Title: Quantum simulation for materials modeling

Speakers: Alexandre Cooper-Roy

Collection/Series: Waterloo-Munich Joint Workshop

Subject: Quantum Information

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Towards Quantum Simulation for Materials Modeling with Rydberg Atom Arrays

Alexandre Cooper-Roy
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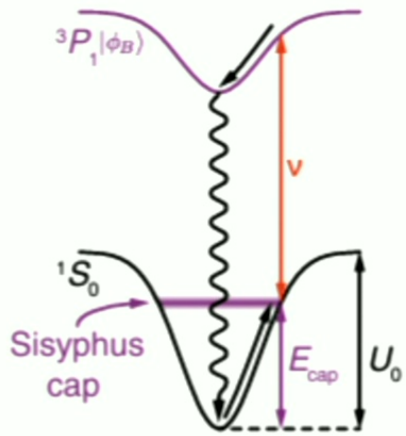
Institute for Quantum Computing
University of Waterloo
October 2nd, 2024

Cooling and localization of atoms in laser-induced potential wells

R. Taïeb, R. Dum, J. I. Cirac, P. Marte, and P. Zoller
Phys. Rev. A **49**, 4876 – Published 1 June 1994



Sisyphus Cooling in Sr-88
PHYSICAL REVIEW X **8**, 041055 (2018)
Caltech (2018)

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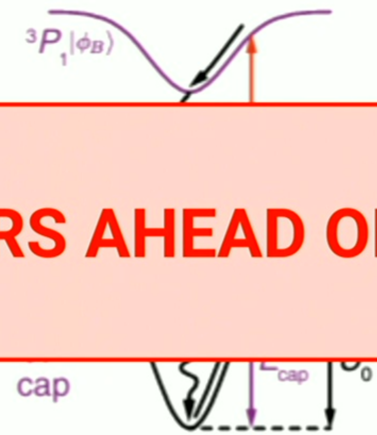
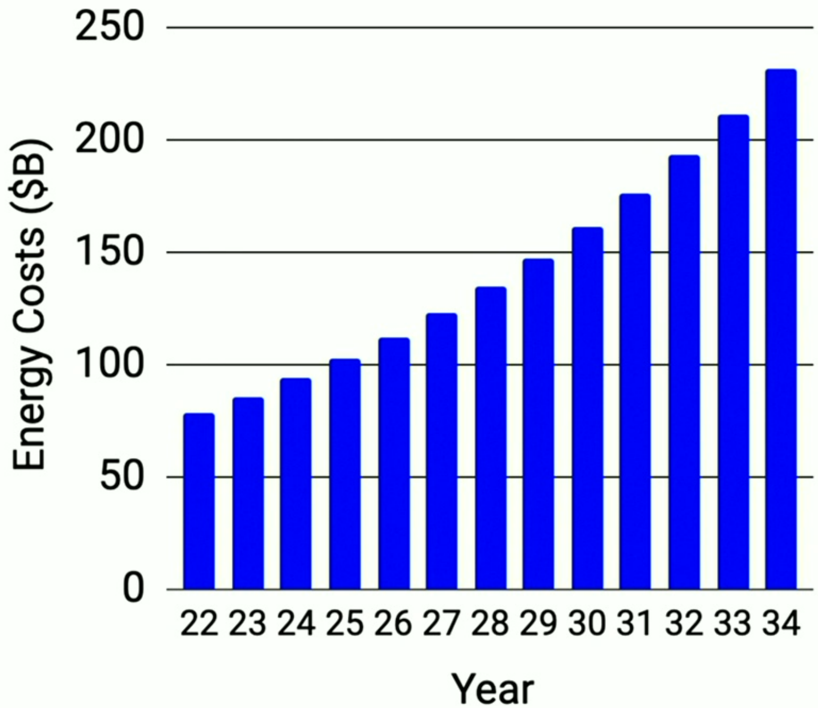


25 YEARS AHEAD OF TIME!

Sisyphus Cooling in Sr-88
PHYSICAL REVIEW X **8**, 041055 (2018)
Caltech (2018)

Exploding worldwide energy demand for processing information



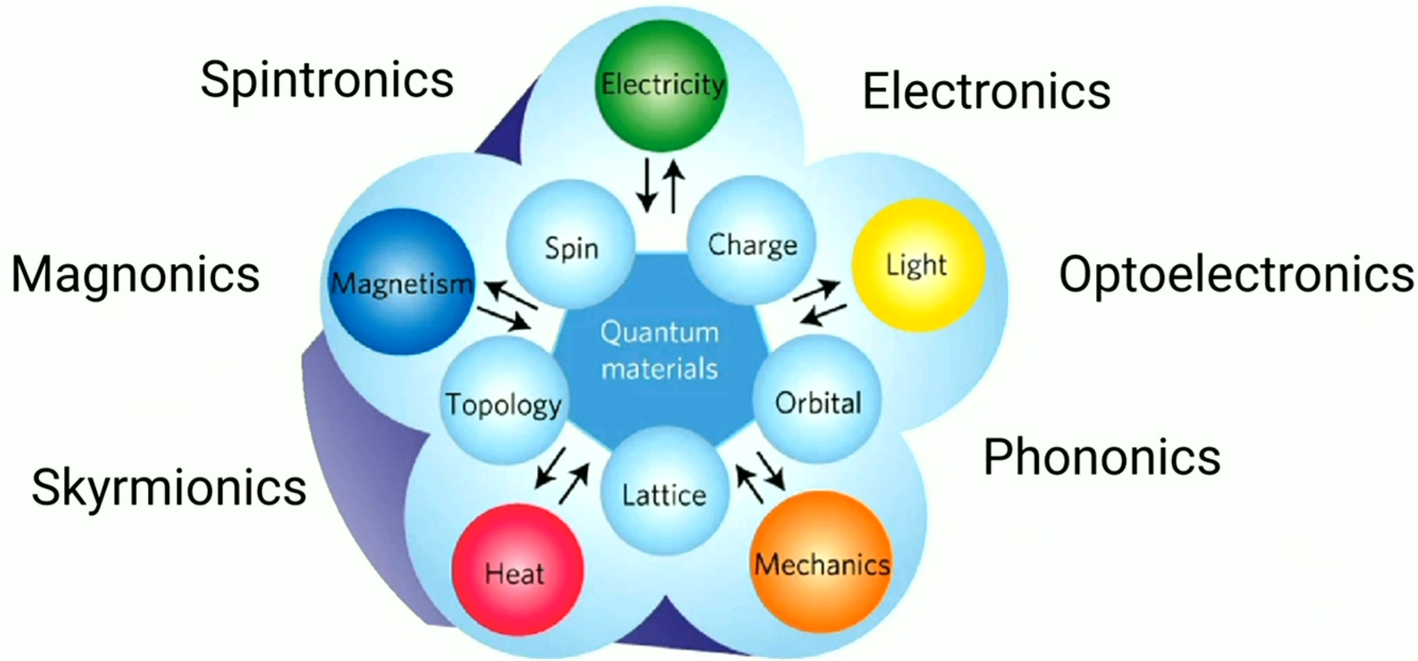
Source: International Energy Agency

Urgent need for groundbreaking innovation driven by fundamental physics

- **Solar panels** for energy harvesting,
- **Nuclear fusion** for energy production,
- **High-Tc superconductors** for lossless transmission,
- **Spintronic logic devices** for energy-efficient processing,
- any many more …

***** MATERIALS *****

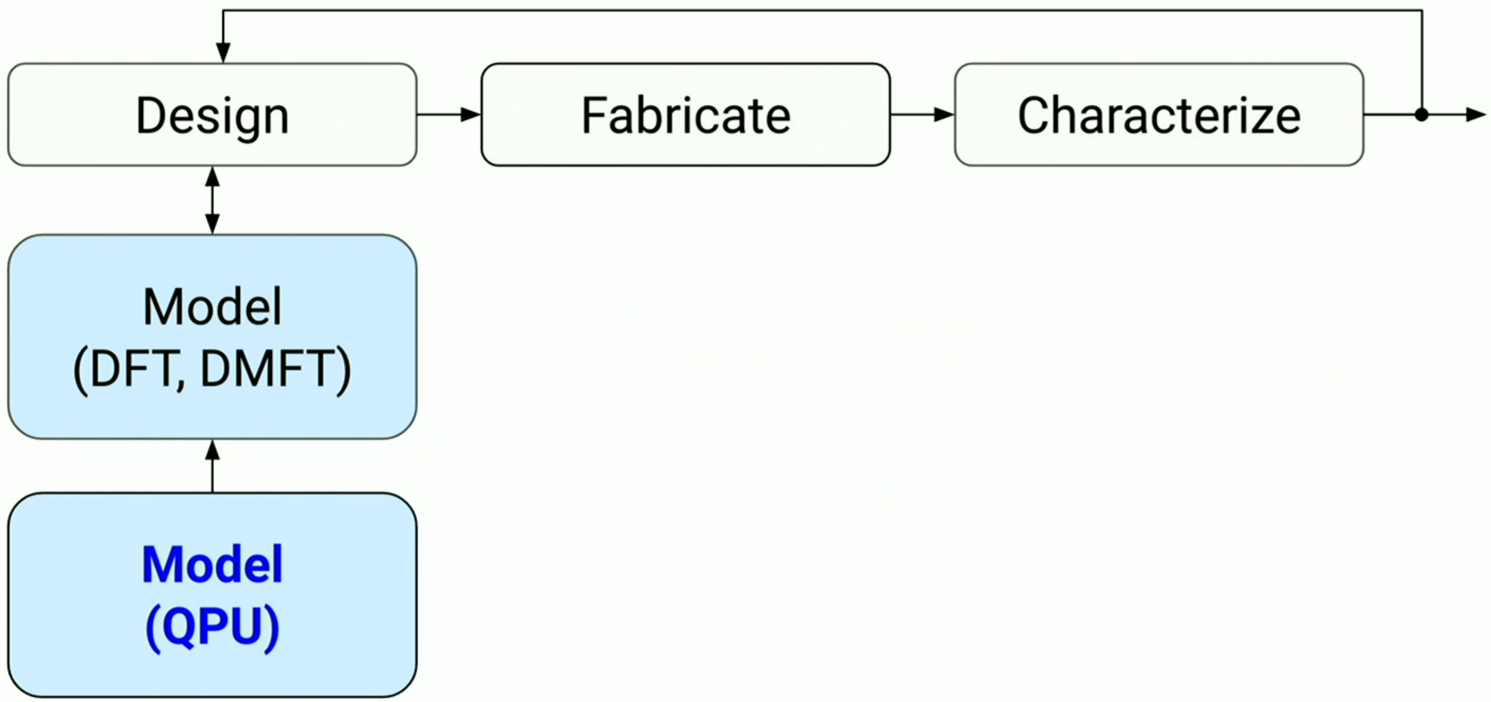
Quantum materials for emerging technologies



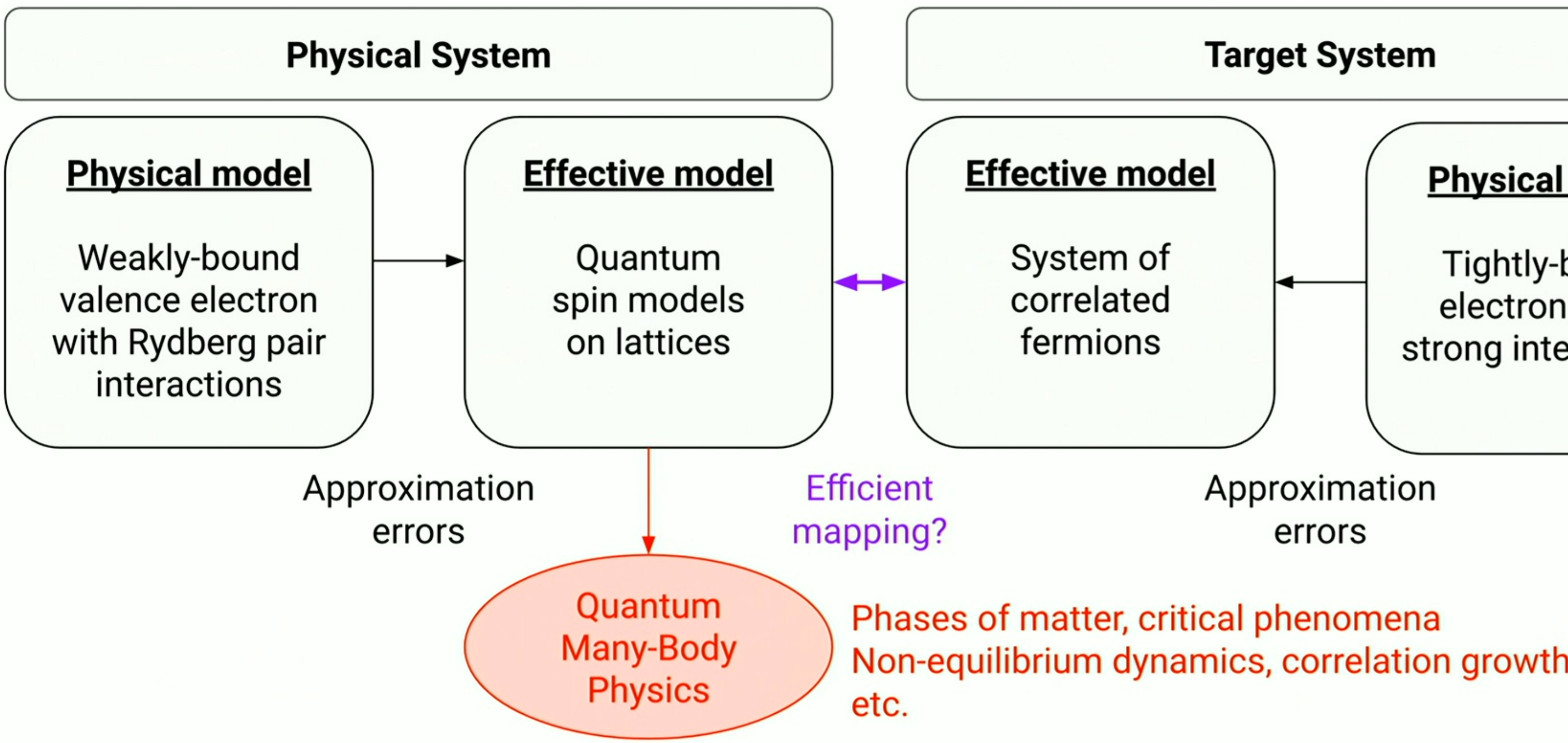
Source: Nature Physics 13, 1056–1068 (2017)

