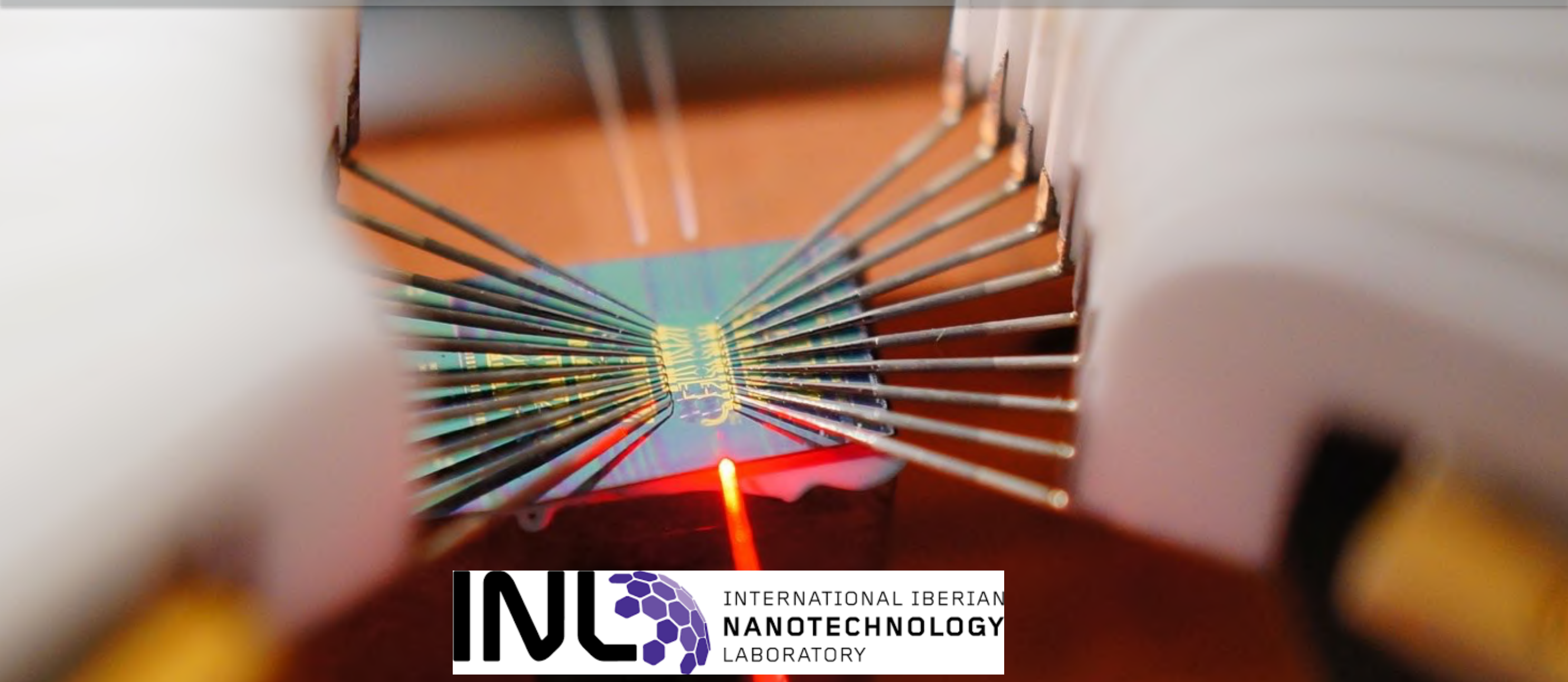
Witness assisted variational eigensolver



INL INTERNATIONAL IBERIAN NANOTECHNOLOGY LABORATORY

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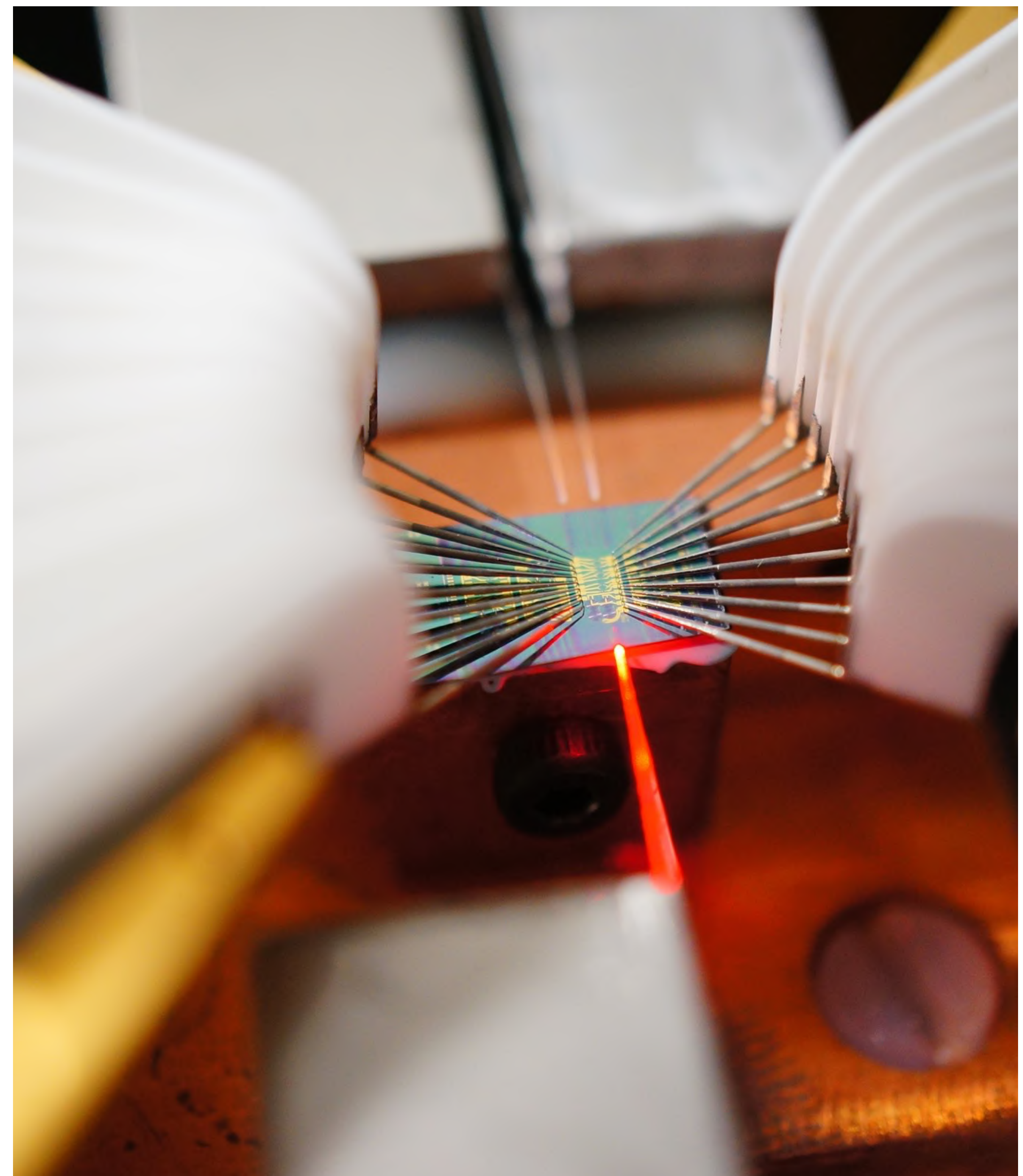
Content

- Variational quantum eigensolvers
- Experimental implementations
- WAVES
- Experimental and simulation results
- (Optional) A bit of photonic quantum hardware



Variational quantum eigensolver

Given $\hat{H}$ we want to find $|\psi\rangle$ s.t. $\hat{H}|\psi\rangle = \lambda|\psi\rangle$.

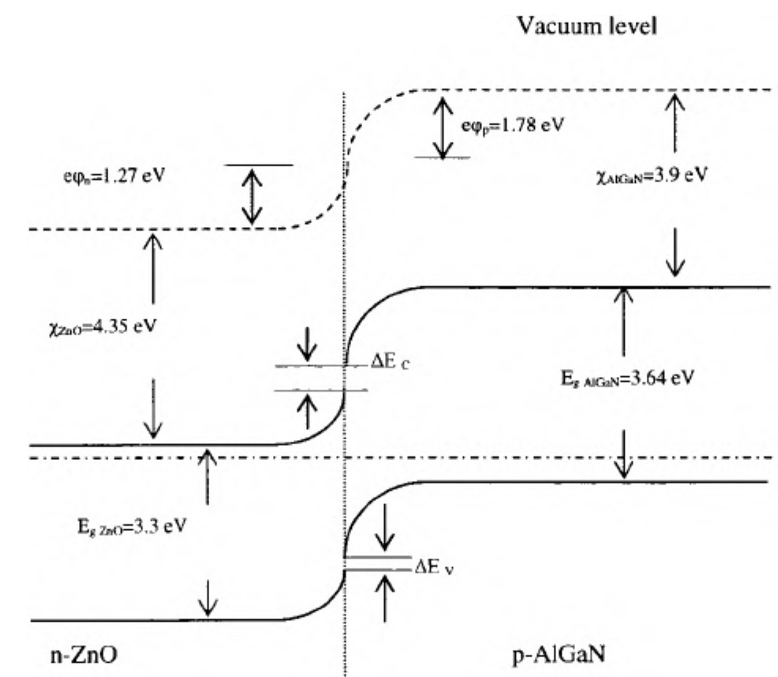
High precision estimation of λ

Agriculture -> 100-200 qubits -> Design catalysts for efficient conversion of Ni to fertilizer

Carbon Capture -> 100-200 qubits -> Catalysts to extract carbon dioxide from air with less energy

Battery design -> 10^3 qubits

Drug discovery -> Molecular docking



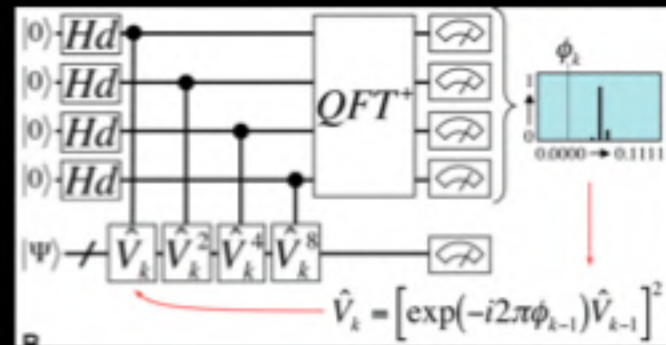
Feynman, R. P. Int. J. Theor. Phys. 21, 467 (1982).
Lloyd, S. Science 273, 1073–1078 (1996).
Aspuru-Guzik, A. et. al. Science 309, 1704 (2005).

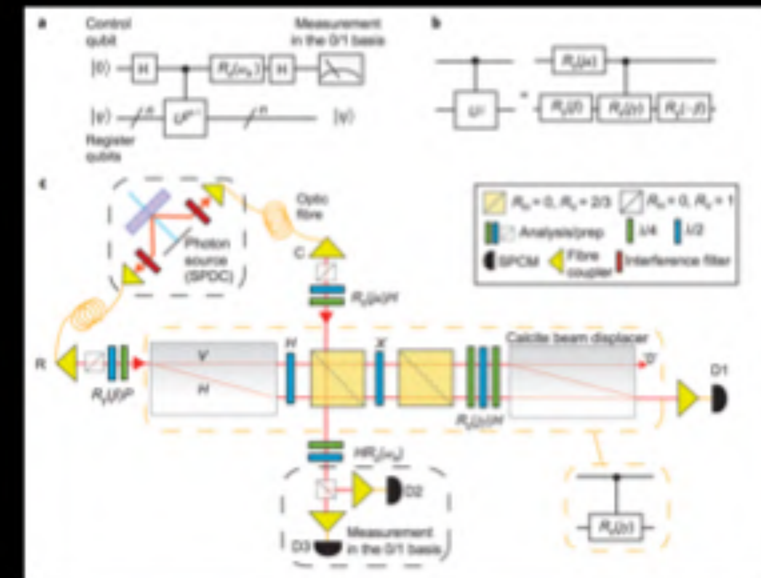
Canonical methods

Adiabatic state preparation

↓

PEA



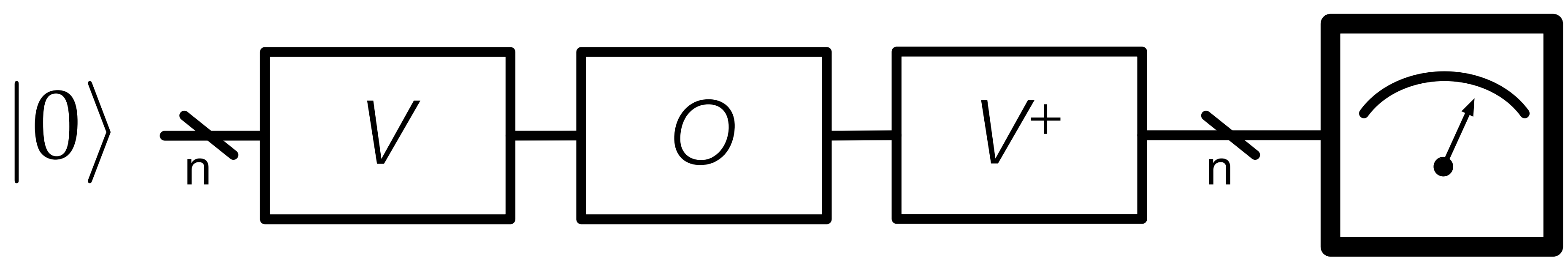


A. Aspuru-Guzik, Love,A. D. Dutoi Science (2005)

Lanyon et al. Nat Chem. (2010)

Measuring expectation values

$$\langle O \rangle_{|\Psi\rangle} = \frac{\langle \Psi | O | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$



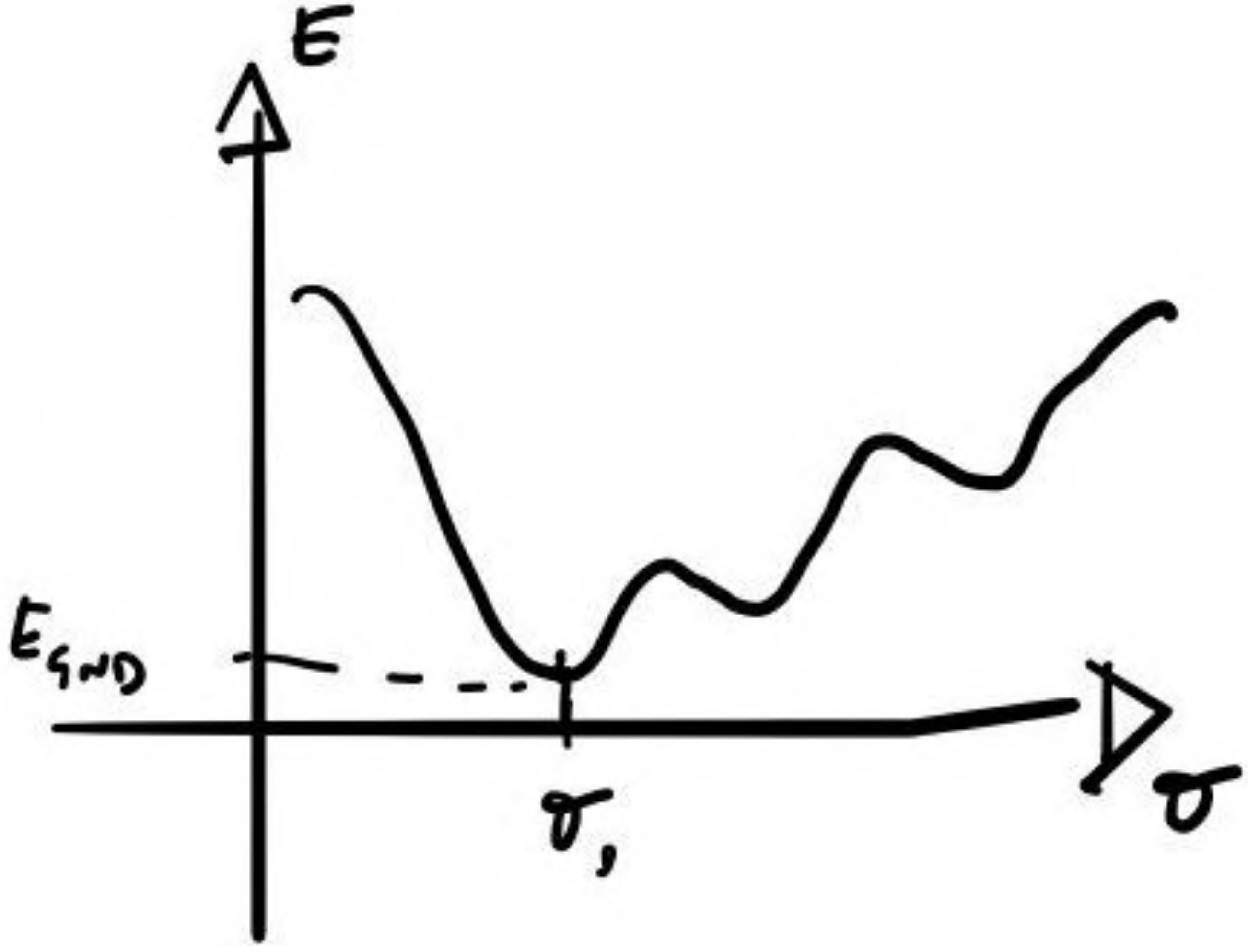
Scalable if $$O = \sum_{\alpha} h_{\alpha} O_{\alpha}$$ With a poly number of O_α

Variational Principle

$$\langle \mathcal{H} \rangle(\vec{\theta}) = \langle \psi(\vec{\theta}) | \mathcal{H} | \psi(\vec{\theta}) \rangle \geq E_{gnd}.$$

In VQE, we want to find the set of parameters that minimize the expectation value of the energy. If our state preparation routine is general enough and the minimization protocol good enough we should find our ground state

