Simulating Quantum Chemistry with a Fully Coupled Quantum Processor

Molecular Collision of Na and He

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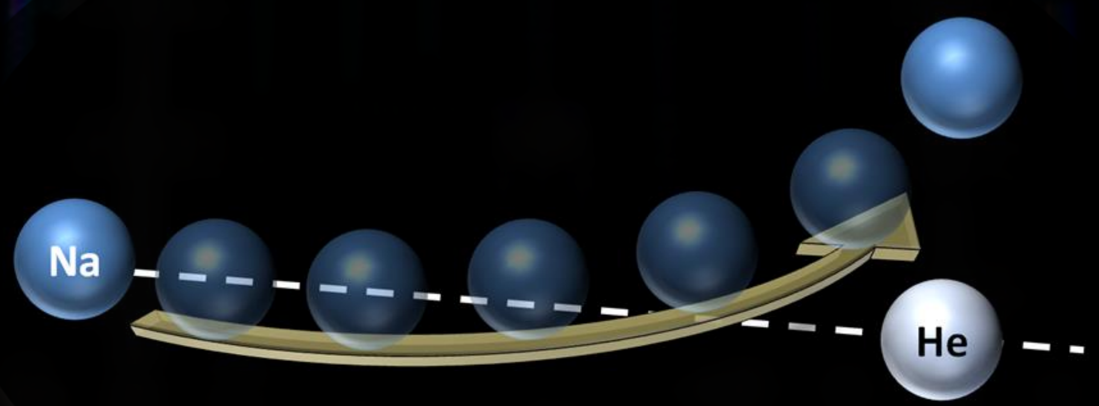
Google



Big Data

10^6 cores

10^{12} transistors/core

Really Big Data

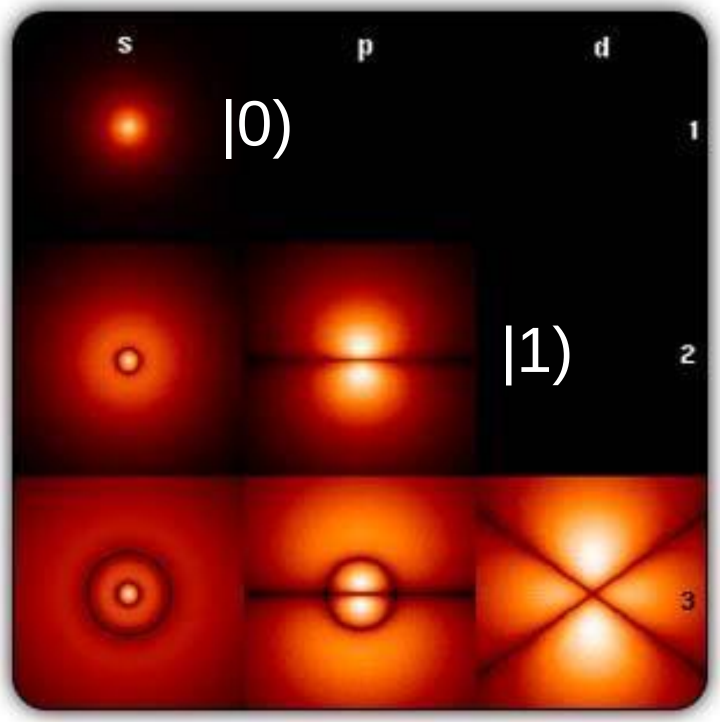
$$(|0\rangle + |1\rangle)^{300}$$

more states than

atoms in universe

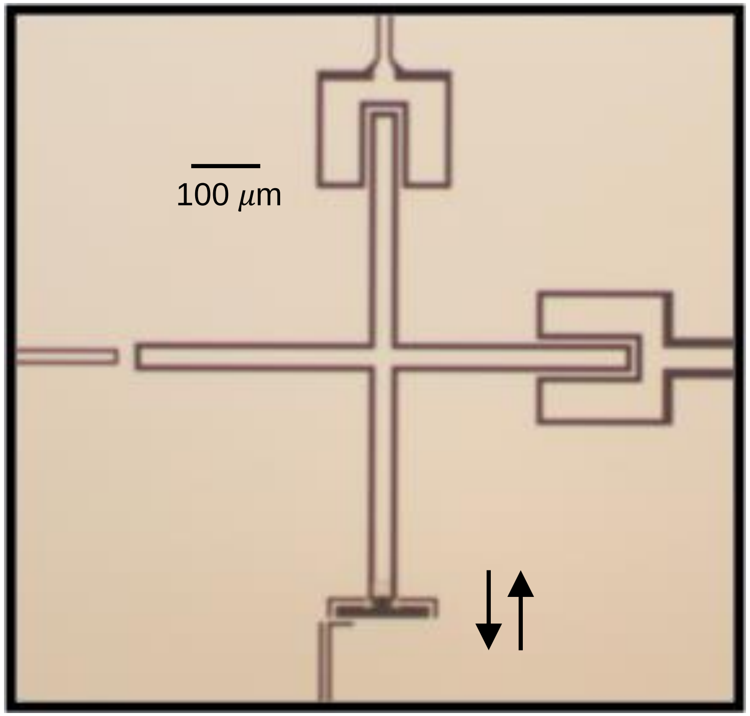
Encoding of quantum bits

H atom:



orbitals

quantum circuit:



6 GHz microwave oscillator

Technology Challenges

- Software - need special algorithms (only n output bits)
  Quantum chemistry
  Machine learning

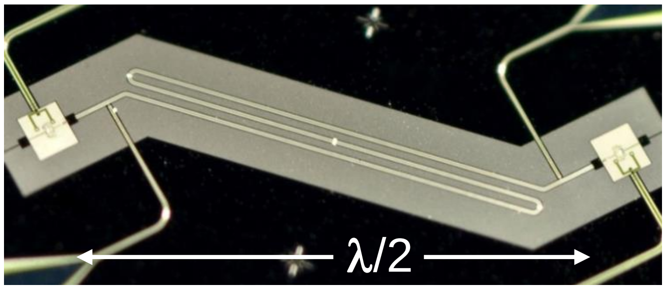
- Hardware - qubits need coherence, scalable, good control …
  Quantum IC with superconductors

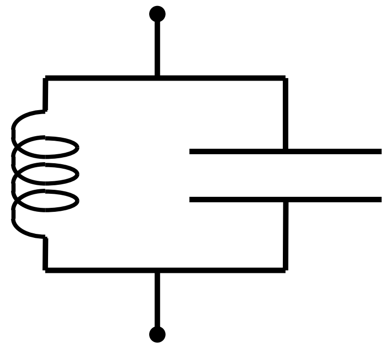
  Analog quantum annealing
  Analog quantum simulation
  Digital quantum computation – need error correction

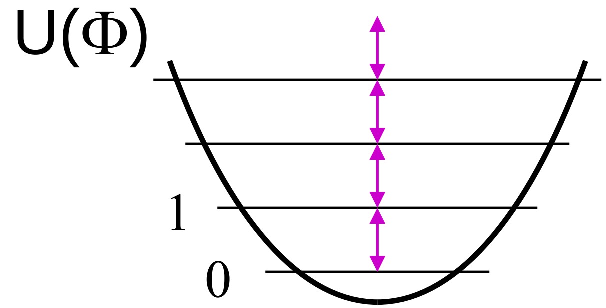
Superconducting Qubits

- Quantum circuit: quantize I and V,   5 GHz >> 20 mK

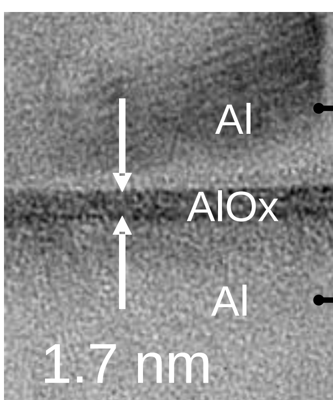
- LC oscillator (linear): memory and communication