8

Quantum simulation for materials design and screening



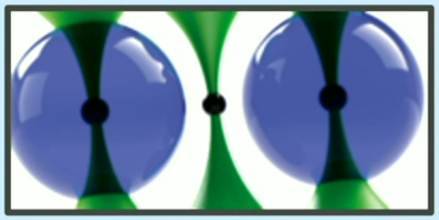
Quantum simulation for materials design and screening



14

Quantum simulation for accelerating materials development cycle

A) Platform development towards realizing quantum control at scale



B) Quantum Many-Body Physics
B1) Perfect transport
B2) Scalable Spin Squeezing
B3) Anomalous Chiral Edge Flow

C) Practical applications
C1) Metrology
C2) Sensing
C3) Computing

17

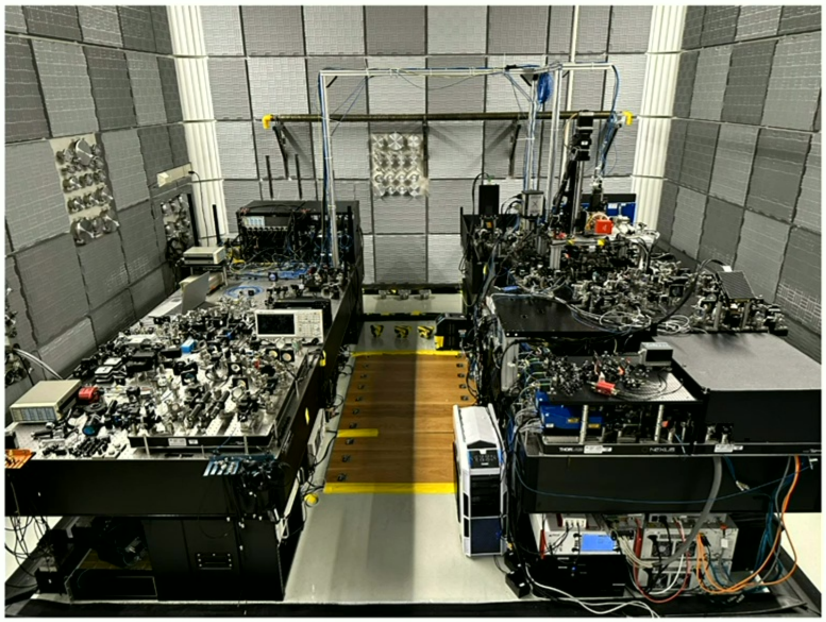
A) Quantum information processing with Rydberg atom arrays

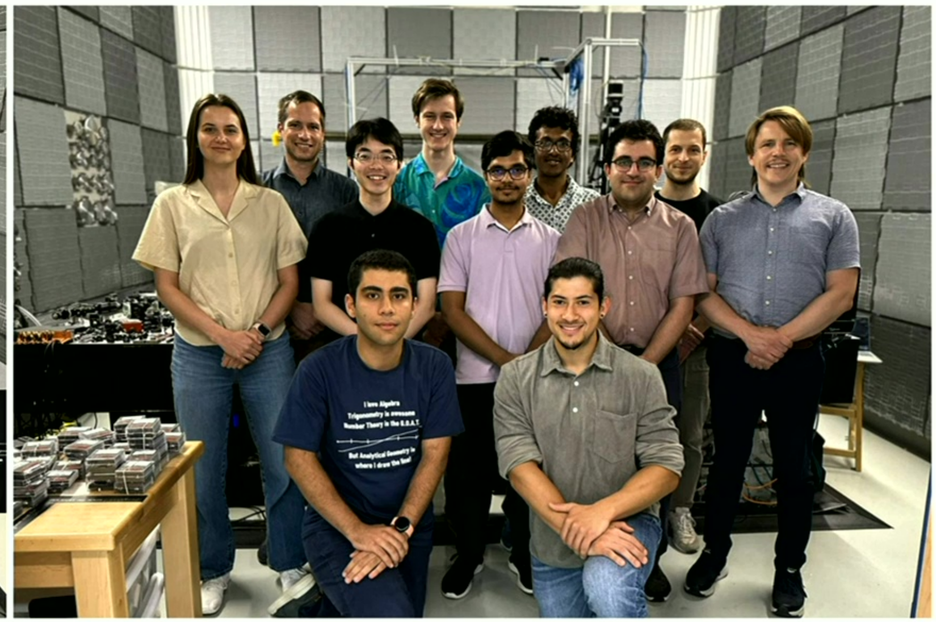
- Long-lived qubits
- Strong, tunable Rydberg-Rydberg interactions
- Quantum spin models on lattices
- Programmable geometry with defects and disorders
- Spin-selective control and readout
- Coherent displacement of atoms for dynamic connectivity
- etc.

Anastasiia Mashko, Artem Zhutov, Soroush Khoubyarian, Kent Ueno

A) Quantum processor based on Rydberg atom arrays

1	1 H	
2	3 Li	4 Be
3	11 Na	12 Mg
4	19 K	20 Ca
5	37 Rb	38 Sr
6	55 Cs	56 Ba
7	87 Fr	88 Ra

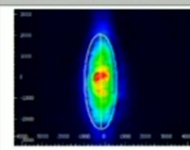
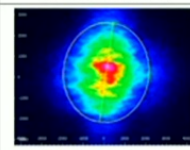
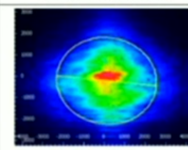
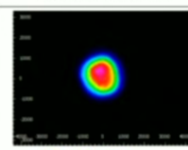


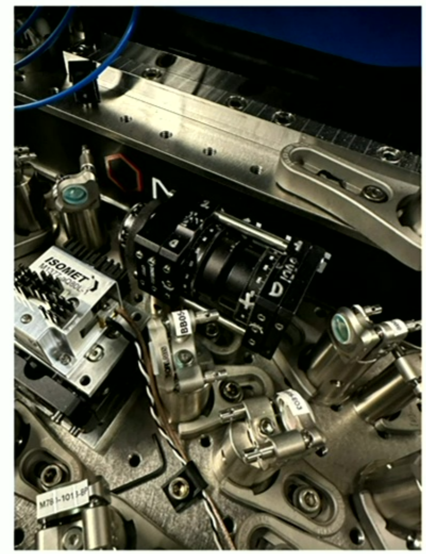


Anastasiia Mashko, Artem Zhutov, Soroush Khoubyarian, Kent Ueno

19

A1) Tunable lens assembly for circularizing elliptical laser beams

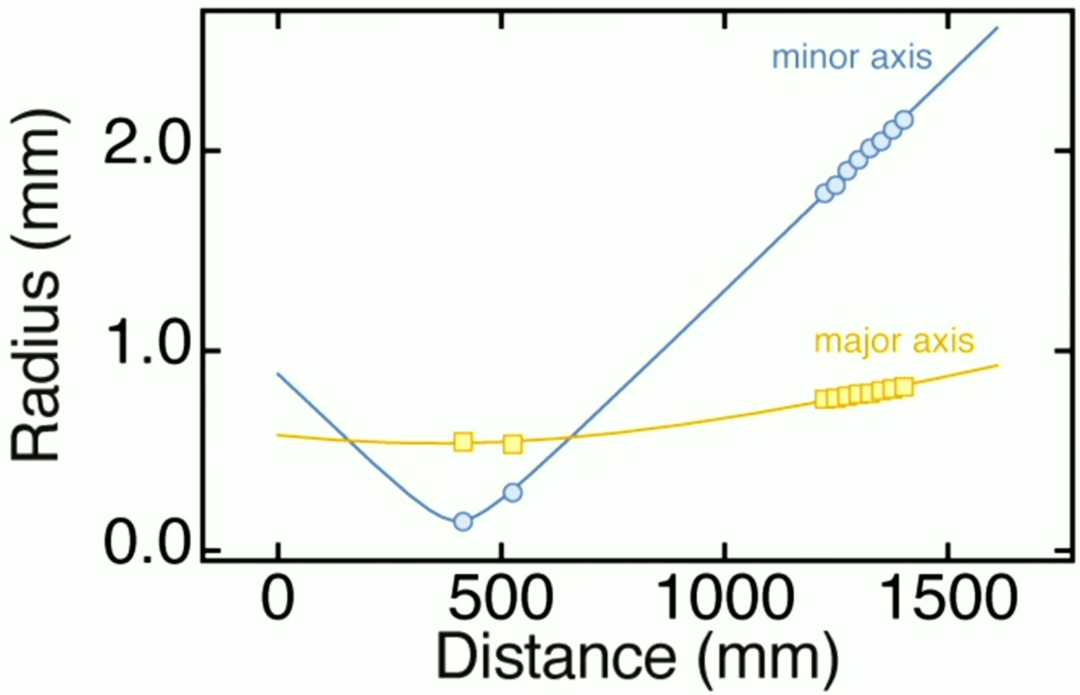
Method	Beam Intensity Profile	Circularity[a]	M^2 Values
Collimated Source Output (No Circularization Technique)	 Click to Enlarge Scale in Microns	0.36	X Axis: 1.28 Y Axis: 1.63
Cylindrical Lens Pair	 Click to Enlarge Scale in Microns	0.84	X Axis: 1.90 Y Axis: 1.93
Anamorphic Prism Pair	 Click to Enlarge Scale in Microns	0.82	X Axis: 1.60 Y Axis: 1.46
Spatial Filter	 Click to Enlarge Scale in Microns	0.93	X Axis: 1.05 Y Axis: 1.10



Source: Thorlabs.com

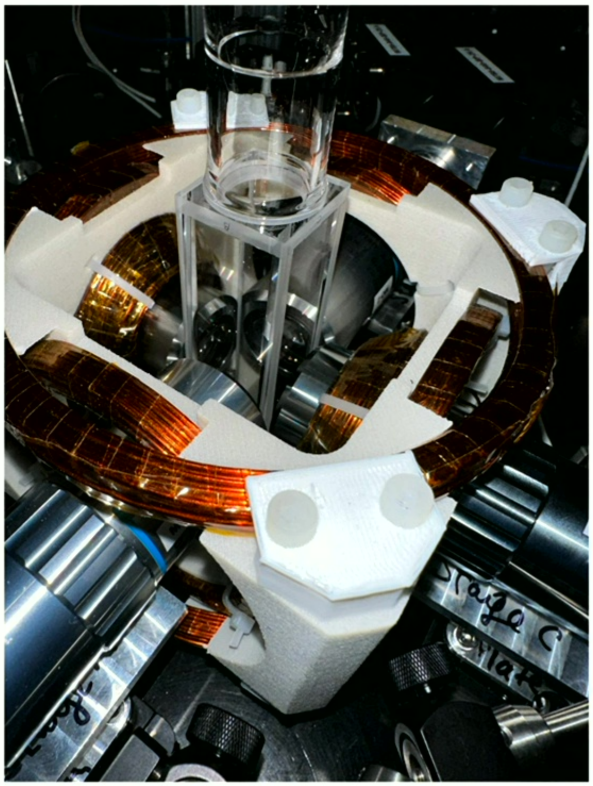
20

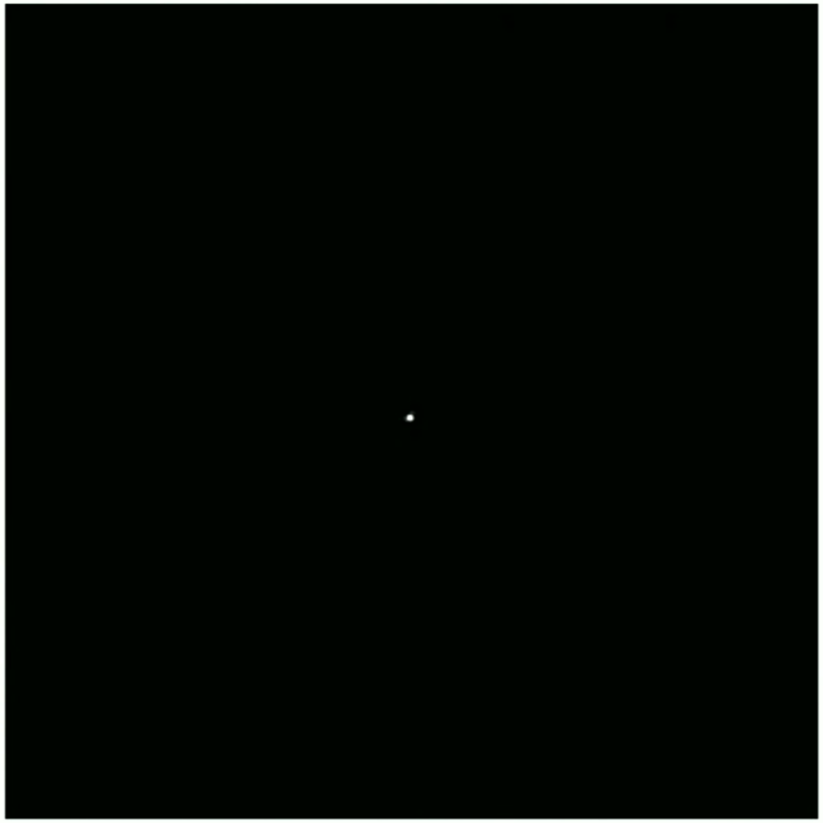
A1) Tunable lens assembly for circularizing elliptical laser beams

