QUANTUM COMPUTATION AND SIMULATING QUANTUM SYSTEMS

WORK PACKAGE 5

Quantum Information National Laboratory
HUNGARY

Nemzeti Kutatási, Fejlesztési és Innovációs Hivatal

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Structure of WP5

Task 5.1 **Development of quantum algorithms and quantum computational architectures, assessment of quantum information resources**
(Tamás Kiss, Wigner RCP, László Oroszlány, ELTE TTK)

Task 5.2 **Optimization algorithms, machine learning and artificial intelligence in quantum computation**
(Zoltán Zimborás, Wigner RCP, Péter Rakyta ELTE TTK, Tamás Kozsik, ELTE IK)

Task 5.3 **Numerical simulations using tensor factorization of compound systems and quantum chemical applications**
(Örs Legeza, Wigner RCP; collaboration: BME TTK)

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Task 5.1

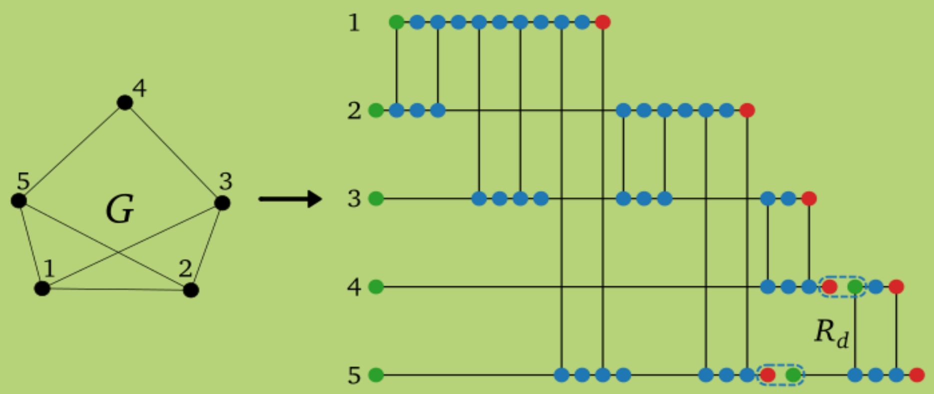
Efficient qudit based scheme for photonic quantum computing

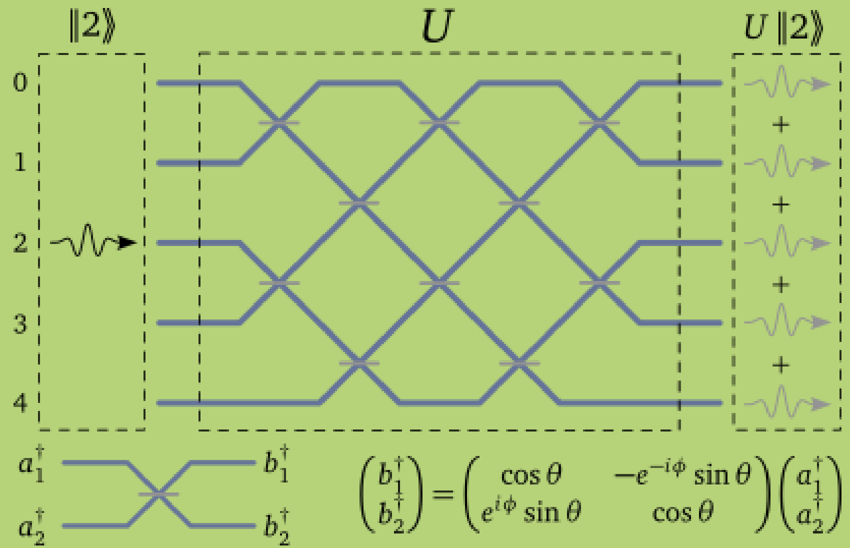
Márton Karácsony, László Oroszlány, Zoltán Zimborás

