HIGH ROBUSTNESS QUANTUM RANDOM WALK SEARCH ALGORITHM WITH QUDIT HOUSEHOLDER TRAVERSING COIN

P. Danev ***H. Tonchev***

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Contents

INTRODUCTION

Discrete time quantum random walk search

Discrete time quantum random walk search algorithm (DTQRWS)

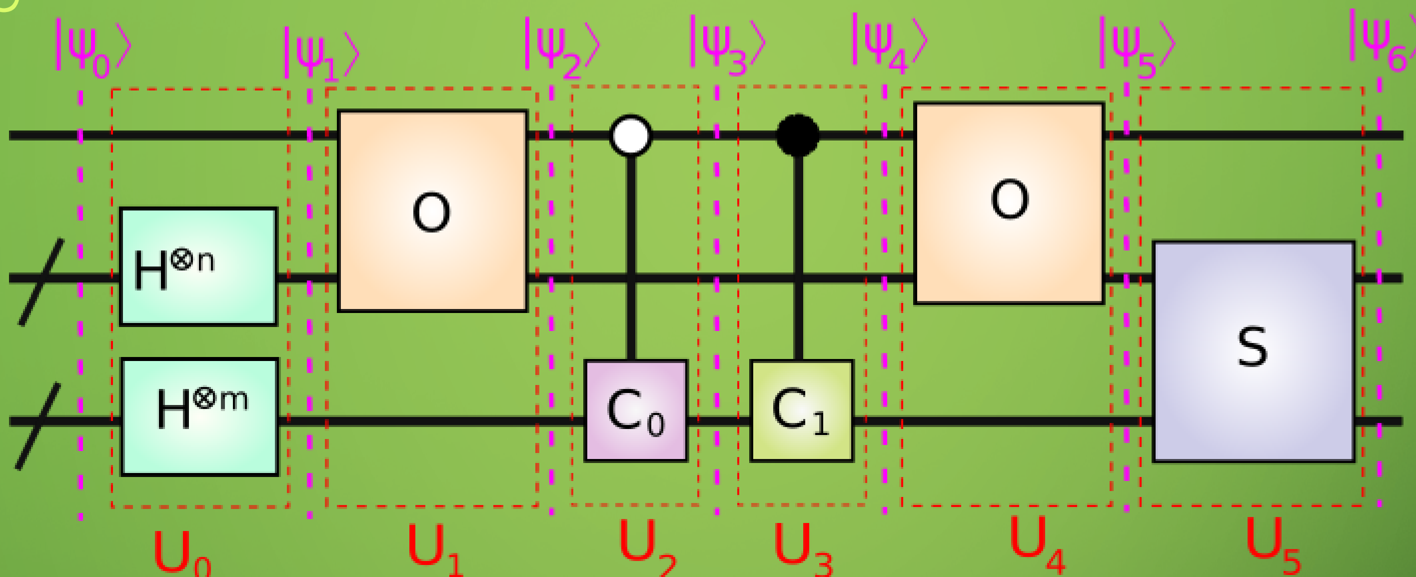
- Uses quantum walk to find searched element in unordered database;
- Quadratically faster than the corresponding classical search algorithms.

Quantum random walk algorithm is large category of quantum algorithms. It is used in variety of quantum information topics:

- quantum simulations;
- quantum algorithms;
- quantum cryptography.

DTQRWS	Grover search algorithm
Search in arbitrary topology	Search only in linear database
Needs more qubits	Needs less qubits
Double Oracle calls	Less Oracle calls

QUANTUM CIRCUIT COMPONENTS



$$|\psi_k\rangle = |con_k, x_k, c_k\rangle = |con_k\rangle \otimes |\, x_k\rangle \otimes |c_k\rangle$$

Dim[$|con_k\rangle$] = 2 Dim[$|x_k\rangle$] = 2^m Dim[$|c_k\rangle$] = m

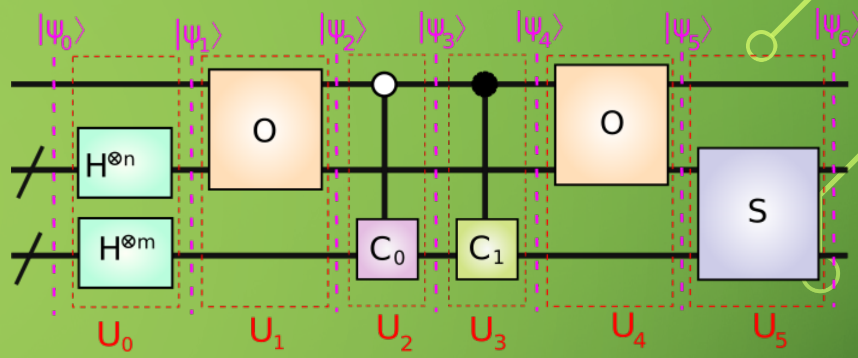
$$|\psi_{k+1}\rangle = U_k|\psi_k\rangle \xrightarrow{\text{yields}} |\psi_6\rangle = U_5U_4U_3U_2U_1U_0|\psi_0\rangle$$

Initial State:

$$|\psi_0\rangle = |0,0,0\rangle$$

$$U_0 = \begin{cases} \hat{I}_2 \otimes \mathrm{H}^{\otimes n} \otimes \mathrm{H}^{\otimes m} & \textit{works on when coin is power of 2} \\ \hat{I}_2 \otimes \mathrm{F}_{2^\wedge m} \otimes \mathrm{F}_m & \textit{works with arbitrary coin size} \end{cases}$$

1) Applying Hadamard Gates:



$$|\psi_0\rangle = |0,0,0\rangle$$

$$w = e^{-2\pi i/m}$$

$$F = \frac{1}{\sqrt{m}}\begin{pmatrix} w^{0*0} & w^{0*1} & \cdots & w^{0*(m-1)} \\ w^{1*0} & w^{1*1} & \cdots & w^{1*(m-1)} \\ \vdots & \vdots & \ddots & \vdots \\ w^{(m-1)*0} & w^{(m-1)*1} & \cdots & w^{(m-1)*(m-1)} \end{pmatrix}$$

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$\hat{I}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$|\psi_1\rangle = U_0|\psi_0\rangle$$

$$|\psi_1\rangle = \left|0, \frac{1}{\sqrt{2^m}}\sum_{j=0}^{2^m-1}|j\rangle, \frac{1}{\sqrt{m}}\sum_{j=0}^{m-1}|j\rangle\right\rangle = \frac{1}{\sqrt{d}}|0\rangle \otimes \sum_{j=0}^{m2^m-1}|j\rangle$$

2) Applying First Oracle

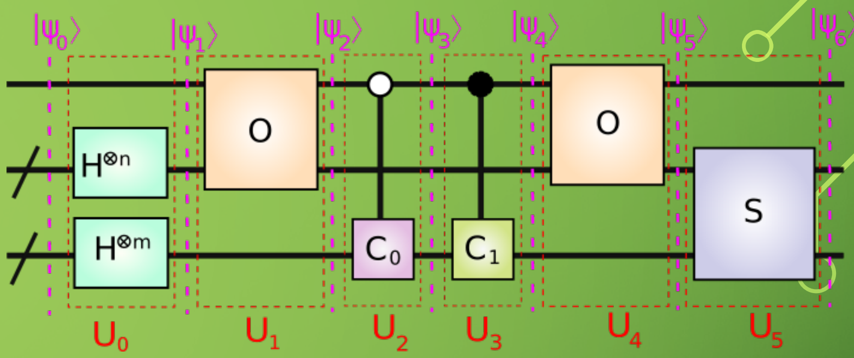
The Oracle marks all solutions, if solutions are $\{h_1, \ldots, h_\lambda\}$:

$$\hat{O} = \hat{I}_{2^{m+1}} - \sum_{i=1}^{\lambda}(|h_i\rangle\langle h_i| + |h_i + 2^m\rangle\langle h_i + 2^m|) + \sum_{i=1}^{\lambda}(|h_i + 2^m\rangle\langle h_i| + |h_i\rangle\langle h_i + 2^m|)$$

$$|\psi_1\rangle = \frac{1}{\sqrt{d}}(0,1) \otimes \sum_{j=0}^{m2^m-1}|j\rangle$$

$$U_1 = \hat{O} \otimes \hat{I}_m$$

$$|\psi_2\rangle = U_1|\psi_1\rangle$$



$$|\psi_2\rangle = \frac{1}{\sqrt{m2^m}}\Big((0,1) \otimes \big(\sum_{j=0}^{d*2^\wedge d-1}|j\rangle - \sum_{i=1}^{\lambda}|h_i\rangle\big) + (1,0) \otimes \big(\sum_{i=1}^{\lambda}|h_i\rangle\big)\Big) \otimes \big(\sum_{j=0}^{m-1}|j\rangle\big)$$

3) Applying Traversing Coin

$$U_2 = \begin{pmatrix} \hat{I}_{m2^m} & \hat{0}_{m2^m} \\ \hat{0}_{m2^m} & \hat{I}_{2^m} \otimes C_0 \end{pmatrix}$$

$$|\psi_3\rangle = U_2|\psi_2\rangle$$

$$C_0(\phi,\chi,\zeta) = e^{i\zeta}\big(I - (1 - e^{i\phi})|\chi\rangle\langle\chi|\big)$$

$$|\chi\rangle = \frac{1}{\sqrt{N}}\sum_{j=0}^{N-1}|j\rangle$$

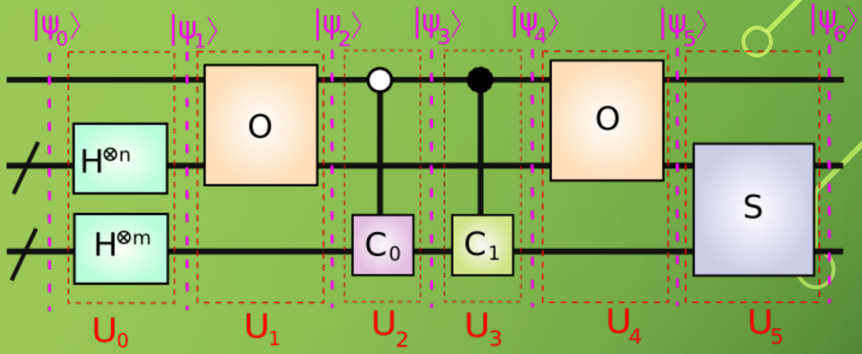
$$\zeta = -2\,\phi + 3\pi + \alpha\sin(2\phi)$$

4) Applying Marking Coin

$$U_3 = \begin{pmatrix} \hat{I}_{2^m} \otimes C_1 & \hat{0}_{m2^m} \\ \hat{0}_{m2^m} & \hat{I}_{m2^m} \end{pmatrix}$$

$$|\psi_3\rangle = U_2|\psi_2\rangle$$

$$C_1 = -\hat{I}_2$$



5) Applying Second Oracle

$U_4 = U_1$

$|\psi_5\rangle = U_4|\psi_4\rangle$

6) Applying Shift Operator

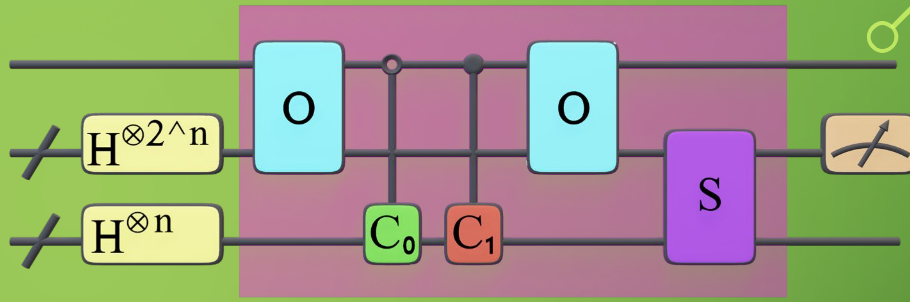
$$S = \sum_{d=0}^{m-1} \sum_{x=0}^{2^m-1} |x^d, d\rangle \langle x, d|$$

Where x^d is the vector x with d^{th} bit flipped

$U_5 = \hat{I}_2 \otimes S$

$|\psi_6\rangle = U_5|\psi_5\rangle$

7) Measurement of the node register



$$\rho_{\psi_k} = |\psi_k\rangle\langle\psi_k| = |con_k, x_k, c_k\rangle\langle con_k, x_k, c_k|$$

If ρ_{ψ_k} is separatable:

$$\rho_{\psi_k} = |con_k, x_k, c_k\rangle\langle con_k, x_k, c_k|$$
$$= |con_k\rangle\langle con_k| \otimes |x_k\rangle\langle x_k| \otimes |c_k\rangle\langle c_k| = \rho_{con_k} \otimes \rho_{x_k} \otimes \rho_{c_k}$$

$$Tr_{\rho_{con_k}} Tr_{\rho_{c_k}} [\rho_{\psi_k}] = \sum_i \langle i|\rho_{con_k}|i\rangle \otimes \rho_{x_k} \otimes \sum_j \langle j|\rho_{c_k}|j\rangle = \rho_{x_k}$$

When ρ_{ψ_k} is not separatable:

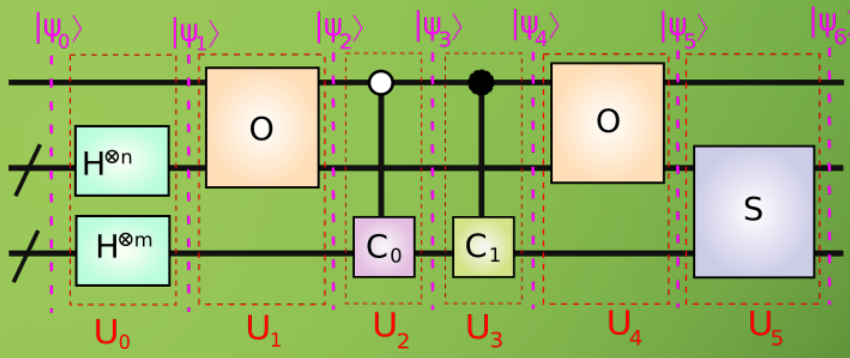
$$Tr_{\rho_{con_k}}[\rho_{\psi_k}] = \sum_j \left(\langle j|_{\rho_{con_k}} \otimes \hat{I}_{\rho_{x_k}\otimes\rho_{c_k}}\right) \rho_{\psi_k} \left(|j\rangle_{\rho_{con_k}} \otimes \hat{I}_{\rho_{x_k}\otimes\rho_{c_k}}\right)$$

$$[\rho_{x_k}] = Tr_{\rho_{c_k}}\left[Tr_{\rho_{con_k}}[\rho_{\psi_k}]\right]$$
$$= \sum_j \left(\hat{I}_{\rho_{x_k}} \otimes \langle j|_{\rho_{c_k}}\right) Tr_{\rho_{con_k}}[\rho_{\psi_k}] \left(\hat{I}_{\rho_{x_k}} \otimes |j\rangle_{\rho_{c_k}}\right)$$

