Quantum algorithms and the Schrödinger equation

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Structure of the talk

1. Motivation: energy spectrum of dense Hamiltonians
2. Grover's algorithm
3. Amplitude amplification
4. Generalized eigenvalue problem
5. Collocation method for the Schrödinger equation
6. Costs and improvements

Main problem

What are the quantum algorithms that offer **speedup**,

as measured in the **asymptotic** regime,

for the energy finding of a Hamiltonian H?

$$H\left|E_i\right\rangle = E_i\left|E_i\right\rangle$$

disclaimer: there are no quantum computers (yet)

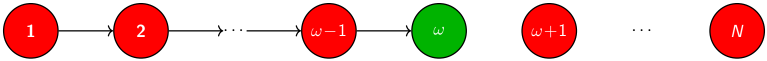
we aim for

fault-tolerant era usefulness

Problem statement – Search for a single instance of a list

We have an unsorted list of N elements with a single marked element ω, with a "marking" function f, such that $f(\beta) = \delta_{\omega\beta}$. The goal is to find the value of ω.

classically, the above problem scales **linearly** as $\mathcal{O}(N)$



while there exists a **quantum** algorithm[1]
that achieves that with optimal[2] scaling $\mathcal{O}(\sqrt{N})$

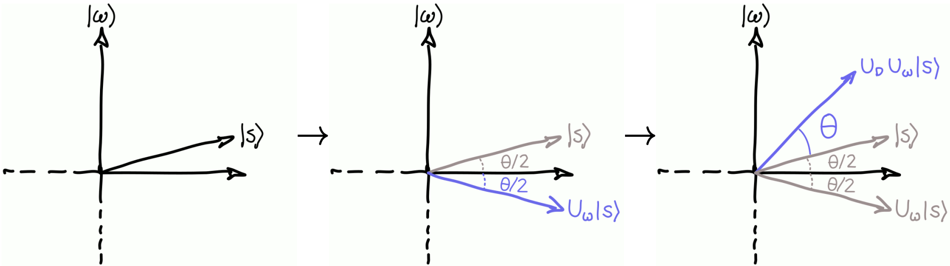
[1] L. K. Grover. In: *Proceedings of the twenty-eighth annual ACM symposium on Theory of computing - STOC '96*. STOC '96. ACM Press, 1996, pp. 212–219.

[2] C. H. Bennett et al. In: *SIAM Journal on Computing* 26.5 (Oct. 1997), pp. 1510–1523.

Amplitude amplification

1. prepare a starting state is an **equal superposition** $|s\rangle = \sum_i |i\rangle$
2. reflect around the state **perpendicular to marked** $|\omega\rangle$ via $U_\omega = \mathbb{I} - 2|\omega\rangle\langle\omega|$
3. reflect around the **starting state** via $U_\omega = \mathbb{I} - 2|s\rangle\langle s|$

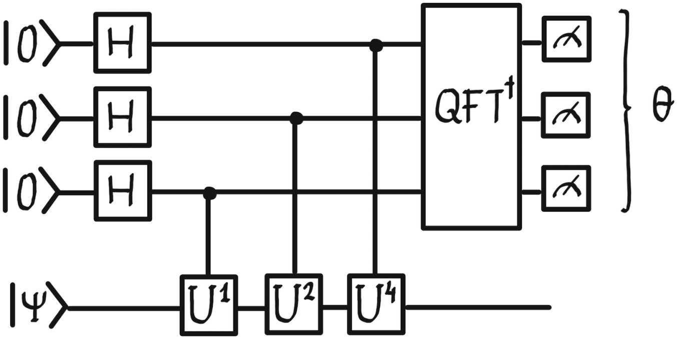
iterate $\frac{\pi}{4}\sqrt{N}$ times



https://pennylane.ai/qml/demos/tutorial_grovers_algorithm

Second useful subroutine: quantum phase estimation

Quantum phase estimation finds the eigenvalues of a given matrix U without inversion, via controlled powers $U, U^2, U^4, \ldots$ and quantum Fourier transform.



