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Quantum Feature Maps for Graph Machine Learning on a Neutral Atom Quantum Processor

QTML 2023 22/11/2023

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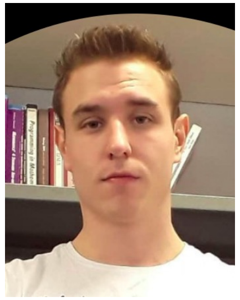
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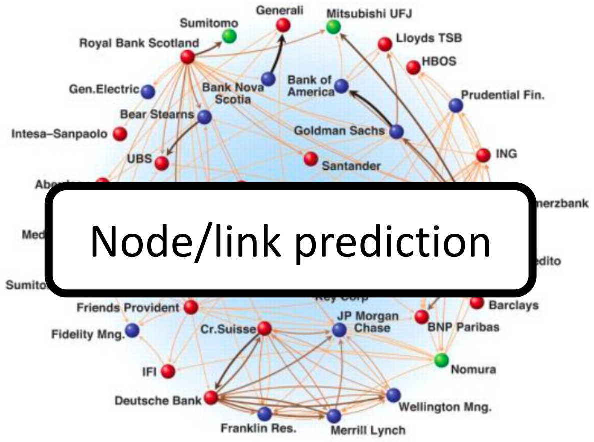
Graph-structured data

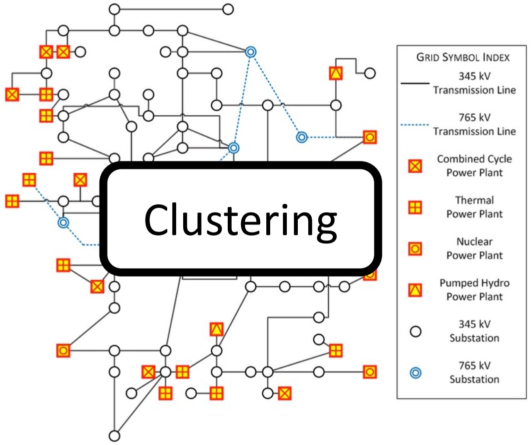
Machine learning tasks on graph-structured data



Node/link prediction

Economic networks

Anticipating new partnerships



Clustering

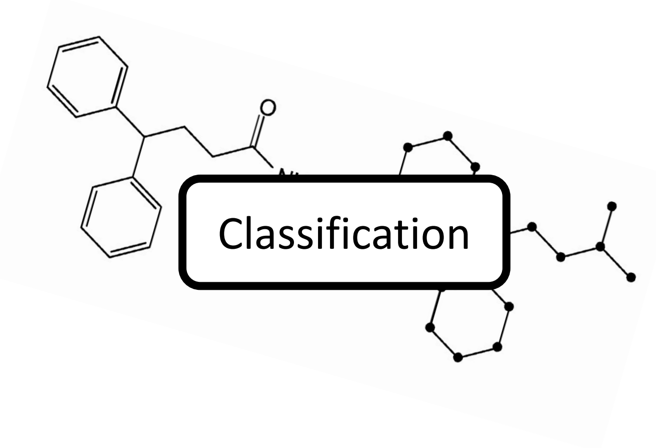
Power grid

Segmenting highly-connected zones

Community detection

Social networks

Marketing to like-minded users



Classification

Molecules

Predicting toxicity of compounds

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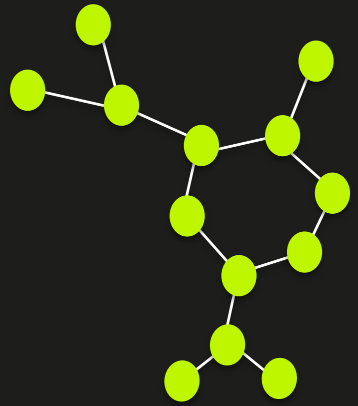
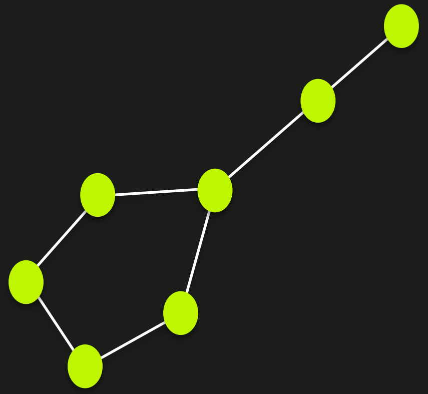
Toxicity screening on a QPU

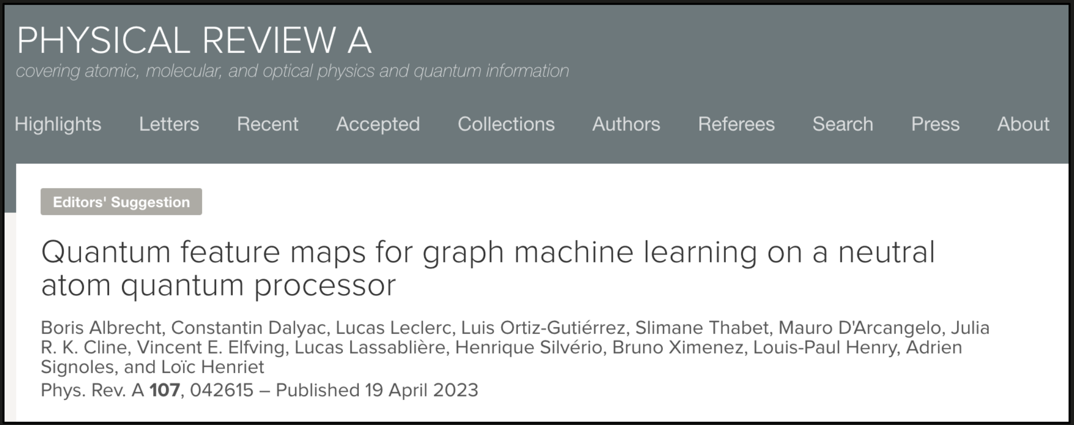
Predictive Toxicity Challenge on Female Mice [1,2]





# of registers # of qubits	Control	Runtime
288 registers, up to 32 qubits	Global analog, constant pulses	~4 days continuous measurement

- First graph QML implementation on a real dataset of such size.



