Boosting ground states preparation with double-bracket quantum algorithms

PART 1: Introducing and optimizing double-bracket quantum algorithms

Matteo Robbiati

28 November 2024

A couple of references

Double-bracket quantum algorithms for diagonalization

Marek Gluza

This work proposes double-bracket iterations as a framework for obtaining diagonalizing quantum circuits. Their implementation on a quantum computer consists of interlacing evolutions generated by the input Hamiltonian with diagonal evolutions which can be chosen variationally. No qubit overheads or controlled-unitary operations are needed but the method is recursive which makes the circuit depth grow exponentially with the number of recursion steps. To make near-term implementations viable, the proposal includes optimization of diagonal evolution generators and of recursion step durations. Indeed, thanks to this numerical examples show that the expressive power of double-bracket iterations suffices to approximate eigenstates of relevant quantum models with few recursion steps. Compared to brute-force optimization of unstructured circuits double-bracket iterations do not suffer from the same trainability limitations. Moreover, with an implementation cost lower than required for quantum phase estimation they are more suitable for near-term quantum computing experiments. More broadly, this work opens a pathway for constructing purposeful quantum algorithms based on so-called double-bracket flows also for tasks different from diagonalization and thus enlarges the quantum computing toolkit geared towards practical physics problems.

Comments: Manuscript accepted in Quantum. Minor finalization changes
Subjects: **Quantum Physics (quant-ph)**
Cite as: arXiv:2206.11772 **[quant-ph]**

Check out this because:

1. Marek is a very nice and smart guy;
2. it contains math foundations of this talk;

Strategies for optimizing double-bracket quantum algorithms

Li Xiaoyue, Matteo Robbiati, Andrea Pasquale, Edoardo Pedicillo, Andrew Wright, Stefano Carrazza, Marek Gluza

Recently double-bracket quantum algorithms have been proposed as a way to compile circuits for approximating eigenstates. Physically, they consist of appropriately composing evolutions under an input Hamiltonian together with diagonal evolutions. Here, we present strategies to optimize the choice of the double-bracket evolutions to enhance the diagonalization efficiency. This can be done by finding optimal generators and durations of the evolutions. We present numerical results regarding the preparation of double-bracket iterations, both in ideal cases where the algorithm's setup provides analytical convergence guarantees and in more heuristic cases, where we use an adaptive and variational approach to optimize the generators of the evolutions. As an example, we discuss the efficacy of these optimization strategies when considering a spin-chain Hamiltonian as the target. To propose algorithms that can be executed starting today, fully aware of the limitations of the quantum technologies at our disposal, we finally present a selection of diagonal evolution parametrizations that can be directly compiled into CNOTs and single-qubit rotation gates. We discuss the advantages and limitations of this compilation and propose a way to take advantage of this approach when used in synergy with other existing methods.

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Subjects: **Quantum Physics (quant-ph)**; Optimization and Control (math.OC)
Cite as: arXiv:2408.07431 **[quant-ph]**

And this because:

1. We delve deeper into the optimization of DBQAs;
2. we base the optimization of the next talk on these studies.

arXiv:2206.11772

Ingredients

1. Input Hamiltonian $\hat{H}_0$ (here 1D XXZ);
2. an anti-hermitian ($(i\hat{W})^\dagger = -i\hat{W}$) rotation generator $\hat{W}_0 = [\hat{D}_0, \hat{H}_0]$;
3. point 2. is used to build a unitary operation:

$$\hat{R}_0 \equiv e^{s\hat{W}_0},$$

with s stepsize or flow duration;

4. $\hat{R}_0$ applied to $\hat{H}_0$ as *double-bracket rotation*:

$$\hat{H}_1 = e^{s\hat{W}_0}\hat{H}_0 e^{-s\hat{W}_0}.$$

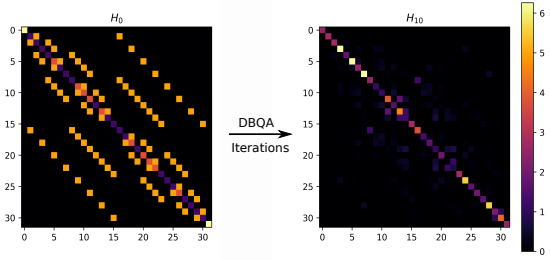


Figure 1: Ten DBQA rotations to a 5 qubit 1D XXZ.