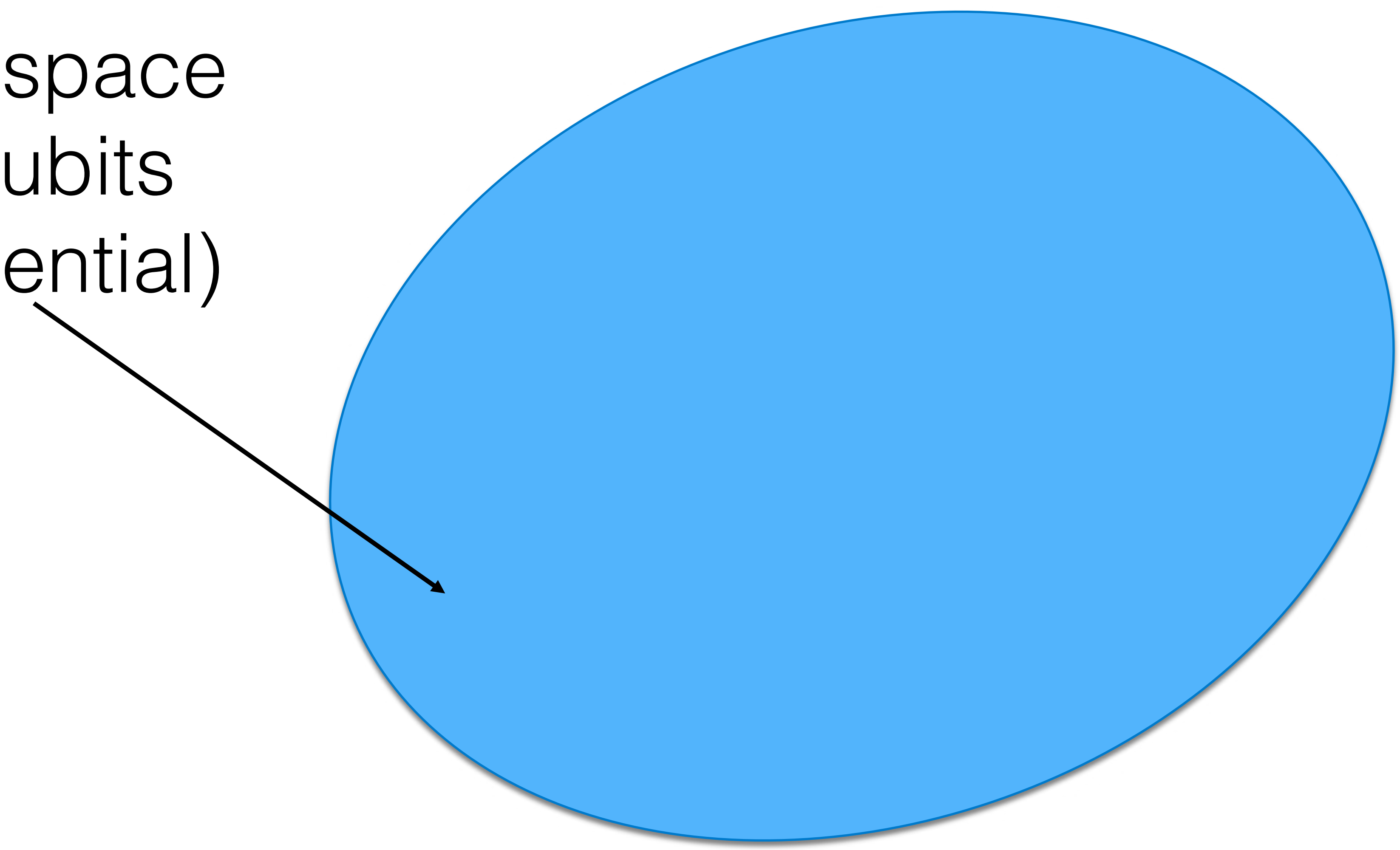
VQE



Variational Principle

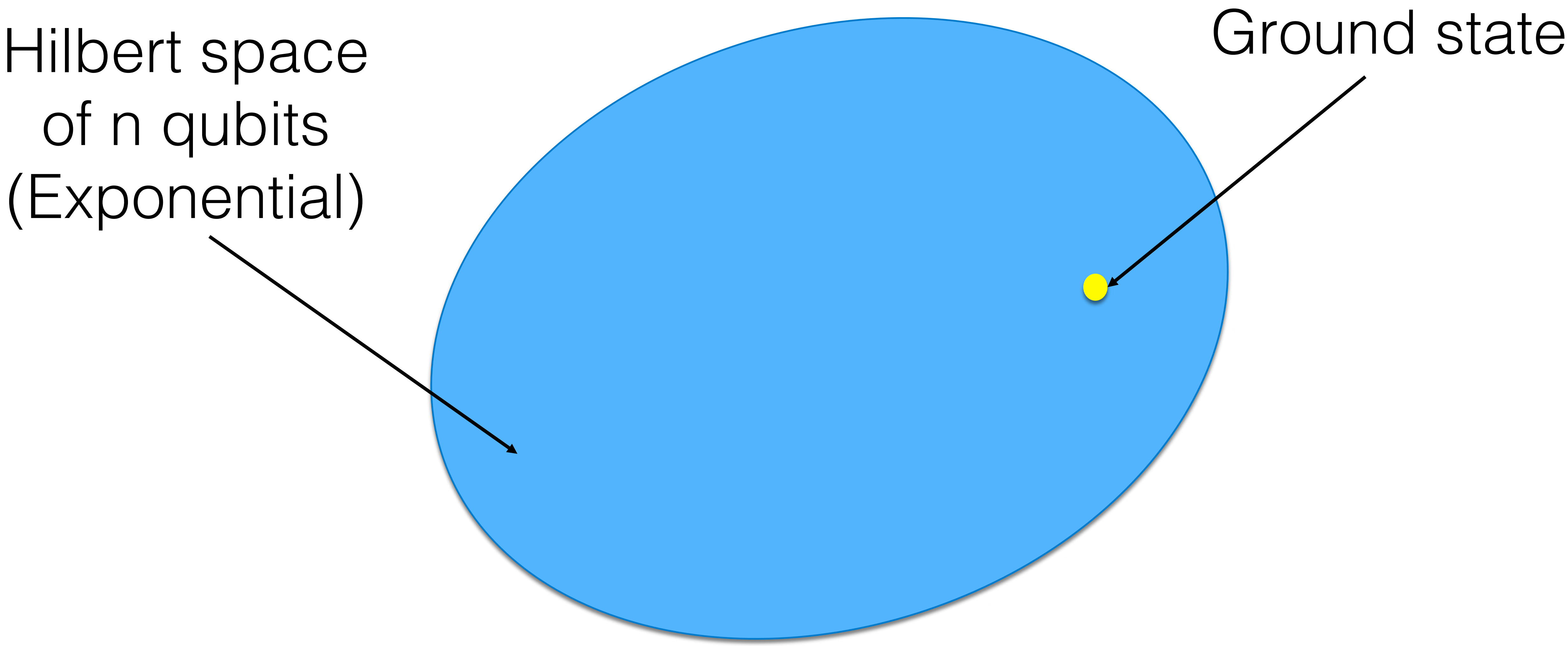
$$\langle \mathcal{H} \rangle(\vec{\theta}) = \langle \psi(\vec{\theta}) | \mathcal{H} | \psi(\vec{\theta}) \rangle \geq E_{gnd}.$$

Hilbert space
of n qubits
(Exponential)



Variational Principle

$$\langle \mathcal{H} \rangle (\vec{\theta}) = \langle \psi(\vec{\theta}) | \mathcal{H} | \psi(\vec{\theta}) \rangle \geq E_{gnd}.$$



Variational Principle

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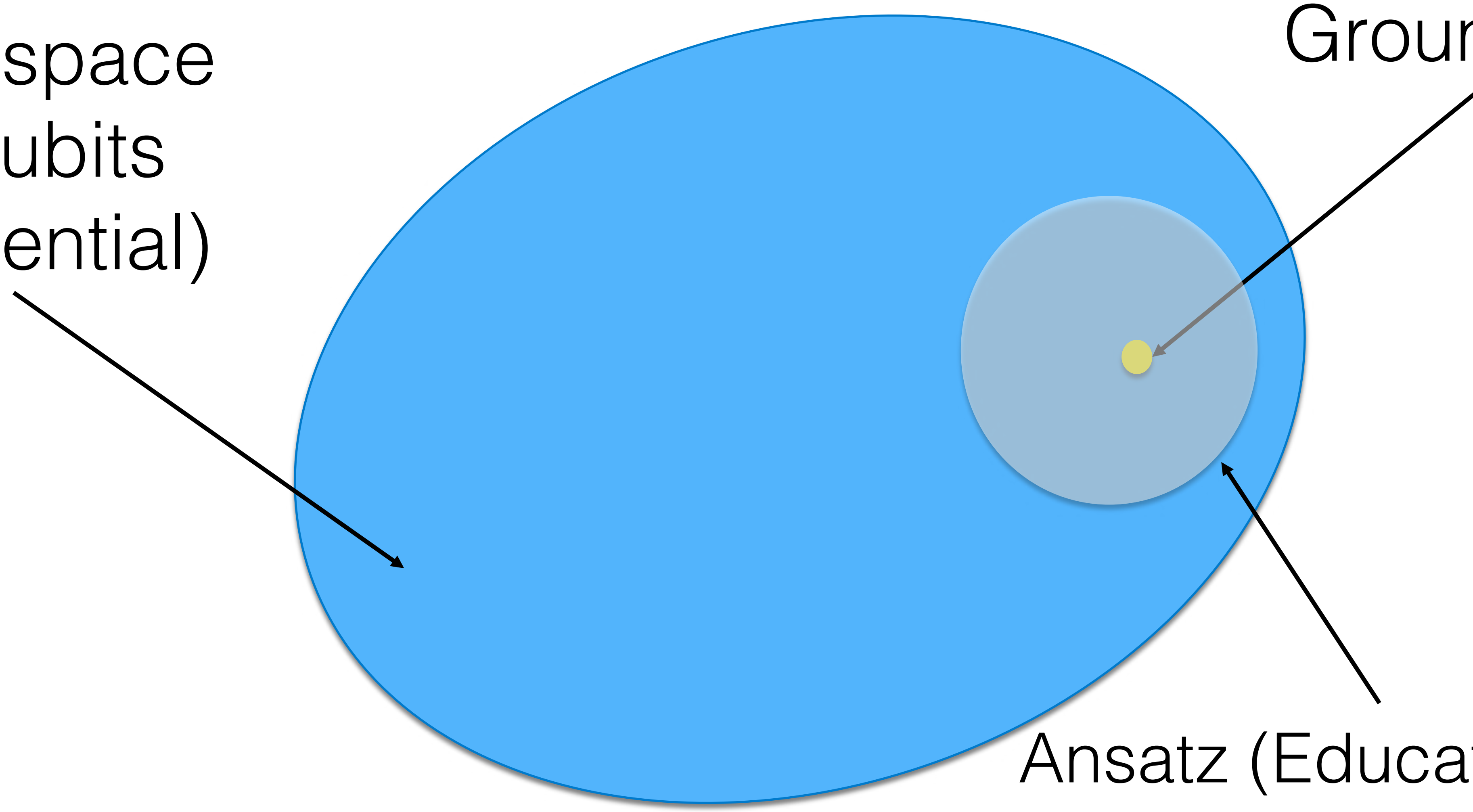
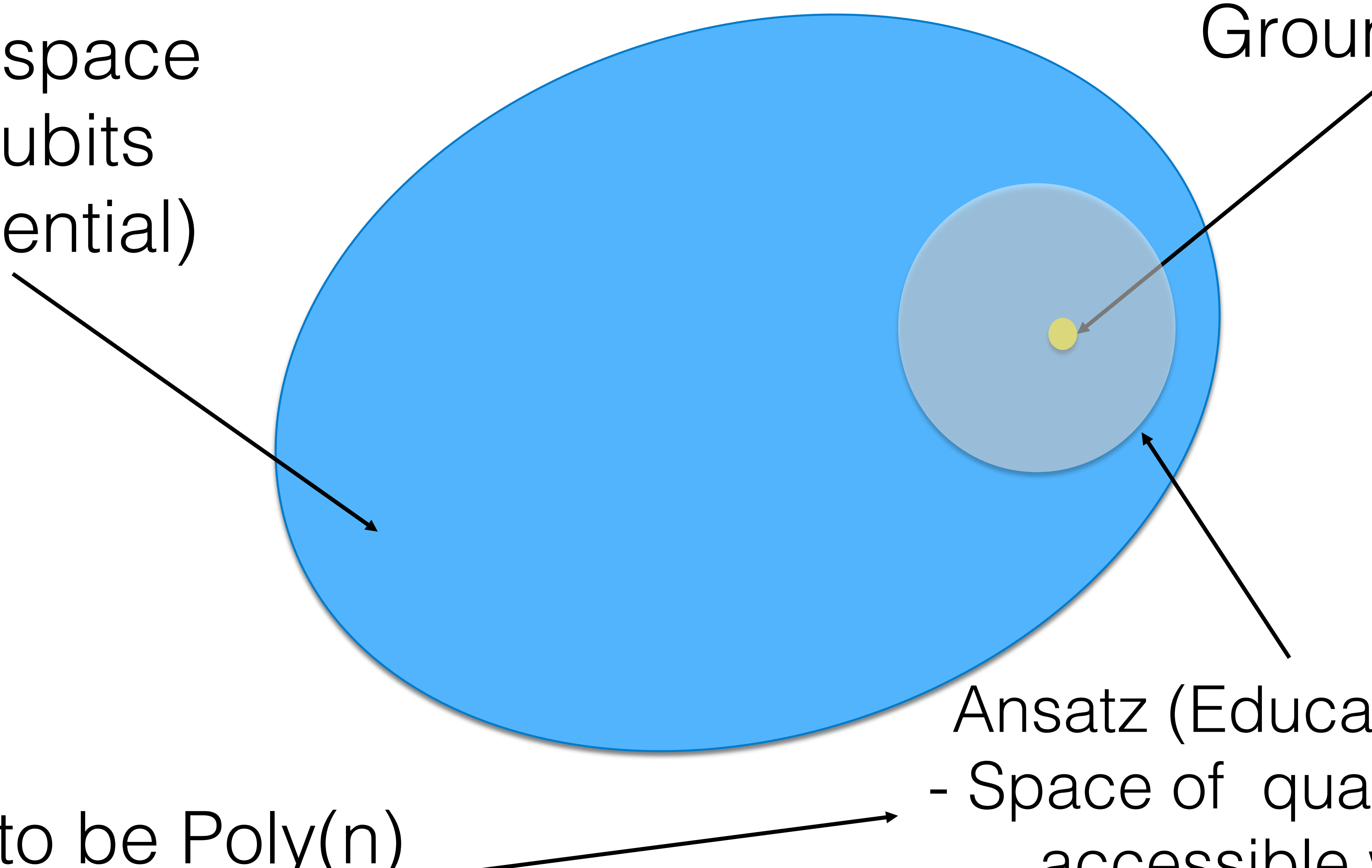


Variational Principle

$$\langle \mathcal{H} \rangle (\vec{\theta}) = \langle \psi(\vec{\theta}) | \mathcal{H} | \psi(\vec{\theta}) \rangle \geq E_{gnd}.$$



Ansatz

Unitary coupled cluster

$$| \Psi \rangle = e^{T - T^\dagger} \ | \Phi \rangle_{\text{ref}}$$

$(T - T^\dagger)$ Anti-hermitian

$$T = T_1 + T_2 + \ldots$$

$$T_1 = \sum_{pr} t_p^r \hat{a}_p^\dagger \hat{a}_r$$

$$T_2 = \sum_{pqrs} t_{pq}^{rs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

Jordan-Wigner

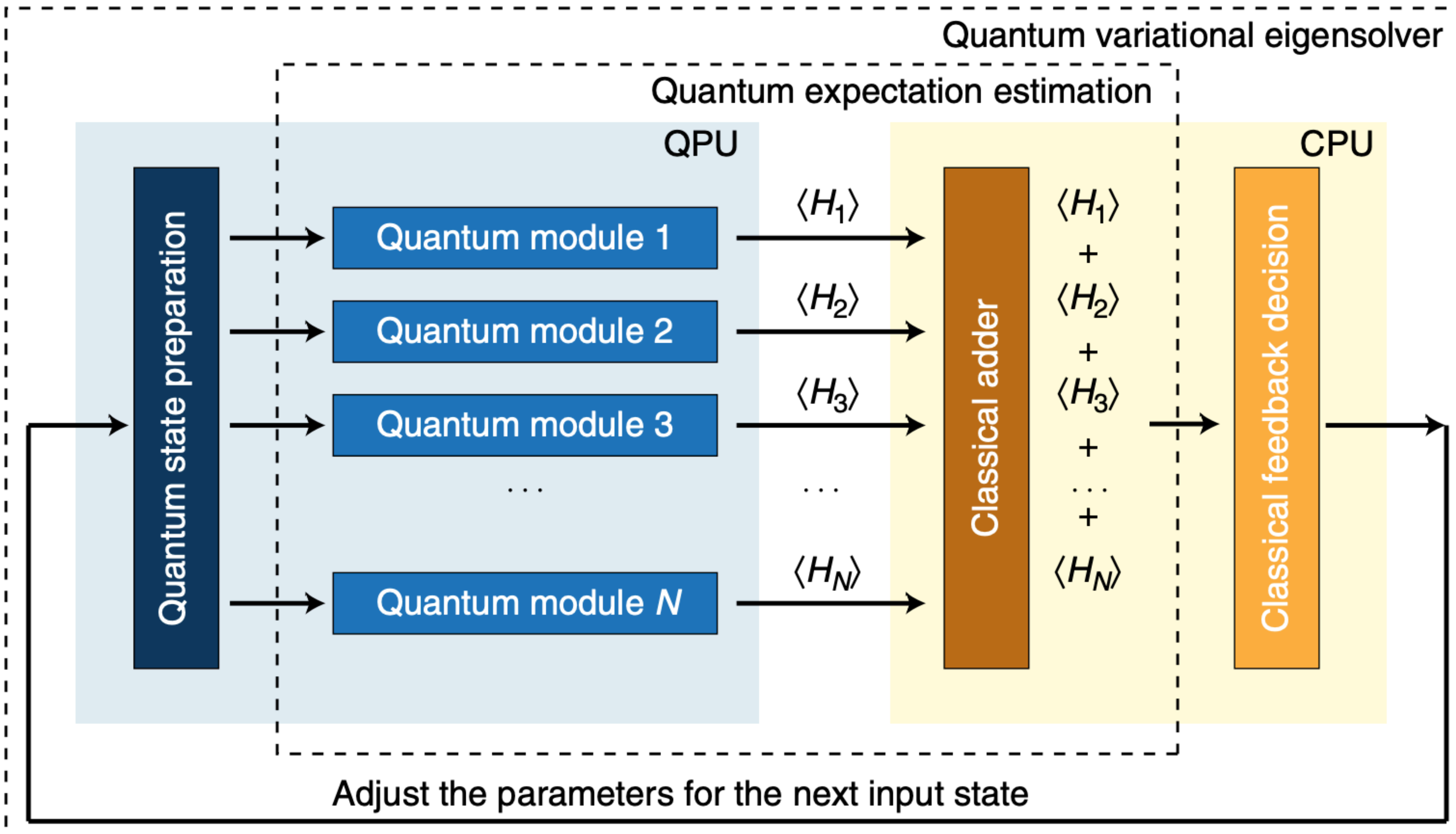
$$\hat{a}_j \rightarrow I^{\otimes j-1} \otimes \sigma_+ \otimes \sigma_z^{\otimes N-j}$$

$$\hat{a}_j^\dagger \rightarrow I^{\otimes j-1} \otimes \sigma_- \otimes \sigma_z^{\otimes N-j}$$

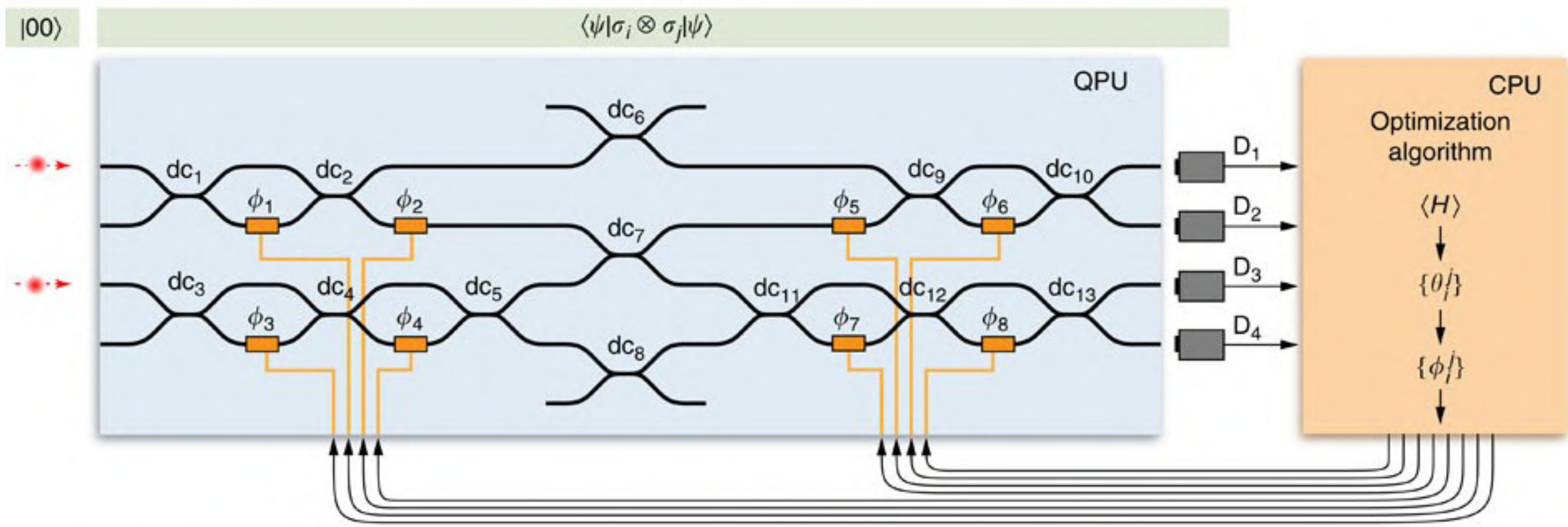
VQE

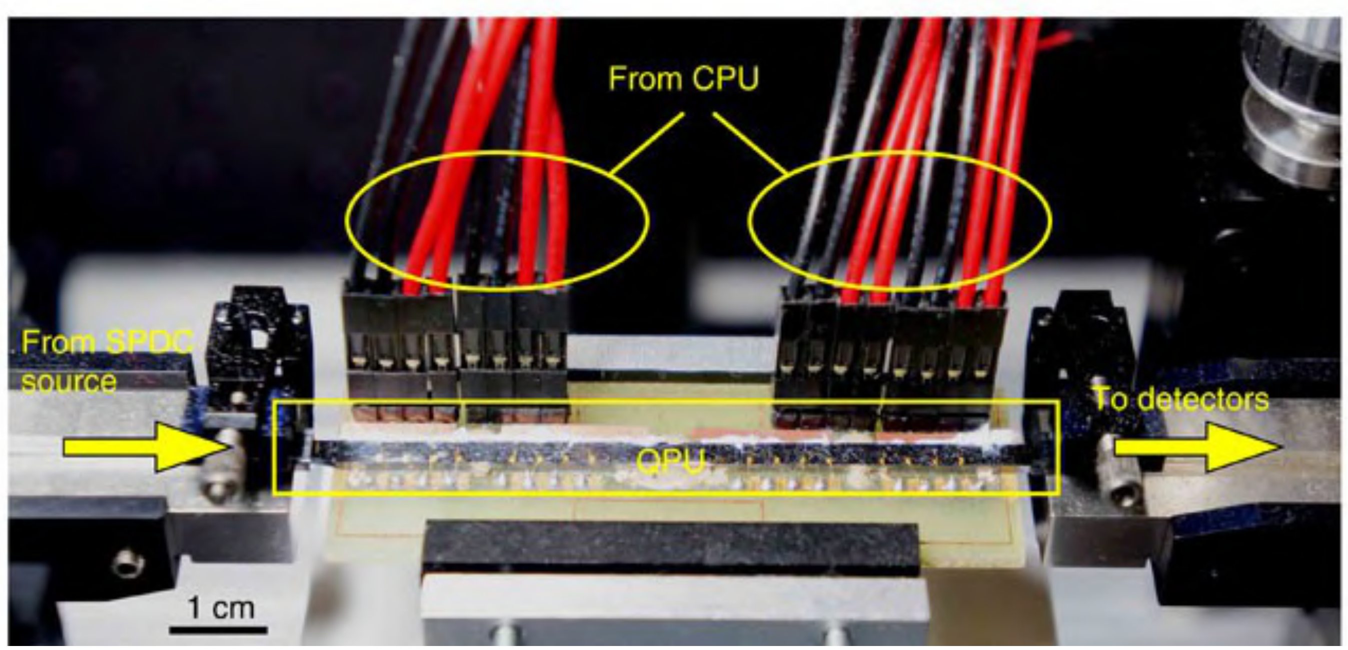
$$\langle \mathcal{H} \rangle (\vec{\theta}) = \langle \psi(\vec{\theta}) | \mathcal{H} | \psi(\vec{\theta}) \rangle \geq E_{gnd}.$$

$$\mathcal{H} = \sum_{i\alpha} h^i_\alpha \sigma^i_\alpha + \sum_{ij\alpha\beta} h^{ij}_{\alpha\beta} \sigma^i_\alpha \sigma^j_\beta + \ \dots$$