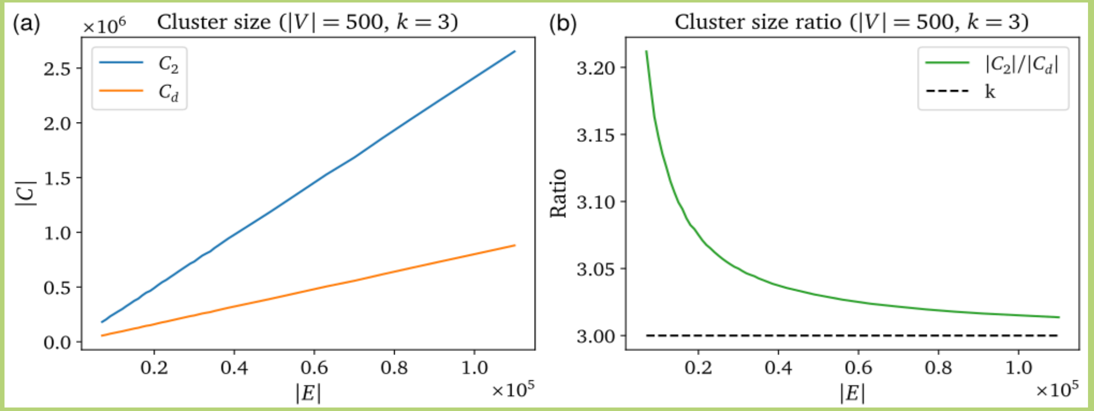
arXiv:2302.07357

Poster 28

- ➢ Locally optimal success rates achieved for some non-deterministic two-quDit gates.
- ➢ Non-deterministic gates can be used for state preparation (e. g. cluster states).
- ➢ QuDit cluster states provide a resource efficient way to implement D-ary optimization problems.