PHYSICAL REVIEW A

covering atomic, molecular, and optical physics and quantum information

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Editors' Suggestion

Quantum feature maps for graph machine learning on a neutral atom quantum processor

Boris Albrecht, Constantin Dalyac, Lucas Leclerc, Luis Ortiz-Gutiérrez, Slimane Thabet, Mauro D'Arcangelo, Julia R. K. Cline, Vincent E. Elfving, Lucas Lassablière, Henrique Silvério, Bruno Ximenez, Louis-Paul Henry, Adrien Signoles, and Loïc Henriet

Phys. Rev. A **107**, 042615 – Published 19 April 2023

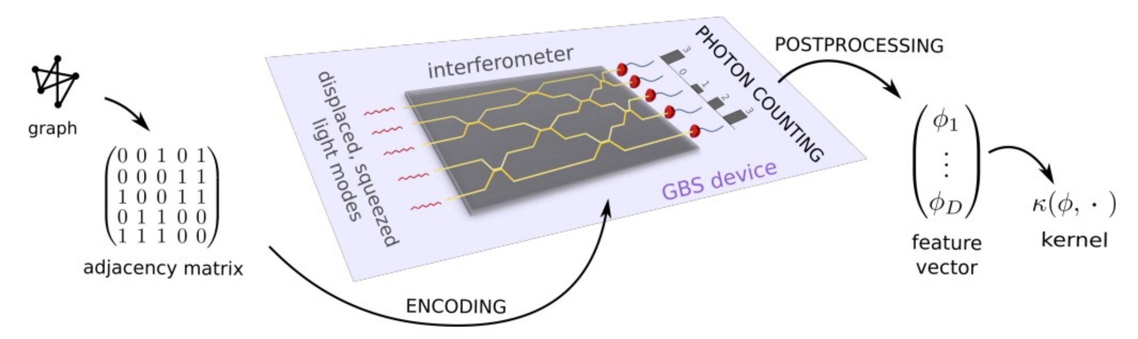
[1] Helma, et al., Bioinformatics, 01, 1, 107-108 (2001)

[2] Data taken from the GraKeL library

Previous work about using quantum computing for graph classification

Measuring the similarity of graphs with a Gaussian Boson Sampler

Maria Schuld,[1,2,*] Kamil Brádler,[1,†] Robert Israel,[1] Daiqin Su,[1] and Brajesh Gupt[1]
[1]*Xanadu, Toronto, Canada*
[2]*University of KwaZulu-Natal, South Africa*
(Dated: October 17, 2019)



Quantum Graph Neural Networks

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Outline

I. Neutral atom Quantum Processing Units

II. Graph Machine Learning with neutral atom QPUS

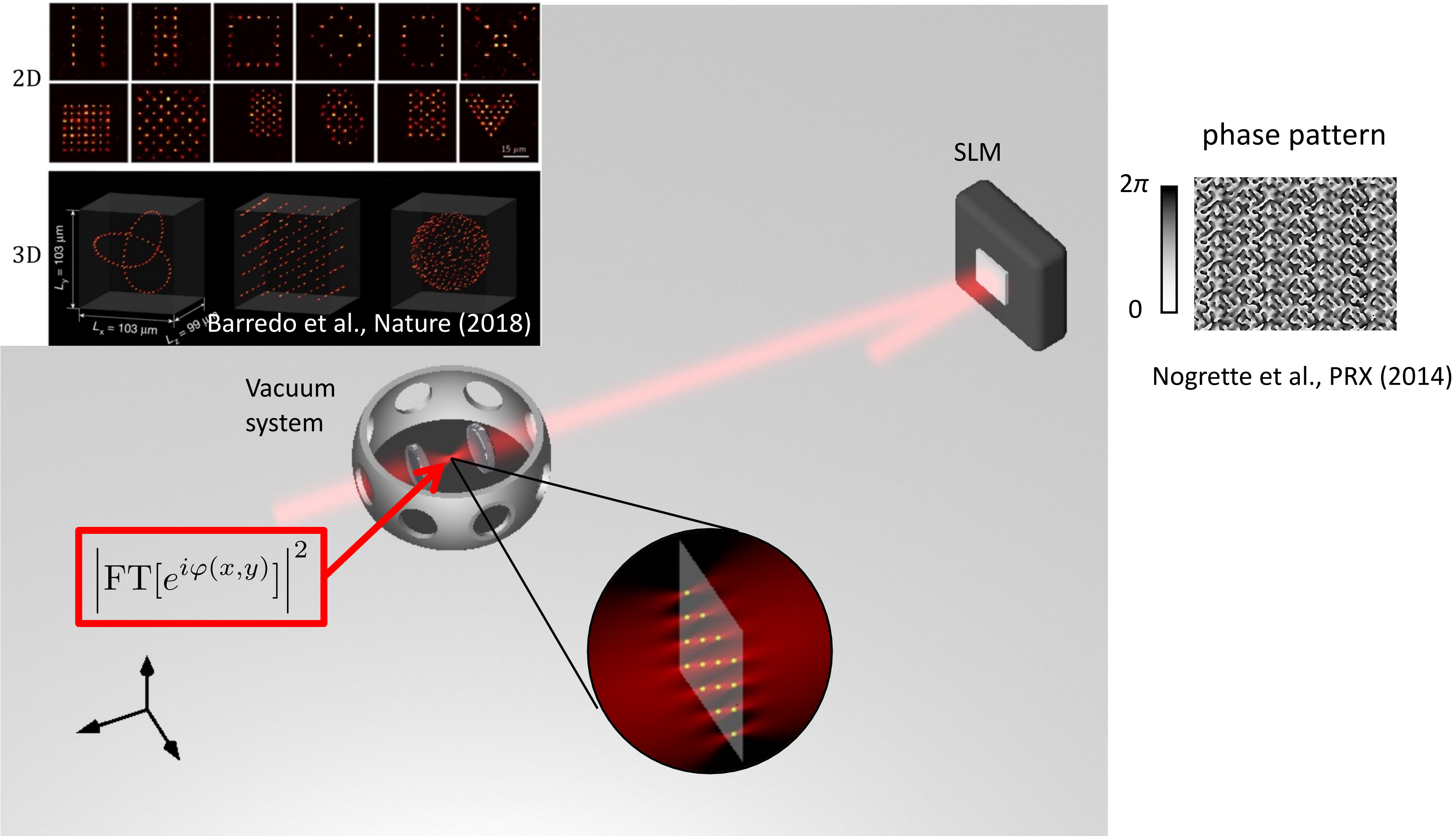
III. Toxicity screening on a QPU

Neutral atom Quantum Processing Units

Trapping atoms in vacuum

Spin out of IOGS:
Trapped Rb atoms in an array of optical tweezers[1]

