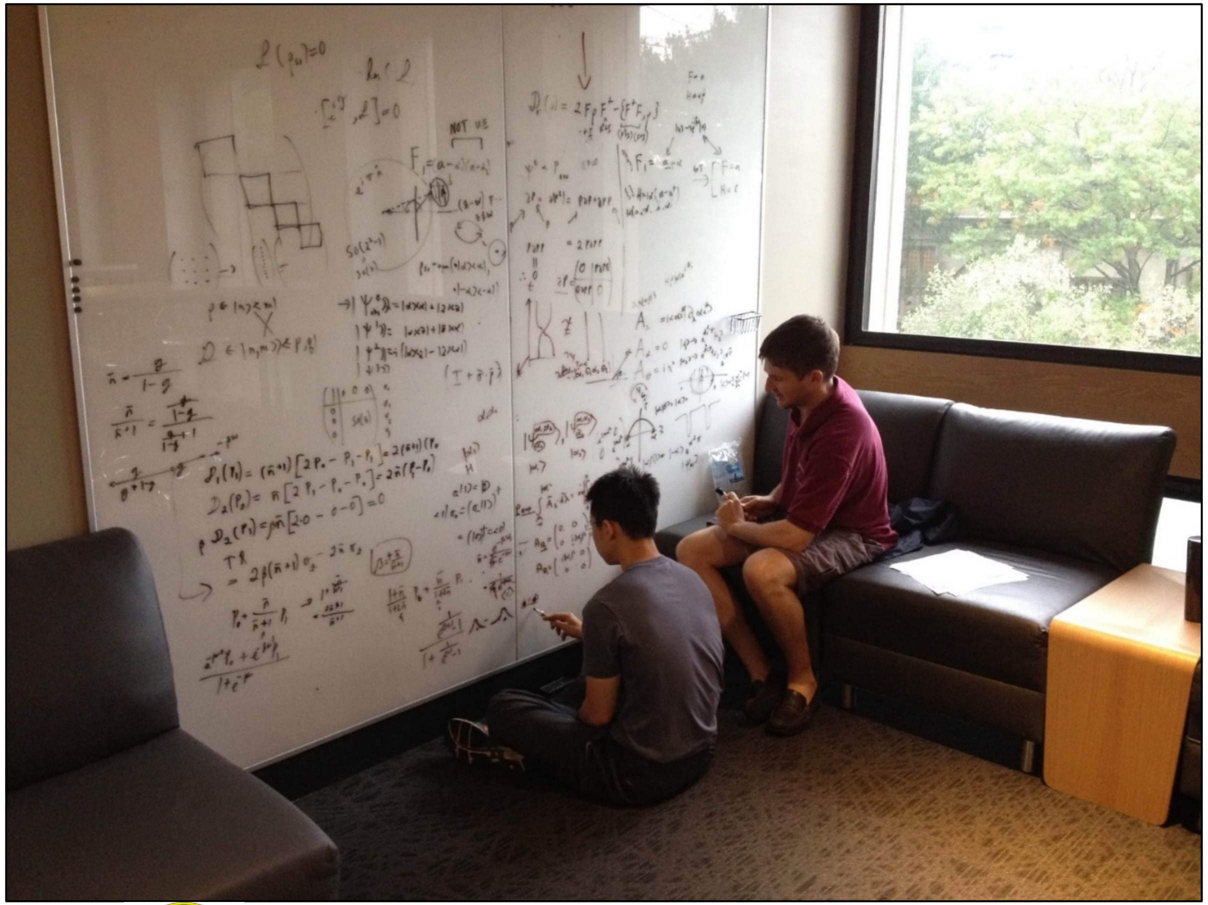
Experimental Simulation of Atomic Vibrational Spectra Using Efficient Boson Sampling

Steven Girvin
Yale Quantum Institute

Experiment
Michel Devoret
Luigi Frunzio
Rob Schoelkopf

Chris Wang
Jacob Curtis
Luyan Sun
Yvonne Gao
Brian Lester
Andrei Petrenko
Nissim Ofek
Reinier Heeres
Philip Reinhold
Yehan Liu
Zaki Leghtas
Brian Vlastakis
+…..



Theory
SMG
Liang Jiang
Leonid Glazman
M. Mirrahimi
Shruti Puri

Baptiste Royer
Shraddha Singh
Kevin Smith
Micheline Soley
Yaxing Zhang
José Lebreuilly
Victor Albert
Kjungjoo Noh
Changling Zou
Richard Brierley
Claudia De Grandi
Zaki Leghtas
Juha Salmilehto
Matti Silveri
Uri Vool
+…..

Research supported by ARO

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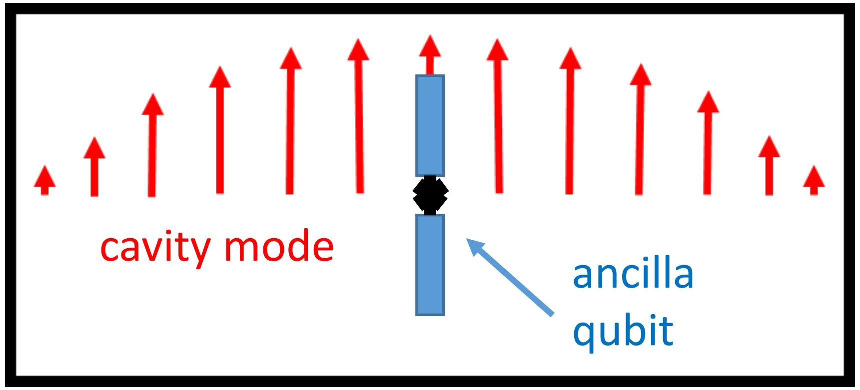
Programmable quantum simulator desiderata:

1. Universal control
    - Create initial non-classical states
    - Synthesize arbitrary Hamiltonian dynamics

2. Efficient and non-trivial measurements
    - Probe the simulation results
    - State tomography beyond capabilities typically available in the system being simulated

Universal control and measurement of hybrid qubit-oscillator systems in circuit QED.



Qubit-Cavity Strong Dispersive Coupling

$$\omega_c \neq \omega_q$$

$$H = \omega_c a^\dagger a + \frac{\omega_q}{2}\sigma^z + \chi\,\sigma^z\, a^\dagger a$$

Permits several possible instruction sets

Example 1: SNAP gate set:

Cavity-controlled qubit rotations + Cavity displacements:

$$U_{\text{SNAP}}(\vec{\theta}) \equiv e^{i\sigma^z \sum_{n=0}^{n_{\max}} \theta_n \hat{P}_n}$$

$$\hat{P}_n = |n\rangle\langle n|$$

$$\vec{\theta} = (\theta_0, \theta_1, \ldots, \theta_{n_{\max}})$$

$$\mathcal{D}(\alpha) = e^{\alpha a^\dagger - \alpha^* a}$$

ISA Example 2: Qubit-Controlled Cavity Displacement + Qubit Rotations

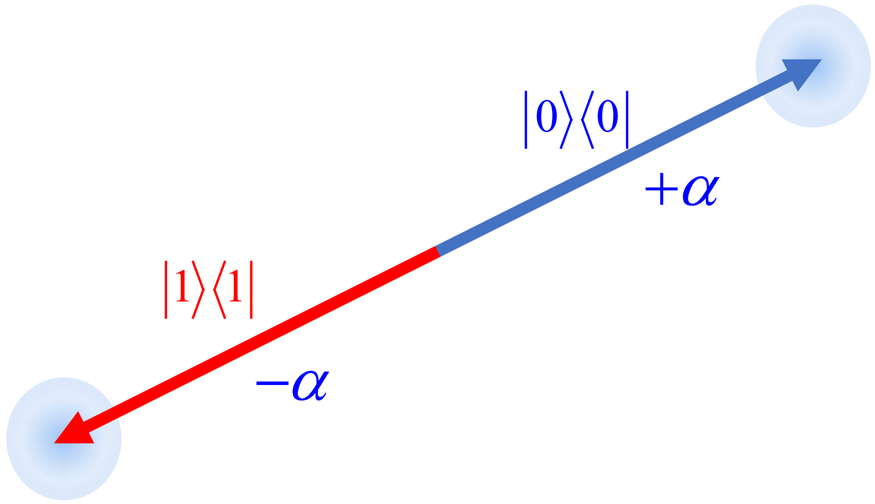
Fast Universal Control of an Oscillator with Weak Dispersive Coupling to a Qubit, A. Eickbusch et al. (Devoret Lab)
arXiv:2111.06414

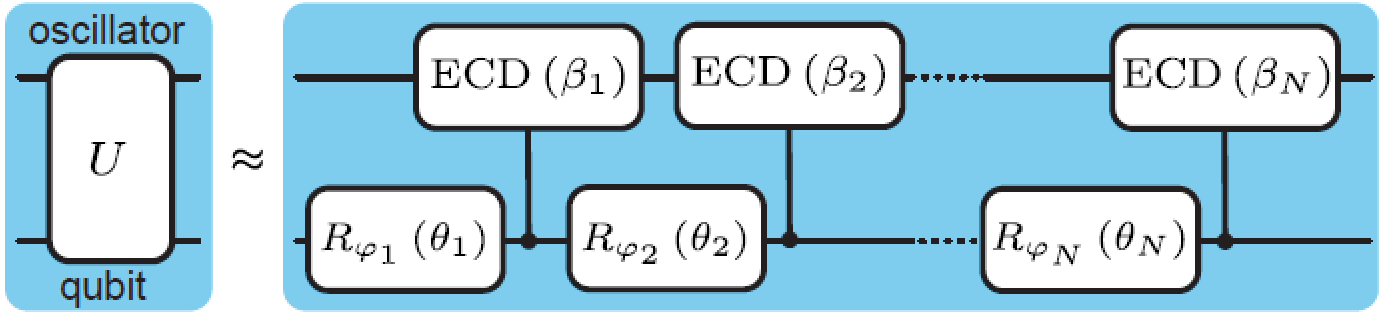
Conditional Displacement Gate

$$\mathcal{D}_c(\alpha) = |0\rangle\langle 0|\mathcal{D}(\alpha) + |1\rangle\langle 1|\mathcal{D}(-\alpha)$$