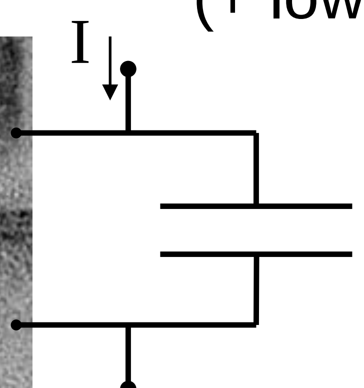


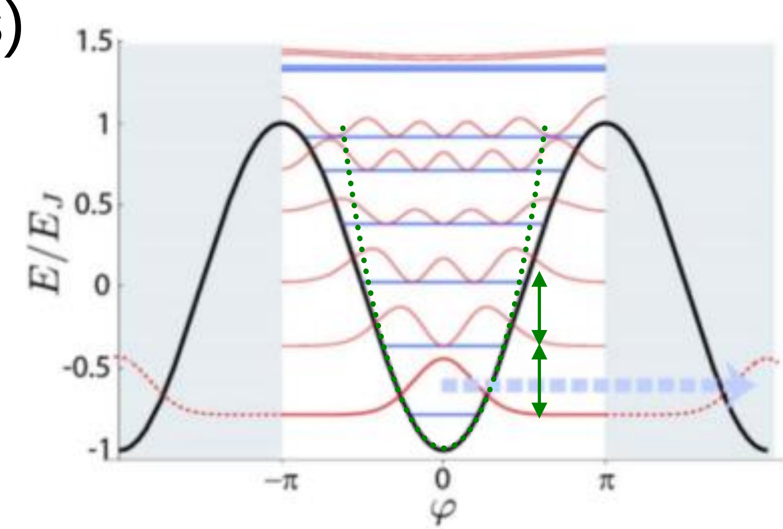




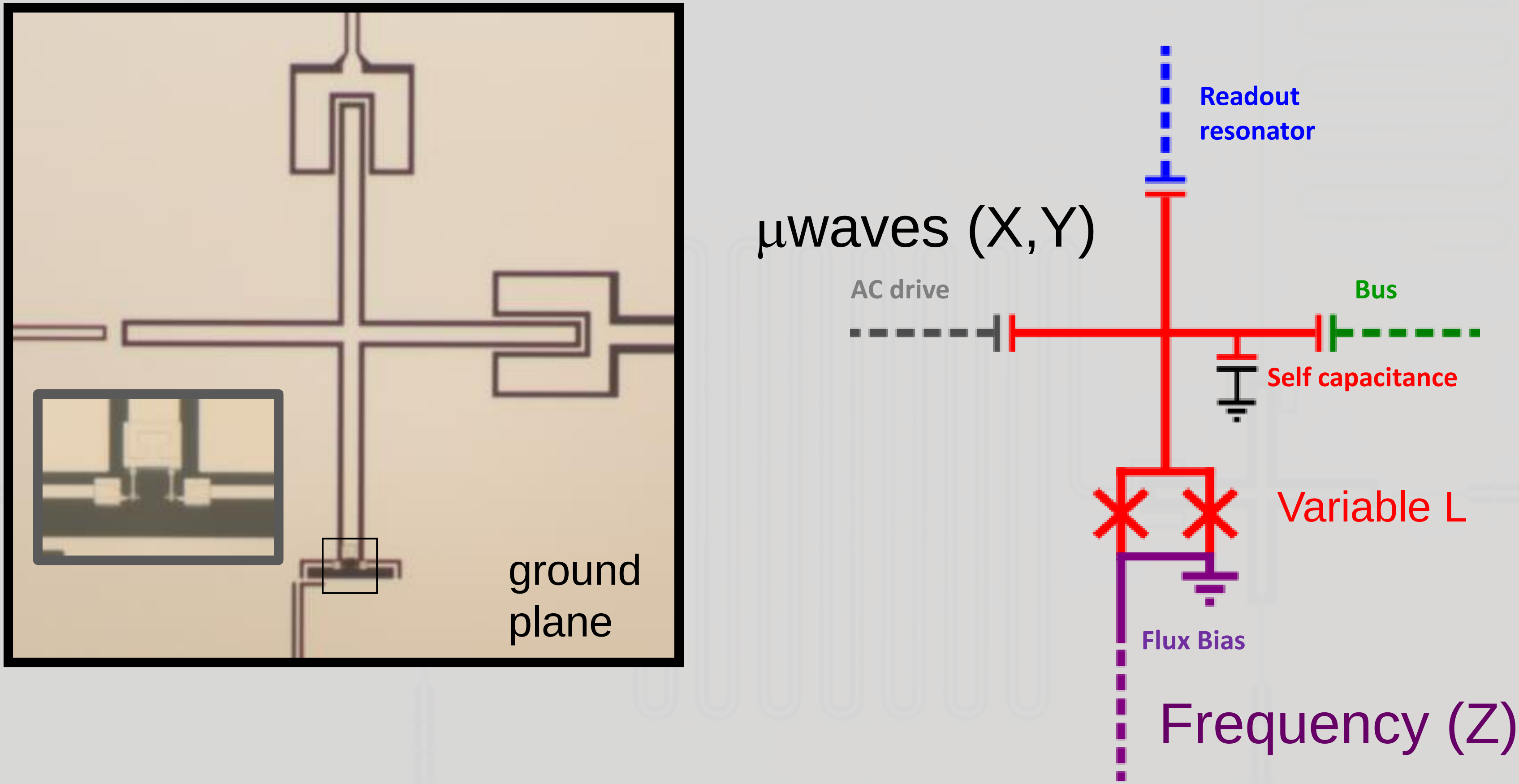
- Josephson junction: non-linear inductance with 1 photon
  (+ low loss)







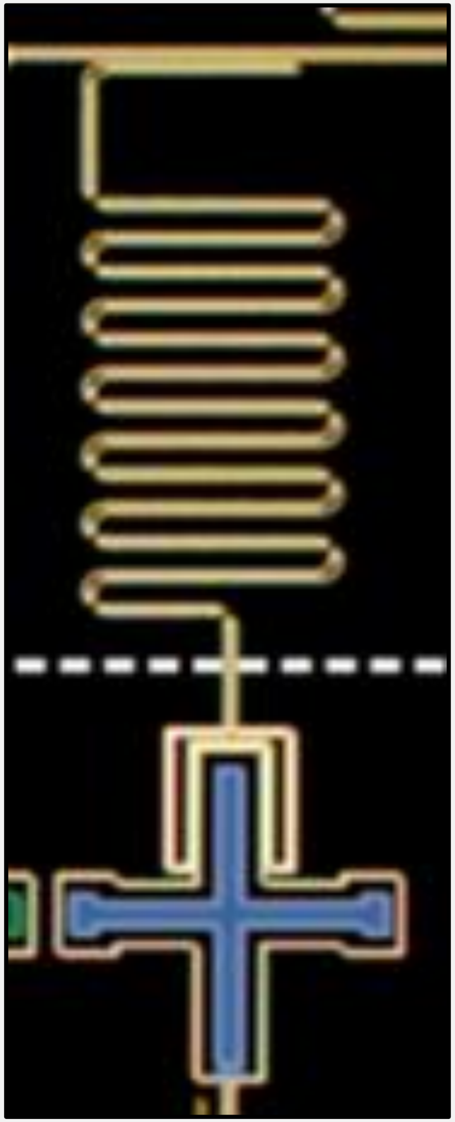
Xmon Circuit



Transmon is non-linear LC oscillator

Measurement: Single Shot, QND, Hi-Fi, Mux'd

Microwave tone measures qubit



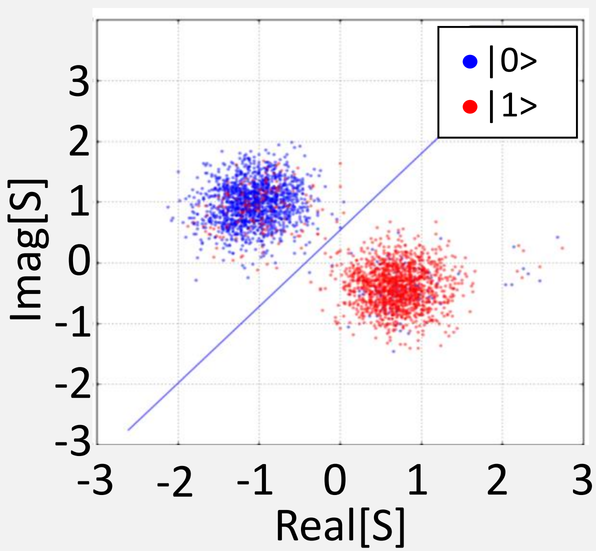
readout S

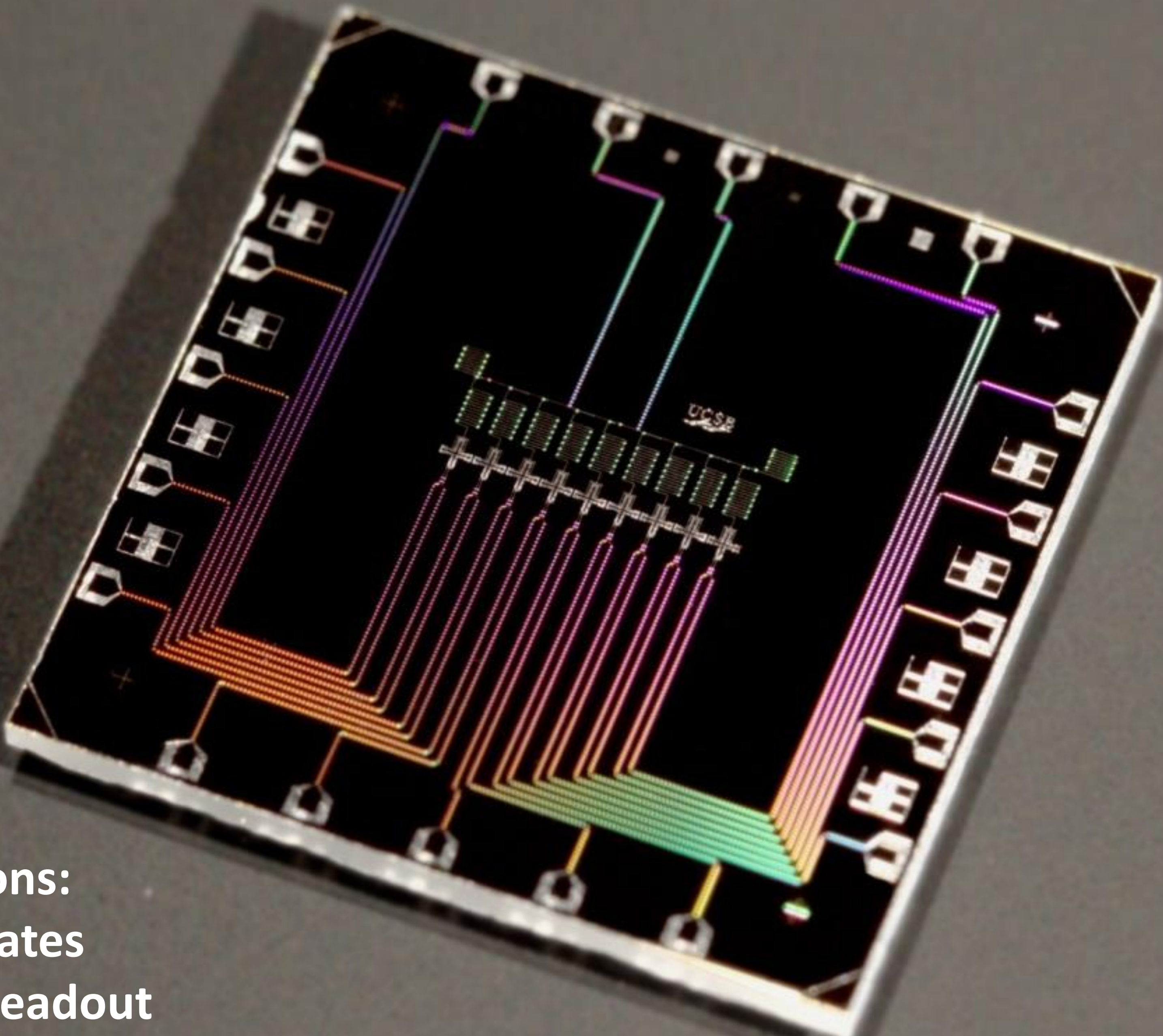
λ/2 resonator (7 GHz)

xmon (5.8 / 6 GHz)

