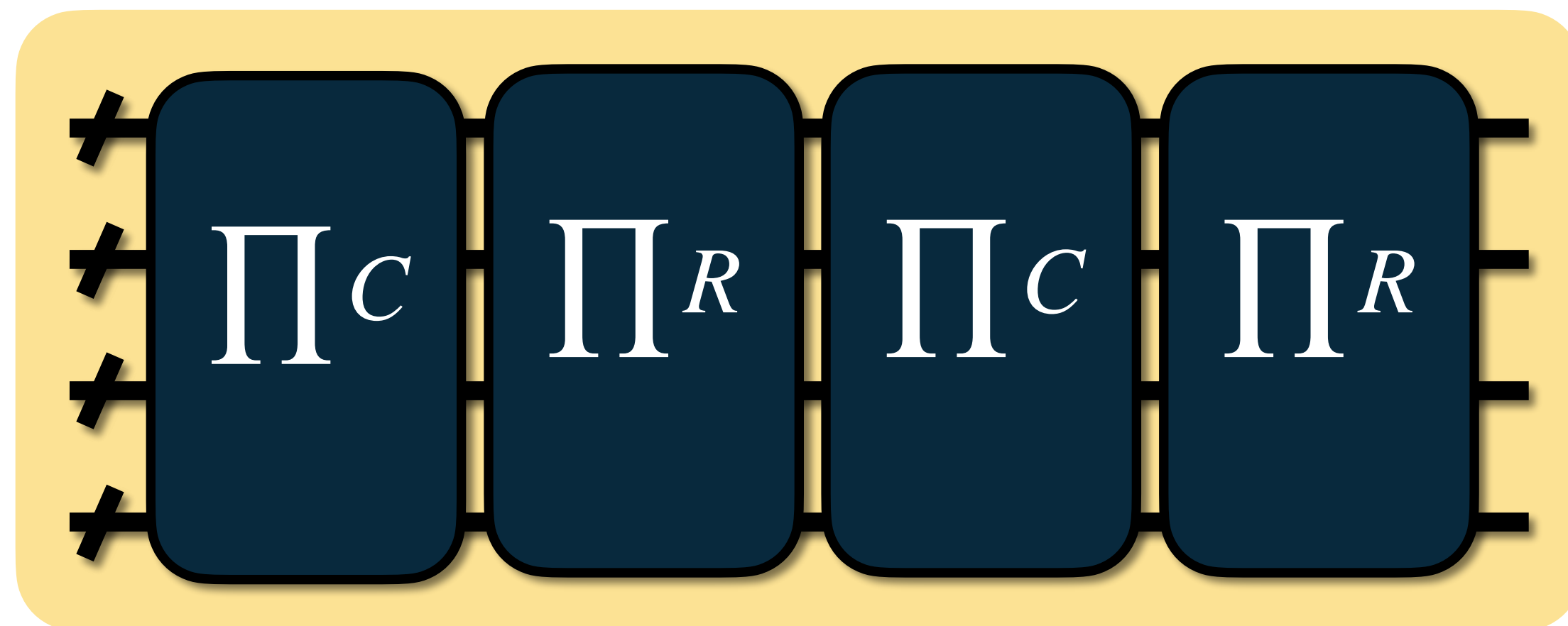
UpCCGSD
parameters: 18
cnots: 66 — 188

k-UpCCGSD: Lee, JCTC, 2018

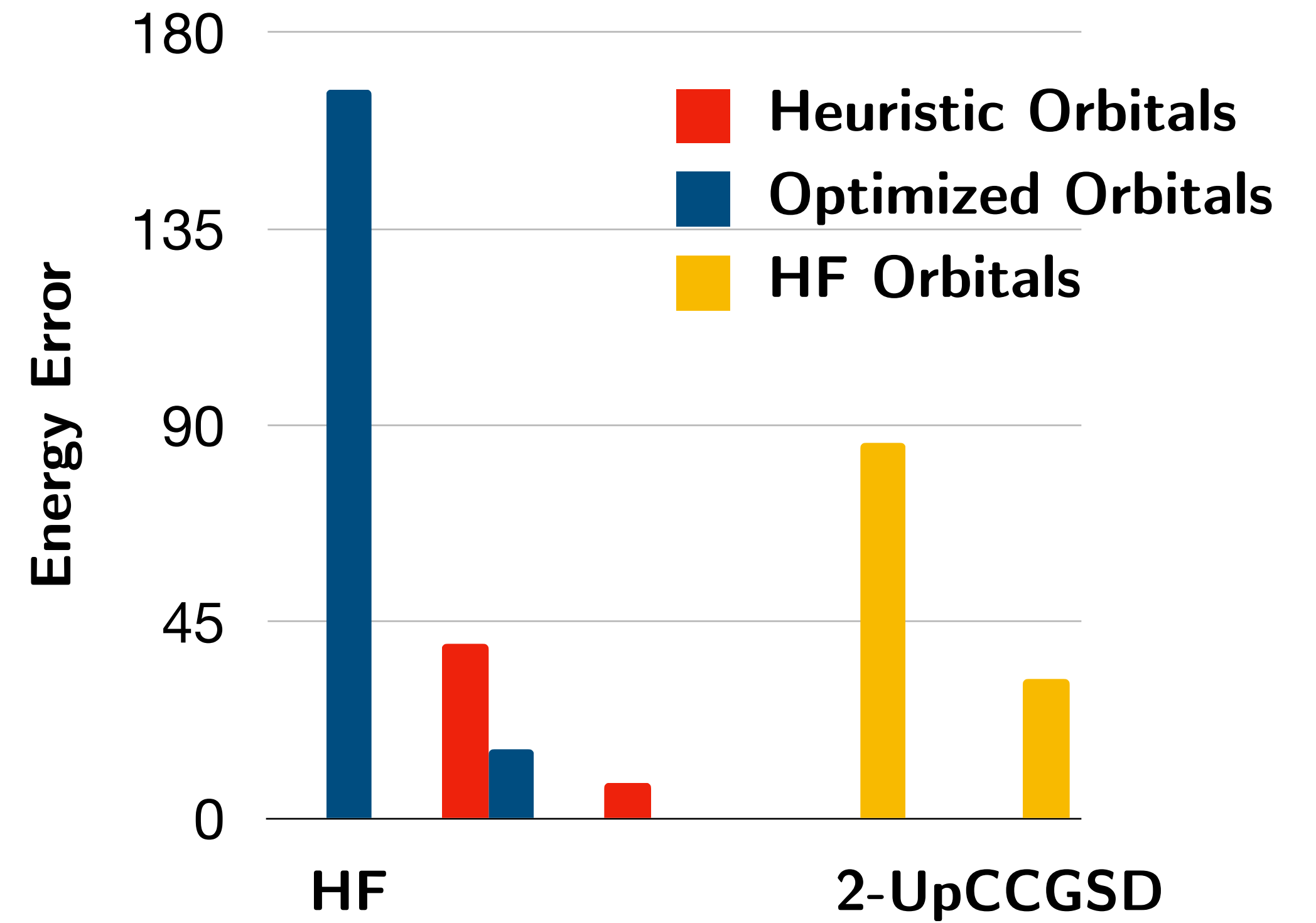


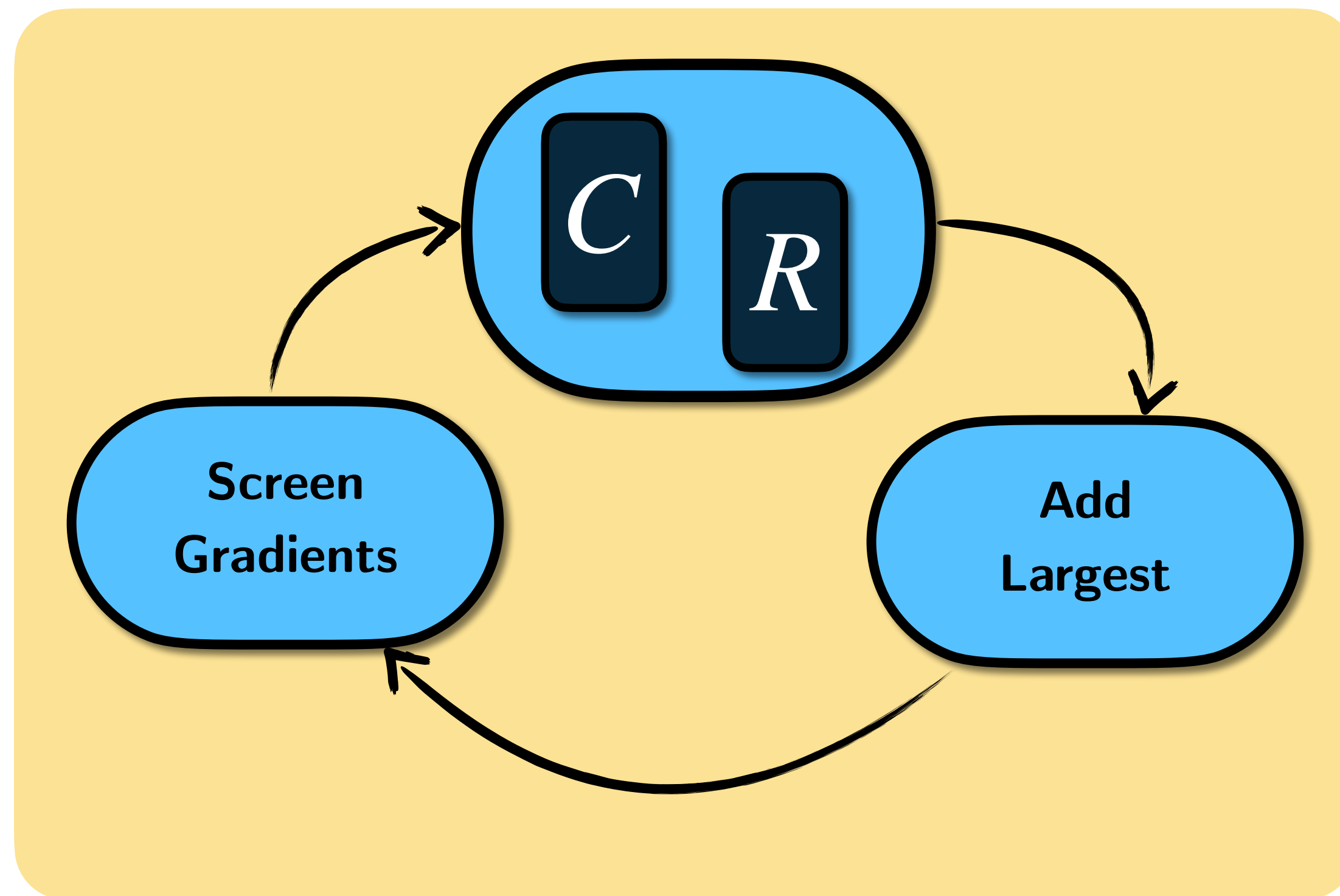


parameters: 6