Nomenclature reason

The presented framework satisfies a Heisenberg equation involving two, not one, brackets:

$$\partial_s \hat{H}_0(s) = [\hat{H}_0(s), [\hat{H}_0(0), \hat{D}_0]].$$

arXiv:2206.11772

1. We care of diagonal $\hat{D}_k$ in $\hat{W}_k = [\hat{D}_k, \hat{H}_k]$. A natural choice is the canonical generator[1]:

$$\hat{W}_k^{\text{can}} = [\hat{H}_k, \hat{\Delta}(\hat{H}_k)], \qquad \text{with} \qquad \begin{cases} \hat{\Delta}(\hat{H}_k) = \text{diag}(\hat{H}_k), \\ \hat{H}_k = \hat{\Delta}(\hat{H}_k) + \hat{\sigma}(\hat{H}_k), \end{cases}$$

   but - as we will see - many choices can be done here.
2. **Lemma**[2]: given $\sigma(\hat{H}_0(s))$ off-diagonal restriction of $\hat{H}_0(s)$ and s small enough:

$$\partial_s \|\sigma(\hat{H}_0(s))\|_{\text{HS}}^2 = -2 \langle \hat{W}_0, [\hat{H}_0, \sigma(\hat{H}_0(s))] \rangle_{\text{HS}} .$$

3. If $\hat{D}_0 = ... = \hat{D}^*$, as long as $s_0 = ... = s^*$ are sufficiently small and $\hat{D}^*$ non degenerate, the recursion converges to a fixed point $\hat{H}_\infty$ with $[\hat{H}_\infty, \hat{D}^*]$[3];

2. $\rightarrow$ If $\hat{D}_0$ is diagonal, then $\hat{H}_1$ will be more diagonal than $\hat{H}_0$,
3. $\rightarrow$ the discrete DBI can converge arbitrary well,
3. $\rightarrow$ *analytically motivated* methods work in some setups but they can be slow.

[1] See Renormalization of Hamiltonians, Glazek and Wilson, 1993 and Flow-equations for Hamiltonians, Wegner, 1994 for extras.

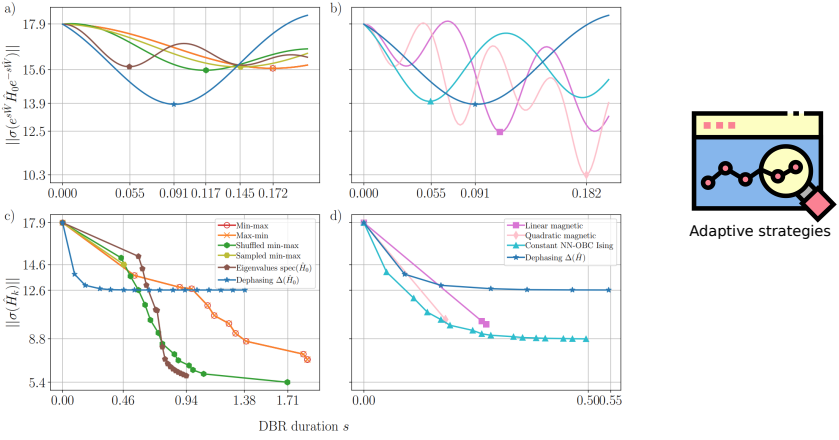
[2] Definition and proof of Lemma 2 in Double-bracket quantum algorithms for diagonalization, M. Gluza, 2024

[3] **If you are really brave:** Optimization and Dynamical Systems [Ch. 2.3], Uwe Helmke , John B. Moore, 1994.