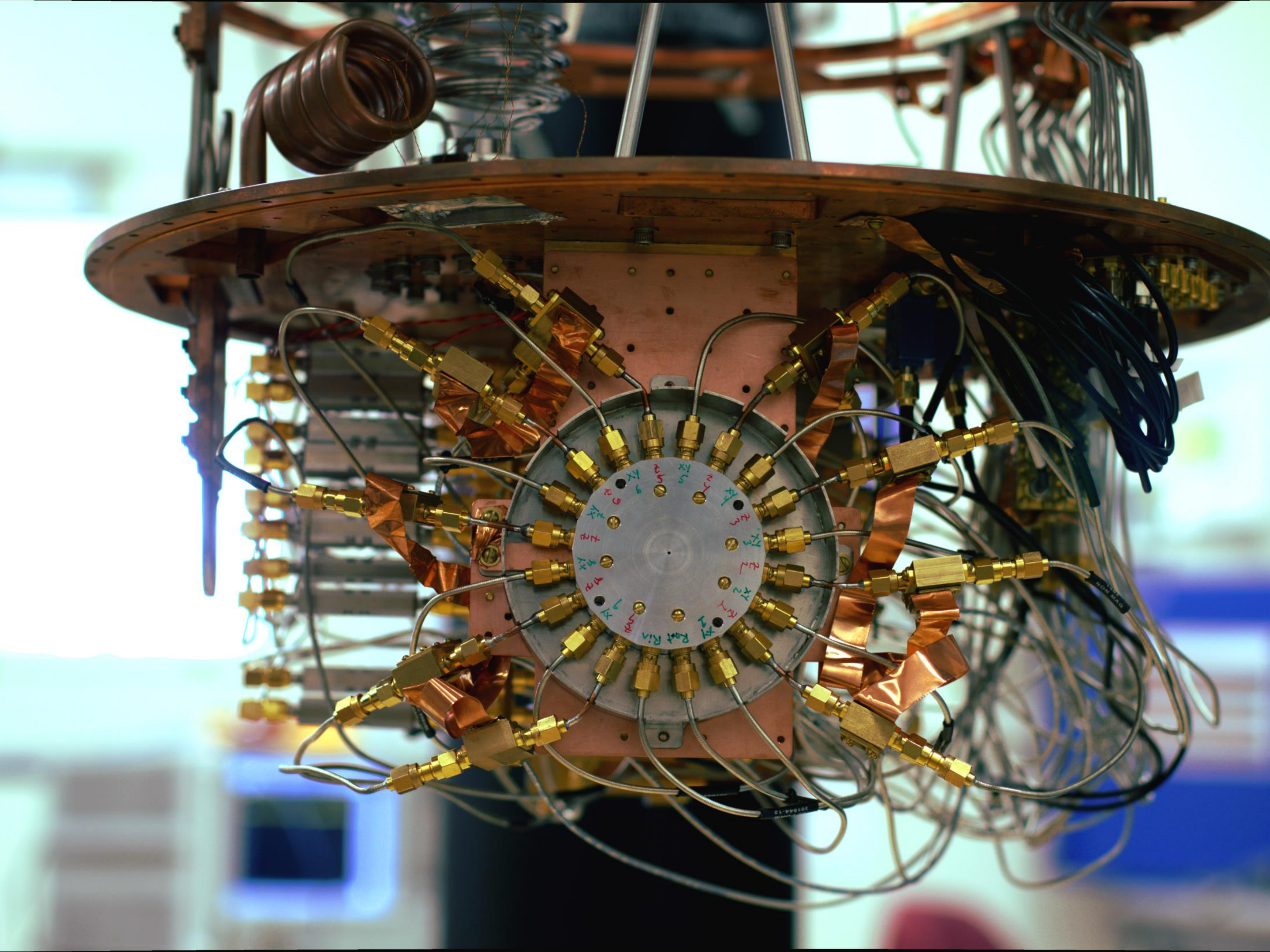
For coupled oscillators:

- Change in qubit frequency shifts resonator frequency
- Measure frequency by change in phase from microwave tone





9 Xmons:
- hifi gates
- fast readout
- surface code compatible

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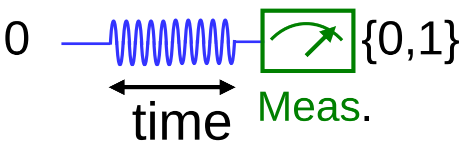
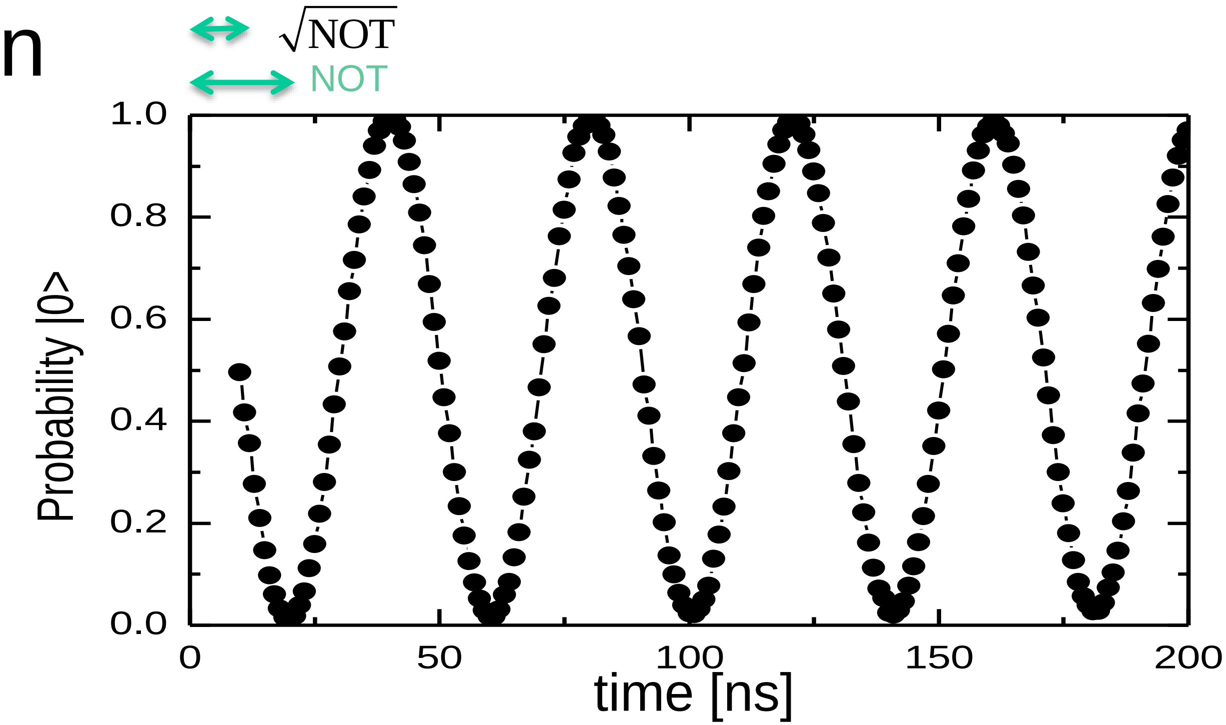
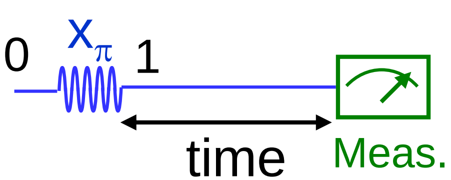
Qubit Operation

