The hybrid classical-quantum computing.

The case of the Hybrid Quantum algorithm to classify Hermitian matrix definiteness

HPCQC-2021
Dec. 15th, 2021

XUNTA DE GALICIA
Xacobeo 21·22
GOBIERNO DE ESPAÑA
MINISTERIO DE CIENCIA E INNOVACIÓN
CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS
Unión Europea
Fondo Europeo de Desarrollo Regional
"Una manera de hacer Europa"

Mission:

Contribute to the advancement of Science and Technical Knowledge, by means of research and application of high performance computing and communications, as well as other information technologies resources, in collaboration with other institutions, for the profit of society

Services:

Adaptation to technological evolution and the needs of researchers / users of all branches of knowledge and the productive sector

Challenges

Big Data,

Research data,

Industry 4.0

AI: ML & DL

(MANUFACTURING 4.0/5.0)

Quantum Technologies

Polo de Tecnologías Cuánticas

Objectives

Vision	Mission
"To be a European reference in Quantum Technologies by 2030"	"To achieve a disruptive impulse of quantum technologies in computing and communications, in Galicia and in Spain, for the improvement of knowledge, the advancement of technology and the consolidation of the economy for the benefit of society"

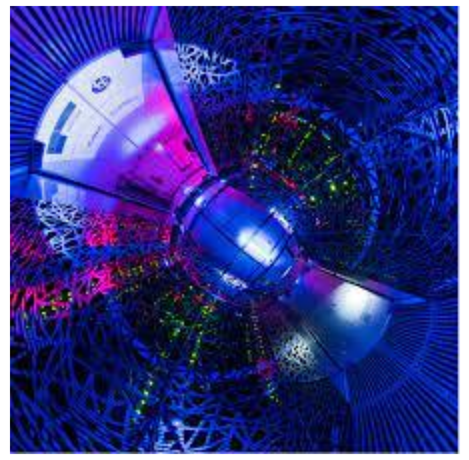
Strategy based on:

- Four pillars
  - The Academy
  - Research & Technological Centers, and Singular entities
  - The enterprises & the economy
  - Society
- Coordination and collaboration
- Singular projects

Polo de Tecnologías Cuánticas

First infrastructure (2023)

A Quantum Computer (QPU)



A new Classical Simulator of QC
(currently, an ATOS QLM 30 qubits)

A HPC system for Quantum Computing

A QRNG (deployed in 2021)

DESPREGAMENTO DUNHA INFRAESTRUTURA BASEADA
EN TECNOLOXÍAS CUÁNTICAS DA INFORMACIÓN QUE
PERMITA IMPULSAR A I+D+I en GALICIA

Apoiar a transición cara a unha economía dixital

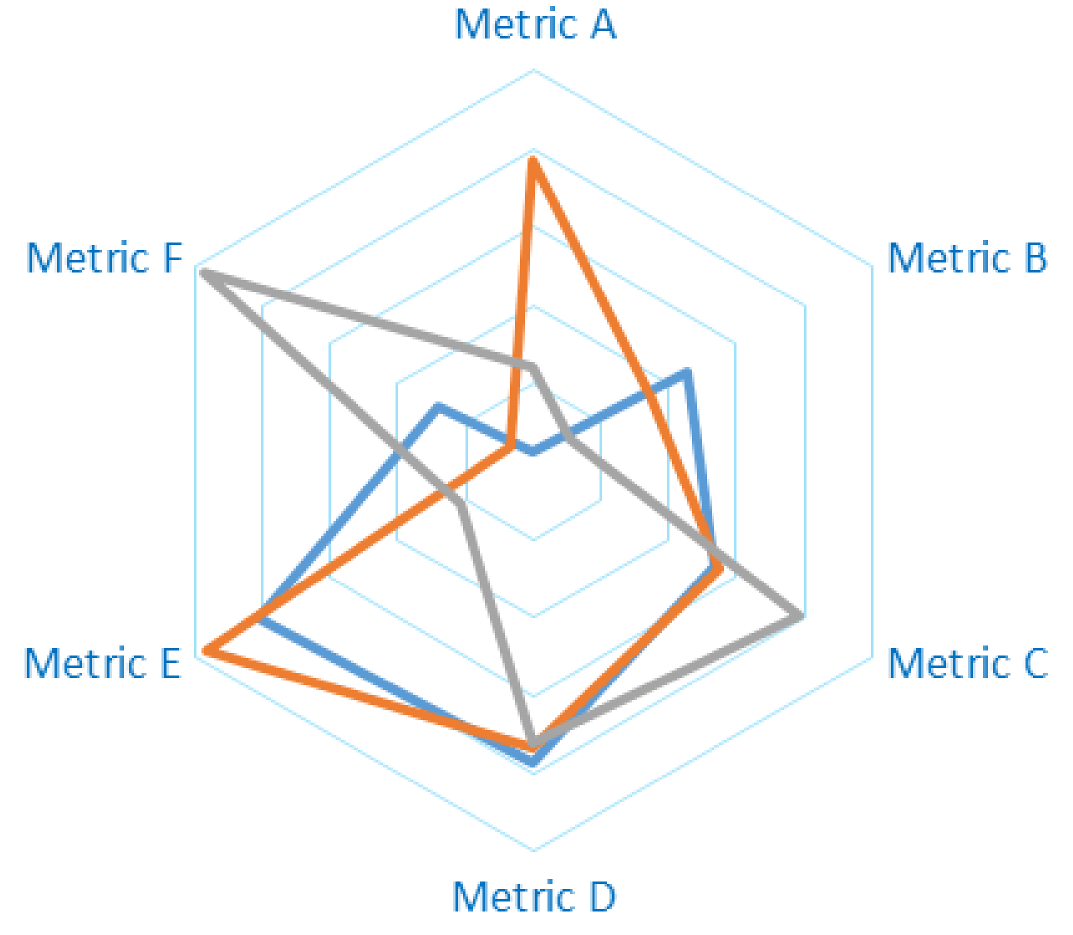
Operación financiada pola Unión Europea, a través do
FONDO EUROPEO DE DESENVOLVEMENTO REXIONAL (FEDER),
como parte da resposta da Unión á pandemia da COVID-19

