



*Quantum computing and simulation
with ultracold Rydberg atoms*

Servaas Kokkelmans

Nikhef Seminar, October 2021

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Outline

Introduction

Quantum Inspire demonstrator projects KAT-1

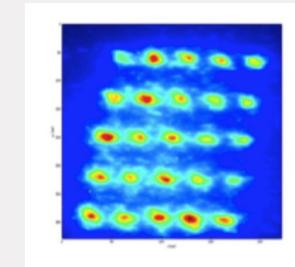
Quantum computing vs quantum simulation



Ultracold Rydberg atoms

Long-range interaction

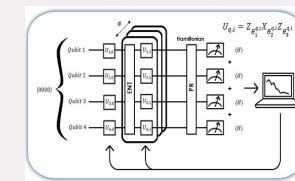
Different types of qubits



Hybrid quantum computing

Rydberg atoms in optical tweezers

Variational Quantum Eigensolver



KAT-1 quantum computing and simulation

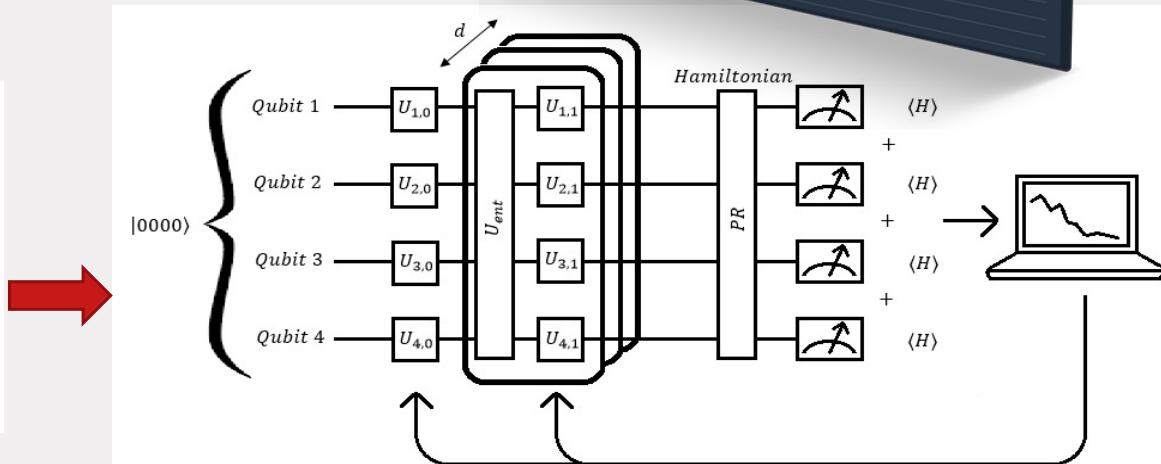
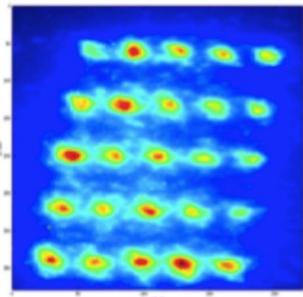
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Hybrid quantum computer

- Variational algorithms
- Ultracold atom based
- Rydberg atoms

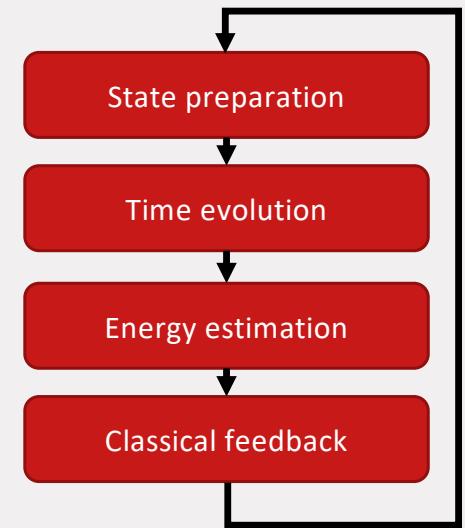
Quantum co-processor



Solve problems in Quantum Chemistry

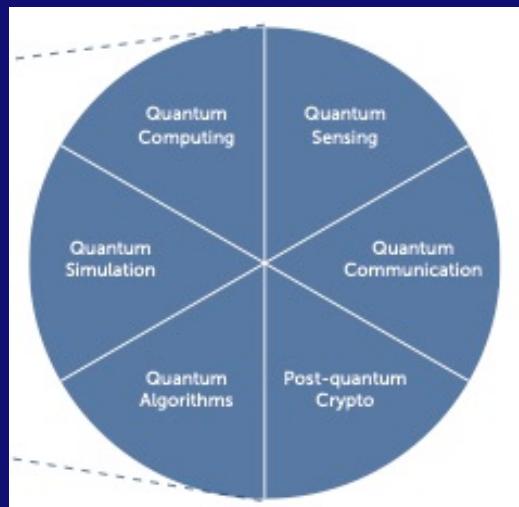
Involved@QT/e:
Servaas Kokkelmans
Edgar Vredenbregt
Sectorplan position
Eugenio Cantatore

Involved@QDeltaNL
Florian Schreck - UvA
Richard Versluis - TNO

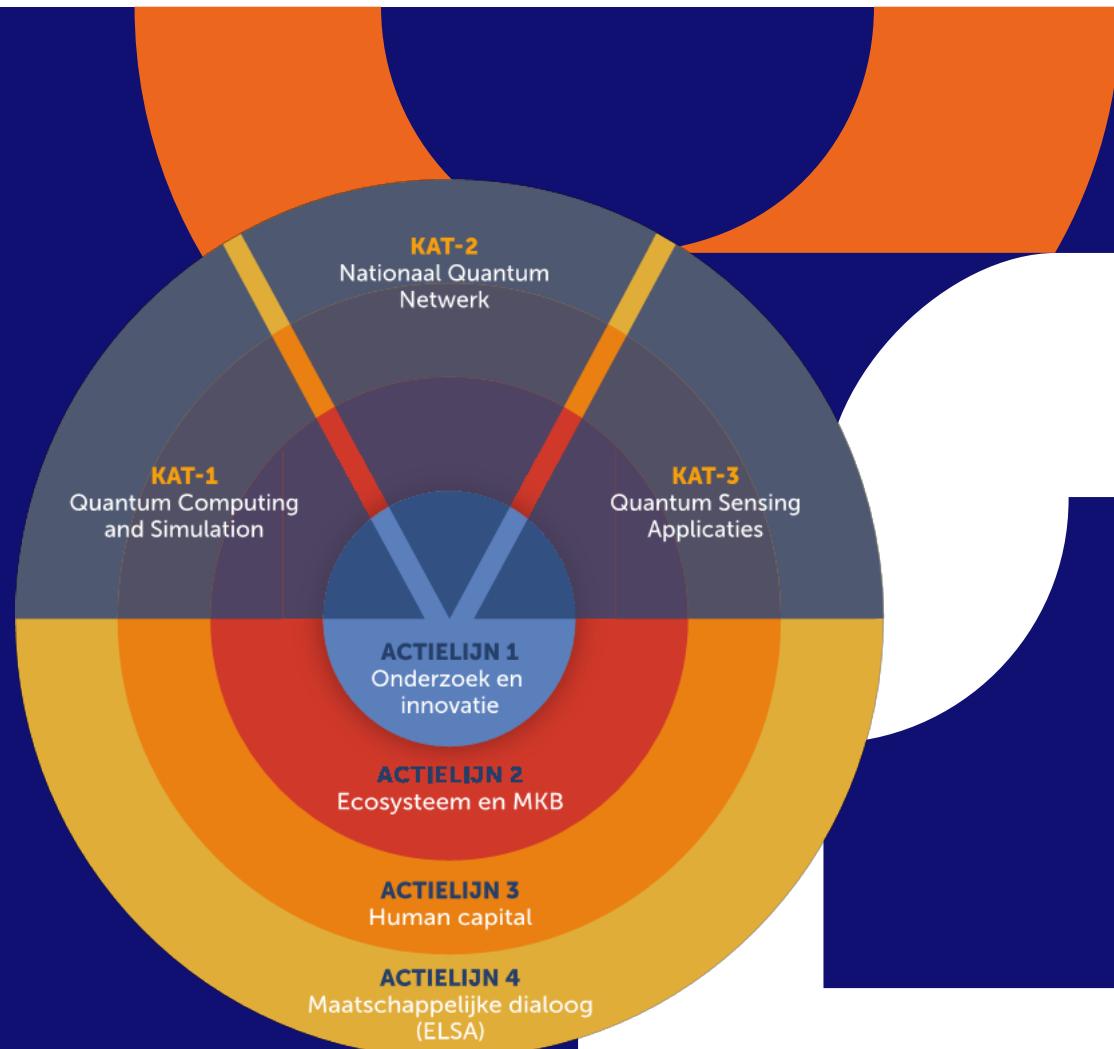




Quantum Delta Nederland

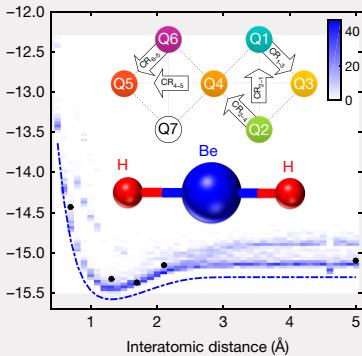


Four Action Lines
With three demonstrator projects
This is the lead for QT in the Netherlands!