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Task 5.1

Single-photon sources

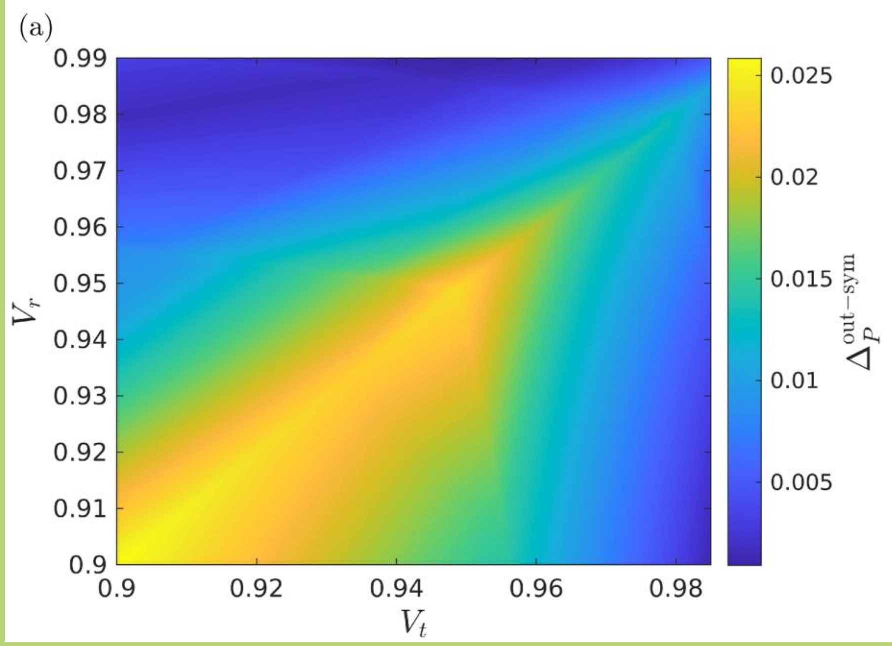
Péter Ádám, Wigner RCP

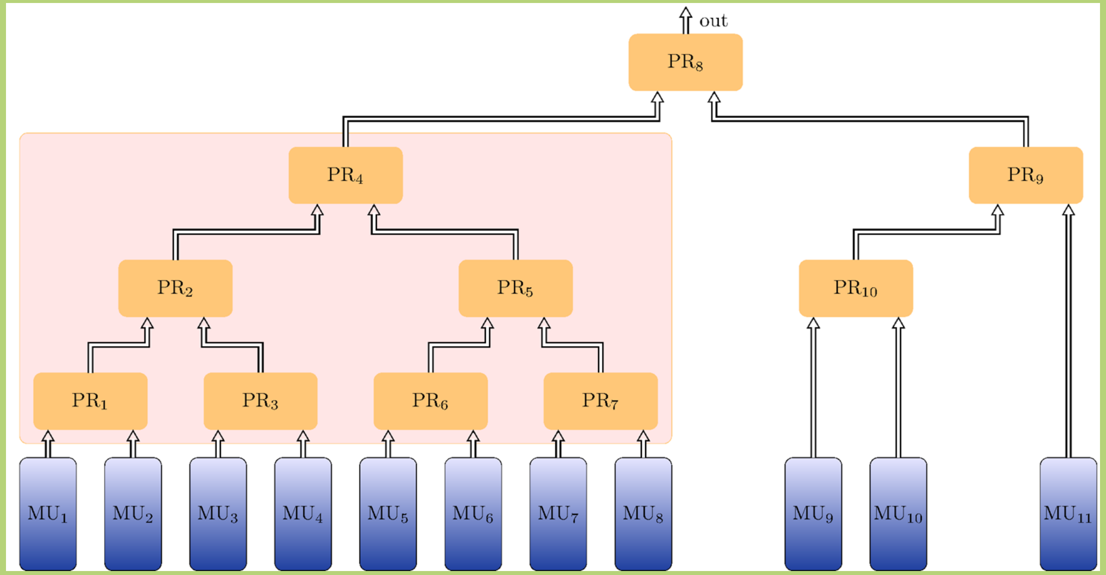
Poster 36

- Novel types of spatially multiplexed single-photon sources based on incomplete binary-tree multiplexer
- Achievable single-photon probabilities higher than 0.93
- Improved performance for suboptimal system sizes relevant in experiments

P. Ádám, F. Bódog, M. Mechler, Optics Express 30, 6999-7016 (2022)

P. Ádám, F. Bódog, M. Koniorczyk, M. Mechler, Phys. Rev. A 105 063721, (2022)





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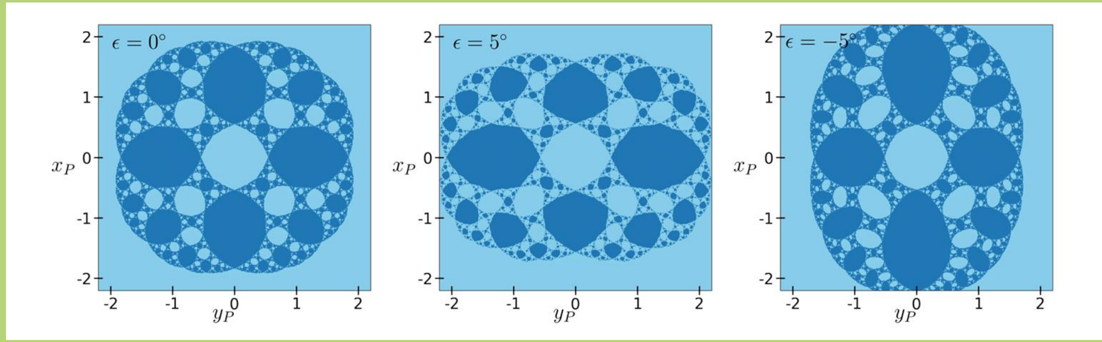
Task 5.1