Qubit Rotation Gate

$$R_\varphi(\theta) = e^{-i\frac{\theta}{2}\left[\cos\varphi\,\sigma^x + \sin\varphi\,\sigma^y\right]}$$



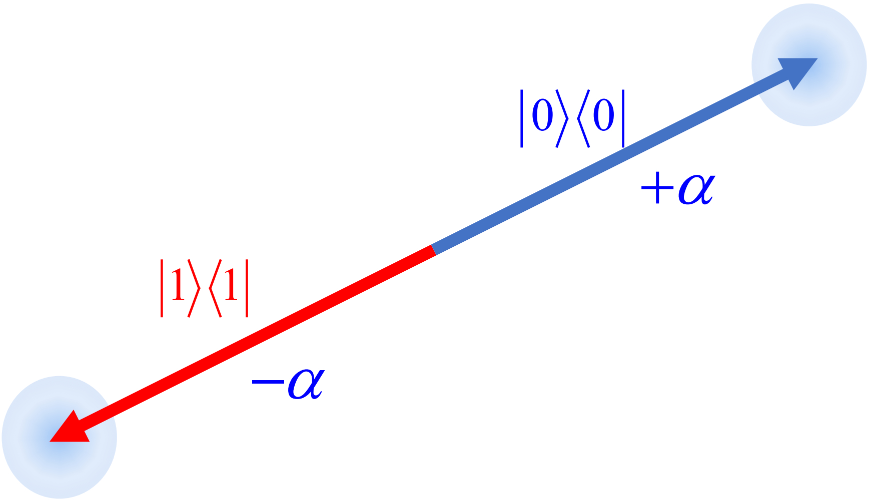


Circuit depth →

ISA Example 2: Qubit-Controlled Cavity Displacement + Qubit Rotations

Non-Commuting Geometry of Oscillator Phase Space $\otimes$ Bloch Sphere: Conditional Displacements

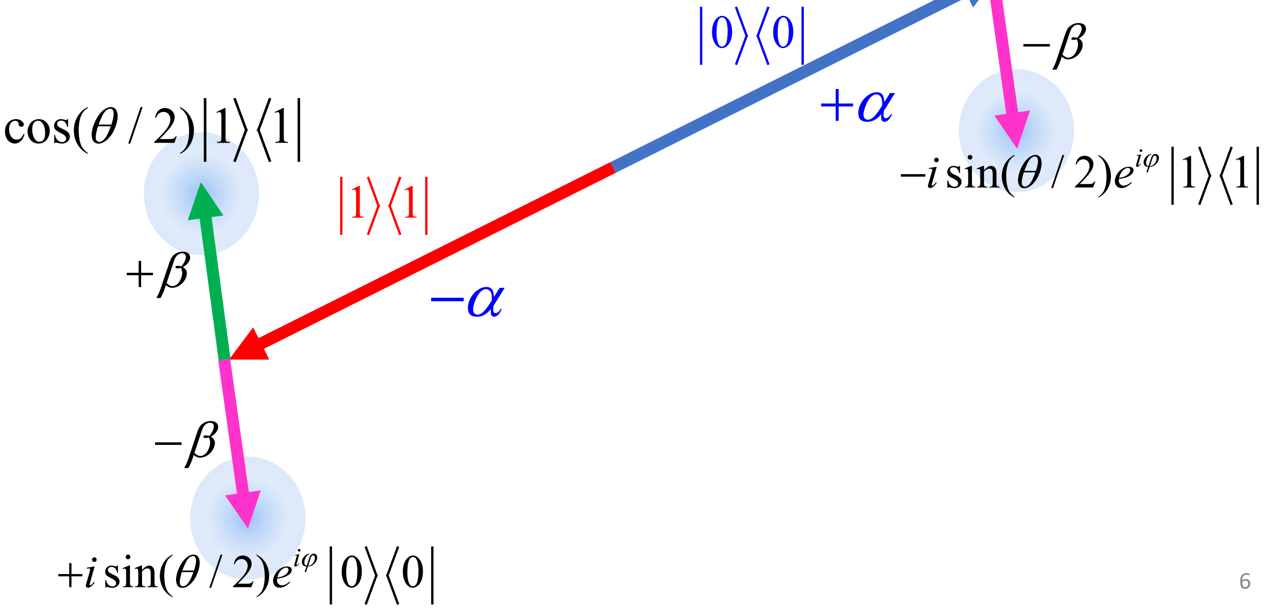
$$\mathcal{D}_c(\alpha) = |0\rangle\langle 0|\mathcal{D}(\alpha) + |1\rangle\langle 1|\mathcal{D}(-\alpha)$$



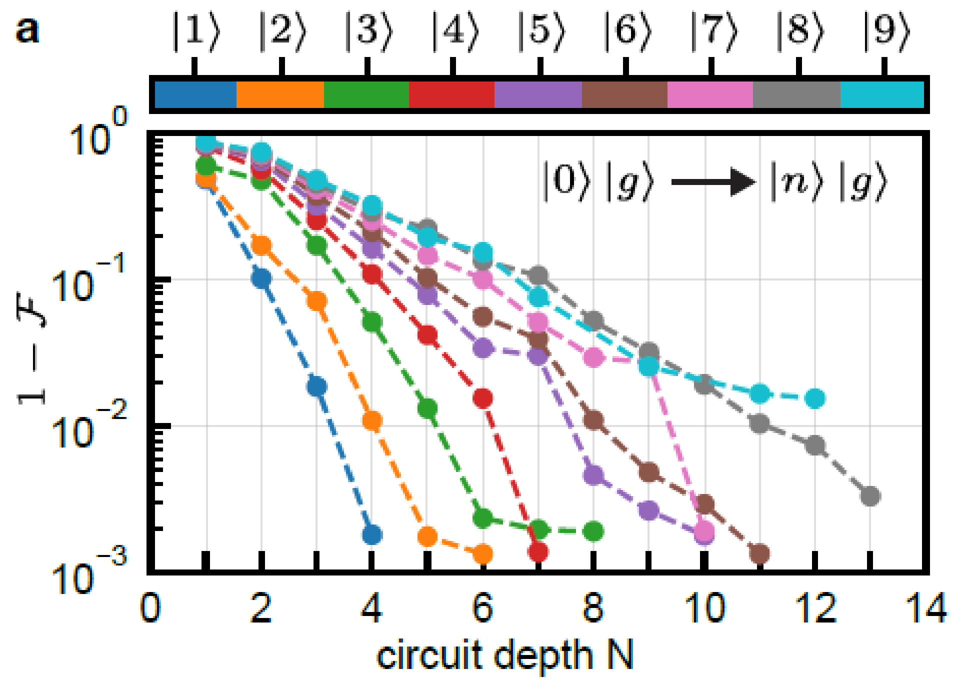
Universal Gate Set:
Composing conditional displacements and qubit rotations

$$\mathcal{D}_c(\beta)R_\varphi(\theta)\mathcal{D}_c(\alpha)$$

$$R_\varphi(\theta) = e^{-i\frac{\theta}{2}\left[\cos\varphi\,\sigma^x + \sin\varphi\,\sigma^y\right]}$$



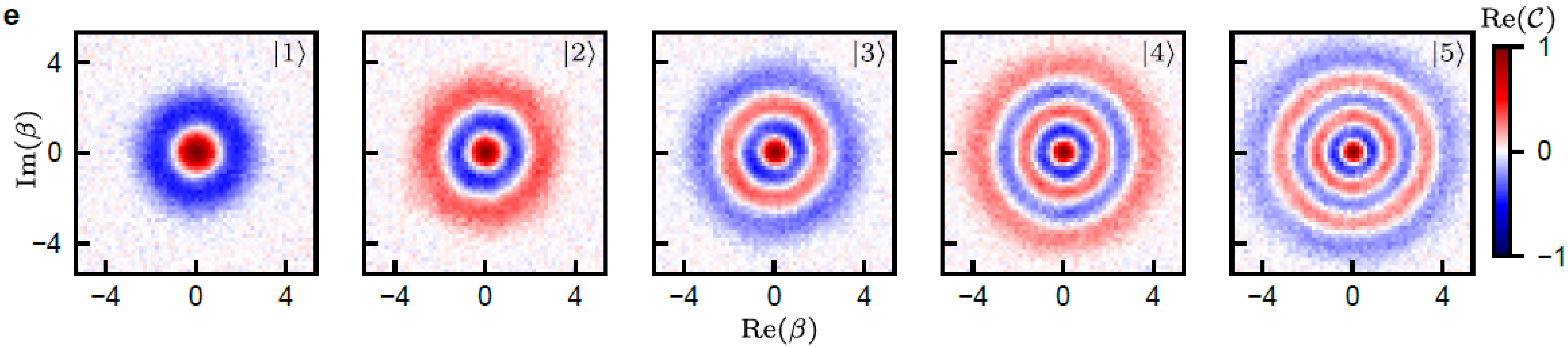
(Echoed) Controlled-Displacement ISA:



Fast Universal Control of an Oscillator with Weak Dispersive Coupling to a Qubit, A. Eickbusch et al. (Devoret Lab) [arXiv:2111.06414](https://arxiv.org/abs/2111.06414)

[Wigner function and characteristic function phase space tomography plots will be explained in Lecture 4.]