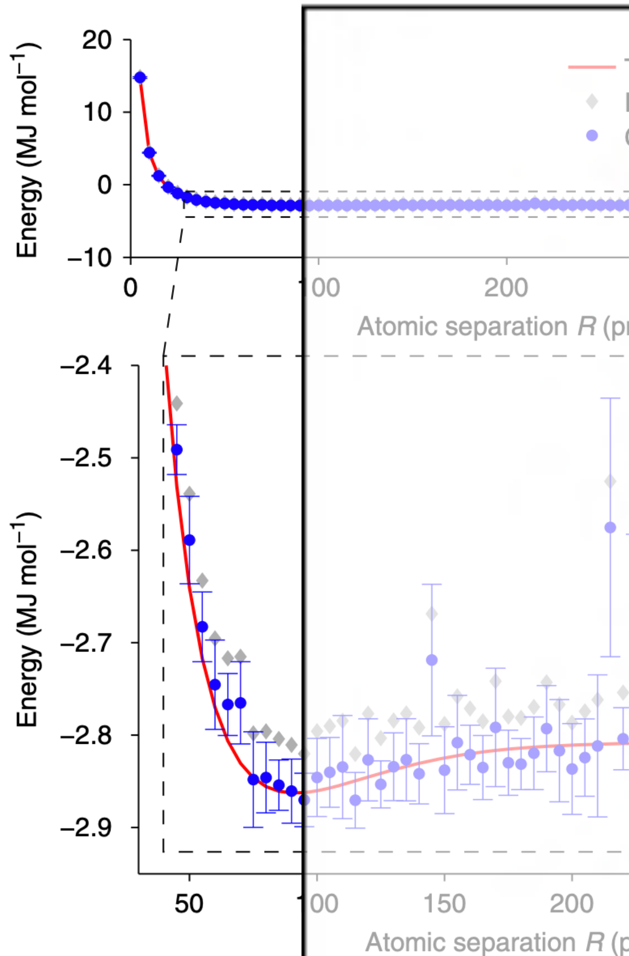


First experimental dem.



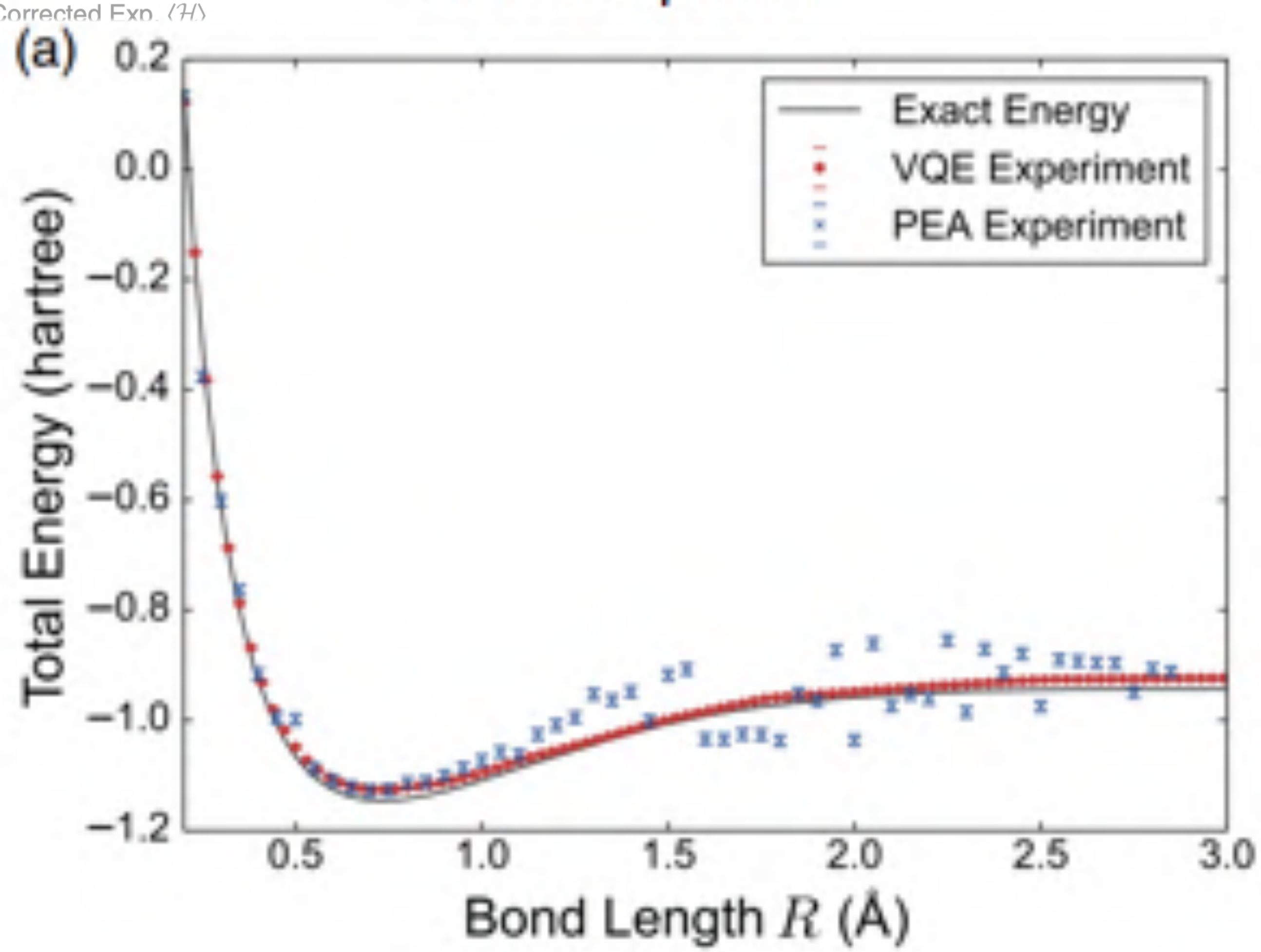


VQE experiment



A. Peruzzo et al. *Nat Commun* 5,

Example:



P. J. J. O'Malley, R. Babbush *et al.*, Phys. Rev. X **6**,031007 (2016)

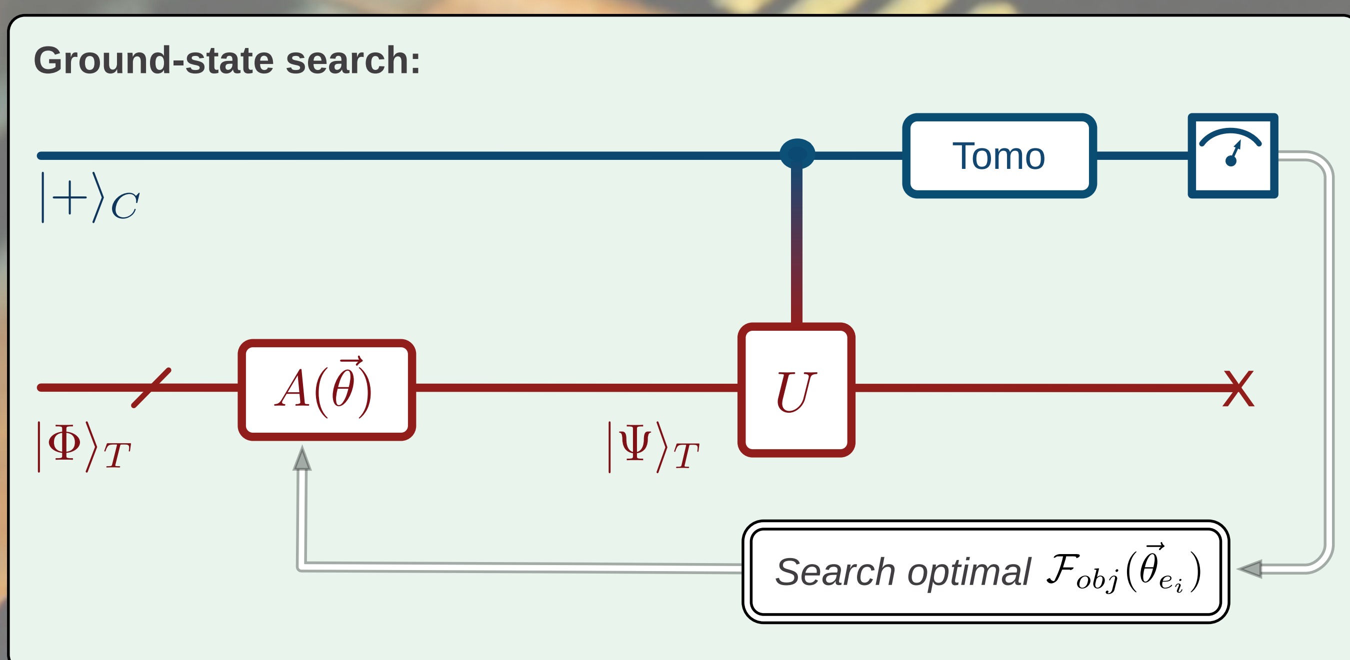
VQE summary

- VQE is great for noise resilience
- It is expected to be applied to pre-threshold devices
- As it is, it can target only the ground state but excited states are equally fundamental
- So far main solution was to use an expensive folding spectra method

WAVES - Wittness Assisted Variational Eigenstate Solver

Ground-state search using $\mathcal{F}_{obj}$ and $\hat{E}_{p_0} = \hat{I}$ → Excited-states search using $\mathcal{S}$ and guessed $\hat{E}_{p_i}$ → Eigenvalues estimation using *IPEA*

$$U = e^{-iHt}$$



$$\hat{U} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$$

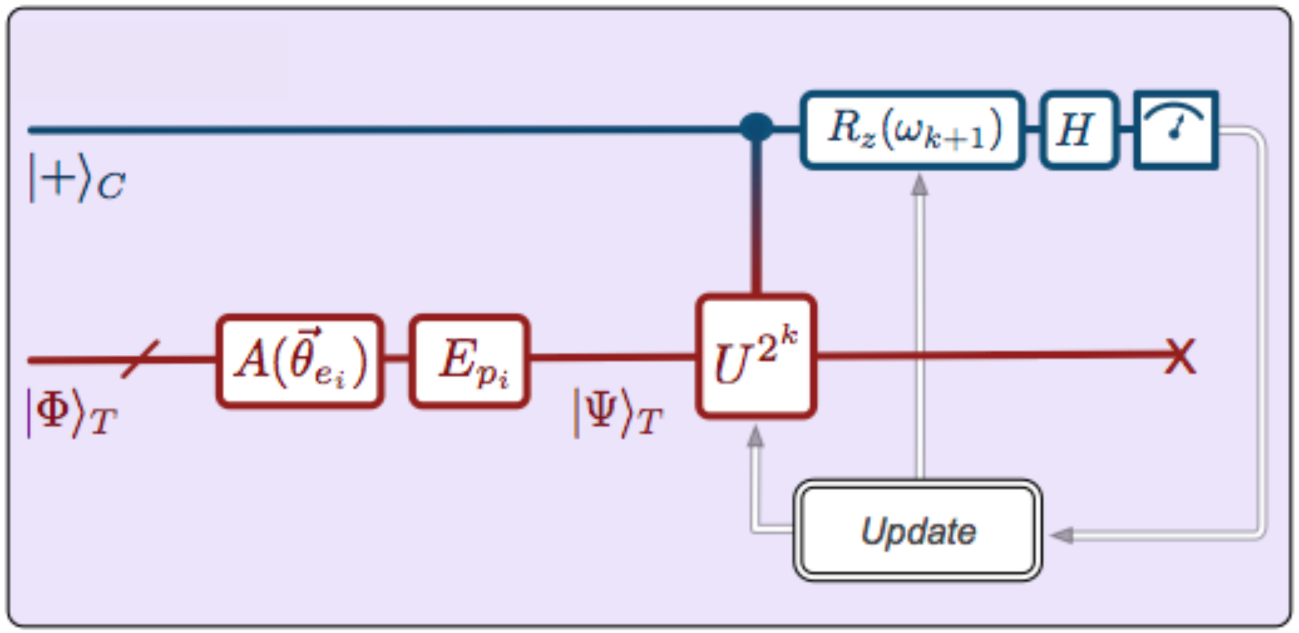
$$|+\rangle_C \to |0\rangle + e^{i\phi}|1\rangle$$

From the phase we can estimate the eigenvalue (i.e. the energy)

Santagati, Wang et al. Sc. Adv. 2018

WAVES - Wittness Assisted Variational Eigenstate Solver

If P is 1 |ΨT> is eigenstate
If P is <1 |ΨT> is NOT eigenstate



The purity can be used as eigenstate witness.

Helmholtz free energy

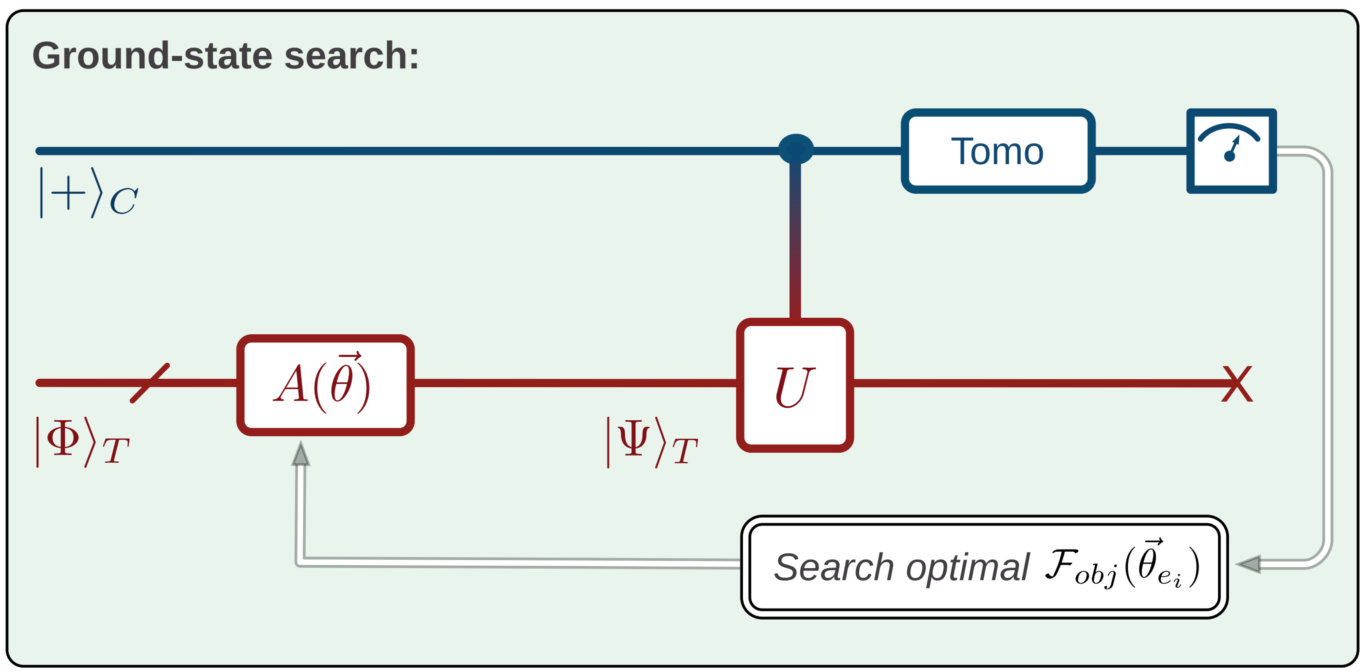
$$\mathcal{F}'_{obj}(\mathcal{S},\mathcal{E}) = \mathcal{E} + T\mathcal{S}(\rho)$$

$$\mathcal{F}_{obj}(\mathcal{P},\mathcal{E}) = \mathcal{E} - T\mathcal{P}$$

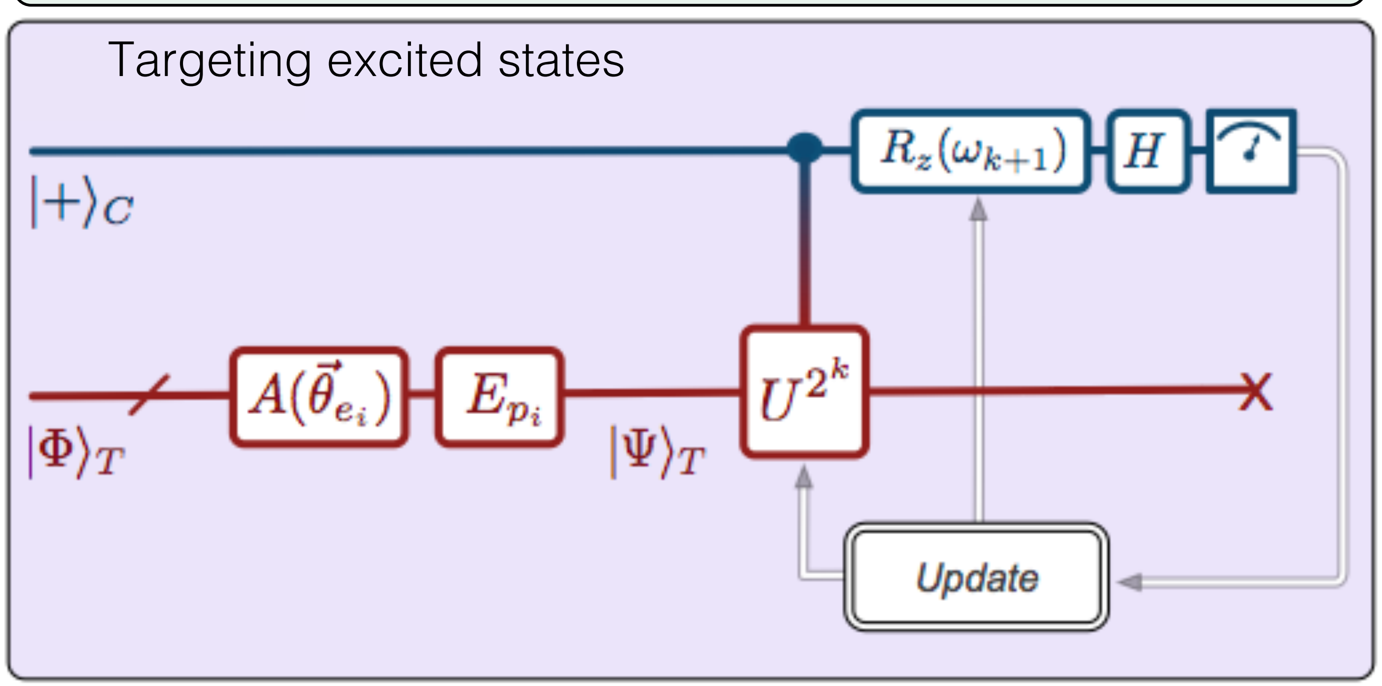
$S = -Tr(\rho \ln \rho)$ $\quad S = 1 - Tr(\rho^2)$

