Joint Center for Quantum Information and Computer Science

University of Maryland 1856

Precisely identifying Hamiltonians from dynamical data

Dominik Hangleiter

QLCI RQS Workshop
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Joint work with . . .

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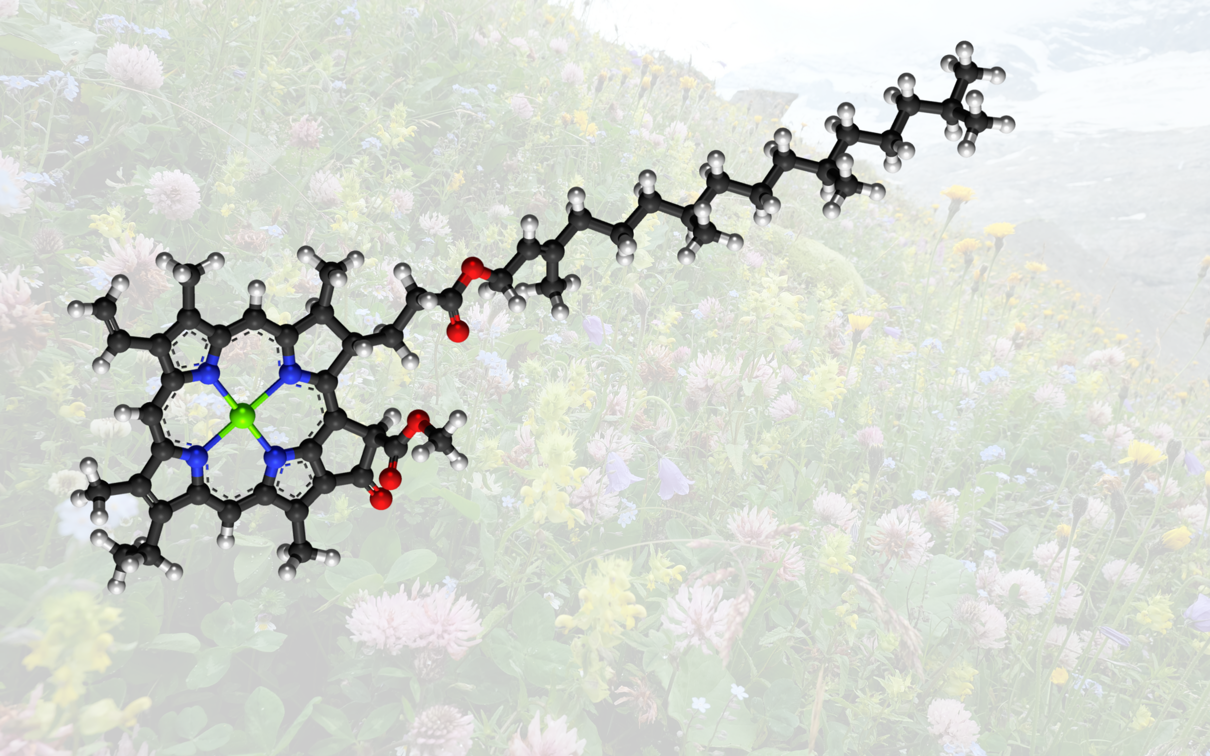
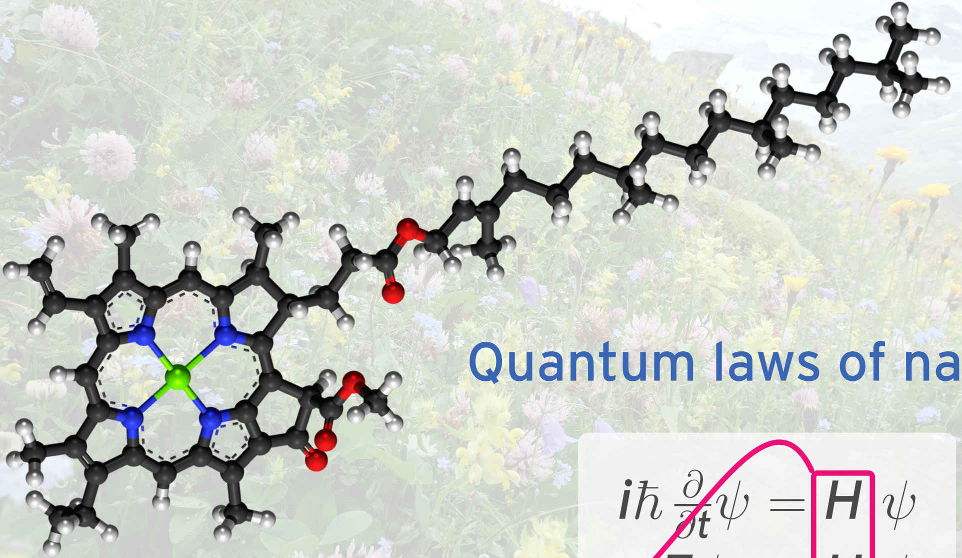