PROGRAMA OPERATIVO
FEDER GALICIA
2014-2020

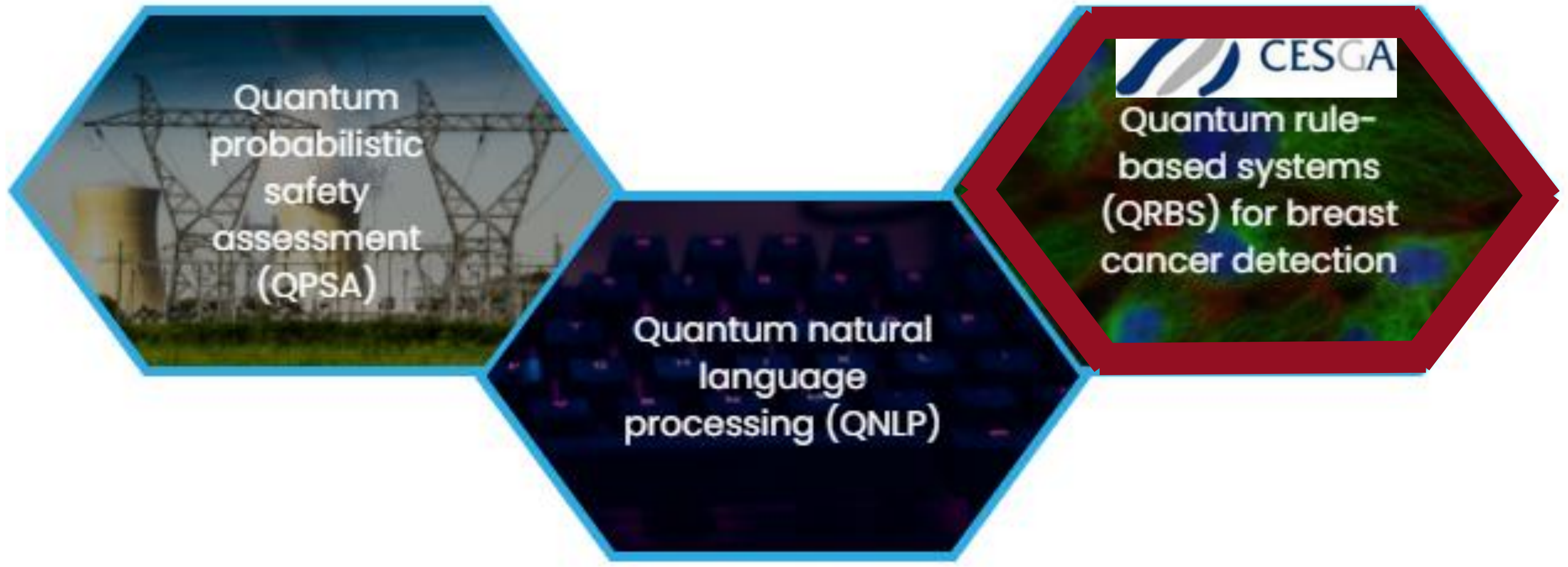
Unha maneira de facer Europa

AXENCIA GALEGA DE INNOVACIÓN
UNIÓN EUROPEA
Xacobeo 21·22
CESGA
Centro de Supercomputación de Galicia

The NEASQC benchmark suite (TNBS)