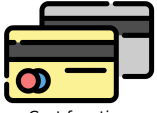
Cost functions and parametrization strategies

arXiv:2408.07431

Analytically motivated strategies



Adaptive strategies



Cost functions

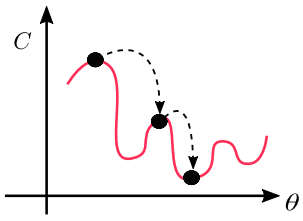
Function	Off-diagonal norm (f_1)	Least-squares (f_2)	Energy (f_3)	Energy fluctuation (f_4)
Formula	$\|\|\sigma(\hat{H}_k)\|\|_{\text{HS}}$	$\frac{1}{2}\|\|\hat{D}_k\|\|^2_{\text{HS}} - \text{Tr}(\hat{H}_k\hat{D}_k)$	$\langle\psi\|\hat{H}\|\psi\rangle$	$\sqrt{(\langle\psi\|\hat{H}_k^2\|\psi\rangle - \langle\psi\|\hat{H}_k\|\psi\rangle^2)}$
Utility	Diagonalization	Diagonalization	Ground state preparation	Eigenstate preparation

$$\hat{H}_{k+1} = e^{s_k \hat{W}_k(\vec{\alpha},\vec{\beta})} \hat{H}_k e^{-s_k \hat{W}_k(\vec{\alpha},\vec{\beta})}$$

$$\hat{D}_k = \sum_{i=1}^{L} \left(\alpha_i \hat{Z}_i + \beta_i \hat{Z}_i \hat{Z}_{i+1} \right)$$

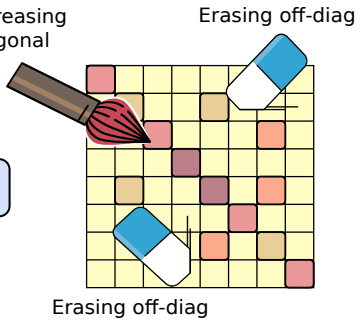
Update DBI

Apply DBI



$$\theta = [s_k, \vec{\alpha}, \vec{\beta}]$$

Compute cost function (can be off-diag norm)



The heart of the compilation of DBQAs is one of the **group commutator formulas** introduced by Dawson and Nielsen in their Solovay-Kitaev algorithm:

$$\hat{V}^{\mathrm{GC}}(\hat{A},\hat{B}) = e^{i\hat{A}}e^{i\hat{B}}e^{-i\hat{A}}e^{-i\hat{B}}, \qquad \hat{A},\hat{B} \text{ hermitian},$$

by means of which:

$$e^{-[\hat{A},\hat{B}]} = \hat{V}^{\mathrm{GC}}(\hat{A},\hat{B}) + \hat{E}^{\mathrm{GC}},$$

where

$$\hat{E}^{\mathrm{GC}} \leq \|[\hat{A},[\hat{A},\hat{B}]]\| + \|[\hat{B},[\hat{B},\hat{A}]]\|$$

in any unitarily invariant norm (e.g. Hilbert-Schmidt norm).

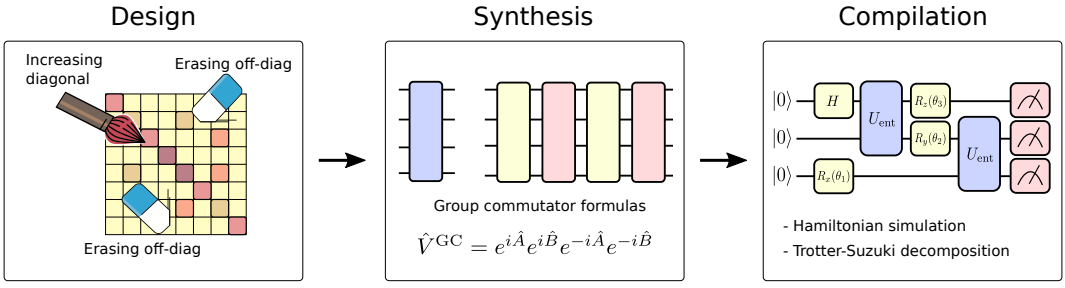
How about DBI?

$$e^{-s[\hat{D}_0,\hat{H}_0]} = e^{i\sqrt{s_0}\hat{H}_0}e^{-i\sqrt{s_0}\hat{D}_0}e^{-i\sqrt{s_0}\hat{H}_0}e^{i\sqrt{s_0}\hat{D}_0} + O(s_0^{3/2}).$$

This is compilable into a sequence of local Hamiltonian evolutions.