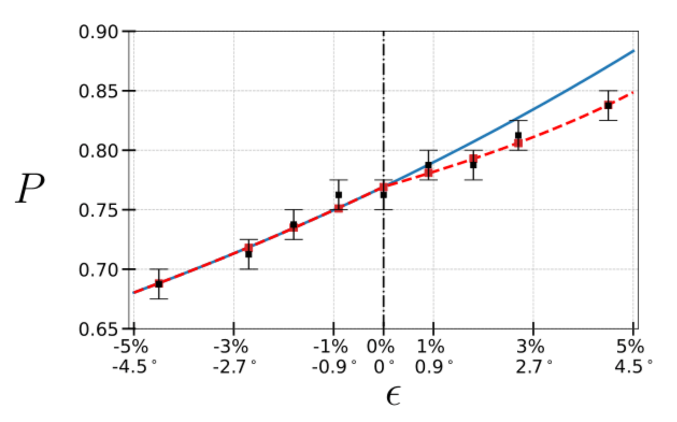
Posters 33 & 38

Iterated nonlinear quantum protocols and benchmarks for quantum computers

Orsolya Kálmán, Adrian Ortega, Wigner RCP

Effect of coherent gate errors

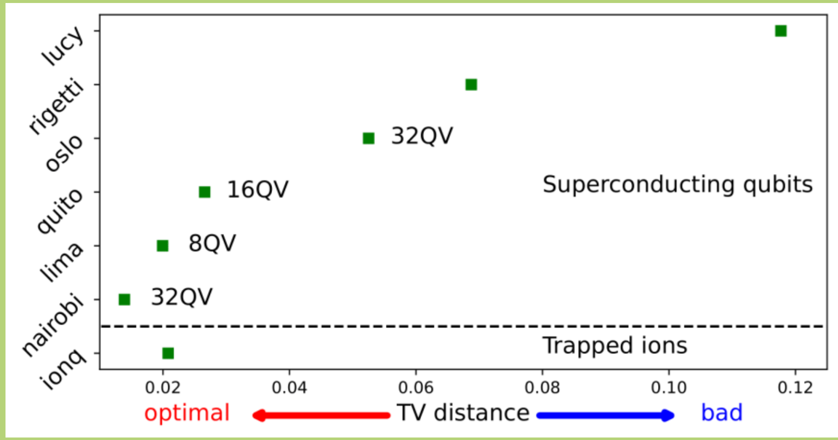




- small coherent errors do not destroy the characteristic features of iterated nonlinear quantum protocols

A. Portik, O. Kálmán, I. Jex, T. Kiss, *Phys. Lett. A* 431 127999 (2022)

Benchmarking quantum computers



- tested freely and commercially available superconducting and trapped ion QCs
- **collaboration: ion QC laboratory of Norbert Linke @ Duke University**

A. Ortega, O. Kálmán, T. Kiss, *Phys. Scr.* 98 024006 (2023)

OpenSuperQPlus

Task 5.1

Quantum correlations, quantum optimization

Mátyás Koniorczyk, Wigner RCP

Posters 40 & 41

- Our REST API logically implementing no-signalling correlations is now in production regime:

```
curl -get https://nonlocalbox.wigner.hu/api/v1/useBox?apiKey=$ALICE_KEY&boxID=4&transactionID=202209140101&x=1
{"a":0,"boxID":4,"status":0}
```

https://nonlocalbox.wigner.hu

Koniorczyk et al. Simulating nonlocal no-signaling boxes, arXiv:2212.06769 (2022) *See also the respective poster.*

Use cases:

- education (mobile app will be released soon: gamification of Bell inequalities)
- business applications?
- design and testing of device-independent quantum cryptography protocols

Ottó Hanyecz, Mátyás Koniorczyk: Simulation of device-independent quantum key distribution protocols, QCRYPT 2023

András Bodor, Orsolya Kálmán, and Mátyás Koniorczyk: Error-free interconversion of nonlocal boxes, Phys. Rev. A 106, 012223 (2022)

- Quantum optimization and applications
  - Koniorczyk et al.: Application of a Hybrid Algorithm Based on Quantum Annealing to Solve a Metropolitan Scale Railway Dispatching Problem
    EUROpt 2023, Budapest, Corvinus University
  - **Statistical quality assessment of Ising-based annealer outputs**
    K Domino, M Koniorczyk, Z Puchała
    Quantum Information Processing 21 (8), 288 (2022)

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Task 5.1

Efficiency of adiabatic quantum computing

Róbert Juhász, Wigner RCP

- The efficiency of adiabatic quantum computing is determined by the minimal energy gap along the annealing path.
- The required annealing time is given by the inverse square of the minimal energy gap.
- The one-dimensional Ising machine is a frequently used model for testing the efficiency of quantum annealing schemes.