SYMBOLIC AI AND GRAPH ALGORITHMICS



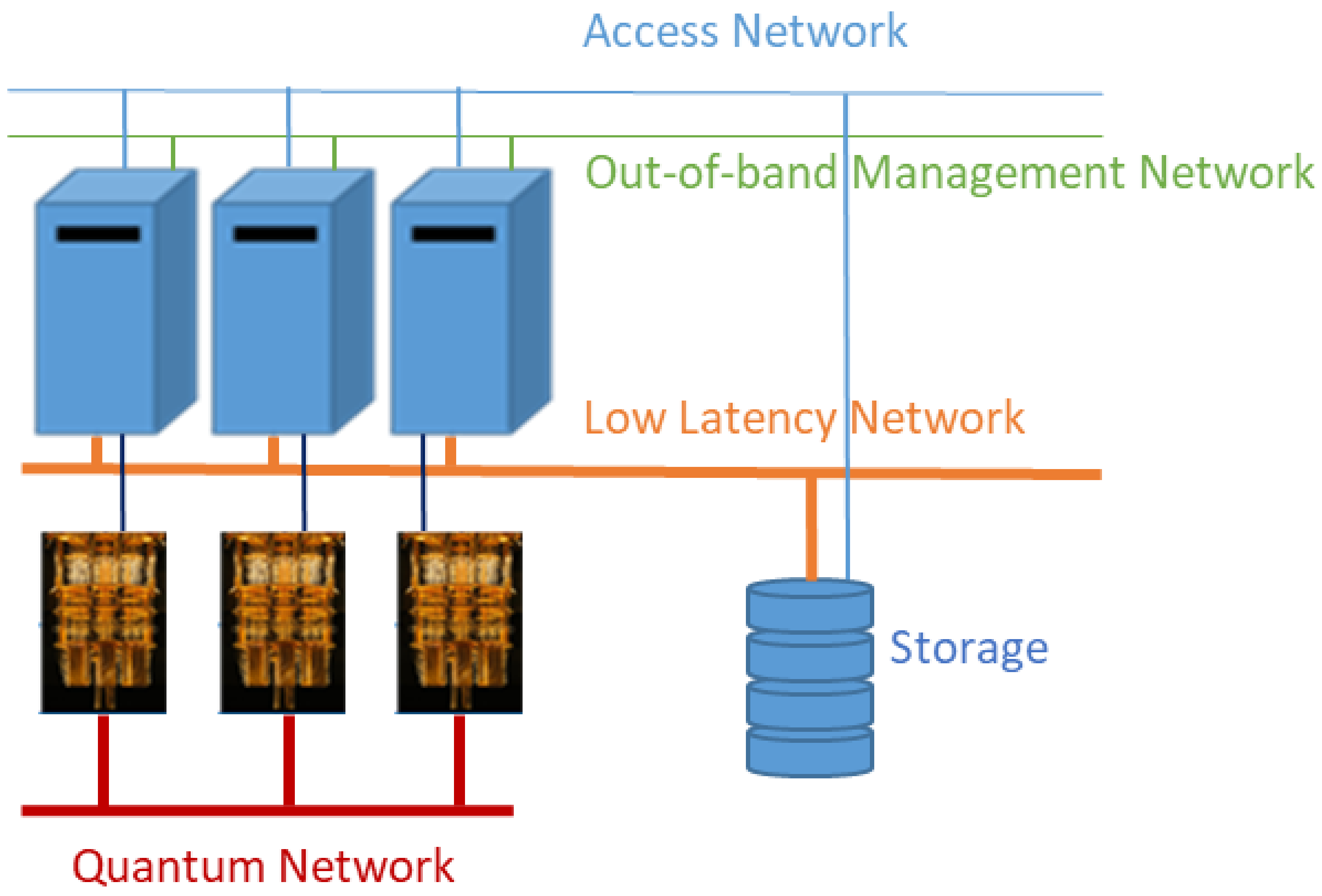
CHEMISTRY

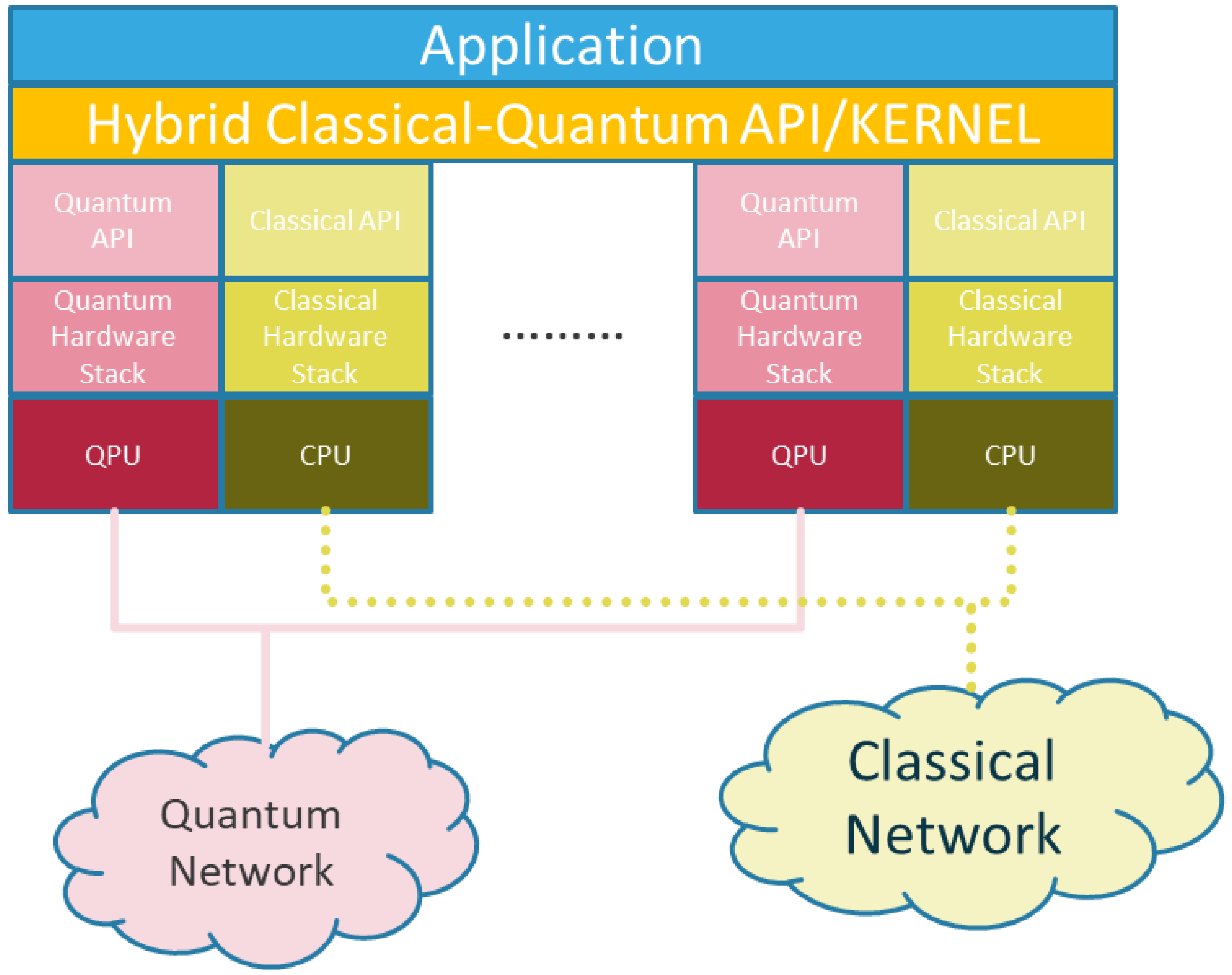
MACHINE LEARNING & OPTIMISATION

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 951821.

The hybrid classical-quantum computer

The new HPC infrastructure forecast





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Hybrid Quantum algorithm to classify Hermitian matrix definiteness

Problem:

Being $M \in \mathbb{C}^{N\times N}$ a general Hermitian matrix, which is its definiteness?

i.e.