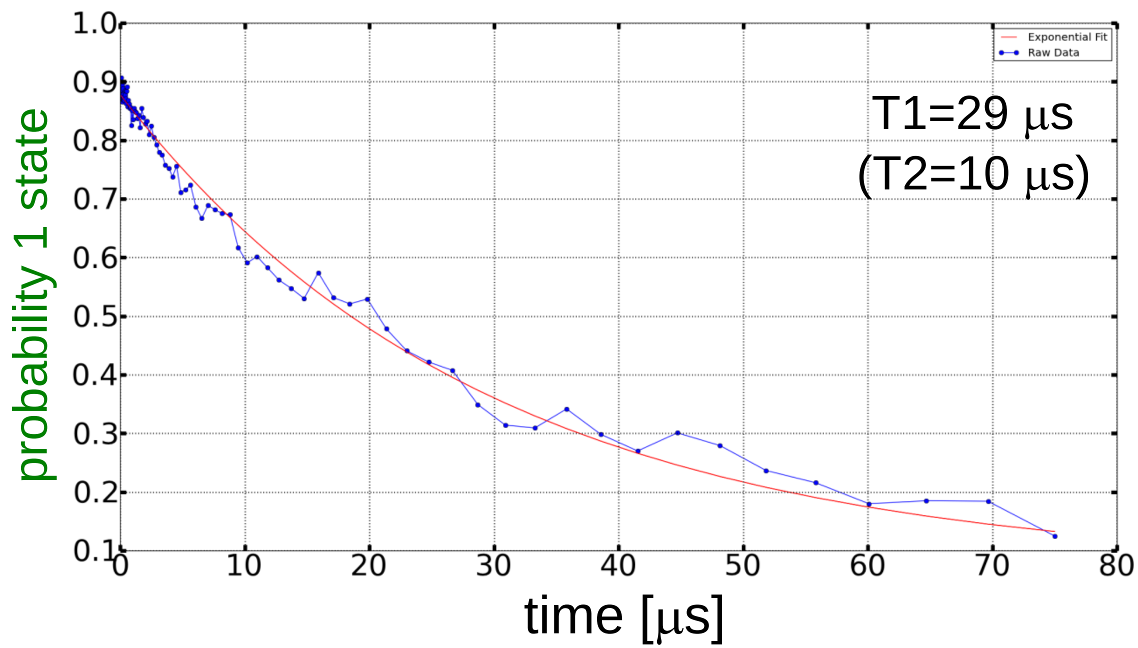
Rabi





lifetime





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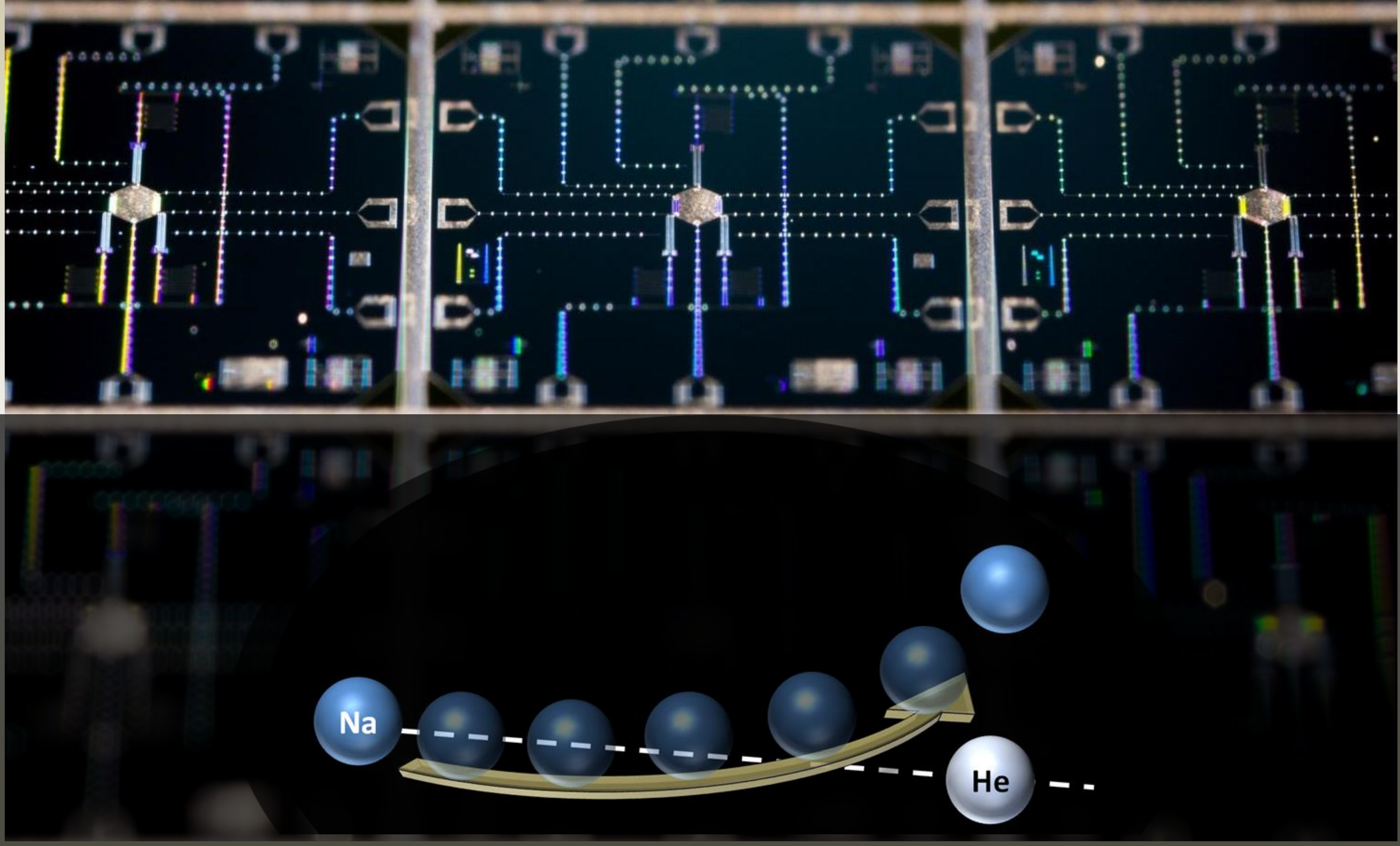
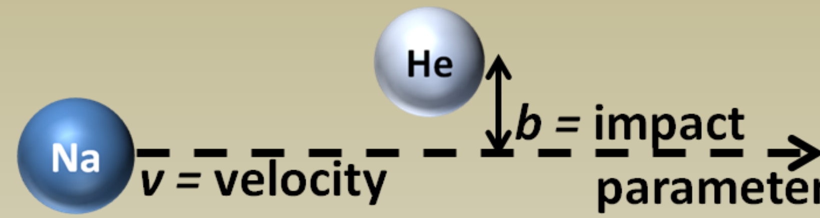
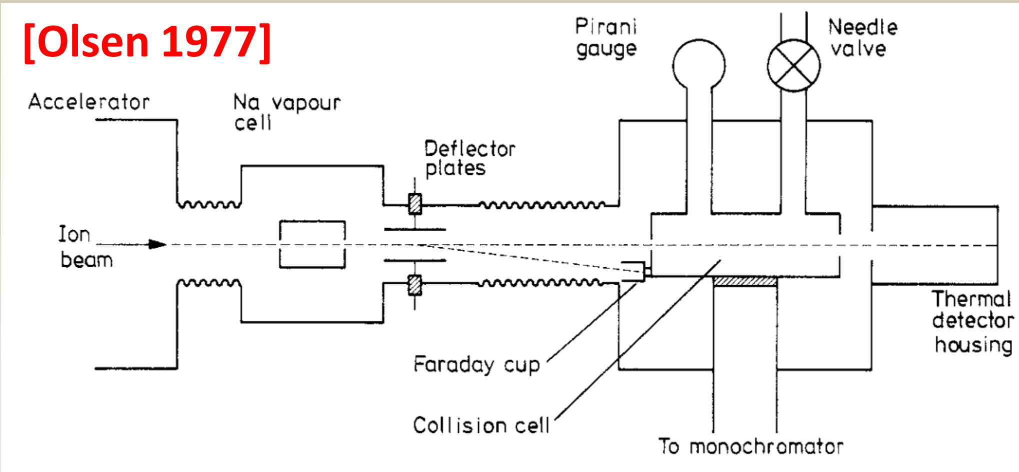
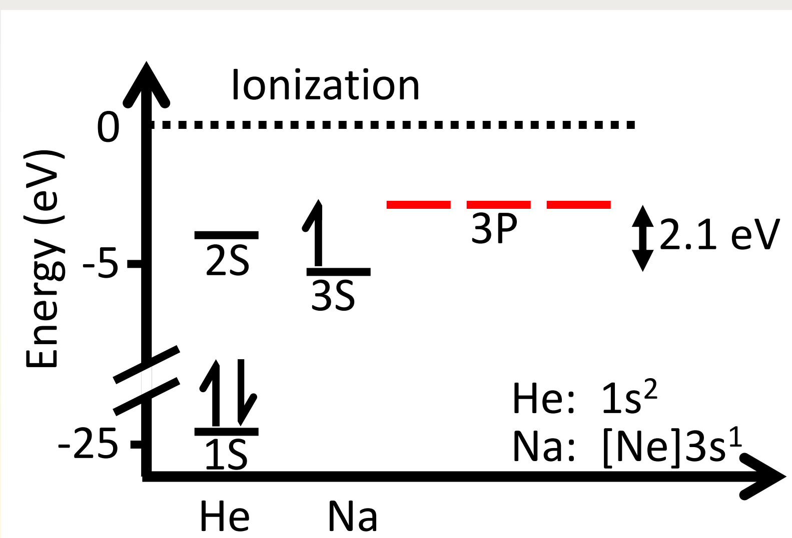