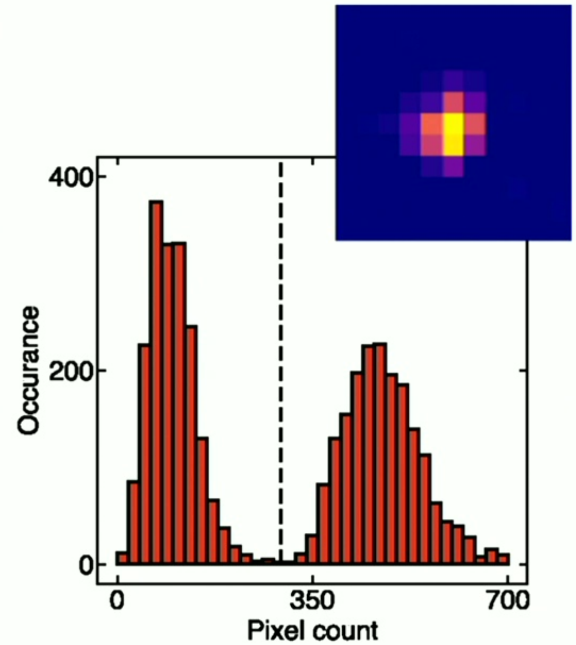


Soroush Khoubyarian, Anastasiia Mashko

A2) Diffractive optical elements for creating large arrays of optical traps

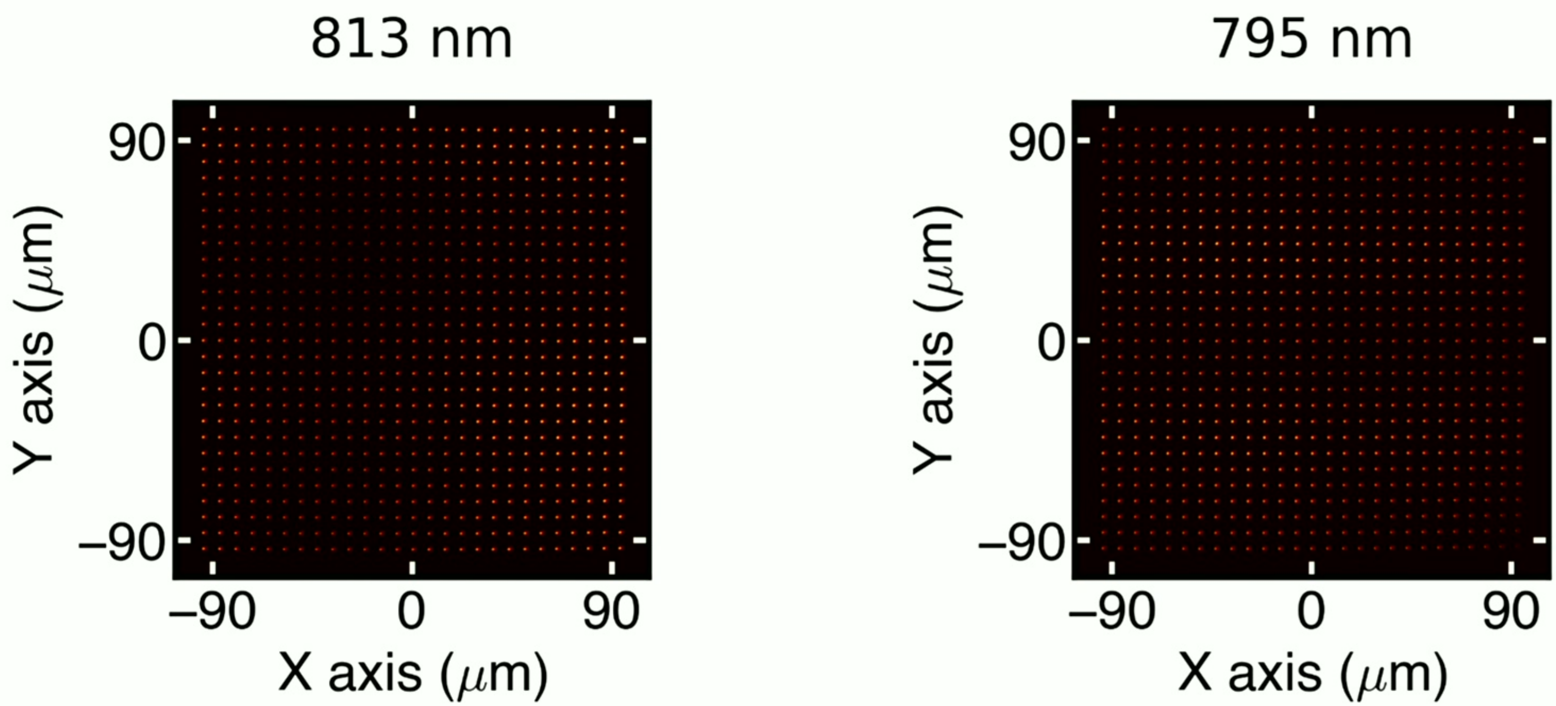






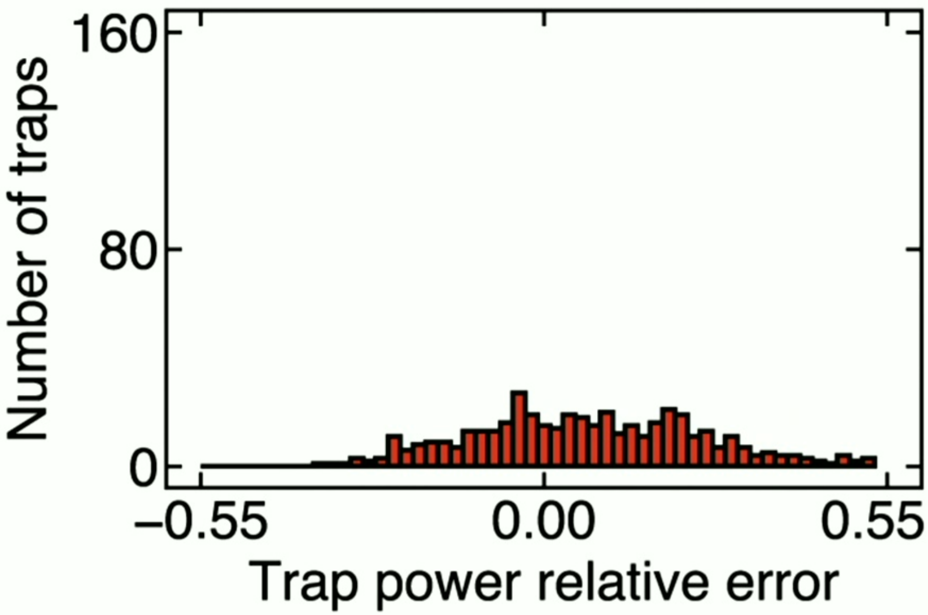
23

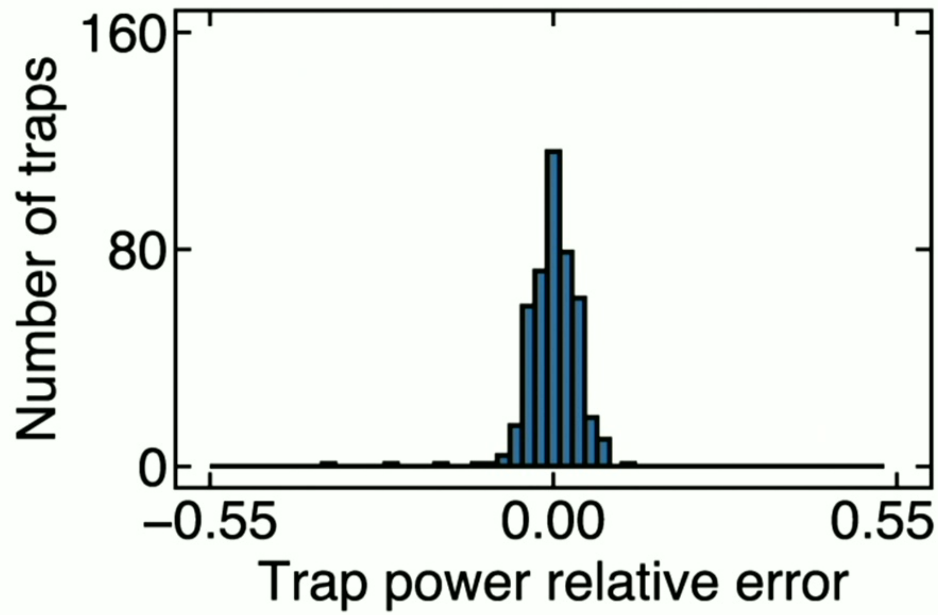
A2) Diffractive optical elements for creating large arrays of optical traps



26

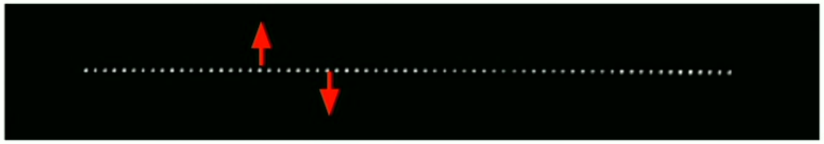
A3) Closed-loop feedback system for creating homogeneous arrays of optical traps

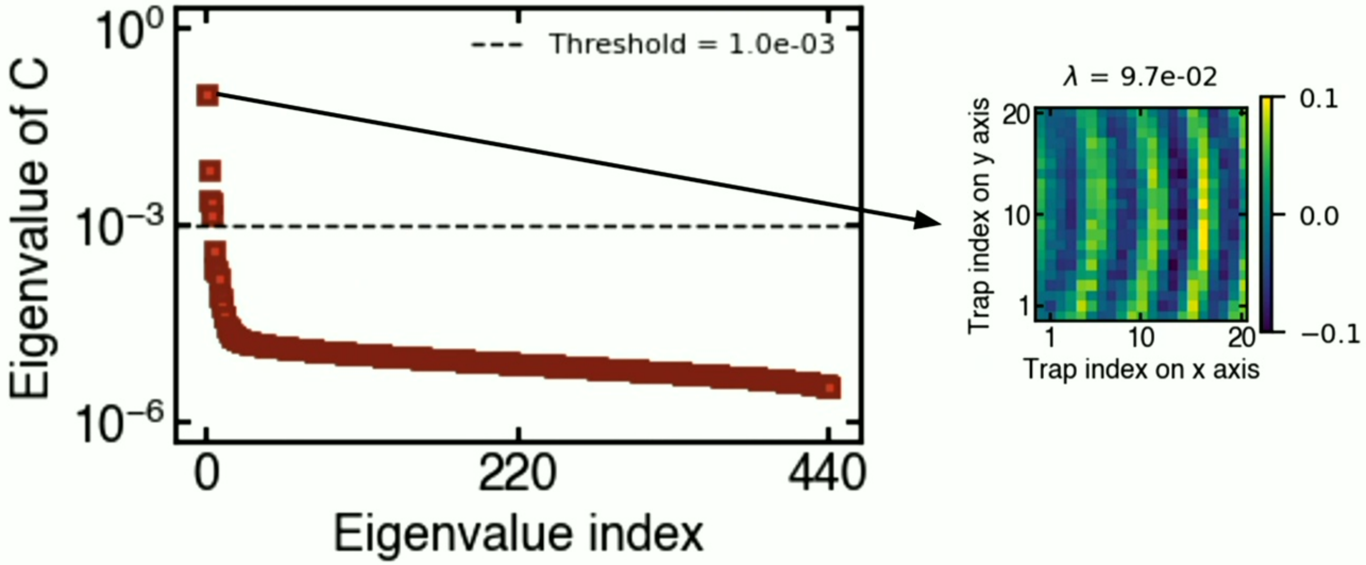




S. Khoubyarian

A3) Closed-loop feedback system for creating homogeneous arrays of optical traps



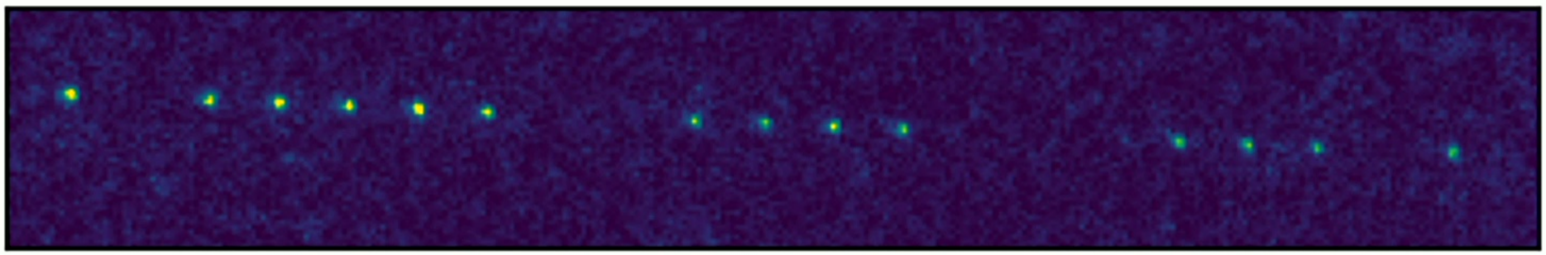


S. Khoubyarian

28

A4) Efficient algorithms for solving atom reconfiguration problems

Trial 3/51 (Cycle 1/2)



Physical Review A 108 (2), 023107 (2023), Physical Review A 108 (2), 023108 (2023)
Collaborators: Prof. Naomi Nishimura (Waterloo), Prof. Izzat El Hajj (AUB), Prof. Amer Mouawad (AUB)

29

A4) Efficient algorithms for solving atom reconfiguration problems

Minimizing distance:

- O(N^2) on uniformly-weighted grids,
- O(N^3) on arbitrary edge-weighted graphs

Minimizing number displacements:

- NP-Hard (Steiner tree problem)
- O(N^α) for 3-approx

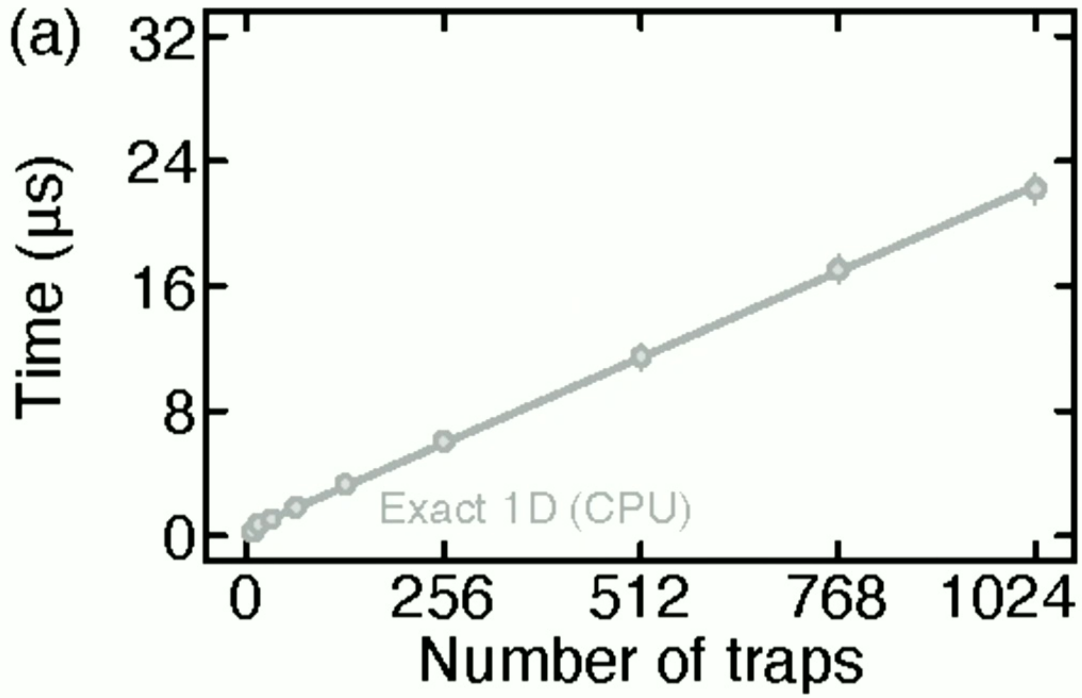
Algorithmica 86, 3284–3308 (2024)
Collaborators: Prof. Naomi Nishimura (Waterloo), Prof. Izzat El Hajj (AUB), Prof. Amer Mouawad (AUB)

A4) Efficient algorithms for solving atom reconfiguration problems

Algorithm	Graph	Configuration	Complexity
exact 1D	Paths/Chains	Arbitrary	$O(n^2)$
red-rec	Grids	Arbitrary	$O(n\sqrt{n})$
aro	Grids	Arbitrary	$O(n^4)$
bird	Grids	Center-compact	$O(n\sqrt{n})$

Fiouani et al. (in preparation)
Collaborators: Prof. Naomi Nishimura (Waterloo), Prof. Izzat El Hajj (AUB), Prof. Amer Mouawad (AUB)

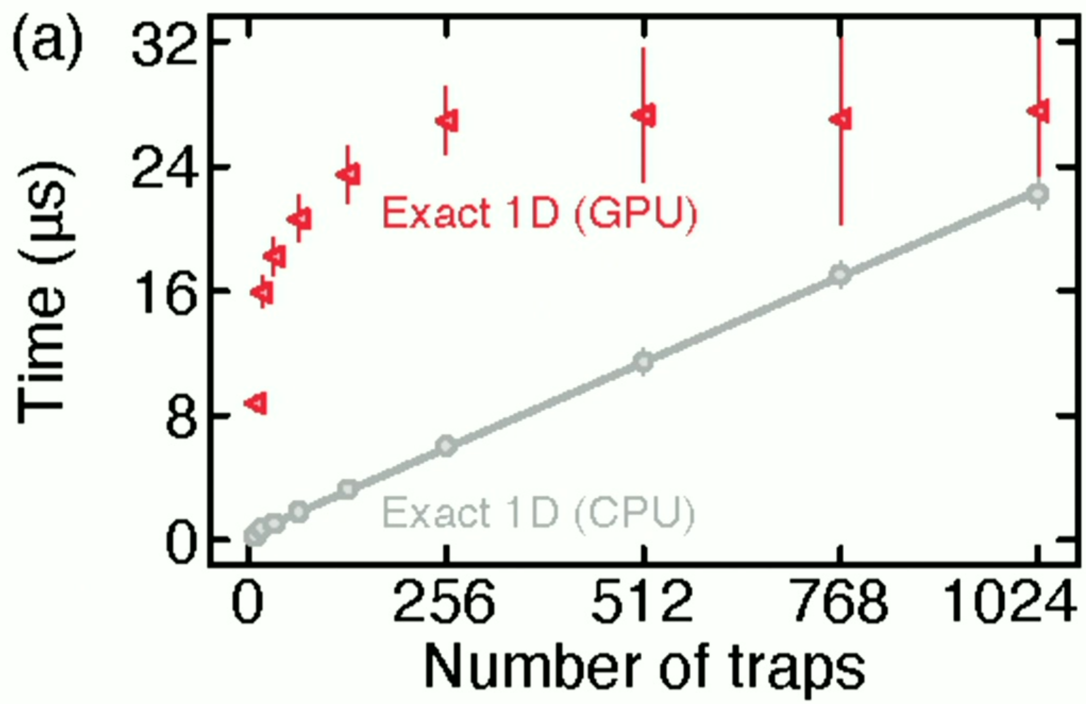
A5) Efficient implementations of atom reconfiguration algorithms on CPUs & GPUs



Dadpour et al. (in preparation)
Collaborators: Prof. Izzat El Hajj (AUB), Prof. Amer Mouawad (AUB)

34

A5) Efficient implementations of atom reconfiguration algorithms on CPUs & GPUs



Dadpour et al. (in preparation)
Collaborators: Prof. Izzat El Hajj (AUB), Prof. Amer Mouawad (AUB)

A5) Efficient implementations of atom reconfiguration algorithms on CPUs & GPUs

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CPUs outperform GPUs for small relevant problem sizes

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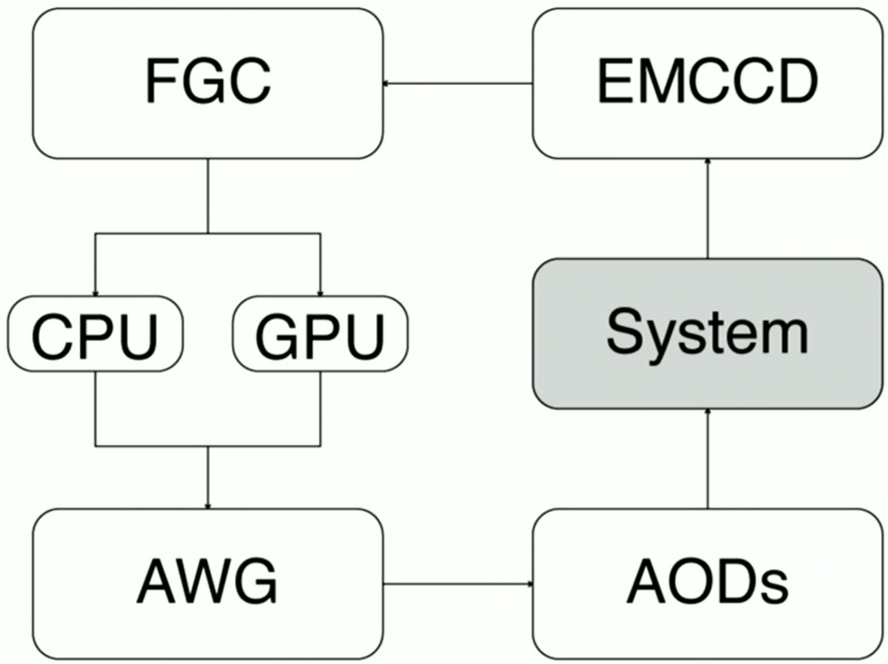
Collaborators: Prof. Izzat El Hajj (AUB), Prof. Amer Mouawad (AUB)

37

A6) Low-latency reconfiguration system for preparing defect-free atom configurations



Open source: https://github.com/TQT-RAAQS/LLRS/
Collaborators: Prof. Izzat El Hajj (AUB), Prof. Amer Mouawad (AUB)

38

A6) Low-latency reconfiguration system for preparing defect-free atom configurations

	Reconfiguration cycle time (ms)		
	Exact 1D $N_a = 1 \times 32$ $N_t = 1 \times 64$ ROI = 16 × 1024	red-rec $N_a = 16 \times 16$ $N_t = 16 \times 32$ ROI = 256 × 512	red-rec $N_a = 32 \times 32$ $N_t = 32 \times 64$ ROI = 512 × 1024
I. Imagree acquisition	25.454± 0.695	30.850± 0.588	46.250± 0.707
I.1 Exposure*	20.000	20.000	20.000
I.2 Vertical frame transfer* (4 .33 μs / px)	4.499	4.499	4.499
I.3 Frame readouts* (30 Mpxps)	0.677	5.923	20.549
I.4 DMA data transfer	0.278	0.428	1.202
II. Image processing	0.259± 0.108	0.281± 0.158	0.277± 0.084
II.1 Deconvolution	0.259	0.279	0.269
II.2 Thresholding	0.001	0.002	0.007
III. Problem solving	0.008± 0.001	0.059± 0.005	0.177± 0.014
III.1 Solving	0.005	0.035	0.100
III.2 Batching	0.003	0.024	0.077
IV. Synthesis & Waveform loading	0.630± 0.268	0.663± 0.117	0.635± 0.247
IV.1 Lookup waveforms (2 × 32 = 64 wfms)	0.078	0.046	0.038
IV.2 Upload waveforms (2 segments)	0.553	0.593	0.574
IV.3 Configure sequence memory	0.000	0.025	0.023
V. Concurrent load & stream	0.746± 0.004	2.765± 0.392	8.496± 0.577
V.1 Streaming time*	0.640± 0.000	2.667± 0.355	8.392± 0.533
V.2 Other	0.106± 0.004	0.098± 0.191	0.104± 0.231
Total	27.097± 1.076	34.618± 1.260	55.835± 1.629

Open source: https://github.com/TQT-RAAQS/LLRS/

Collaborators: Prof. Izzat El Hajj (AUB), Prof. Amer Mouawad (AUB)

40

A6) Low-latency reconfiguration system for preparing defect-free atom configurations

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Runtime limited by camera and displacement speed

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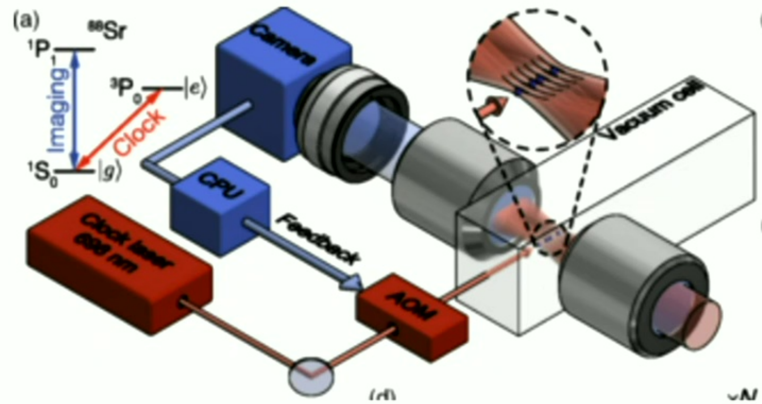
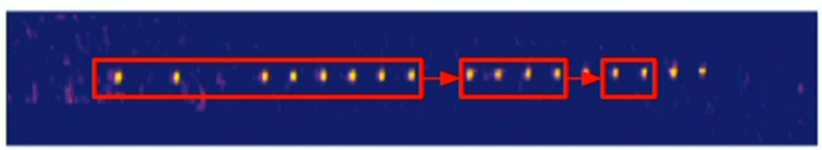
Open source: https://github.com/TQT-RAAQS/LLRS/

Collaborators: Prof. Izzat El Hajj (AUB), Prof. Amer Mouawad (AUB)