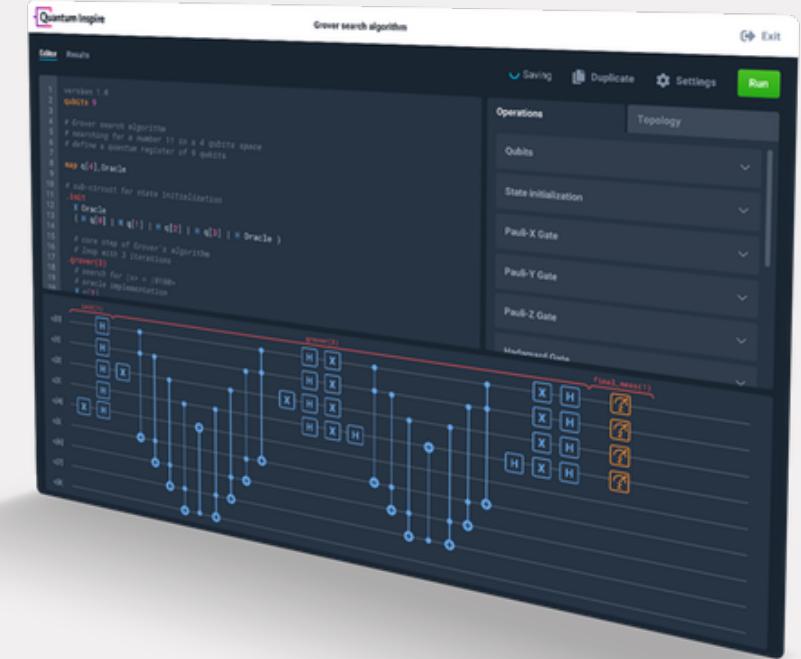


Demonstrator - Rydberg hybrid quantum computer

Interesting use cases in the field of quantum chemistry:



Artificial photosynthesis
Nitrogen fixation
Quantum medicine



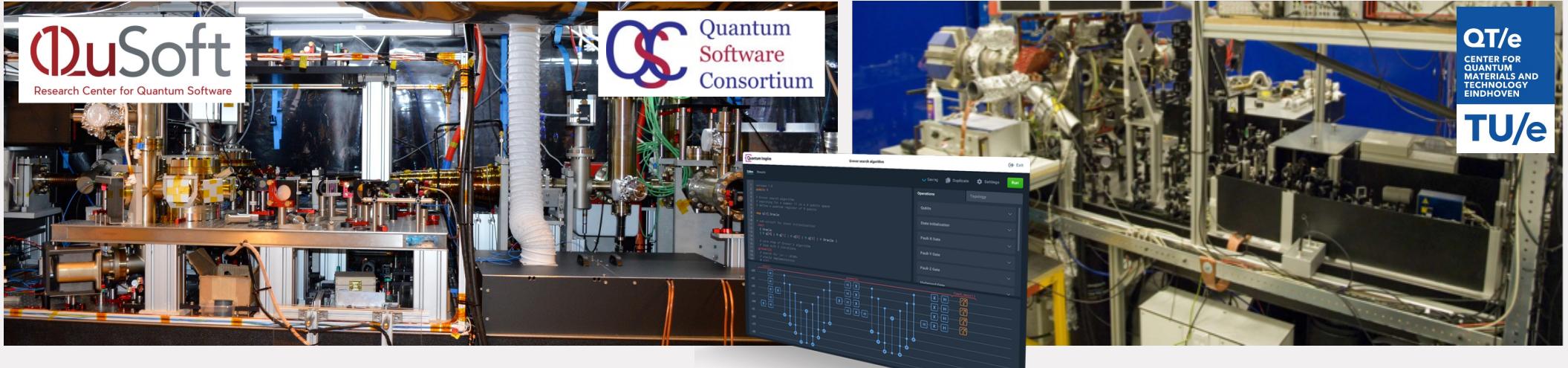
- Setup Rydberg platform as a robust demonstrator, scale-up from few 10s to 100 noisy qubits
- Hookup Rydberg platform to **Quantum Inspire** with 24/7 online access, system ready for hybrid classical-quantum calculations
- Collaboration between QT/e and experimental Rydberg lab at QuSoft on next generation Rydberg platforms



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KAT-1 Rydberg Quantum Inspire team



Alex Urech
QSC PhD



Thies
Plassman
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Spreuw



Florian
Schreck



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Servaas
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Edgar
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Rensburg
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Rik
van Herk
master



Lotte
Boer
bachelor



Marijn
Venderbosch
master

TU/e

Theory

Special thanks to
Jasper Postema
Robert de Keijzer
Gijs Groeneveld
Madhav Mohan
Marcin Plodzien



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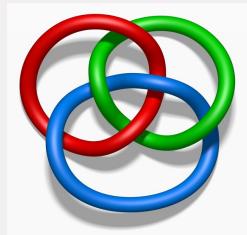
 **FOM**

 **NWO**
Netherlands Organisation
for Scientific Research

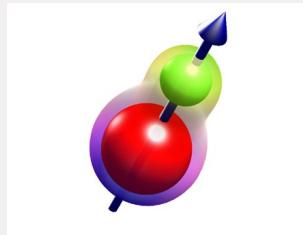
 **MOQS**
Molecular
Quantum Simulations

 **Quantum Delta
Nederland**

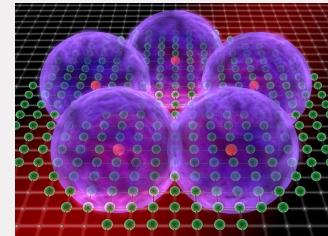
Strong interactions at different ranges



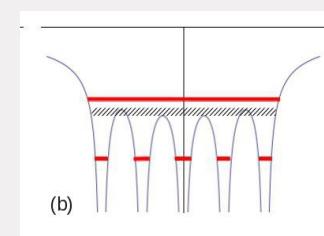
short range



dipolar molecules



Rydberg atoms



quantum plasmas



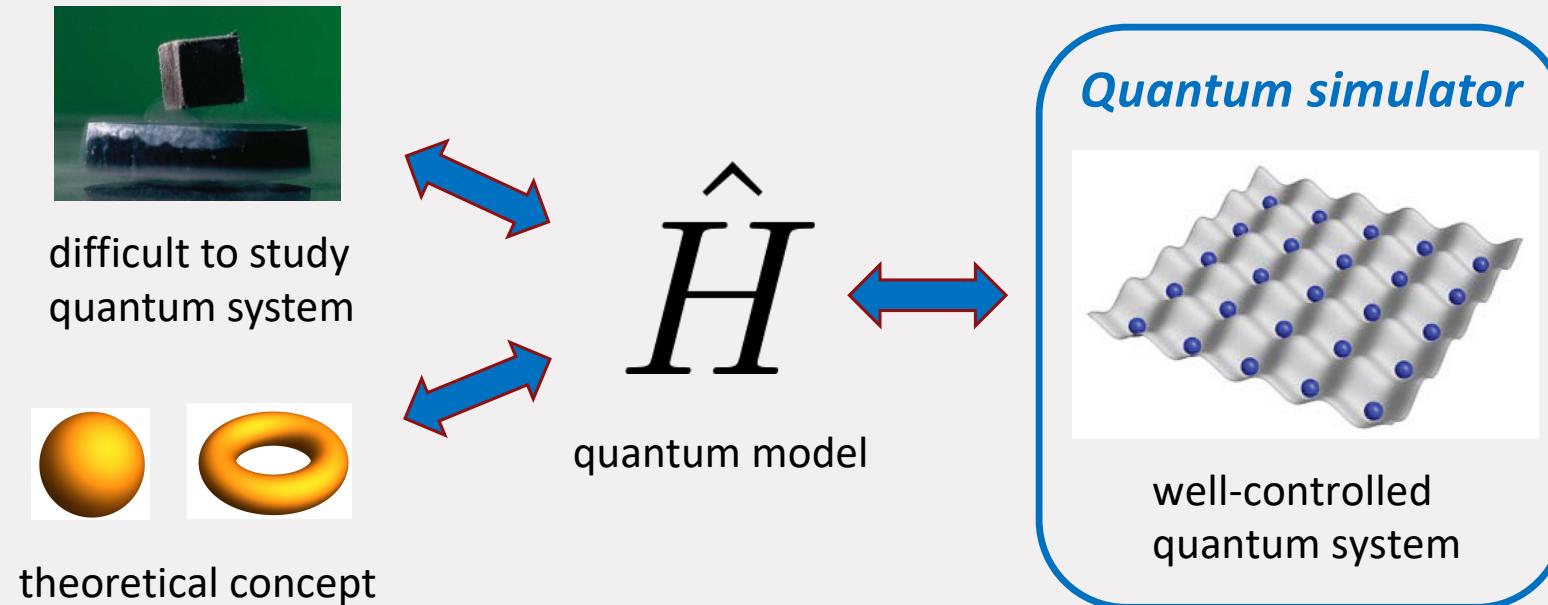
long range

quantum gases

quarks
electrons and ions

M^N scaling, for all these quantum physics problems!

Quantum simulation – analog quantum computing

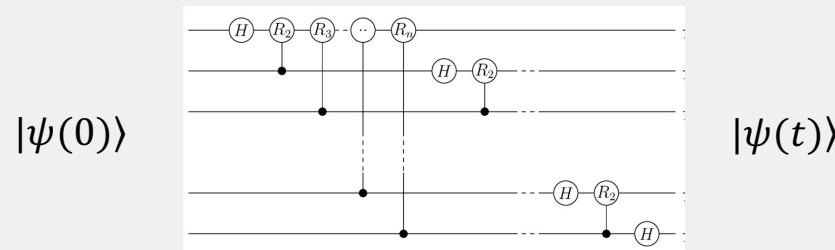


Digital quantum computing?

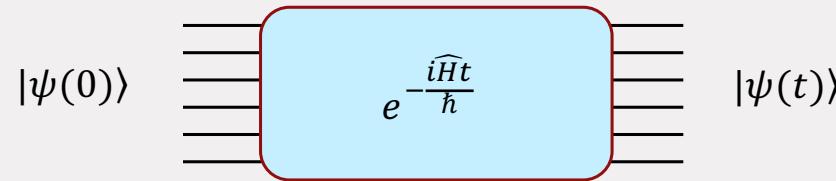
Currently in the NISQ regime

Noisy Intermediate Scale Quantum computers (Preskill)