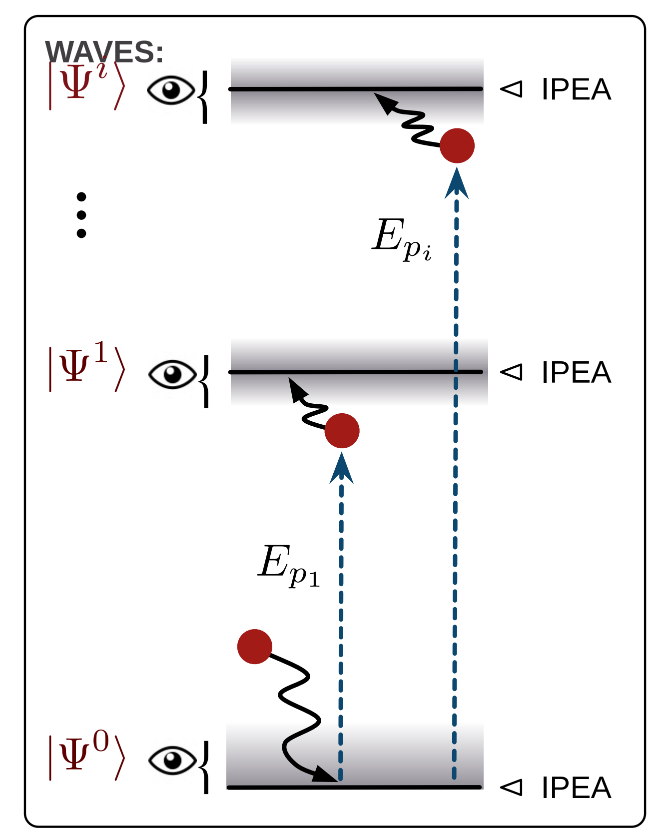
WAVES - Wittness Assisted Variational Eigenstate Solver

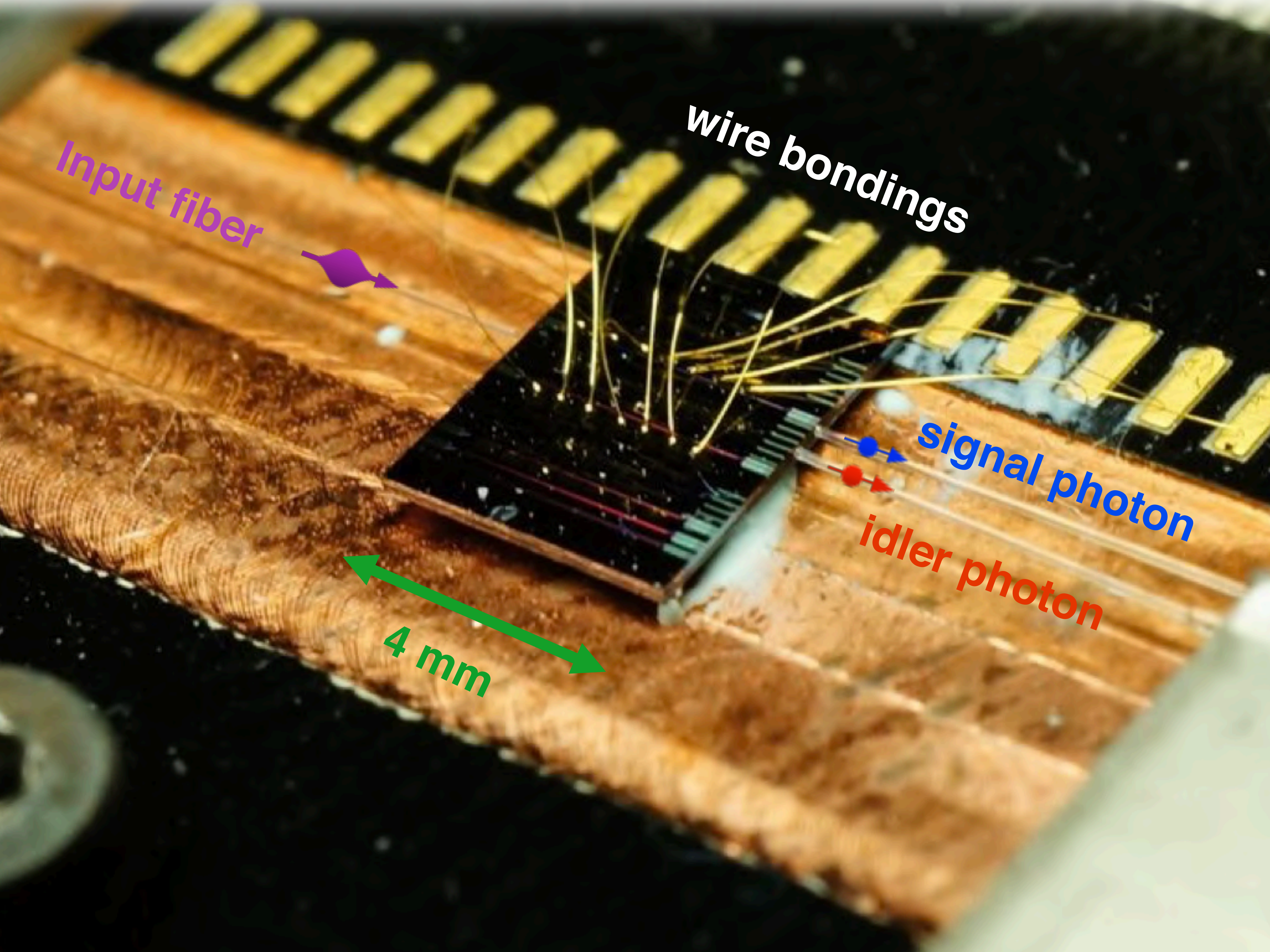
Ground-state search using $\mathcal{F}_{obj}$ and $\hat{E}_{p_0} = \hat{I}$ → Excited-states search using $\mathcal{S}$ and guessed $\hat{E}_{p_i}$ → Eigenvalues estimation using *IPEA*



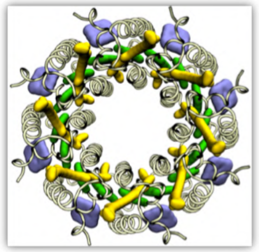
$$\mathcal{F}_{obj} = \mathcal{E} + T\mathcal{S}$$
$$T \to \infty$$





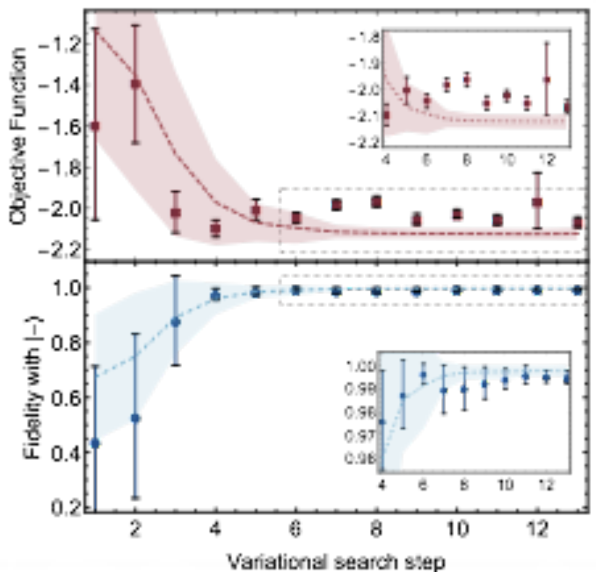

wire bondings
Input fiber
signal photon
idler photon
4 mm

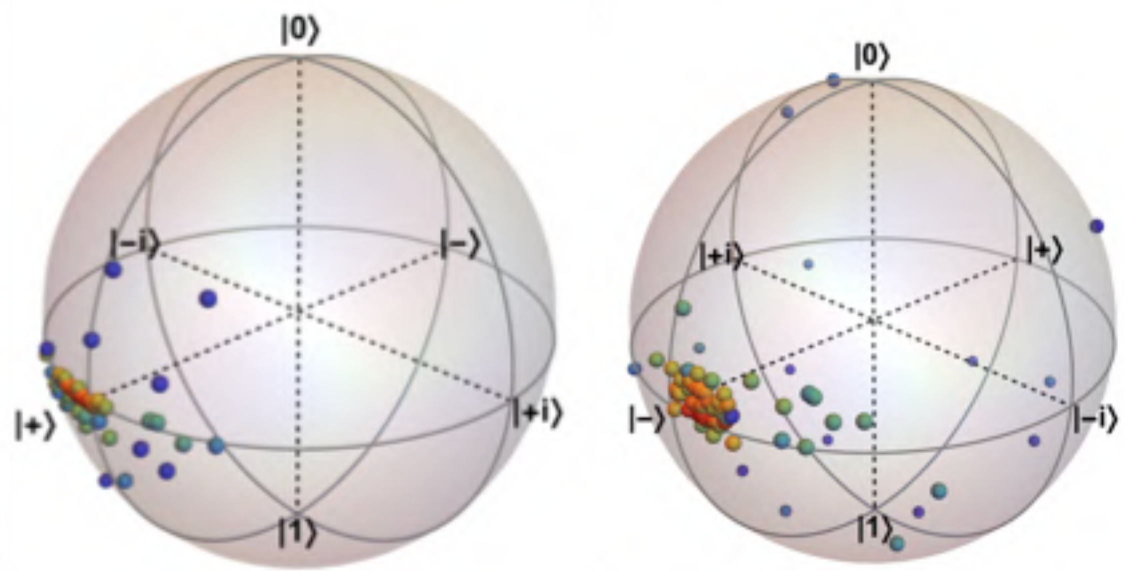
Experiment

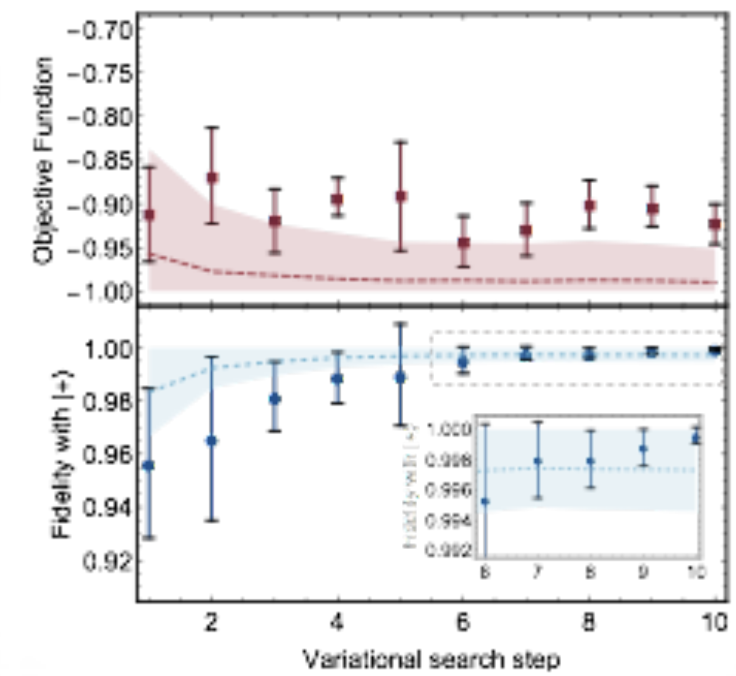


Ground-state search using $\mathcal{F}_{obj}$ and $\hat{E}_{p_0} = \hat{I}$

Excited-states search using $\mathcal{S}$ and guessed $\hat{E}_{p_i}$







$\mathcal{F}'_{obj}(\mathcal{S},\mathcal{E}) = \mathcal{E} + T\mathcal{S}(\rho)$

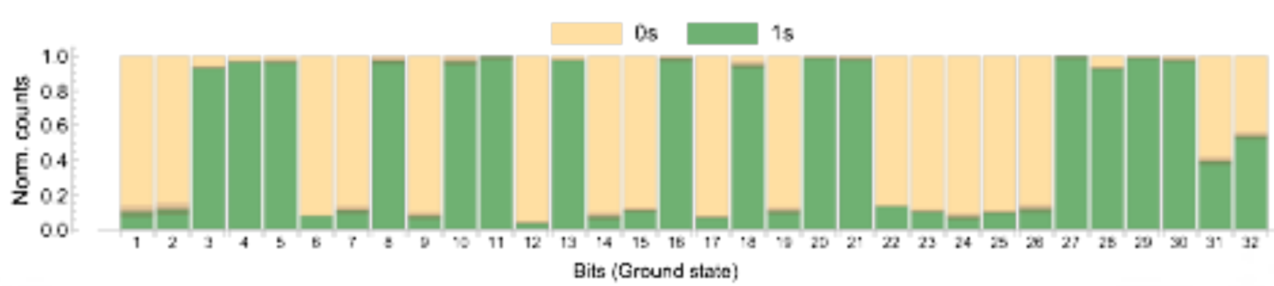
F=99.5%

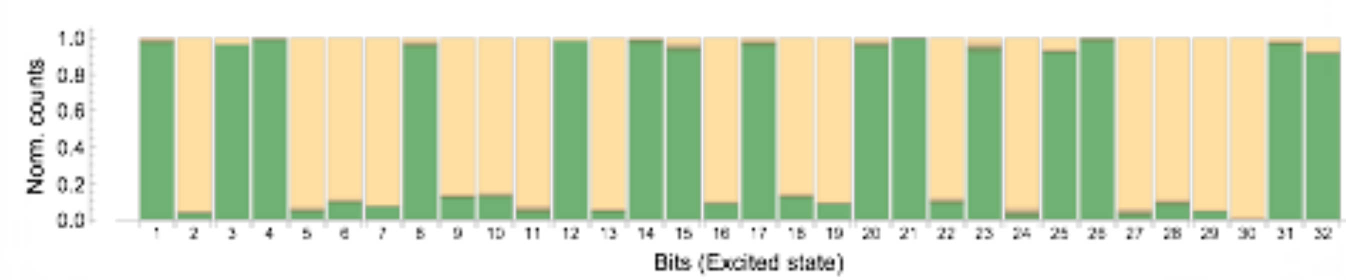
Santagati et. al (2016) in preparation

F=99.9%

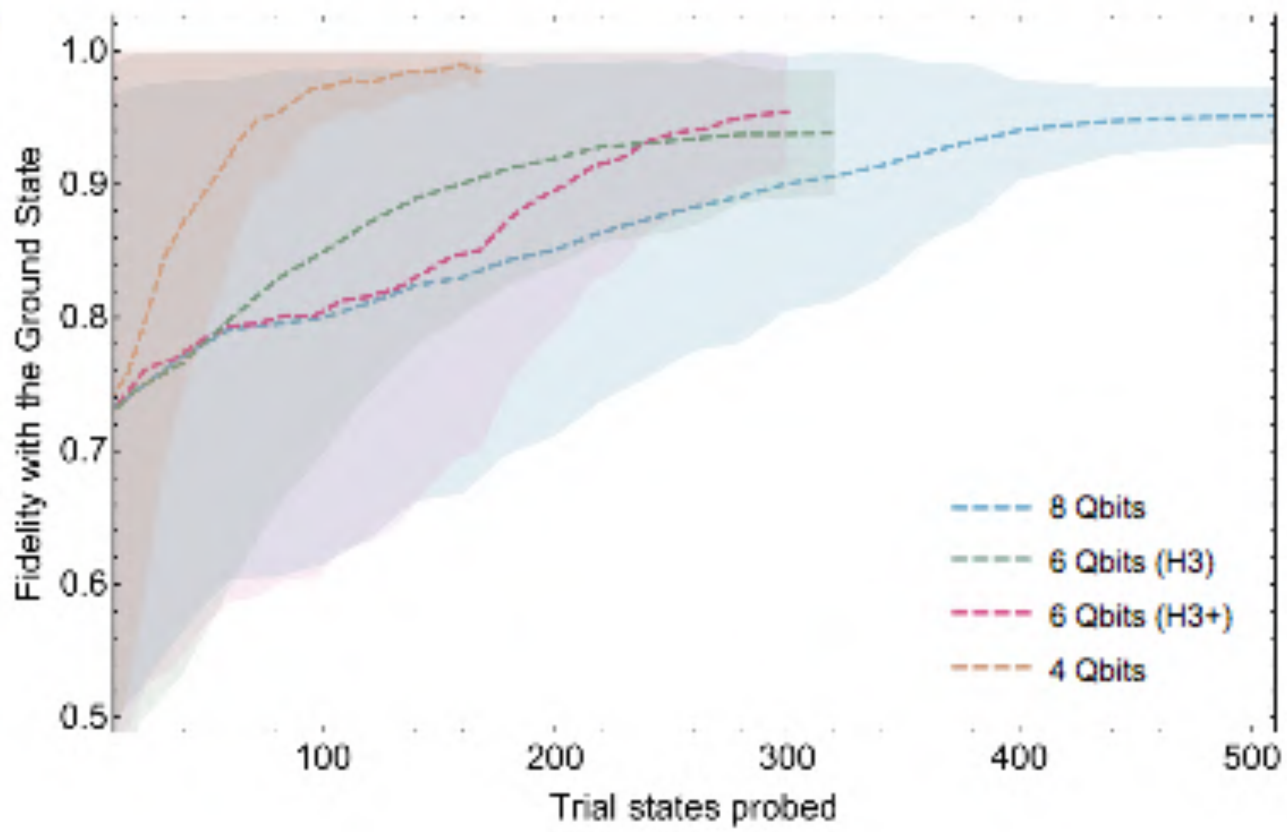
IPEA

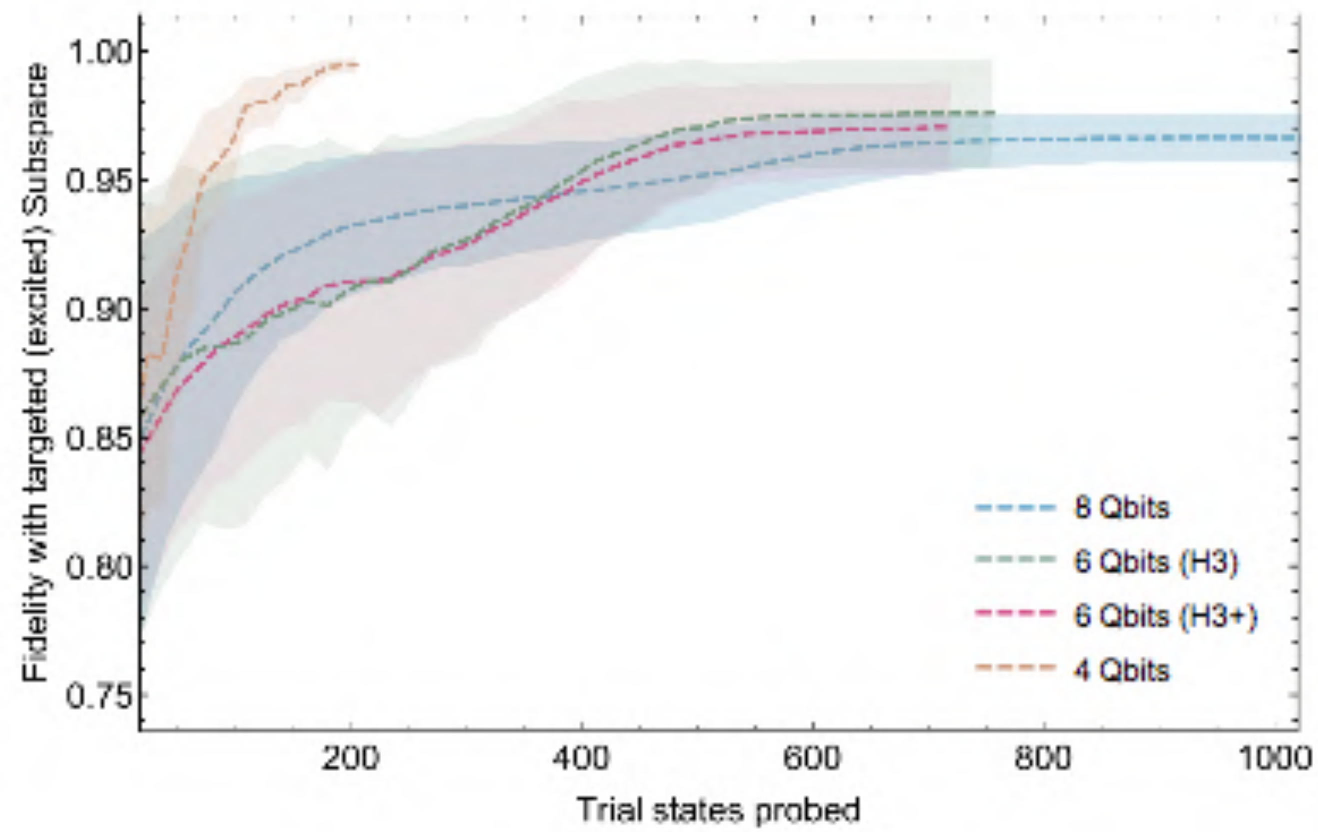
32 bits





WAVES: Simulations





Simulating H2, H3, H3+ and H4 with 4,6 and 8 qubits

Restrictions on the ansatz state preparation seems to limit the initial fidelity

Ansatz: UUCC

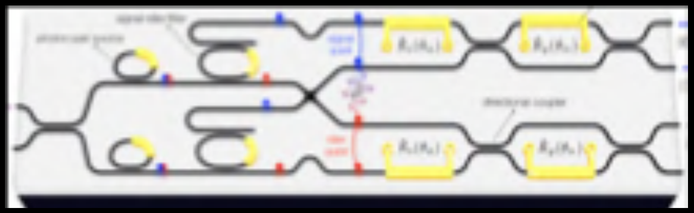
$$U(\vec{t}) = \exp\left[\sum_{ij} t_{ij}(a_i^\dagger a_j - a_j^\dagger a_i) + \sum_{ijkl} t_{ijkl}(a_i^\dagger a_j a_k^\dagger a_l - a_l^\dagger a_k a_j^\dagger a_i)\right]$$