M$[\rho_{x_k}]$ - измерване на регистъра на върховете

EXAMPLE

Example For Coin Size 2, solutions {2}, for walk coin is used Hadamard gate and for marking coin is used -I



$$\hat{I}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad H= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$|\psi_0\rangle = (1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0)^T$$

$$U_0 = \hat{I}_2 \otimes (\mathrm{H} \otimes \mathrm{H}) \otimes \mathrm{H}$$

$$|\psi_1\rangle = 1/\sqrt{8}(1,1,1,1,1,1,1,1,0,0,0,0,0,0,0,0)^T$$

$$U_1 = O \otimes \hat{I}_2$$

$$|\psi_2\rangle = 1/\sqrt{8}(1,1,0,01,1,1,1,0,0,1,1,0,0,0,0)^T$$

$$U_2 = \mathrm{Diag}[\hat{I}_8, \hat{I}_4 \otimes C_0]$$

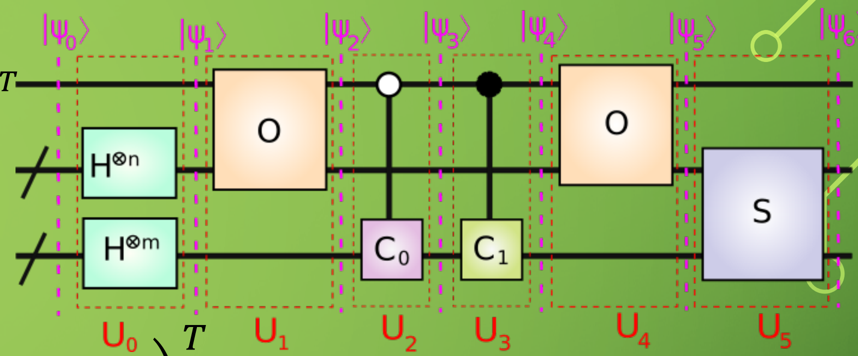
$$|\psi_3\rangle = \left(\frac{1}{2},0,0,0,\frac{1}{2},0,\frac{1}{2},0,0,0,\frac{1}{\sqrt{8}},\frac{1}{\sqrt{8}},0,0,0,0\right)^T$$

$$O= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\hat{I}_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$|\psi_3\rangle = \left(\frac{1}{2},0,0,0,\frac{1}{2},0,\frac{1}{2},0,0,0,\frac{1}{\sqrt{8}},\frac{1}{\sqrt{8}},0,0,0,0\right)^T$$

$$U_3 = \text{Diag}[\hat{I}_4 \otimes C_1,\ \hat{I}_8]$$



$$|\psi_4\rangle = \left(\frac{1}{2},0,0,0,\frac{1}{2},0,\frac{1}{2},0,0,0,\frac{-1}{\sqrt{8}},\frac{-1}{\sqrt{8}},0,0,0,0\right)^T$$

$$C_1 = -\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

$$U_4 = O \otimes \hat{I}_2$$

$$|\psi_5\rangle = \left(\frac{1}{2},0,\frac{-1}{\sqrt{8}},\frac{-1}{\sqrt{8}},\frac{1}{2},0,\frac{1}{2},0,0,0,0,0,0,0,0,0\right)^T$$

$$U_5 = \hat{I}_2 \otimes S$$

$$S=\begin{pmatrix}0&0&0&0&1&0&0&0\\0&0&0&1&0&0&0&0\\0&0&0&0&0&0&1&0\\0&1&0&0&0&0&0&0\\1&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&1\\0&0&1&0&0&0&0&0\\0&0&0&0&0&1&0&0\end{pmatrix}$$

$$|\psi_6\rangle = \left(\frac{1}{2},\frac{-1}{\sqrt{8}},\frac{1}{2},0,\frac{1}{2},0,\frac{-1}{\sqrt{8}},0,0,0,0,0,0,0,0,0\right)^T$$

$$\text{M}[|\psi_6\rangle] = \left(\frac{3}{8},\frac{2}{8},\frac{2}{8},\frac{1}{8}\right)$$

ROBUSTNESS OF QRWS WITH MODIFIED COIN

Modification of the walk coin

We study the following walk coin:

$$C_0(\phi,\chi,\zeta) = \underbrace{e^{i\zeta}}_{Phase\ gate} \times \underbrace{\left(I-(1-e^{i\phi})|\chi\rangle\langle\chi|\right)}_{Generalized\ Householder\ reflection}$$

Both Generalized Householder reflection and phase gate can be done efficiently in some physical Quantum circuit implementations like the ion traps.

To have equal probability to go at each direction χ must be equal weight superposition of the basis vectors $|j\rangle$

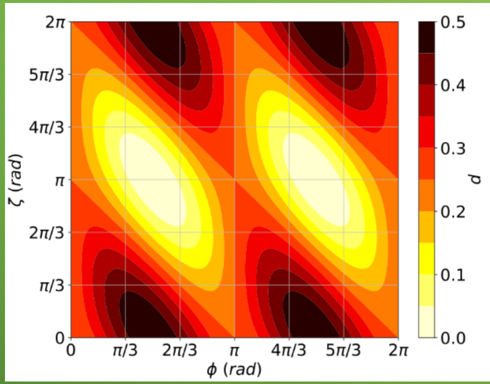
$$|\chi\rangle = \frac{1}{\sqrt{m_n}} \sum_{j=0}^{m_n-1} |j\rangle$$

The probability to find solution $p = p(\zeta, \phi, \mathrm{n})$ depends on ζ, ϕ and coin register size n.

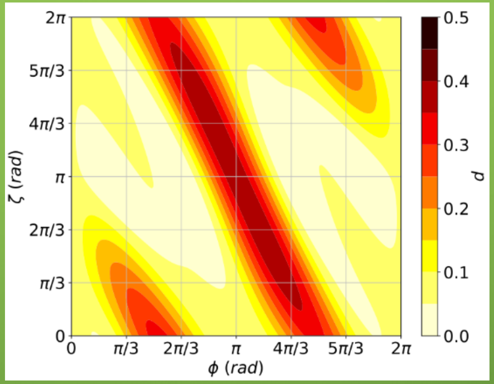
Monte Carlo simulations of the algorithm

MC simulations of p(ζ, ϕ) of QRWS for Hypercube
In each run n is fixed and for $\zeta, \phi \in [0, 2\pi)$ are taken random values

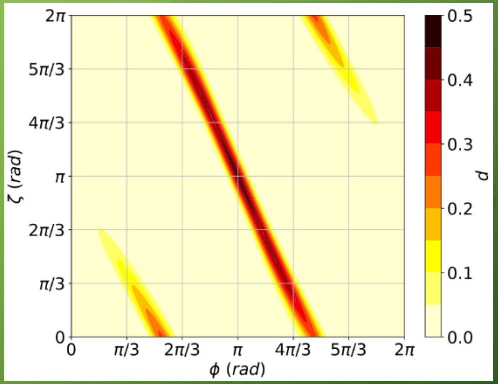
One qubit coin



Two qubit coin



Three qubit coin



There exist connected areas in (ϕ, ζ) plane with high probability to find solution!

Robustness of $p(\zeta,\phi)$

In order to make QRWS more robust to change in the phases, we search for areas in the plane defined by (ϕ, ζ) that give high probability to find solution when one or both of the parameters vary:

$$p(\phi \in (\phi_{max} - \varepsilon, \phi_{max} + \varepsilon)) \cong p_{max} = p\ (\phi_{max})$$

In our case p can be expressed as function of just one of the phases:

$$\zeta = \zeta(\phi) \Longrightarrow p(\zeta(\phi), \phi\ , \mathrm{n} = \mathrm{const}) \longrightarrow p(\phi)$$

Different functions $\zeta(\phi)$ were fitted to MC data points, to find the one that makes the algorithm as robust as possible

Note: For Grover coin both phases ϕ and ζ are equal to π, and $|\chi\rangle$ is equal weight superposition

Improvement of algorithm's stability

Examples for linear functions:

Best linear approximation:
$\zeta = -2\,\phi + 3\pi$

ζ =const
$\zeta = \pi$

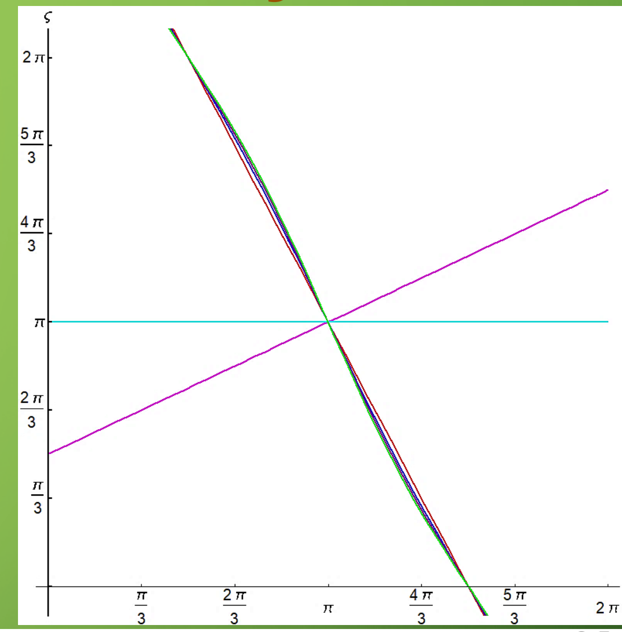
Nonlinear functions:

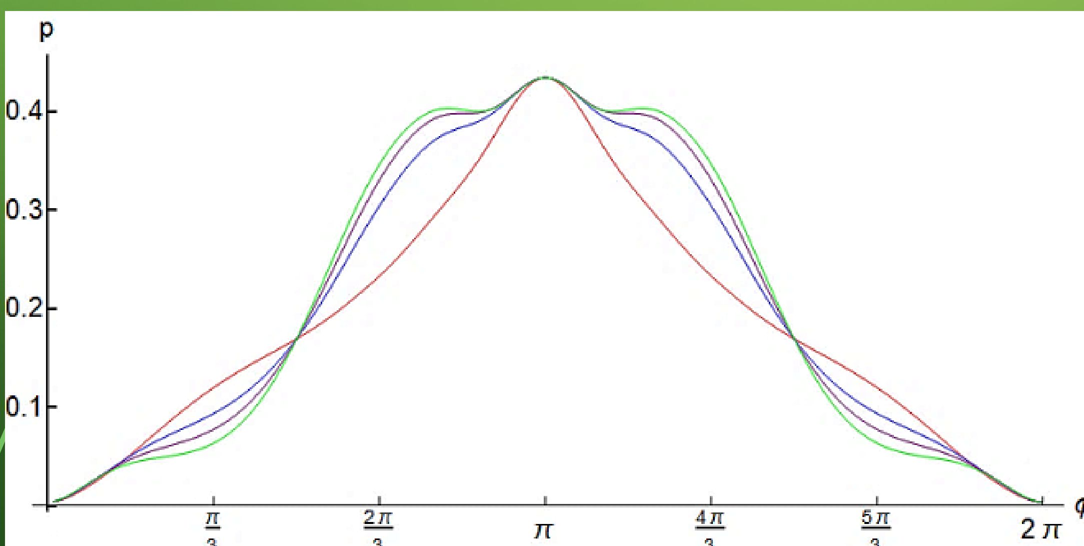
Almost linear:
$\zeta = -2\,\phi + 3\pi + \alpha \sin(2\phi)$

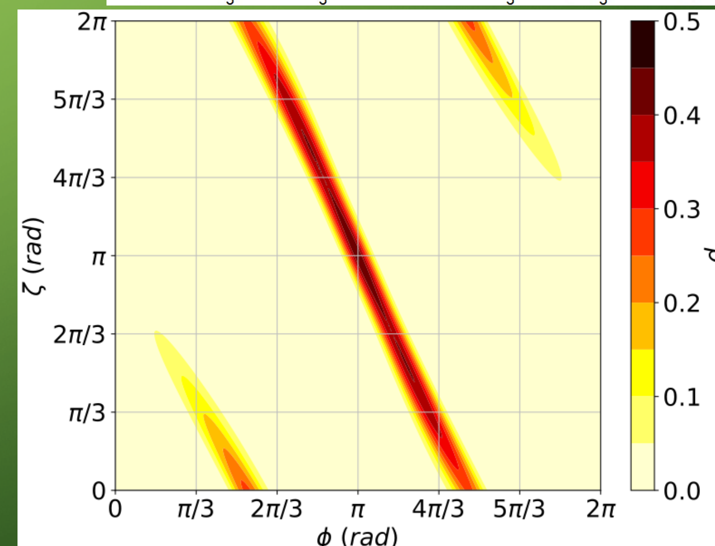
$\alpha = 0.204$

$\alpha = 1/(2\pi)$

$\alpha = 1/(3\pi)$







Coin size $n = 3$

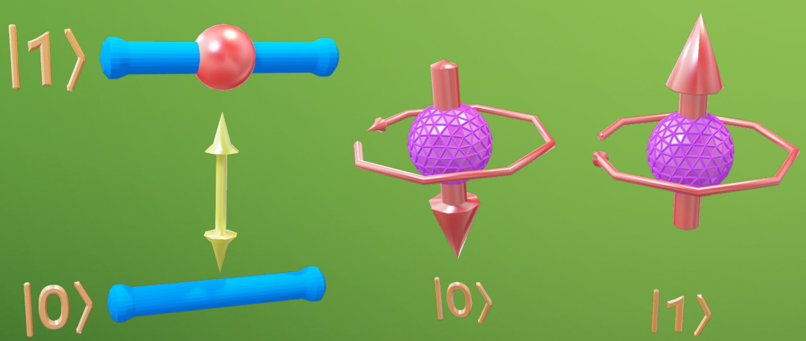
ROBUSTNESS OF QRWS WITH QUDIT COIN

Qubits vs Qudits

One qubit can be any two level quantum system:

1. Levels of electron in ions;
2. Spins of quantum dots;
3. Others.

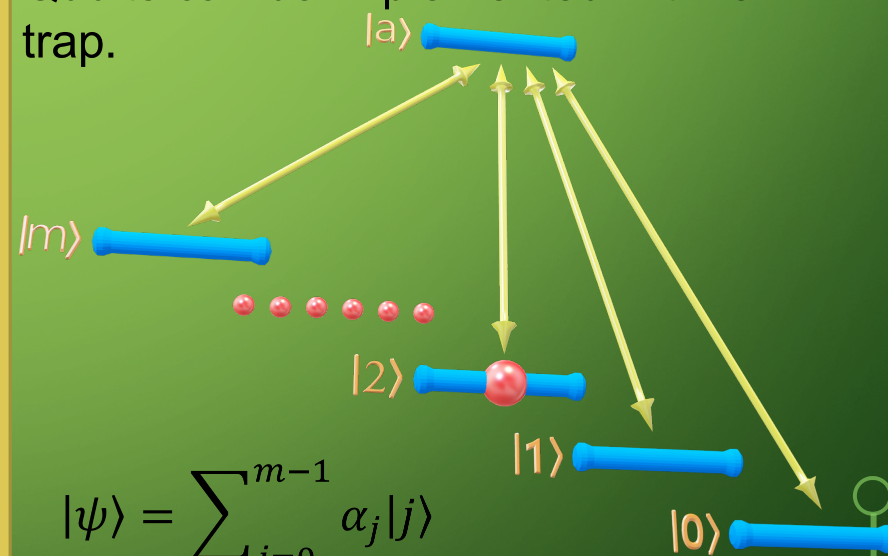
Qubit states $|\psi\rangle = \alpha_0\ |0\rangle + \alpha_1\ |1\rangle$



Qubit coin register can have only power of two number of states – 2; 4; 8; 16; 32…

$m = 2^k$ k= $Integer$

Qudits can be implemented by using any system with d levels, e.g. hyperfine states of one split level due to external electric or magnetic field. All those levels should be metastable. Qudits can be implemented with ion trap.



$$|\psi\rangle = \sum_{j=0}^{m-1} \alpha_j |j\rangle$$

Often transitions between levels are made by using ancilla state.