- Digital simulation



- Analog simulation



Ultracold Rydberg atoms

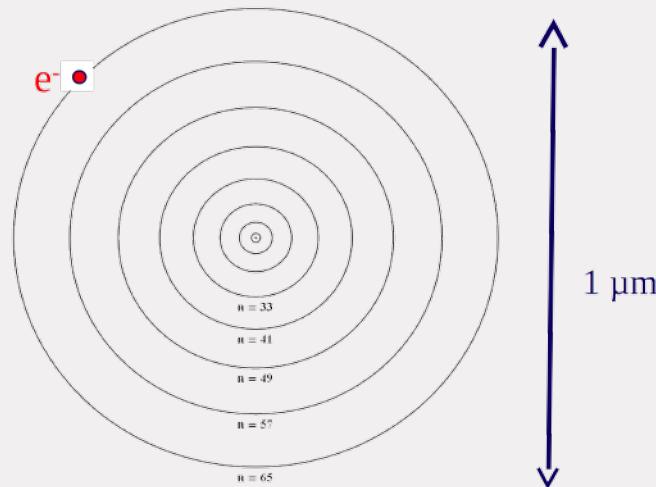
High principal quantum number n

Extreme properties

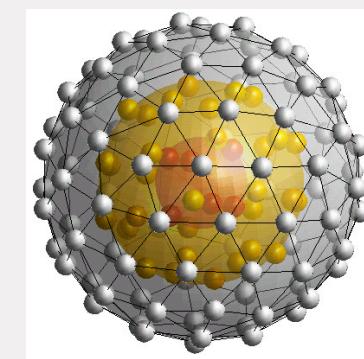
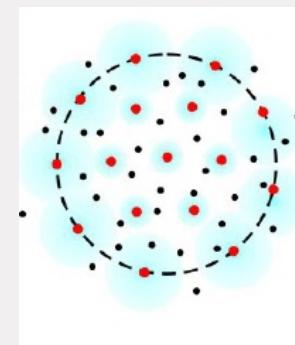
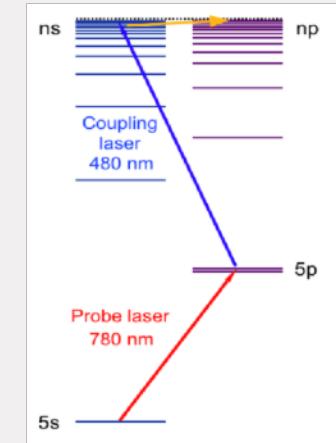
long lifetime $\sim n^3$

Size: order of micrometer

Very strong van der Waals interaction

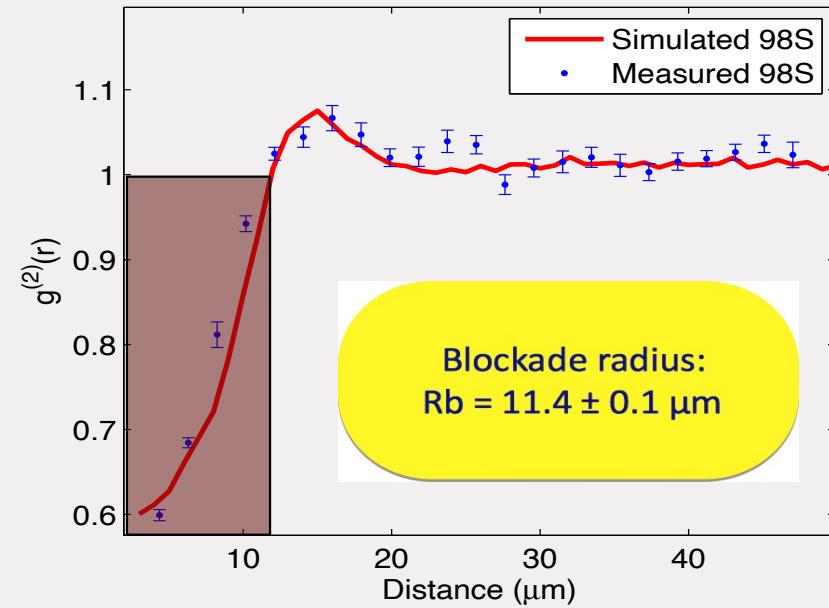
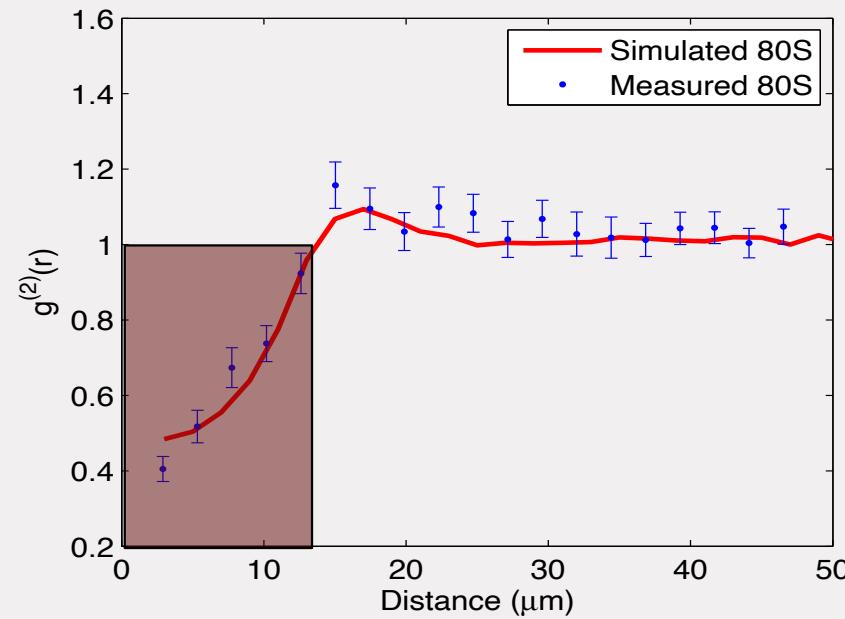


$$C_6 \sim n^{11}$$

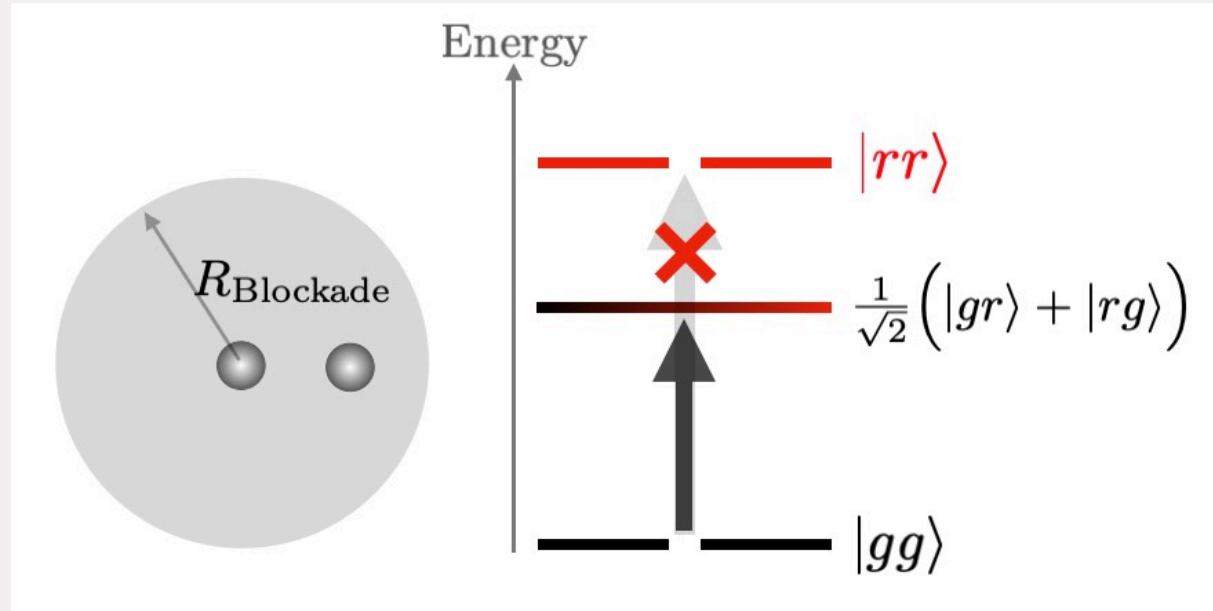


Rydberg blockade: correlations

$$g^{(2)}(r_1 - r_2) = \frac{G^2(r_1 - r_2)}{\sqrt{G^2(r_1 - r_2')G^2(r_1 - r_2')}}$$



Rydberg blockade effect



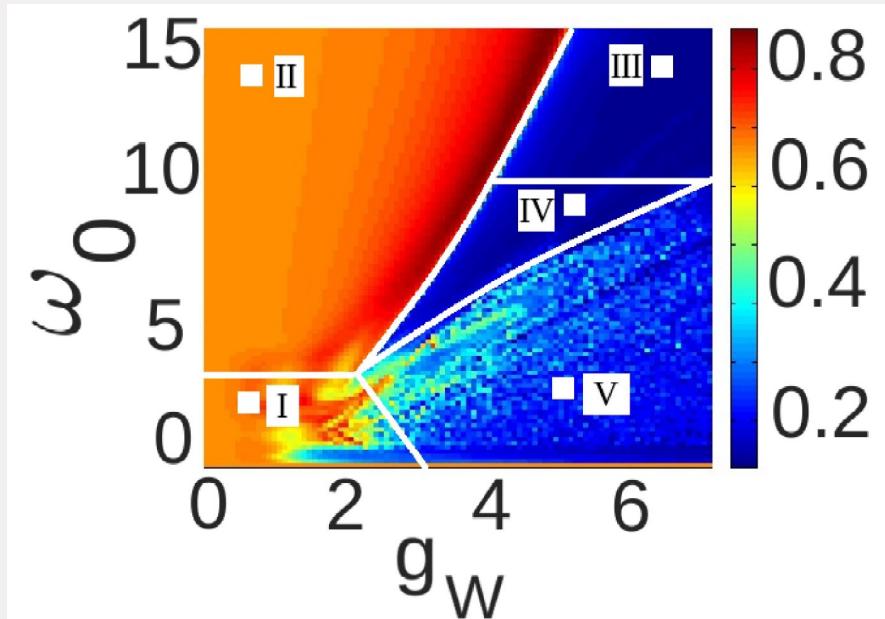
$$H = \frac{\hbar\Omega(t)}{2} \sum_i \sigma_i^x - \frac{\hbar\delta(t)}{2} \sum_i \sigma_i^z + \sum_{i < j} U_{ij} n_i n_j$$