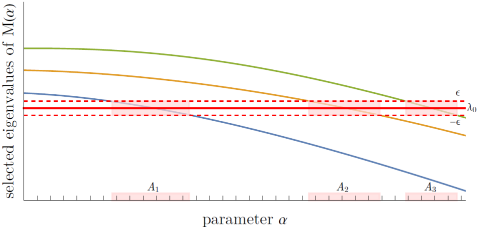
https://pennylane.ai/qml/demos/tutorial_qpe

Quantum landscape scanning

classically we find eigenvalues of matrices of size N with costs **at least** $\widetilde{\mathcal{O}}(N)$

Quadratic speedup for finding eigenvalues in a region

Theorem. Hermitian matrices $\boldsymbol{M}(\alpha) = \boldsymbol{M}_0 + \alpha \boldsymbol{M}_1$ on a grid formed by K points $\{\alpha_i\}$. There exists a quantum algorithm that finds a set of the parameters α' such that matrices $\boldsymbol{M}(\alpha')$ have eigenvalues in a region $[\lambda_0 - \varepsilon, \lambda_0 + \varepsilon]$ with $\widetilde{\mathcal{O}}(\zeta\sqrt{K}\sqrt{N}/\varepsilon)$ calls to block-encoded matrices $\boldsymbol{M}_j$, which all have their max-norms upper-bounded by ζ.



Search for the lowest eigenvalue: [Kerzner et al 2024 Quantum Sci. Technol. **9** 045025]

Collocation method

the continuous-system Hamiltonian $\hat{H} = \hat{K} + \hat{V}$ is **discretized** by expanding the solution in a **basis set** $\{|\phi_n\rangle\}_{n=0,\ldots,N-1}$ on a **physical grid** with points q

Time-independent Schrödinger equation in the collocation language

$$(\boldsymbol{B}'' + \boldsymbol{V}^{\text{diag}}\boldsymbol{B})\boldsymbol{U} = \boldsymbol{BUE}$$

where $\boldsymbol{U}$ is the matrix formed by the **approximate Hamiltonian's eigenvectors.**

Notation: $\boldsymbol{B}_{kn} = \phi_n(q_k)$, $\boldsymbol{B}''_{kn} = (\hat{K}\phi_n)(q)|_{q=q_k}$, $\boldsymbol{V}^{\text{diag}}_{kn} = \delta_{kn}V(q_k)$, and $\boldsymbol{E} = \text{diag}(E_0, \ldots, E_D)$ is the diagonal matrix of eigenvalues.

Inversion of matrices (standard) vs. landscape scanning

$(\boldsymbol{B}'' + \boldsymbol{V}^{\text{diag}}\boldsymbol{B})\boldsymbol{U} = \boldsymbol{BUE} \mapsto$

$$\underbrace{(\boldsymbol{B}^\dagger\boldsymbol{B})^{-1}(\boldsymbol{B}^\dagger\boldsymbol{B}'' + \boldsymbol{B}^\dagger\boldsymbol{VB})}_{\widetilde{\boldsymbol{H}}}\boldsymbol{U} = \widetilde{\boldsymbol{H}}\boldsymbol{U} = \boldsymbol{UE},$$

and diagonalize $\widetilde{\boldsymbol{H}}$

vs.

$(\boldsymbol{B}'' + \boldsymbol{V}^{\text{diag}}\boldsymbol{B})\boldsymbol{U} = \boldsymbol{BUE} \mapsto$

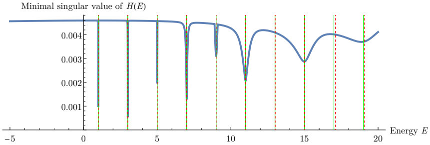
$$\underbrace{(\boldsymbol{B}'' + \boldsymbol{V}^{\boldsymbol{diag}}\boldsymbol{B} - E\boldsymbol{B})}_{\boldsymbol{M}(E)}u_i = 0.$$

and find E_i such that u_i is in kernel of $\boldsymbol{M}(E_i)$

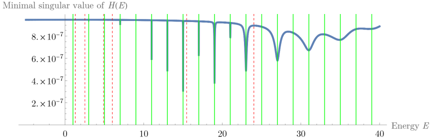
Condition number $\kappa = ||\boldsymbol{A}|| \, ||\boldsymbol{A}^{-1}||$ of matrix $\boldsymbol{A}$

determines the **sensitivity of the matrix inversion**

Small perturbation $\boldsymbol{A}'$ with $||\boldsymbol{A} - \boldsymbol{A}'|| \leq \epsilon$.
Then, the error of the matrix inversion is of the order of $\kappa^2 \epsilon$.