❗ Higher-order formulas can be implemented to reduce the approximation error.

Warming start the new talk



Boosting ground states preparation with double-bracket quantum algorithms

PART 2: Interfacing DBQAs with other techniques

Matteo Robbiati

5 December 2024

A couple of references

Double-bracket quantum algorithms for diagonalization

Marek Gluza

This work proposes double-bracket iterations as a framework for obtaining diagonalizing quantum circuits. Their implementation on a quantum computer consists of interlacing evolutions generated by the input Hamiltonian with diagonal evolutions which can be chosen variationally. No qubit overheads or controlled-unitary operations are needed but the method is recursive which makes the circuit depth grow exponentially with the number of recursion steps. To make near-term implementations viable, the proposal includes optimization of diagonal evolution generators and of recursion step durations. Indeed, thanks to this numerical examples show that the expressive power of double-bracket iterations suffices to approximate eigenstates of relevant quantum models with few recursion steps. Compared to brute-force optimization of unstructured circuits double-bracket iterations do not suffer from the same trainability limitations. Moreover, with an implementation cost lower than required for quantum phase estimation they are more suitable for near-term quantum computing experiments. More broadly, this work opens a pathway for constructing purposeful quantum algorithms based on so-called double-bracket flows also for tasks different from diagonalization and thus enlarges the quantum computing toolkit geared towards practical physics problems.

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Double-bracket quantum algorithms for high-fidelity ground state preparation

Matteo Robbiati, Edoardo Pedicillo, Andrea Pasquale, Xiaoyue Li, Andrew Wright, Renato M. S. Farias, Khanh Uyen Giang, Jeongrak Son, Johannes Knörzer, Siong Thye Goh, Jun Yong Khoo, Nelly H.Y. Ng, Zoë Holmes, Stefano Carrazza, Marek Gluza

Ground state preparation is a key area where quantum computers are expected to prove advantageous. Double-bracket quantum algorithms (DBQAs) have been recently proposed to diagonalize Hamiltonians and in this work we show how to use them to prepare ground states. We propose to improve an initial state preparation by adding a few steps of DBQAs. The interfaced method systematically achieves a better fidelity while significantly reducing the computational cost of the procedure. For a Heisenberg model, we compile our algorithm using CZ and single-qubit gates into circuits that match capabilities of near-term quantum devices. Moreover, we show that DBQAs can benefit from the experimental availability of increasing circuit depths. Whenever an approximate ground state can be prepared without exhausting the available circuit depth, then DBQAs can be enlisted to algorithmically seek a higher fidelity preparation.

Comments: 5 pages + appendix, 4 figures, code available at: this https URL
Subjects: **Quantum Physics (quant-ph)**
Report number: TIF-UNIMI-2024-6
Cite as: arXiv:2408.03987 **[quant-ph]**

And this because:

1. we will follow this paper for the numerical results;
2. there are some nice figures :)

Let's remember what a DBI is

Ingredients

1. Input Hamiltonian $\hat{H}_0$ (here 1D XXZ);
2. an anti-hermitian ($(i\hat{W})^\dagger = -i\hat{W}$) rotation generator $\hat{W}_0 = [\hat{D}_0, \hat{H}_0]$;
3. point 2. is used to build a unitary operation:

$$\hat{R}_0 \equiv e^{s\hat{W}_0},$$

with s stepsize or flow duration;

4. $\hat{R}_0$ applied to $\hat{H}_0$ as *double-bracket rotation*:

$$\hat{H}_1 = e^{s\hat{W}_0}\hat{H}_0 e^{-s\hat{W}_0}.$$

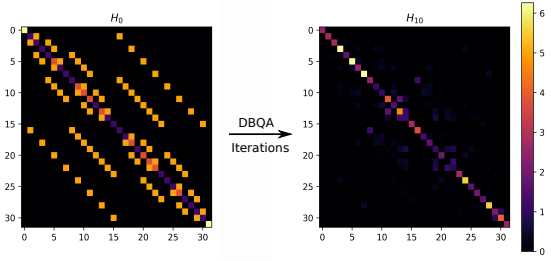


Figure 2: Ten DBQA rotations to a 5 qubit 1D XXZ.