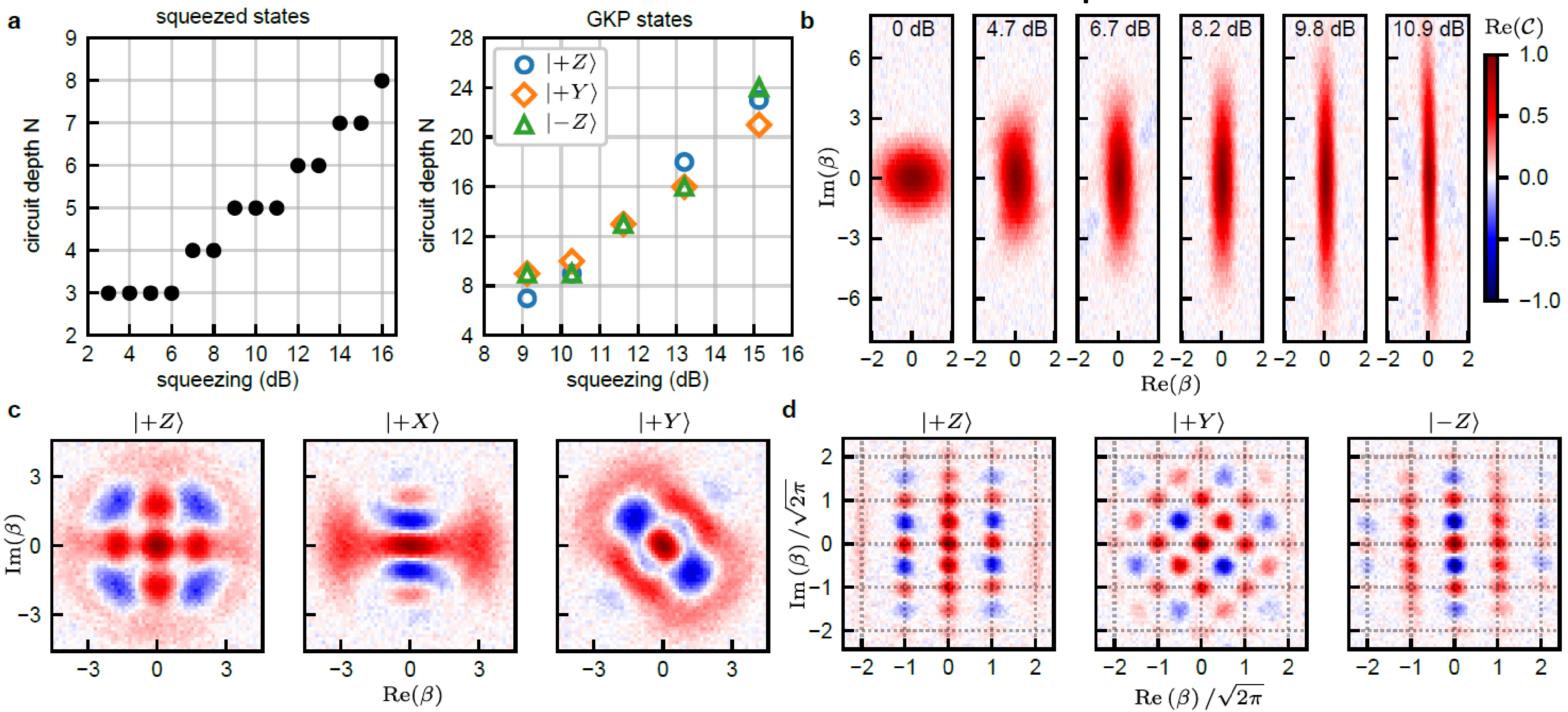
Photon Fock State Generation



(Echoed) Controlled-Displacement ISA:

Fast Universal Control of an Oscillator with Weak Dispersive Coupling to a Qubit, A. Eickbusch et al. arXiv:2111.06414

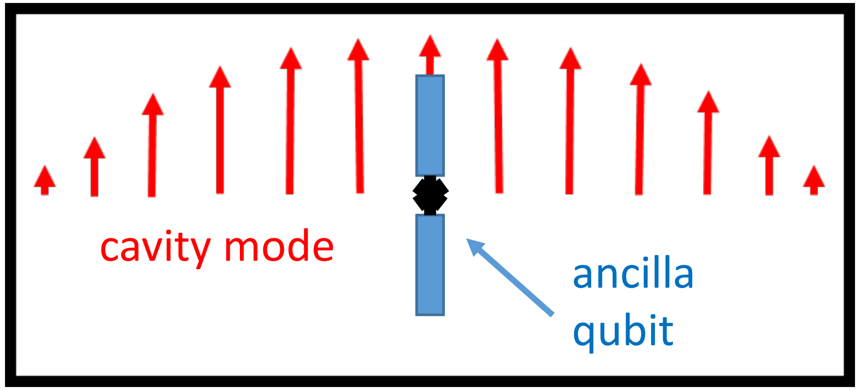
Squeezed states



Binomial QEC code word states

GKP QEC code word states

Universal control and measurement of hybrid qubit-oscillator systems in circuit QED.



Is the photon number equal to
1? Yes or no?
13? Yes or no?

[If there are, say, 256 possible photon numbers, the answer is likely to be 'no' most of the time.]

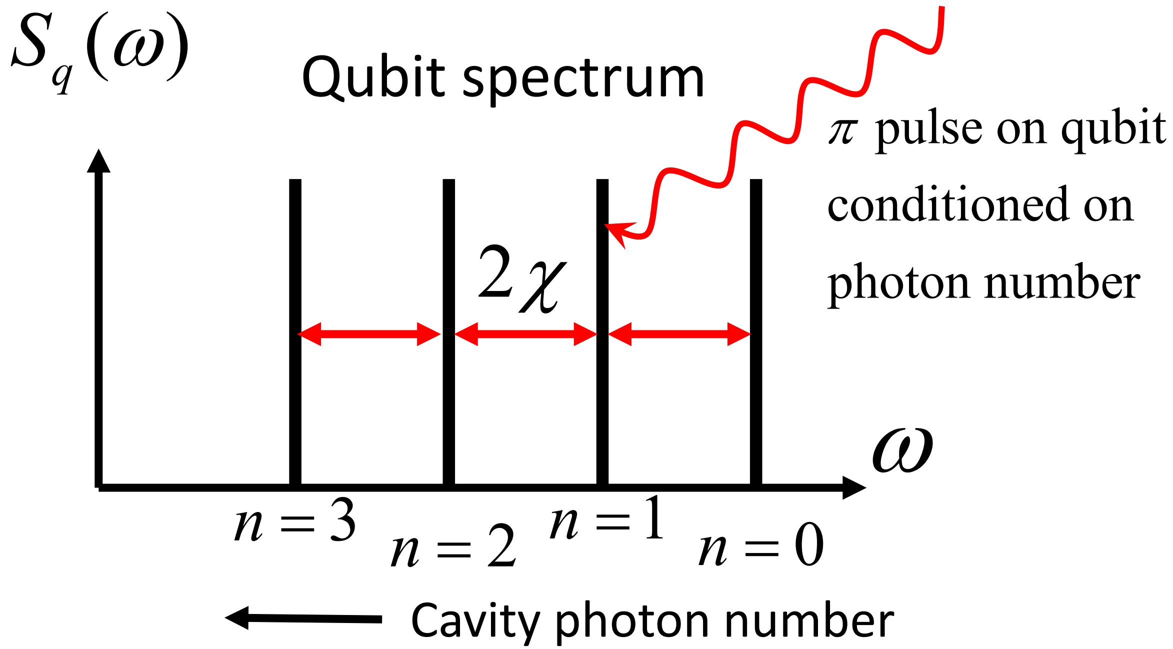
Inefficient sampling implies
large query complexity.]

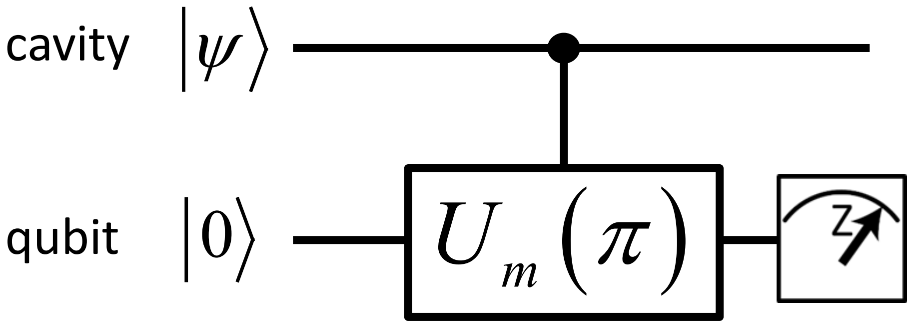
Qubit-Cavity Strong Dispersive Coupling

$$\omega_c \neq \omega_q$$

$$H = \omega_c a^\dagger a + \frac{\omega_q}{2}\sigma^z + \chi\,\sigma^z\, a^\dagger a$$

Measure cavity photon number by its effect qubit transition frequency. [QND]

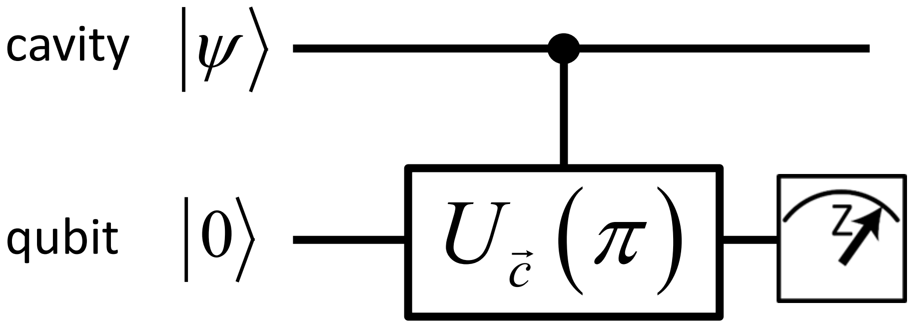


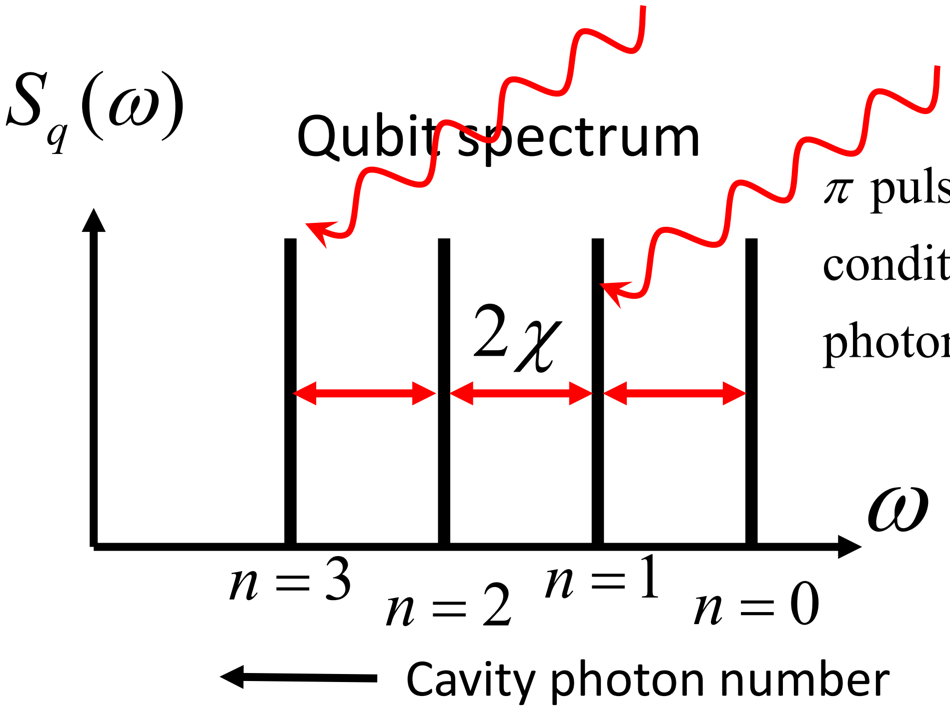


$$U_m(\pi) = e^{-i\frac{\pi}{2}\sigma^x \hat{P}_m} \qquad \hat{P}_m \equiv |m\rangle\langle m|$$

Measure <u>any arbitrary binary function</u> of the photon number. [QND]

Is the photon number equal to either 1 or 3?
Yes or no?