Inelastic Scattering of Na & He: **Experiment**







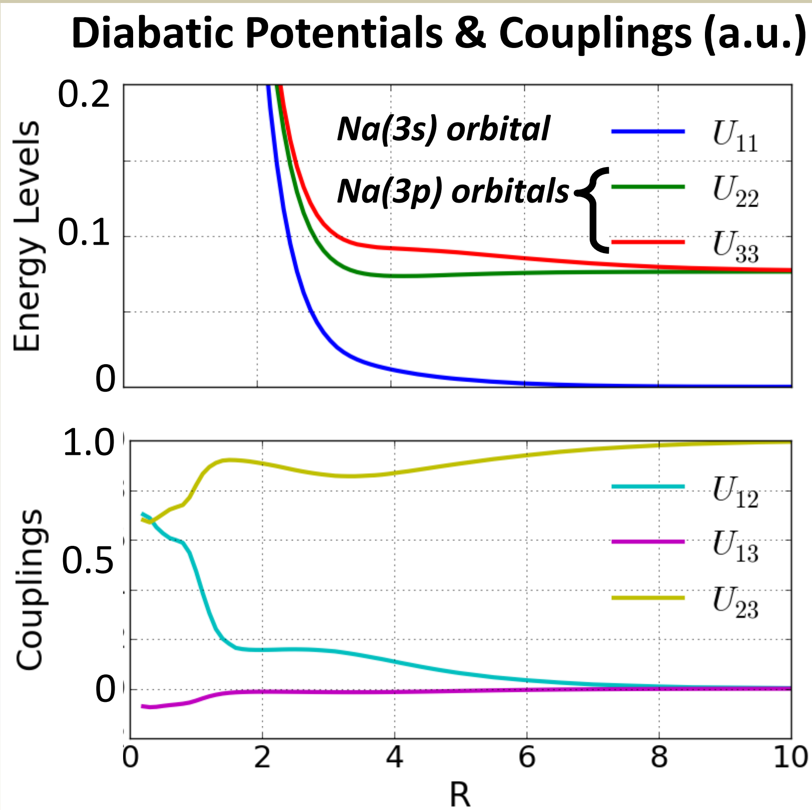
$$\mathrm{Na}(3s) + \mathrm{He}(1s^2) \quad [1\,^2\Sigma^+] \rightarrow |1\rangle_{\mathrm{Sim}}$$

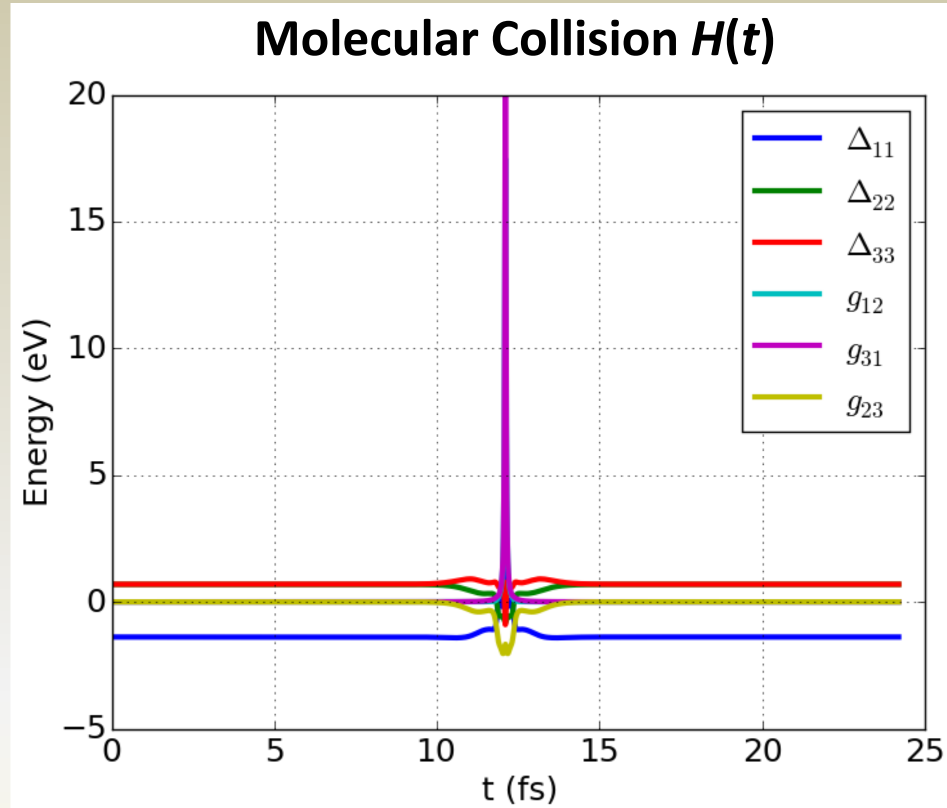
$$\mathrm{Na}(3p) + \mathrm{He}(1s^2) \quad [1\,^2\Pi] \rightarrow |2\rangle_{\mathrm{Sim}}$$

$$\mathrm{Na}(3p) + \mathrm{He}(1s^2) \quad [2\,^2\Sigma^+] \rightarrow |3\rangle_{\mathrm{Sim}}$$

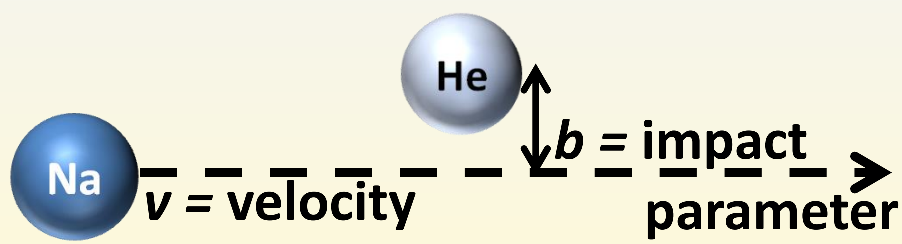
Inelastic Scattering of Na & He: **Numerical Computation**

$$H(t)=\begin{bmatrix}\Delta_{11} & g_{12} & g_{13}\\ g_{21} & \Delta_{22} & g_{23}\\ g_{31} & g_{32} & \Delta_{33}\end{bmatrix}$$





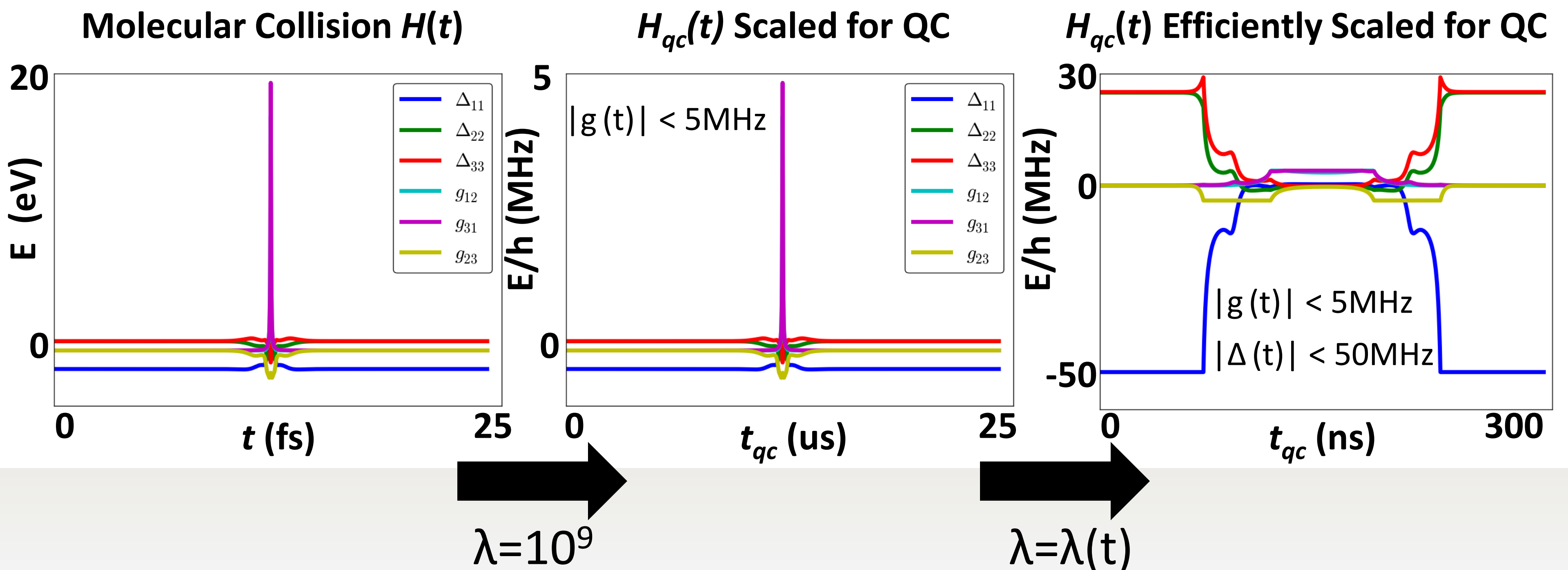
$$R(t)=\sqrt{b^2+v^2(t-t_{collision})^2}$$