Nomenclature reason

The presented framework satisfies a Heisenberg equation involving two, not one, brackets:

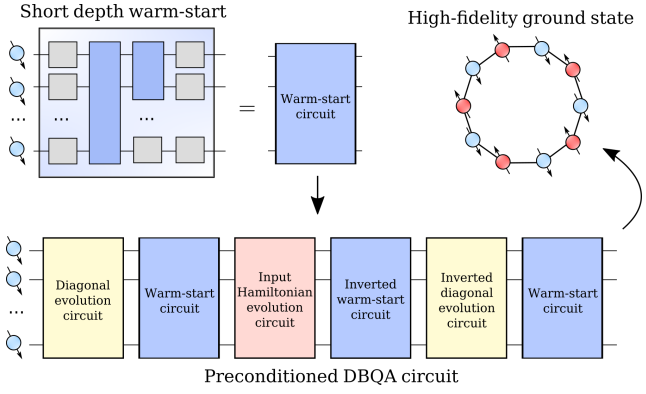
$$\partial_s \hat{H}_0(s) = [\hat{H}_0(s), [\hat{H}_0(0), \hat{D}_0]].$$

How to make this work in practice?

We left the last session with an approximation:

$$e^{-s[\hat{D},\hat{H}]} \approx e^{i\sqrt{s_k}\hat{H}_k} e^{i\sqrt{s_k}\hat{D}_k} e^{-i\sqrt{s_k}\hat{H}_k} e^{-i\sqrt{s_k}\hat{D}_k}.$$

Today, we will see how this is costly in practice, and propose the synergistic usage of more methods together.



Interfacing a warm start approximation with DBIs

Let me apply a little modification to our input Hamiltonian:

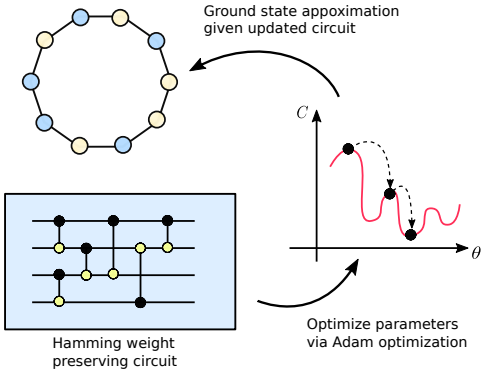
$$\hat{A}_0 = \hat{U}_\theta^\dagger \hat{H}_0 \hat{U}_\theta,$$

where $\hat{U}_\theta$ is a variational unitary operator introduced to approximate the ground state preparation (VQE here).

VQE in a nutshell

1. Define a good parametric circuit ansatz $\hat{U}_\theta$ (Hamming-weight preserving here);
2. we want the circuit to approximate the ground state of a target $\hat{H}_0$;
3. the cost function is the expval of $\hat{H}_0$ over the final state given by the circuit:

$$C = \langle 0 | \hat{U}_\theta^\dagger \hat{H}_0 \hat{U}_\theta | 0 \rangle .$$



Interfacing a warm start approximation with DBIs

Let me apply a little modification to our input Hamiltonian:

$$\hat{A}_0 = \hat{U}_\theta^\dagger \hat{H}_0 \hat{U}_\theta .$$

One step of this group commutator iteration (GCI):

$$\hat{A}_1 = \hat{V}_1^\dagger \hat{U}_\theta^\dagger \hat{H}_0 \hat{U}_\theta \hat{V}_1 \qquad \text{with} \qquad \hat{V}_1 = e^{-i\sqrt{s_0}\hat{D}_0} \hat{U}_\theta^\dagger e^{-i\sqrt{s_0}\hat{H}_0} \hat{U}_\theta e^{i\sqrt{s_0}\hat{D}_0}.$$