Quantum laws of nature

$$i\hbar \frac{\partial}{\partial t}\psi = H\psi$$
$$E\psi = H\psi$$

THE HAMILTONIAN

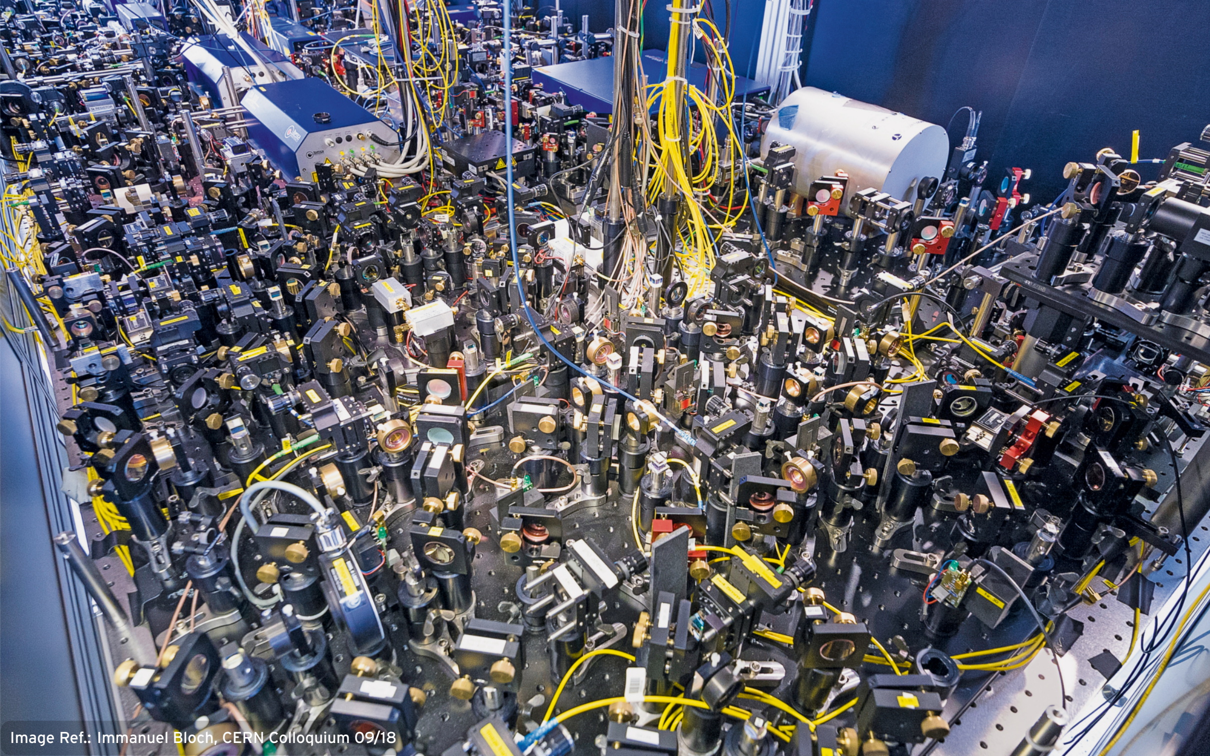
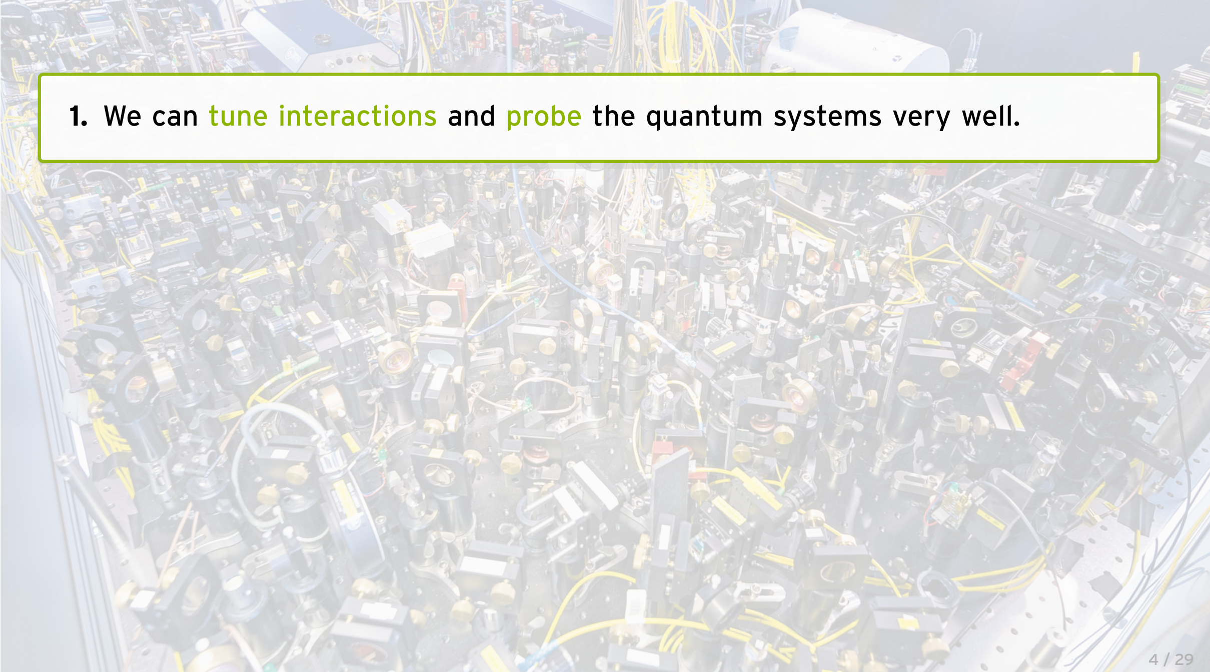