41

C1) Measurements and feed-forward for quantum-enhanced atom-array optical clocks

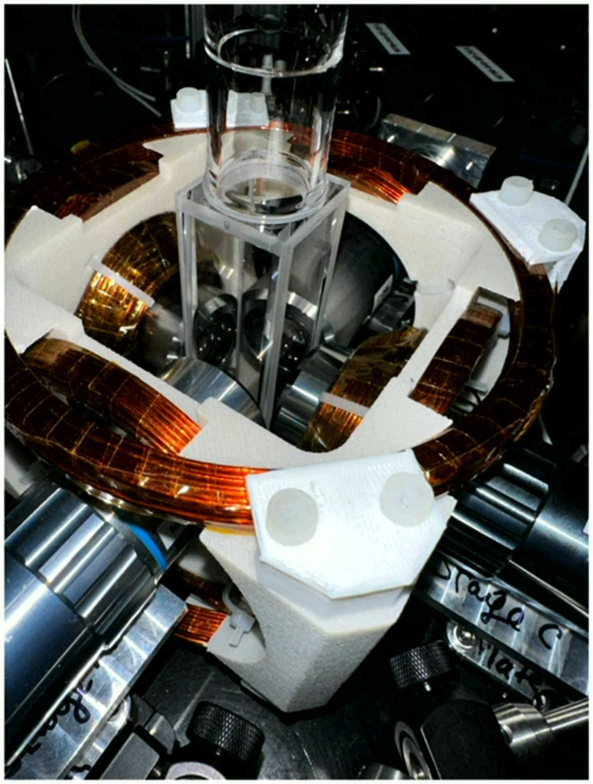


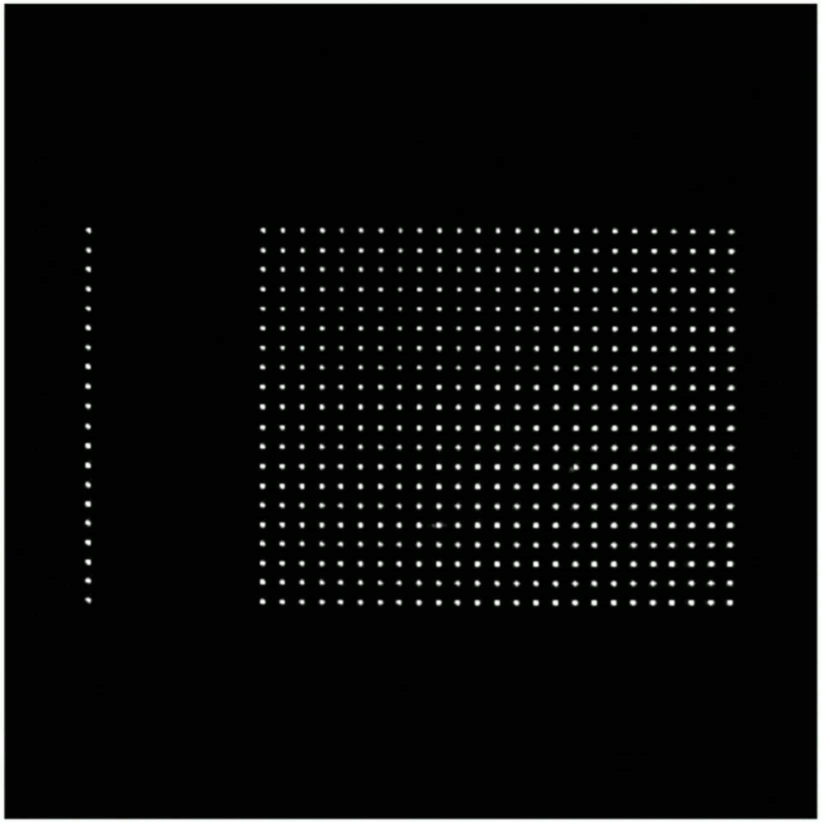


Caltech: Phys. Rev. X 9, 041052 (2019)

42

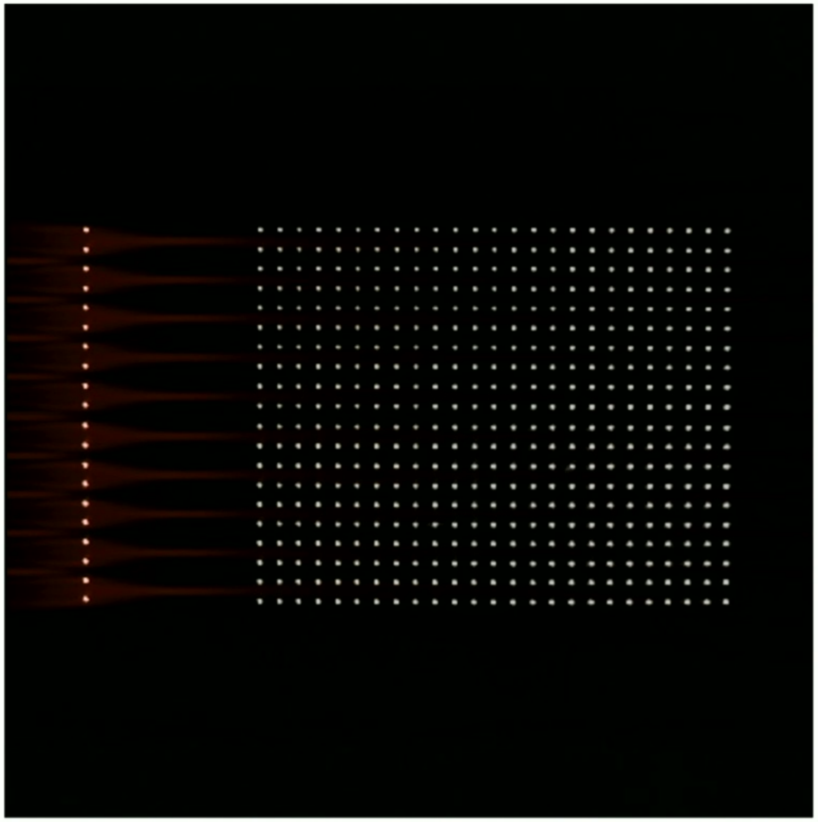
A8) Diffractive optical elements for creating atom-selective coherent control gates

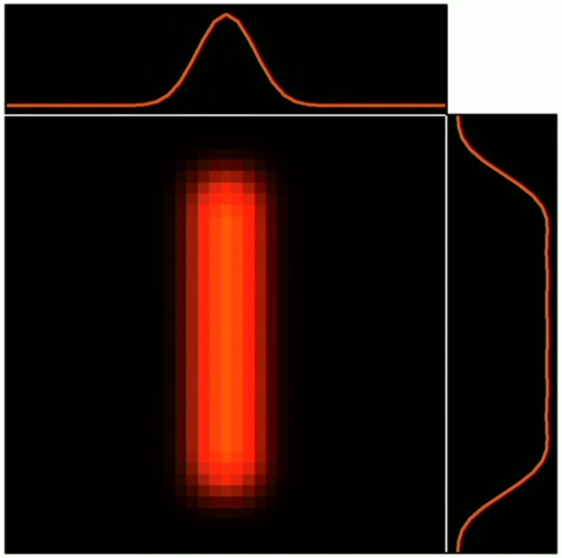




44

A8) Diffractive optical elements for creating atom-selective coherent control gates





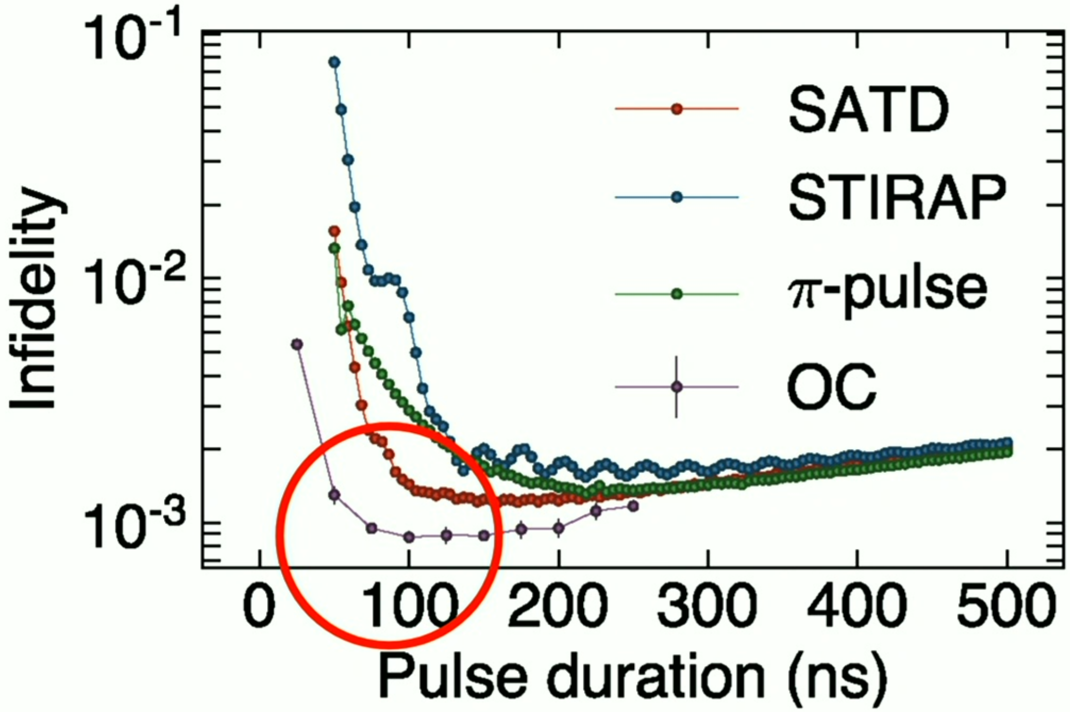
45

A8) Diffractive optical elements for creating atom-selective coherent control gates

Transverse-field Ising Hamiltonian with Site-Selective Parameters

$$\hat{\mathcal{H}} = \sum_{i}^{L} \boxed{\frac{\Omega_i}{2}} \hat{\sigma}_x^i - \sum_{i}^{L} \Delta_i \hat{\sigma}_{rr}^i + \sum_{i<j} V_{ij} \hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j$$

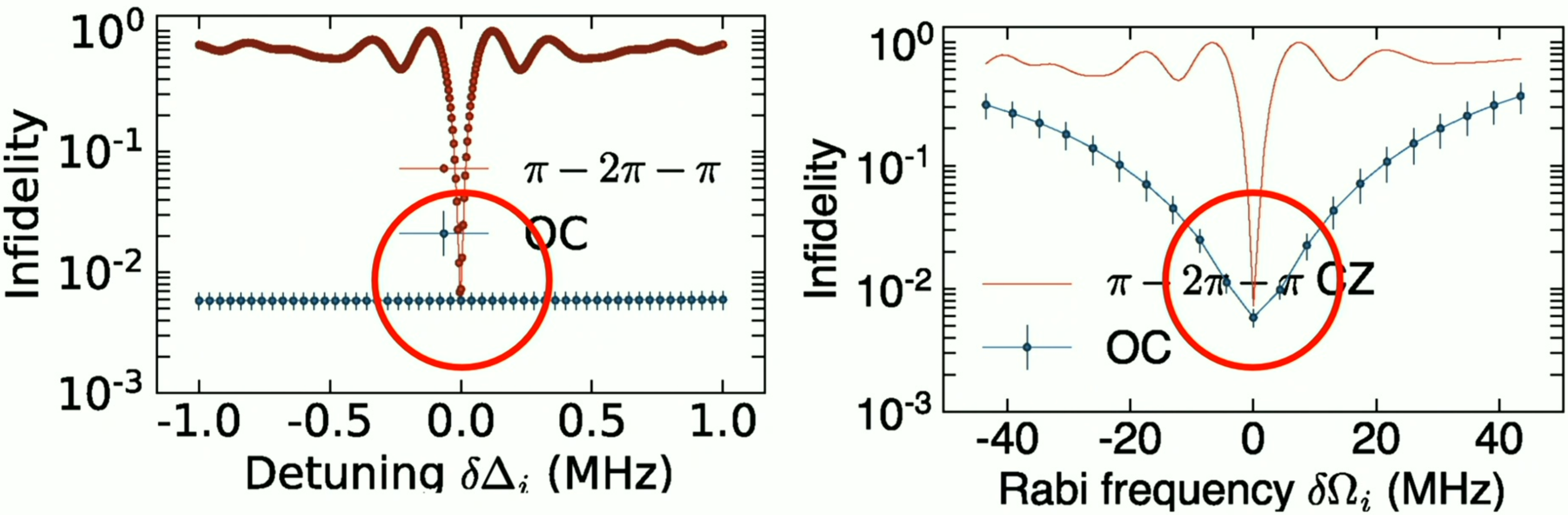
A9) Optimal control pulses for fast and robust entangling gates