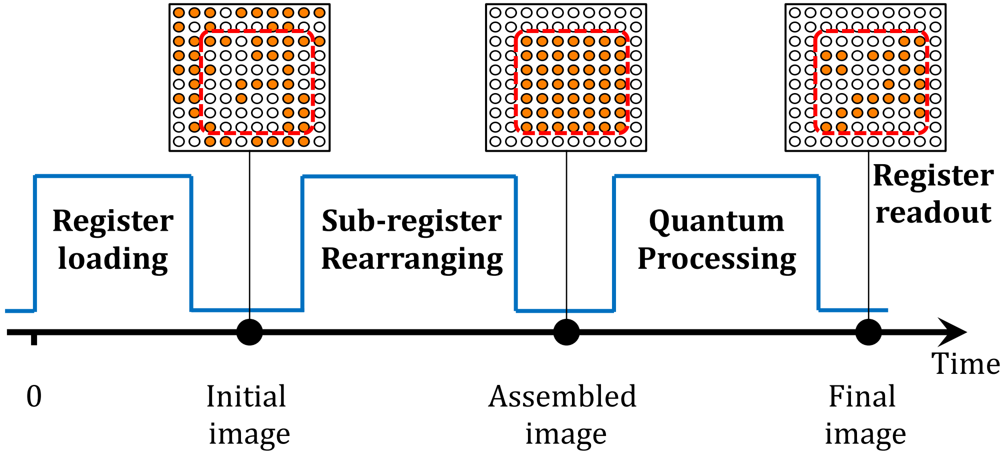
Using a SLM, one can reconfigure the geometry of the qubit register



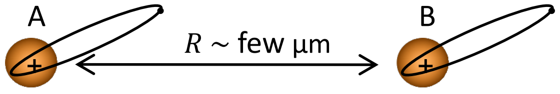
[1] Quantum computing with neutral atoms, Quantum 4, 327 (2020)

Processing quantum information

Qubit registers made of individual atoms



Rydberg interaction as entanglement resource



Jaksch et al., PRA (2000)
Saffman, RMP (2010)
Browaeys & Lahaye, Nat. Phys. (2020)

$$H_{ising} = \frac{\hbar\Omega}{2}\sum_{i=1}^{N}\sigma_i^x - \hbar\delta\sum_{i=1}^{N}\sigma_i^z + \sum_{j<i}\frac{C_6}{r_{ij}^6}n_i n_j, \quad n_i = \frac{\sigma_i^z + 1}{2}$$

$$H_{XY} = \frac{\hbar\Omega}{2}\sum_{i=1}^{N}\sigma_i^x - \frac{\hbar\delta}{2}\sum_{i=1}^{N}\sigma_i^z + 2\sum_{j<i}\frac{C_3}{r_{ij}^3}(\sigma_i^+\sigma_j^- + \sigma_i^-\sigma_j^+)$$

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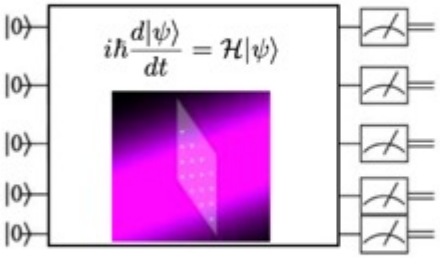
Two controls modes

Quantum resources can be used in two different modes:

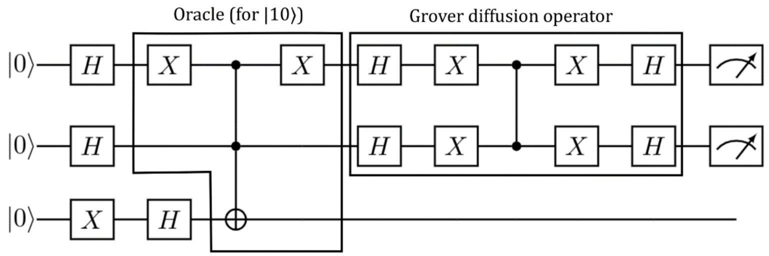
ANALOG CONTROL
programming a Hamiltonian sequence



$$H = \sum_j [\hbar\delta(t)\,\sigma_j^z + \hbar\Omega(t)\,\sigma_j^x] + \sum_{i,j} U_{i,j}\,\sigma_i^z\sigma_j^z$$

The Hamiltonian faithfully describes the dynamics of a physical system or the constraints of an operational case. Parameters can be tuned continuously.

DIGITAL CONTROL
programming a quantum circuit with digital quantum gates



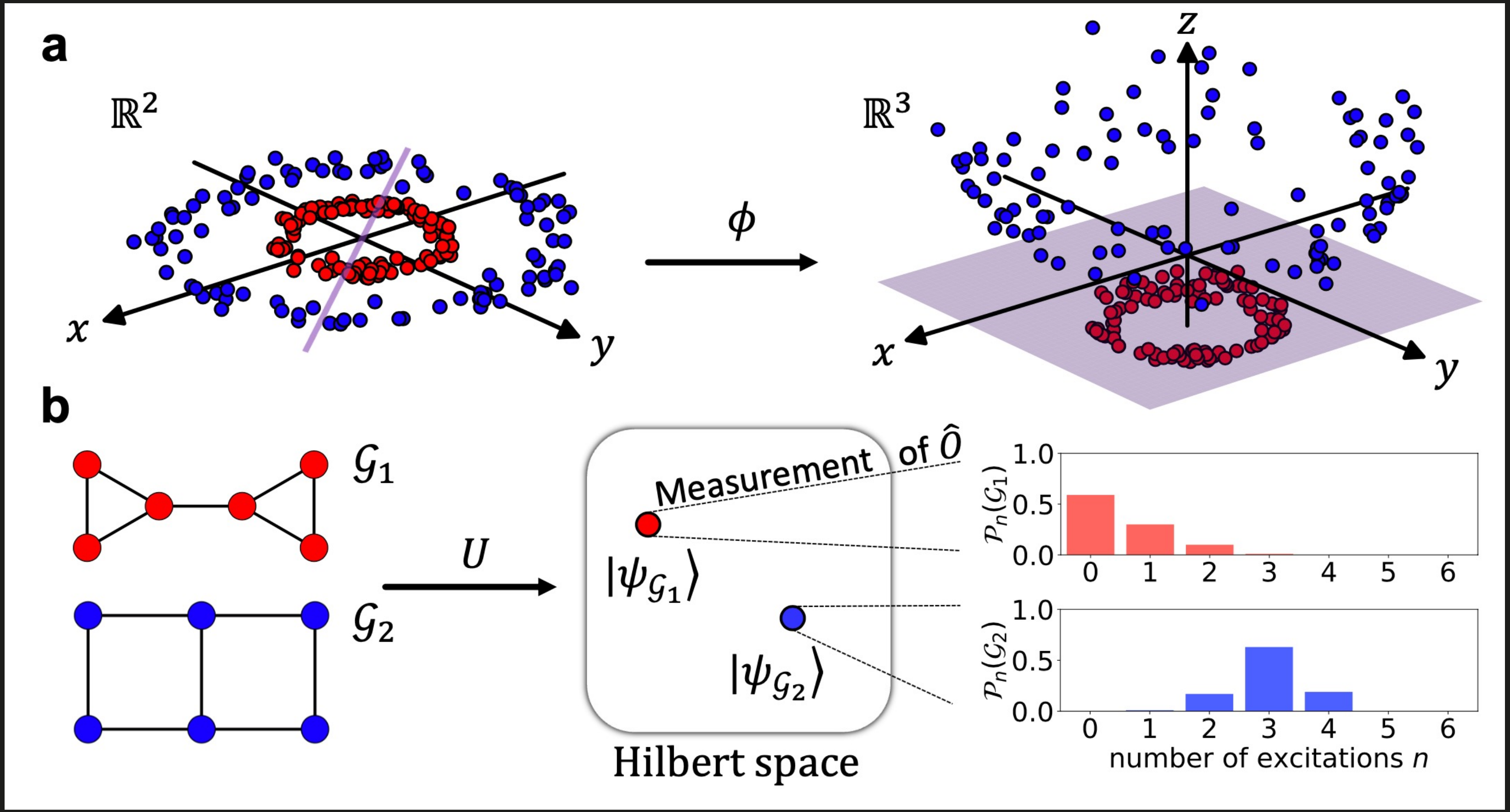
Elementary operations are discrete digital quantum gates, that can act either on individual qubits, or on several qubits at the same time.