Rydberg platform: a dedicated quantum device

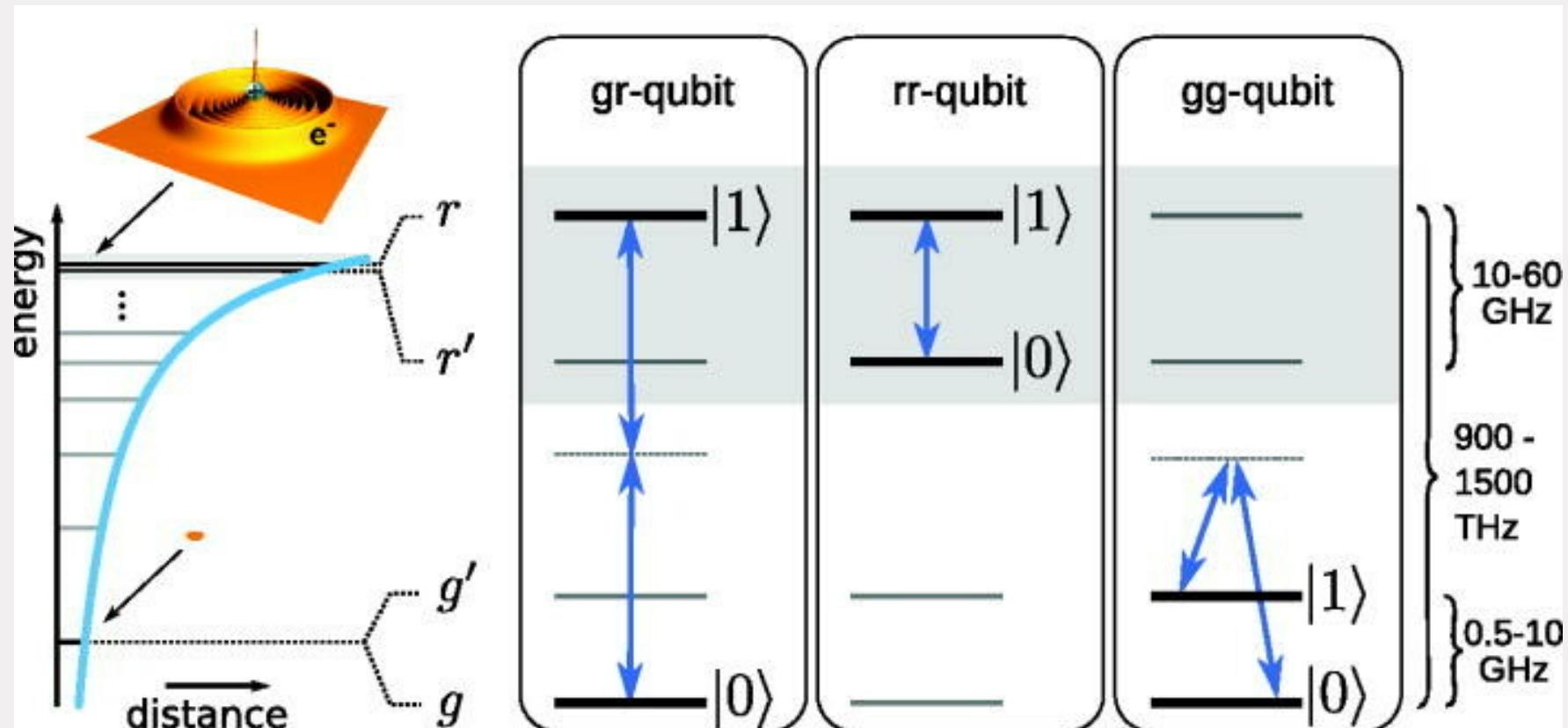
SSH model, Davydov soliton

[M. Płodzień, T. Sowiński, and S. Kokkelmans, Simulating polaron biophysics with Rydberg atoms, Scientific Reports. 8, 9247 (2018)]

Energy transport (solitons)



Rydberg atom qubits



[M. Morgado and S. Whitlock, arXiv:2011.03031]

Rydberg dressing

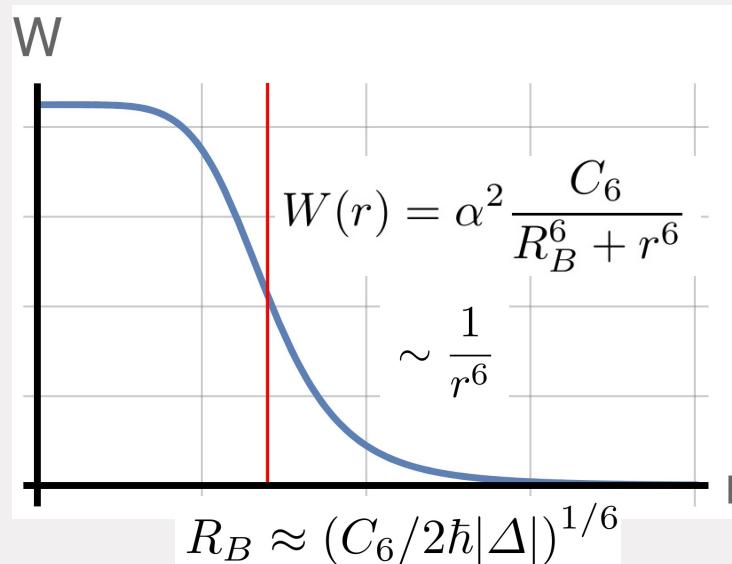
Admixture properties of Rydberg state to atom ground state

$$|\psi\rangle \approx |g\rangle + \alpha|nS\rangle$$

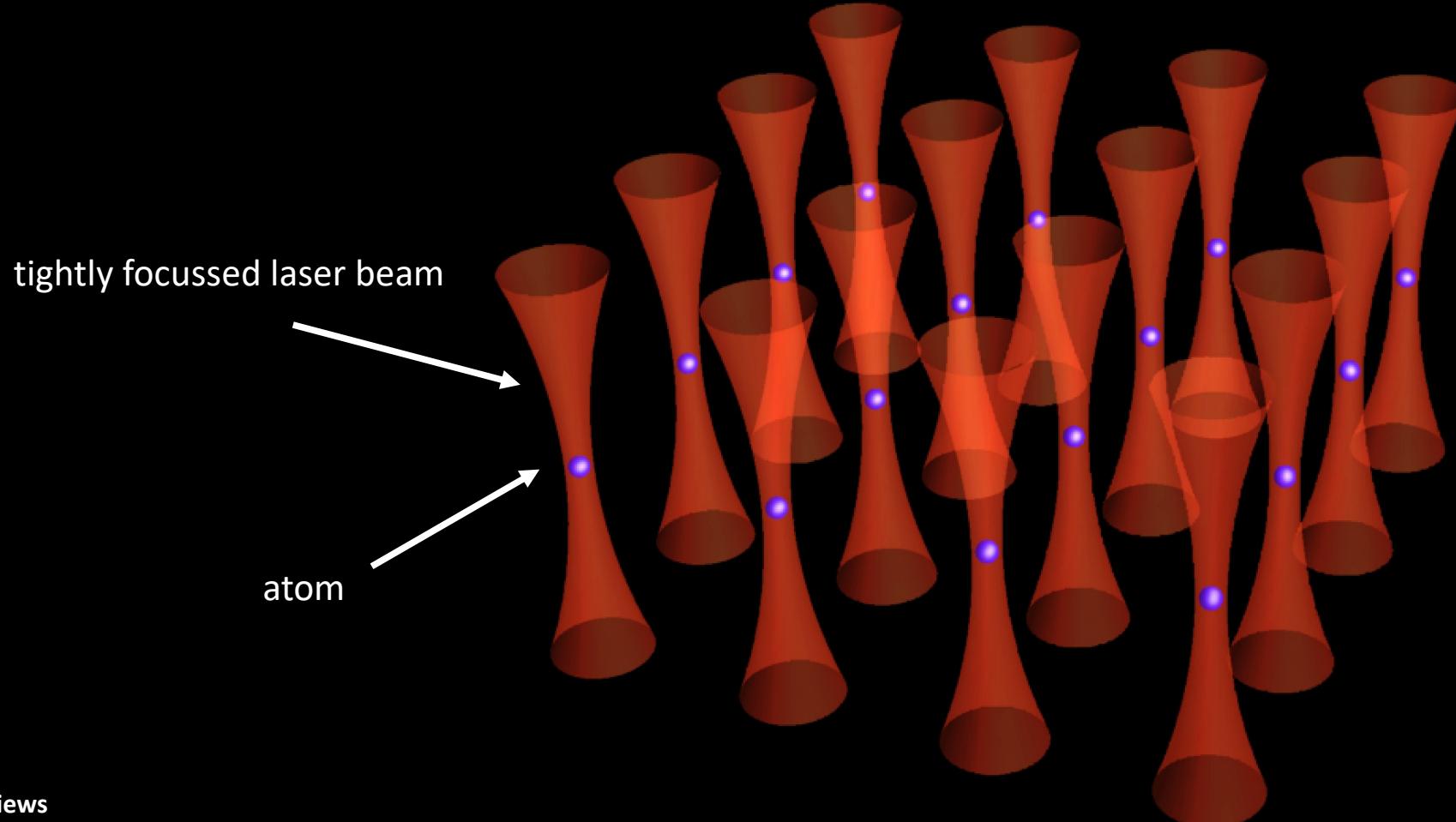
$$\alpha = \frac{\Omega}{2|\Delta|}$$

Dressed state acquires life-time:

$$\tau_{eff}^{-1} = \left(\frac{\Omega}{2\Delta}\right)^2 \tau_{|nS\rangle}^{-1} + \left(\frac{\Omega_1}{2\Delta_1}\right)^2 \Gamma_{5P_{3/2}}$$



Quantum simulation based on single atoms



Reviews

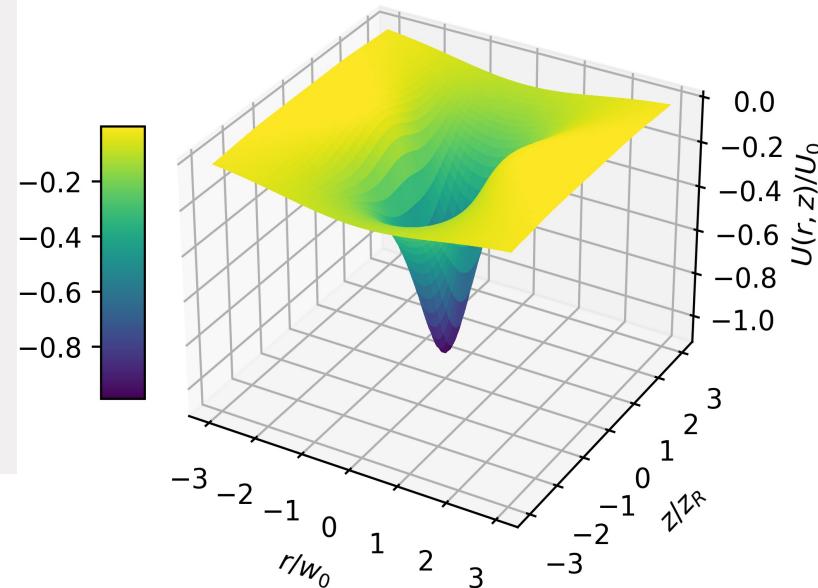
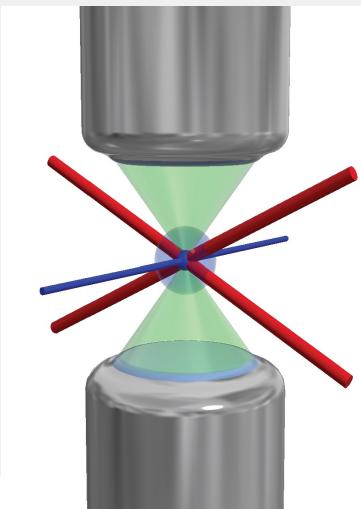
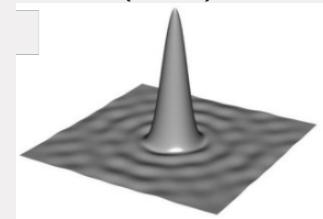
Quantum computing with neutral atoms, *Quantum* 4, 327 (2020)