If $\lambda_i \in \mathbb{R}, i = 0, \dots, N$ are the eigenvalues of M:

- Positive definite, if $\lambda_i > 0, \forall i$
- Positive semi-definite, if $\lambda_i \geq 0, \forall i$
- Negative semi-definite, if $\lambda_i \leq 0, \forall i$
- Negative definite, if $\lambda_i < 0, \forall i$
- Indefinite, otherwise (some $\lambda_i \leq 0$ and others $\lambda_i \geq 0$)

Quantum solution: Use Quantum Phase Estimation

The hybrid classical-quantum computer

Hybrid Quantum algorithm to classify Hermitian matrix definiteness

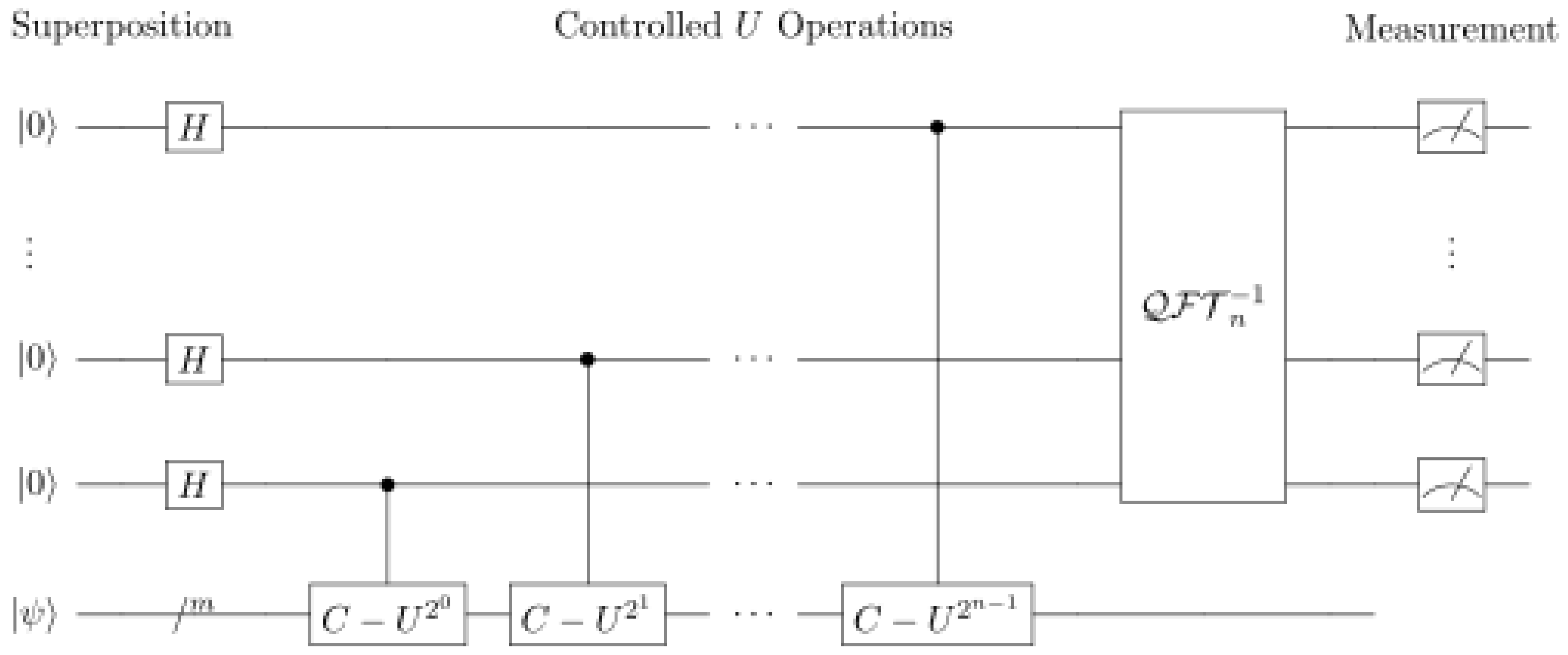
Quantum solution: Use Quantum Phase Estimation

a. If λ_i is an eigenvalue of $M \in \mathbb{C}^{N\times N}$ with eigenvector e_i, then $e^{i\lambda_i}$ is an eigenvalue of $U = e^{iM}$ with the same eigenvectors $e_i \to |e_i\rangle$

b. But:
   i. λ_i could be higher than 1, and QPE "needs" $\phi \in [0,1]$
   - Divide M by **a**, so $\frac{\lambda_i}{a} < 1$. But, which **a**?
   - What's happen if $\lambda_i < 0$ for some i?

   ii. $|e_i\rangle$ are unknown.

   iii. Even if you know e_i, you have to calculate all λ_i
   - Lucky, quantum parallelism if $|\psi\rangle = \sum_i a_i |e_i\rangle$