$m = Integer$

Advantages of using Qudits

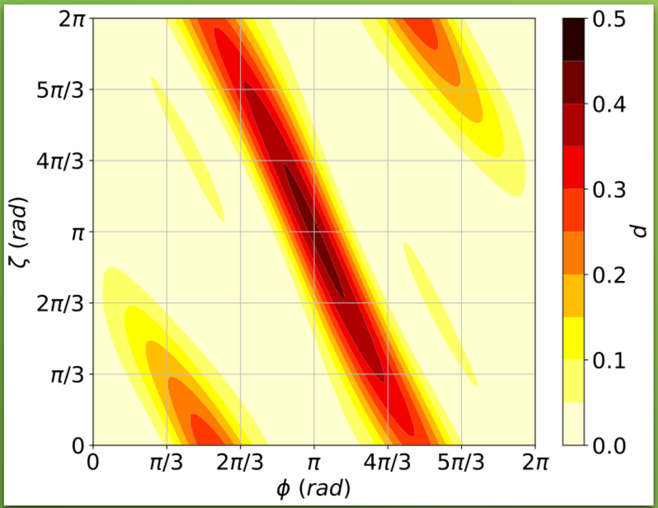
Using qudits instead of qubits gives various advantages for the quantum algorithms:

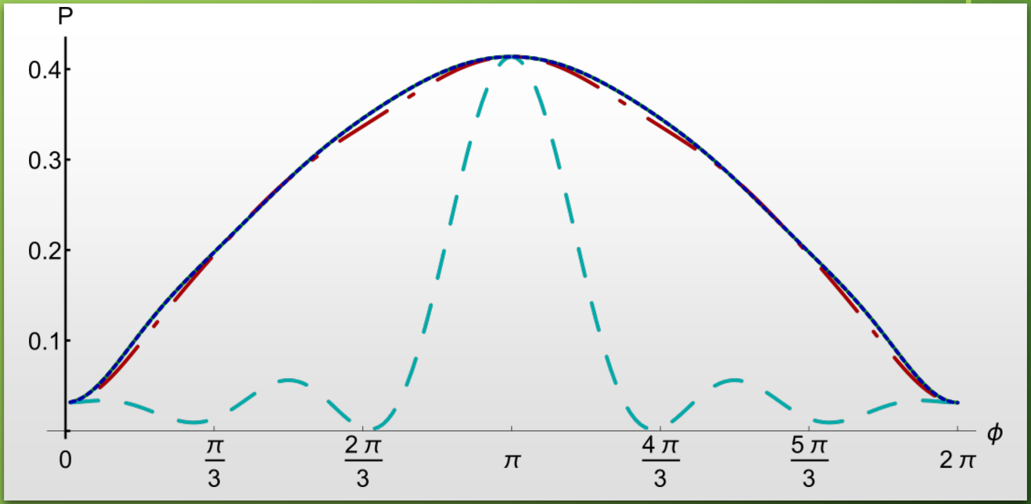
- They are more robust against noise and give more dependable quantum computations;
- The coin can have arbitrary dimension not only power of 2;
  - Allow us to make much more reliable extrapolations for quantum random walk search algorithm's stability for larger coin sizes;
- Increasing the size of the coin state space;
- More efficient construction of various quantum gates;
- New quantum error correction protocols.

QRWS with Qudit coin

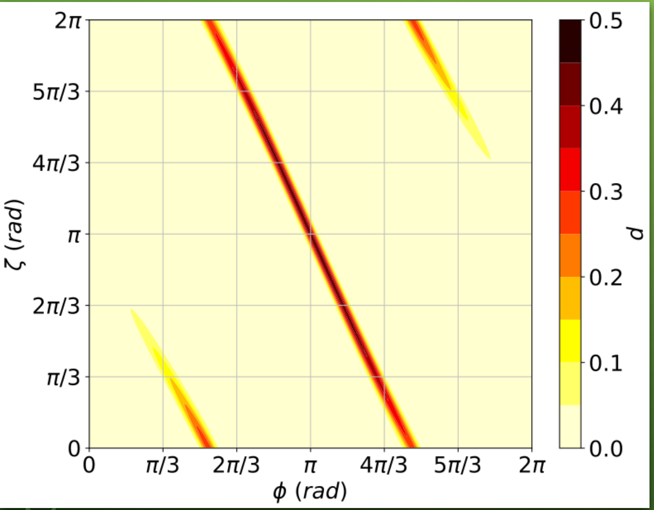
MC simulations of the algorithm with different qudit size

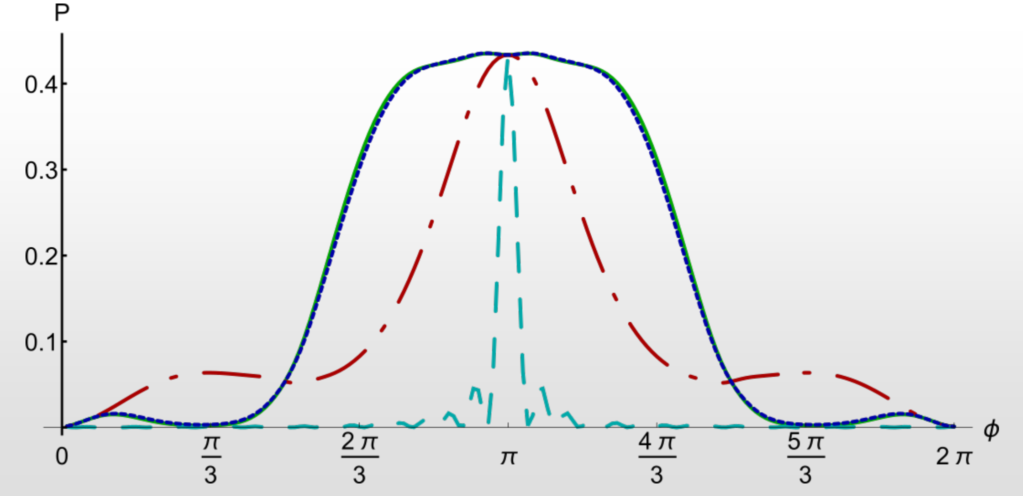
m=5



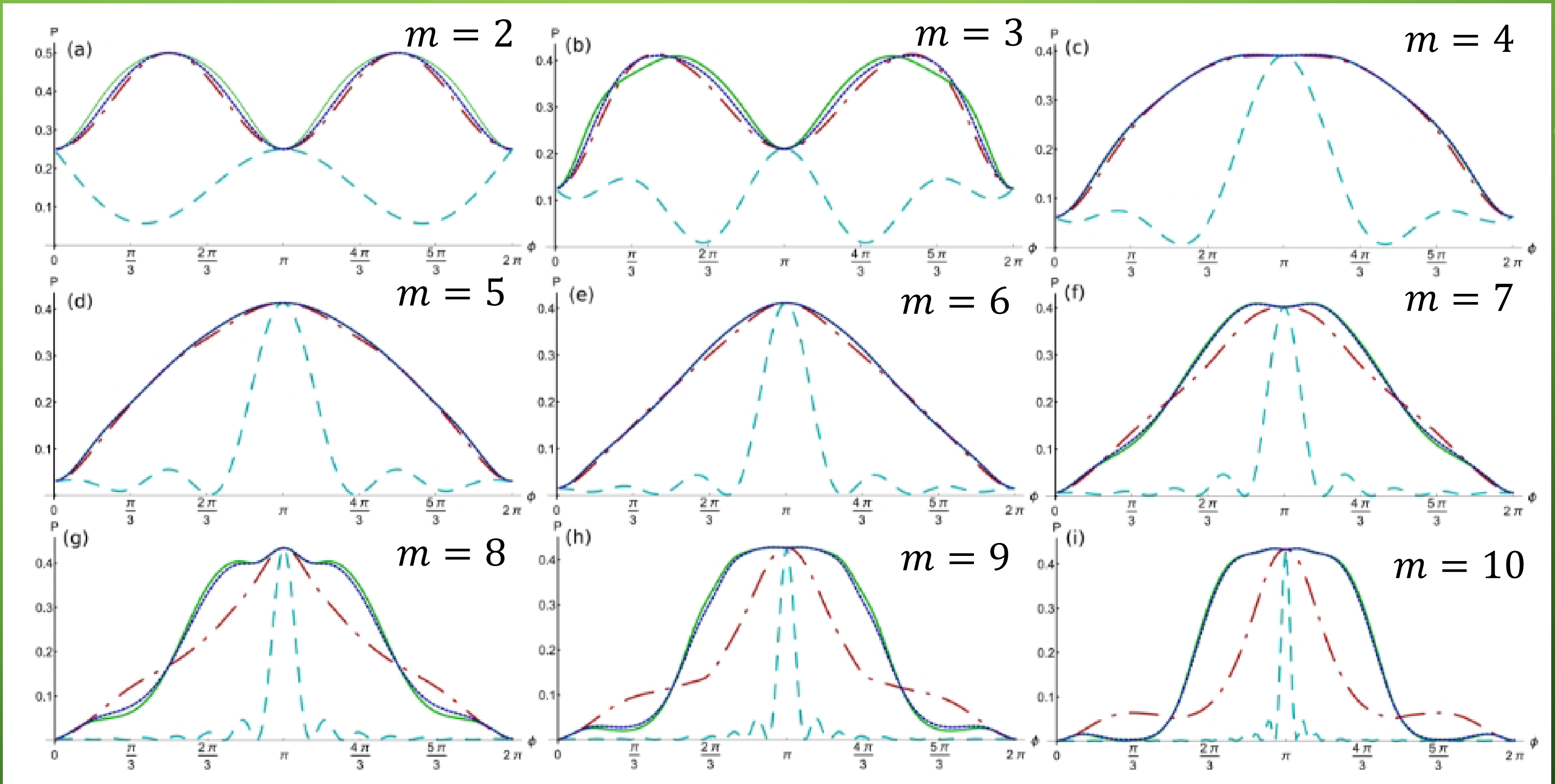


m=10





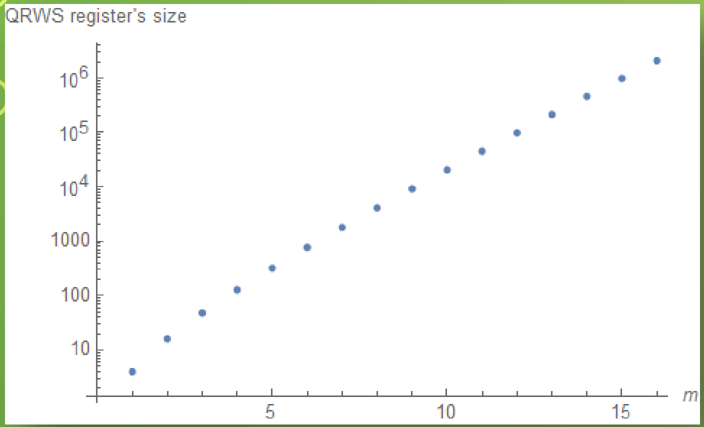
MC simulations with different qudit size



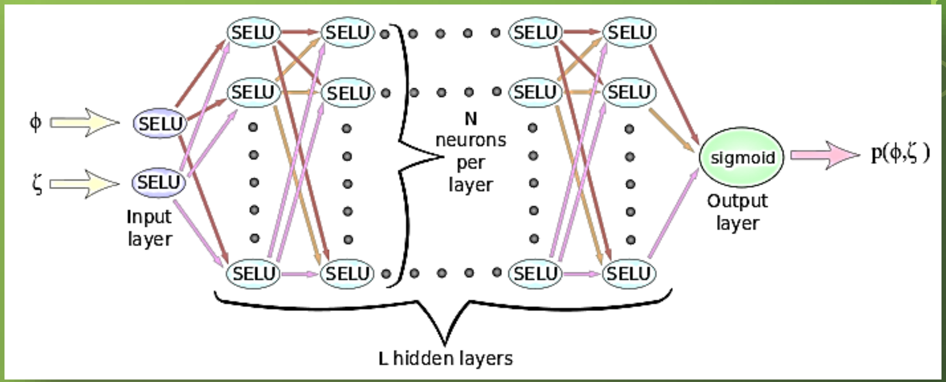
- For $m \geq 3$ central plateau area becomes more wide for higher coin size;
- The optimized coins with parameter relations

$\zeta = -2\,\phi + 3\pi + \alpha \sin(2\phi)$ give more robust algorithm.

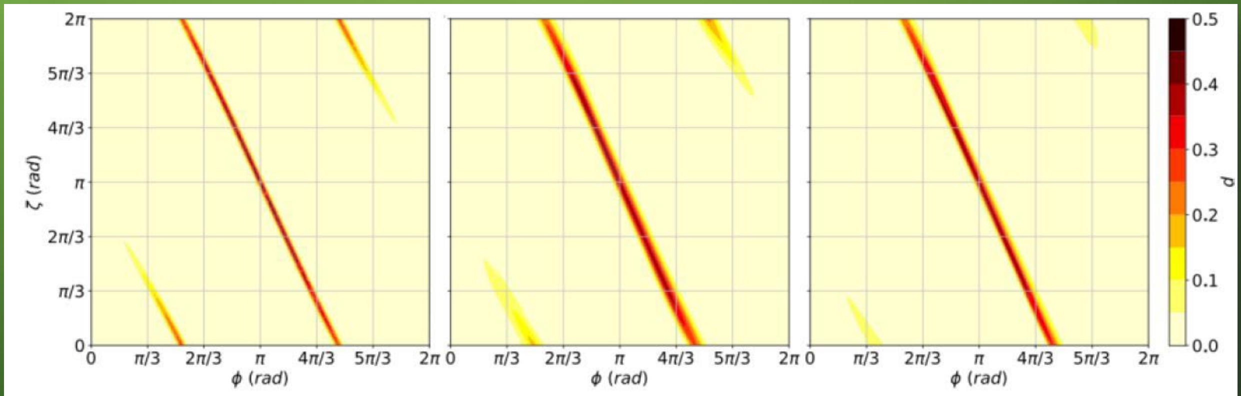
Machine learning assisted optimization



Register scaling



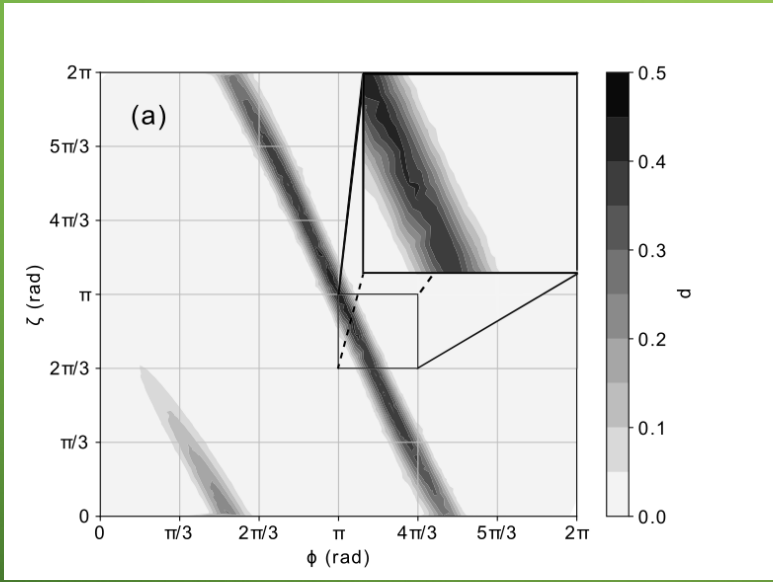
Dense feedforward DNN used for predictions