(a) 26 basis functions



(b) 36 basis functions

1D Harmonic oscillator – comparison of exact energies (solid green) estimation for the inversion method (dashed red) and the landscape method (blue curve)

How to input non-unitary matrices into circuits?

Block-encoding of a matrix A

With extension via ancillary qubits, we define the block-encoding U_A as a matrix with a submatrix equal to the desired A:

$$\langle 0|_{\text{anc}} \, U_A \, |0\rangle_{\text{anc}} = A.$$

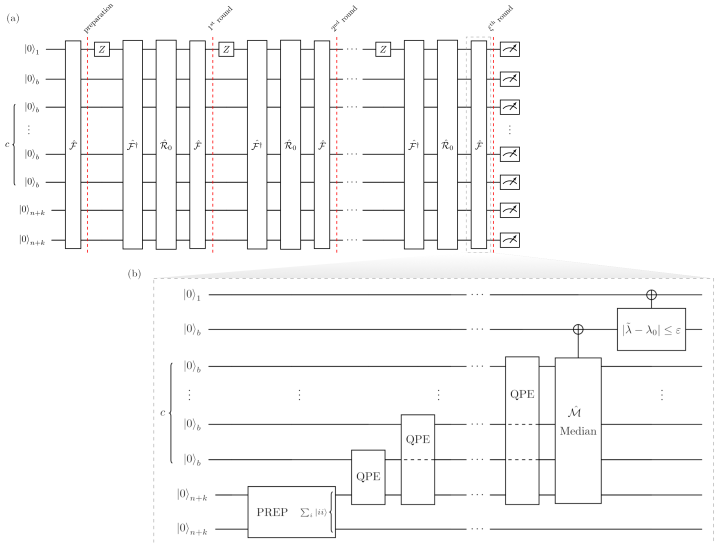
In other words,

$$U_A \left(|0\rangle_{\text{anc}} \, |\psi\rangle \right) = |0\rangle_{\text{anc}} \, A \, |\psi\rangle$$

$$U_A = \begin{bmatrix} A & \star \\ \star & \star \end{bmatrix}$$

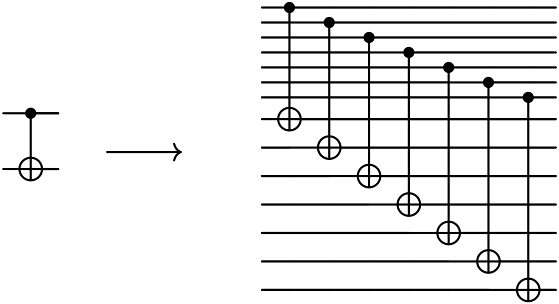
possible problem: **norm of *H***

Quantum phase estimation + amplitude amplification



Fault-tolerant era

transversal logical gate – **logical** operation achieved by broadcasting the **same** operation over the **physical qubits**



Eastin-Knill theorem

No quantum error correcting code can transversally implement a universal gate set.[a]

[a] B. Eastin et al. In: *Physical Review Letters* 102.11 (Mar. 2009).

Costs in the fault-tolerant era

the standard codes allow for transversal implementation of
the universal gate set **apart from the T gate**

$$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$$

T gate is $\approx 100 - 1000$ times more expensive[3] than CNOT

T-count

The number of **appearances of T gate** in the algorithm

[3] C. Gidney et al. In: *Quantum* 3 (Apr. 2019), p. 135.

how to deal with T gates? Magic states: distillation, factories, injection.

Improvements for the quantum algorithm

classical		quantum
matrix inversion	landscape scanning	
$\boldsymbol{N}^{2.371} \log(\kappa) + N^2 \kappa^{\frac{1}{2}} \log(1/\varepsilon)$	$K \boldsymbol{N}^2 \log(1/\varepsilon)$	$M_{\max} \frac{\sqrt{K}}{\varepsilon} \boldsymbol{N}^{1/2} \operatorname{polylog}(N/\varepsilon)$
condition number problem	—	—

Table: **Computational complexities** $\mathcal{O}$ for different methods solving the collocation Schrödinger equation. For the classical computing algorithms it is the **number of floating-point operations**, for quantum algorithm it is the **T-count** number of non-Clifford T-gates. Here N **is the number of basis functions**, K is the number of grid points in the landscape method, ε is the error in the determination of the energies, $M_{\max}$ is the maximal element of all matrices, and κ is condition number of $\boldsymbol{B}^\dagger \boldsymbol{B}$.