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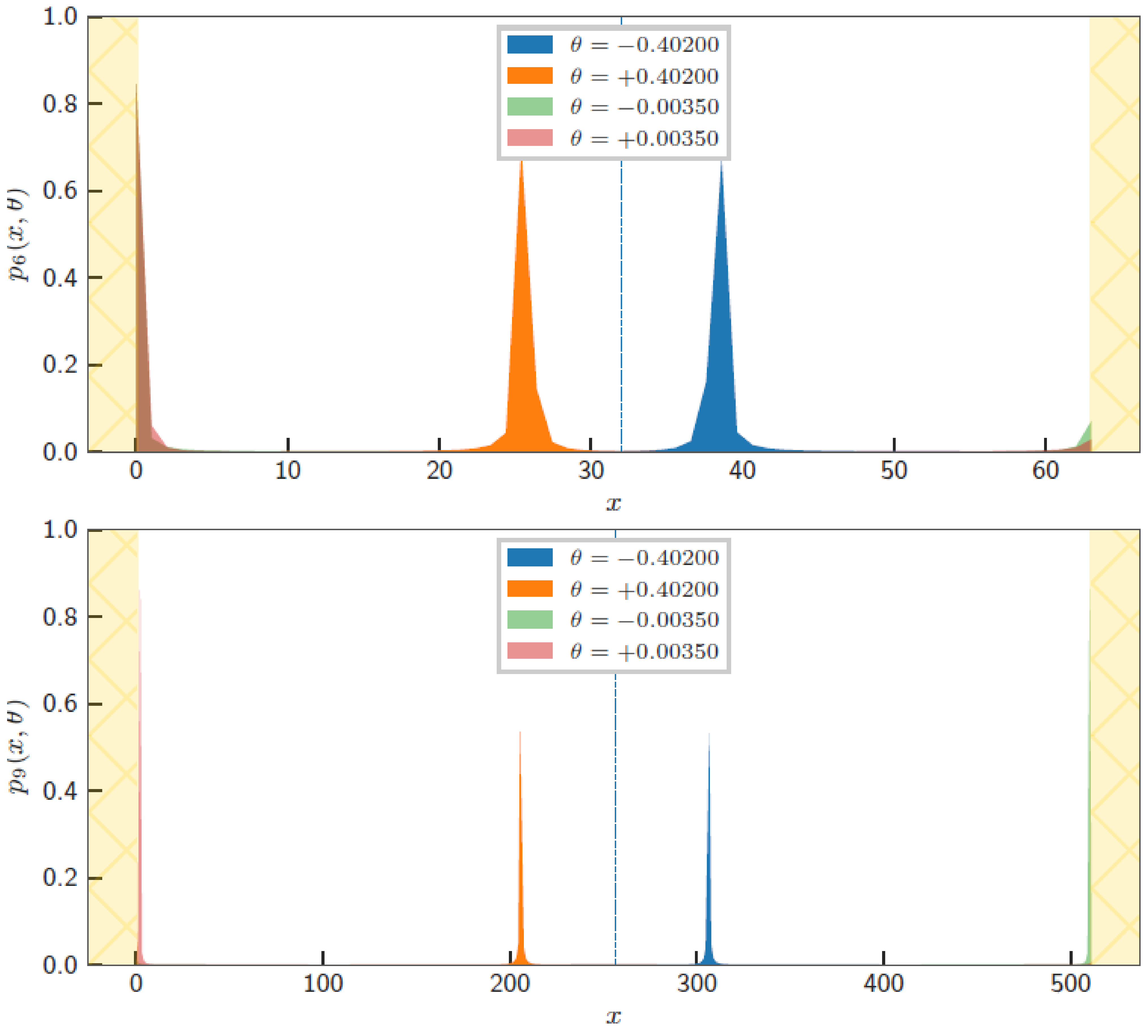
Hybrid Quantum algorithm to classify Hermitian matrix definiteness

Quantum solution: Use Quantum Phase Estimation

"What's happen if $\lambda_i < 0$ for some i?"

- Well, really QPE **can work for $\boldsymbol{\phi} \in [-\mathbf{0.5}, \mathbf{0.5})$**
- So, now we need that $\frac{|\lambda_i|}{a} < 0.5$. But, which a?



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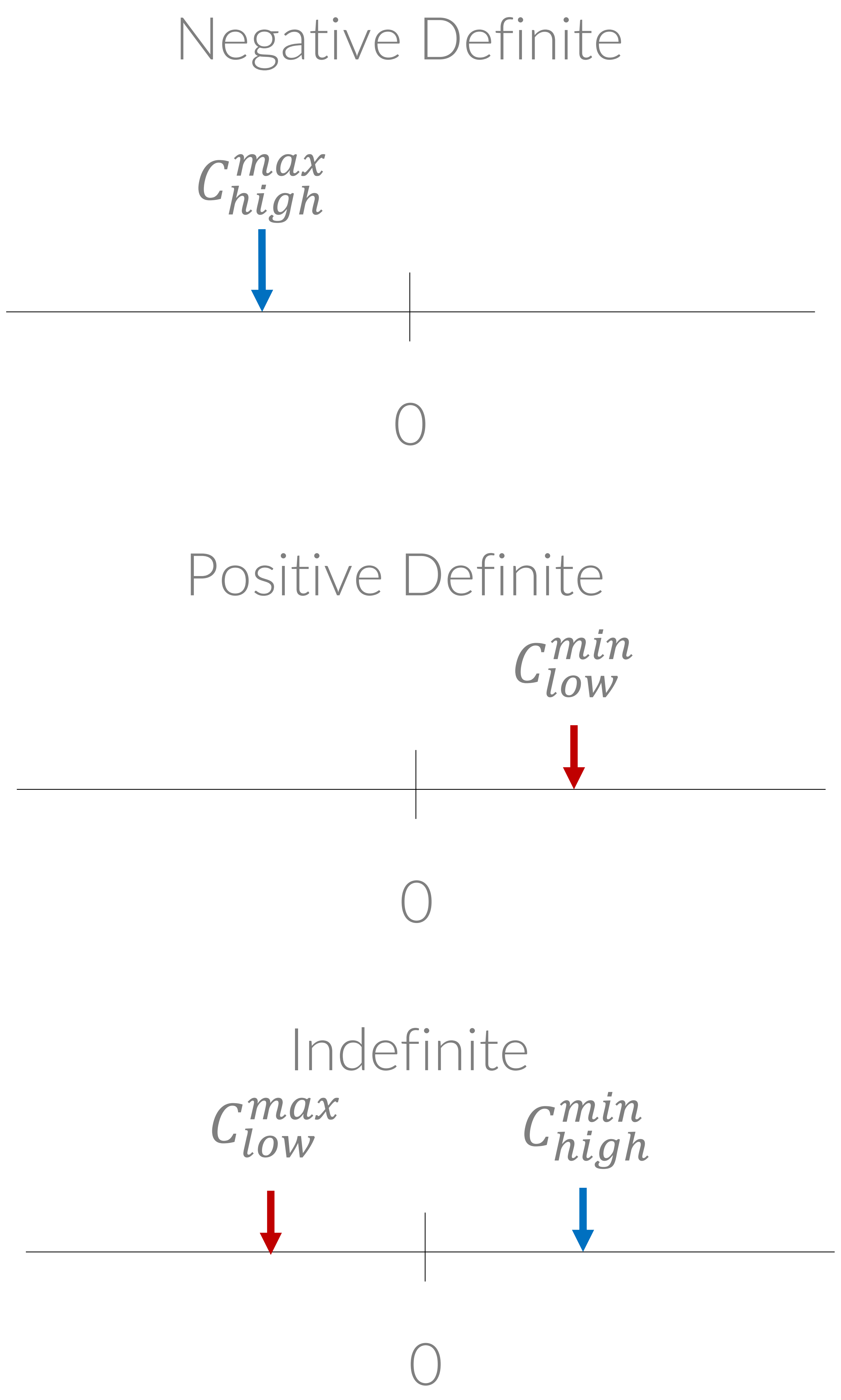
Hybrid Quantum algorithm to classify Hermitian matrix definiteness