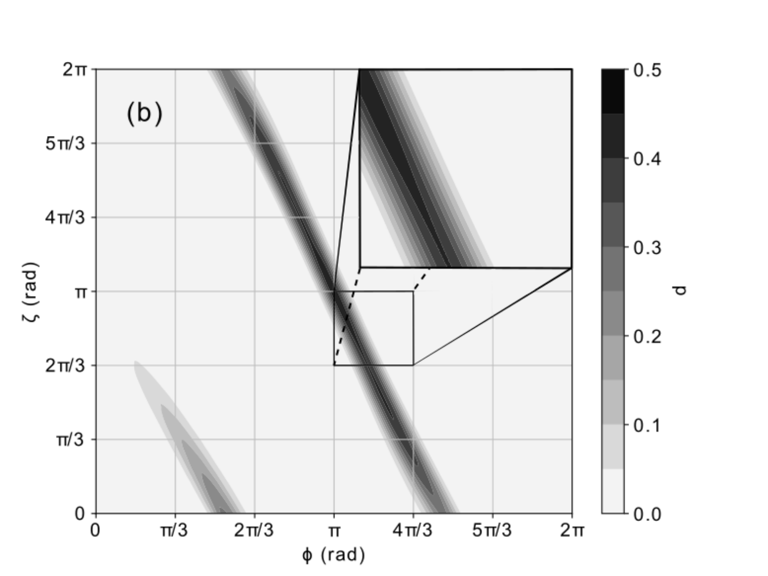
MC, $m = 11$ ML, $m = 11$ ML, $m = 16$

Augmenting data by machine learning

Interpolation of data within the training area



MC, $m = 8$



ML, $m = 8$

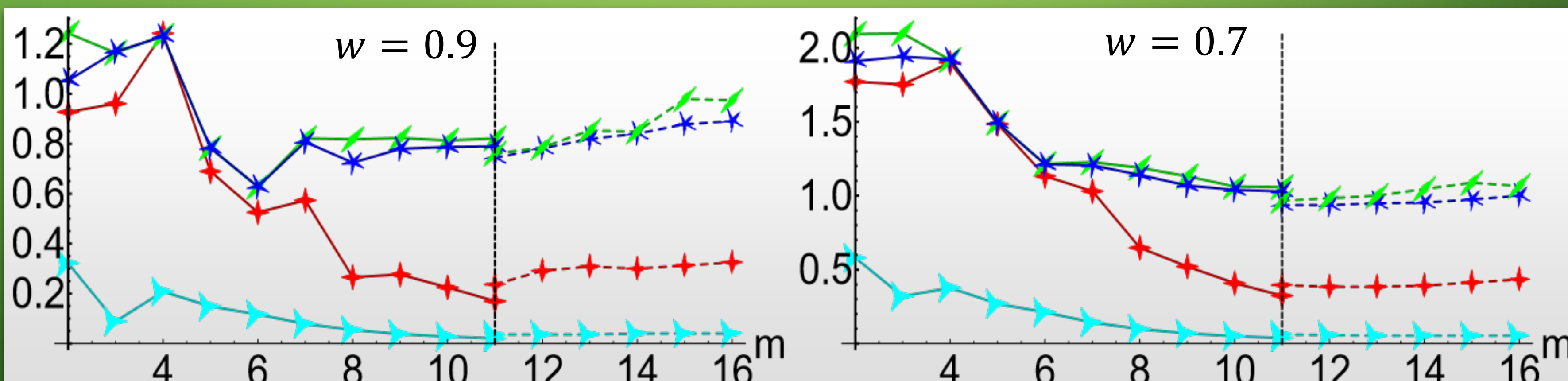
Stability interval for different $\zeta(\phi)$

Interval ε depends on the function that is used and the acceptable probability $w \cdot p_{max}$

$$p(\phi \in (\phi_{max} - \varepsilon, \phi_{max} + \varepsilon)) \cong w \cdot p_{max}$$

$$\Longrightarrow \varepsilon = \varepsilon(m, \alpha, w)$$

Interval ε for different functions: found from Monte Carlo data for coin size 2-11 and by DNN – for coin size 11-16. Best value for $\alpha = \alpha_{ML}(m)$ is found by ML. When for $\zeta(\phi)$ is used nonlinear function, ε deceases slower with increasing the coin size.



$\zeta = -2\,\phi + 3\pi + \alpha \sin(2\phi)$

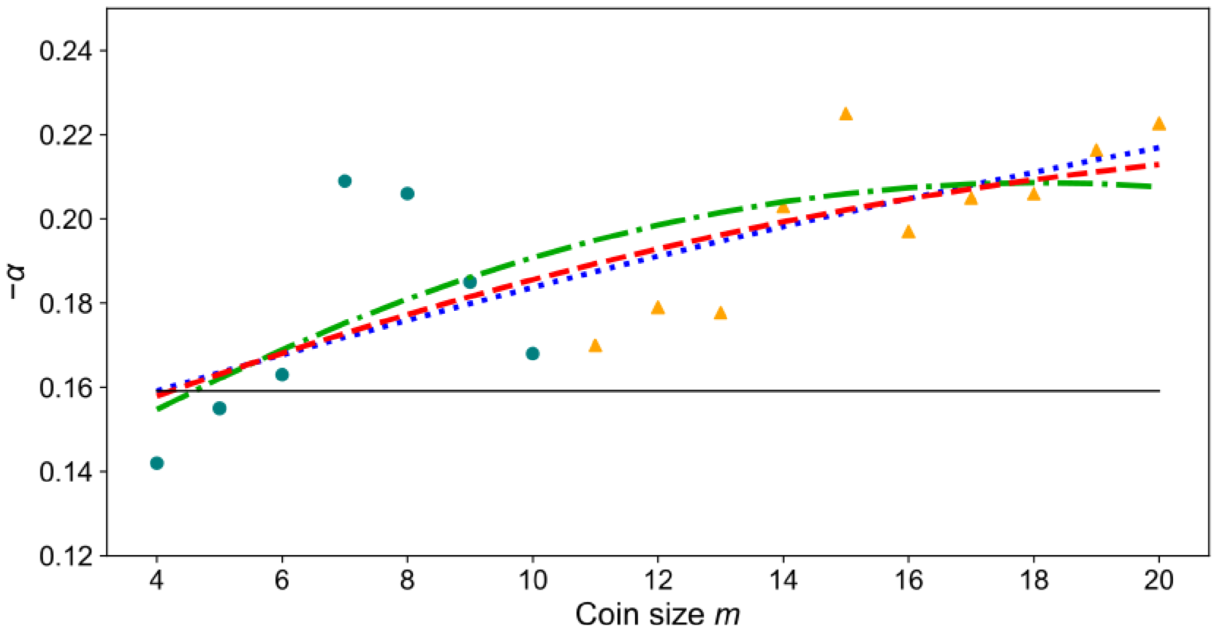
$\alpha = \alpha_{ML}(m)$

$\zeta = -2\,\phi + 3\pi$

$\alpha = 1/(2\pi)$

$\zeta = \pi$

Study of the nonlinear parameter α behavior



$\zeta = -2\,\phi + 3\pi + \alpha \sin(2\phi)$

● – from simulations
▲ – from ML

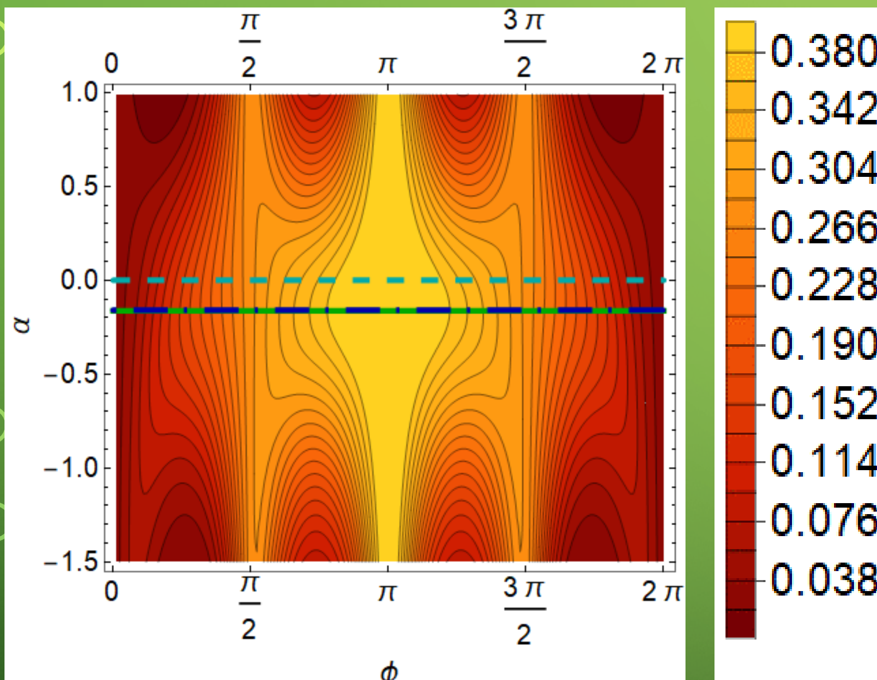
$\alpha(m) = am^2 + bm + c$	a	b	c
$\alpha_1(m)$	4.85×10^{-5}	-4.78×10^{-3}	-1.41×10^{-1}
$\alpha_2(m)$	2.71×10^{-4}	-9.82×10^{-3}	-1.20×10^{-1}
$\alpha_3(m)$	1.17×10^{-4}	-6.24×10^{-3}	-1.35×10^{-1}

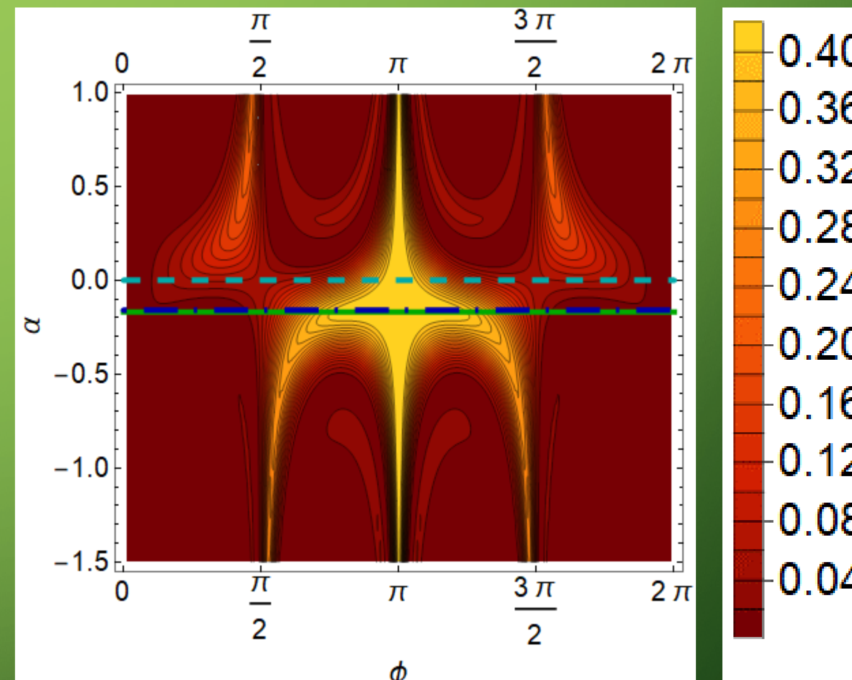
Robustness analysis including all coin parameters

Most promising results were achieved with relation:

$$\zeta = -2\,\phi + 3\pi + \alpha \sin(2\phi)$$
$$\Rightarrow p = p(\zeta(\alpha,\phi),\phi) = p(\alpha,\phi)$$

Probability to find solution $p = p(\alpha,\phi)$ for coin size 5 and 10





$\zeta = -2\,\phi + 3\pi$

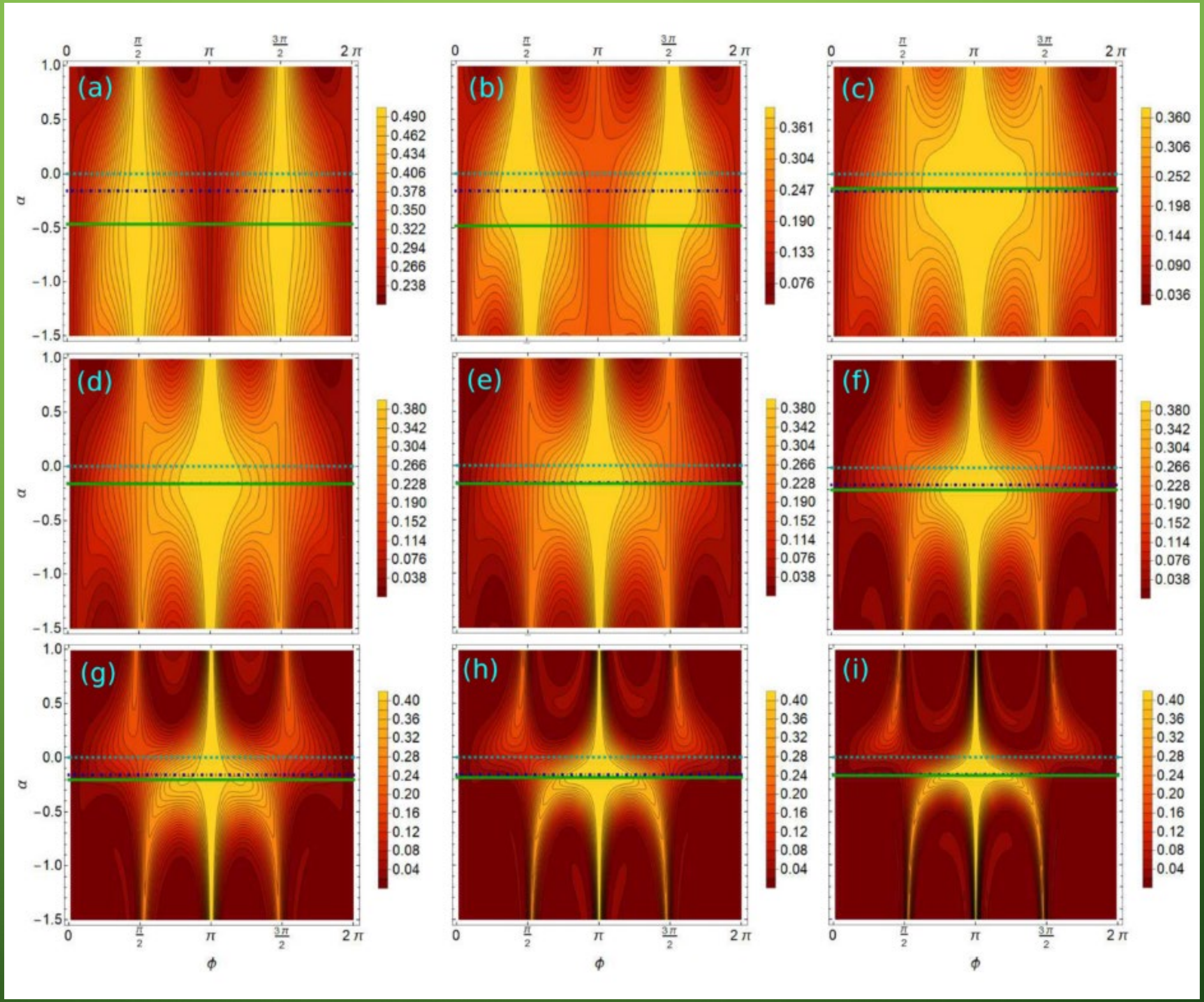
$\zeta = -2\,\phi + 3\pi + \alpha \sin(2\phi)$