M. Troyer (Microsoft), A. J. Daley (Strathclyde), I. Bloch (MPQ) and P. Zoller (Innsbruck), comparing the **requirements to simulate the same quantum dynamics** of a 10x10 2D Hubbard model system using an **analogue vs digital** modes: with typical <u>error level of 1%</u> of the analogue mode → <u>10^6 gate operations</u> are required with 1-F < 10^6

Graph Machine Learning with neutral atom QPUs

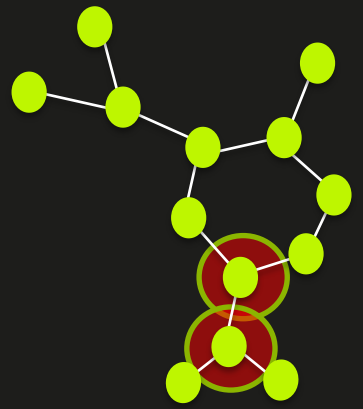
Using the quantum dynamics to embed the data

The quantum dynamics is expected to introduce a richer feature map, with characteristics that are hard to access for classical methods



Quantum feature map

The graph topology is encoded in the dynamics through the Hamiltonian of the system

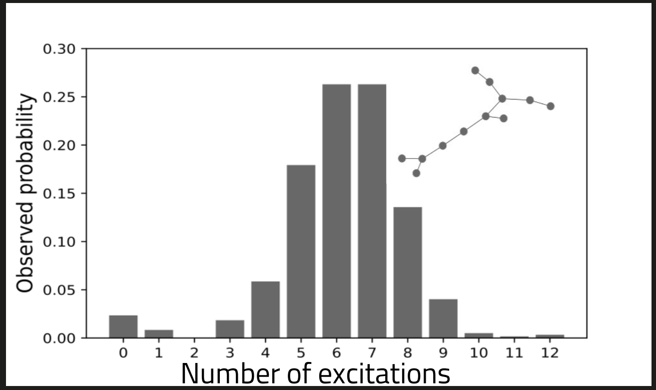


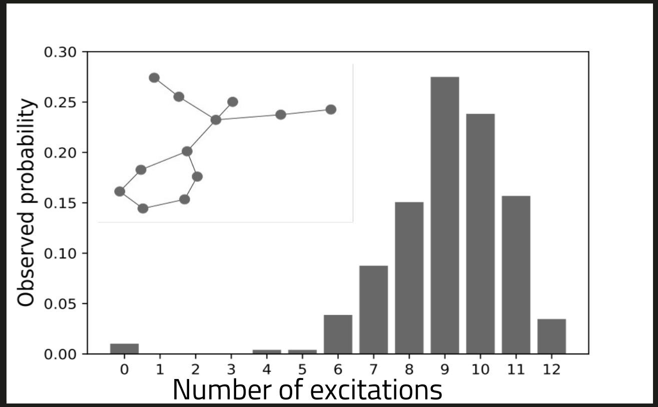
Creates an edge if $r_{ij} < r_0$

$$G = (V, E)$$

$$H_G \sim \sum_{(i,j)\in E} \frac{C_6}{r_{ij}^6} n_i n_j$$

The measurement histograms enable us to build a similarity measure between graphs

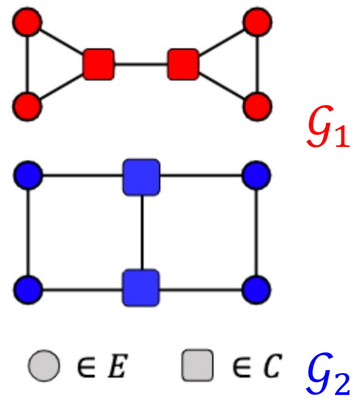




Henry, L. P., Thabet, S., Dalyac, C., & Henriet, L. (2021). Quantum evolution kernel: Machine learning on graphs with programmable arrays of qubits. *Physical Review A*, *104*(3), 032416.

Distinguishing graphs with quantum dynamics

Interactions induce graph-dependent quantum dynamics

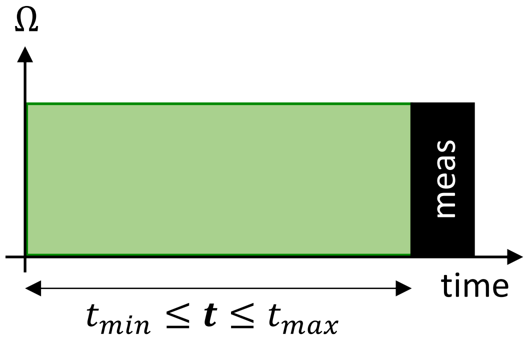


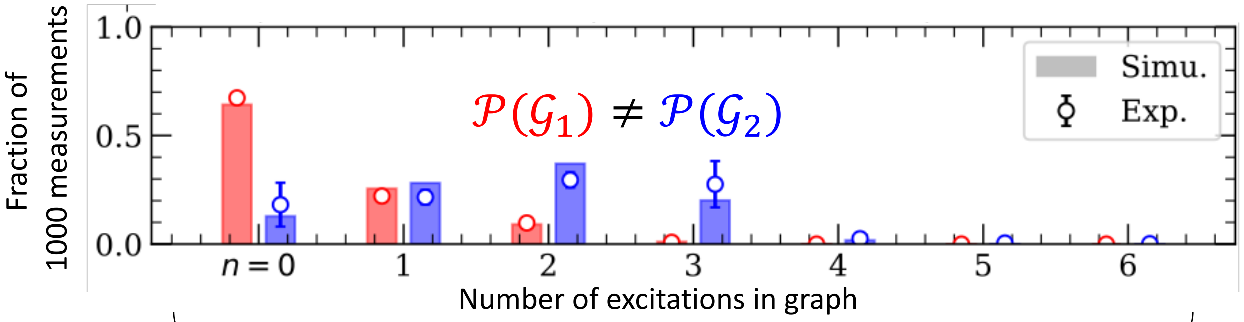
Two graphs
locally similar
but non isomorphic