Artem Zhutov, Dr. Jeremy Flannery

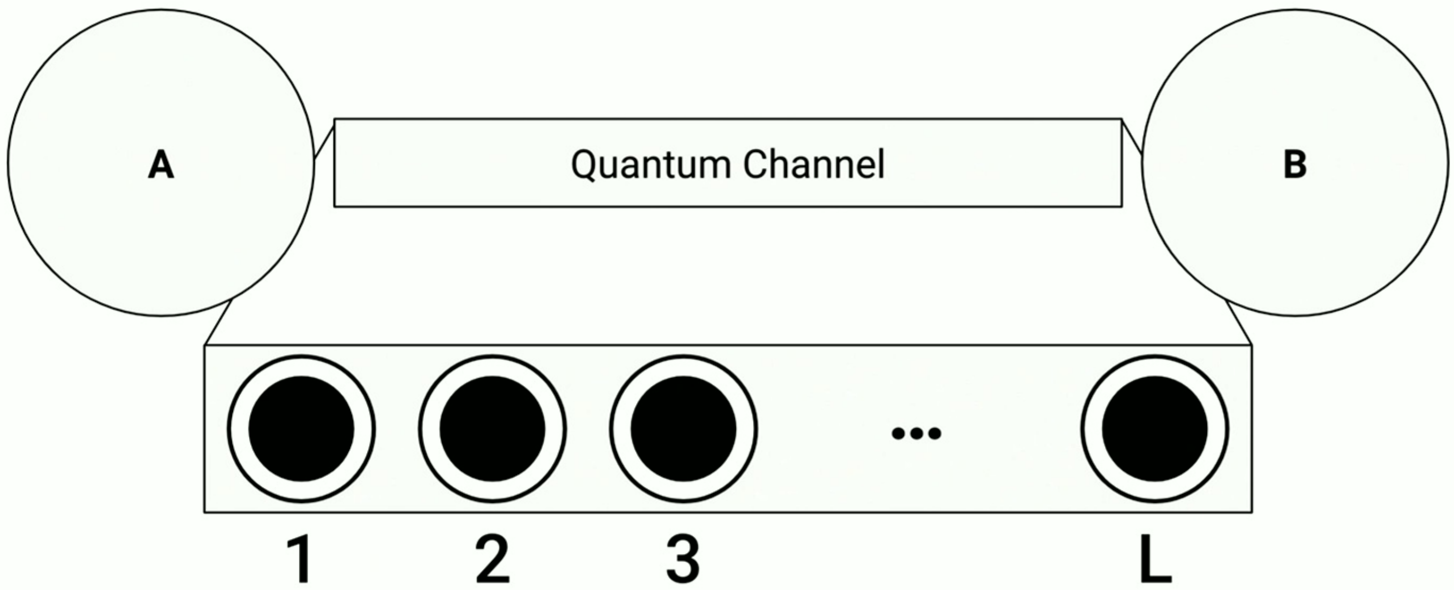
47

A9) Optimal control pulses for fast and robust entangling gates



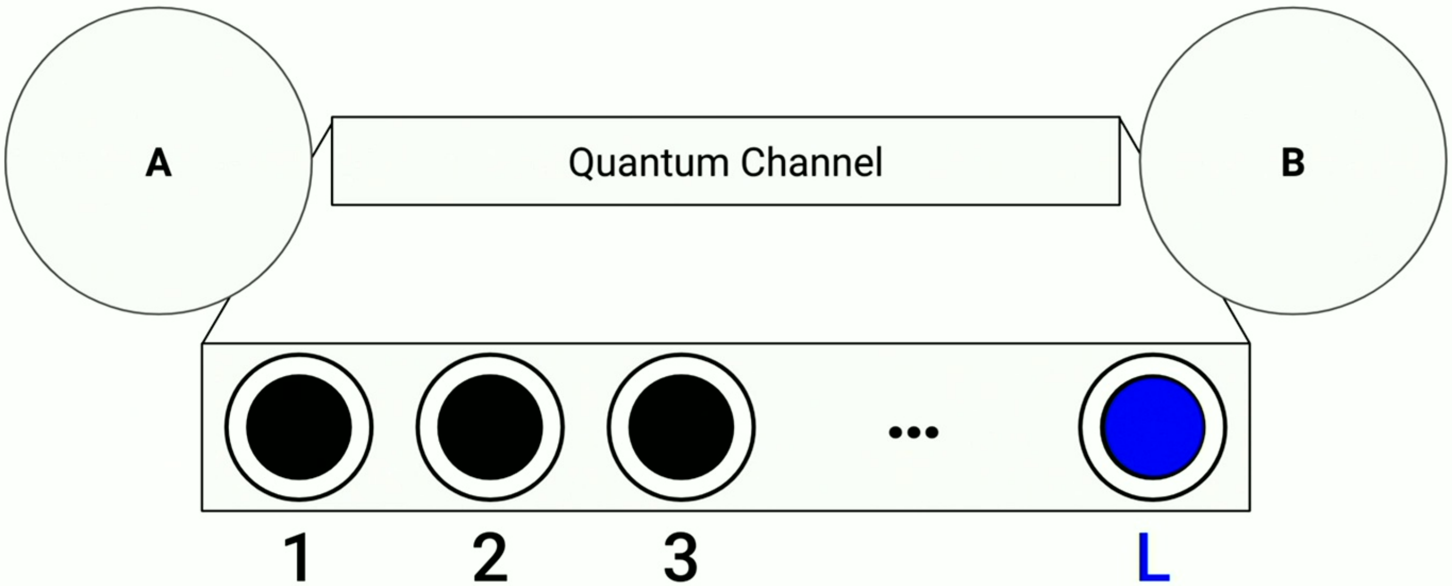
Artem Zhutov, Dr. Jeremy Flannery

B1) Perfect transport of single Rydberg excitations in chains of neutral atoms



51

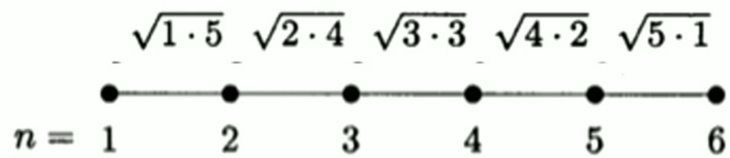
B1) Perfect transport of single Rydberg excitations in chains of neutral atoms

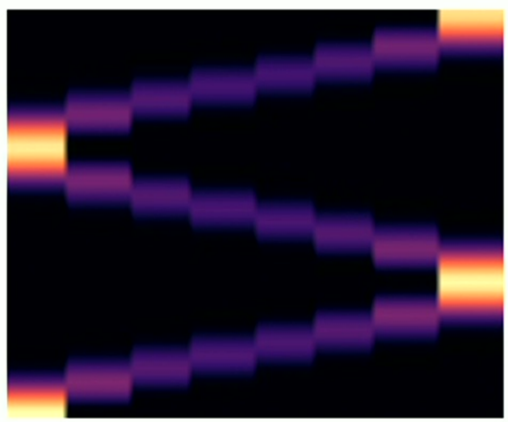


53

B1) Perfect transport of single Rydberg excitations in chains of neutral atoms

$$\hat{\mathcal{H}}_{\text{eff}} = \sum_i \mu_i \hat{\sigma}_+^i \hat{\sigma}_-^i + \sum_{i<j} J_{ij} \left(\hat{\sigma}_+^i \hat{\sigma}_-^j + \hat{\sigma}_+^j \hat{\sigma}_-^i \right)$$





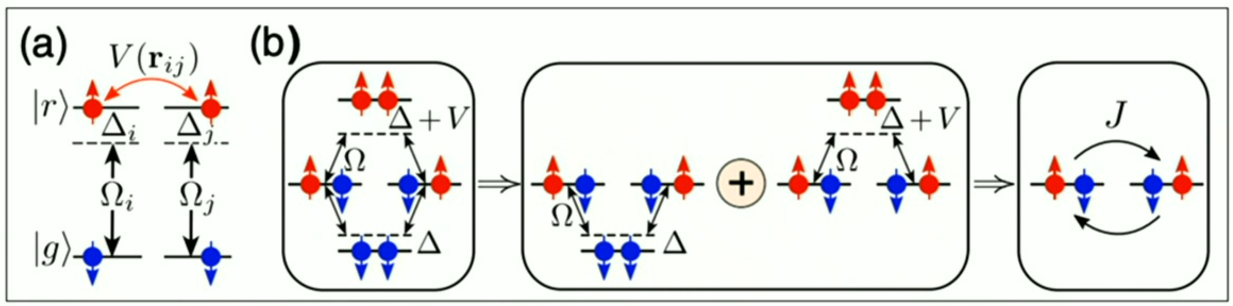
Quantum Speed Limit!

$$t_\pi(L) = \frac{\pi \bar{L}}{4 J_{\max}}$$

Kent Ueno

B1) Perfect transport of single Rydberg excitations in chains of neutral atoms

$$\hat{\mathcal{H}} = \sum_i^L \frac{\Omega_i}{2}\hat{\sigma}_x^i - \sum_i^L \Delta_i \hat{\sigma}_{rr}^i + \sum_{i<j} V_{ij}\hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j$$



$$\hat{\mathcal{H}}_{\text{eff}} = \sum_i \mu_i \hat{\sigma}_+^i \hat{\sigma}_-^i + \sum_{i<j} J_{ij}\left(\hat{\sigma}_+^i \hat{\sigma}_-^j + \hat{\sigma}_+^j \hat{\sigma}_-^i\right)$$

See Yang2019, Phys. Rev. Lett. 123, 063001 (2019)
Kent Ueno

B1) Perfect transport of single Rydberg excitations in chains of neutral atoms

$$\hat{\mathcal{H}} = \sum_{i}^{L} \frac{\Omega_i}{2}\hat{\sigma}_x^i - \sum_{i}^{L} \Delta_i \hat{\sigma}_{rr}^i + \sum_{i<j} V_{ij}\hat{\sigma}_{rr}^i \hat{\sigma}_{rr}^j$$

Hierarchy of approximations

1) 2nd order perturbation theory
2) Nearest-neighbor approximation

$$\hat{\mathcal{H}}_{\text{eff}} = \sum_{i} \mu_i \hat{\sigma}_+^i \hat{\sigma}_-^i + \sum_{i<j} J_{ij}\left(\hat{\sigma}_+^i \hat{\sigma}_-^j + \hat{\sigma}_+^j \hat{\sigma}_-^i\right)$$

See Yang2019, Phys. Rev. Lett. 123, 063001 (2019)
Kent Ueno

B1) Perfect transport of single Rydberg excitations in chains of neutral atoms

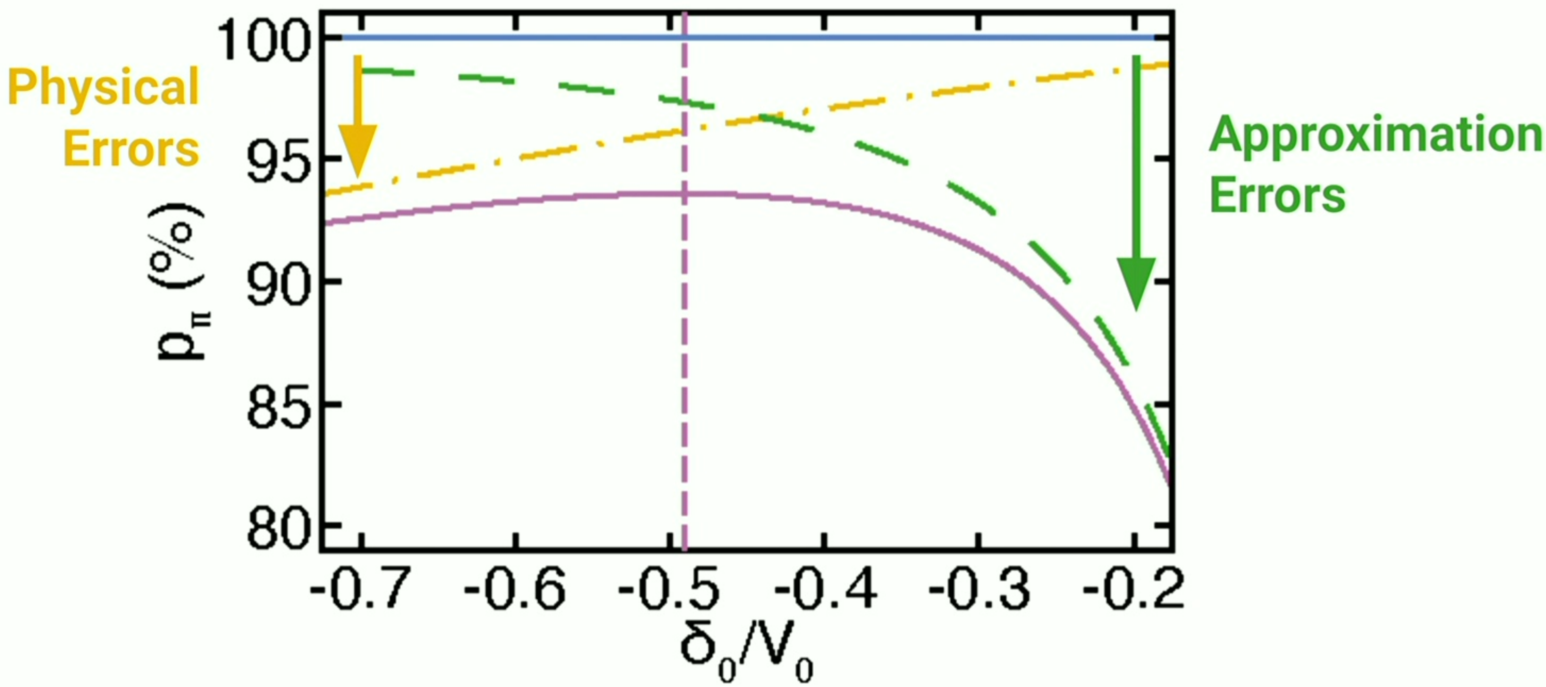
Approximation Errors ⟷ **Tradeoff** ⟷ **Physical Errors**

Large detuning to increase validity of perturbation theory → Slower transport → High probability of radiative decay

Injection of spin excitations ← Faster transport ← Small detuning to reduce transport time w/r to radiative decay

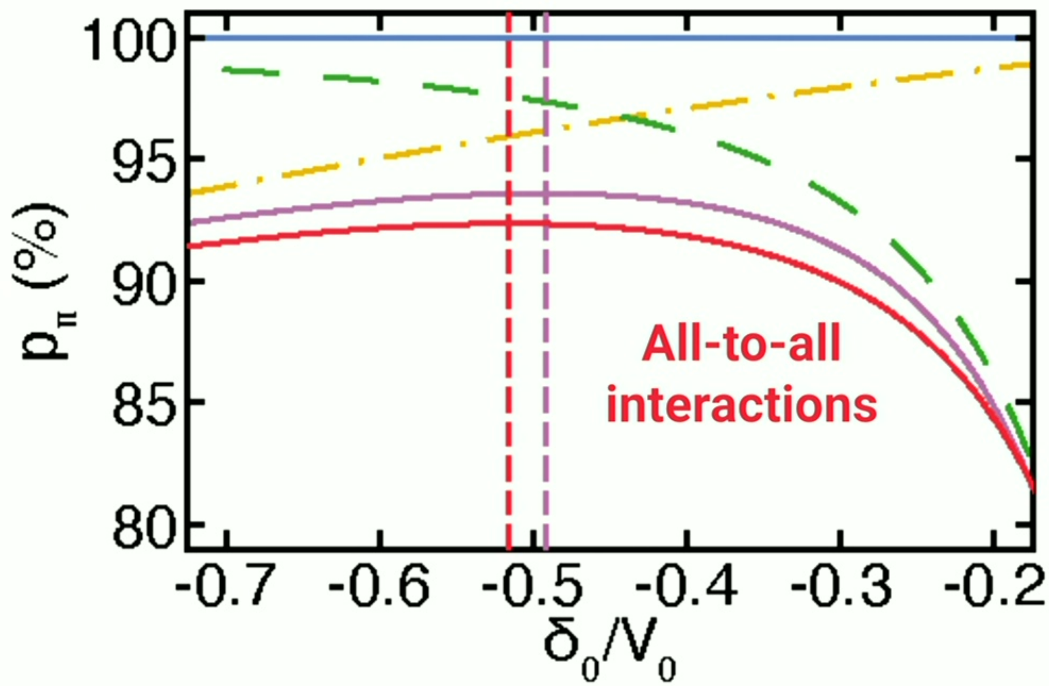
Kent Ueno (manuscript in preparation)