Quantum simulation and computing with Rydberg-interacting qubits, arXiv:2011.03031 (2020)

Optical tweezer

- Highly focussed laser beam
- Diffraction limit: $d = 0.61 \frac{\lambda}{\text{NA}}$
- AC stark shift causes $U_{dip} \propto \frac{I(r, z)}{\delta}$
- Attractive force for $\delta < 0$
- Radial and axial confinement

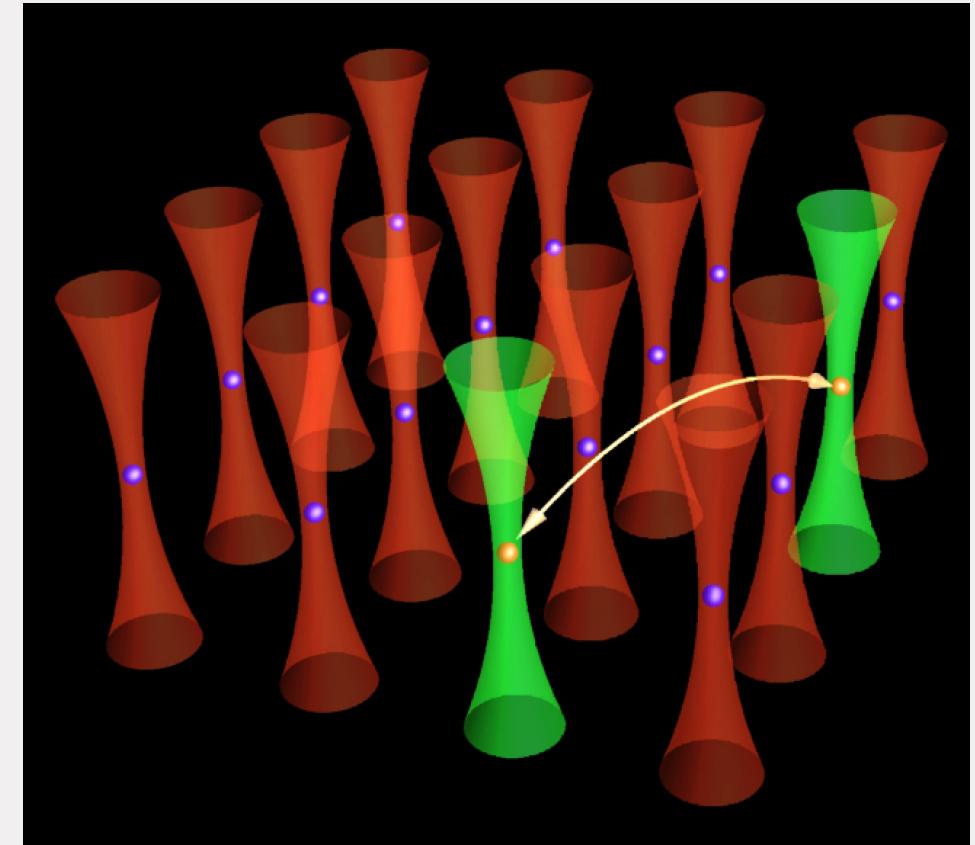
Magn. Reson. Med. **82**, 527–550 (2019)



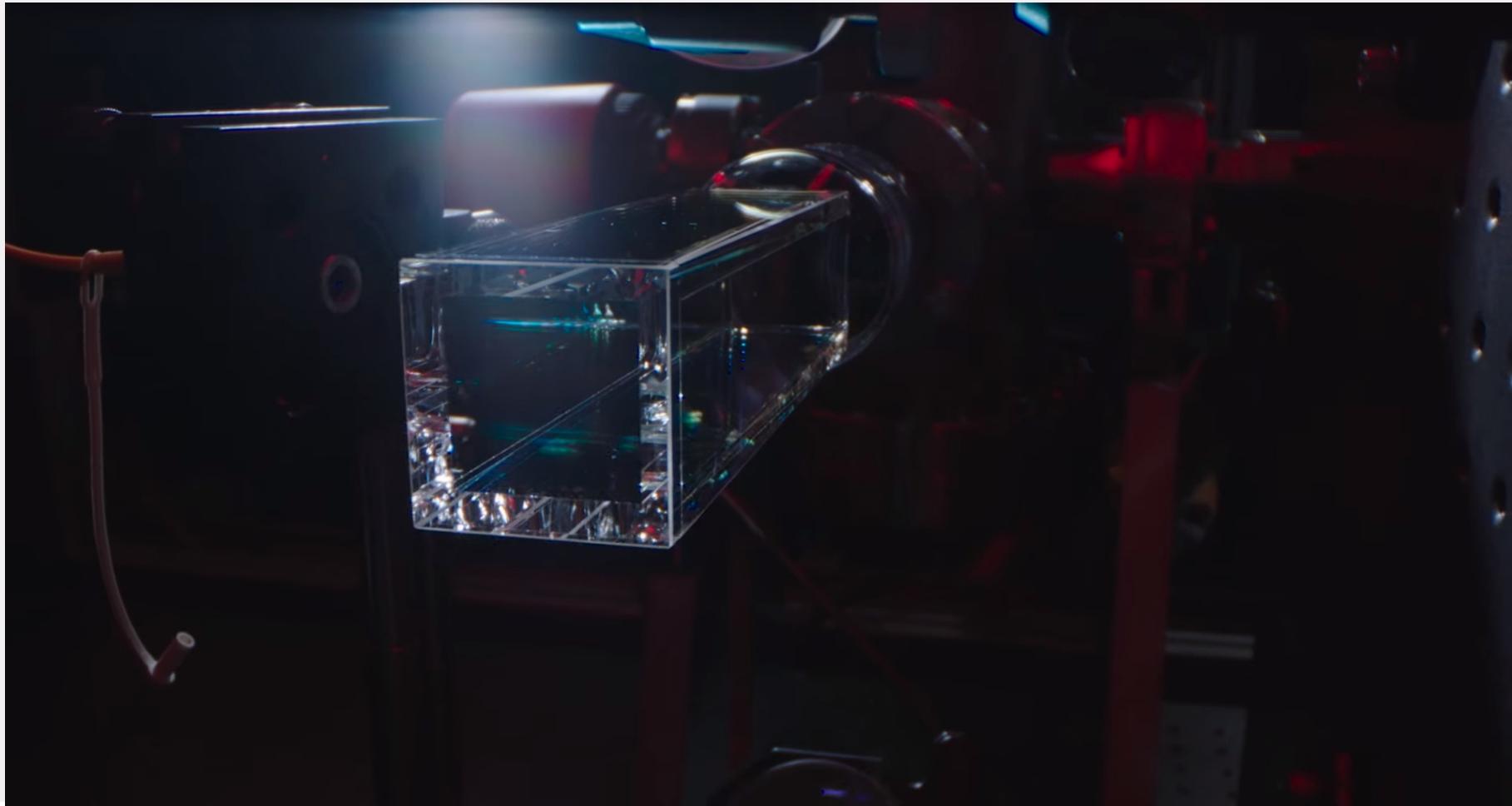
Control of the qubits (atoms) via tweezers

$$H = \frac{\hbar}{2} \sum_i \Omega_i(t) \sigma_i^x - \frac{\hbar}{2} \sum_i \delta(t) \sigma_i^z + \sum_{i < j} U_{ij} n_i n_j$$