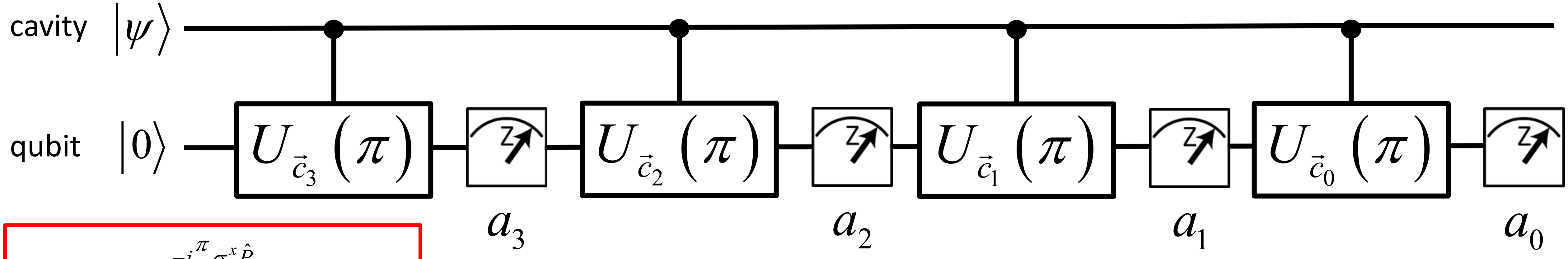


$$U_{\vec{c}}(\pi) = e^{-i\frac{\pi}{2}\sigma^x \hat{P}_{\vec{c}}}$$

$$\hat{P}_{\vec{c}} \equiv \sum_{m=0}^{n_{\max}} c_m \hat{P}_m \,, \quad c_j \in \{0,1\}$$

Example: binary search for photon number

More convenient than phase estimation—
no feedforward required + obtain most significant bits first



$$U_{\vec{c}}(\pi) = e^{-i\frac{\pi}{2}\sigma^x \hat{P}_{\vec{c}}}$$

$$\hat{P}_{\vec{c}} \equiv \sum_{m=0}^{n_{\max}} c_m \hat{P}_m \,, \quad c_j \in \{0,1\}$$

$$\vec{c}_0 = [1010101010101010]$$ Parity

$$\vec{c}_1 = [1100110011001100]$$

$$\vec{c}_2 = [1111000011110000]$$

$$\vec{c}_3 = [1111111100000000]$$

Walsh-Hadamard transform

circuit cost: $\log_2 n_{\max}$
efficient boson sampling
(exponential gain)

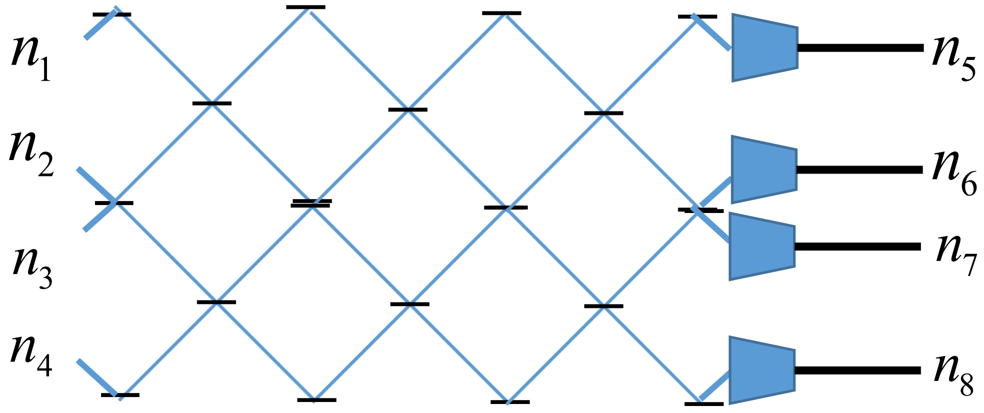
Binary digits in measured photon number

$$[b_3 b_2 b_1 b_0]$$
$$b_3 = a_3$$
$$b_2 = a_3 \oplus a_2$$
$$b_1 = a_3 \oplus a_2 \oplus a_1$$
$$b_0 = a_3 \oplus a_2 \oplus a_1 \oplus a_0$$

Using this control and measurement toolbox for hardware-efficient simulation of physical models containing bosons.

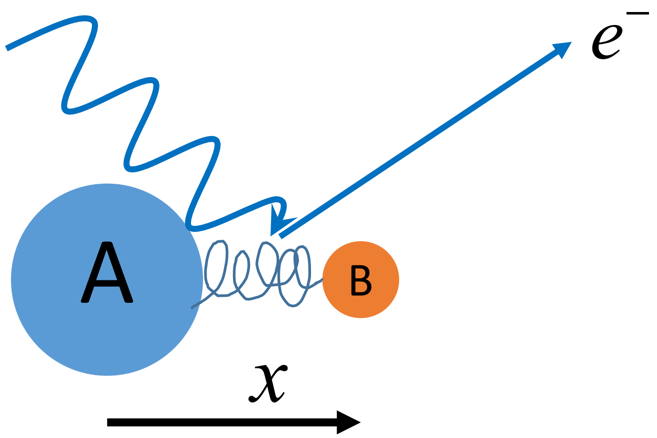
Experimental simulation of the optical spectra of vibrating molecules

Franck-Condon factors as a boson sampling problem



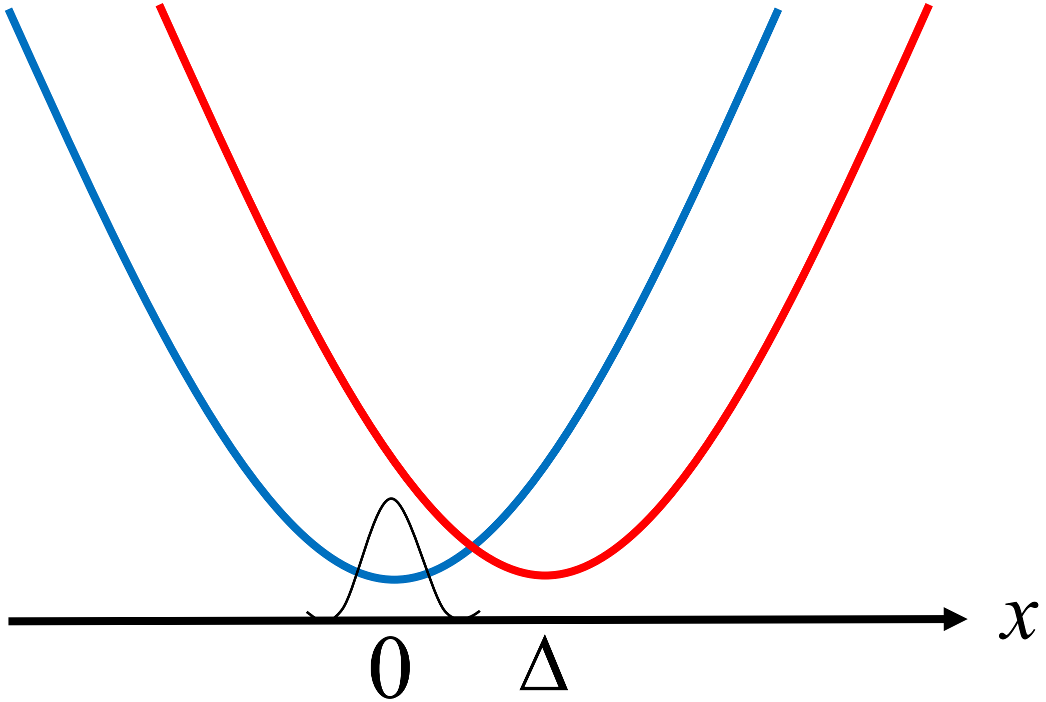
Huh et al. *Nature Photonics* **9** 615 (2015)