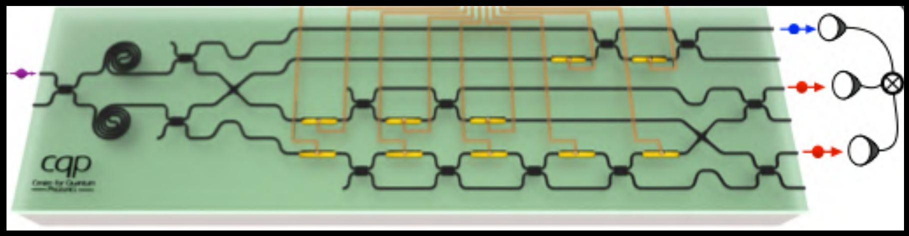
Excitation operators

$$E_{ij} = \exp\left[\frac{\pi}{2}(a_i^\dagger a_j - a_j^\dagger a_i)\right]$$

CONCLUSION

- VQE
- Witness Assisted Variational Eigensolver
- Implementation in silicon quantum photonics

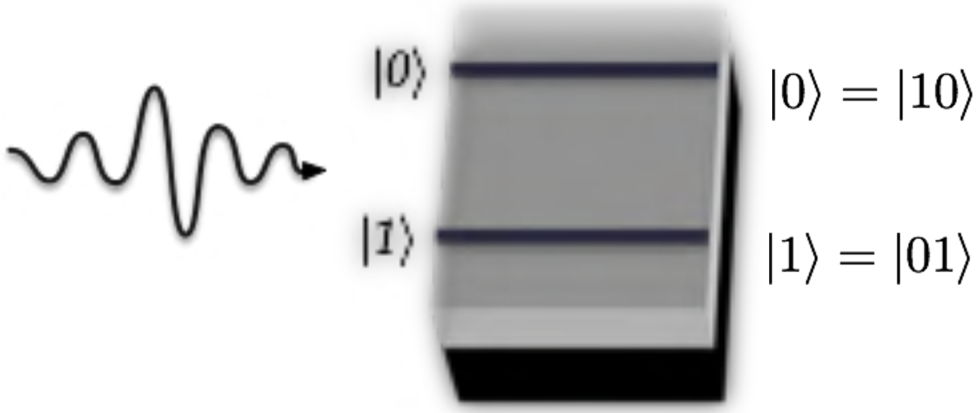




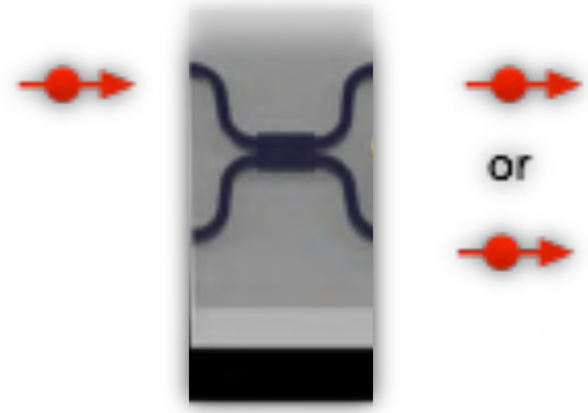

cqp
Barreto
O'Brien
Wilkes
Sinclair
Piekarek
Tyler
Thompson
Kennard
Sibson
Villareal
Bonneau
Santagati
Silverstone
Wang
Gentile
Erven
Adcock
Paesani

Q.I. with integrated photonics

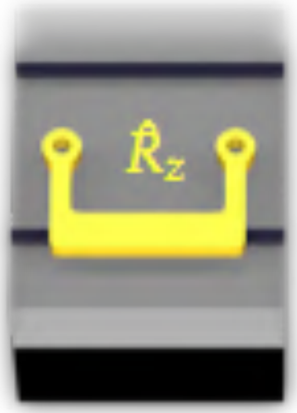
path-encoded qubit



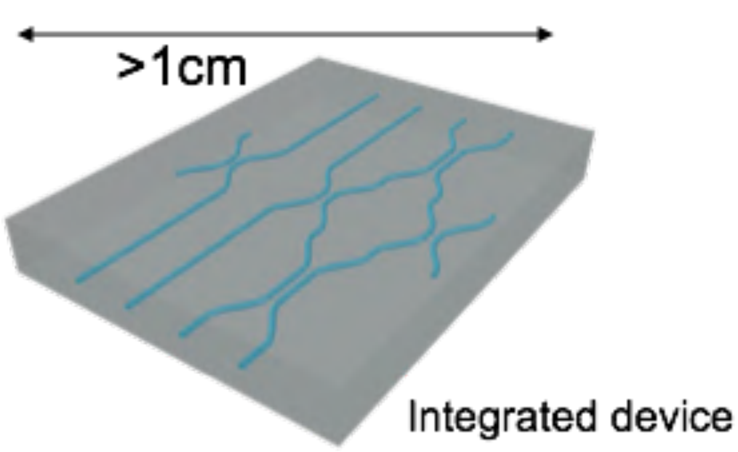
Directional Coupler

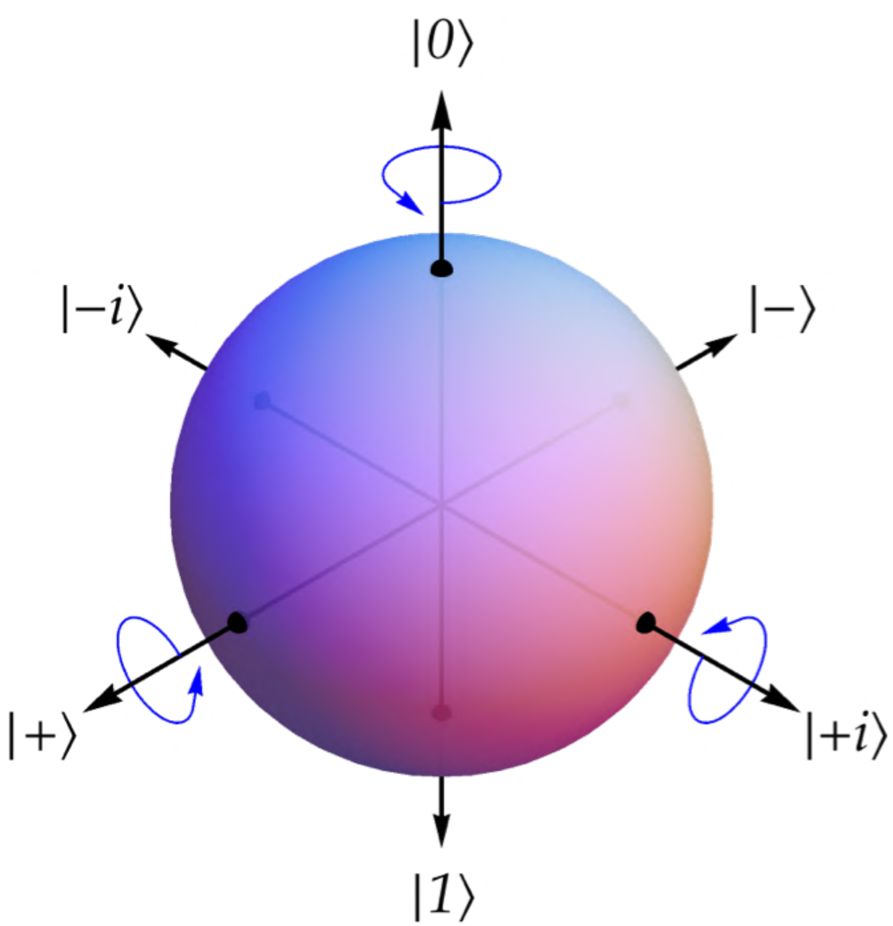


Termal phase shifter

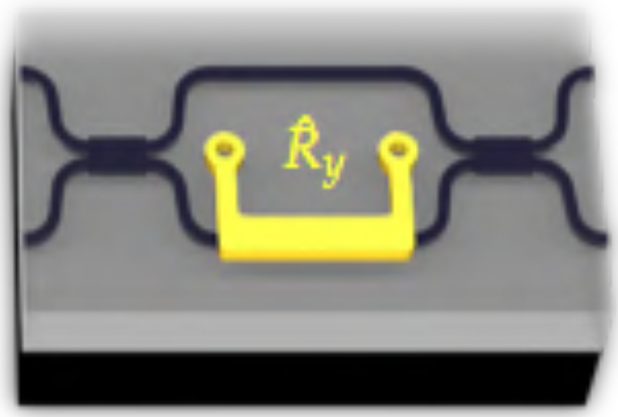


- Path encode qubits
- very long coherence time
- single and 2 qubits gate



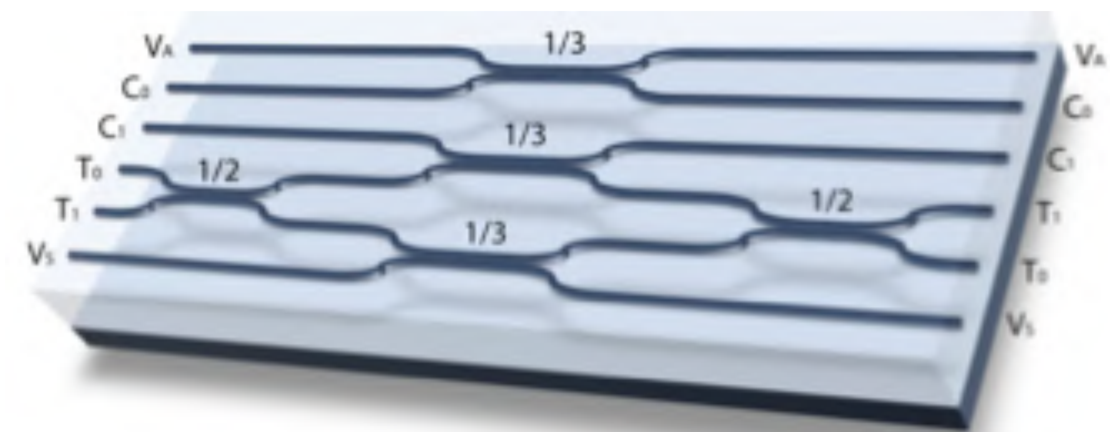


Interferometers



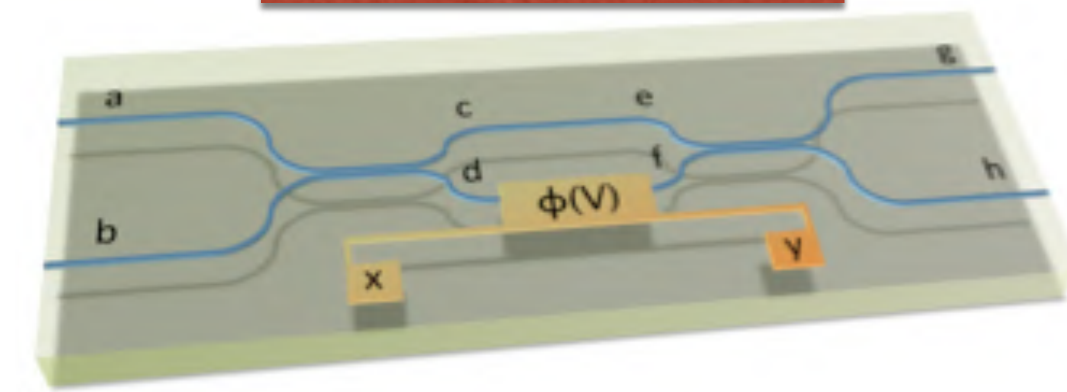
Silica on silicon integrated quantum photonic circuits

CNOT Gate



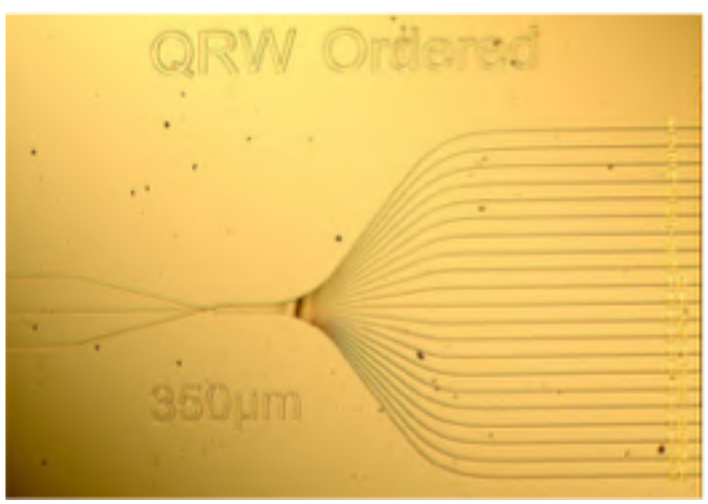
Politi, Cryan, Rarity, Yu, and O'Brien
***Science* 320**, 5876 (2008)

Single qubit Gate



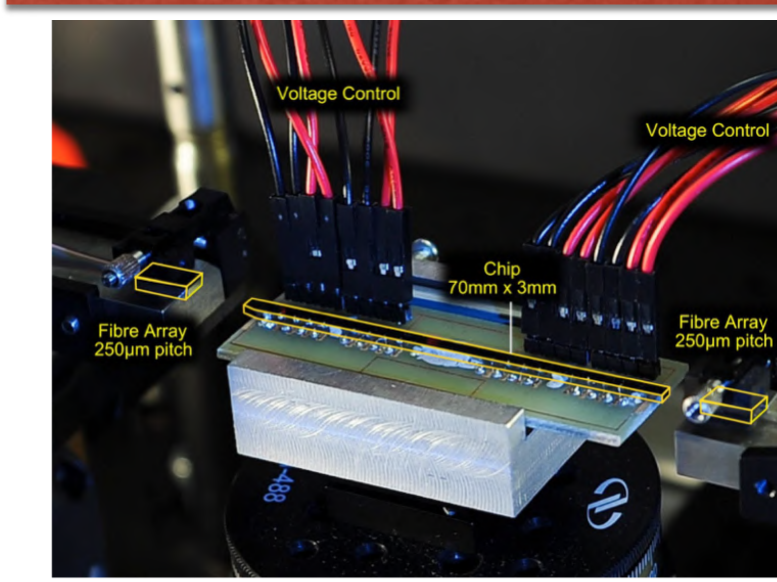
Politi, Cryan, Rarity, Yu, and O'Brien
***Science* 320**, 5876 (2008)

Quantum Walks



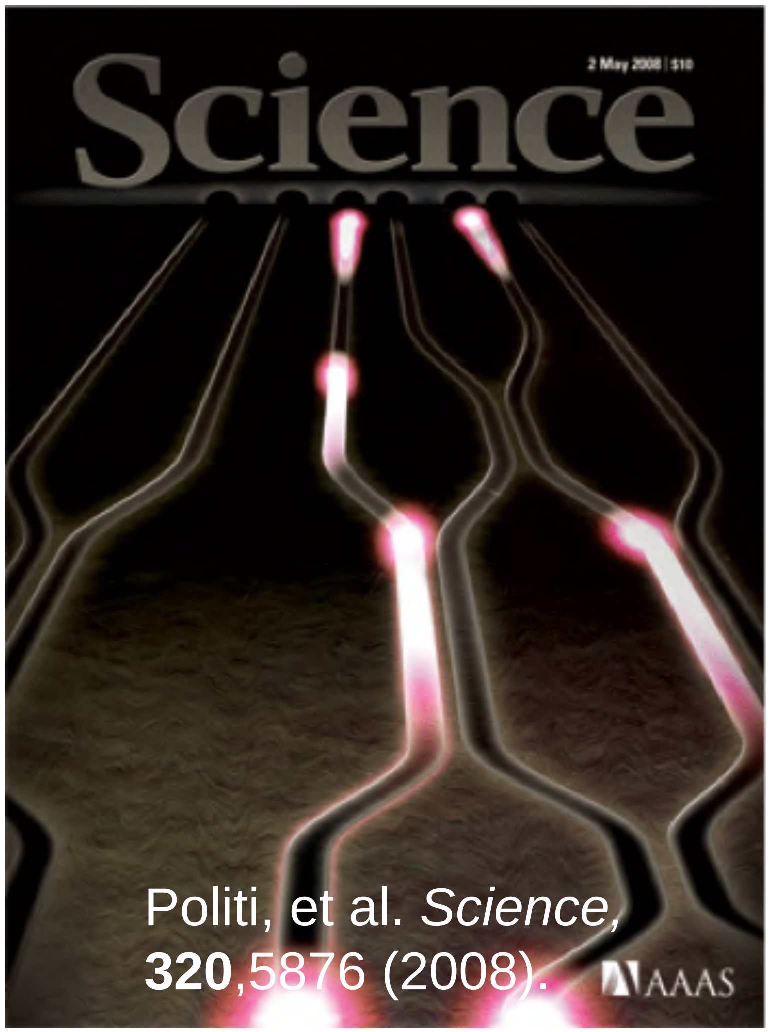
Peruzzo, Lobino, Matthews, Matsuda, *et al.*
***Science* 329** 1500 (2010)

Generate arbitrary states

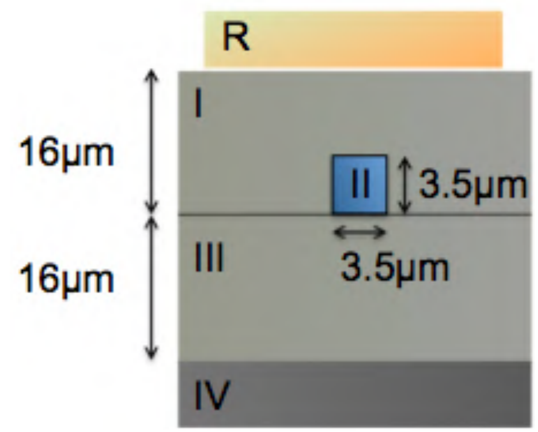


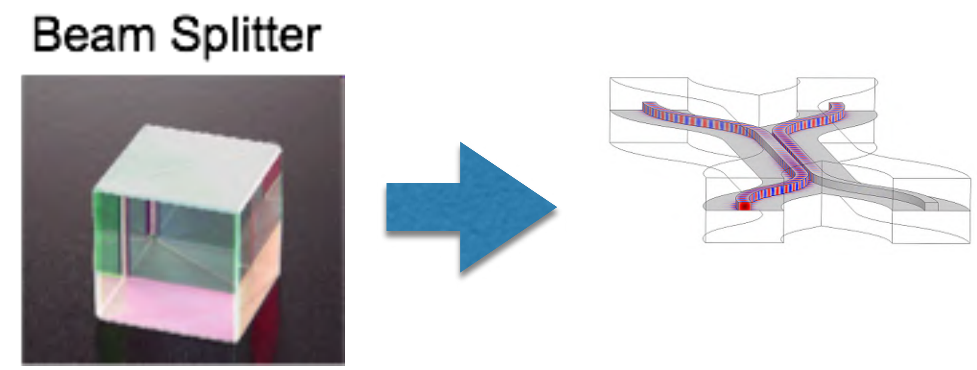
Shadbolt *et al.*
Nature Photonics (2011)