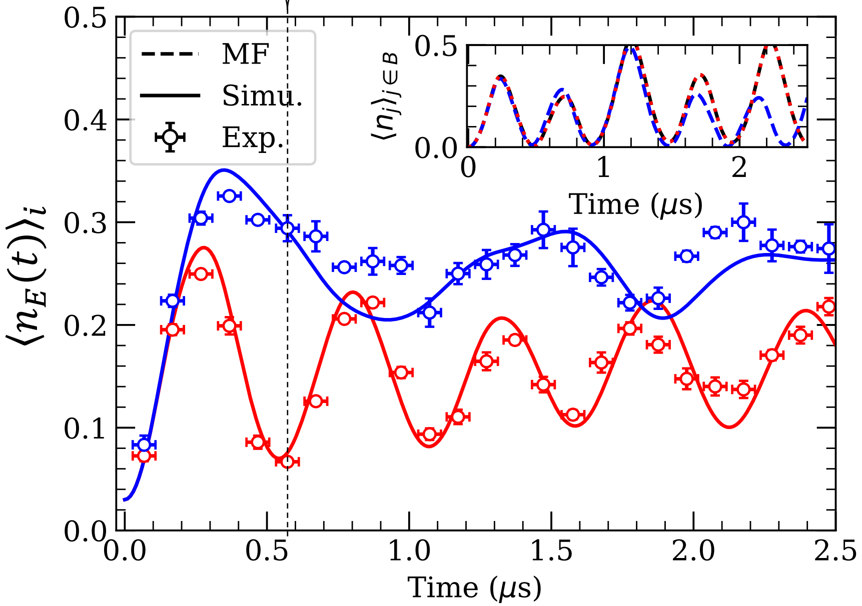
$$U(\mathcal{G};\mathrm{t}) = \; e^{-\mathrm{i}/\hbar\left(H_{\mathcal{G}}+\frac{\Omega}{2}\sum_j \sigma_j^x\right)\mathrm{t}}$$

+

Measuring n_i 1000 times







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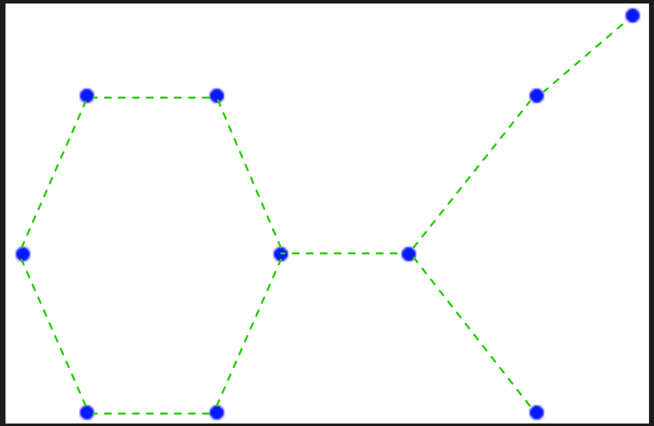
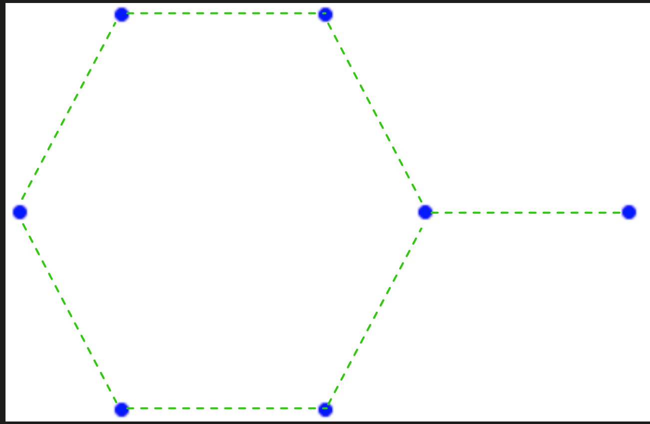
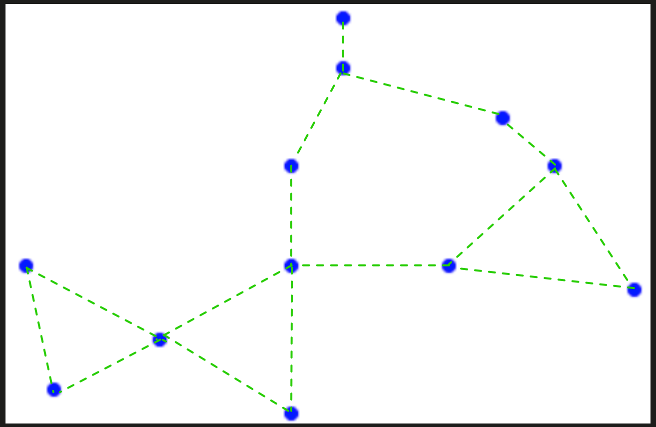
Toxicity screening experiment