Warm up example: the suddenly displaced harmonic oscillator

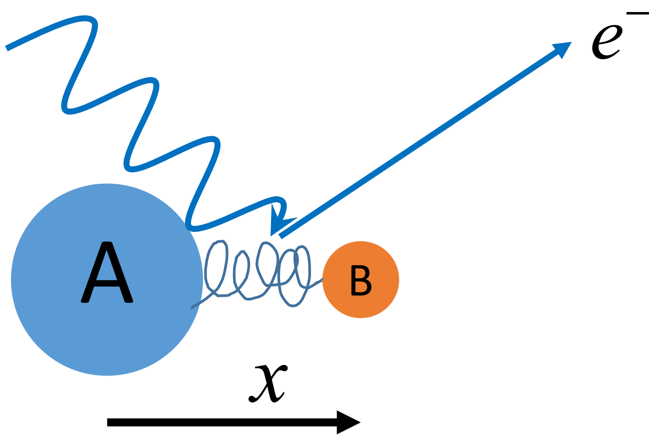


Photon emission ejects a bonding electron suddenly changing the equilibrium spacing of the two nuclei

$$H(t) = \frac{p^2}{2m} + \frac{1}{2}k\left[x - \Delta\theta(t)\right]^2$$



Warm up example: the suddenly displaced harmonic oscillator

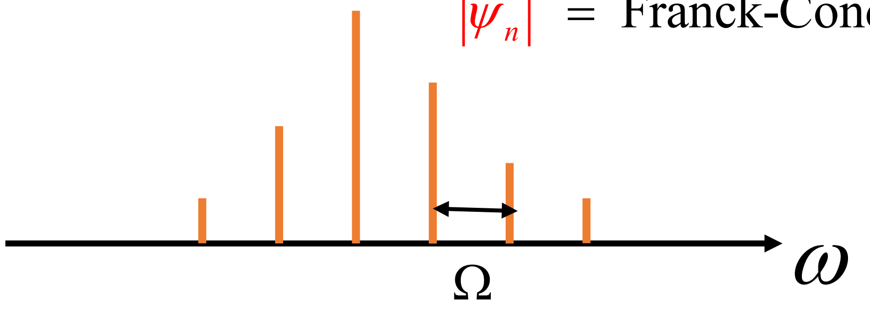


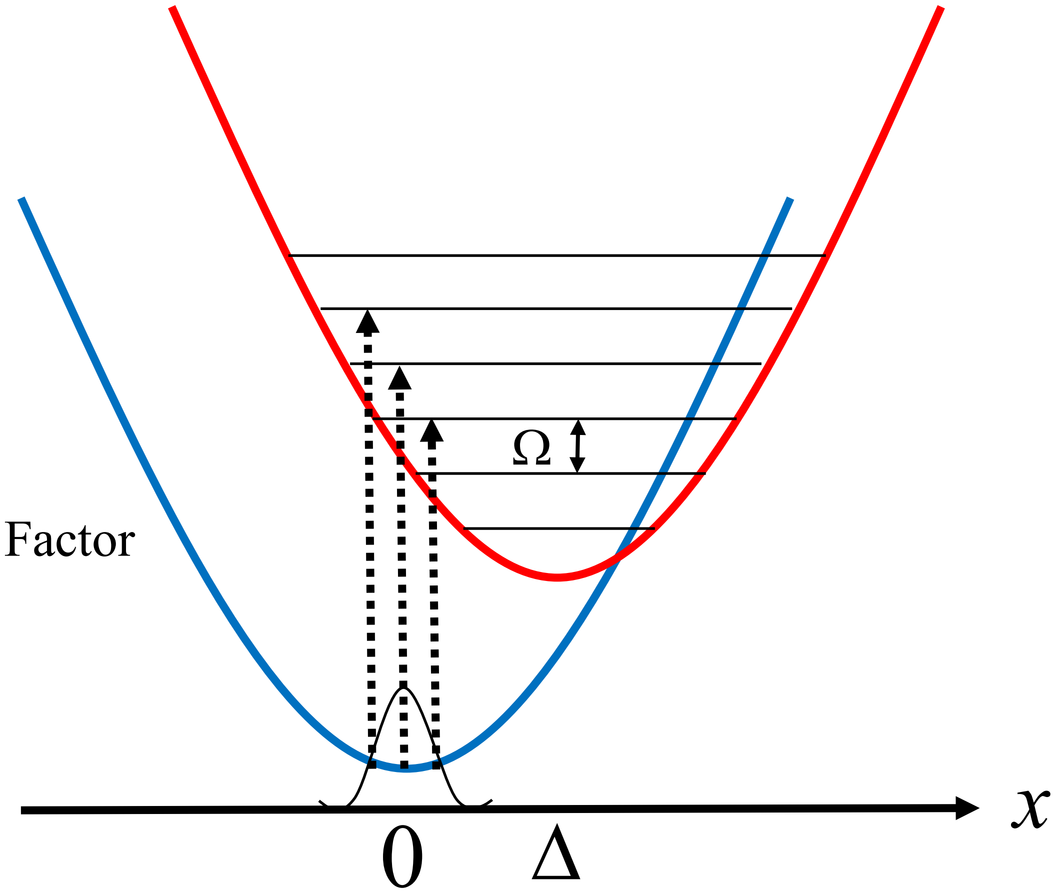
Nuclear wave function has no time to change. Sudden projection onto eigenstates of the new Hamiltonian.

$$|\Psi\rangle = \sum_n \psi_n |n\rangle$$

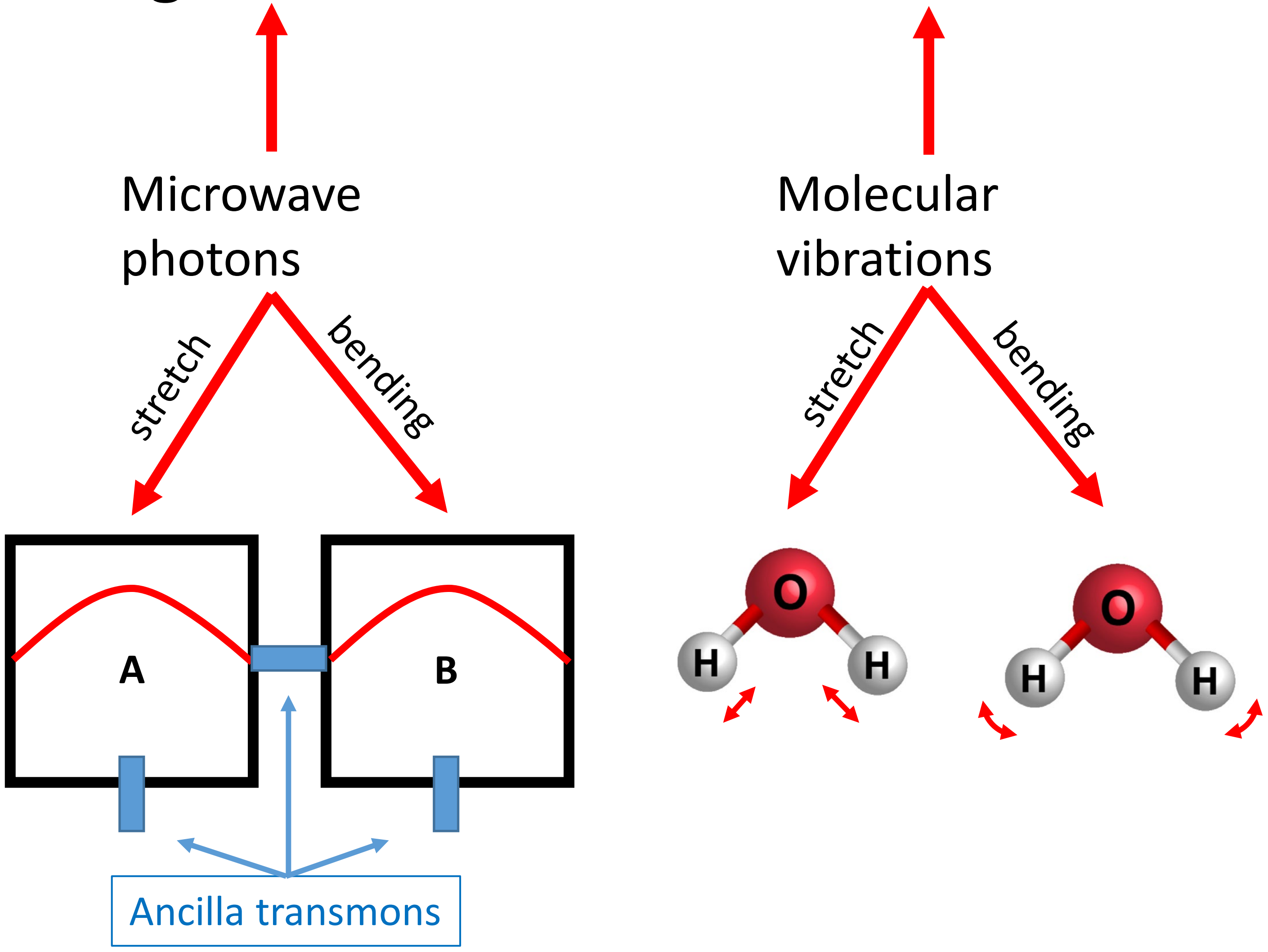
$$S(\omega) = \sum_n |\psi_n|^2 \delta(\omega - n\Omega)$$