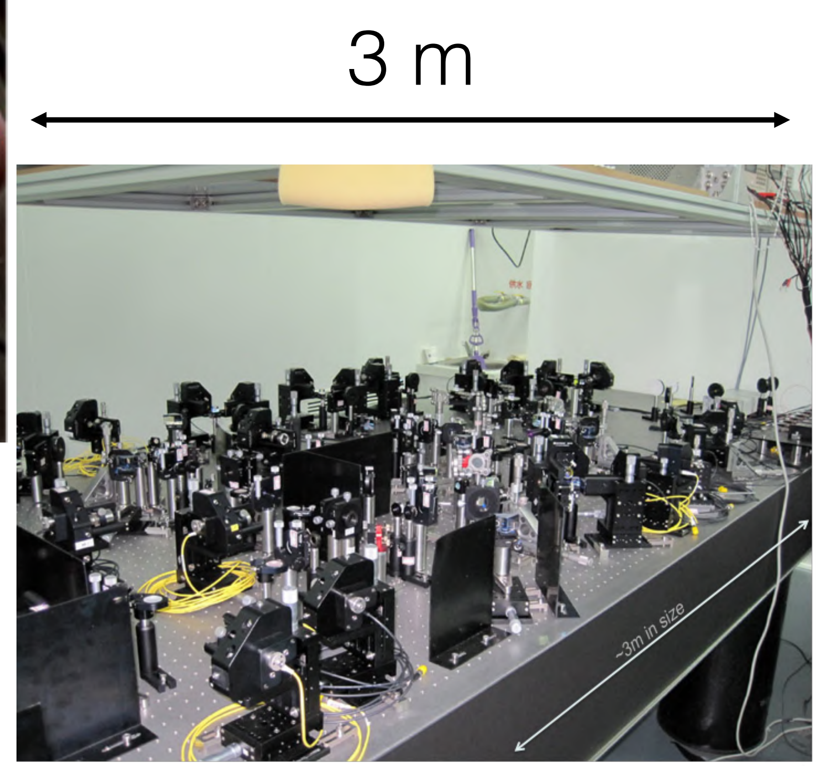
Silica on silicon integrated quantum photonic circuits

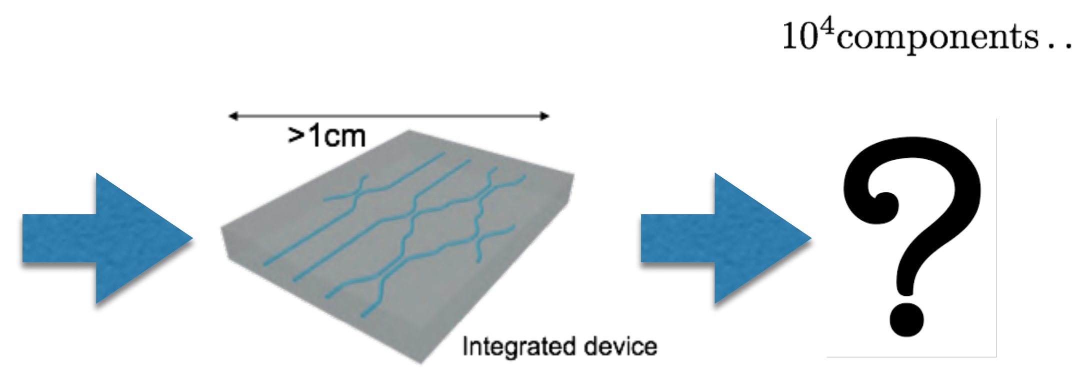


Politi, et al. *Science*, **320**,5876 (2008).







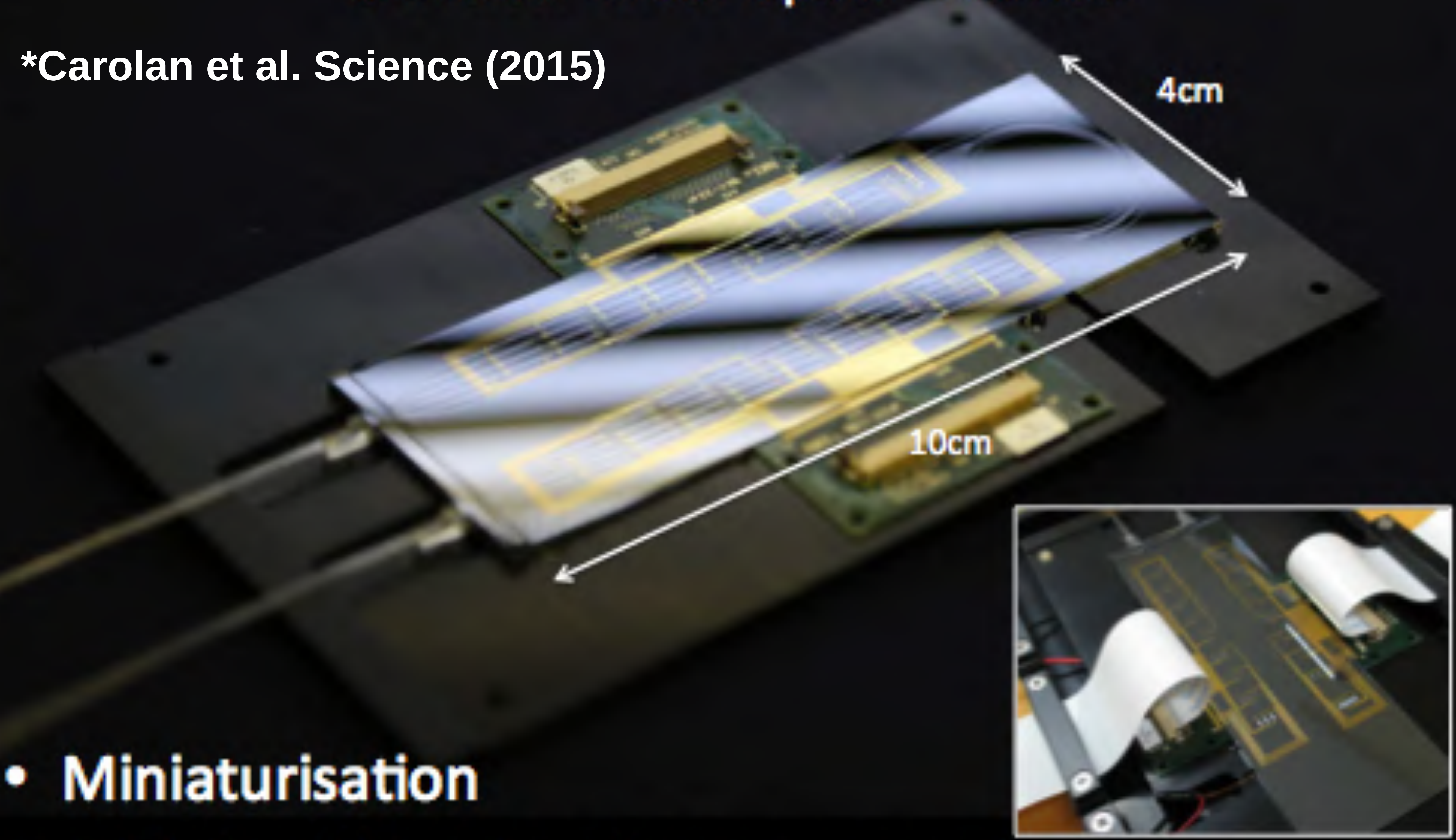


- **Size / Compactness**
- **Stability**
- **Complexity**
- **Route to scalability?**

- Silica waveguide on a silicon wafer
- Photo-lithographically processed with sub μm accuracy
- Low loss coupling to fibre-optics

Universal Linear Optics Processor

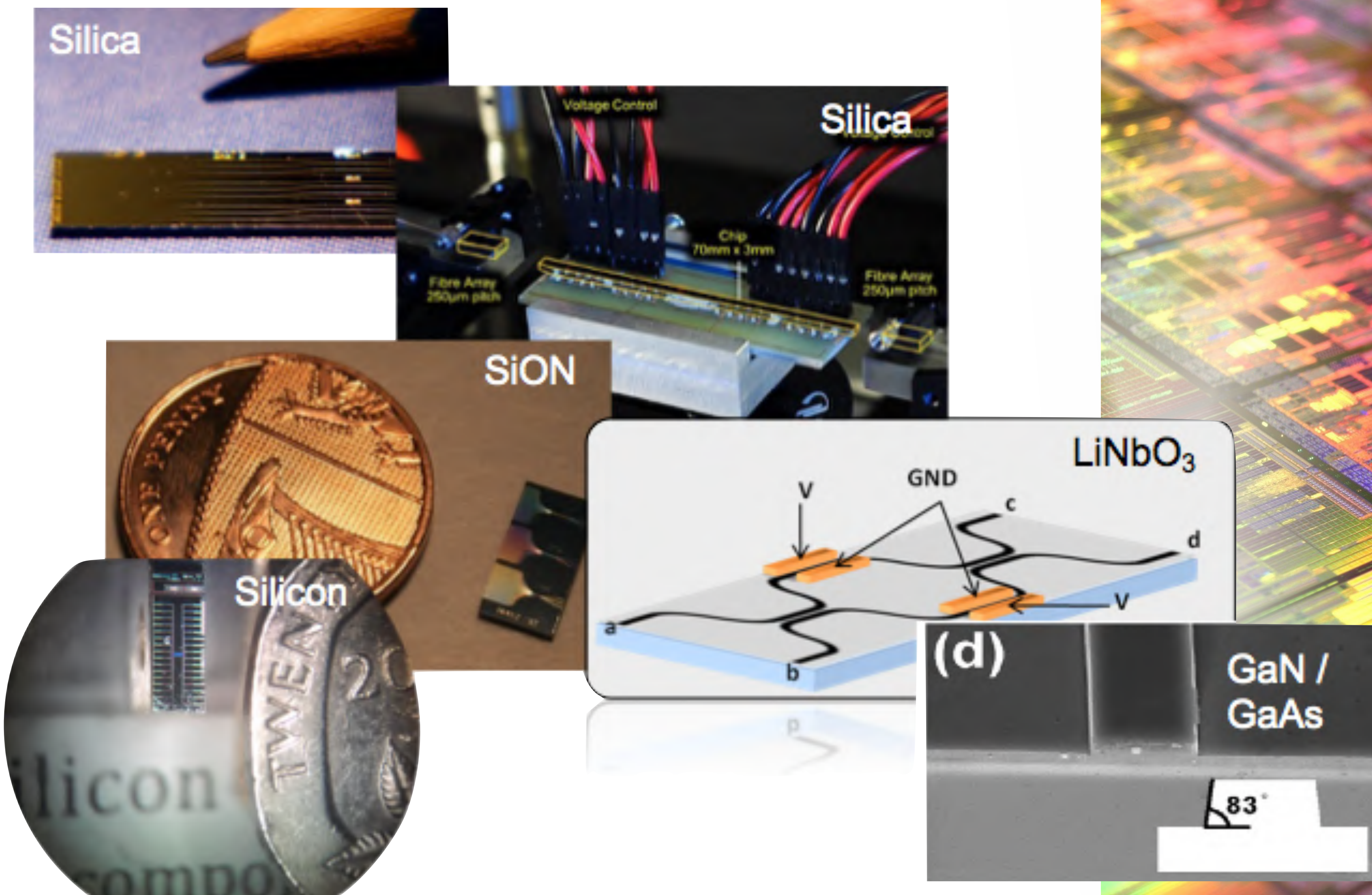
*Carolan et al. Science (2015)

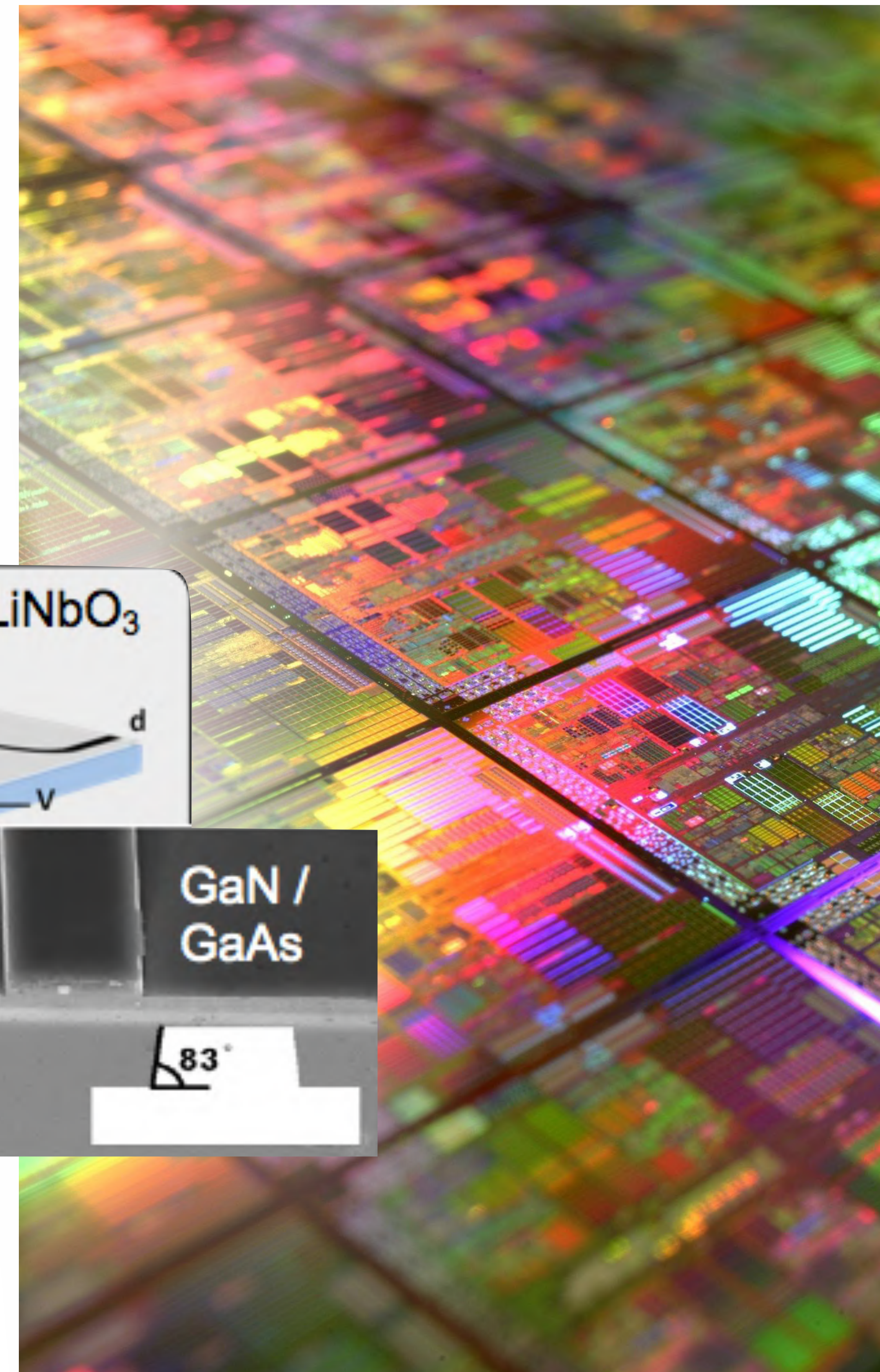


- Miniaturisation
- Additional functionality (sources, detectors)
- Full integration

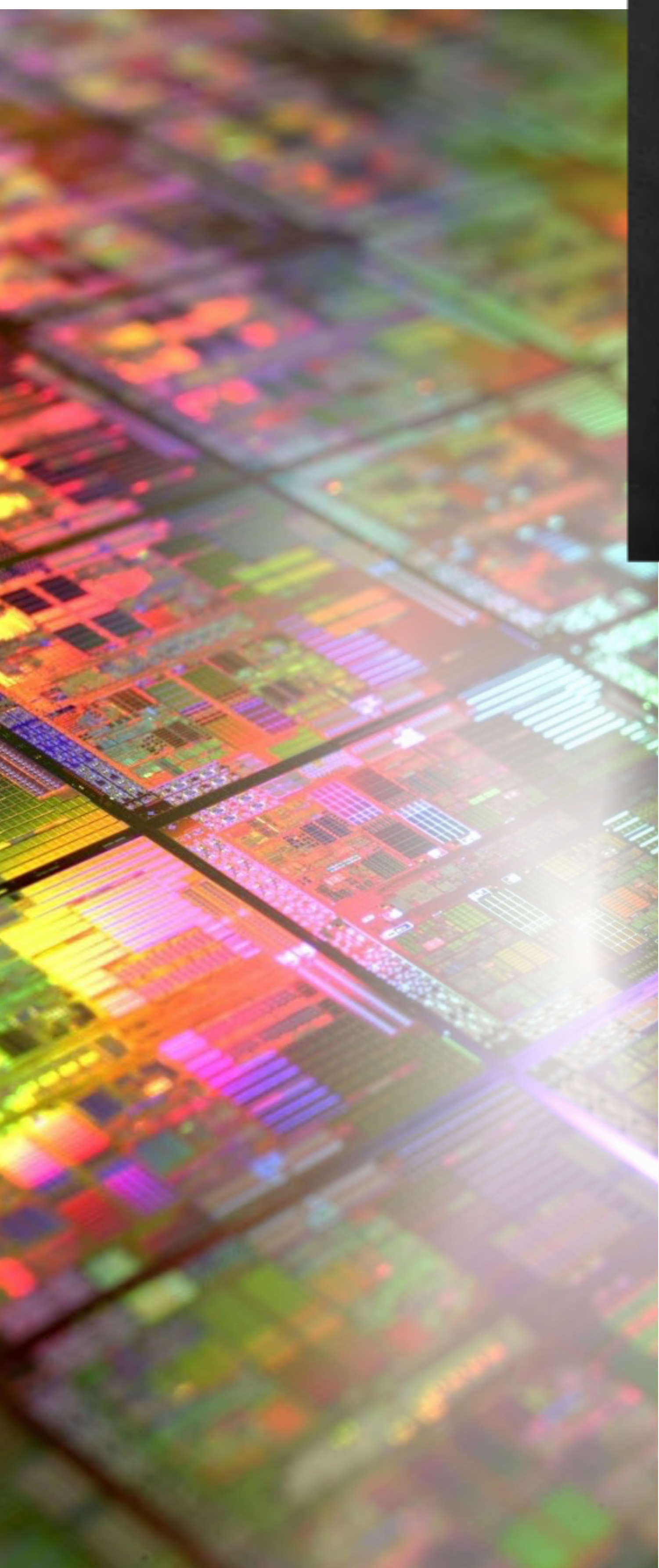
University of BRISTOL

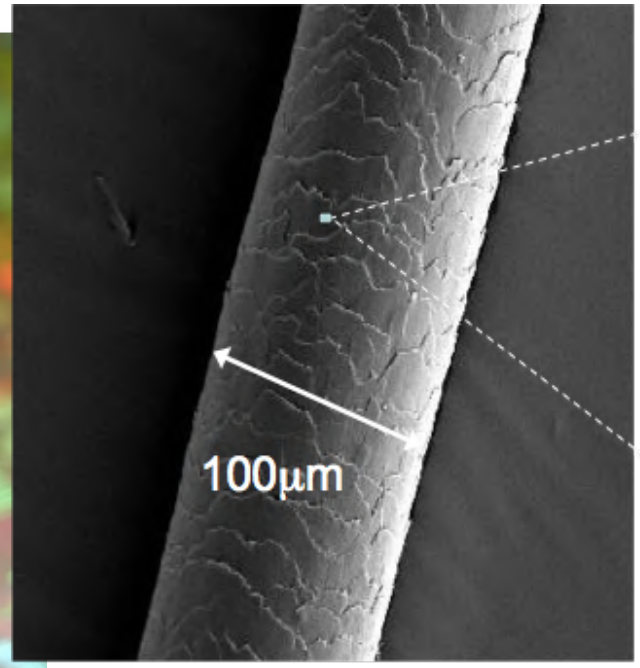
Materials choices





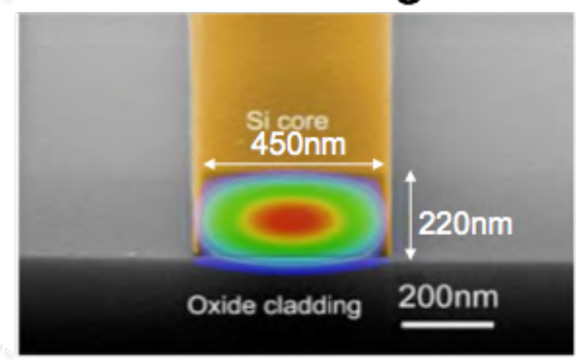
Silicon Quantum photonics





Si waveguide is 200 times smaller

Silicon waveguide

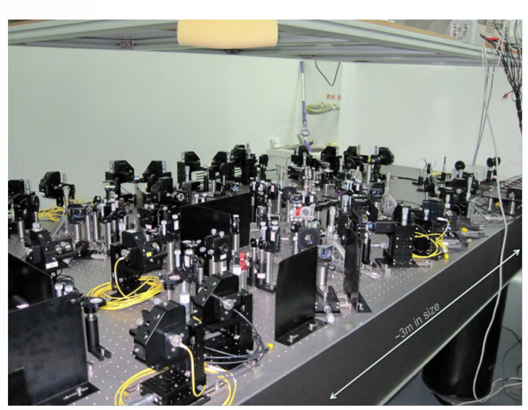


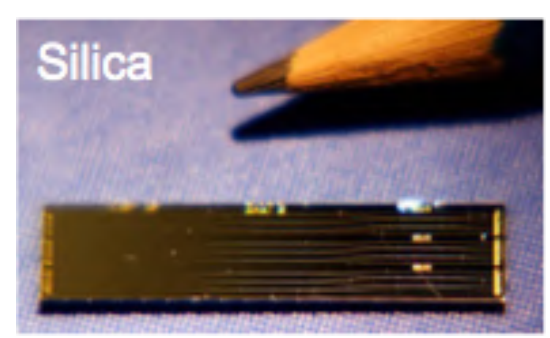
Ultra-high confinement of light

<u>silicon</u>

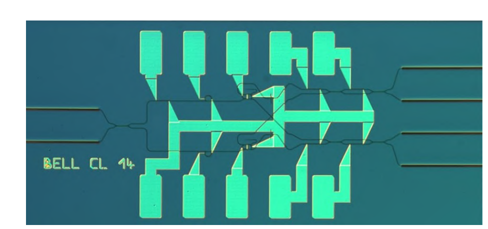
- Ultra-compact waveguides
  - Small bend radius (<1μm)
  - High component density
- Mature semiconductor fabrication processing
- High non-linearity efficient sources
- High confinement efficient detectors
- Filters have been demonstrated
- Integration with electronics