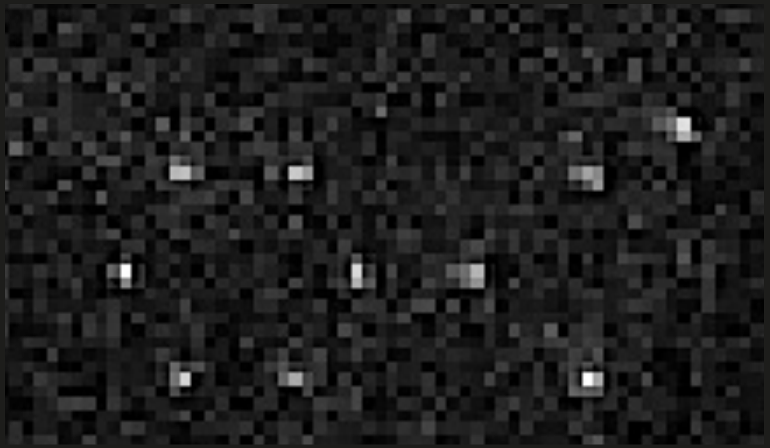
Chemical compounds in PTC-FM

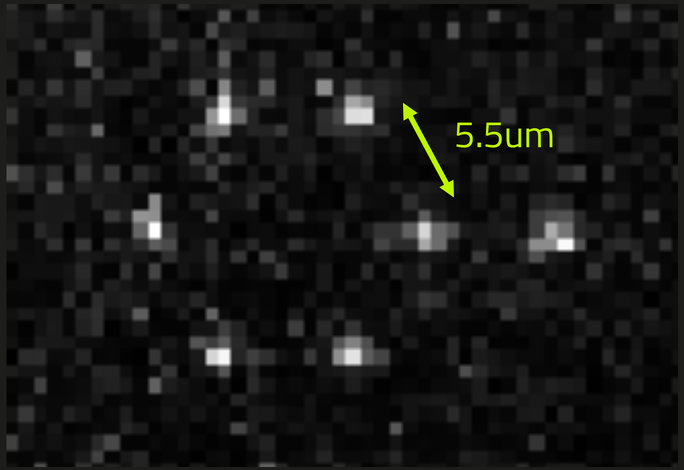






Chemical compounds in PTC-FM

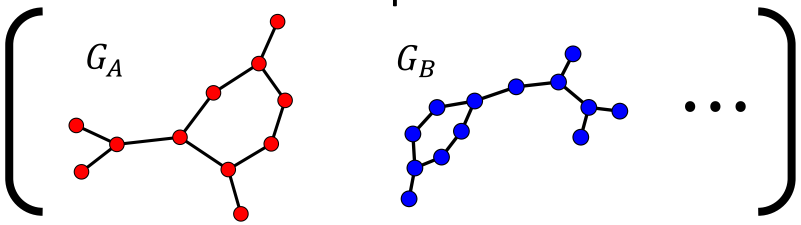




Batching atomic registers

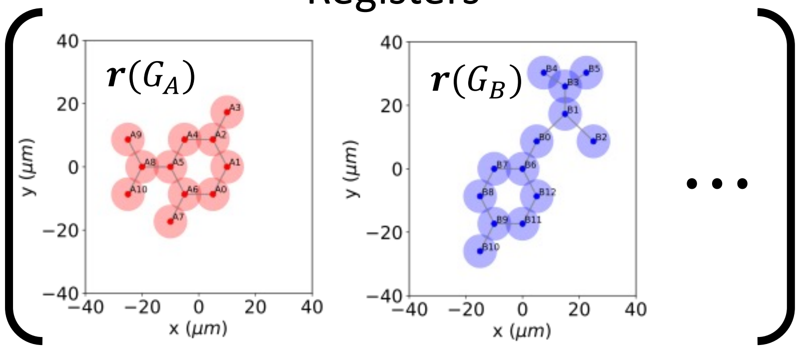
Changing trap layout is resource consuming → Do several registers with one layout