Control over interactions:
global or local, switch or always on



Current setup: explore tweezers with rubidium



Sr atoms in optical tweezers

Work by Alex Urech and Ivo Knottnerus

UvA group: load tweezers

long lifetimes

On to sorting and larger lattices

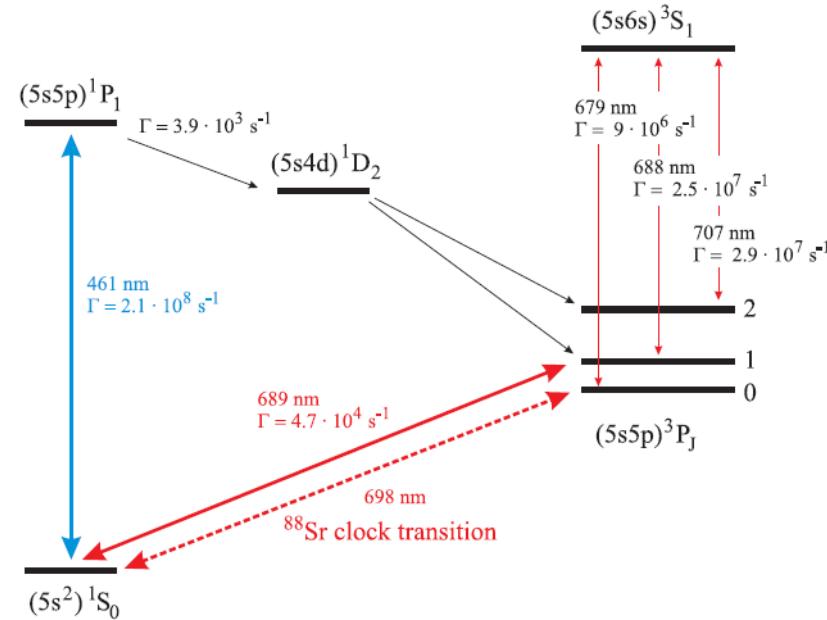
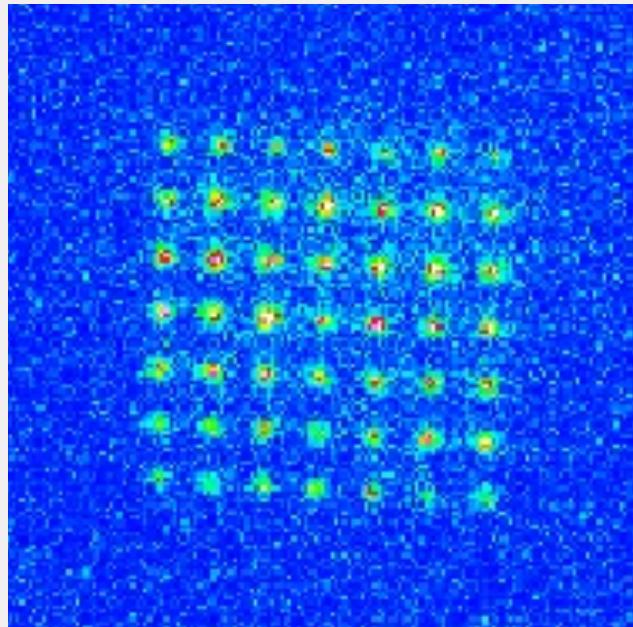
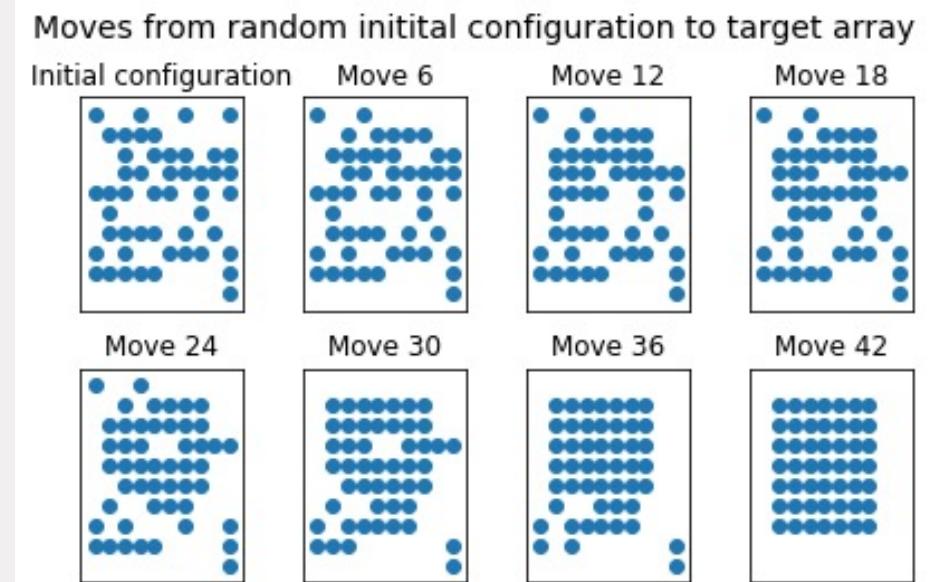
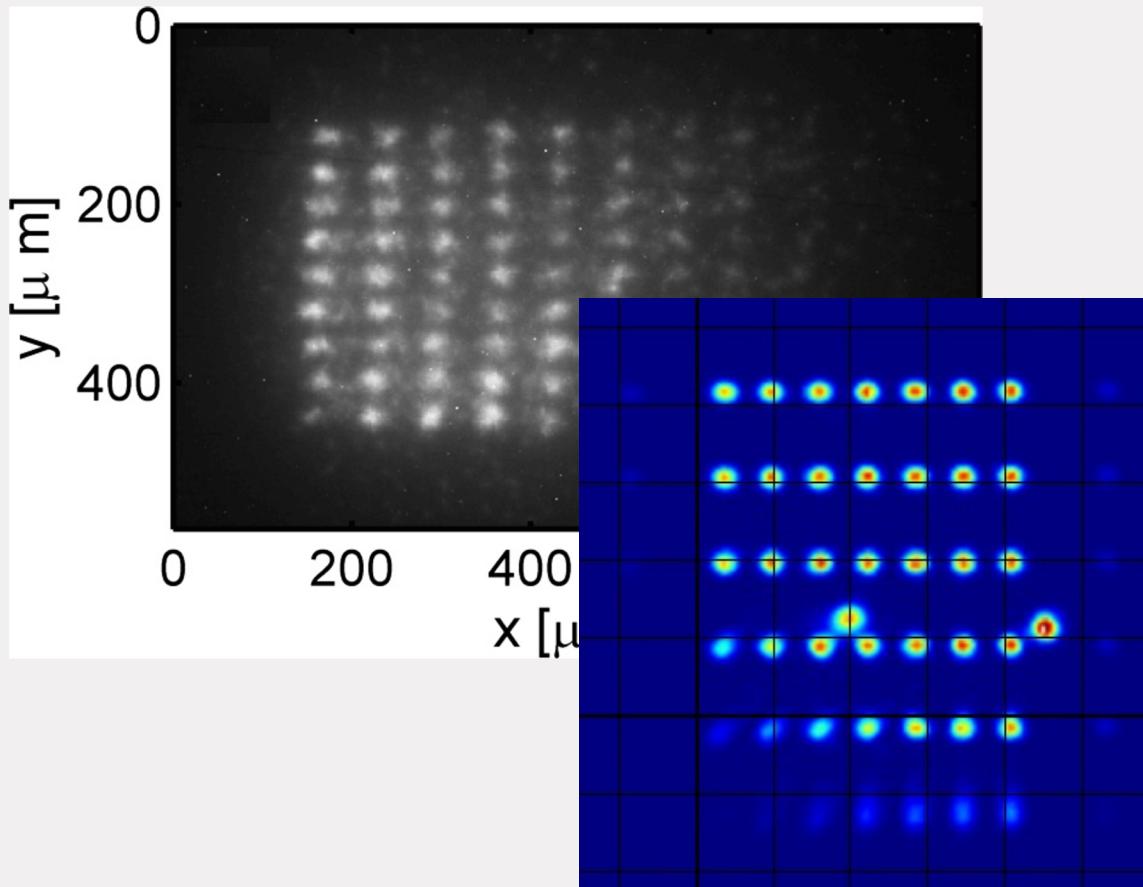


Fig. 1. Partial strontium energy level scheme. Γ denotes the spontaneous decay rate.

2020, Madjarov et al. *Nat. Phys.* 16, 857 (2020): ⁸⁸Sr (gr) pCU_{xy}(π) , fidelity $\geq 0.991(4)$, decoherence time $\approx 2\mu\text{s}$, operation time 51 ns

Build up demonstrator facility in Eindhoven



Work by Marijn Venderbosch, Lotte Boer, Deon JvRensburg, Ivo Knottnerus

Quantum chemistry

Born-Oppenheimer approximation:

Molecular Hamiltonian

$$H = \sum_{p,q=1}^M h_{pq} a_p^\dagger a_q + \sum_{p,q,r,s=1}^M h_{pqrq} a_p^\dagger a_q^\dagger a_r a_s$$

with interaction terms

$$h_{pq} = \int \varphi_p^*(\sigma) \left(\frac{\nabla_r^2}{2} - \sum_i \frac{Z_i}{|R_i - r|} \right) \varphi_q(\sigma) d\sigma, \quad \text{[One-electron term]}$$

$$h_{pqrs} = \int \frac{\varphi_p^*(\sigma_1) \varphi_q^*(\sigma_2) \varphi_s(\sigma_1) \varphi_r(\sigma_2)}{|r_1 - r_2|} d\sigma_1 d\sigma_2.$$

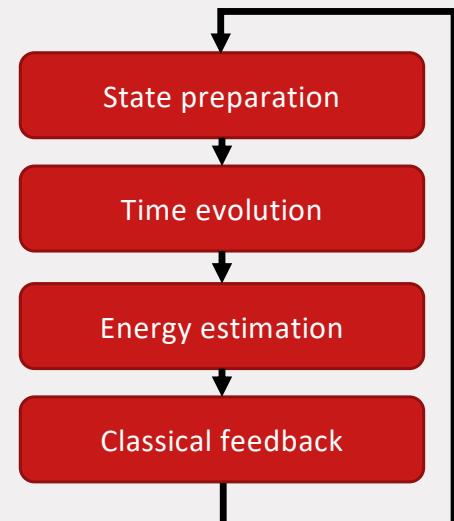
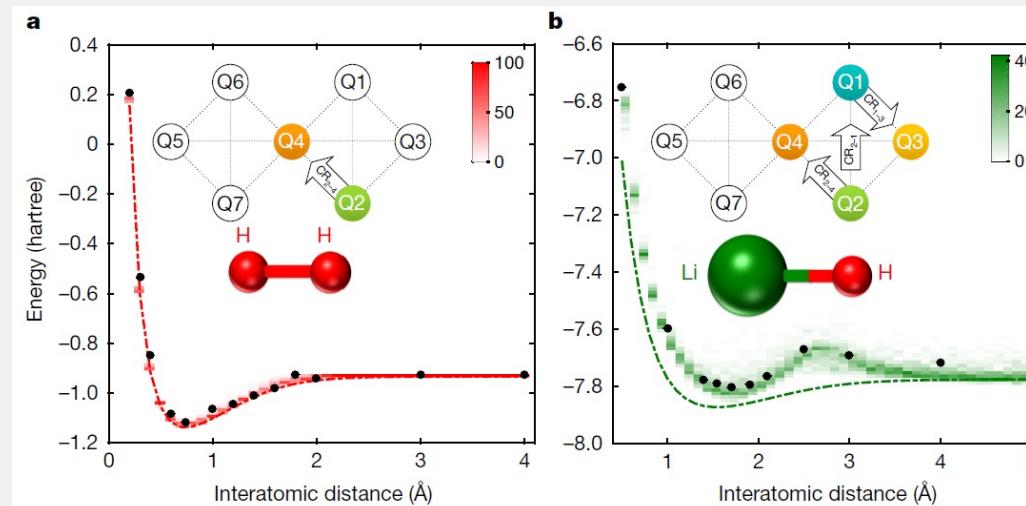
[Two-electron term]