B1) Perfect transport of single Rydberg excitations in chains of neutral atoms



Kent Ueno

B1) Perfect transport of single Rydberg excitations in chains of neutral atoms



Kent Ueno

B1) Perfect transport of single Rydberg excitations in chains of neutral atoms

Physical Parameters ⟷ **Tradeoff** ⟷ **Physical Errors**

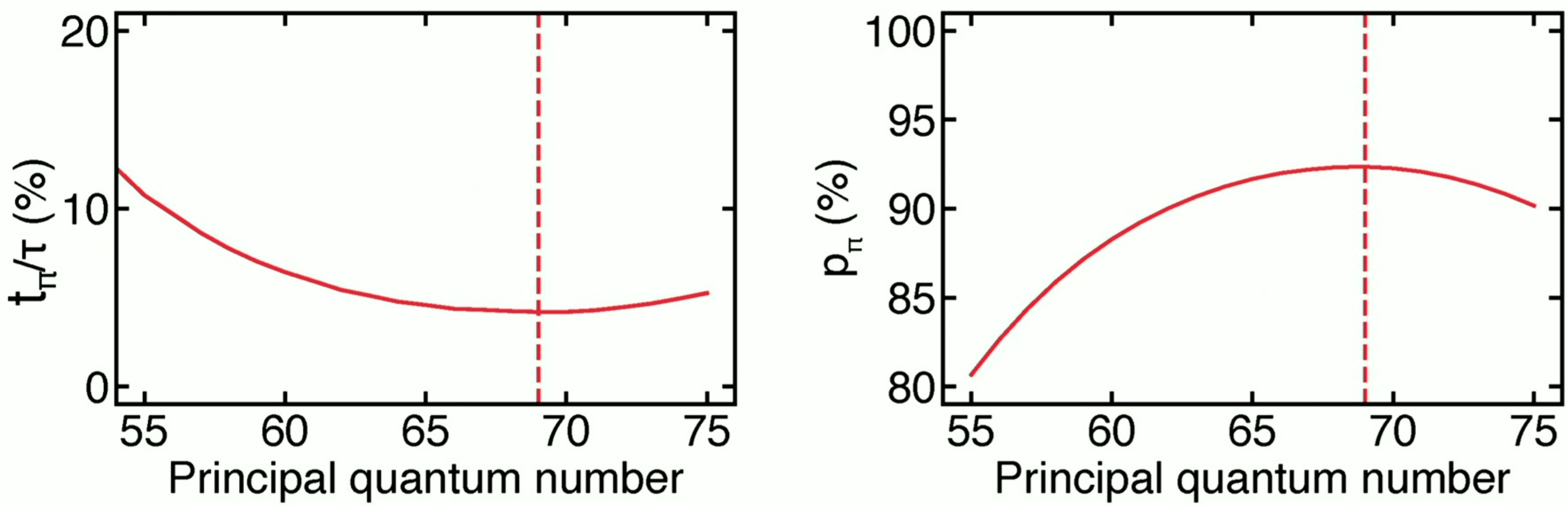
Interaction strength
$C6 \sim n^{11}$

Rabi frequency
$\Omega \sim n^{-3}$

Radiative lifetime
$\tau \sim n^3$

Kent Ueno

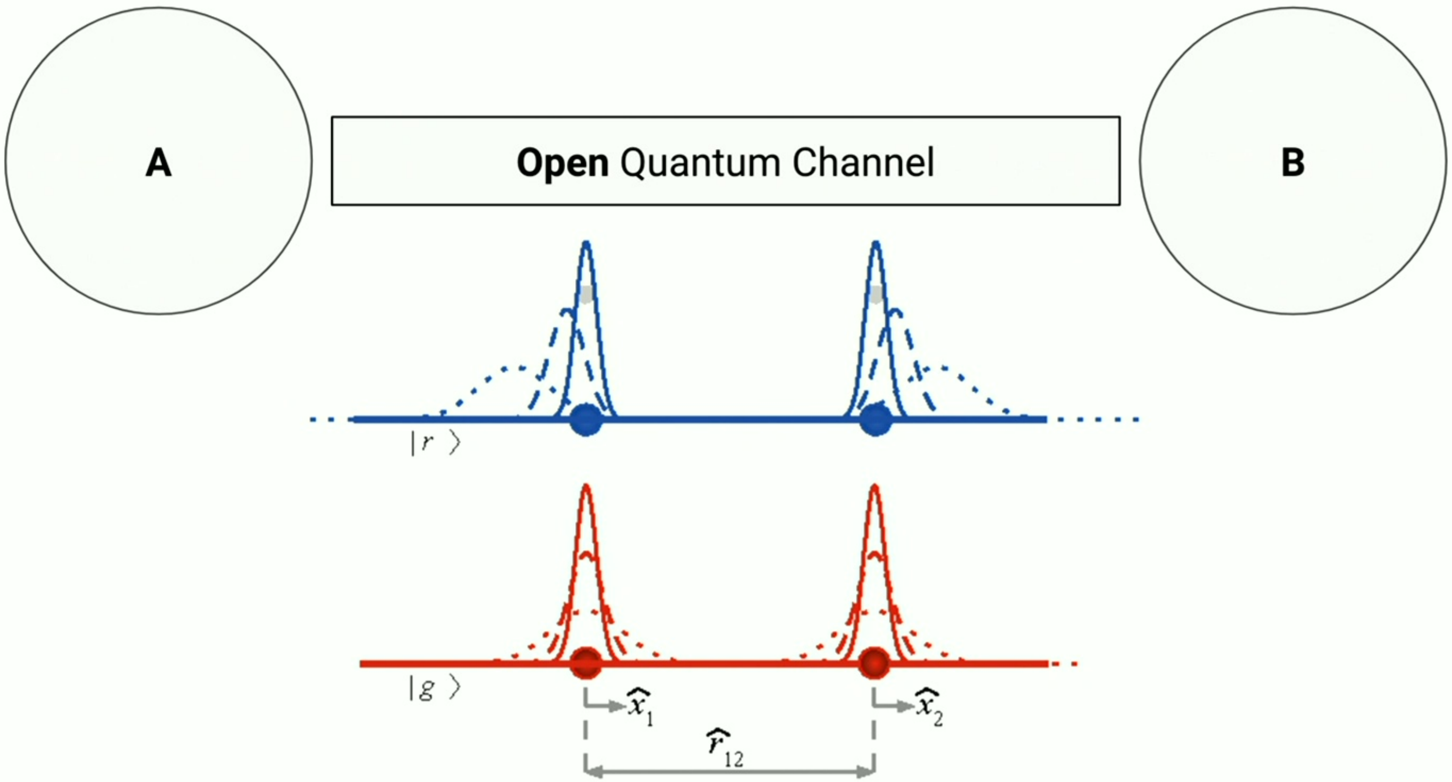
B1) Perfect transport of single Rydberg excitations in chains of neutral atoms



Kent Ueno

66

B2) Quantum channel for modeling spin-motion dephasing in Rydberg chains



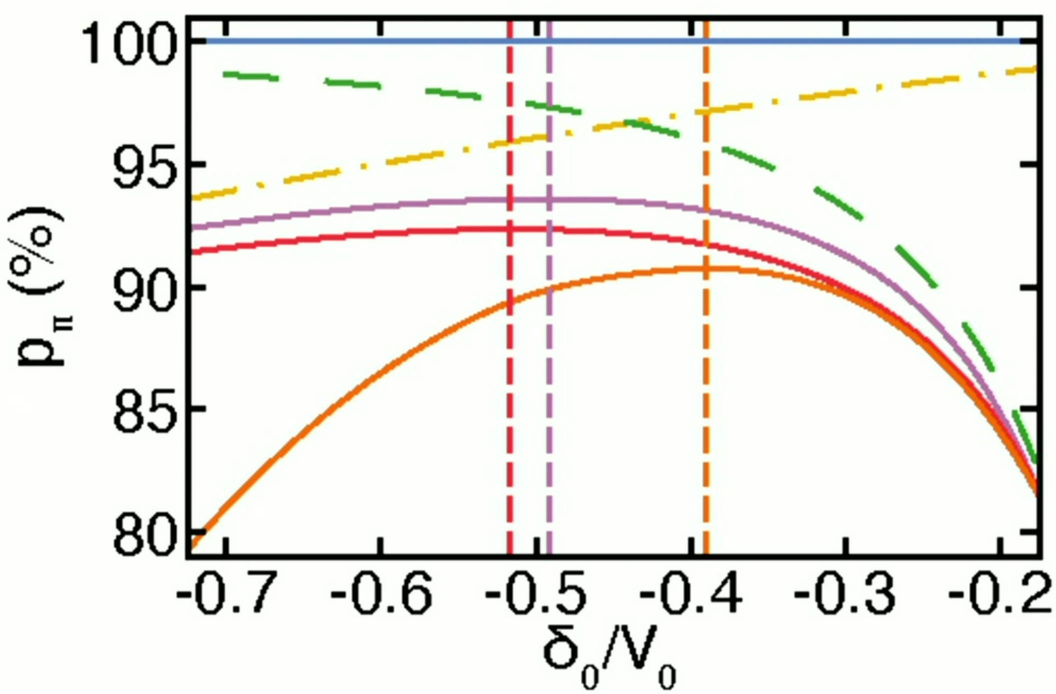
69

B2) Quantum channel for modeling spin-motion dephasing in Rydberg chains

$$\rho'_{nm}(t) = \Gamma_{nm}(t)\rho^{\mathrm{fga}}_{nm}(t),$$
$$\Gamma_{nm}(t) = C^*_n(t)C_m(t)\gamma_{nm}(t)$$

Dr. Chris Wyenberg (manuscript in preparation)

B2) Quantum channel for modeling spin-motion dephasing in Rydberg chains



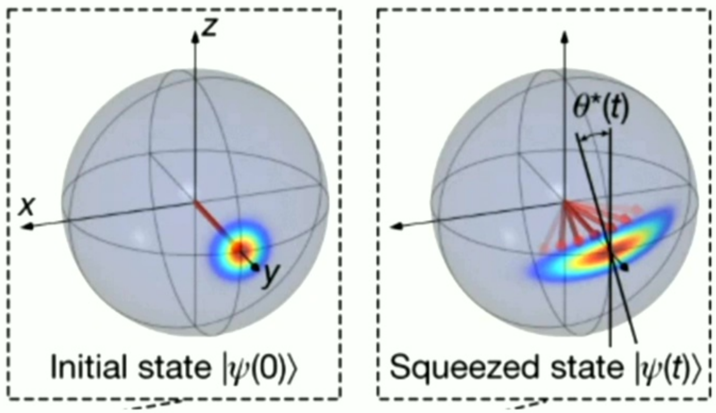
Kent Ueno, Dr. Chris Wyenberg

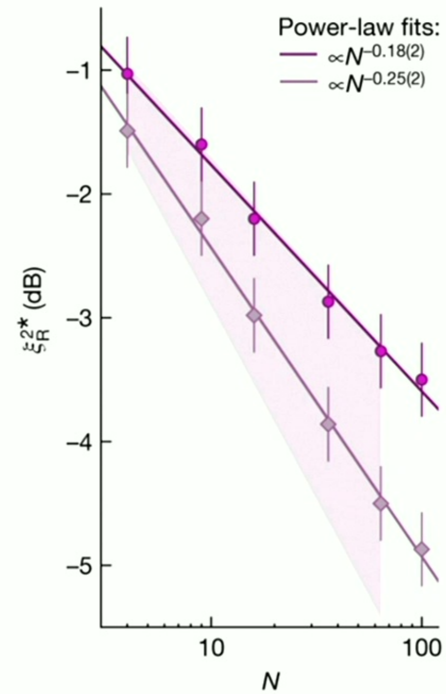
71

B3) Scalable spin squeezing in two-dimensional dipolar spin lattices

$$\mathcal{H} = -\frac{J_d}{2}\sum_{i\neq j}\frac{1}{r_{ij}^3}\left(S_i^x S_j^x + S_i^y S_j^y\right)$$

$$\mathcal{H} = \chi J_z^2$$





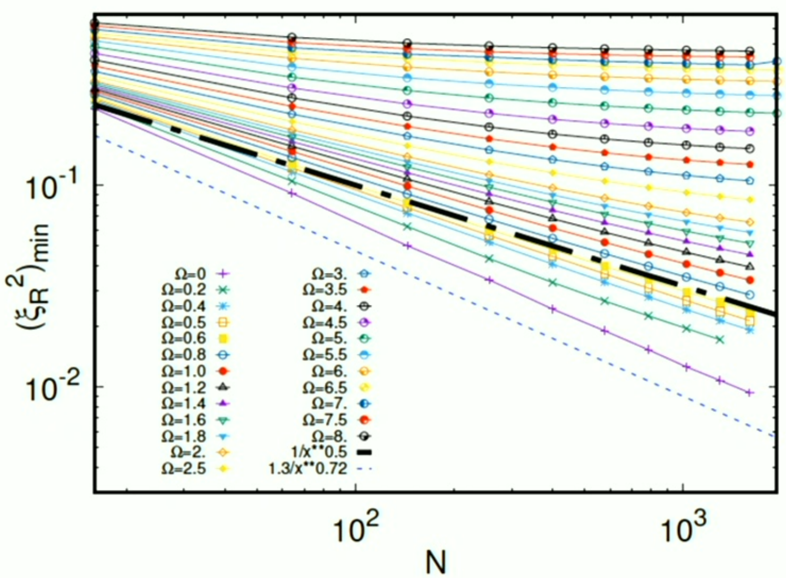
Inspired from *Nature* **621**, 728–733 (2023) from A. Browaeys
Collaborators: Dr. Meenu Kumari (NRC), Profs. Fabio Mezzacapo and Tommaso Roscilde (ENS Lyon)