Hybrid solution (draft: arxiv:2009.04117, under review):

1. Step 1: Classical. Use Wolkowicz and Styan[1] result.
   - $r = \frac{Tr(M)}{N}$ and $s^2 = \frac{Tr(M^2)}{N} - r^2$
   - $C_{low}^{min} = r - s\sqrt{N-1} \leq \lambda_{low} \leq C_{low}^{max} = r - \frac{s}{\sqrt{N-1}}$
   - $C_{high}^{min} = r + \frac{s}{\sqrt{N-1}} \leq \lambda_{high} \leq C_{high}^{max} = r + s\sqrt{N-1}$
   - Operations $O(N^2)$

2. Step 2 if Step 1 does not work. Quantum Phase Estimation for:
   - $U = e^{i2\pi tM}$
   - $t = \frac{1}{2\max\left(|C_{low}^{min}|, C_{high}^{max}\right)}$
   - MEASURE only the sign, i.e., $< \sigma_z >_{n-1}$
   - Because $|e_i\rangle$ are unknown, init with 3 to 5 random vectors $|v_j\rangle = \sum \beta_i |e_i\rangle$ and calculate $\overline{< \sigma_z >_{n-1}}$



1 Henry Wolkowicz and George P.H. Styan. Bounds for eigenvalues using traces. Linear Algebra and its Applications, 29:471–506, feb 1980.

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Hybrid Quantum algorithm to classify Hermitian matrix definiteness

BUT QPE Classical step: Decompose M in unitary operators:

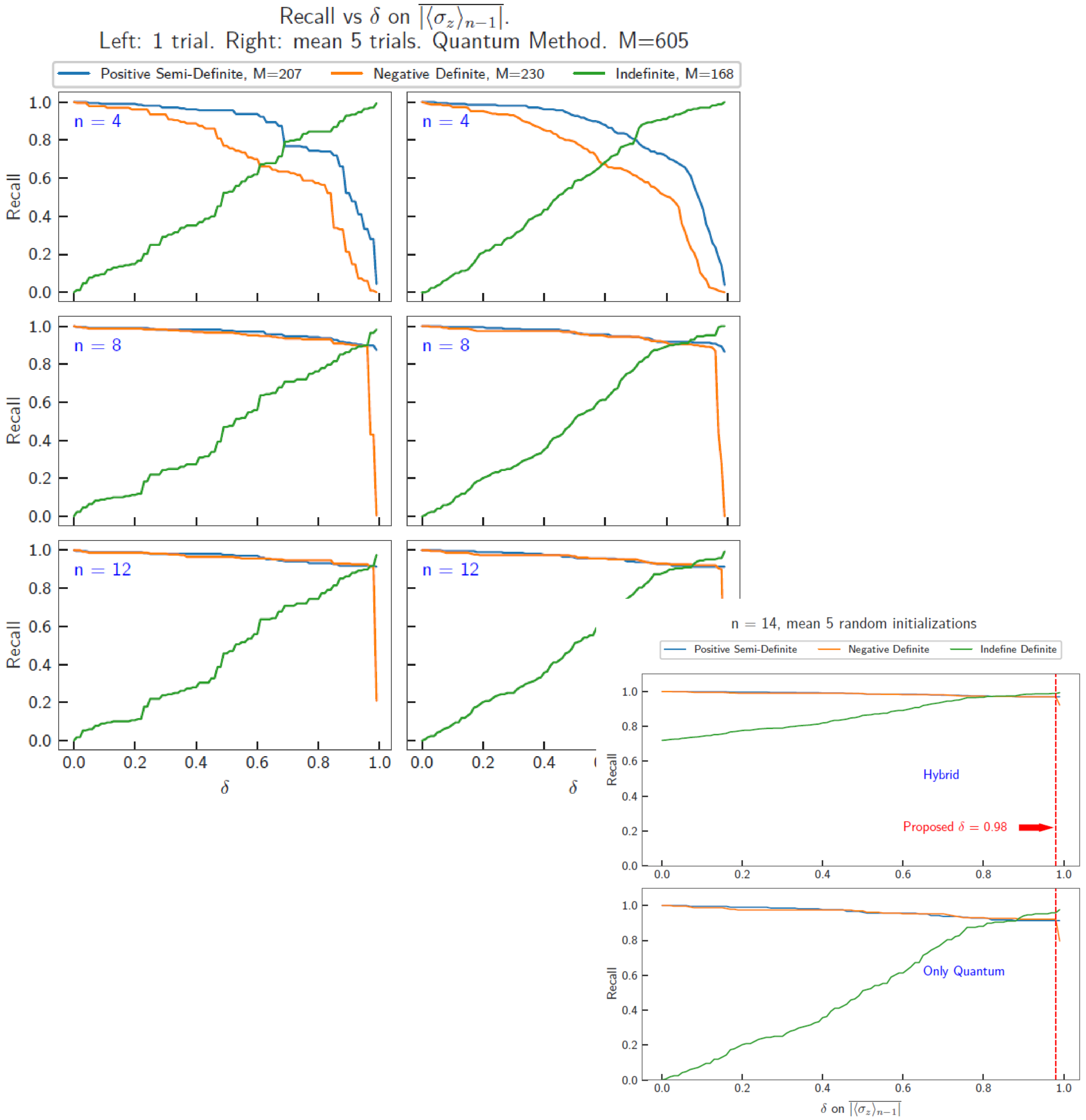
- $M = \sum a_{ij\ldots m}\sigma_i \otimes \sigma_j \otimes \cdots \otimes \sigma_m$
- This needs $O(N^3)$ operations to calculate all $a_{ij\ldots m}$