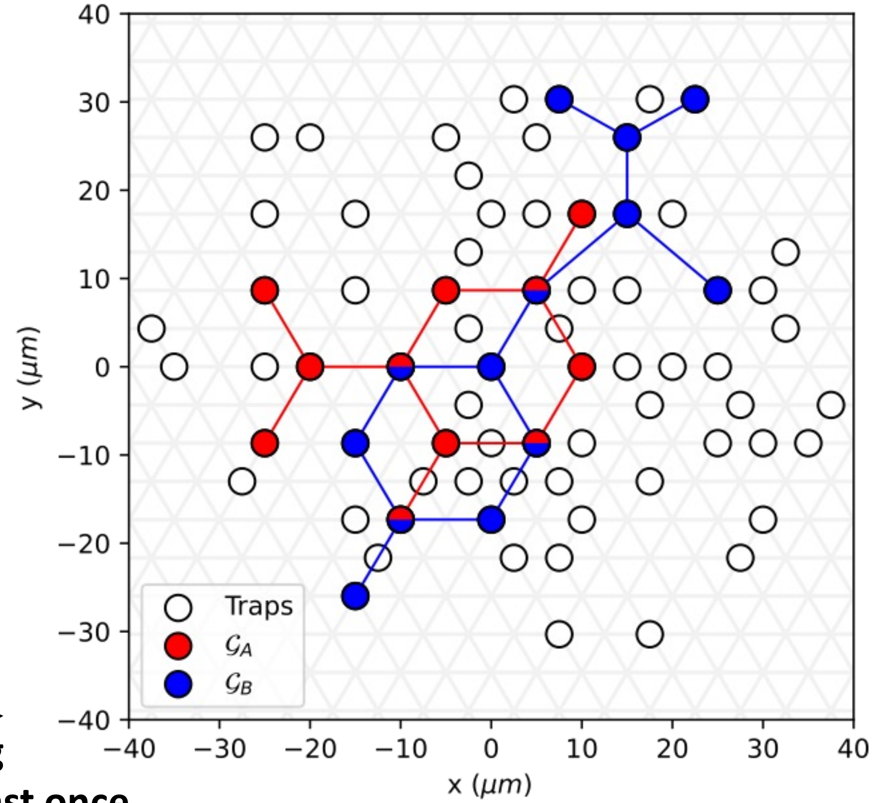
Graphs



Mapping to underlying triangular pattern

Registers





Batching and keeping only traps used at least once

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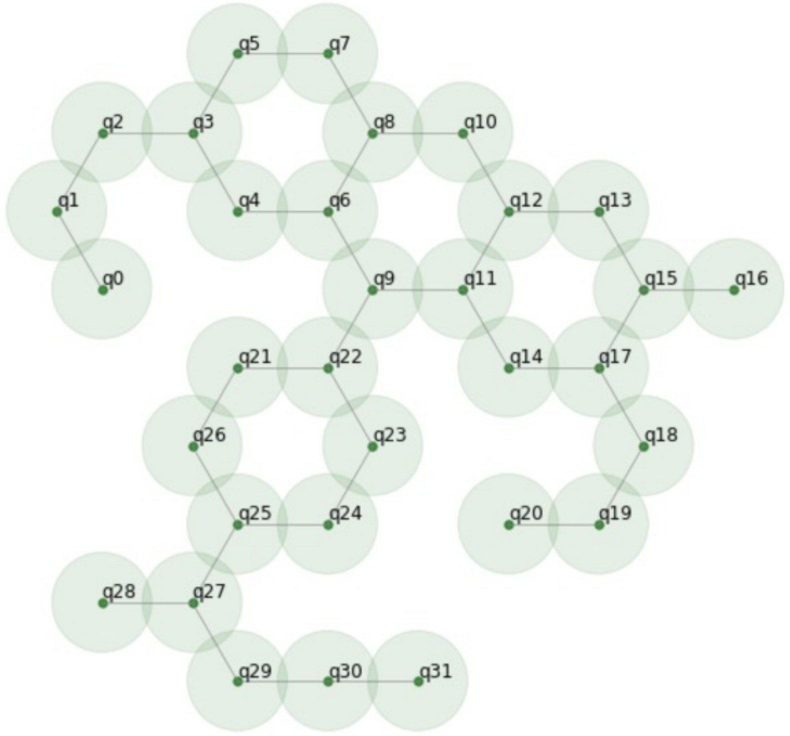
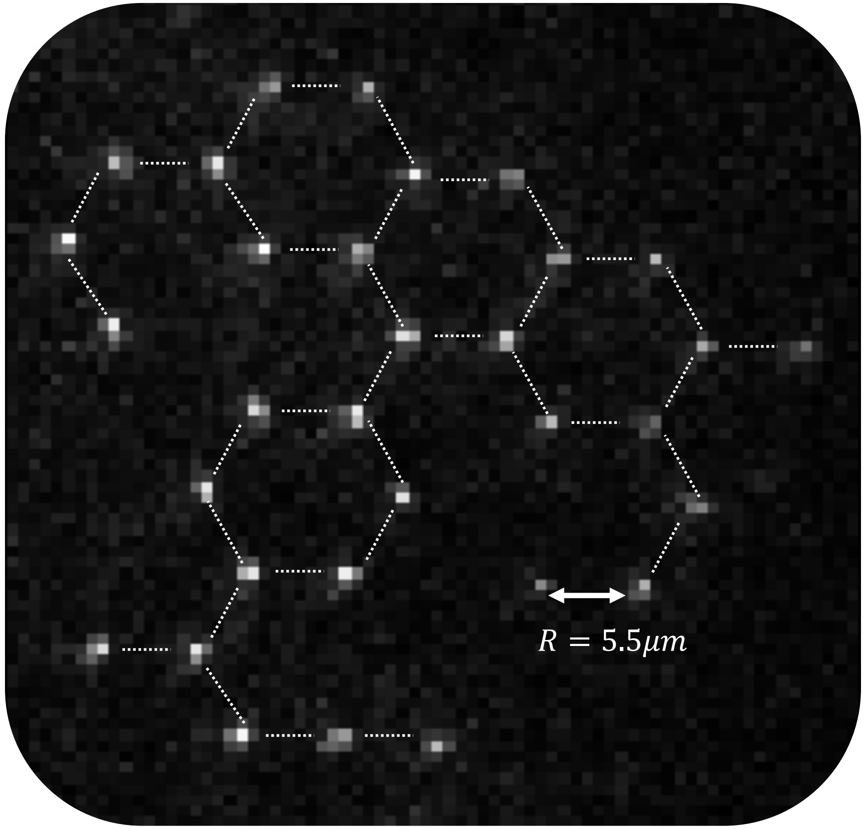
Large atom number registers

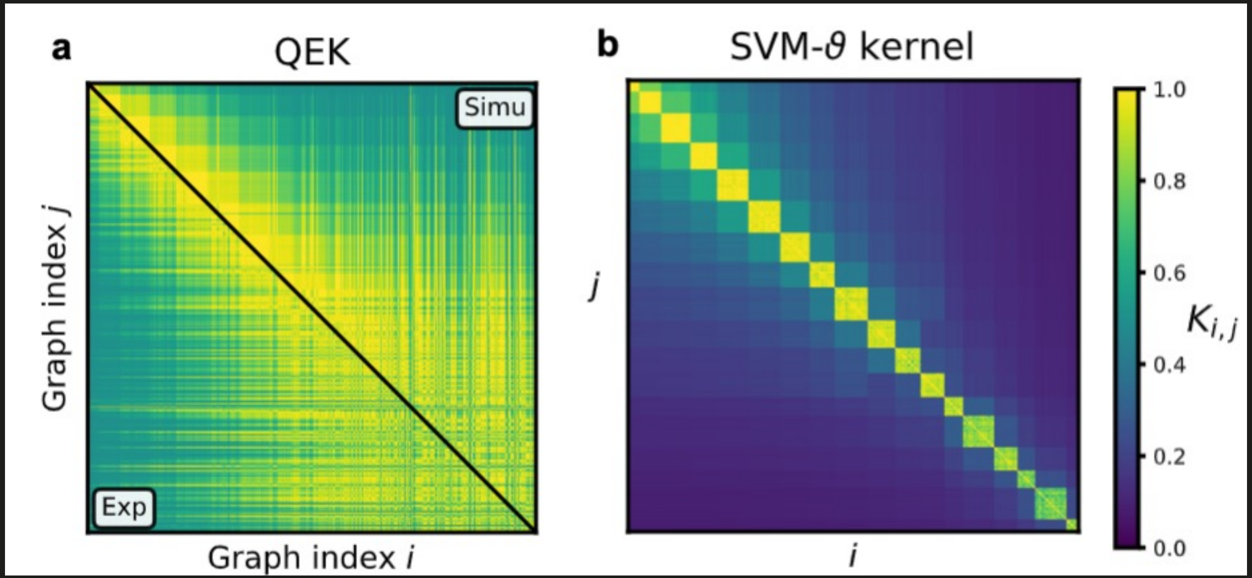


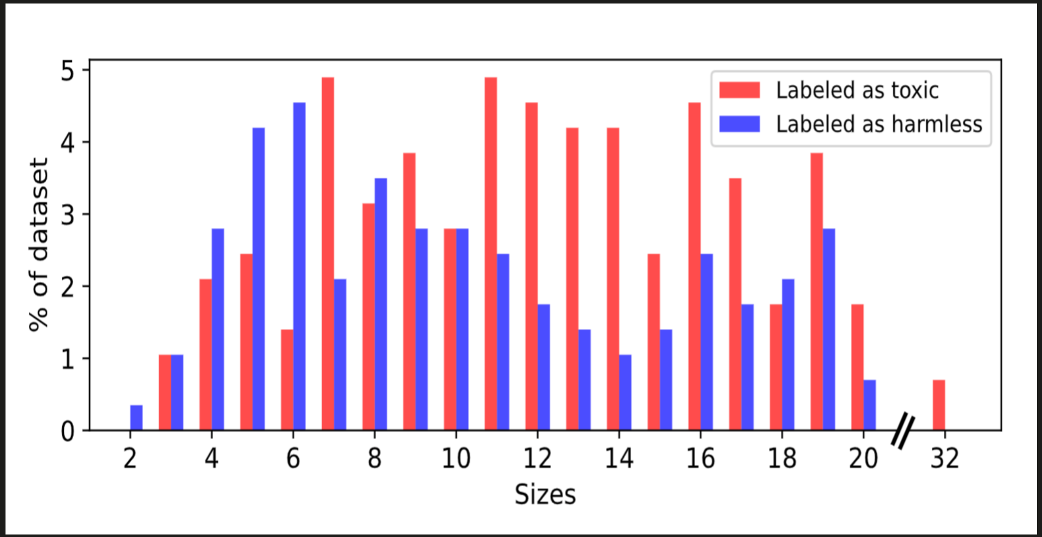


Experimental results on par with classical kernel

Classification results on par with the best classical kernels on this dataset

Kernel	F_1-score (%)
QEK	60.4 ± 5.1
SVM-ϑ	58.2 ± 5.5
Graphlet Sampling	56.9 ± 5.0
Random Walk	55.1 ± 6.9
Shortest Path	49.8 ± 6.0





Assessing the general potential of QEK

Strong evidence that the quantum feature map perceives data in an original way, which is hard to replicate using classical kernels

We use the recently introduced geometric difference [1].

$$g_{12} = \sqrt{||\sqrt{K_2}\,(K_1)^{-1}\,\sqrt{K_2}||_\infty}$$

- Small g_{12} (wrt sqrt size of the dataset) → no underlying function mapping the data to the targets such that K_1 outperforms K_2
- Large g_{12} (wrt sqrt size of the dataset) → such a map exists.