C. Y. Lin *et al*, Phys. Rev. A 78, 052706 (2008)

Inelastic Scattering of Na & He: **Scaling *H(t)* for QC**

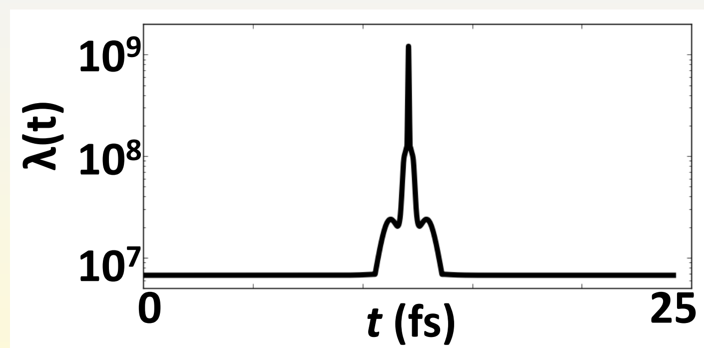
$$H(t) = \begin{bmatrix} \Delta_{11} & g_{12} & g_{13} \\ g_{21} & \Delta_{22} & g_{23} \\ g_{31} & g_{32} & \Delta_{33} \end{bmatrix}$$



$$U(t) = e^{-i \int H(t')dt'}$$

$$H_{qc} = H(t) / \lambda$$

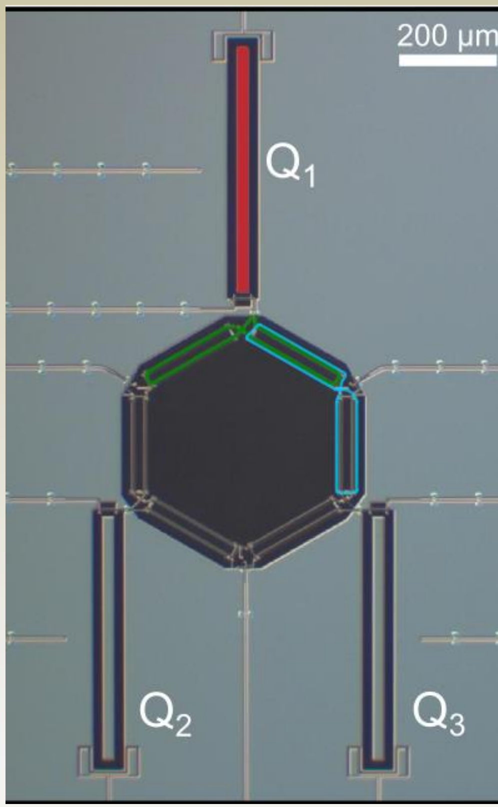
$$dt_{qc} = dt * \lambda$$



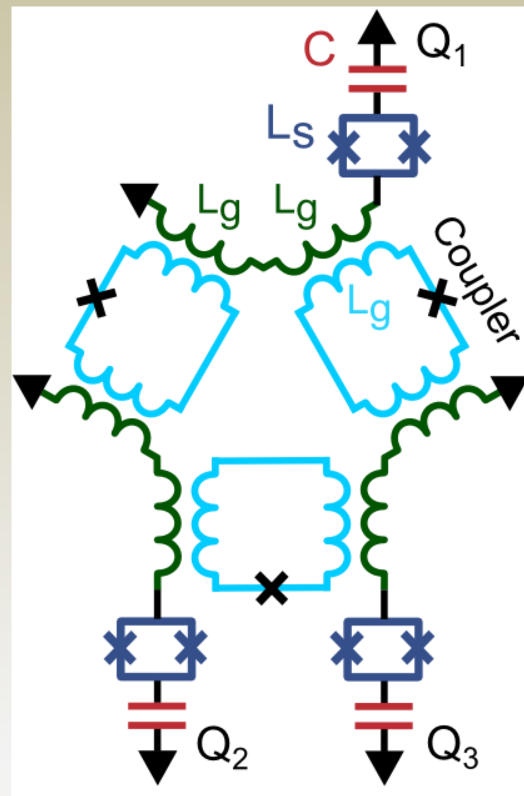
Pritchet *et al*, arXiv:1008.0701 (2010)

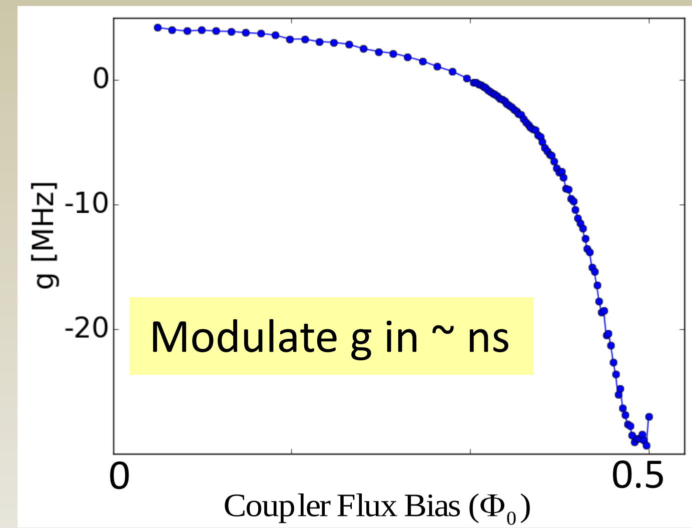
3 Qubit Quantum Processor

with Full Connectivity & Full Controllability



C. Neill *et al.* In preparation





gmon Architecture

High Coherence: T1~20us

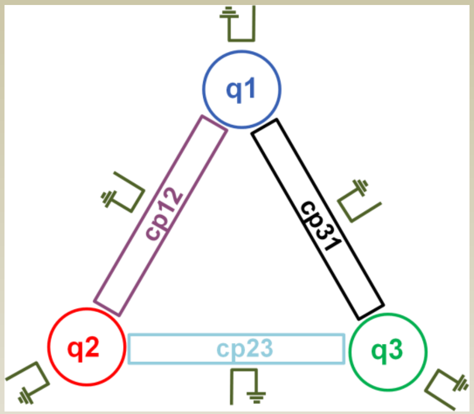
T2~12us

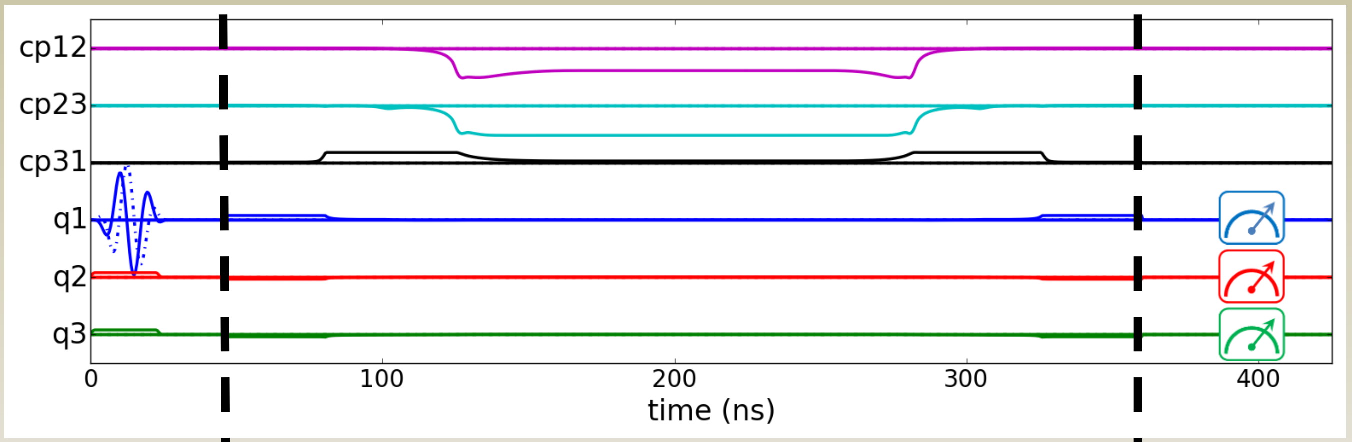
Tunable qubit frequency ***Tunable coupling***

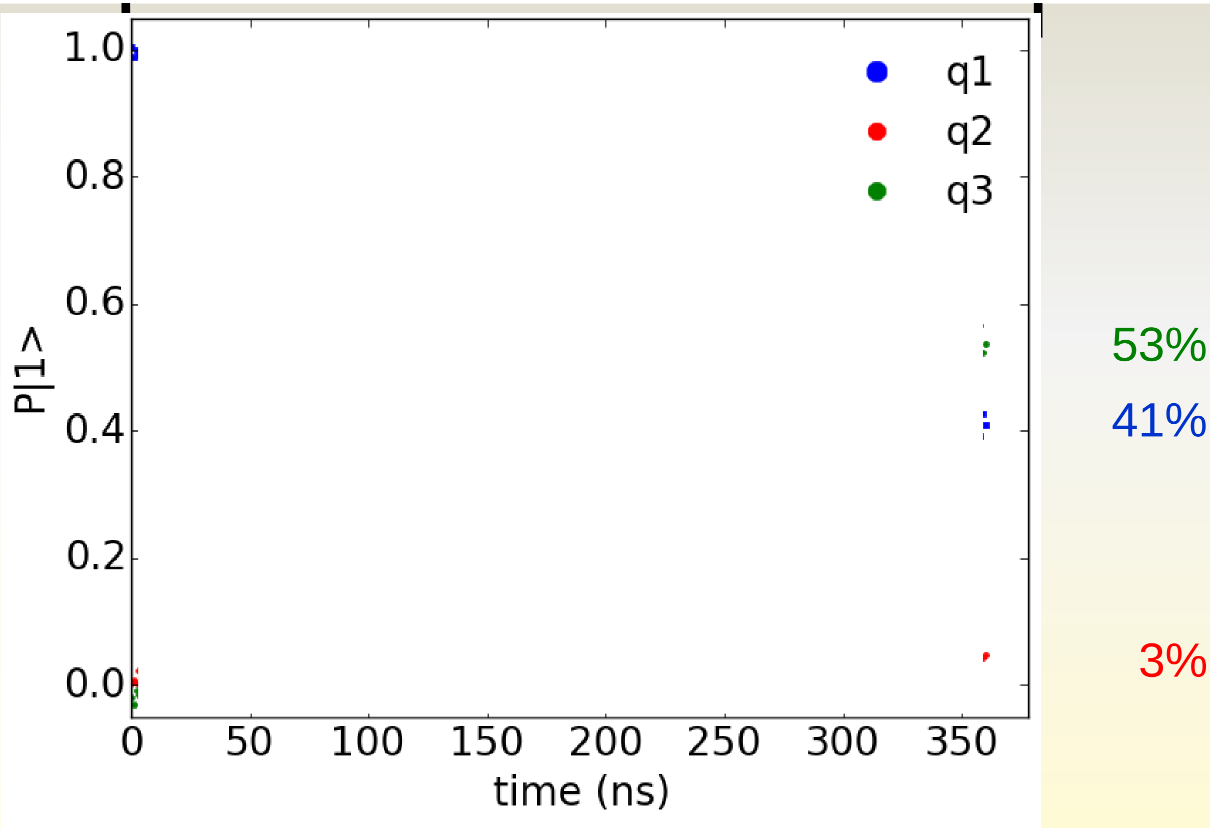
$$H = \sum_{Qubits} H_x(t)\,\sigma^x + H_y(t)\,\sigma^y + H_z(t)\,\sigma^z - \sum_{i\neq j} g_{i,j}(t)\,(\sigma_i^X\sigma_j^X + \sigma_i^Y\sigma_j^Y)$$