Image Ref.: Immanuel Bloch, CERN Colloquium 09/18

Identifying the Hamiltonian of analog quantum simulators



1. We can tune interactions and probe the quantum systems very well.

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2. Hamiltonian identification is crucial for
   (a) Engineering and making quantum simulators more precise.
   (b) Certifying they are doing the right thing.

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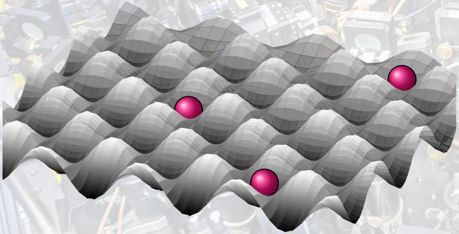
WE NEED IT AND WE CAN DO IT

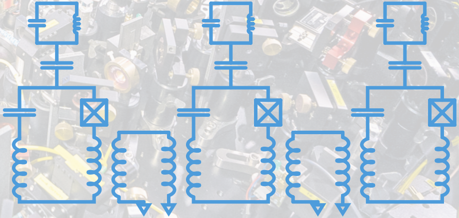
Identifying the Hamiltonian of analog quantum simulators

Bose-Hubbard physics

$$H = -\sum_{\langle i,j \rangle} J_{i,j} \left(b_i^\dagger b_j + b_j^\dagger b_i \right) + \sum_i \mu_i b_i^\dagger b_i + U \sum_i b_i^\dagger b_i^\dagger b_i b_i$$



Cold atoms in optical lattices



Superconducting qubits

Identifying the Hamiltonian of analog quantum simulators

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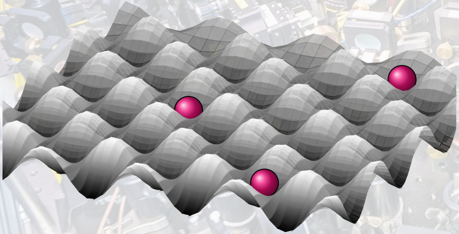

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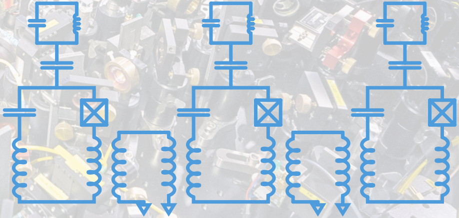

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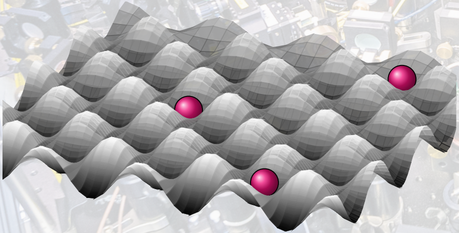

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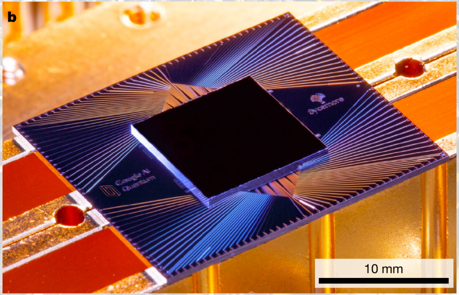

Superconducting qubits

THEORY LAND

Approaches to Hamiltonian identification

Theory

- [Qi and Ranard, 2019] : Local Hamiltonians can generically be identified from two-point correlations on a single eigenstate.
- [Anshu *et al.*, 2020] : Local Hamiltonians can be identified from polynomially many measurements on $\exp(-\beta H)$.
- [Li *et al.*, PRL (2020)] : Generalized conservation of energy fixes the Hamiltonian.
- [Yu *et al.*, 2201.00190] : Pauli-sparse Hamiltonians can be efficiently identified (SPAM-robustly).