QPE (for this algorithm) needs, for n aux qubits:

- $O(2^{n+2}\log_2(N)N^2)$ operations

So, classical step can be dominant in the scalability.

Of course. This algorithm is probabilistic.

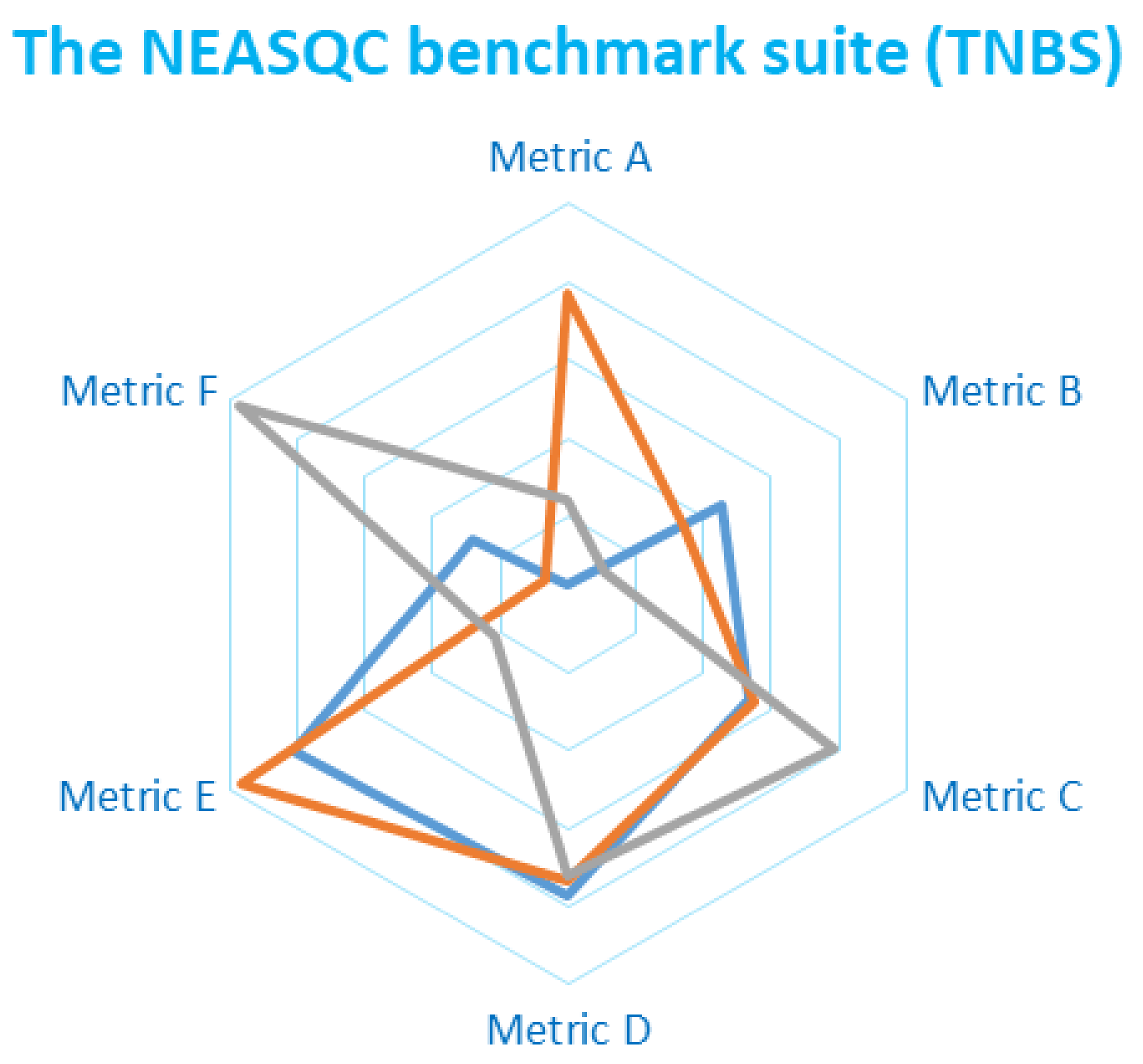


$$\overline{\langle\sigma_z\rangle}_{n-1} \in \begin{cases} [\delta, 1] & \rightarrow \text{ positive semi-definite} \\ [-1, -\delta] & \rightarrow \text{ negative definite} \\ (-\delta, +\delta) & \rightarrow \text{ indefinite} \end{cases}$$

The hybrid classical-quantum computer

The NEASQC Benchmark Suite (TNBS)

- Based on needs of real applications from use cases.
- Under development.
- The defined objectives of this suite are:
  - **Objective 1**: the test cases which compose the suite must help computer architects, programmers and researchers to design future quantum computers, taking into account the variability in the performance introduced by the different components of the stack.
  - **Objective 2**: they must help to understand the evolution of quantum computers (more qubits, better topologies) or to improve the current one (reduction of noise, better compilers, etc.).
  - **Objective 3**: they must allow to compare the performance of different platforms. Currently, there are many different proposals (as transmons, ions, neutral atoms, etc.) which use different one- and two-qubit gates. The benchmarks must allow users and researchers to compare the performance of different platforms, and find their bottlenecks. For users, they should allow them to find the best platforms for their application.
  - **Objective 4**: They should consider other metrics which may be important to understand the quantum computing advantage (as energy consumption, throughput or better scalability).