$|\psi_n|^2$ = Franck-Condon Factor



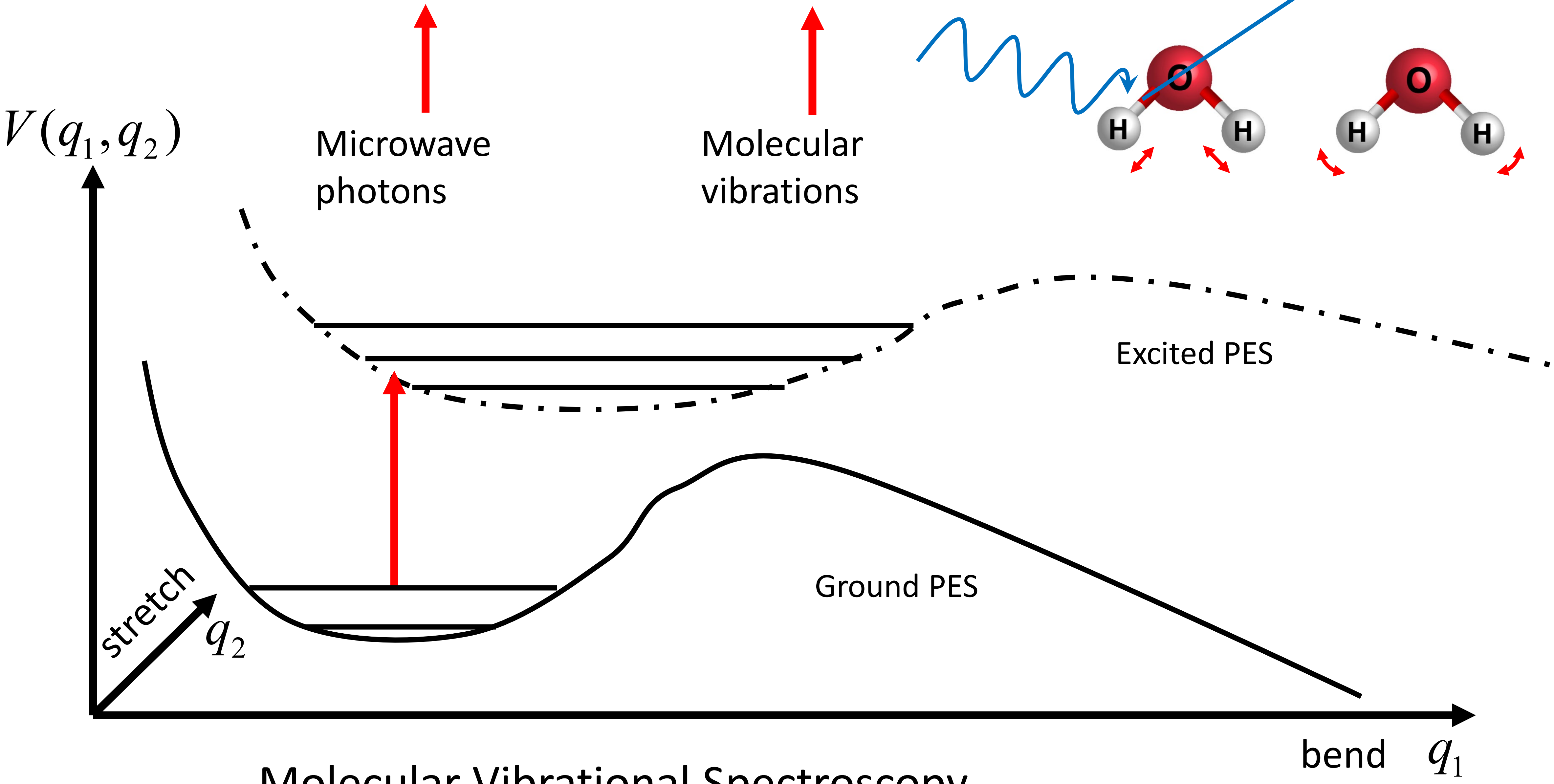


Using Bosons to Simulate Bosons

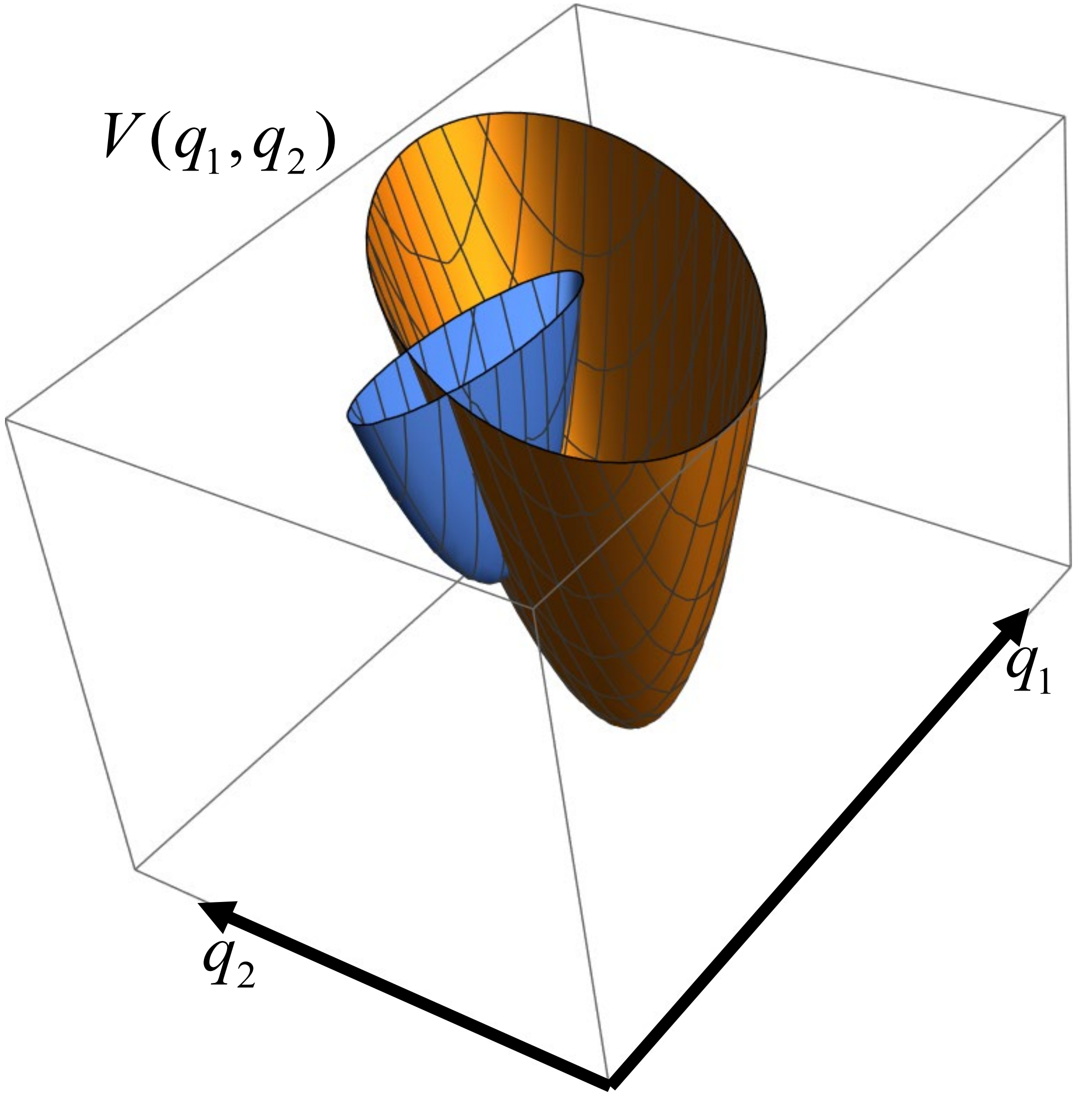


Molecular Vibrational Spectroscopy

Using Bosons to Simulate Bosons



Molecular Vibrational Spectroscopy



First-generation experiment:
Chris Wang (Schoelkopf lab)
Phys. Rev. X 10, 021060 (2020)

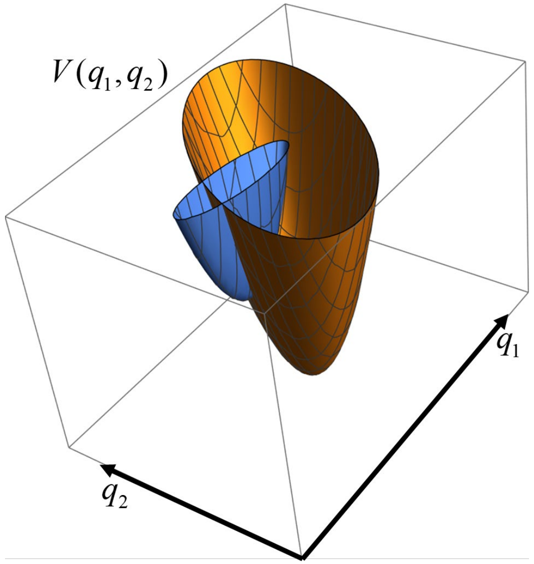
1. Obtain nuclear PES from solving fermionic problem on classical computer.

2. Approximate nuclear PES as quadratic

3. But allow for different frequencies, displacement, squeezing, and orientation of symmetry axes of PES between electronic ground and excited states.

4. Sudden approximation: Perform unitary transformation between eigenstates of ground and excited state Hamiltonians.

Doktorov et al. *J. Mol. Spec.* **64** 302-326 (1977)



Requirements:

(rotations between modes)

- ❑ bosonic modes
- ❑ Gaussian operations: beamsplitters, squeezing, displacements Gao et al. *PRX* **8** 2 (2018)
- ❑ non-Gaussian state preparation Heeres et al. *Nat. Comm.* **8** 1 (2017)
- ❑ number-resolved detection Wang et al. Phys. Rev. X 10, 021060 (2020)

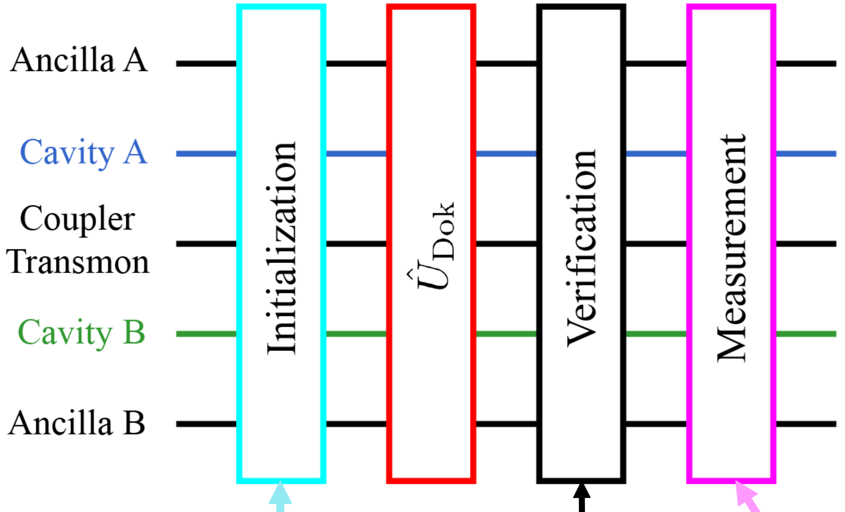
Challenging in conventional quantum optics