$\alpha = 1/(2\pi)$

$\alpha = \alpha_{ML}(m)$

Stability area in (ϕ, α) plane

$(2 \leq m \leq 10)$

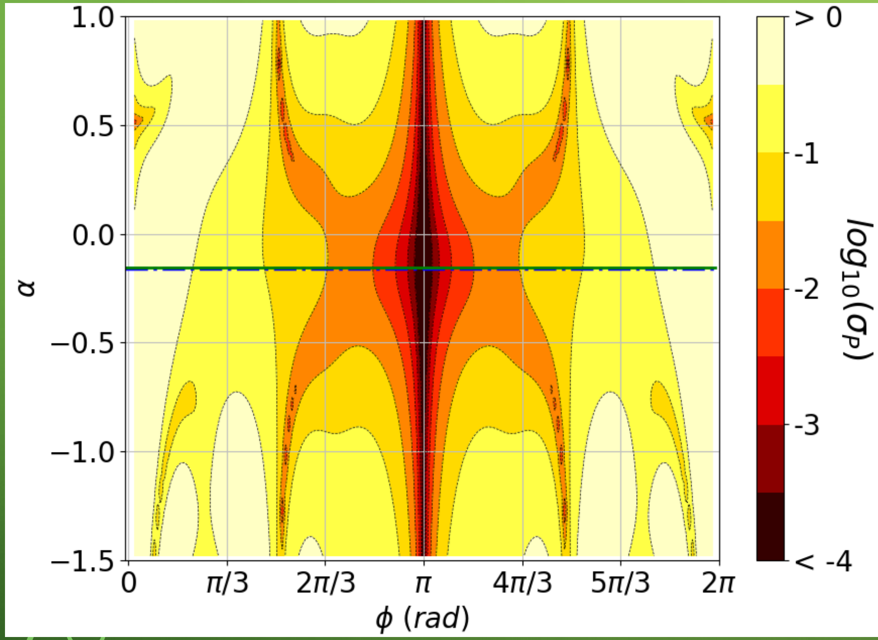


Root-mean-square deviation of p

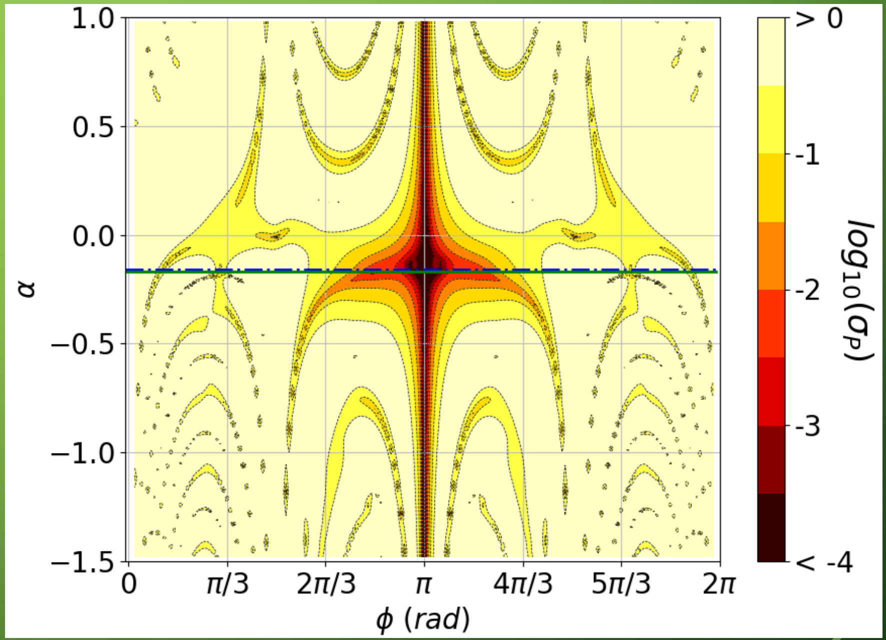
Increased robustness of the QRWS algorithm can be evaluated by using root-mean-square deviation of the probability $p(\phi, \alpha, m)$:

$$\sigma_p^{ij}(m) = \frac{1}{p^{ij}} \sqrt{\left(\frac{\partial p^{ij}}{\partial \phi^i}\right)^2 \sigma_\phi^2 (\phi^i - \pi)^2 + \left(\frac{\partial p^{ij}}{\partial \alpha^j}\right)^2 \sigma_\alpha^2 (\alpha^j - \alpha_{ML}(m))^2}, \sigma_\phi = \sigma_\alpha = 0.1$$

m=5



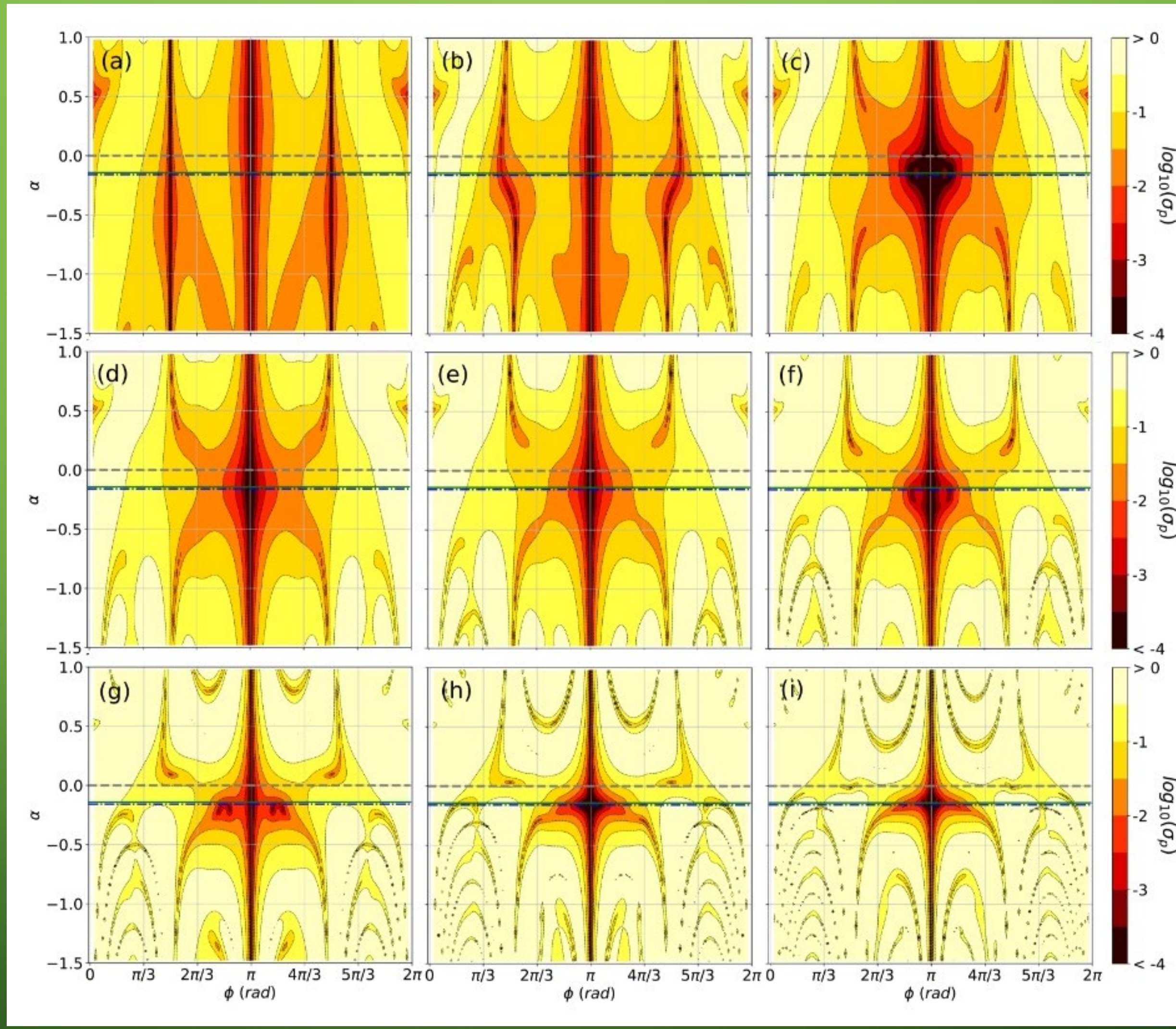
m=10



The large dark central area shows high stability of the QRWS algorithm near the optimal value of α.
The robustness against changes in the phase ϕ is preserved

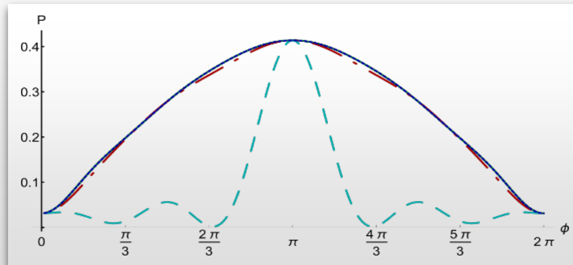
R.M.S. deviation of QRWS

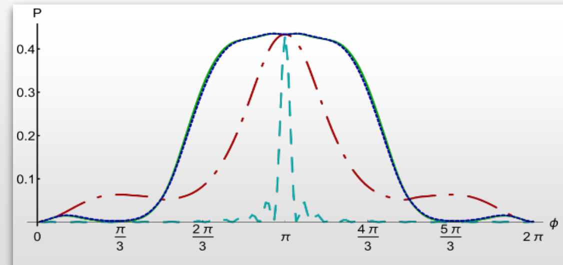
$(2 \leq m \leq 10)$

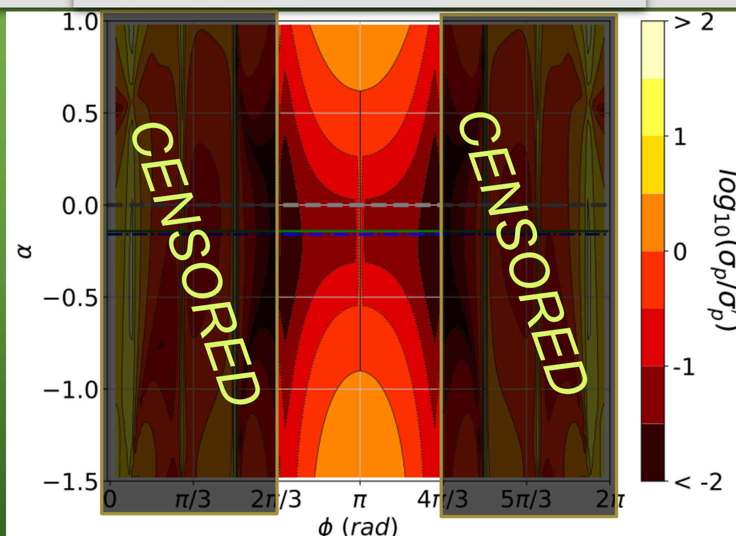


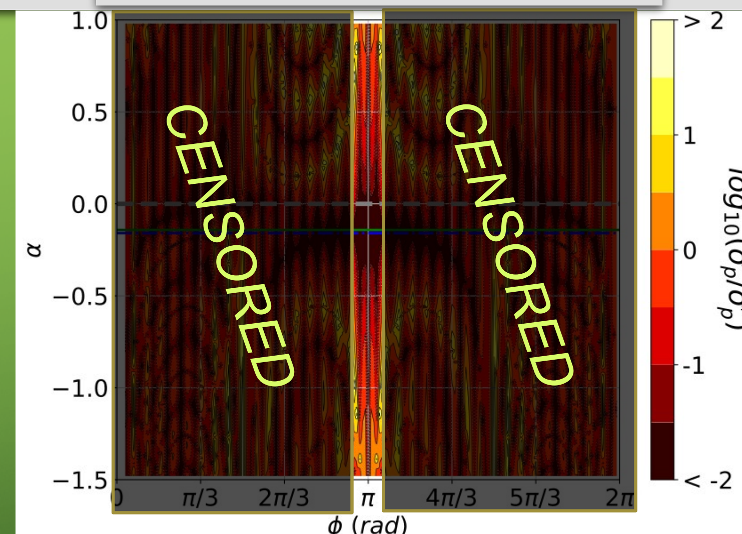
Comparison of stability between standard and optimized coin

$$\sigma'^{i}_{p} = \frac{1}{p'^{i}} \left| \frac{\partial p'^{i}}{\partial \phi^{i}} \sigma_{\phi} (\phi^{i} - \pi) \right|$$



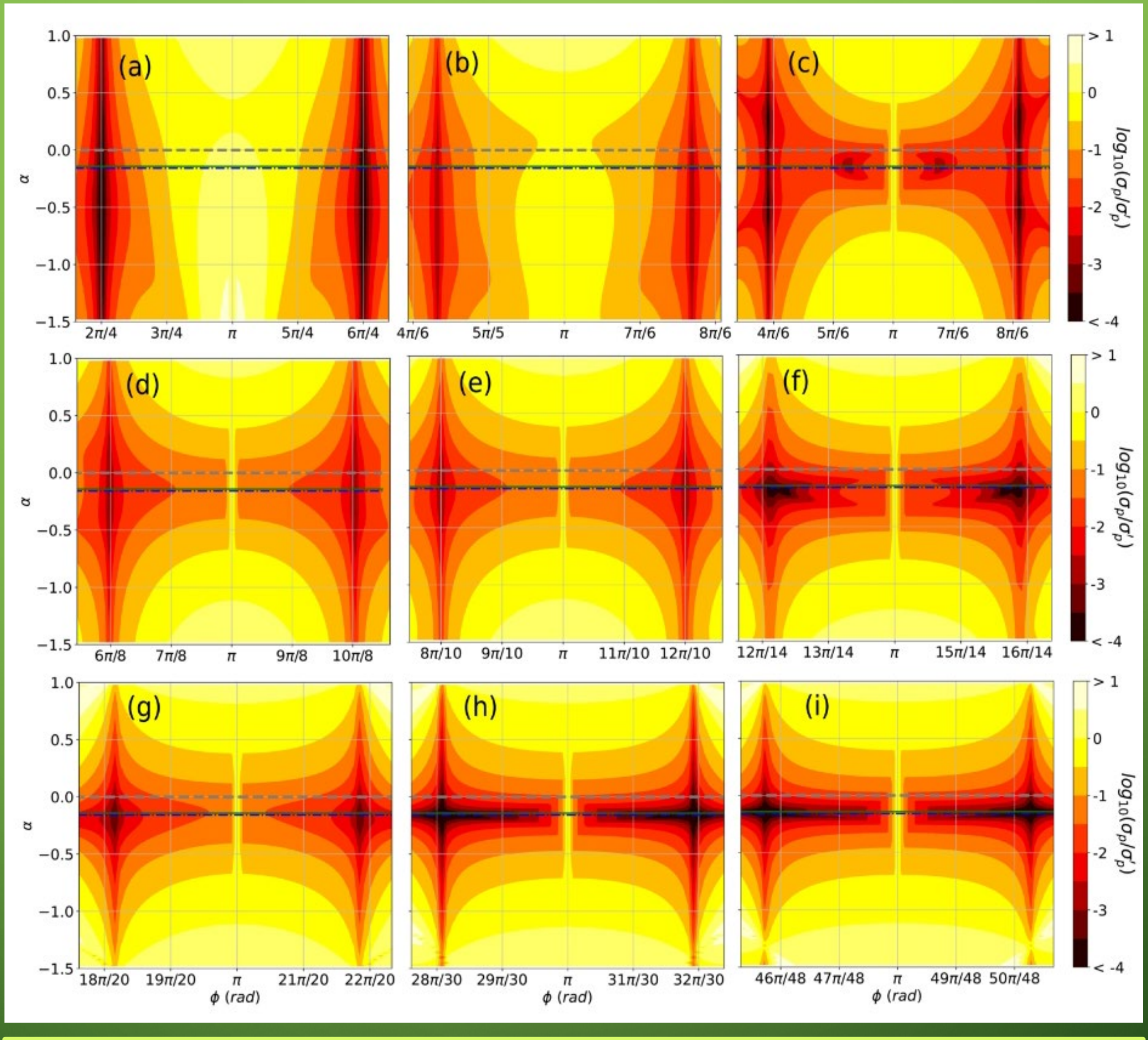






High stability of nonlinear coin in central region compared to standard coin with $\zeta = \pi$

Relative robustness of QRWS $(2 \leq m \leq 10)$



The relative stability of the modified algorithm increases with increasing the coin size!

Conclusion

- The discrete time quantum random walk search is quantum algorithm able to search in unordered database with arbitrary topology. It is quadratically faster than the corresponding classical search algorithms;
- A modification of the algorithm with walk coin constructed by Generalized Householder reflections and a phase gate could be made extremely robust to deviations in the coin parameters if a proper relations between the parameters is maintained;
- Using qudits for walk coin register give the possibility to increase even more algorithm's stability;
- Quantitative numerical analysis of quantum random walk search algorithm's robustness to all coin parameters have been done;
- With Monte Carlo and machine learning methods we made predictions for the stability of algorithm's implementation with larger coin size.

