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.

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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

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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.

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*:

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

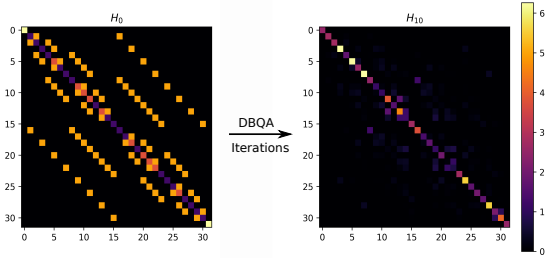


Figure 1: Ten DBQA rotations to a 5 qubit 1D XXZ.

Nomenclature reason

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

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

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:

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

   but - as we will see - many choices can be done here.
2. **Lemma**[1]: 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 $[\hat{H}_\infty, \hat{D}^*]$[2];

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.

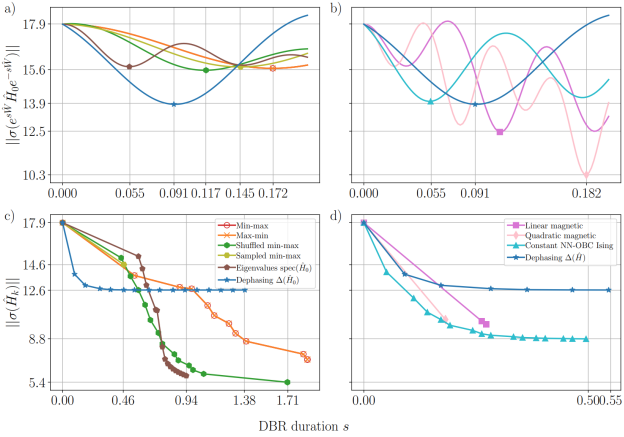
[1] Definition and proof of Lemma 2 in Double-bracket quantum algorithms for diagonalization, M. Gluza, 2024

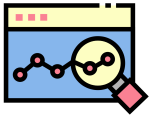
[2] **If you are really brave:** Optimization and Dynamical Systems [Ch. 2.3], Uwe Helmke , John B. Moore, 1994.

Cost functions and parametrization strategies

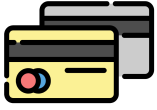
arXiv:2408.07431

Analytically motivated strategies





Variational strategies



Cost functions

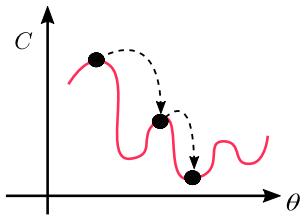
Function	Off-diagonal norm (f_1)	Least-squares (f_2)	Energy (f_3)	Energy fluctuation (f_4)
Formula	$\|\|\sigma(\hat{H}_k)\|\|_{\text{HS}}$	$\frac{1}{2}\|\|\hat{D}_k\|\|^2_{\text{HS}} - \text{Tr}(\hat{H}_k\hat{D}_k)$	$\langle\psi\|\hat{H}\|\psi\rangle$	$\sqrt{(\langle\psi\|\hat{H}_k^2\|\psi\rangle - \langle\psi\|\hat{H}_k\|\psi\rangle^2)}$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

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

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

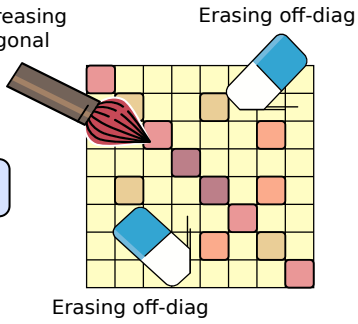
Update DBI

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?

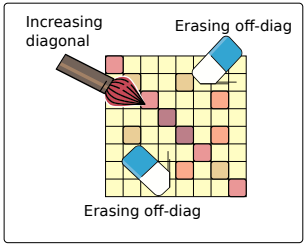
$$e^{-s[\hat{D}_0,\hat{H}_0]} = e^{i\sqrt{s_0}\hat{H}_0}e^{-i\sqrt{s_0}\hat{D}_0}e^{-i\sqrt{s_0}\hat{H}_0}e^{i\sqrt{s_0}\hat{D}_0} + O(s_0^{3/2}).$$

This is compilable into a sequence of local Hamiltonian evolutions.

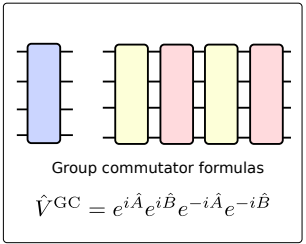
❗ Higher-order formulas can be implemented to reduce the approximation error.

Sum up

Design



Synthesis



Compilation