$$\mathcal{H}(t) = -\sum_{ij} J_{ij}\sigma_i^x\sigma_j^x - h(t)\sum_i \sigma_i^z$$

- There is no general, explicit expression for the energy gap.
- Based on a relationship with random walks, we derived exact lower and upper bounds on the energy gap, which are explicit in the parameters.

$$\epsilon_1 > \frac{1}{\sqrt{\tau_1}} = \left[\sum_{l=1}^{L}\sum_{m=1}^{l}\frac{1}{h_l^2}\prod_{i=m}^{l-1}\frac{J_i^2}{h_i^2}\right]^{-\frac{1}{2}}$$

$$\epsilon_1 < \frac{1}{\sqrt{\tau_s}} = \left[\sum_{n=1}^{L}\prod_{i=1}^{n-1}\frac{h_i^2}{J_i^2}\right]^{\frac{1}{2}}\left[\sum_{n=1}^{L}\left(\prod_{i=1}^{n-1}\frac{h_i^2}{J_i^2}\right)\sum_{l=n}^{L}\sum_{m=1}^{l}\frac{1}{h_l^2}\prod_{j=m}^{l-1}\frac{J_j^2}{h_j^2}\right]^{-\frac{1}{2}}$$

Using these bounds, we have demonstrated that,
by applying appropriately chosen heterogeneous driving fields,
the gap closing can be mitigated and thus
the quantum annealing can be made more accurate.

R. Juhász, Phys. Rev. B 106, 064204 (2022)

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Task 5.2

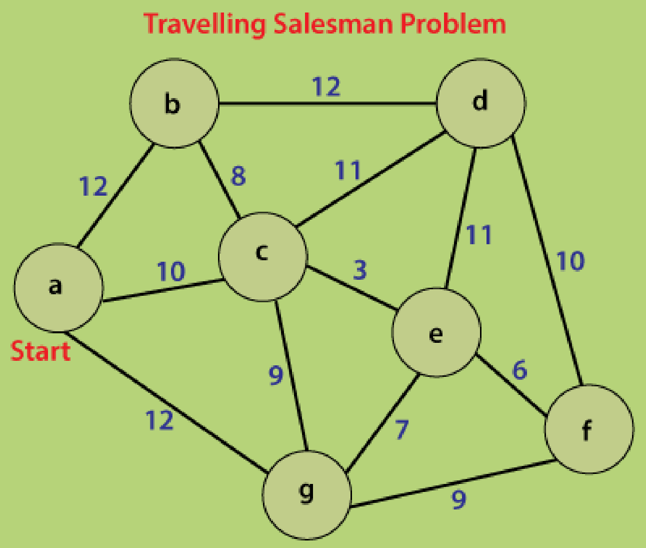
Optimization algorithms, machine learning and artificial intelligence in quantum computation

Posters 31 & 32

Zoltán Zimborás, Wigner RCP, Péter Rakyta ELTE TTK, Tamás Kozsik, ELTE IK

Optimal Quantum Circuit Design for the Travelling Salesperson Problem (TSP)

- TSP is one of the most well-known paradigmatic combinatorial optimization problems.



- Task: Find the shortest path that goes through all the cities and returns to the start.

2 talks @ QIP 2022 & 2023

- In recent years, there has been great interest and progress in making the quantum optimization algorithms for TSP increasingly efficient.
- Further improving our previous HOBO technique (npj Quantum Information 8, 39 (2022)), we have designed a variational quantum circuit (coined FUNC-QAOA) that **surpasses all the other prior circuit designs in all the circuits metrics simultaneously** and **matches** (up to log corrections) **the theoretical optima** (arXiv:2209.03386).