Provide block-encodings of matrices B, B'', and V in a doubly-extended space $\begin{pmatrix} 0 & B^\dagger \\ B & 0 \end{pmatrix}$ ⤳ Extend by index Hilbert space $\mathbb{I} \otimes (B'' + VB) - \mathrm{diag}(\alpha_1, ..., \alpha_K) \otimes B$ ⤳ Apply QPE and AA using region oracle, finally measure a single “good” index α

a quantum algorithm achieving up to

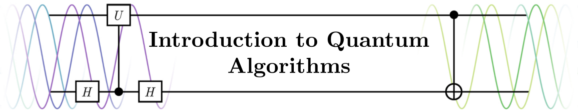
fourth power improvement in T-gate complexity

no **condition number** problem

exact speedup is potential- and basis-dependent

requires QPE: **fault-tolerant** algorithm

Introduction to Quantum Algorithms



Faculty of Mathematics and Computer Science,
Jagiellonian University

We invite you to participate in the lecture

Introduction to Quantum Algorithms

during the winter term of 2025/2026. In this course, we will introduce participants to the fundamentals of quantum computing and quantum information. We will discuss contemporary topics related to the use of quantum techniques and algorithms and present the prospects for their future applications. Special focus will be placed on fault-tolerant quantum computing, which will become crucial for both commercial and research applications, such as simulations of processes in molecular physics.

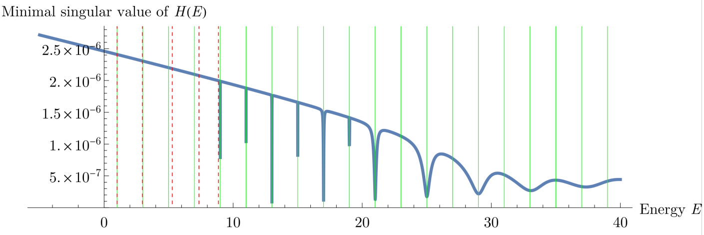
Time: Wednesdays 2–4 PM
Room 0086, Maths Faculty, UJ

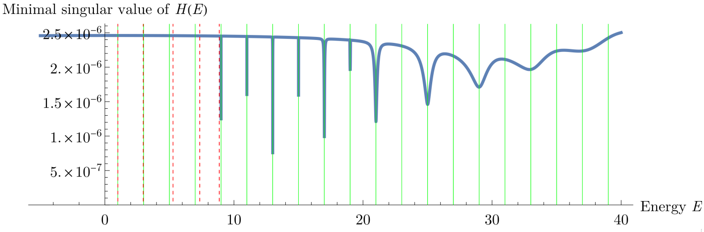
Lecturers:
Jan Tułowiecki
Grzegorz Rajchel-Mieldzioć
Emil Żak

BEIT Kraków

More information:

Background removal

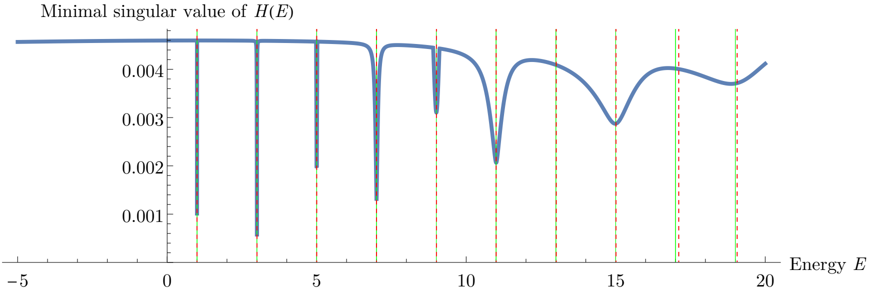




In the above, the minimal singular value is found straightforwardly, while below, we remove the slope.

(harmonic oscillator potential with 26 basis functions and 80 grid points.)

Few basis functions



Harmonic oscillator potential with 26 basis functions and 80 grid points.