73

B3) Scalable spin squeezing in two-dimensional dipolar spin lattices

$$\mathcal{H} = -\frac{J_d}{2}\sum_{i\neq j}\frac{1}{r_{ij}^3}\left(S_i^x S_j^x + S_i^y S_j^y\right) + \Omega\sum S_i^x$$

$$\mathcal{H} = \chi J_z^2 + \Omega J_x$$



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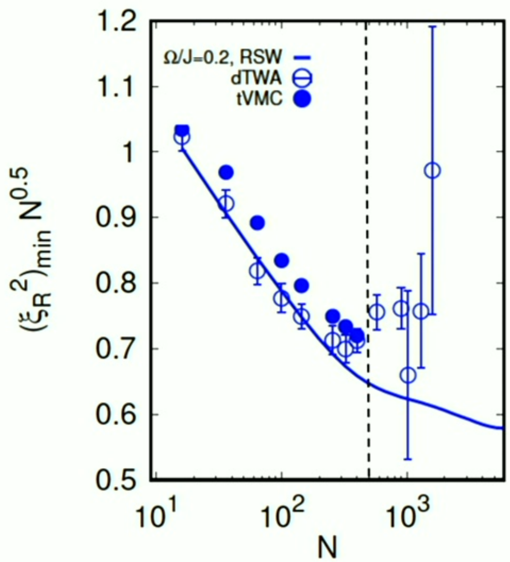
B3) Scalable spin squeezing in two-dimensional dipolar spin lattices

$$\mathcal{H} = -\frac{J_d}{2}\sum_{i\neq j}\frac{1}{r_{ij}^3}\left(S_i^x S_j^x + S_i^y S_j^y\right) + \Omega\sum_i S_i^x$$

$$\mathcal{H} = \chi J_z^2 + \Omega J_x$$



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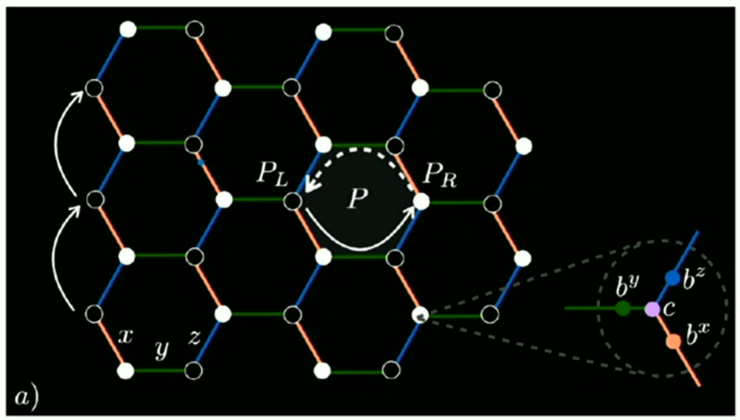
Collaborators: Dr. Meenu Kumari (NRC), Profs. Fabio Mezzacapo and Tommaso Roscilde (ENS Lyon)

75

B4) Anomalous chiral edge flow in Kitaev Honeycomb model

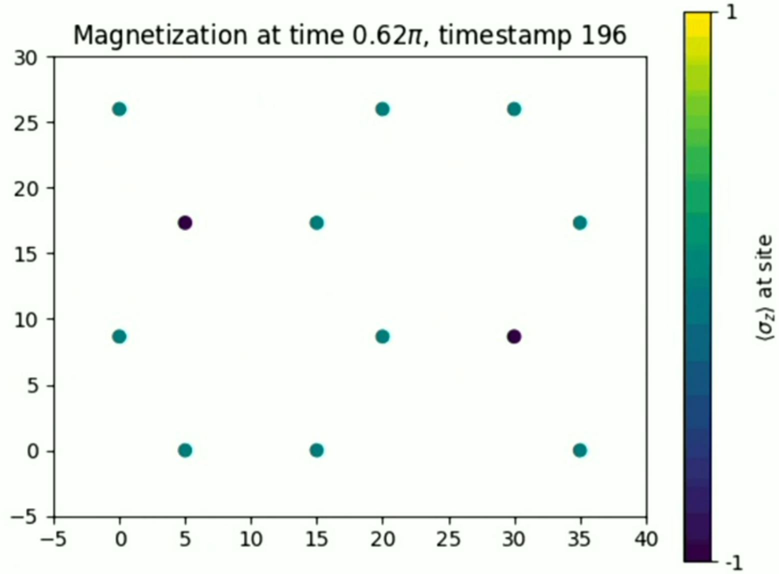
$$\mathcal{H} = \mathcal{H}_{XX} + \mathcal{H}_{YY} + \mathcal{H}_{ZZ}$$

$$\exp(-it\mathcal{H}) \approx \exp(it\mathcal{H}_F) = \sum_{n=1}^{N} \exp(-i\frac{t}{N}\mathcal{H}_{XX})\exp(-i\frac{t}{N}\mathcal{H}_{YY})\exp(-i\frac{t}{N}\mathcal{H}_{ZZ})$$



Collaborators: Dr. Jacob Lin (Maryland)

B4) Anomalous chiral edge flow in Kitaev Honeycomb model

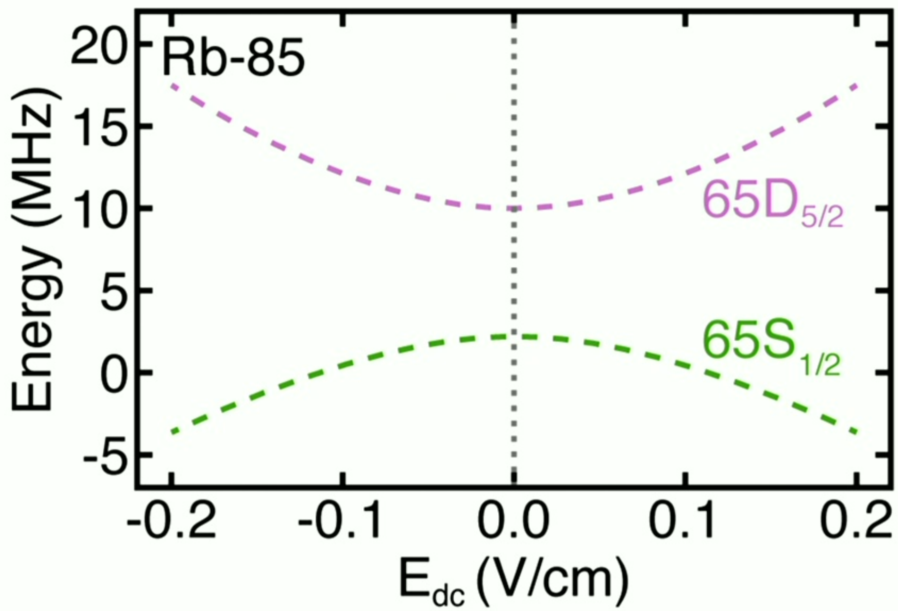


$$\mathcal{H}(t) = \mathcal{H}(t+T)$$

$$T = \frac{3\pi}{4J}$$

Collaborators: Dr. Jacob Lin (Maryland)

C2) Rydberg DC electrometry using bichromatic Floquet engineering



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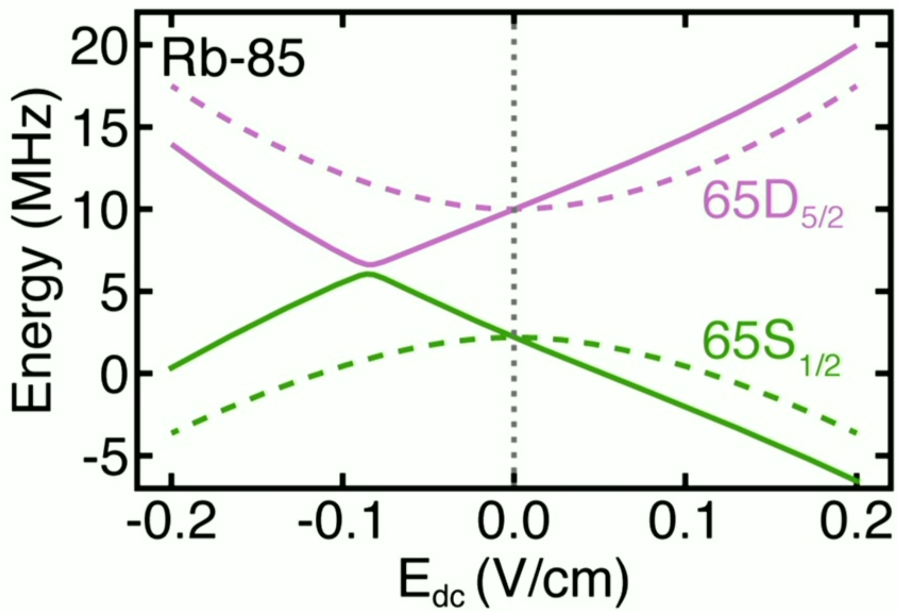
78

C2) Rydberg DC electrometry using bichromatic Floquet engineering



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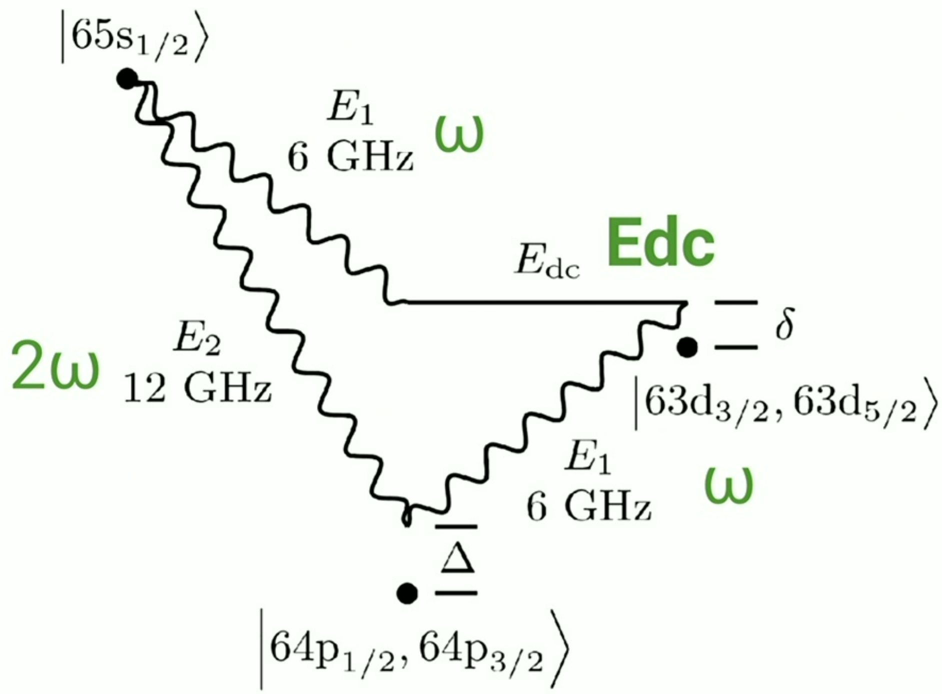
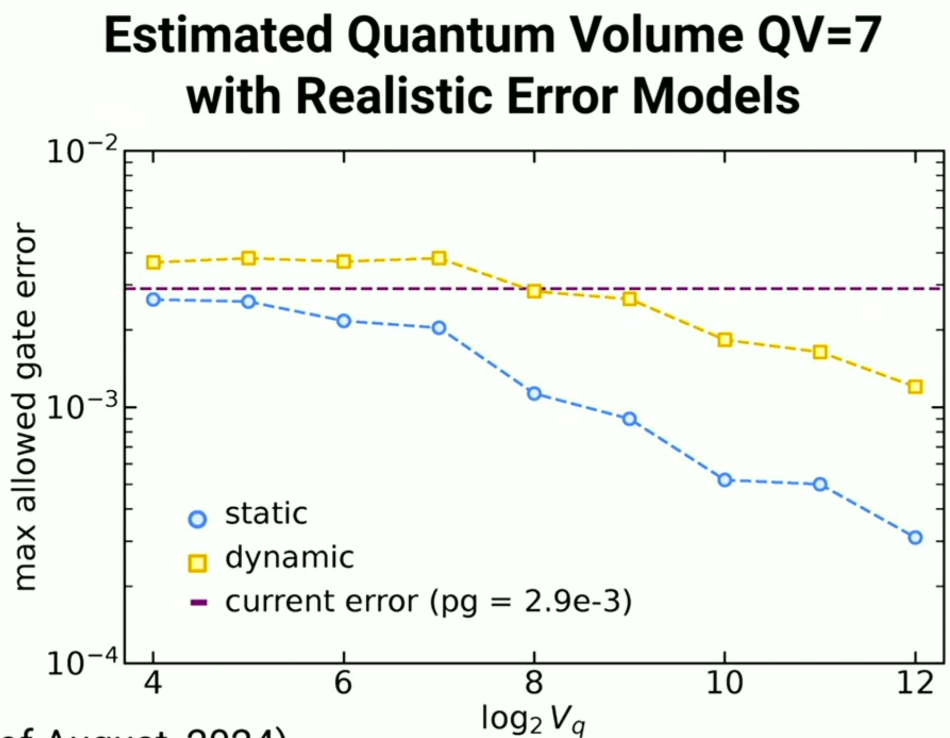
79

C2) Rydberg DC electrometry using bichromatic Floquet engineering



Dr. Chris Wyenberg, Prof. Jim Martin (Waterloo)

C3) Performance of quantum processors with dynamic connectivity



See: Quantinuum (QV=21 as of August, 2024)
Parth Padia, Shreya JVS, Dr. Anton Borissov

81

So... what's next?

- Mention us as **collaborators** in your grant applications!
- Let's co-apply for Germany-Canada **funding**!
- Let's **exchange** students and postdocs!
- Visit our lab in RA2 before your leave!
- Visit our website: quantum-simulators.com
- Use our code: https://github.com/TQT-RAAQS/LLRS/