Quantum chemistry

Jordan-Wigner transformation: $a_p^\dagger, a_p \rightarrow I, X, Y, Z$

$$a_p = I^{p-1} \otimes \frac{1}{2}(X + iY) \otimes Z^{N-p}$$

$$a_p^\dagger = I^{p-1} \otimes \frac{1}{2}(X - iY) \otimes Z^{N-p}$$

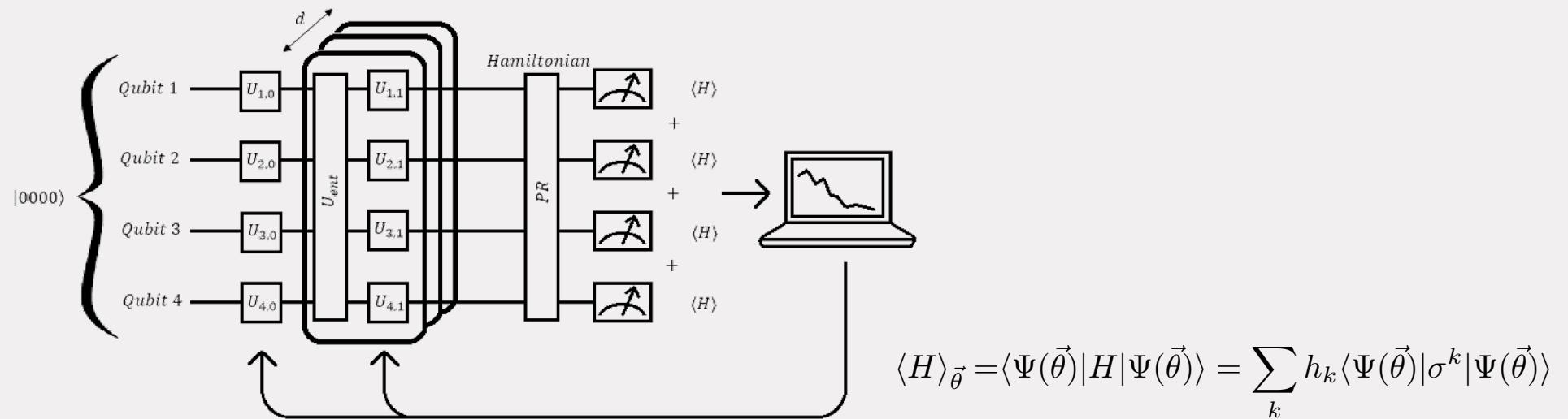


[Kandala et al, Nature 549, 242 (2017)]

VQE: Simulating the wave function

$$|\Psi(\vec{\theta})\rangle = \prod_{q=1}^m U_{q,d}(\vec{\theta}) \times U_{ent} \times \prod_{q=1}^m U_{q,d-1}(\vec{\theta}) \times U_{ent} \times \dots \times \prod_{q=1}^m U_{q,0}(\vec{\theta}) |\psi_{init}\rangle$$

$$U_{q,i}(\vec{\theta}) = Z_{\theta_1^{q,i}} X_{\theta_2^{q,i}} Z_{\theta_3^{q,i}}$$

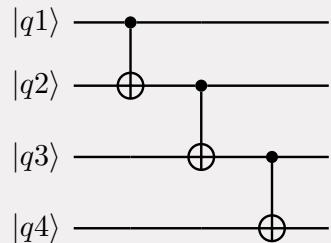


Specific architecture

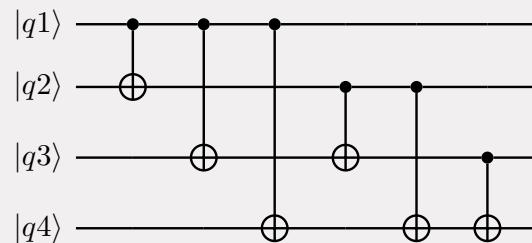
Investigate hardware-specific entanglement

- NISQ area: optimize every step!

Chain



pairs

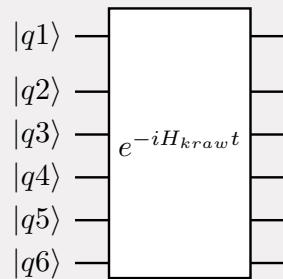


Specific architecture

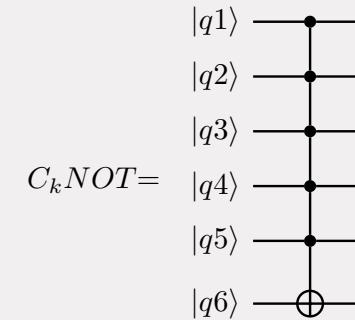
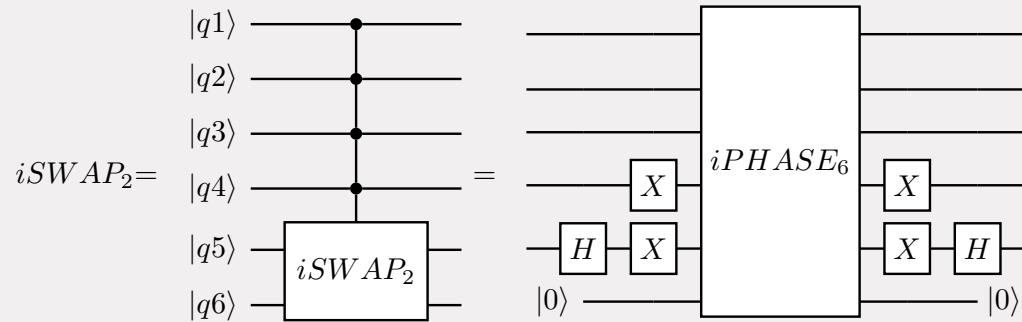
Krawtchouk chain

Multi-qubit gate

$$H^K = -\frac{J}{4} \sum_{j=1}^{N-1} \sqrt{j(N-j)} (\sigma_j^X \sigma_{j+1}^X + \sigma_j^Y \sigma_{j+1}^Y)$$



Work by Jasper Postema
implementation with
Rydberg atoms

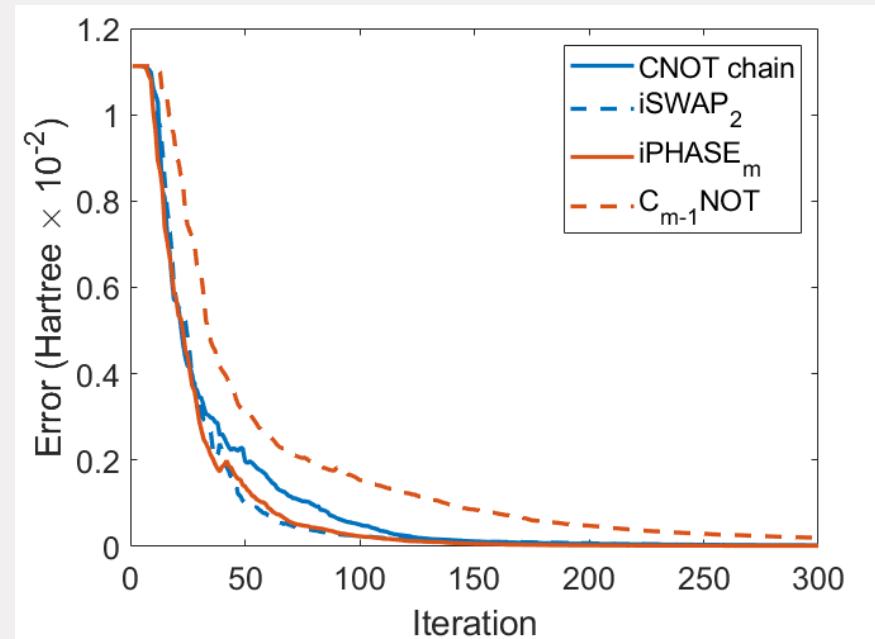


LiH molecule

VQE problem: LiH molecule (6 qubits) at depth 6, classical optimization SPSA

Compare different entangling methods

- $i\text{PHASE}_m$, $C_{m-1}\text{NOT}$ and $i\text{SWAP}_2$,
standard CNOT chain



[Optimization of the Variational Quantum Eigensolver, R. J. P. T. de Keijzer, V. E. Colussi, B. Skoric, and S. J. J. M. F. Kokkelmans, arXiv:2102.01781]

Pulse based vs gate based

Several proposals for quantum gates. Not always trivial and timeconsuming...

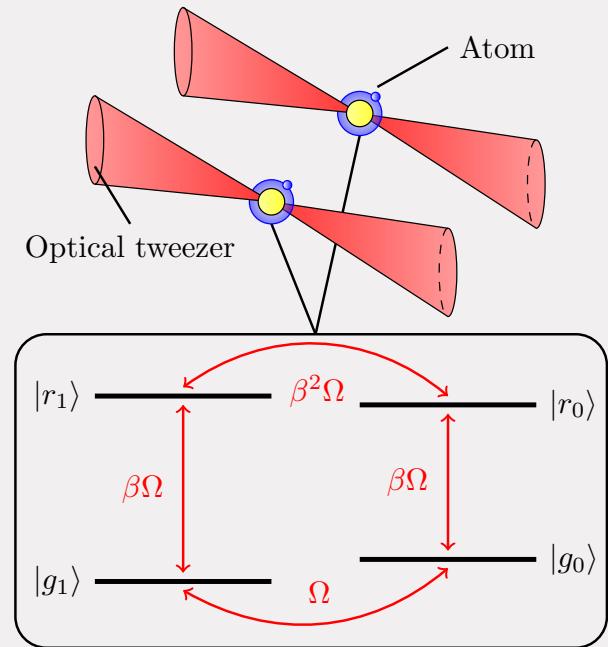
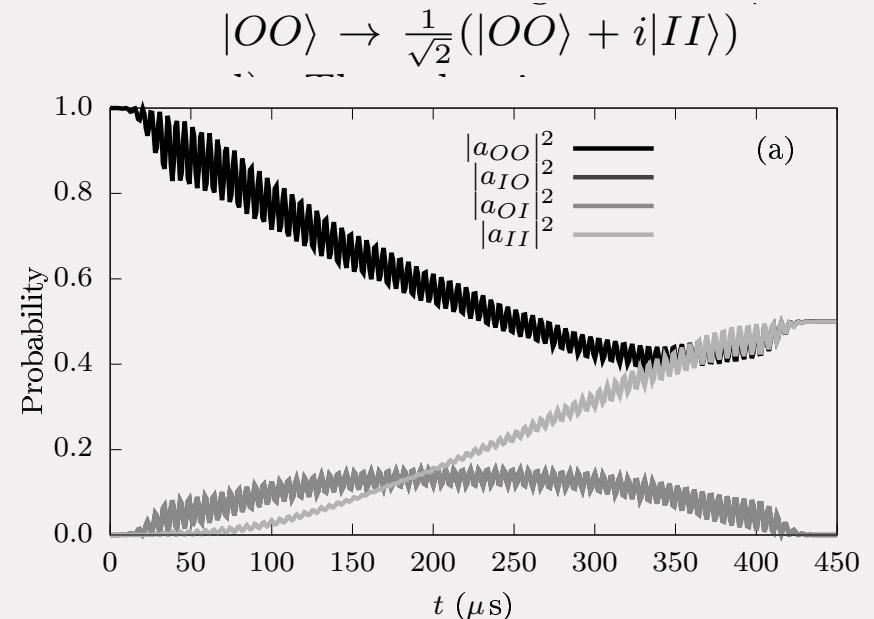


FIG. 1. Excitation scheme for using dressed qubits. The useful quantum states for qubits are the 'cross-dressed' states $|O\rangle = (|g_0\rangle + \beta|r_1\rangle)/\sqrt{1+\beta^2}$ and $|I\rangle = (|g_1\rangle + \beta|r_0\rangle)/\sqrt{1+\beta^2}$.