cnots: 116



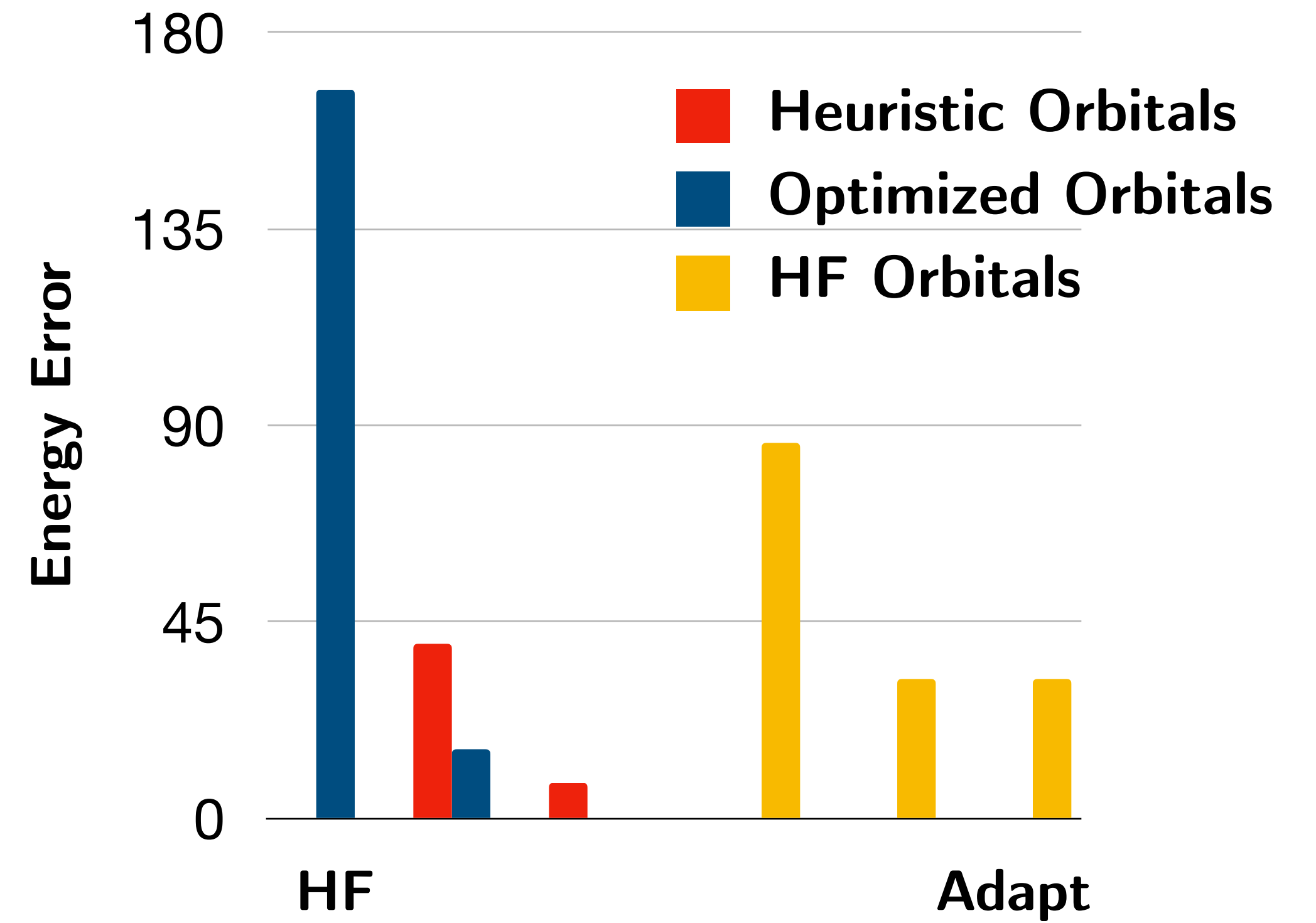
2-UpCCGSD
parameters: 36
cnots: 432



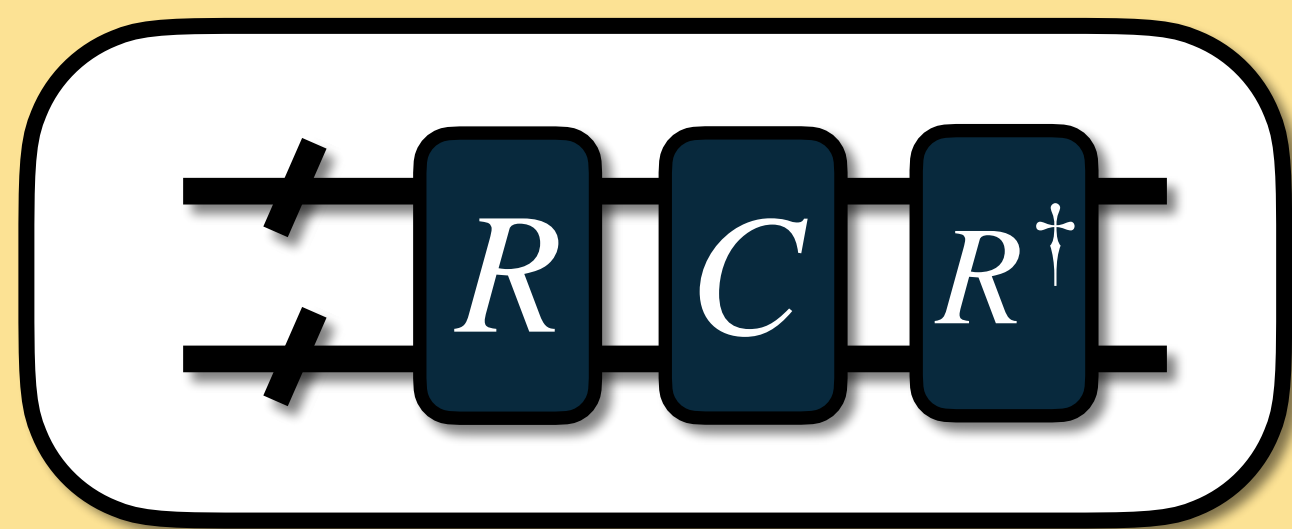


2-UpCCGSD
parameters: 36
cnots: 432

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