3 m





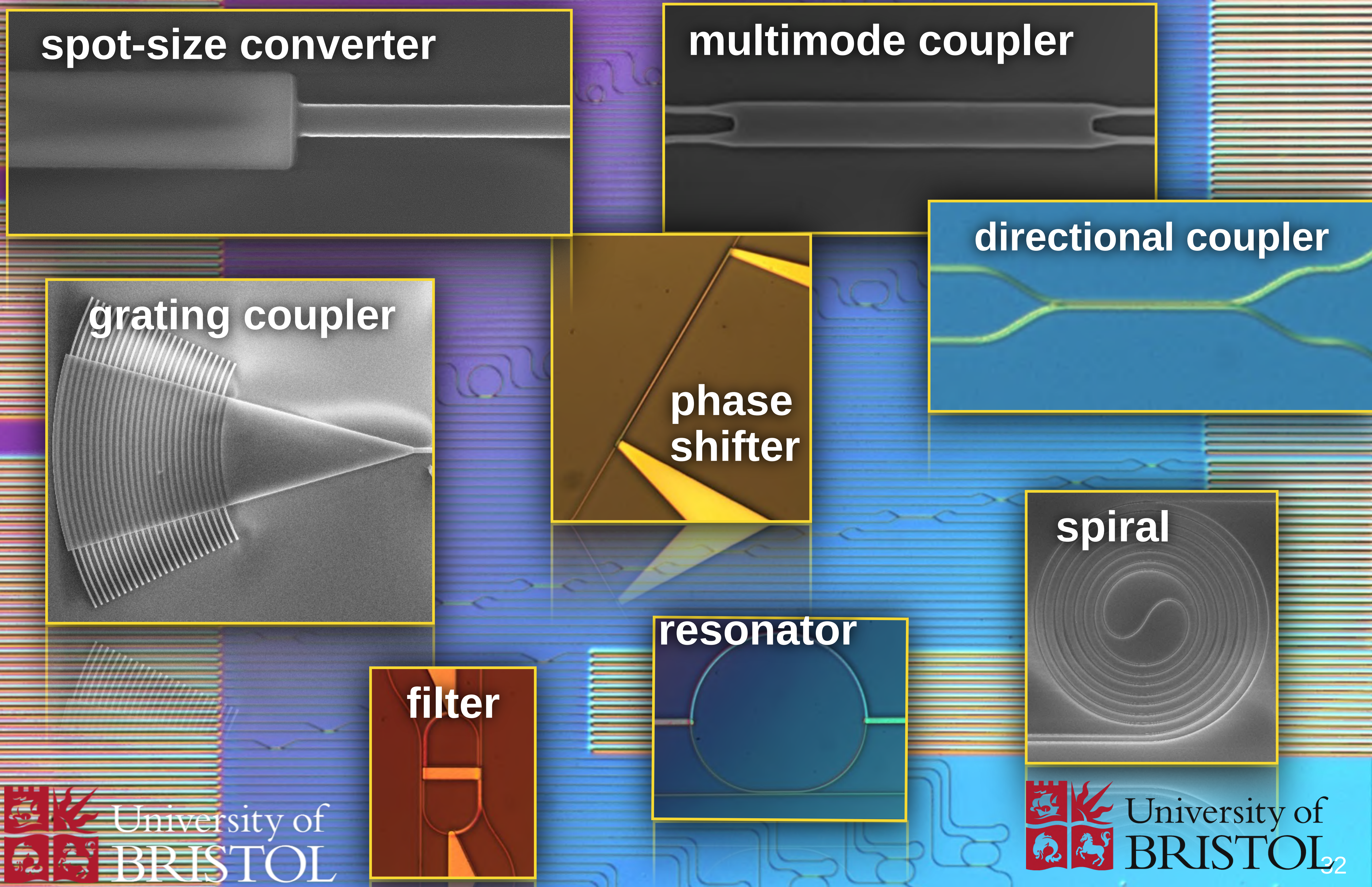
> 1 cm



1.4 mm

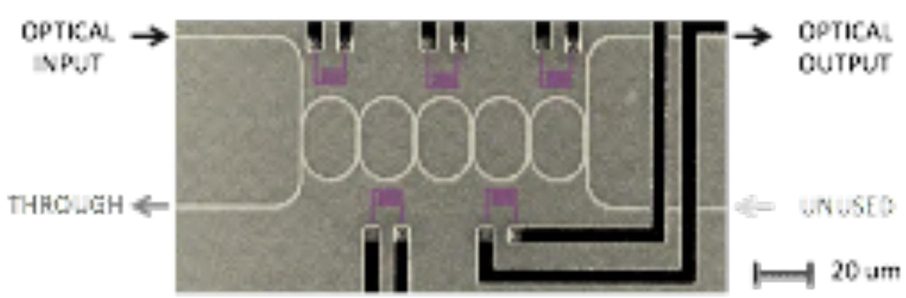
J. Silverstone et al., IEEE J. Select. Topics Quantum Electron. 1 (2016).

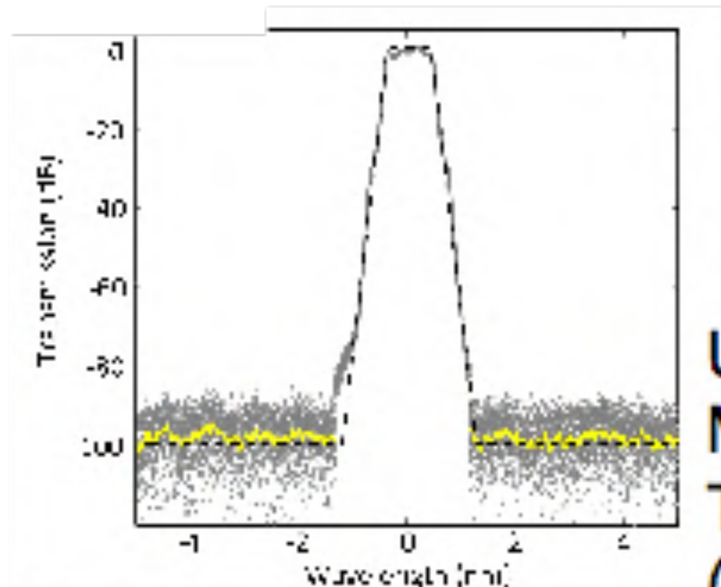
Silicon photonics components



Integrated filters in SOI

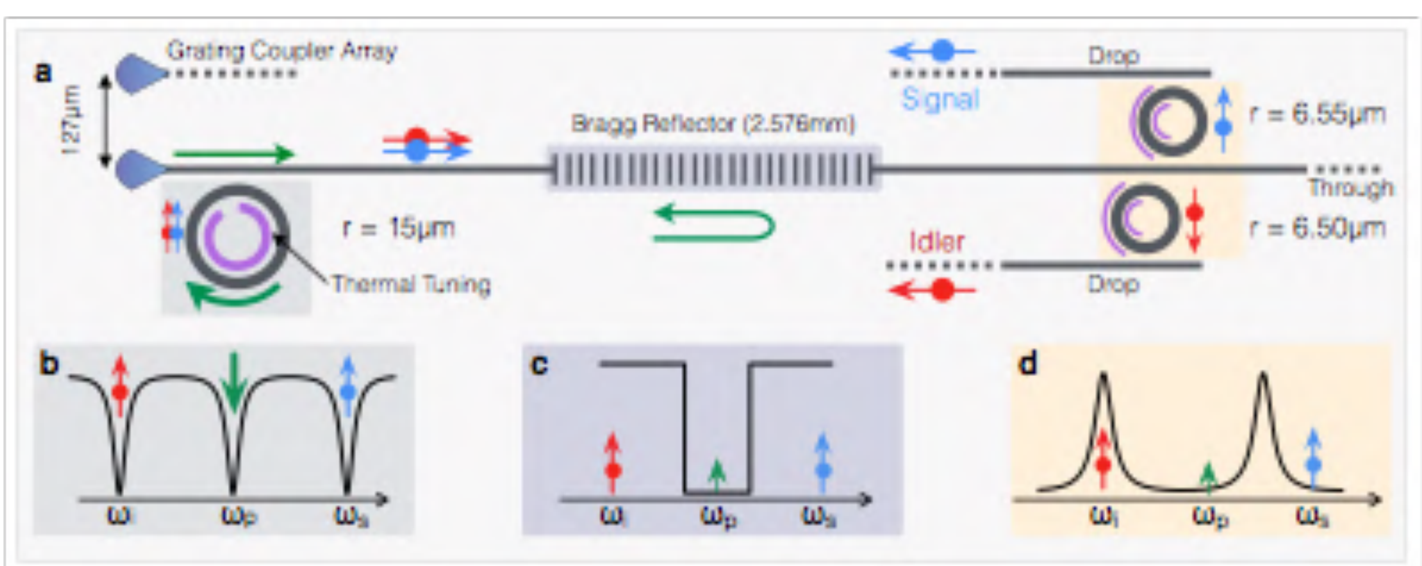
>100 dB extinction ratio

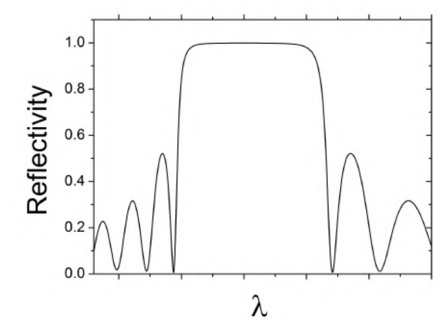




UCSD: Ong, Kumar, Mookherjea, IEEE Photon. Technol. Lett. **25**, 1543 (2013).

Integration with photon source





95 dB
CAR 50Hz

MIT: Harris, D. Grassani, Simbula, Pant, Galli, Baehr-Jones, Hochberg, Englund, Bajoni, Galland, (2014).

J. Silverstone et al., IEEE J. Select. Topics Quantum Electron. 1 (2016).

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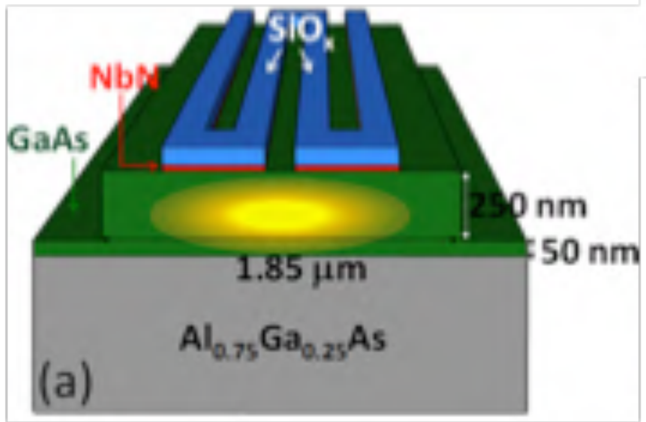
Detectors

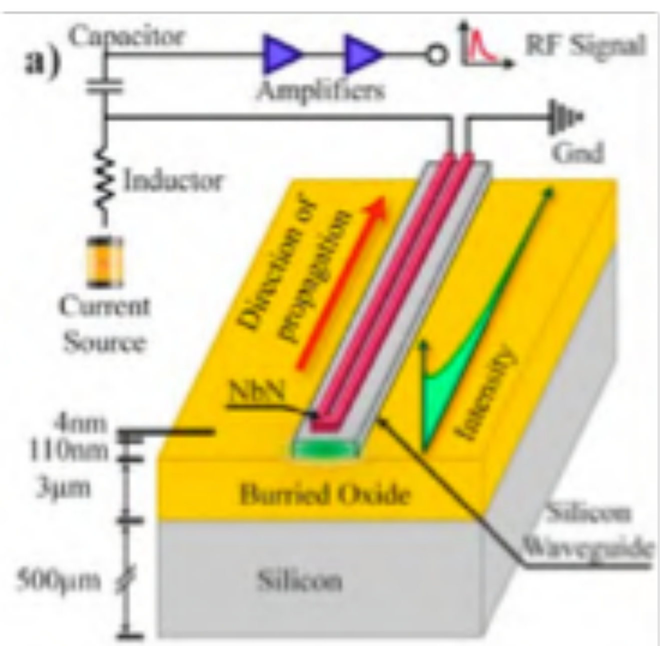
GaAs waveguide superconducting detector



η=20%

Sprengers, Gaggero, Sahin, Jahanmirinejad, Frucci, Mattioli, Leoni, Beetz, Lermer, Kamp, Höfling, Sanjines, Fiore, Appl. Phys. Lett. **99**, 181110 (2011)

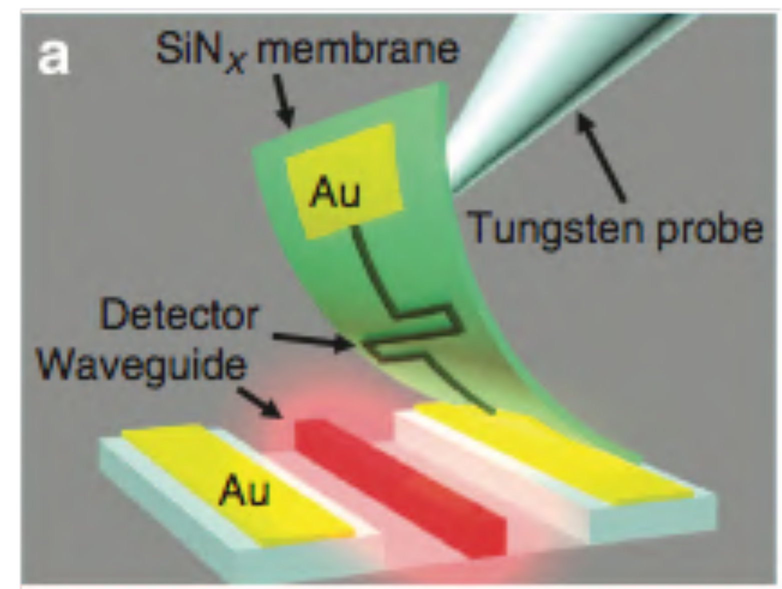
Silicon waveguide superconducting detector



η=91%

Pernice, Schuck, Minaeva, Gol'tsman, Sergienko, Tang, Nat Comms **3**, 1325 (2012)

Flip-chip integration



Najafi, Mower, Harris, Bellei, Dane, Lee, Hu, Kharel, Marsili, Assefa, Berggren, Englund, Nat Comms **6**, 5873 (2015).

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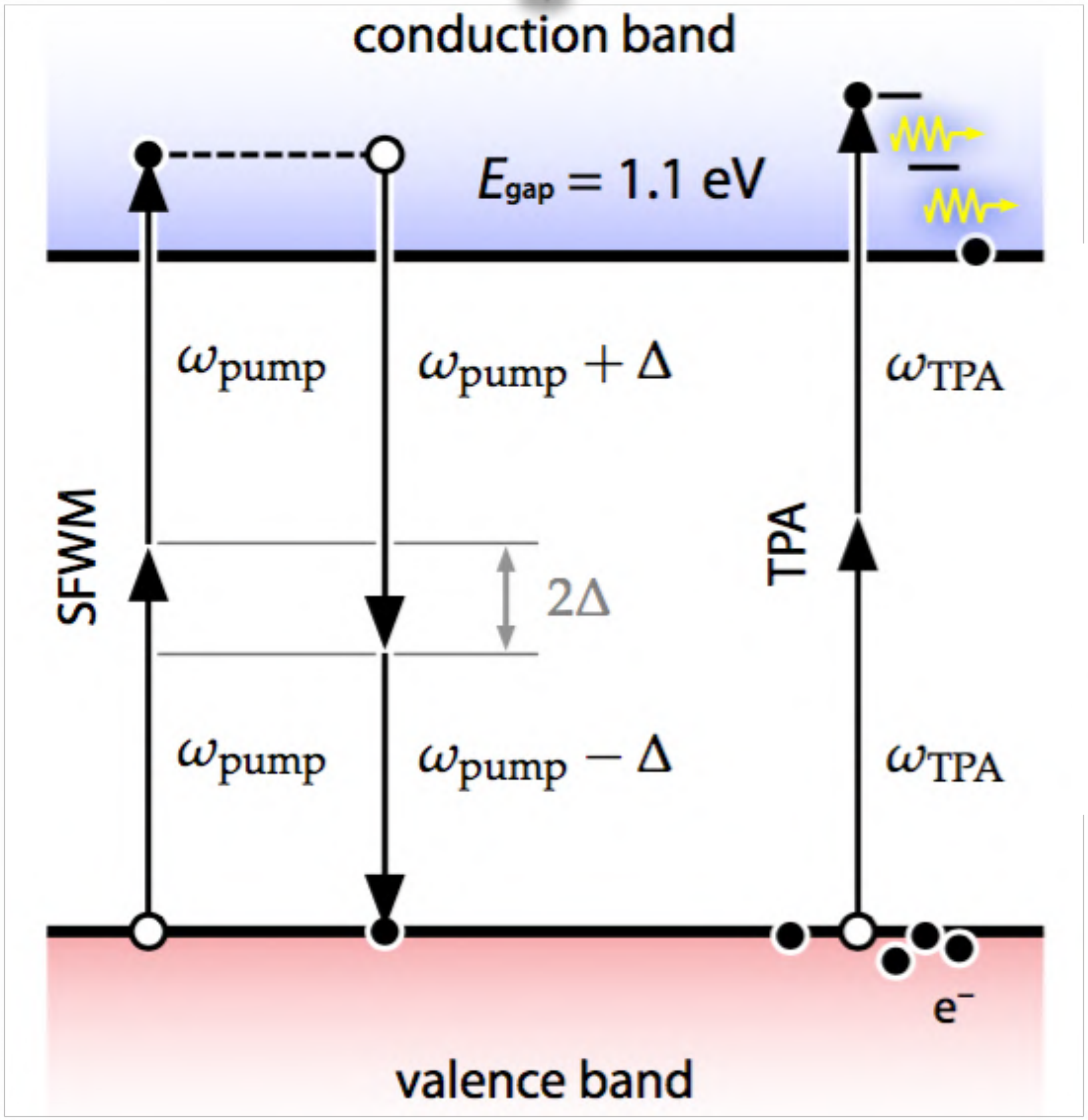
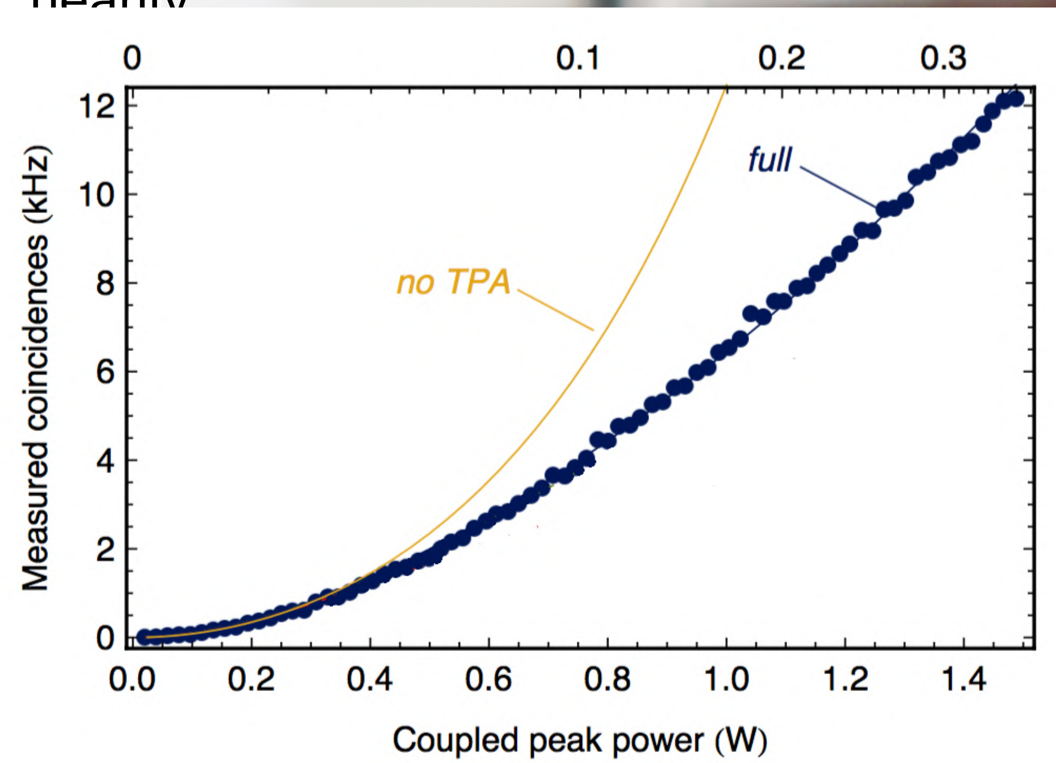
FWM