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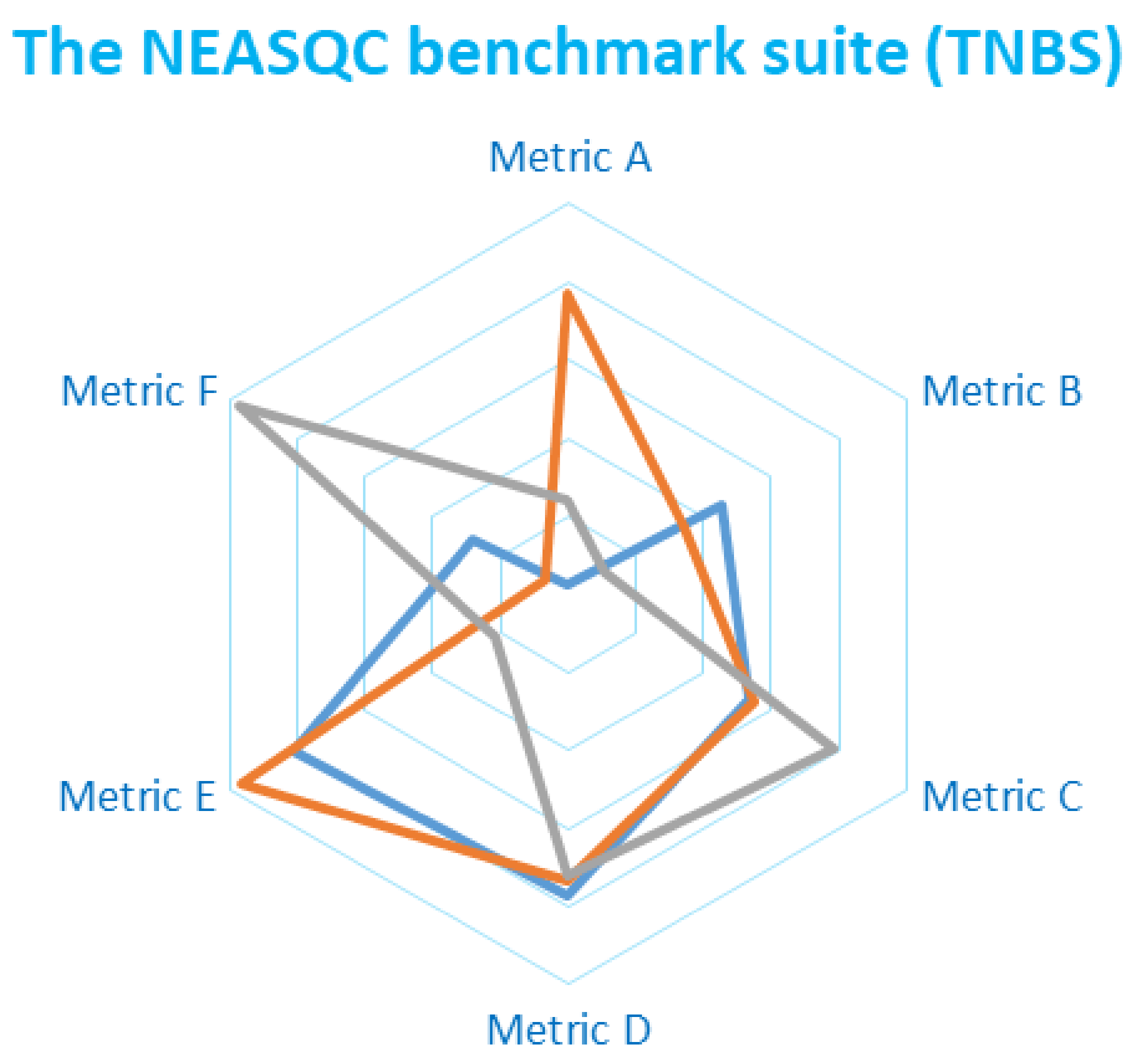
The NEASQC Benchmark Suite (TNBS)

- No single metric. A set of metrics.

- Reporting using JSON format:
  - Description of the hardware. Include multi-QPU/CPU (i.e., clusters).
  - Date ant time of execution.
  - Description of software stack and compilation flags/steps.
  - For each microbenchmark, for each used number of qubits:
    - the used placement, list of QPUs used (the benchmark allows to use more than one QPU for executing it),
    - Total elapsed time in seconds and its sigma,
    - Total time for executing the quantum algorithm in seconds and its sigma,
    - Total time for executing the classical part of the algorithm in seconds and its sigma,
    - Information about additional metrics for the case (to compare quality of the result, for example, fidelity).



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Final remarks

- Quantum Computers probably will be Quantum Accelerators for HPC systems.

- Quantum computers can help HPC to:
  - Solve problems without classical known possibilities (“Quantum Supremacy”).
  - Solve problems faster, even when classical algorithm Works (“Speed Quantum Advantage”)
  - Provide better solutions, even when classical algorithm exists (“Better Quantum Advantage”)
  - Solve problems with less power consumption (“Power Quantum Advantage”)

- Algorithms will be mainly hybrid, with some parts accelerated by QC.

- Speed-up of a Quantum Algorithm should include the classical part (pre-/post-/other).

- Benchmarking has to take into account the full quantum-classical stack.

CESGA

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