Yu Chen *et al.* PRL (2014)

Inelastic Scattering of Na & He: **Quantum Simulation**





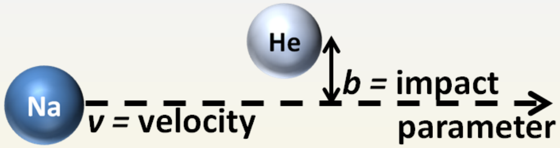


Simulation Conditions

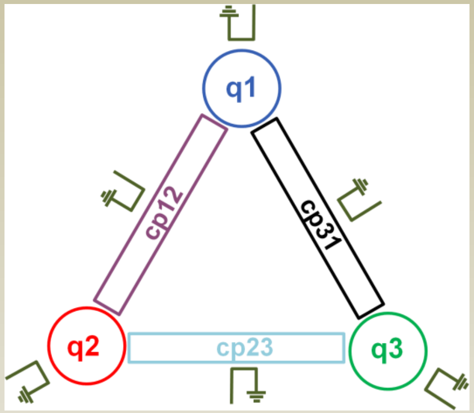
Initial Channel = |1>

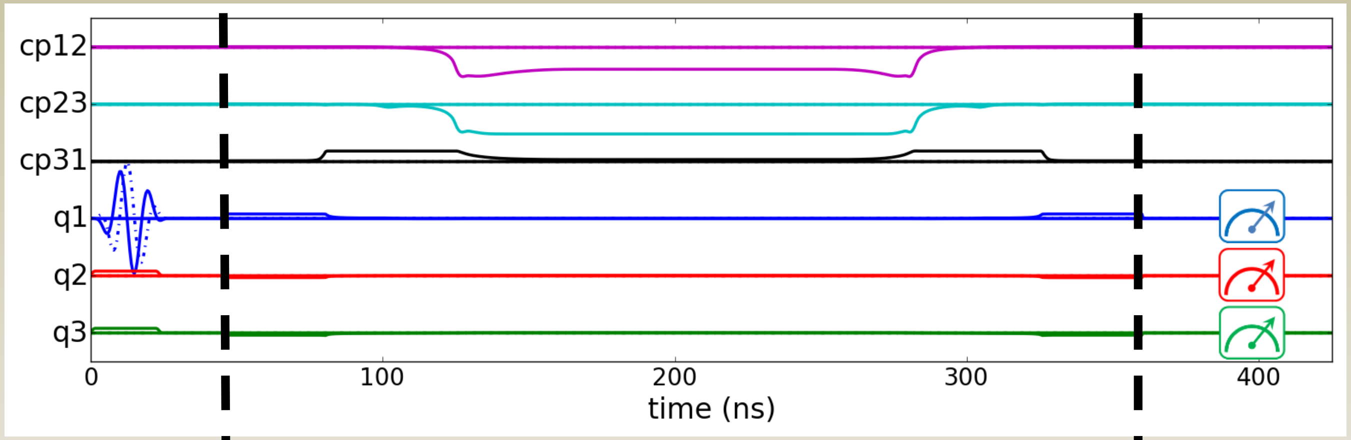
***v/c* = 7.3x10^{-4}**

***b* = 0.053 Å**



Inelastic Scattering of Na & He: **Quantum Simulation**





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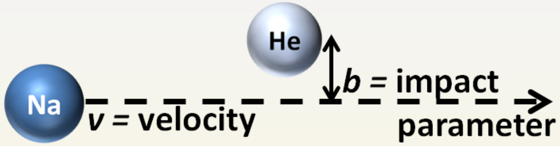
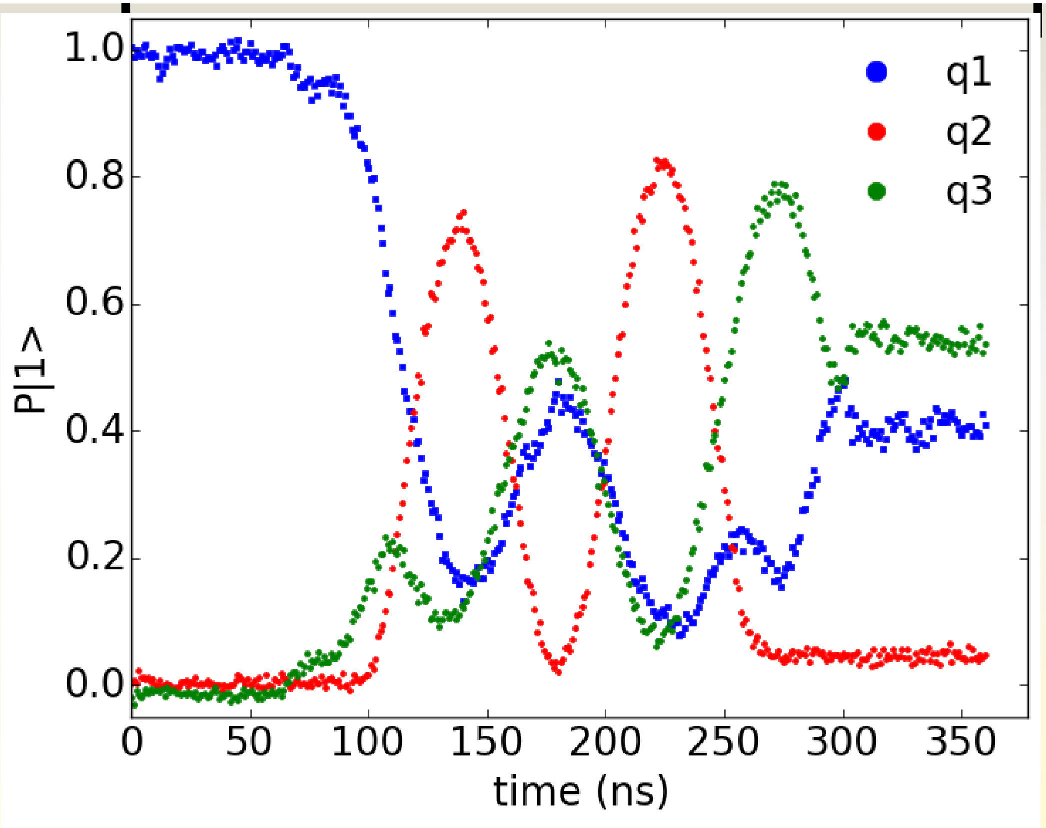
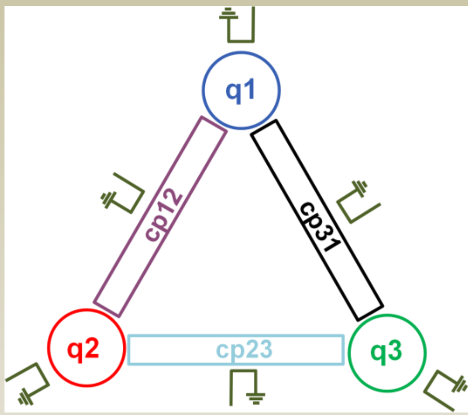
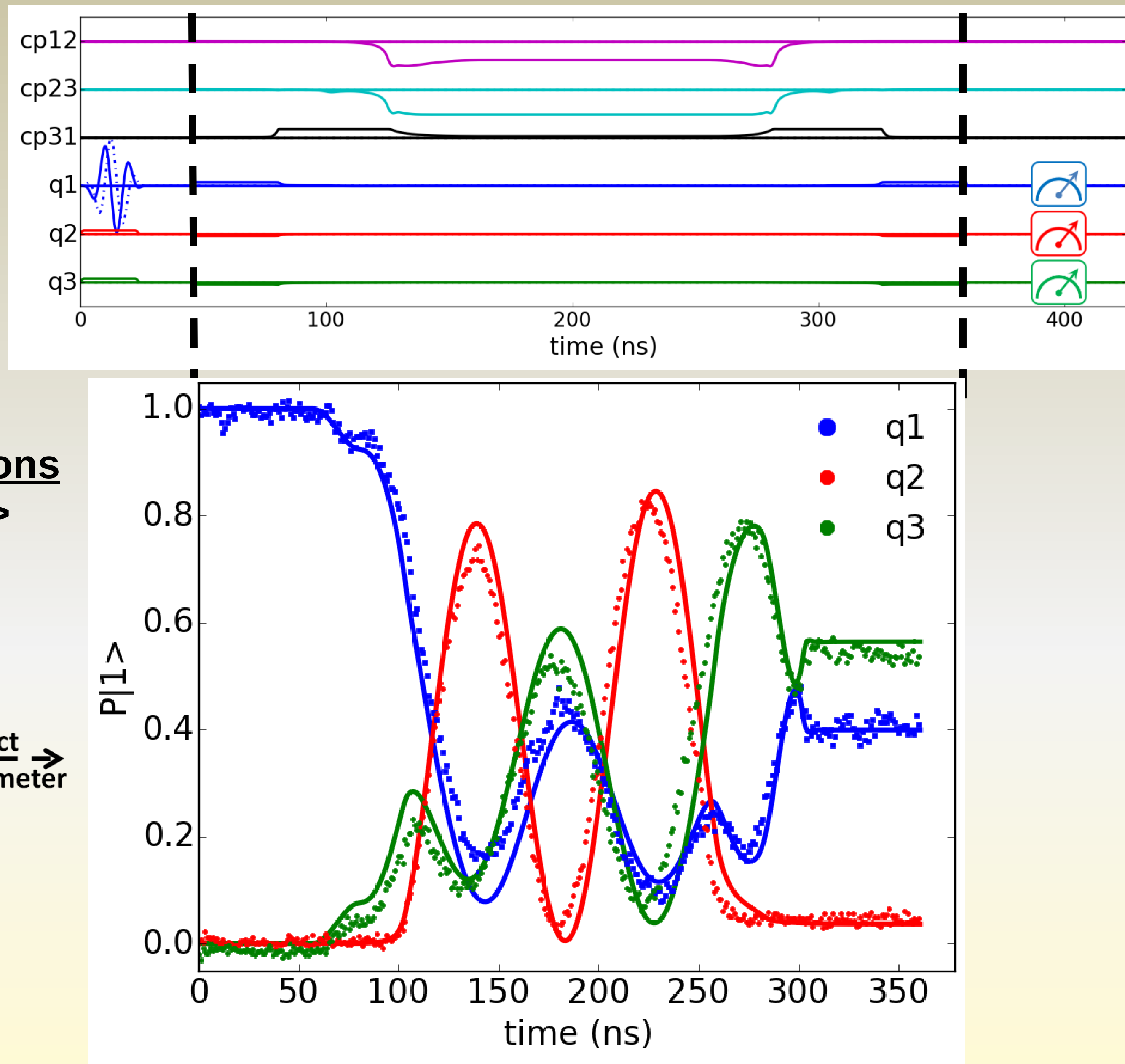