ECAMP14


ECAMP14
14th European
Conference on Atoms
Molecules and Photons
NEW DATE! June 27- July 1, 2022
Vilnius, Lithuania

ECAMP14 at glance

More than:

- 260 participants from 20 countries
- 220 poster presentations
- 9 Plenary lectures and 50 lectures in two parallel sessions

Topics:

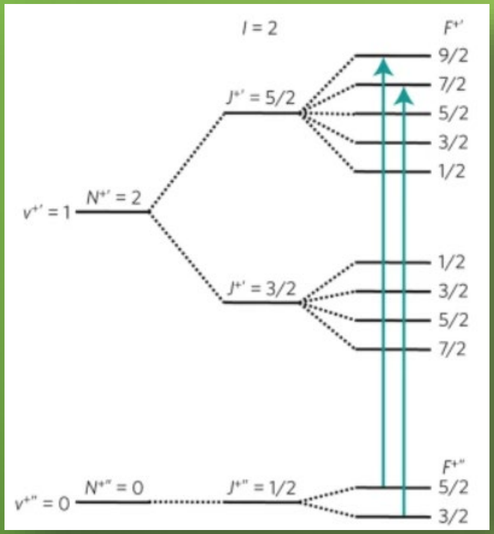
- Atomic and Molecular spectroscopy
- Quantum information and cavity QED
- Fundamental physics, precision measurements and metrology
- Photon induced processes
- Highly charged ions
- Rydberg atoms and ultra-cold plasmas and others

QUANTUM TECHNOLOGIES FOR SINGLE MOLECULAR IONS

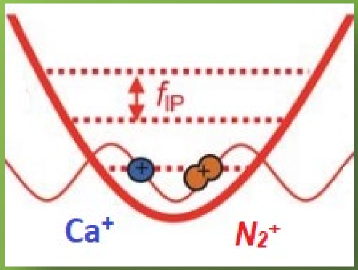
1. Over the past years an impressive progress in the development of experimental methods which enable the control of single isolated quantum systems has been made
2. Molecules offer prospects as novel platforms for:
   - precise determinations of fundamental constants and their possible variations,
   - new frequency standards and clocks,
   - high-fidelity qubits for use in quantum information processing,
   - cold chemistry, etc.

(1) Molecular-ion quantum technologies, M Sinhal, S Willitsch, arXiv preprint arXiv:2204.08814

Precision spectroscopy of N_2^+



Electrical quadrupole transitions in $28N_2^+$ (1)



Trapping of singular nitrogen molecular ion together with Ca^+.

Ca^+ ions are used for:

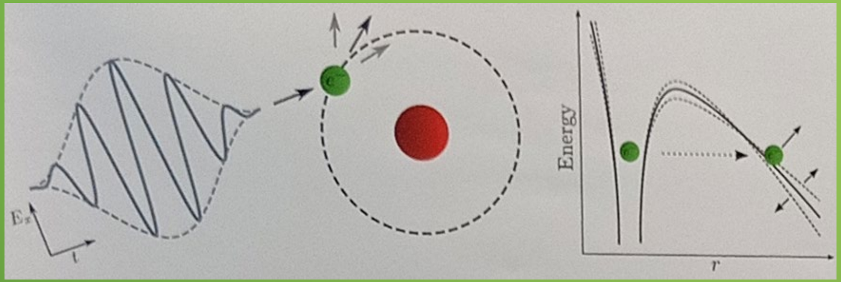
- Sympathetic cooling
- Nondemolition state detection (2)

(1) M. Germann, X. Tong, S. Willitsch, Observation of electric-dipole-forbidden infrared transitions in cold molecular ionsNature Physics 10 (11), 820-824 (2014)

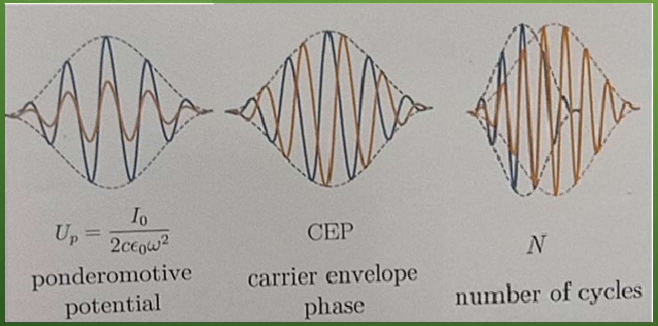
(2) M. Sinhal, Z. Meir, K. Najafian, G. Hegi and S. Willitsch, Quantum-nondemolition state detection and spectroscopy of single trapped molecules, Science 367, 1213 (2020).

Photoelectron momentum distribution of attosecond pulses – machine learning based parameter determination

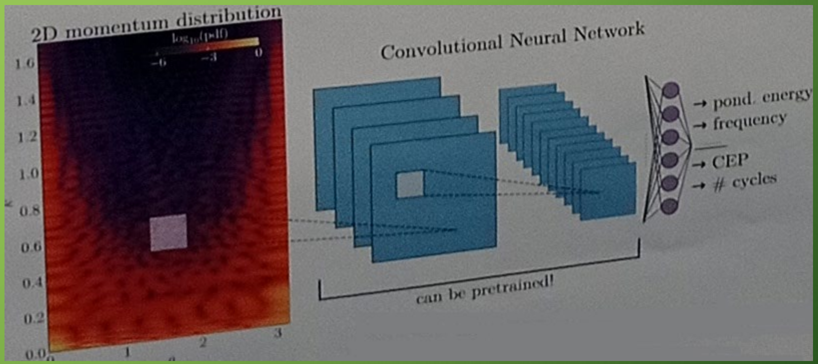
Scattering of electrons with attosecond EM pulses

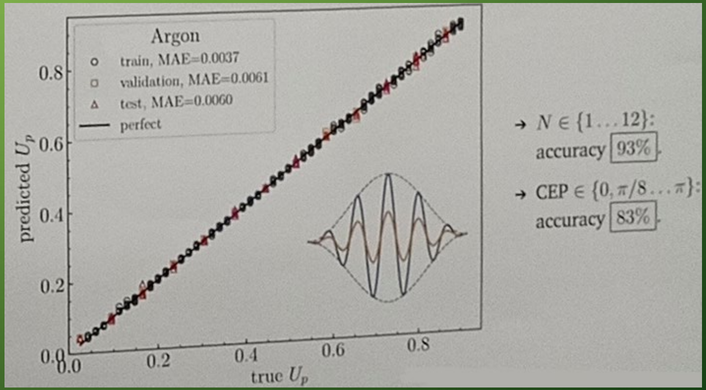


Ultrafast processes are strongly sensitive to pulse parameters wavelength,



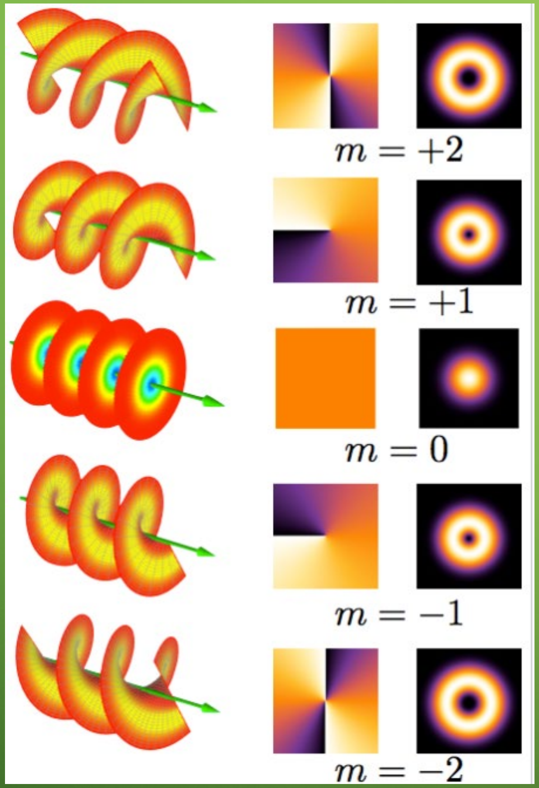
Convolutional network to determine pulse parameters from the 2D plots of the scattered electron distribution – k, θ





High accuracy of CNN (> 99% for pulse intensity)

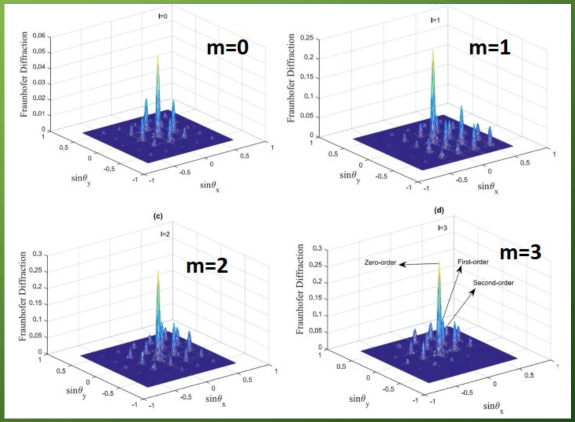
Twisted light
(Structured light, Orbital Angular Momentum of light)



m – angular momentum of light, optical vortex topological charge, winding number

Applications:

- Transfer huge quantities of data through optical fibers – Terabits per second;
- Use in quantum information;
- Inducing high-order multipole transitions;
- Angular momentum transfer,…

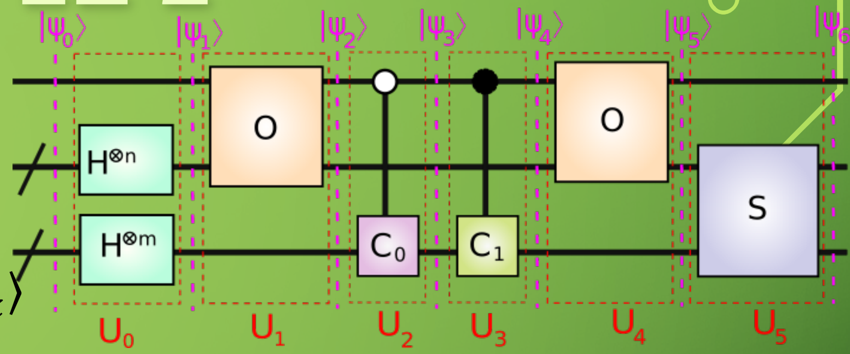


Asadpour, S.H., Kirova, T., Qian, J. et al. Azimuthal modulation of electromagnetically induced grating using structured light, Sci Rep 11, 20721 (2021).

THANK YOU FOR YOUR ATTENTION!

This work was supported by the Bulgarian Science Fund under contract KP-06-M48/2 /26.11.2020.

EXAMPLE 2



Example For Coin Size 3, solutions {2,6} (or x_k=1 & x_k =5), for walk coin is used Grover Coin and for marking coin is used -I

$|\psi_k\rangle = |con_k, x_k, c_k\rangle = |con_k\rangle \otimes |x_k\rangle \otimes |c_k\rangle$

Dim[$|\psi_k\rangle$]=3*2^(3+1)=48

$|\psi_0\rangle = |0, 0,0\rangle$

$$U_0 = \hat{I}_2 \otimes H^{\otimes 3} \otimes \mathrm{F}_3$$

$$F_3 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 1 & 1 \\ 1 & e^{2i\pi/3} & e^{-2i\pi/3} \\ 1 & e^{-2i\pi/3} & e^{2i\pi/3} \end{pmatrix} \qquad \hat{I}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

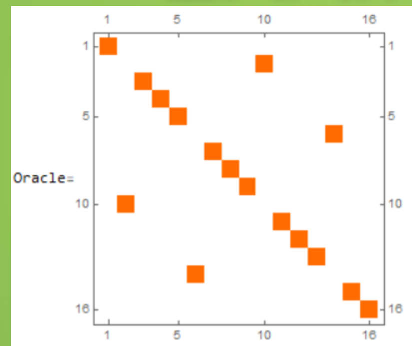
$$H^{\otimes 3} = \left(\frac{1}{\sqrt{2}}\right)^3 \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad \hat{I}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

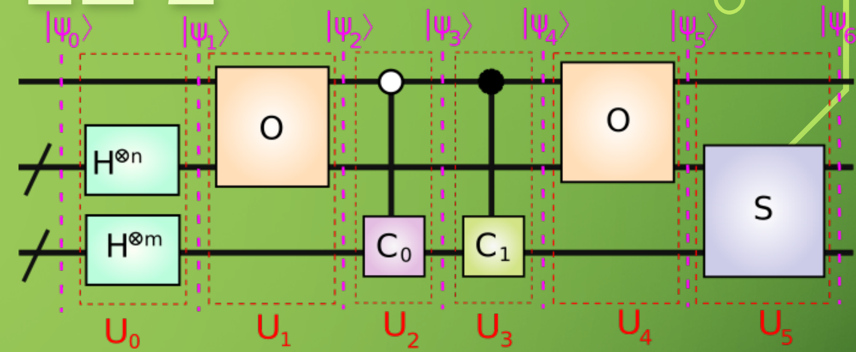
$$|\psi_1\rangle = U_0|\psi_0\rangle = \frac{1}{2\sqrt{6}}|0\rangle \otimes \sum_{j_1=0}^{2^3-1} \sum_{j_2=0}^{2} |j_1\rangle \otimes |j_2\rangle$$

$$\hat{O} = \hat{I}_{16} - (|2\rangle\langle 2| + |10\rangle\langle 10| + |6\rangle\langle 6| + |14\rangle\langle 14|) + (|2\rangle\langle 10| + |10\rangle\langle 2| + |6\rangle\langle 14| + |14\rangle\langle 6|)$$

EXAMPLE 2

$U_1 = O \otimes \hat{I}_3$





$|\psi_2\rangle = U_1|\psi_1\rangle = \frac{1}{2\sqrt{6}}|0\rangle \otimes \sum_{j_1=0}^{2^3-1}\sum_{j_2=0}^{2}|j_1\rangle \otimes |j_2\rangle$- $\frac{1}{2\sqrt{6}}|0\rangle \otimes (|1\rangle + |5\rangle) \otimes \sum_{j_2=0}^{2}|j_2\rangle)$ + $\frac{1}{2\sqrt{6}}|1\rangle \otimes(|1\rangle$+ $|5\rangle) \otimes \sum_{j_2=0}^{2}|j_2\rangle$

U_2 =Diag[$\hat{I}_{24}, \hat{I}_8 \otimes C_0$]

$|\psi_3\rangle = U_2|\psi_2\rangle = |\psi_2\rangle$

$$C_0 = \frac{1}{3}\begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}$$

$C_1 = -\hat{I}_3$

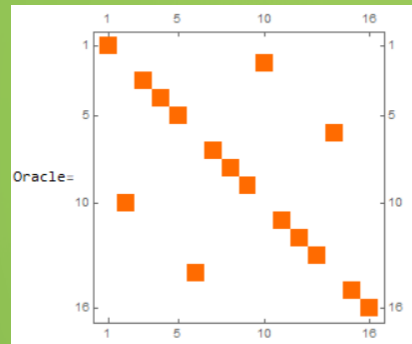
U_3 =Diag[$\hat{I}_8 \otimes C_1, \ \hat{I}_{24}$]

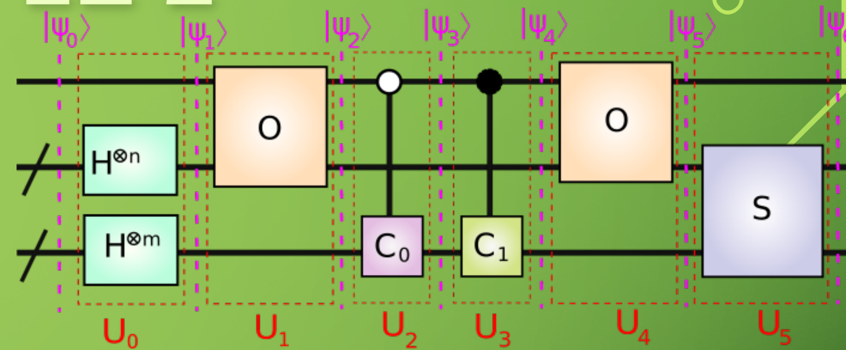
$|\psi_4\rangle = U_1|\psi_1\rangle = \frac{1}{2\sqrt{6}}|0\rangle \otimes (\sum_{j_1=0}^{2^3-1}\sum_{j_2=0}^{2}|j_1\rangle \otimes |j_2\rangle$-$(|1\rangle + |5\rangle) \otimes \sum_{j_2=0}^{2}|j_2\rangle)$ - $\frac{1}{2\sqrt{6}}(|1\rangle \otimes (|1\rangle + |5\rangle) \otimes \sum_{j_2=0}^{2}|j_2\rangle)$