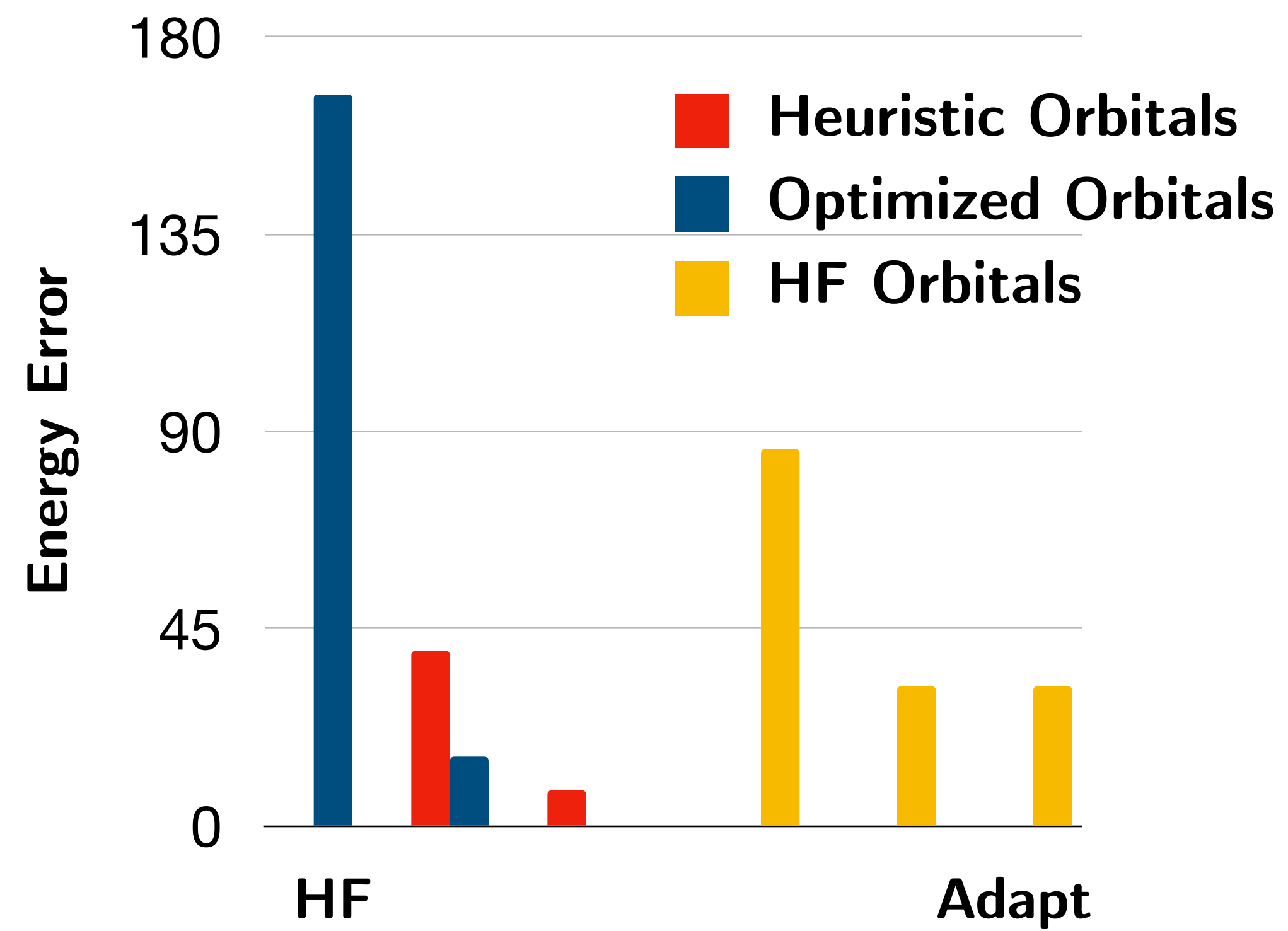


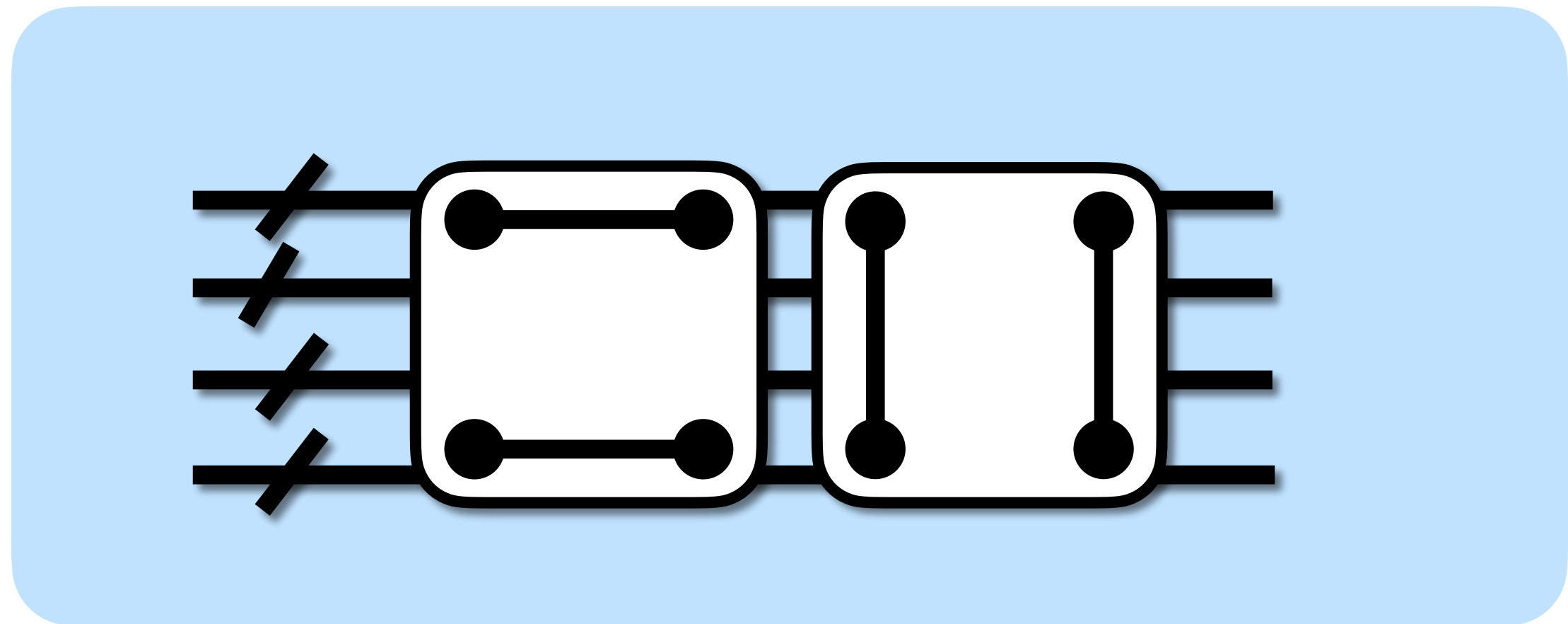
Motif hard to detect locally



2-UpCCGSD
parameters: 36
cnots: 432

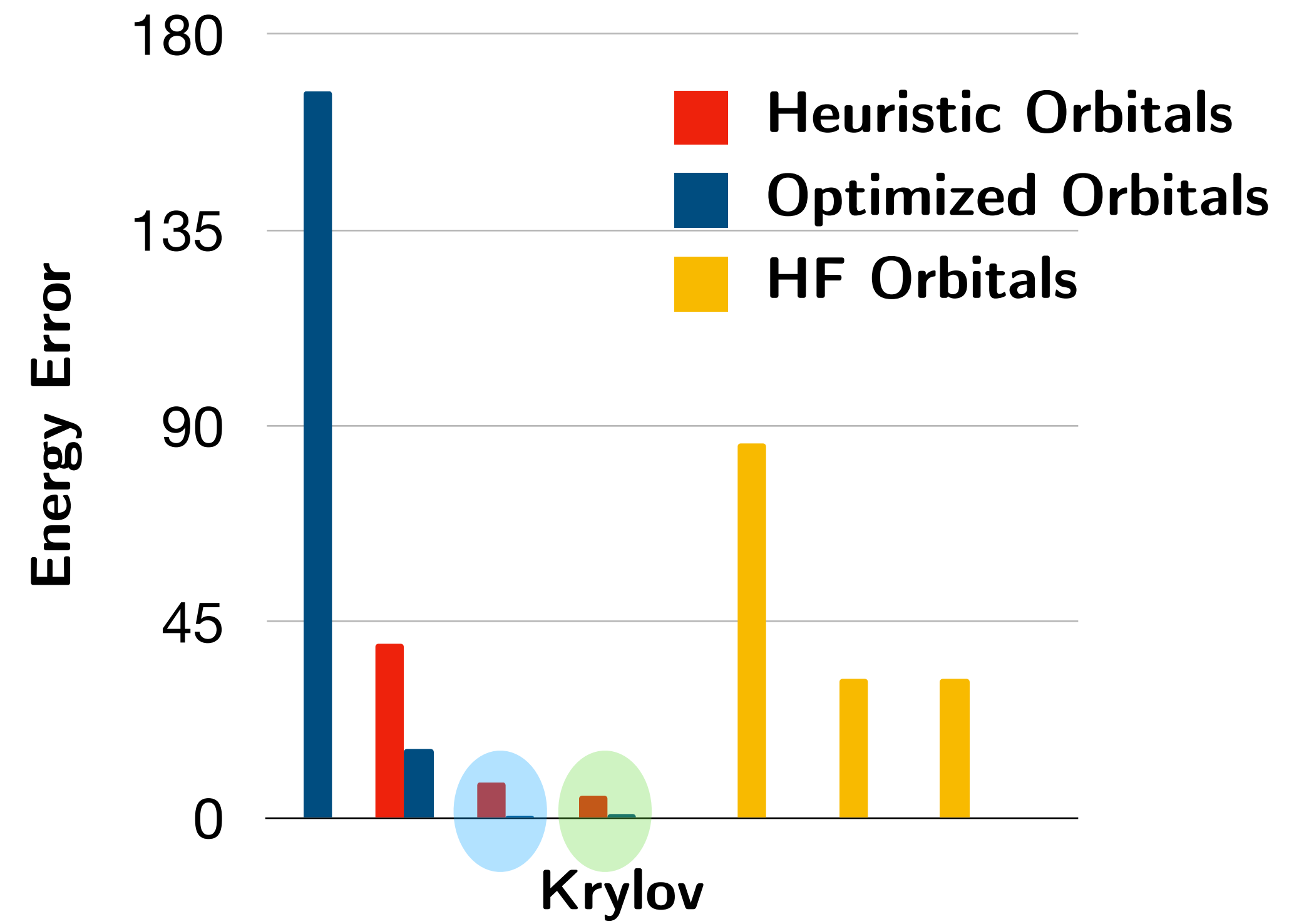