Inelastic Scattering of Na & He: **Q. + Num. Simulation**





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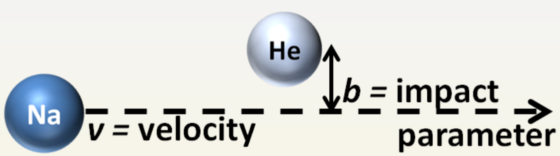
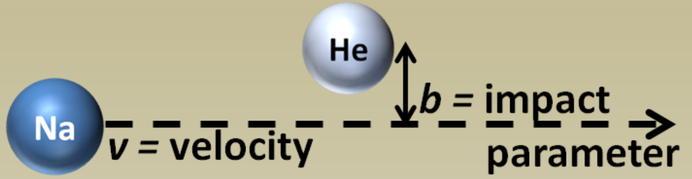
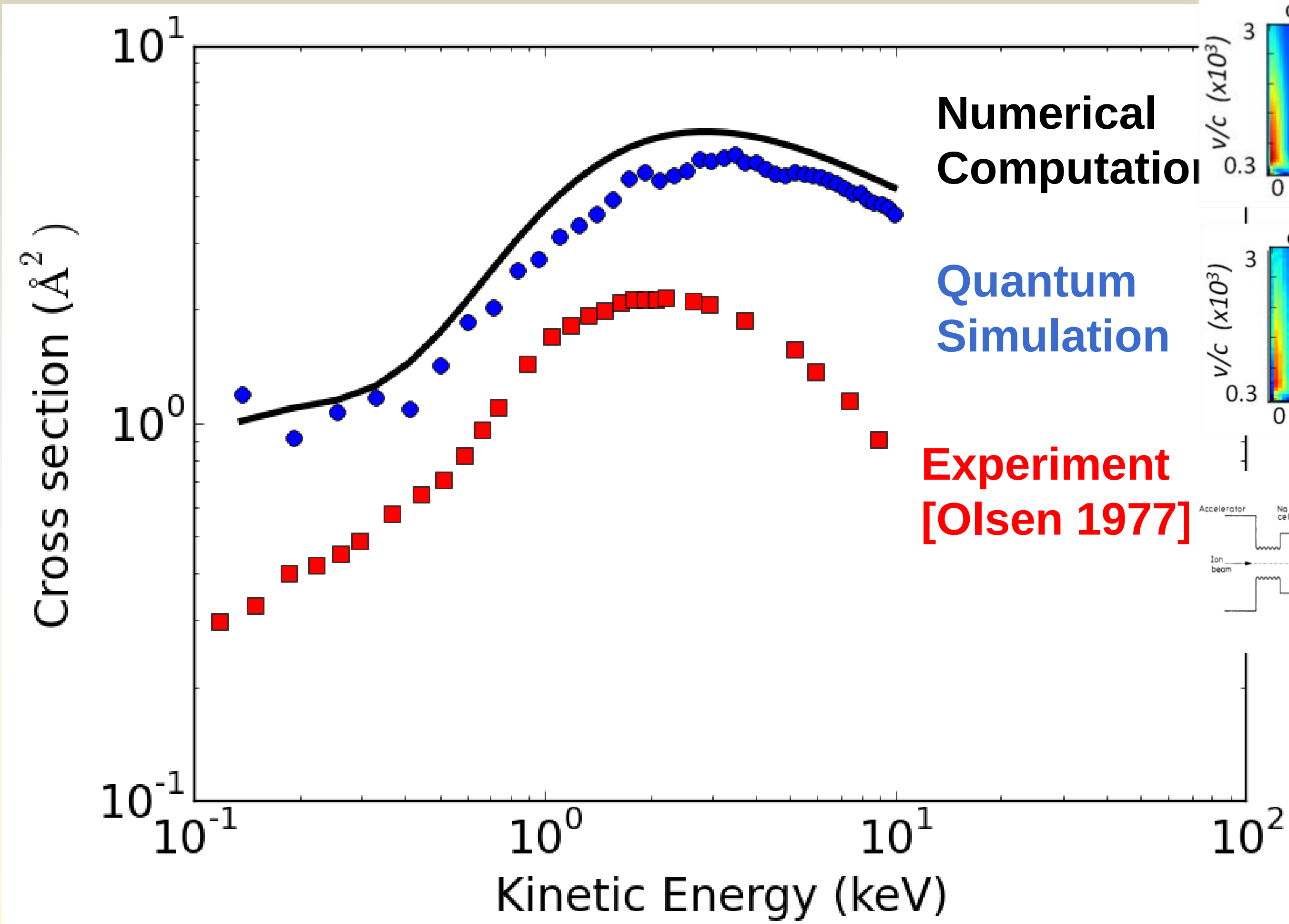


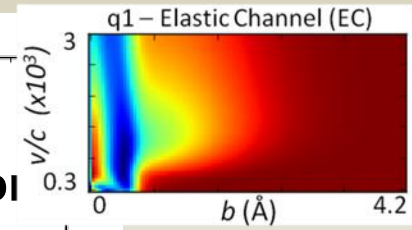
Inelastic Cross Section:

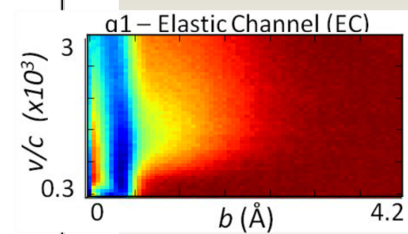
Comparing Simulation to Experiment

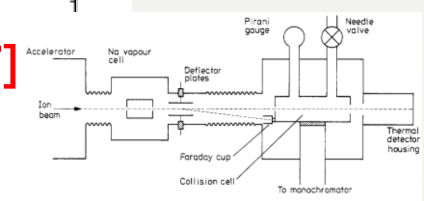


$$\text{Cross section} = 2\pi \int_0^{\infty} b * (1 - P_1(EC))\, db$$

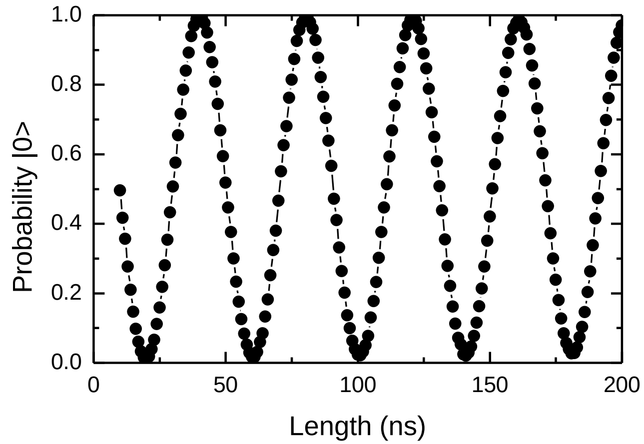








Summary & Outlook



Xmon qubits are high-fidelity technology

- 1 qubit: 99.93(3)%
- 2 qubit: 99.45(5)%
- Repetitive measure: 99%

} all at once

- Improvements ongoing, with scaling

With fidelity and control, perform computations at thresholds

- Digital: Bit-flip error correction
- Analog: Computation power for chemical simulation

Technology in hand to scale up to ~100 qubits, soon…