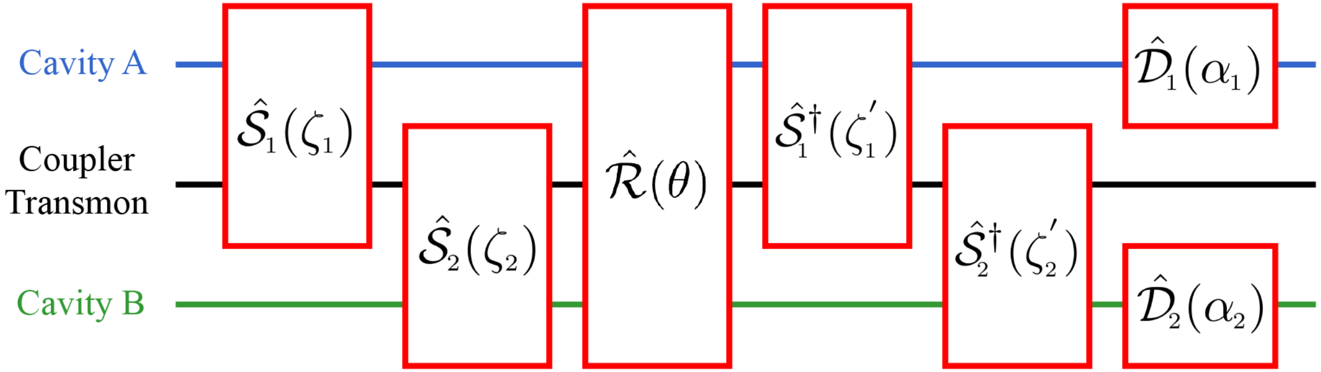
Huh et al. *Nature Photonics* **9** 615 (2015)

Circuit implementation of the Franck-Condon simulation

Phys. Rev. X 10, 021060 (2020)

$\hat{U}_{\text{dok}}$ Unitary basis change between ground and excited PES





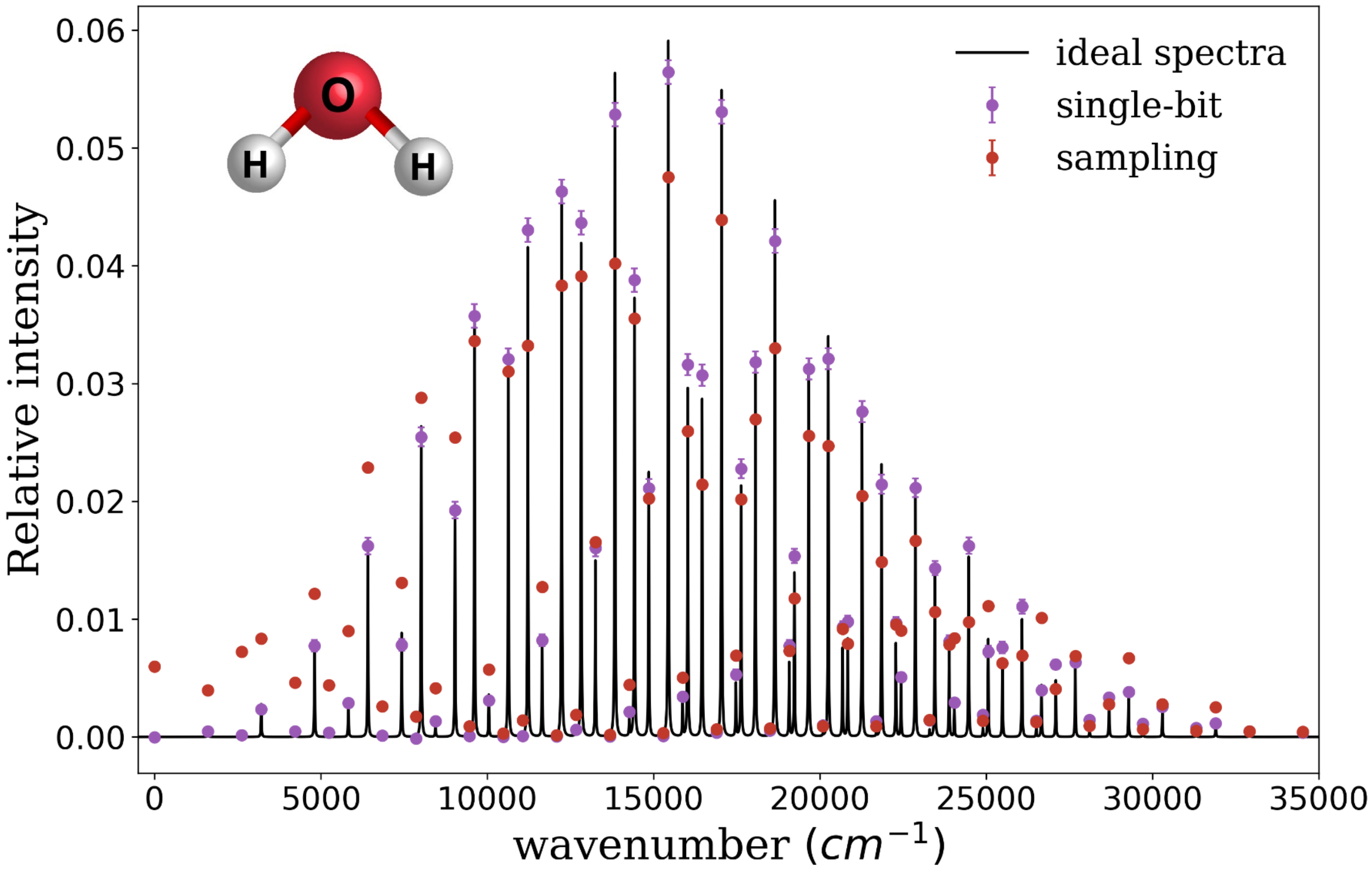
Non-Gaussian state preparation

Check error flags (ancillae)

[Reject 5-10%]

Number-resolving measurements in each cavity

Experimentally simulated photoelectron processes via efficient boson sampling (photons represent phonons)



$$H_2O \rightarrow H_2O^+(\tilde{B}\,^2B_2) + e^-$$

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

L_1 distance between exact and experimental distributions:

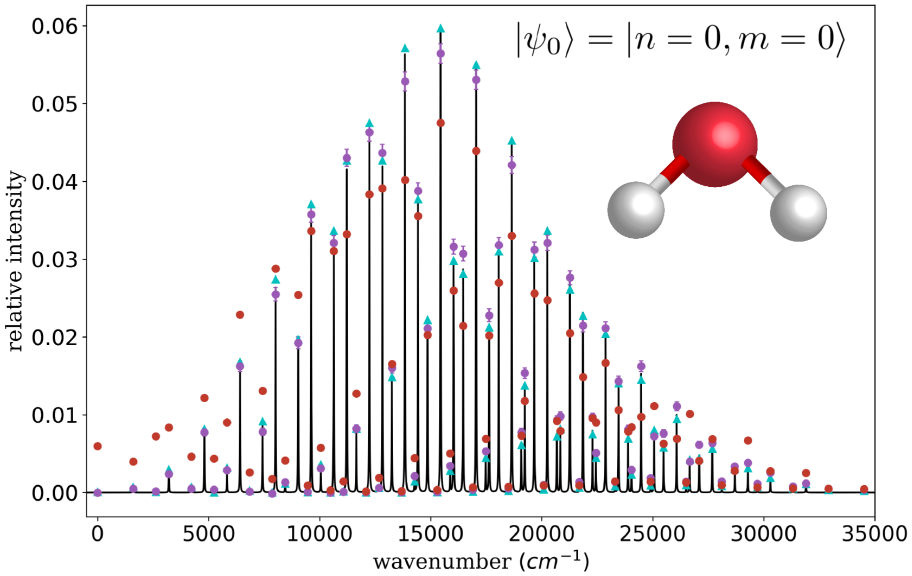
$$D = \frac{1}{2}\sum_{i,j}|p_{ij} - q_{ij}|$$

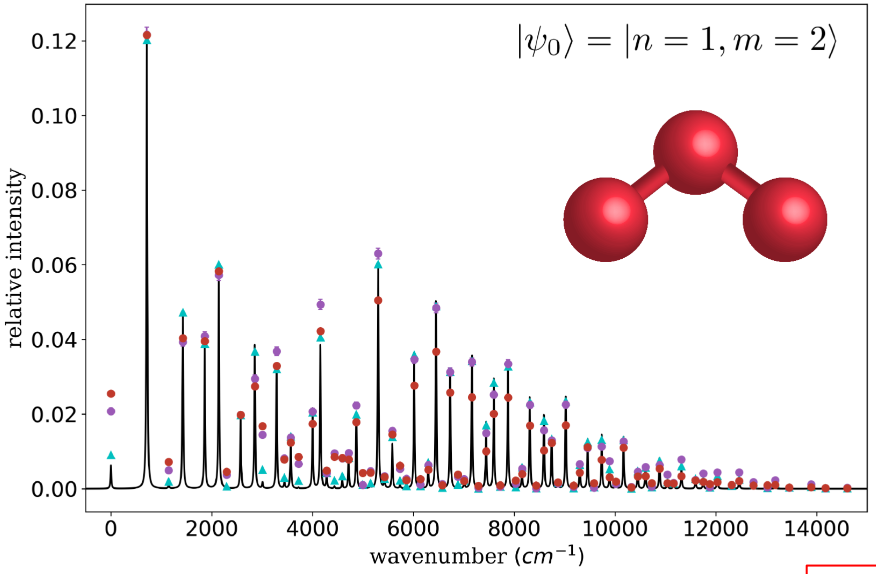
$$D_{\text{single-bit}} = 0.049$$

$$D_{\text{sampling}} = 0.152$$

Phys. Rev. X 10, 021060 (2020)

[Chris Wang]





Phys. Rev. X 10, 021060 (2020)

Typical photodetectors are not number resolving and are destructive.
Here we have efficient QND single-shot boson number sampling.
We measure which of D=256 photon states the two cavities are in by
QND measurement of the 'digits' in the binary representation of the photon number:

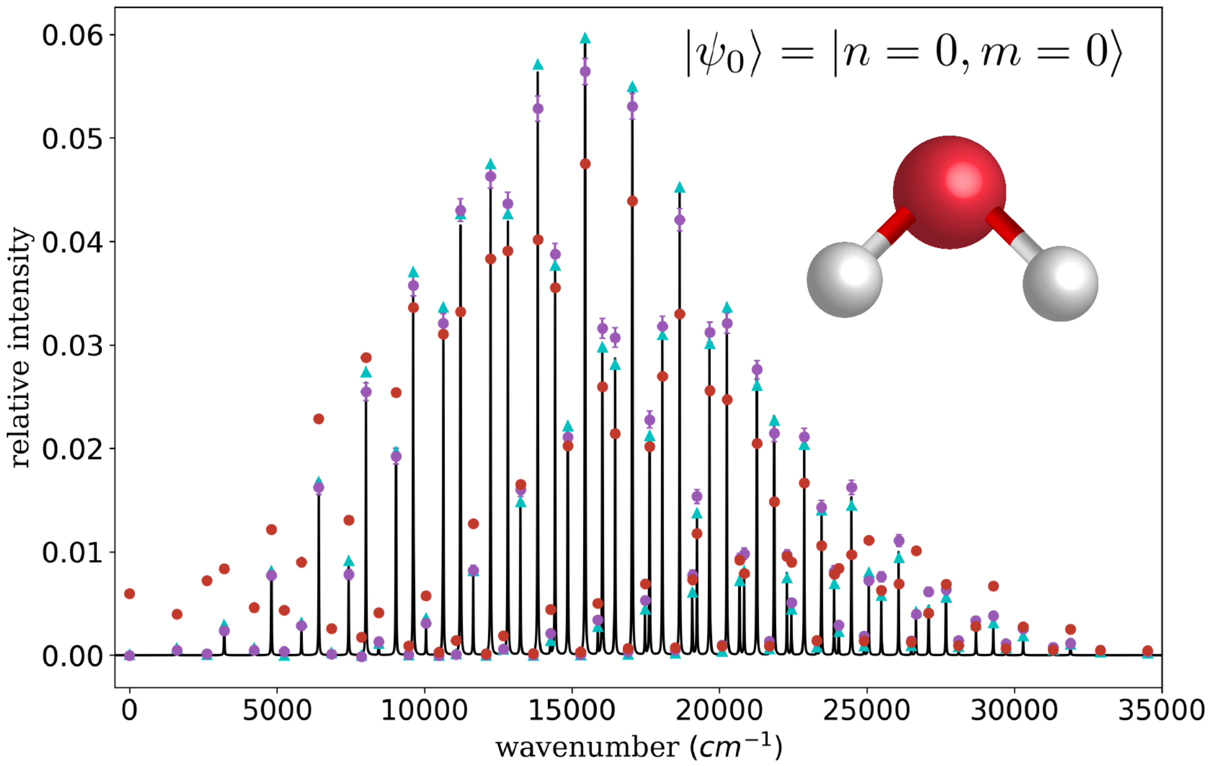
$$[n,m]=[(b_3,b_2,b_1,b_0),(c_3,c_2,c_1,c_0)]$$

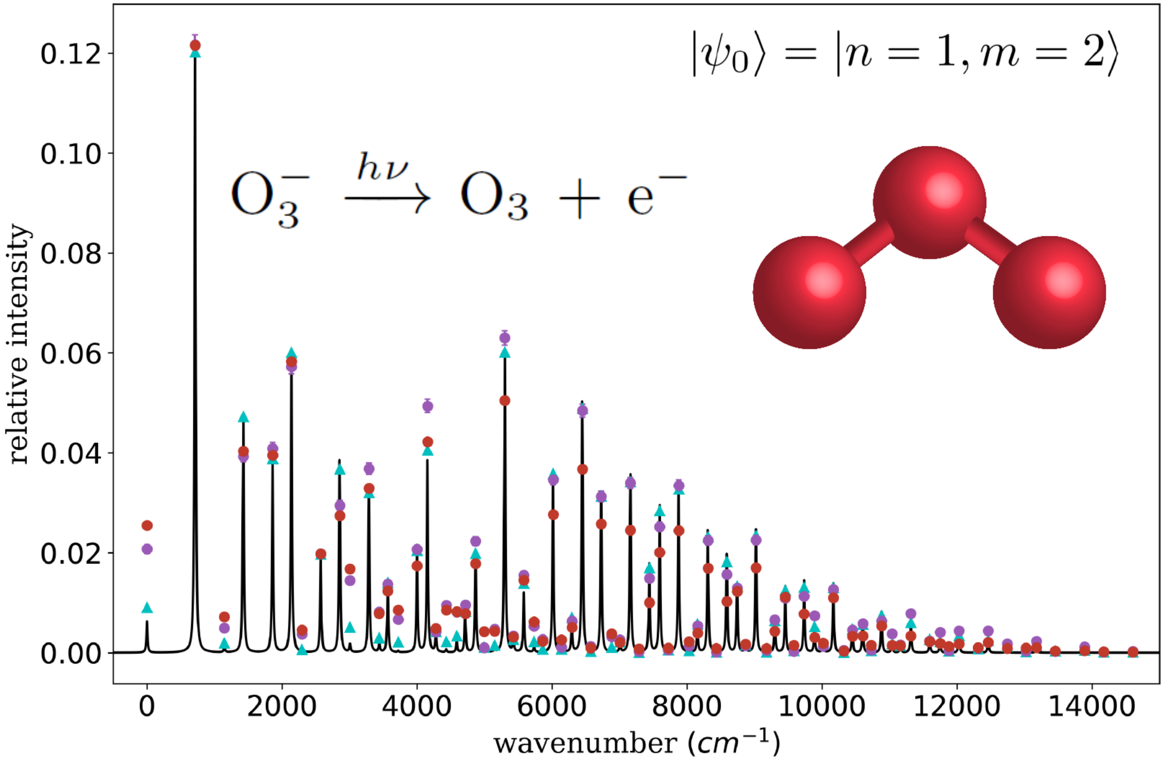
Circuit complexity cost is only log D, not D. (Exponential gain, true boson sampling)

$$H_2O \xrightarrow{h\nu} H_2O^+\left(\tilde{B}\,^2B_2\right) + e^-$$

Phys. Rev. X 10, 021060 (2020)

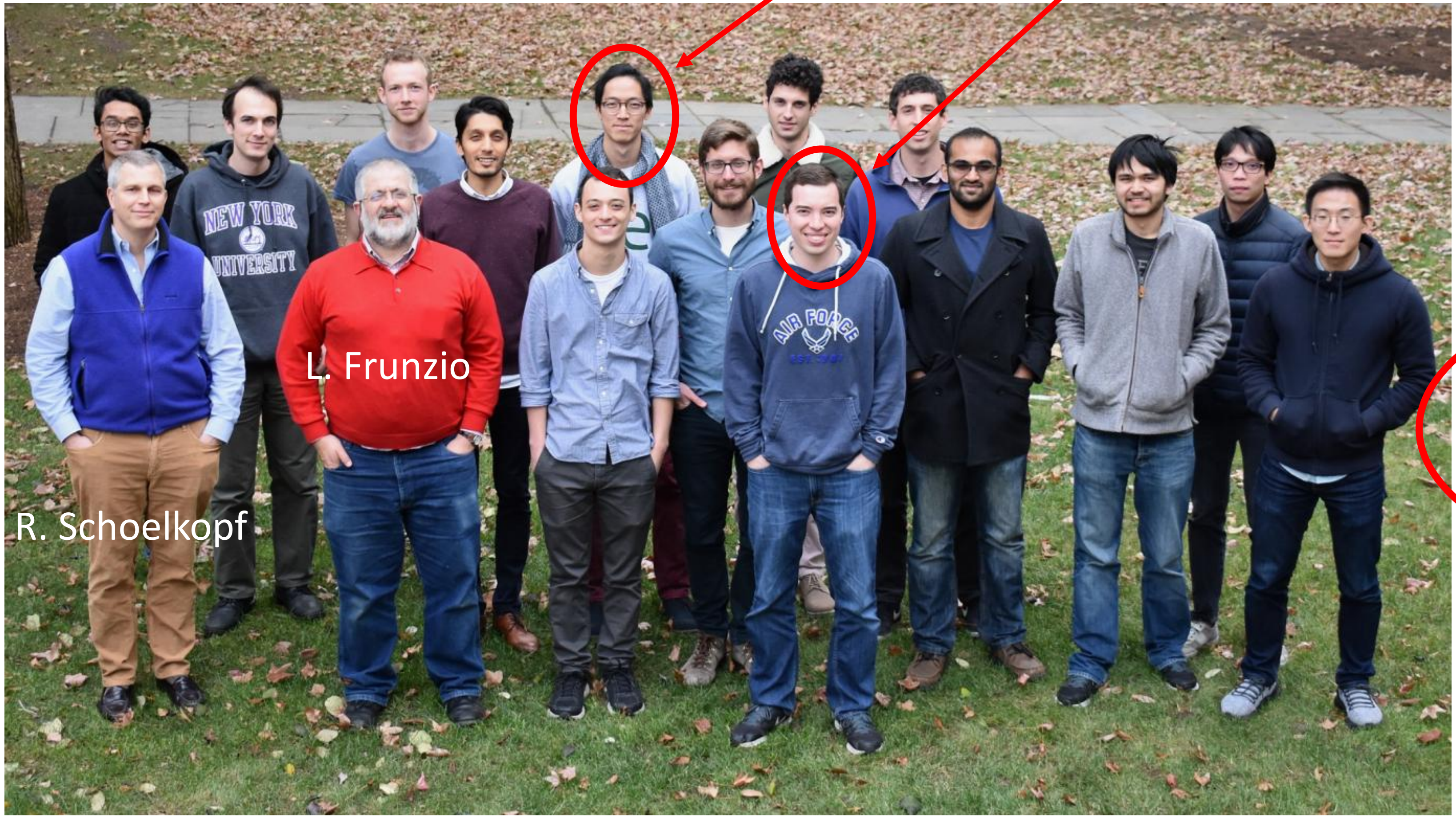
‘exact’ (cyan), single bit extraction (purple) and sampling (red) measurement





Microwave bosons to simulate vibrational bosons is highly advantageous.
Would have required >8 qubits and ~10^3 gates in an ‘ordinary’ quantum computer.

Schoelkopf Lab

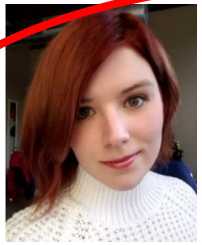


Actual Chemists


B. Lester

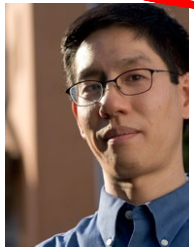

Y. Y. Gao


Y. Zhang


J. Freeze


V. Batista


P. Vaccaro


I. Chuang


L. Jiang


S. Girvin

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& many others!

Devoret Lab