Let me write here a (simplified in notation) full expression for the expval of $\hat{H}_0$:

$$C = \langle 0 | e^{-D_0} U^\dagger e^{H_0} U e^{D_0} U^\dagger H_0 U e^{-D_0} U^\dagger e^{-H_0} U e^{D_0} | 0 \rangle$$

Reduced group commutator formula

$$\hat{V}_k^{(\mathrm{RGC})} = e^{-i\sqrt{s_k}\hat{D}_k} e^{-i\sqrt{s_k}\hat{A}_k} e^{i\sqrt{s_k}\hat{D}_k} \qquad \text{since} \qquad \hat{A}_k = e^{-i\sqrt{s_k}\hat{A}_k} \hat{A}_k e^{i\sqrt{s_k}\hat{A}_k}$$

Cost reduction without any impact on the result calculation.

Two steps

In terms of state preparation (we want to compile it) one VQExDBQA step appears as:

$$U e^{-D_0} U^\dagger e^{-H_0} U e^{D_0} |0\rangle .$$

Adding one more step means applying $\hat{V}_2$ to the system:

$$\begin{aligned}\hat{V}_2 =& e^{-ir_1\hat{D}_1}\hat{V}_1^\dagger e^{-ir_1\hat{A}_0}\hat{V}_1 e^{ir_1\hat{D}_1}\\ =& e^{-i(r_0\hat{D}_0+r_1\hat{D}_1)}\hat{U}_{\boldsymbol{\theta}}^\dagger e^{ir_0\hat{H}_0}\hat{U}_{\boldsymbol{\theta}} e^{ir_0\hat{D}_0}\hat{U}_{\boldsymbol{\theta}}^\dagger e^{-ir_1\hat{H}_0}\hat{U}_{\boldsymbol{\theta}} e^{-ir_0\hat{D}_0}\hat{U}_{\boldsymbol{\theta}}^\dagger e^{-ir_0\hat{H}_0}\hat{U}_{\boldsymbol{\theta}} e^{i(r_0\hat{D}_0+r_1\hat{D}_1)}.\end{aligned}$$

Compiling the hamiltonian evolutions

The XXZ is decomposed into contributions involving two qubits per time $\hat{H}_0 = \sum_{a=1}^{L}\hat{H}^{(a)}$ such that $\hat{H}^{(a)} = \hat{X}_a\hat{X}_{a+1} + \hat{Y}_a\hat{Y}_{a+1} + \hat{Z}_a\hat{Z}_{a+1}$ and then a Trotter-Suzuki decomposition is implemented:

$$e^{-it\hat{H}_0} = \left(\prod_{a=1}^{L} e^{-i\frac{t}{M}\hat{H}^{(a)}}\right)^M + O(M^{-1}).$$

Compiling

Any unitary can be compiled into proper set of gates

1. Euler decomposition for 1-qubit gates;
2. KAK decomposition for 2-qubit gates;
3. Shannon decomposition for n-qubit gates.

Theorem 5. *Every two-qubit quantum gate in* $\mathbf{U}(4)$ *can be realized, up to a global phase, by a circuit consisting of* 15 *elementary one-qubit gates and* 3 CNOT *gates.*

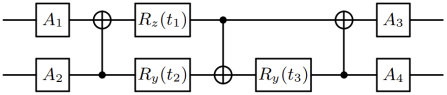


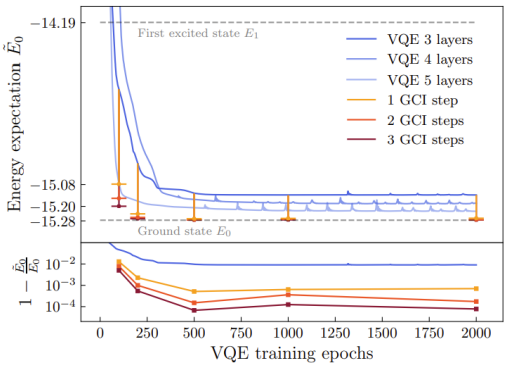
FIG. 7: A circuit for implementing a transform in $\mathbf{U}(4)$.