Adapt(C,R)
parameters: 12
cnots: 448



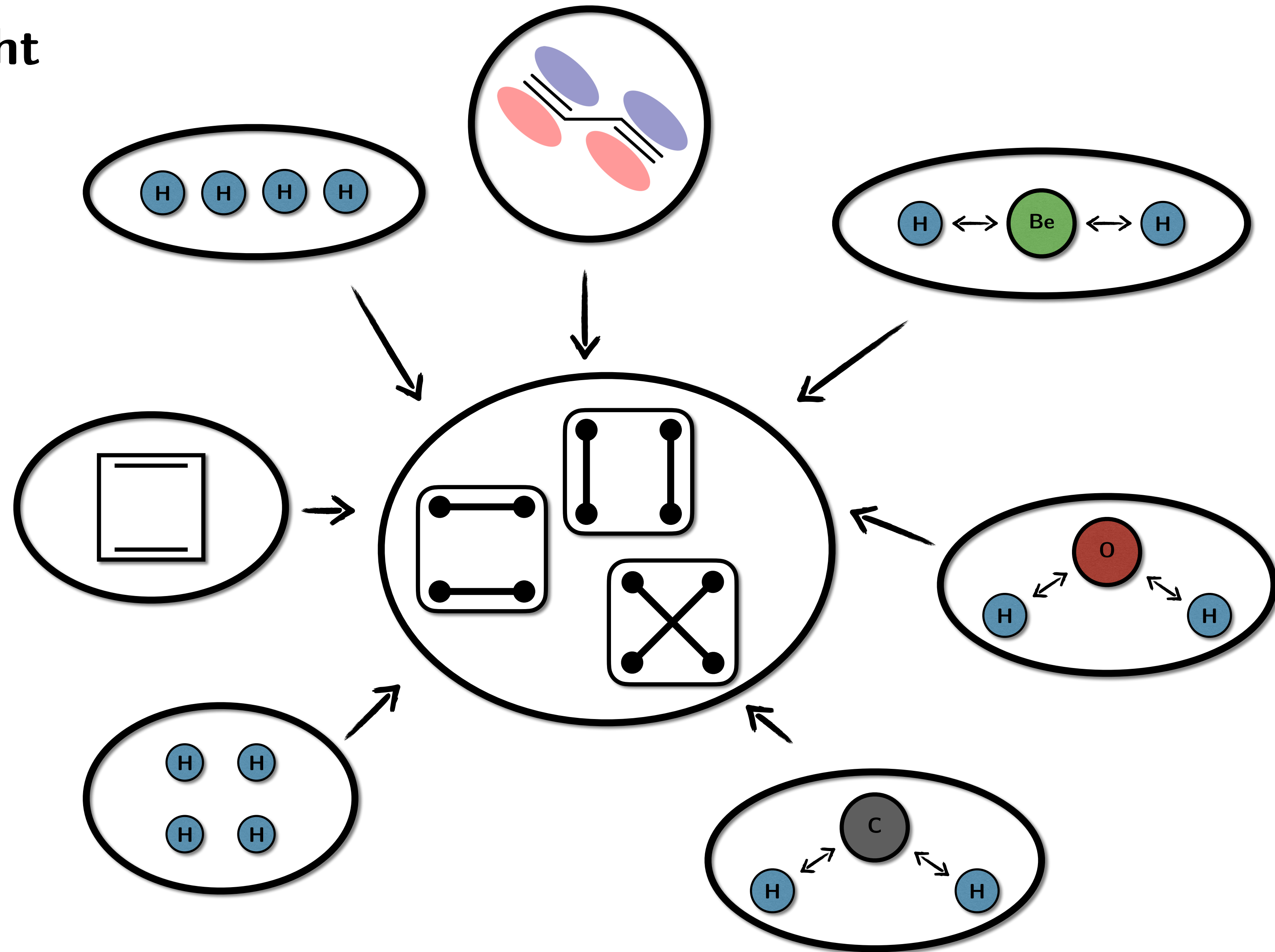


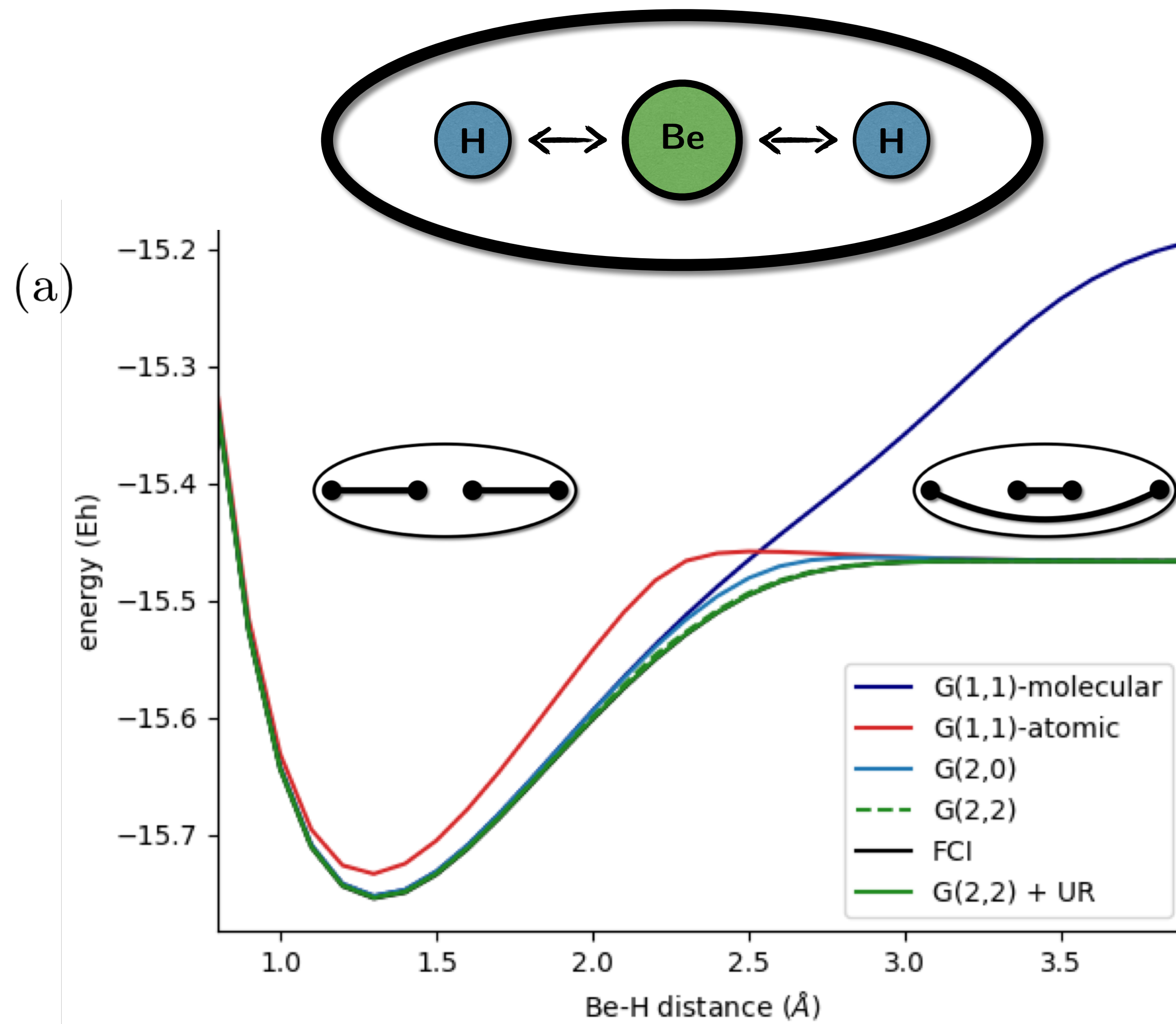
$$a \left| \begin{array}{cc} \bullet & \bullet \\ \bullet & \bullet \end{array} \right\rangle + b \left| \begin{array}{cc} \bullet & \bullet \\ \bullet & \bullet \end{array} \right\rangle$$

A quantum state representation on a light green background. It shows a superposition of two states, each represented by a square box with four dots at the corners. The first state is labeled with coefficient a and the second with coefficient b . The boxes are connected by a plus sign.



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)

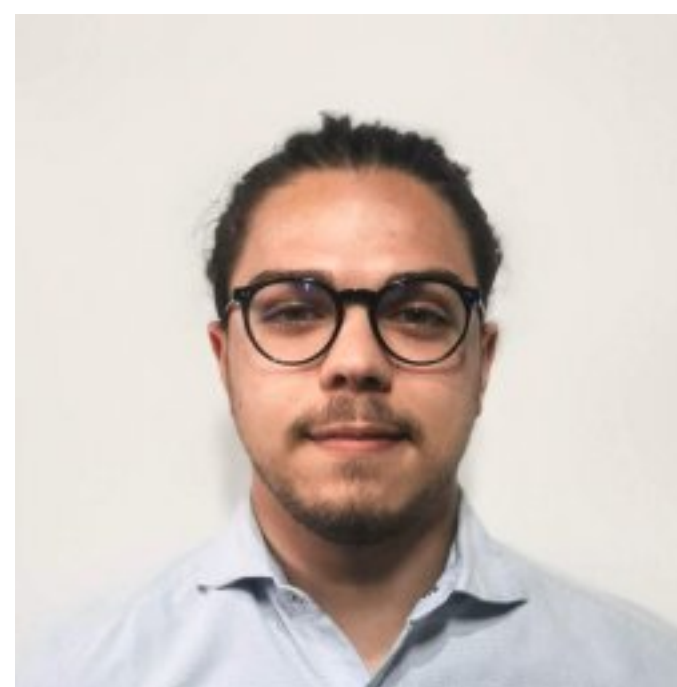
Krylov-Style Multi-Graphs

Compact Effective Basis Generation: Insights from Interpretable Circuit Design

Jakob S. Kottmann¹ and Francesco Scala²



quantum
open-source
foundation



PhD Position Available

code examples online



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



github.com/tequilahub