	optimal	X-QAOA	XY-QAOA	MTZ ILP	HOBO	FUNC-QAOA
qubits	$n\log n$	n^2	n^2	$n^2\log n$	$n\log n$	$n\log n$
gates	n^2	n^3	n^3	n^3	n^3	n^2
depth	n	n	n	$n\log n$	n^2	$n\log n$
depth (LNN)	n	n^2	n^2	$n^2\log n$	$n^2\log n$	$n\log n$
energy span	n	n^3	n^2	n^4	n^2	n
param.gates	n^2	n^3	n^3	n^3	n^3	n^2
eff.space	$n\log n$	n^2	$n\log n$	$n^2\log n$	$n\log n$	$n\log n$

OpenSuperQPlus

Task 5.2

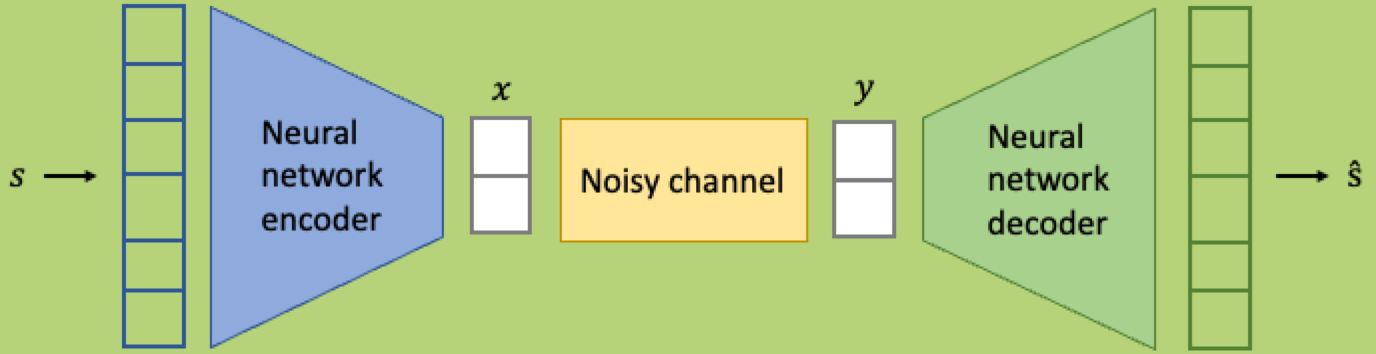
Optimization algorithms, machine learning and artificial intelligence in quantum computation

Zoltán Zimborás, Wigner RCP, Péter Rakyta ELTE TTK, Tamás Kozsik, ELTE IK

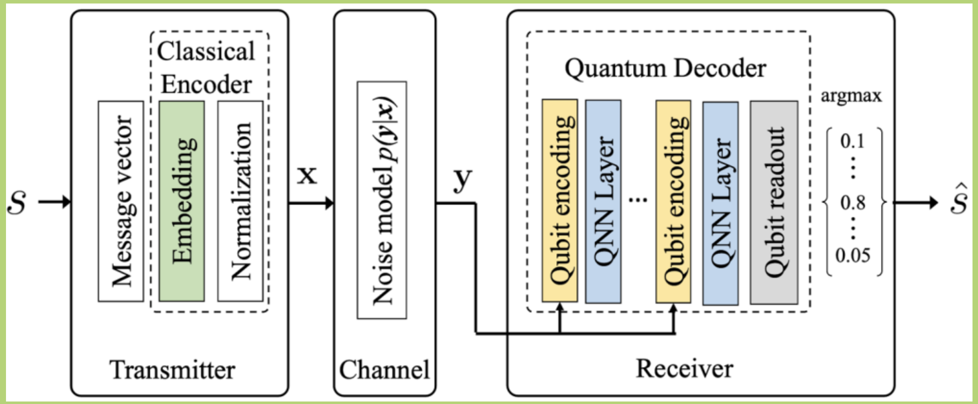
Posters 31 & 32

Hybrid Quantum-Classical Autoencoders (Wigner RCP-Ericsson collaboration)