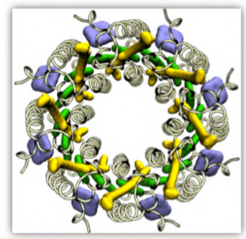
WM
nearity

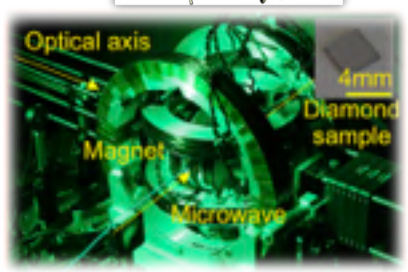


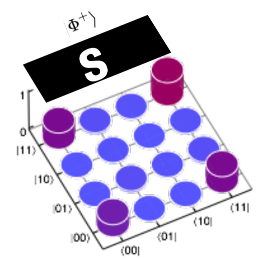
vidth

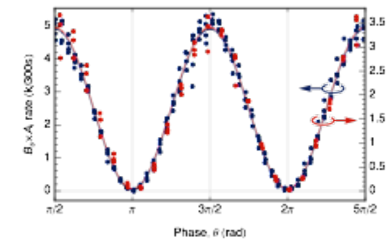
Priem, Dumon, Bogaerts et al. 2005
Silverstone et al. 2016

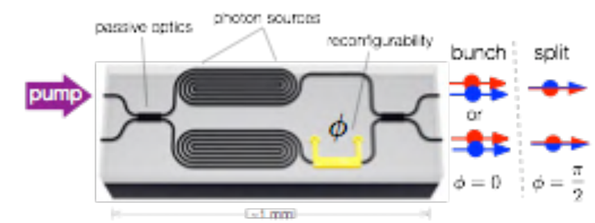
Quantum information processing and communication in Si QP

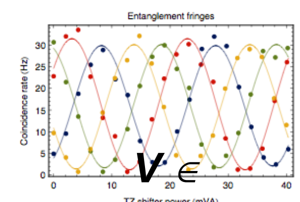




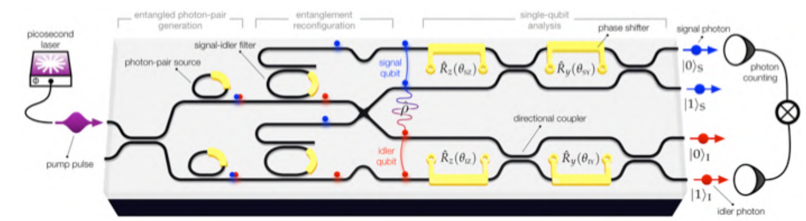


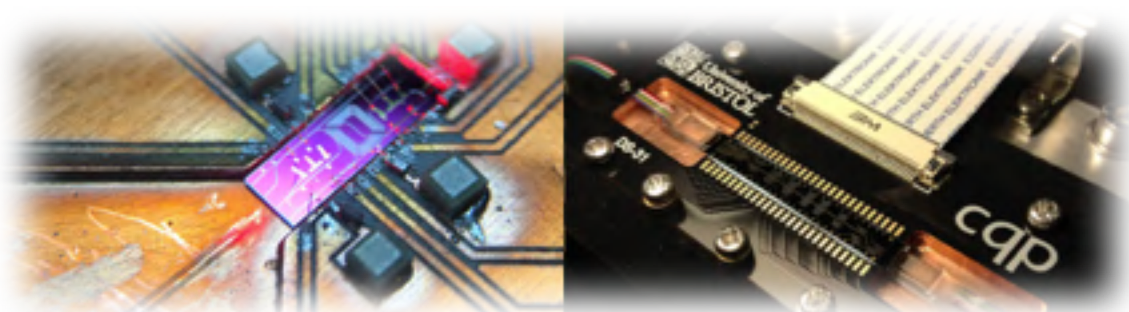




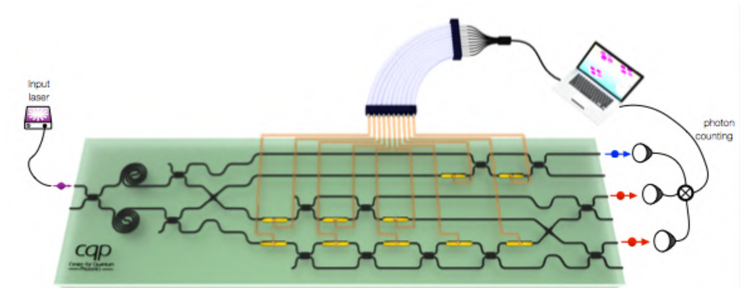


$V \in [93, 96]$ %





- Quantum simulation
- Bayesian Phase Estimation
- Hamiltonian Learning



Santagati et al. (2016)
Paesani et al. (2016)
Wang et al. (2016)

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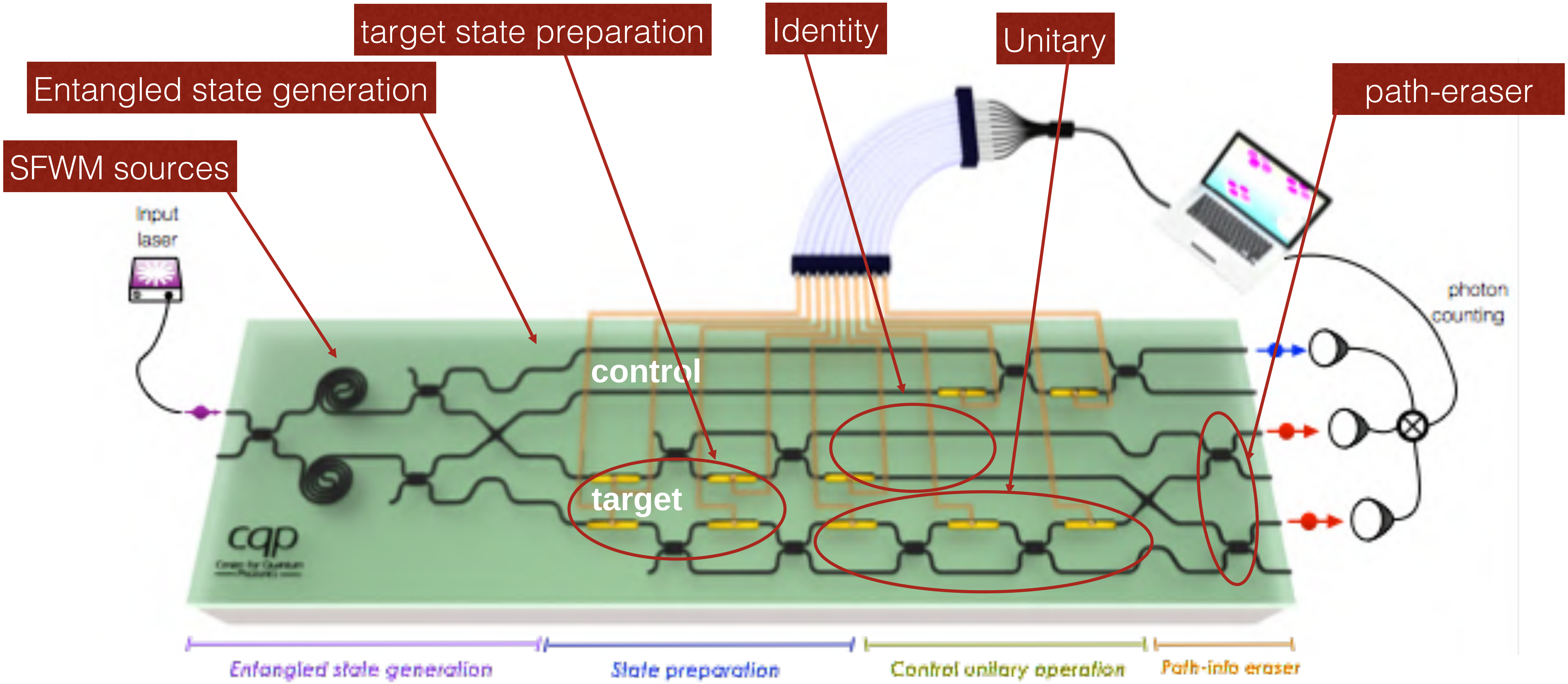
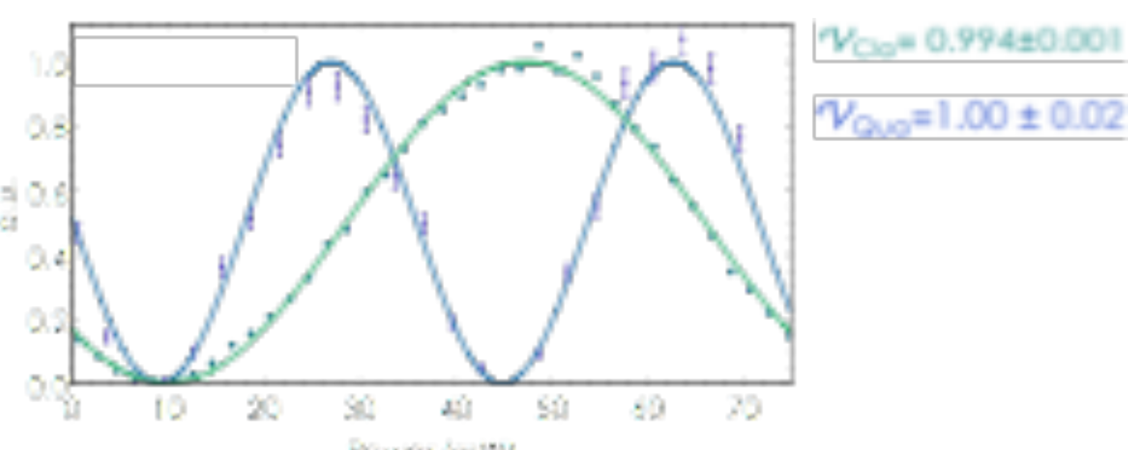
CU in Integrated Optics





$$|0\rangle_C \otimes I|\psi\rangle_T + |1\rangle_C \otimes U|\psi\rangle_T$$

Zou et al. (2013)

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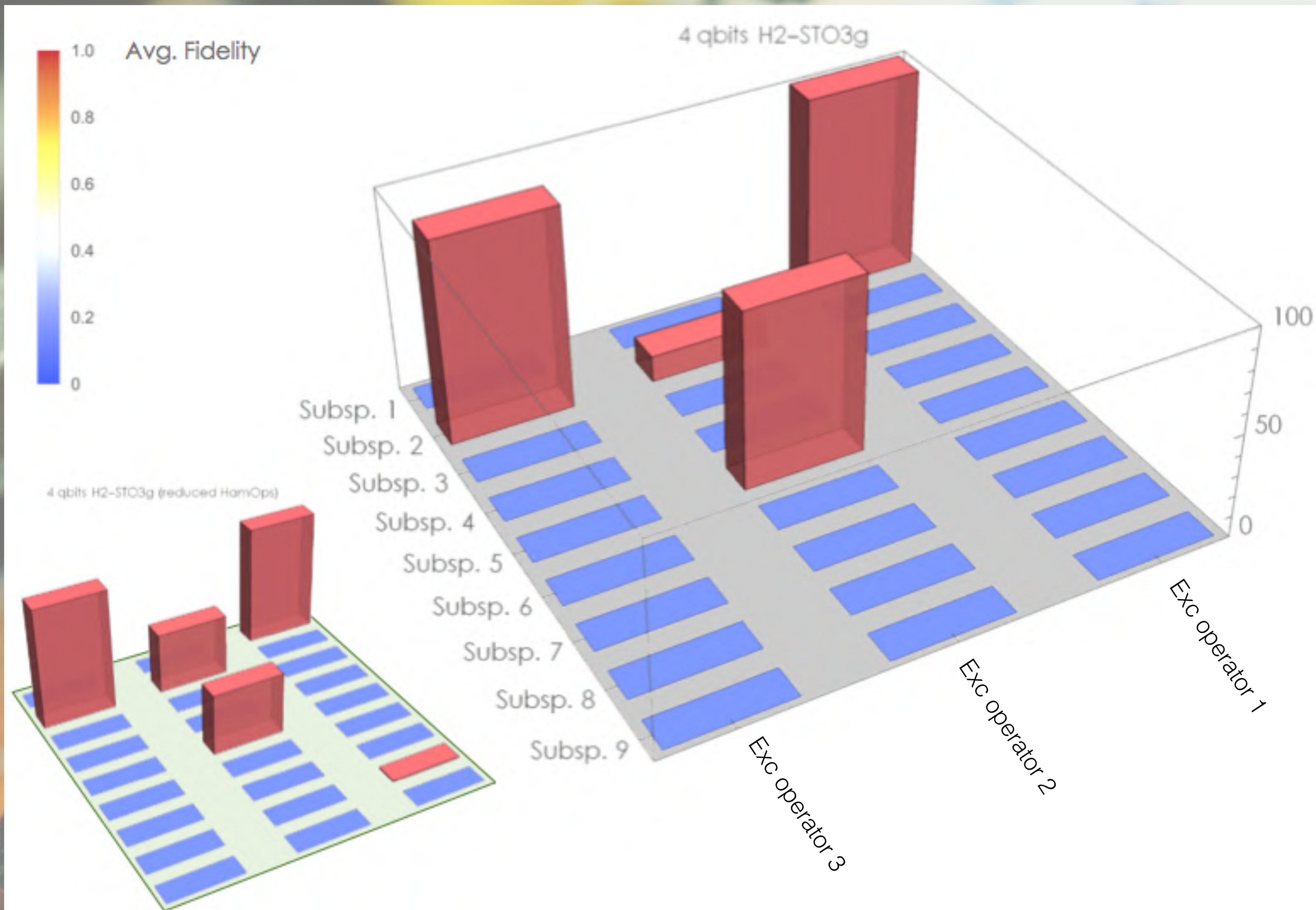
Simulations



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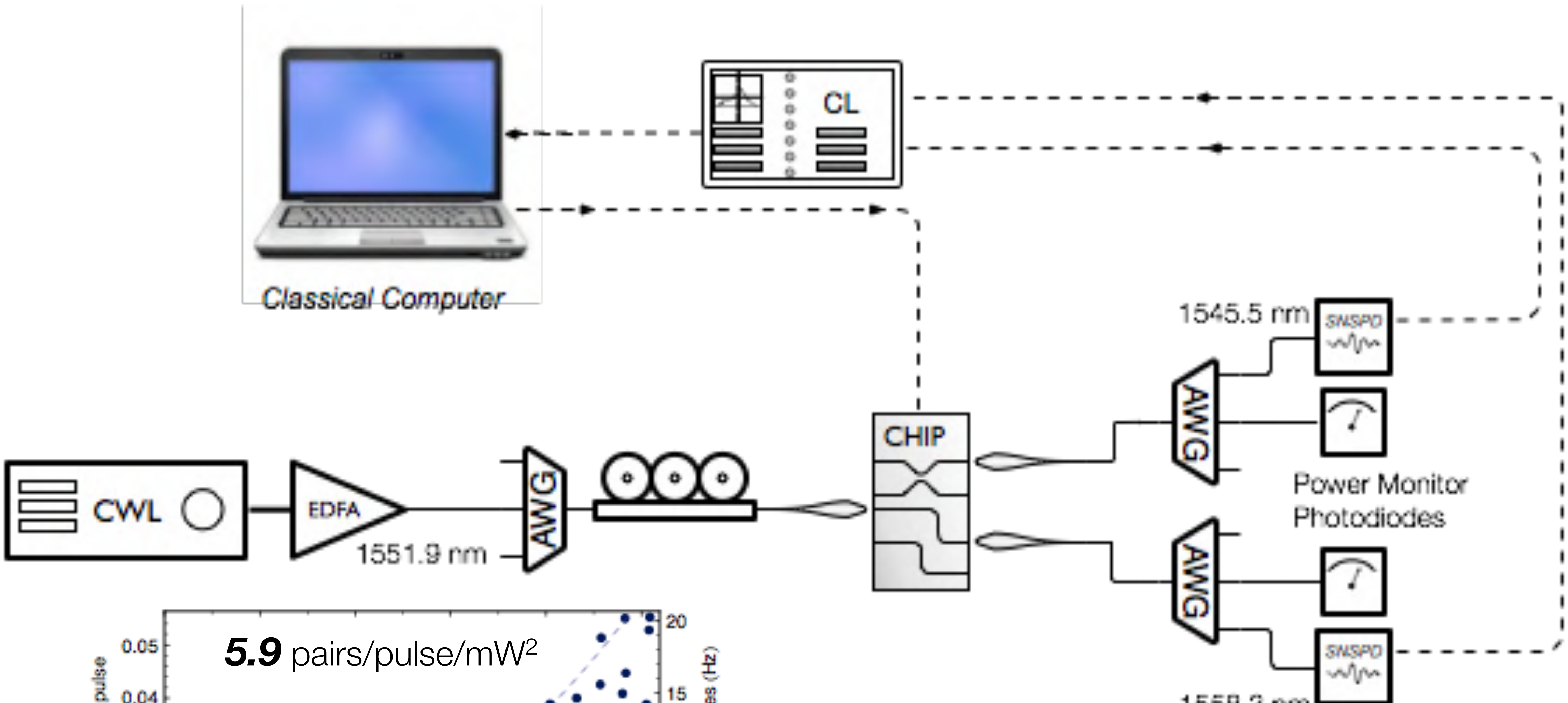
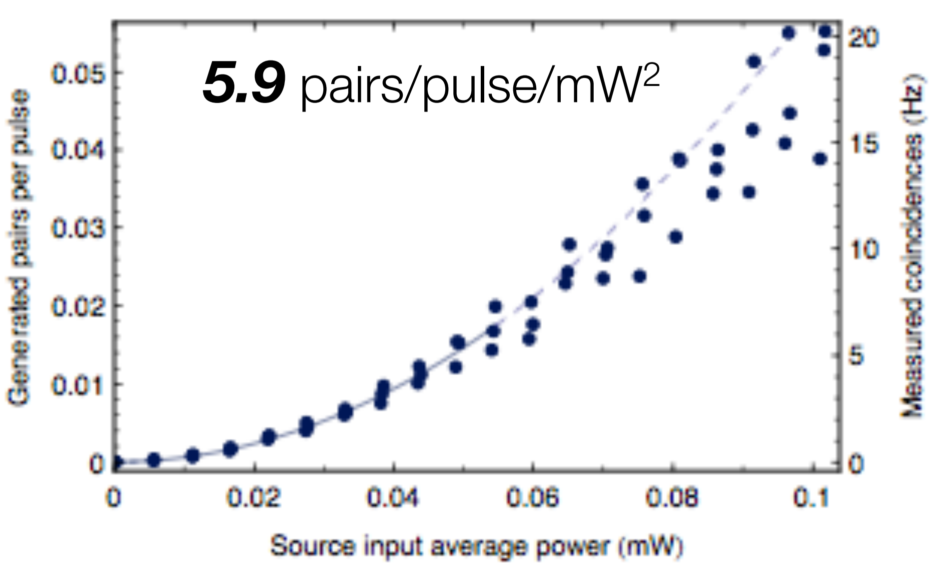
Typical Silicon quantum photonics experiment





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