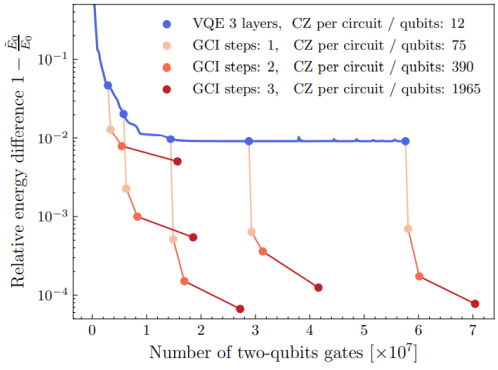
Trotter-Suzuki approximation, combined with compilation, means a quite intense number of required gates.

Interface with a warm start a a couple of DBI steps

If we are able to setup a short-depth first approximation, then we can boost the preparation with DBI.

Boosting 1D XXZ ground state preparation





Two qubit gates count

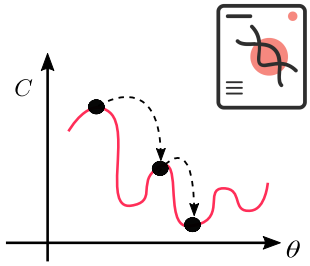
Number of CZ executed considering *i)* VQE training, *ii)* hyper-optimization of the unfolded GCI's parameters.

$$\hat{H}_{k+1} = e^{s_k \hat{W}_k(\vec{\alpha},\vec{\beta})} \hat{H}_k e^{-s_k \hat{W}_k(\vec{\alpha},\vec{\beta})}$$

$$\hat{D}_k = \sum_{i=1}^{L} \left(\alpha_i \hat{Z}_i + \beta_i \hat{Z}_i \hat{Z}_{i+1} \right)$$

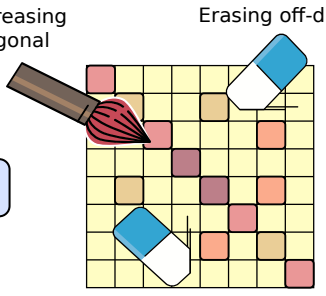
Update DBI

Apply DBI



$$\theta = [s_k, \vec{\alpha}, \vec{\beta}]$$

Compute cost function (can be off-diag norm)



Boosting 1D XXZ ground state preparation

Layers	Warm-start		1 GCI step		2 GCI steps		1 DBI step	Long VQE training	
	$1-\tilde{E}_0/E_0$		$1-\tilde{E}_0/E_0$		$1-\tilde{E}_0/E_0$		$1-\tilde{E}_0/E_0$	$1-\tilde{E}_0/E_0$	
3	0.012 ± 0.004		0.0011 ± 0.0007		0.0005 ± 0.0004		0.0009 ± 0.0006	0.010 ± 0.004	
4	0.008 ± 0.004		0.0006 ± 0.0005		0.0002 ± 0.0002		0.0005 ± 0.0004	0.004 ± 0.002	
5	0.005 ± 0.003		0.0003 ± 0.0002		0.0001 ± 0.0001		0.0002 ± 0.0002	0.003 ± 0.002	
	Depth	Cumulative cost	Depth	Cumulative cost	Depth	Cumulative cost	-	Depth	Cumulative cost
3	12	1.44×10^7	75	1.49×10^7	390	1.69×10^7	-	12	5.76×10^7
4	16	2.56×10^7	95	2.62×10^7	490	2.88×10^7	-	16	10.24×10^7
5	20	4.0×10^7	115	4.07×10^7	590	4.38×10^7	-	20	16.0×10^7

Layers	Warm-start	1 GCI step	2 GCI steps	3 GCI steps
3	0.83 ± 0.06	0.95 ± 0.01	0.993 ± 0.006	0.997 ± 0.003
4	0.89 ± 0.05	0.992 ± 0.007	0.997 ± 0.003	0.998 ± 0.001
5	0.93 ± 0.04	0.996 ± 0.003	0.998 ± 0.002	0.9992 ± 0.0008