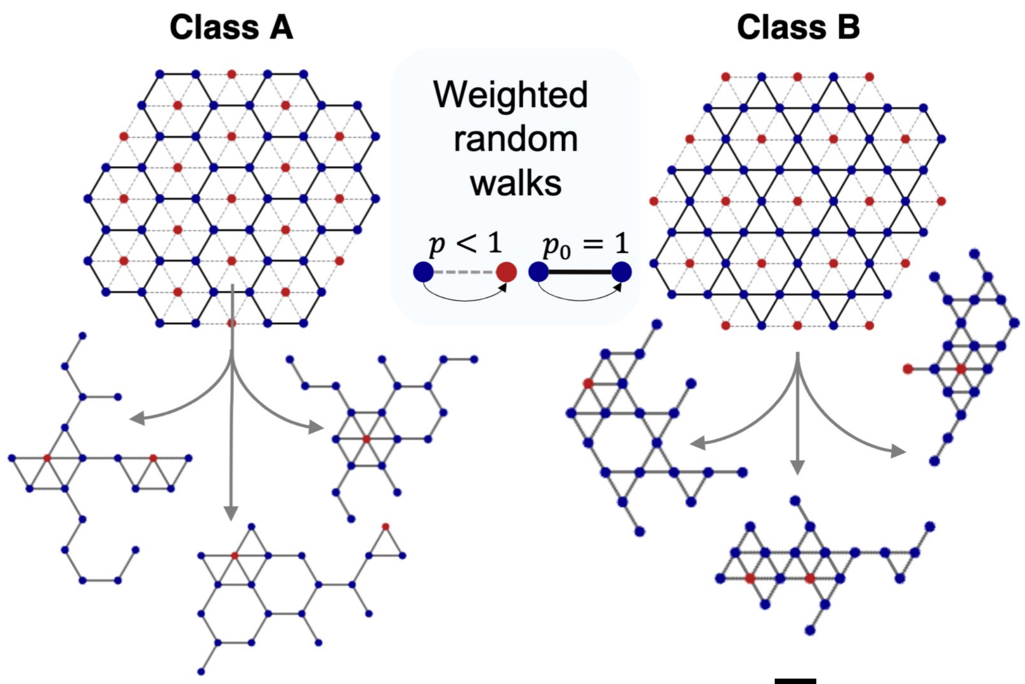
Geometric Difference w.r.t. QEK	
SVM-ϑ	10^3
Size	10^5
Graphlet Sampling	10^4
Random Walk	10^5
Shortest Path	10^5

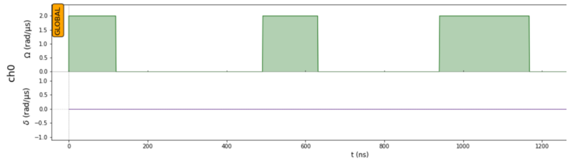
F_1-score gap (%) w.r.t. QEK (relabeled)	
SVM-ϑ	17.2%
Size	17.8%
Graphlet Sampling	20.1%
Random Walk	17.3%
Shortest Path	18.2%

[1] Huang, et al., Nature Communications 12, 1, 2631 (2021)

Performance of QEK

Synthetic dataset

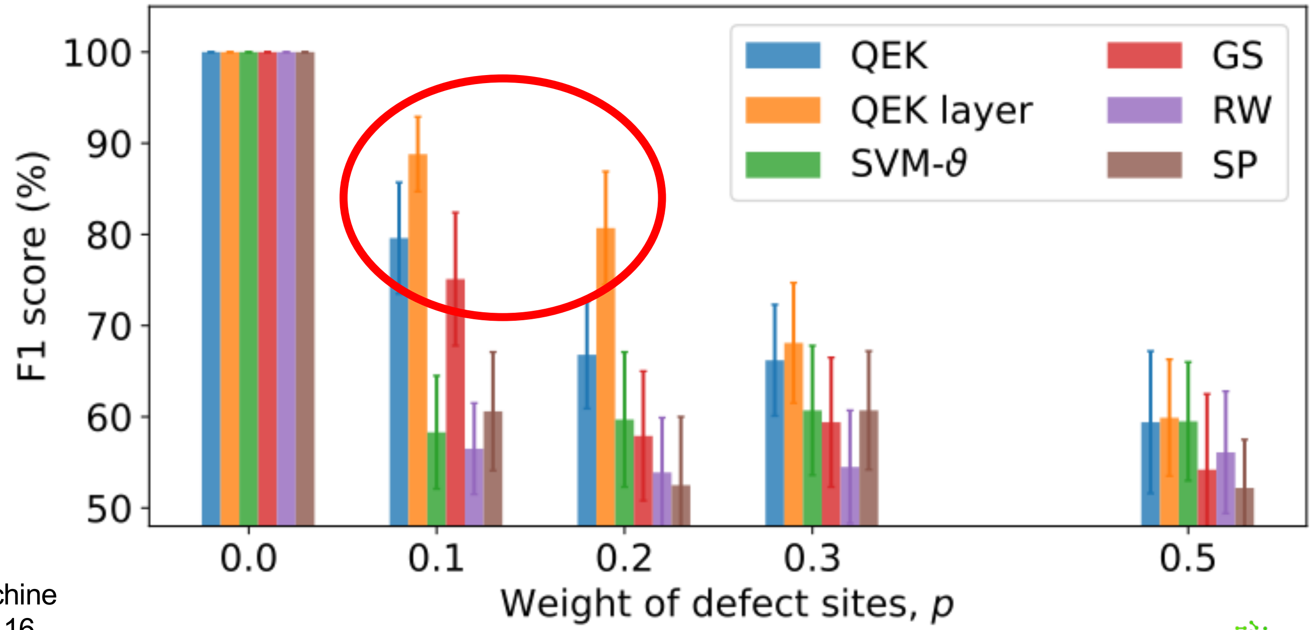




QEK (layer)

- $p = 0 \Longrightarrow A =$ Hexagon, $B =$ Kagome $\Longrightarrow$ Easy to distinguish
- $p \to 1 \Longrightarrow \mathrm{A} \approx B \Longrightarrow$ Impossible to distinguish

For $0.1 \leq p \leq 0.2 \Longrightarrow$ QEK (layer) performs better than class.



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Thanks for your attention

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