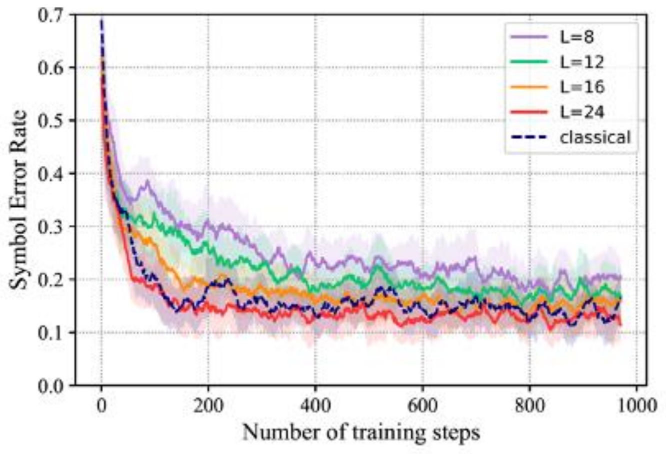
- Neural network approach: train encoder-decoder neural networks to get a good estimate of the original symbol.



- Our idea: use **quantum neural network** decoder (arXiv:2301.026019).



Results



- We introduced a "double data re-uploading" approach, as this significantly improved performance.
- The classical baseline efficiency was reached, we expect a quantum advantage for more complex noise scenarios.

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Task 5.3

Numerical simulations using tensor factorization of compound systems

Poster 39

Örs Legeza, Wigner RCP

[1] Massively Parallel Tensor Network State Algorithms on Hybrid CPU-GPU Based Architectures, *Andor Menczer, Örs Legeza,* arXiv:2305.05581, 2023

[2] Hilbert space multireference coupled clusters tailored by matrix product states, *Ondrej Demel, Jan Brandejs, Jakub Lang, Jiri Brabec, Libor Veis, Ors Legeza, Jiri Pittner,* arXiv:2304.01625

[3] Symmetric carbon tetramers forming chemically stable spin qubits in hBN, *Zsolt Benedek, Rohit Babar, Ádám Ganyecz, Tibor Szilvási, Örs Legeza, Gergely Barcza, Viktor Ivády,* arXiv:2303.14110, 2023

[4] Predicting the FCI energy of large systems to chemical accuracy from restricted active space density matrix renormalization group calculations, *Gero Friesecke, Gergely Barcza, Örs Legeza,* arXiv:2209.14190, 2022

[5] Accurate localization of Kosterlitz-Thouless-type quantum phase transitions for one-dimensional spinless fermions, *Florian Gebhard, Kevin Bauerbach, Örs Legeza,* doi 10.1103/PhysRevB.106.205133, 2022

[6] Combining the in-medium similarity renormalization group with the density matrix renormalization group: Shell structure and information entropy, *A. Tichai, S. Knecht, A. T. Kruppa, Ö. Legeza, C. P. Moca, A. Schwenk, M. A. Werner, G. Zarand,* a arXiv:2207.01438, 2022

[7] Spectroscopic evidence for engineered hadron formation in repulsive fermionic SU(N) Hubbard Models *Miklós Antal Werner, Cătălin Paşcu Moca, Márton Kormos, Örs Legeza, Balázs Dóra, Gergely Zaránd,* arXiv:2207.00994, 2023

Highlighted results:

Numerical simulations based on quantum informational methods for the FeMoCo molecular cluster, which plays an important role in the binding of nitrogen, for heavy nuclei with a large number of protons and neutrons, for point defect qubits in semiconductors, and for strongly correlated solid state systems.

Industrial collaborations:

- **Furukawa Electric Institute of Technology** (numerical simulation of molecular systems containing metal centers)
- **Governmental Agency for IT Development, KIFÜ** (applications for HPC)

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Activities

- **QHungary**: *Z. Zimborás, O. Kálmán (Wigner RCP), J. Asbóth, A. Pályi (BME TTK)* part of the QWorld
  - QBronze course on Quantum Computing, 2 days, 37 participants
  - World Quantum Day, ~100 participants, together with Nokia
  - Active Facebook channel
- **Free public service:** https://nonlocalbox.wigner.hu
- **Conference:** *J. Pittner and Ö. Legeza*, Sat. Meeting on Strong Correlation in Molecules, 20-23th June 2023, Znojmo, Czech Republic https://www.jh-inst.cas.cz/icqc2023sat/

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