EXAMPLE 2

$U_4 = O \otimes \hat{I}_3 = U_4$

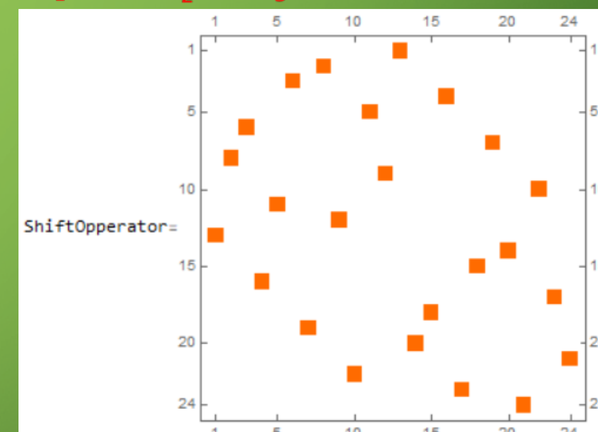
$U_5 = \hat{I}_2 \otimes S$





$$|\psi_5\rangle = U_4|\psi_4\rangle = \frac{1}{2\sqrt{6}}|0\rangle \otimes \sum_{j_1=0}^{2^3-1}\sum_{j_2=0}^{2}|j_1\rangle \otimes |j_2\rangle -$$

$$\frac{2}{2\sqrt{6}}|0\rangle \otimes (|1\rangle + |5\rangle) \otimes \sum_{j_2=0}^{2}|j_2\rangle$$



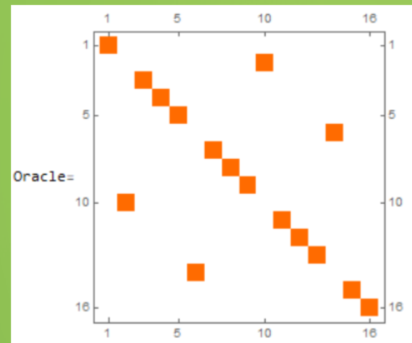
$$S = \sum_{d=0}^{3-1}\sum_{x=0}^{2^3-1}|x^d, d\rangle\langle \mathrm{x}, d|$$

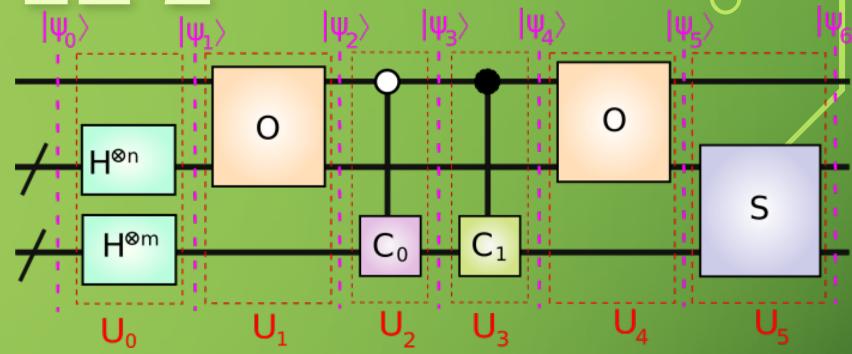
$|\psi_6\rangle = U_5|\psi_5\rangle = \frac{1}{2\sqrt{6}}|0\rangle \otimes (\sum_{j_1=0}^{2^3-1}\sum_{j_2=0}^{2}|j_1\rangle \otimes |j_2\rangle$ - 2*($|0\rangle \otimes |2\rangle$ + $|1\rangle \otimes |0\rangle$ + $|3\rangle \otimes |1\rangle$ +$|4\rangle \otimes |2\rangle$ + $|5\rangle \otimes |0\rangle$ + $|7\rangle \otimes |1\rangle$))

$$\mathrm{M}[|\psi_6\rangle] = \frac{1}{2\sqrt{6}}(1,1,1,1,1,1,1,1)$$

EXAMPLE 2

$U_6 \equiv U_1$
$U_7 \equiv U_2$

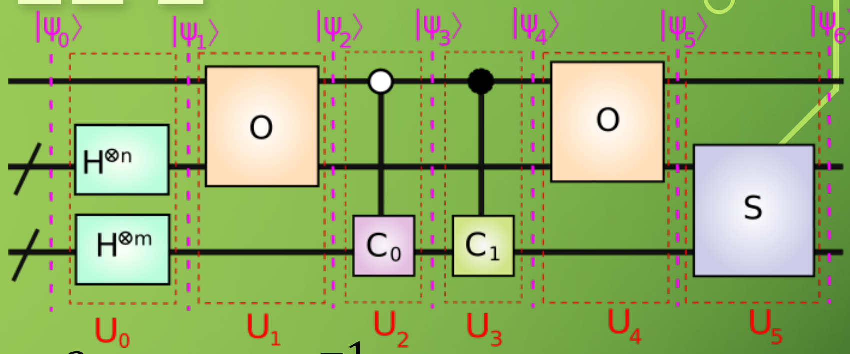




$$|\psi_7\rangle = U_6|\psi_6\rangle = \frac{1}{2\sqrt{6}}|0\rangle \otimes (\sum_{j_1=0}^{2^3-1}\sum_{j_2=0}^{2}|j_1\rangle \otimes |j_2\rangle \text{ - } \frac{1}{2\sqrt{6}}|0\rangle \otimes (|1\rangle + |5\rangle) \otimes \sum_{j_2=0}^{2}|j_2\rangle + \frac{1}{2\sqrt{6}}|1\rangle \otimes (|1\rangle + |5\rangle) \otimes \sum_{j_2=1}^{2}|j_2\rangle - \frac{1}{2\sqrt{6}}|1\rangle \otimes (|1\rangle + |5\rangle) \otimes |0\rangle$$

$$|\psi_8\rangle = U_7|\psi_7\rangle = \frac{1}{2\sqrt{6}}|0\rangle \otimes (|2\rangle + |6\rangle) \otimes \sum_{j_2=0}^{2}|j_2\rangle + \frac{-1}{12\sqrt{6}}|0\rangle \otimes (|0\rangle \otimes |0\rangle + |0\rangle \otimes |1\rangle + |3\rangle \otimes |0\rangle + |3\rangle \otimes |2\rangle + |4\rangle \otimes |0\rangle + |4\rangle \otimes |1\rangle + |7\rangle \otimes |0\rangle + |7\rangle \otimes |2\rangle) + \frac{10}{12\sqrt{6}}|0\rangle \otimes (|0\rangle \otimes |2\rangle + |3\rangle \otimes |1\rangle + |4\rangle \otimes |2\rangle + |7\rangle \otimes |1\rangle) + \frac{1}{2\sqrt{6}}|1\rangle \otimes (|1\rangle + |5\rangle) \otimes \sum_{j_2=1}^{2}|j_2\rangle - \frac{1}{2\sqrt{6}}|1\rangle \otimes (|1\rangle + |5\rangle) \otimes |0\rangle$$

EXAMPLE 2

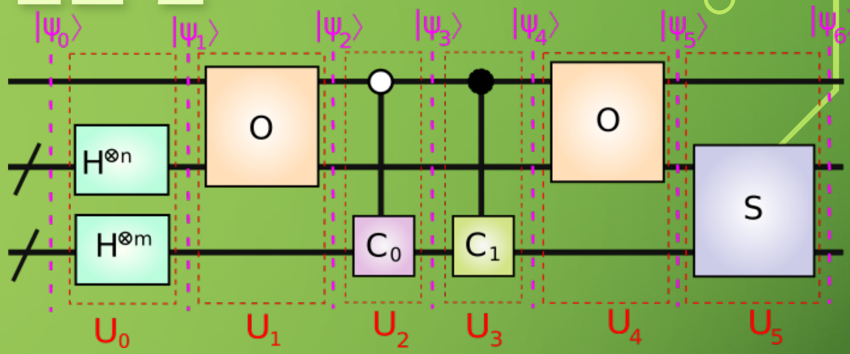


$U_8 \equiv U_3$
$U_9 \equiv U_4$

$$|\psi_9\rangle = U_8|\psi_8\rangle = \frac{1}{2\sqrt{6}}|0\rangle \otimes (|2\rangle + |6\rangle) \otimes \sum_{j_2=0}^{2}|j_2\rangle + \frac{-1}{12\sqrt{6}}|0\rangle \otimes (|0\rangle \otimes |0\rangle + |0\rangle \otimes |1\rangle + |3\rangle \otimes |0\rangle + |3\rangle \otimes |2\rangle + |4\rangle \otimes |0\rangle + |4\rangle \otimes |1\rangle + |7\rangle \otimes |0\rangle + |7\rangle \otimes |2\rangle) + \frac{10}{12\sqrt{6}}|0\rangle \otimes (|0\rangle \otimes |2\rangle + |3\rangle \otimes |1\rangle + |4\rangle \otimes |2\rangle + |7\rangle \otimes |1\rangle) - \frac{1}{2\sqrt{6}}|1\rangle \otimes (|1\rangle + |5\rangle) \otimes \sum_{j_2=1}^{2}|j_2\rangle + \frac{1}{2\sqrt{6}}|1\rangle \otimes (|1\rangle + |5\rangle) \otimes |0\rangle$$

$$|\psi_{10}\rangle = U_9|\psi_9\rangle = \frac{1}{2\sqrt{6}}|0\rangle \otimes (|2\rangle + |6\rangle) \otimes \sum_{j_2=0}^{2}|j_2\rangle + \frac{-1}{12\sqrt{6}}|0\rangle \otimes (|0\rangle \otimes |0\rangle + |0\rangle \otimes |1\rangle + |3\rangle \otimes |0\rangle + |3\rangle \otimes |2\rangle + |4\rangle \otimes |0\rangle + |4\rangle \otimes |1\rangle + |7\rangle \otimes |0\rangle + |7\rangle \otimes |2\rangle) + \frac{10}{12\sqrt{6}}|0\rangle \otimes (|0\rangle \otimes |2\rangle + |3\rangle \otimes |1\rangle + |4\rangle \otimes |2\rangle + |7\rangle \otimes |1\rangle) - \frac{1}{2\sqrt{6}}|0\rangle \otimes (|1\rangle + |5\rangle) \otimes \sum_{j_2=1}^{2}|j_2\rangle + \frac{1}{2\sqrt{6}}|0\rangle \otimes (|1\rangle + |5\rangle) \otimes |0\rangle$$

EXAMPLE 2



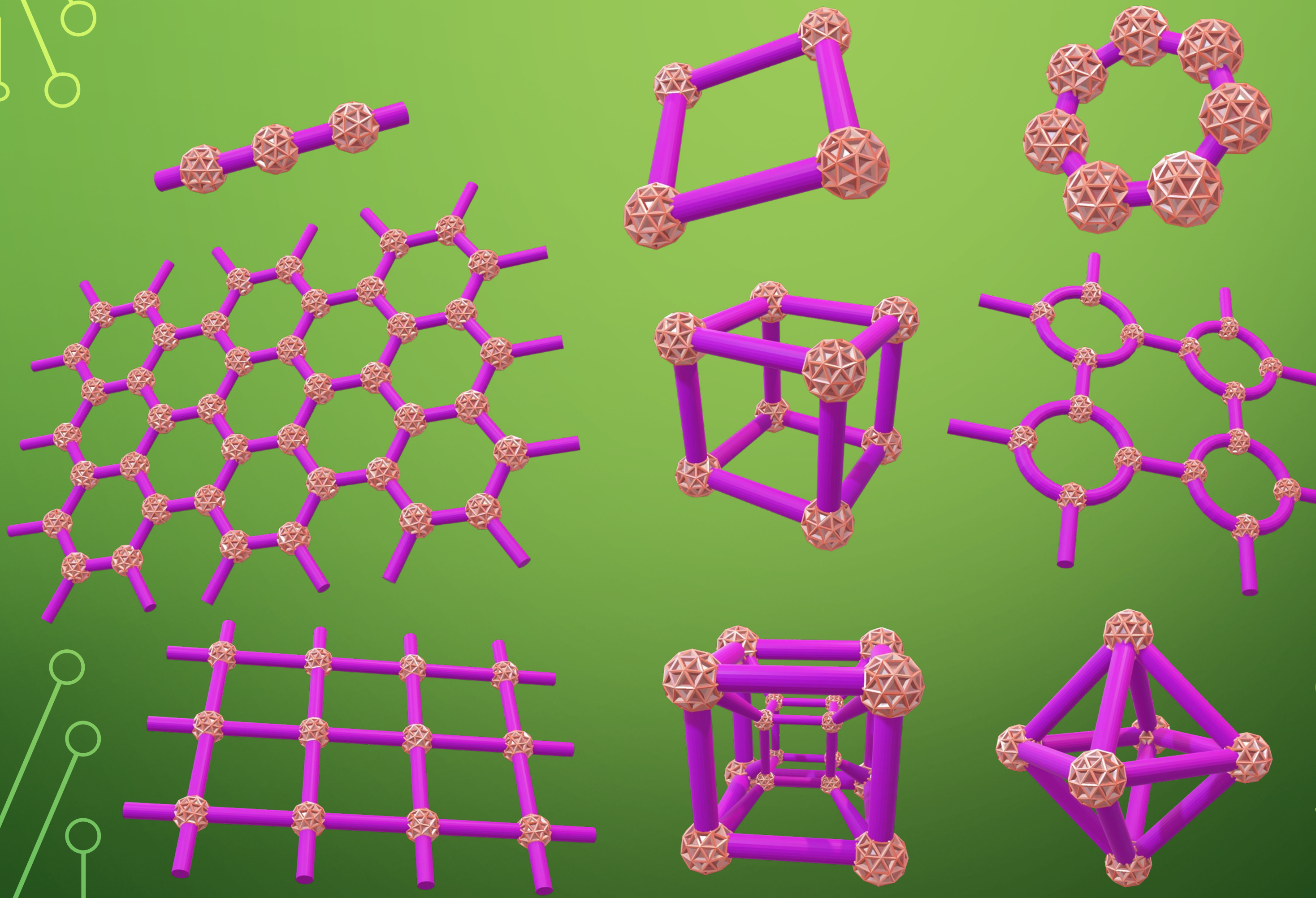
$U_{10} \equiv U_5$

$$|\psi_{10}\rangle = U_9|\psi_9\rangle = \frac{1}{2\sqrt{6}}|0\rangle \otimes (|0\rangle \otimes |1\rangle - |0\rangle \otimes |2\rangle + |1\rangle \otimes |0\rangle + |2\rangle \otimes |0\rangle - |3\rangle \otimes |1\rangle + |3\rangle \otimes |2\rangle + |4\rangle \otimes |1\rangle - |4\rangle \otimes |2\rangle + |5\rangle \otimes |0\rangle + |6\rangle \otimes |0\rangle - |7\rangle \otimes |1\rangle + |7\rangle \otimes |2\rangle) + \frac{-1}{12\sqrt{6}}|0\rangle \otimes (|0\rangle \otimes |0\rangle + |2\rangle \otimes |1\rangle + |2\rangle \otimes |2\rangle + |3\rangle \otimes |0\rangle + |4\rangle \otimes |0\rangle + |6\rangle \otimes |1\rangle + |6\rangle \otimes |2\rangle + |7\rangle \otimes |0\rangle) + \frac{10}{12\sqrt{6}}|0\rangle \otimes (|1\rangle \otimes |1\rangle + |1\rangle \otimes |2\rangle + |5\rangle \otimes |1\rangle + |5\rangle \otimes |2\rangle)$$

$$M[|\psi_{10}\rangle] = (0.0879, 0.2731, 0.0509, 0.0879, 0.0879, 0.2731, 0.0509, 0.0879)$$