[R. V. Skannrup, R. Gerritsma, S. J. J. M. F. Kokkelmans, arXiv:2008.13622]

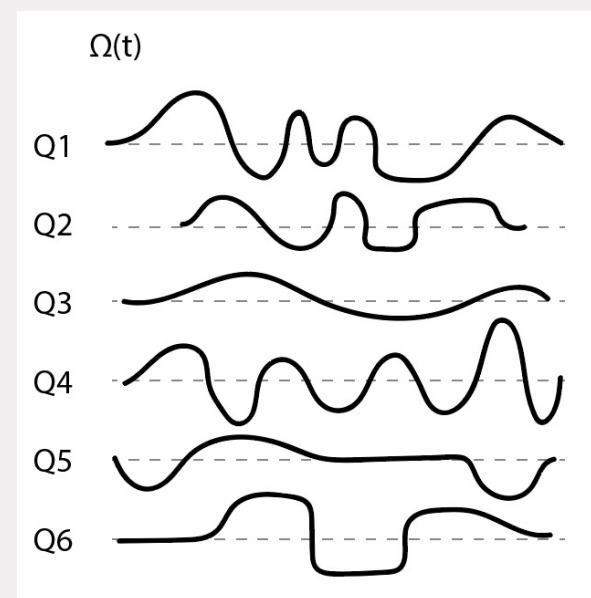
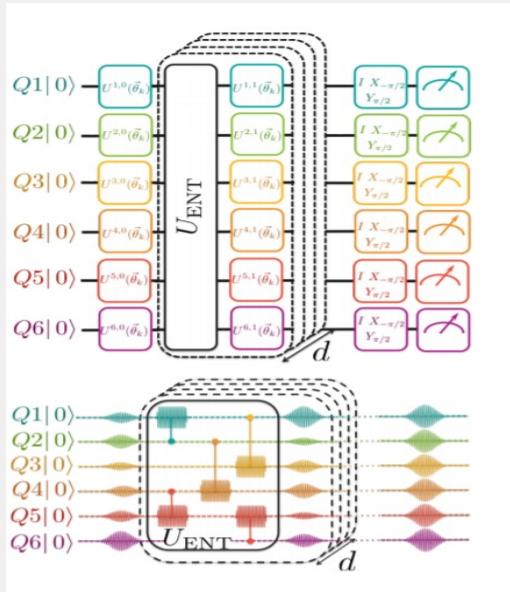
Optimized search through Hilbert space

NISQ regime: hardware-dependent optimisation

Gate-based computing

vs.

Pulse-based computing



Quantum Optimal Control

Multi-qubit entanglement

- Realised by controlled long-range Rydberg-atom interaction

$$|\Psi_{UCCSD}\rangle = e^{\hat{\tau}_1 + \hat{\tau}_2} |0\rangle$$
$$\hat{\tau}_1 = \sum_{ia} \theta_{ia} (a_a^\dagger a_i - a_i^\dagger a_a)$$

$$\hat{\tau}_2 = \sum_{ijab} \theta_{ijab} (a_a^\dagger a_b^\dagger a_i a_j - a_j^\dagger a_i^\dagger a_b a_a)$$

Minimize

$$Tr(U^\dagger(T)\rho_0U(T)H_{mol}) + \lambda \sum_{k=1}^m \frac{1}{2} \int_0^T |Z_k(t)|^2 dt$$

Work by Robert de Keijzer
implementation with
Rydberg atoms

Subject to:

$$i\partial_t U(t) - [H_d + H_{c,Z}(t)]U(t) = 0$$

Individual qubit rotations

$$H_c(t) = \sum_j \left(\frac{\Omega_j(t)}{2} e^{i\nu_j(t)} |0\rangle_j \langle 1|_j + \text{h.c.} \right)$$



$$H_c(t) = \sum_k Z_k(t) |0\rangle_k \langle 1|_k + \overline{Z_k(t)} |1\rangle_k \langle 0|_k,$$

Rydberg interaction: global

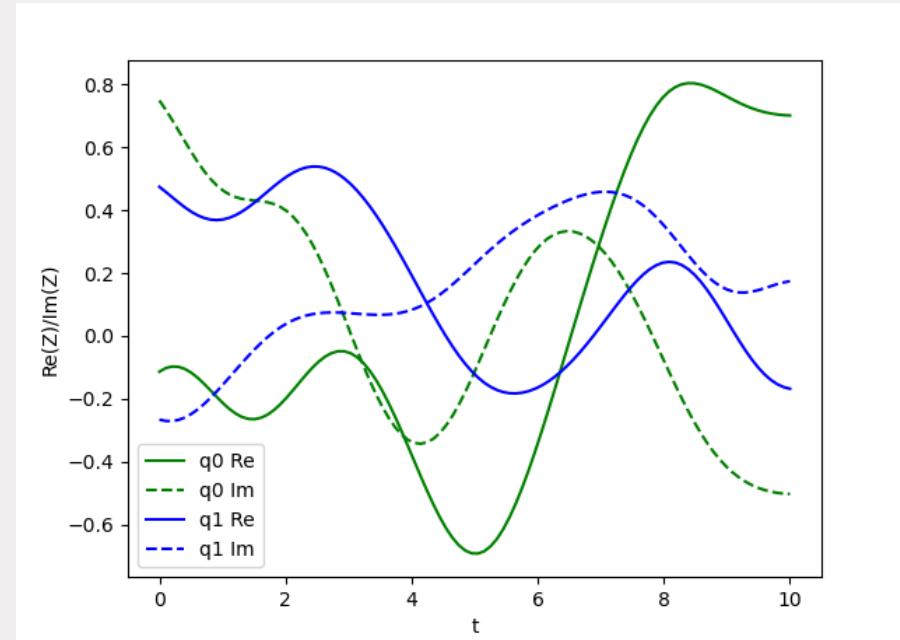
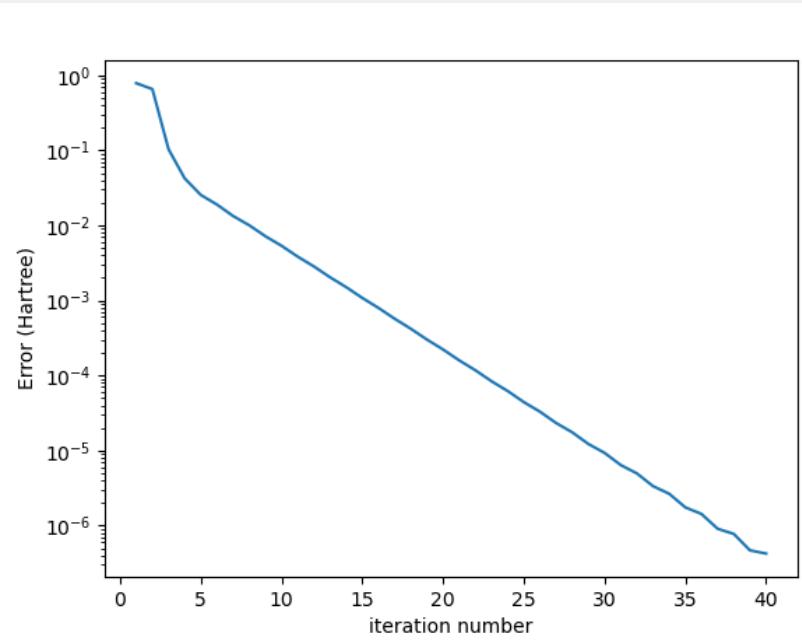
$$H_d = \sum_{ij} \frac{C}{R_{ij}^6} |11\rangle_{ij} \langle 11|_{ij}$$



$$H_d = \sum_{ij} \tilde{Q} |11\rangle_{ij} \langle 11|_{ij},$$

Example with “global” Rydberg coupling

H_2 , two qubits



Quantum Eindhoven building

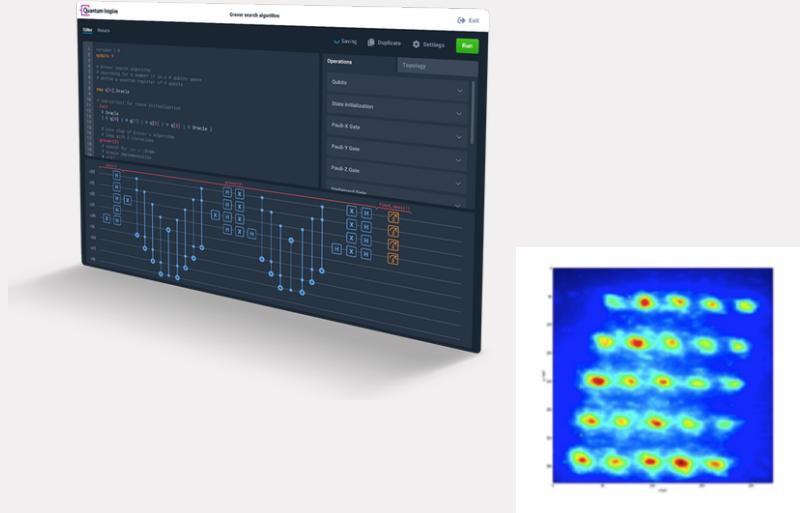
With large underground lab for quantum technology



Summary/Outlook

Hybrid quantum computation:

- Quantum Inspire project QuantumDeltaNL
- Based on ultracold atoms in optical tweezers
- Interaction via Rydberg excitations



Variational quantum Eigensolver

- Investigation of hardware optimized strategies
- Different entanglement schemes: multi-qubit entanglement
- Pulse-based vs gate-based

Thanks!