Shift Operator

Shift operator S defines the topology of the walked object



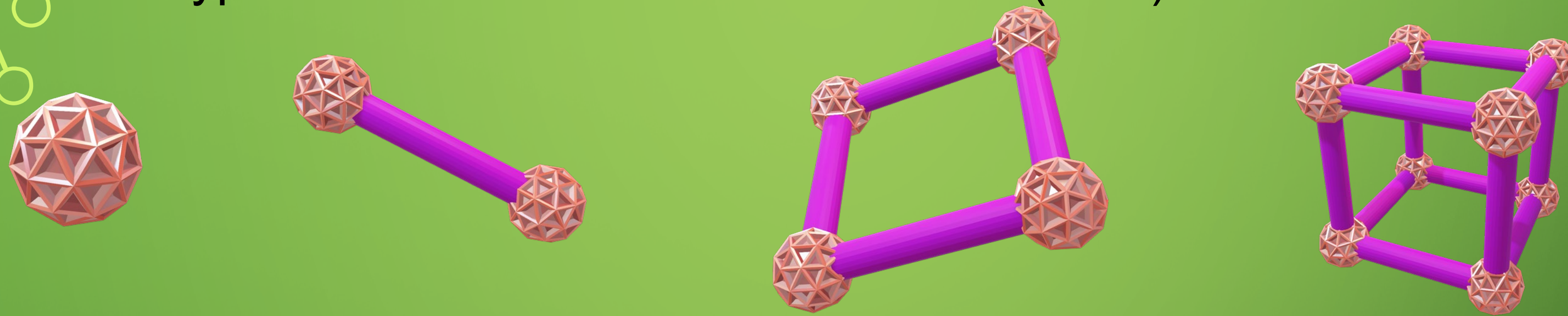
Coin Register Size is 2

Coin Register Size is 3

Coin Register Size is 4

Hypercube and Node Numbering

Hypercubes with different dimensions (0 - 3):

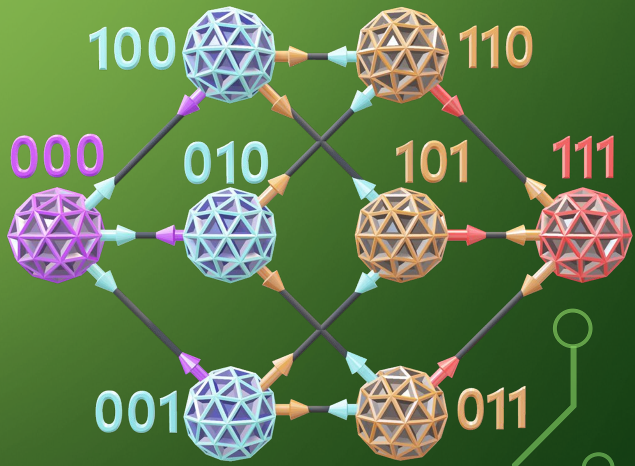


Number of nodes and edges of such Hypercube are:

$E_{0,d} = 2^d$ $\quad\quad$ $E_{1,d} = R2^{d-1}$

Each node (and also edges) can be numbered with binary string label. Zeroth node can be arbitrary chosen.

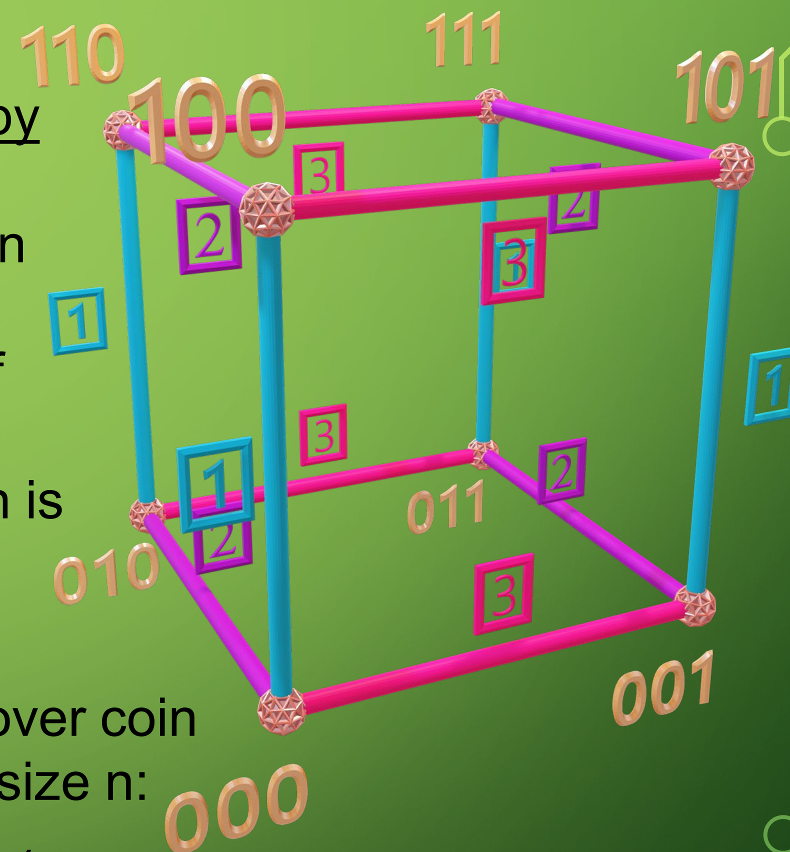
Two nodes in a hypercube are neighbors, if they differ by only one symbol (their Hamming distance is 1).



Walk Coin

Walk coin gives probabilities for transition between nodes connected by an edge.

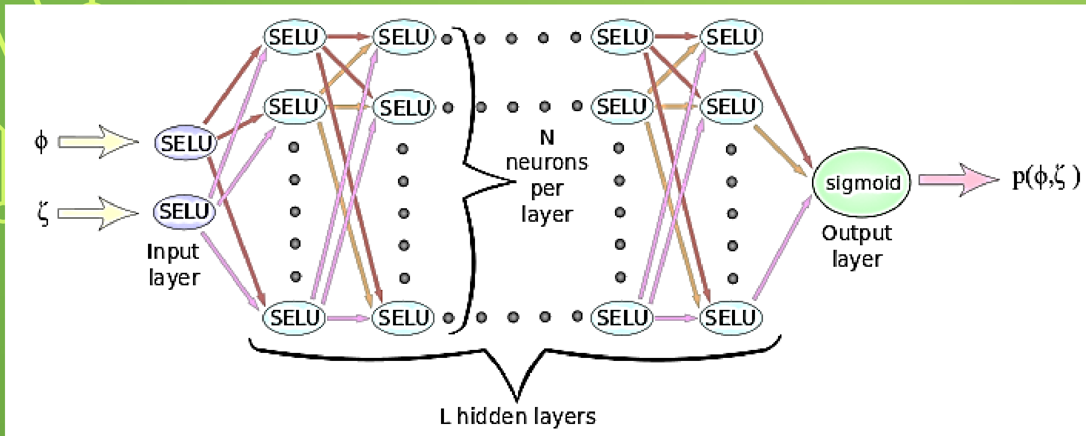
- The system can be in superposition of nodes, so during the evolution it can go to different superposition of states.
- If probability to go in each direction is the same, then off diagonal matrix elements should be the same.



Original QRWS algorithm uses Grover coin G for traversing a graph. For coin with size n:

$$G = \begin{pmatrix} -1 + 2/n & 2/n & \dots & 2/n \\ 2/n & -1 + 2/n & \dots & 2/n \\ \vdots & \vdots & \ddots & \vdots \\ 2/n & 2/n & \dots & -1 + 2/n \end{pmatrix}$$

Machine learning and optimization



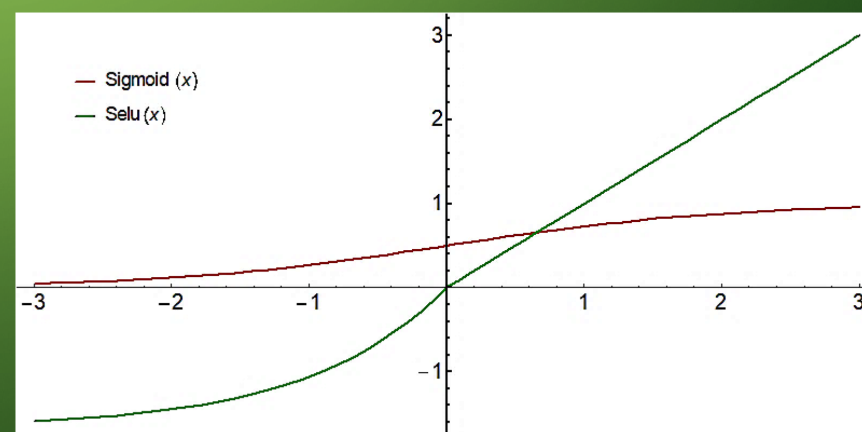
This neural network is used to fit training examples to obtain a ML model that best approximate quantum random walk search algorithm. This model is used to optimize the quantum algorithm

Feed Forward NN – network were information flows from k-th to (k+1)-th layer. No information flows between neurons on the same layer or from (k+1)-th layer to the k-th. Activation Function of neuron – non-linear function, witch result depends on the input

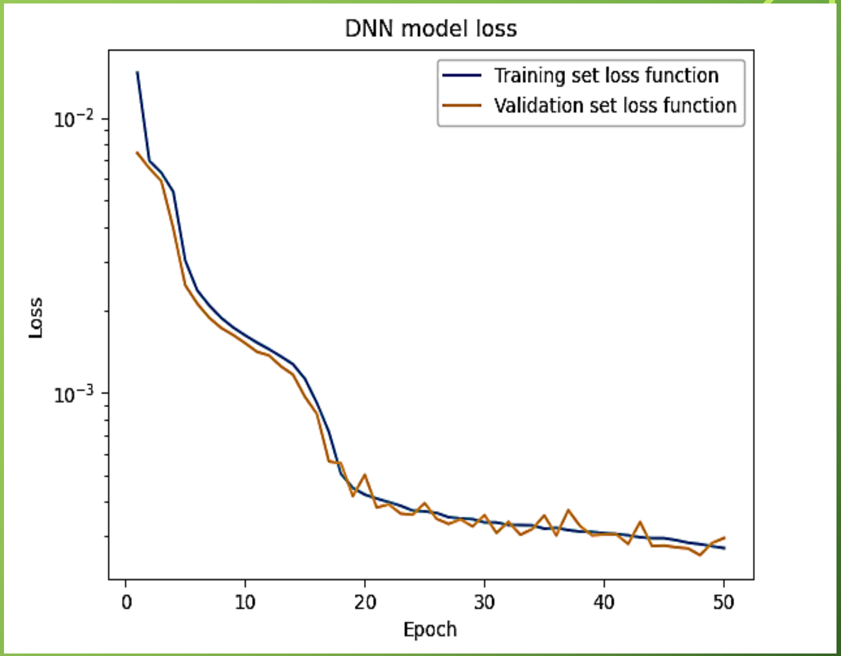
$$SELU(x) = \begin{cases} x & if\ x > 0 \\ 1.673(e^x - 1) & if\ x \le 0 \end{cases}$$

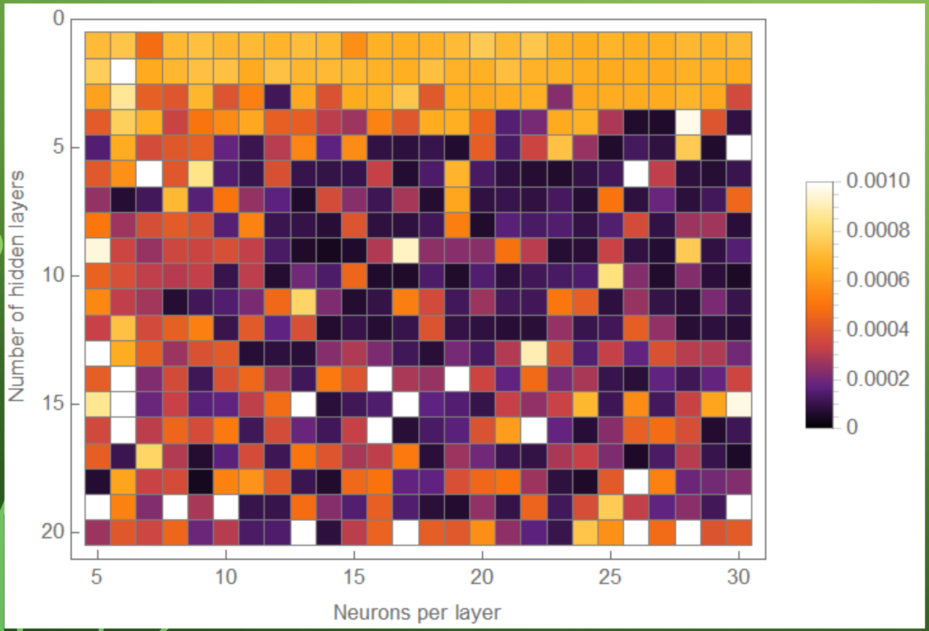
$$Sigmoid(x) = \frac{1}{1 + e^{-x}}$$

Gradient descent is an iterative optimization algorithm for finding a local minimum of a function by making steps at direction of the steepest descent.



Epoch – one run of the neuron network trough training examples. Network update its parameters at end of each epoch.
Batch Gradient Descent – At each epoch, lost function is calculated by smaller portion of training examples (batch). This batch is taken by random training examples. Therefore there is larger uncertainty at the end of the training, lost function oscillate around the minimum.





Training Set – set used to train NN
Validation Set – set used to evaluate NN
Lost function – measure how well ML model fit training examples (depend of network parameters)
Early stopping – stop training of NN when LF on VS starts to worsen trough the epochs
On the left figure darker colors correspond to smaller lost function => better ML model
Adam optimization is a stochastic gradient descent method that is based on adaptive estimation of expected value and variance

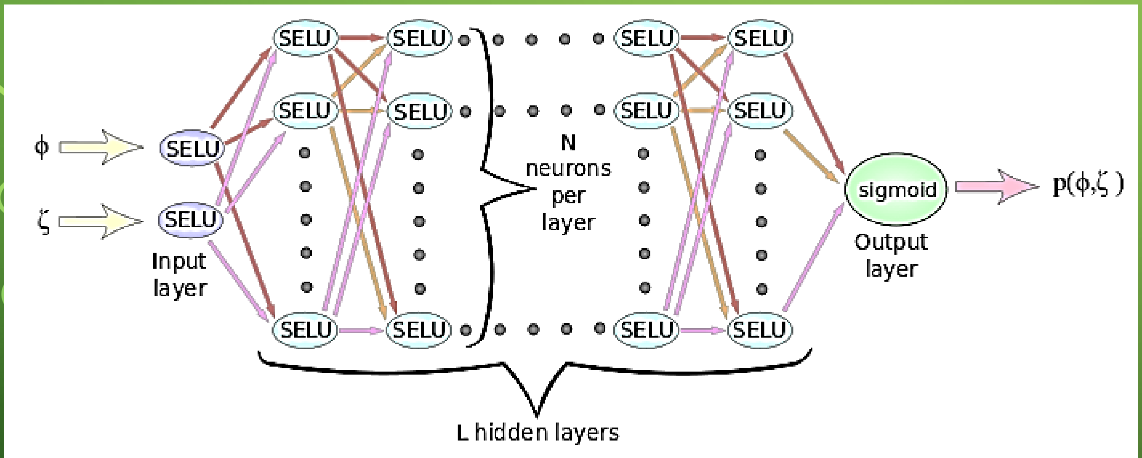
Optimizing walk coin by machine learning

Different functions were fitted to data points, to find the function that makes the algorithm as robust as possible. So for largest possible ε to be fulfilled:

$$p(\phi \in (\phi_{max} - \varepsilon, \phi_{max} + \varepsilon)) \cong p_{max} = p\,(\phi_{max})$$

Best results were obtained with the function: $\zeta = -2\,\phi + 3\pi + \alpha \sin(2\phi)$ where $\phi, \zeta\, \epsilon [0,2\pi]$

For finding the best value of α a feed forward Neural Network is used.



N and L are varied to find the best model. The model is used to fit the above function to the points in the ζ, ϕ plane with highest $p(\zeta, \phi)$. Then extract the corresponding value of α

Neural network Parameters:

1) $N \in [1,20]$
2) $L \in [5,30]$
3) Training Examples 300000 for one and two qubits and 15000 for 3-qubits
4) Batch size is 256 examples
5) Early stopping is used.
6) Training set 80%
7) Validation set 20%
8) Adam optimization