Small-scale experiments using dynamical data

- NMR experiments for up to 3 qubits. Dominant error is decoherence. [e.g. Zhang and Sarovar, 2014; Hou *et al.*, 2017, Chen *et al* (2021)]
- Liouvillian tomography [Samach *et al.*, 2105.02338]

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Approaches to Hamiltonian identification

Challenges

- incoherent + state-preparation and measurement (SPAM) errors, AND
- scalable to intermediate-scale devices, AND
- practically applicable

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"How do we identify our Hamiltonian?"

Small-scale experiments using dynamical data

GOAL: Come up with a scheme that works in practice on Sycamore data!

- Liouvillian tomography [Samach *et al.*, 2105.02338]

The Hamiltonian identification problem

Recoverying dynamical laws from dynamical data

Given dynamical data →

$$y_{m,n}(t) = \langle \psi_n | e^{itH} O_m e^{-itH} | \psi_n \rangle$$

→ identify H.

The Hamiltonian identification problem

Recoverying dynamical laws from dynamical data

Given dynamical data ⟶

$$y_{m,n}(t) = \langle \psi_n | e^{itH} O_m e^{-itH} | \psi_n \rangle$$

⟶ identify H.

1. What data O_m, ψ_n are needed and measurable?
2. How can we identify H from those data?

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CHALLENGES

→ Simulating time evolution

→ Nonlinear reconstruction problem due to e^{-itH}

Keeping it simple: Noninteracting Hamiltonians

$$H = \sum_{i,j=1}^{N} h_{i,j} a_i^\dagger a_j, \qquad [a_i, a_j^\dagger] = \delta_{i,j}$$

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$$a_m(t) = \sum_{j=1}^{N} (e^{-ith})_{m,j}\, a_j$$

$$|\psi_n\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle + |0, \ldots, 0, 1, 0, \ldots, 0\rangle \right) = \frac{1}{\sqrt{2}} \left(|0\rangle + |1_n\rangle \right)$$

n^{th}

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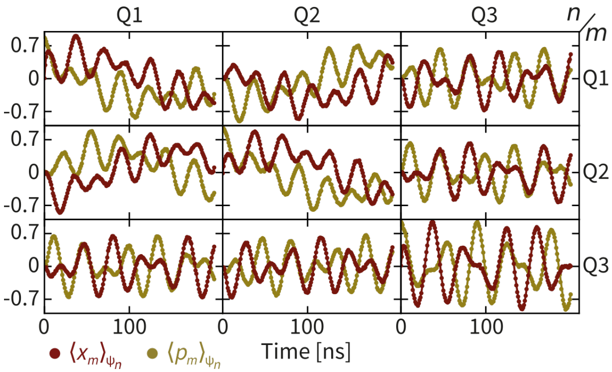
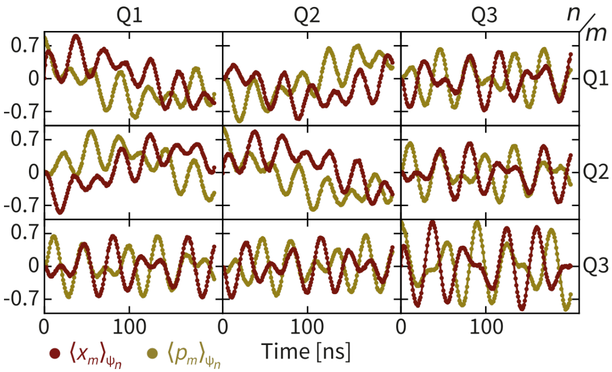
⟶ Measure as $\langle x_m(t)\rangle_{\psi_n} + i\langle p_m(t)\rangle_{\psi_n} = \langle a_m(t)\rangle_{\psi_n}$

Time slices



Q1
Q2
Q3
n
m
0.7
0
-0.7
Q1
Q2
Q3
0
100
Time [ns]
$\langle x_m \rangle_{\psi_n}$
$\langle p_m \rangle_{\psi_n}$

Time slices



Q1
Q2
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n
m
0.7
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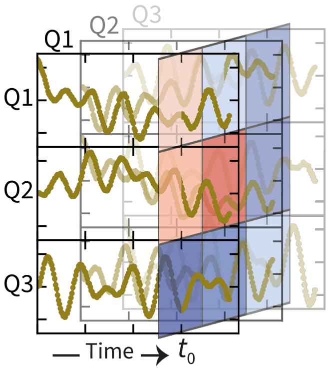
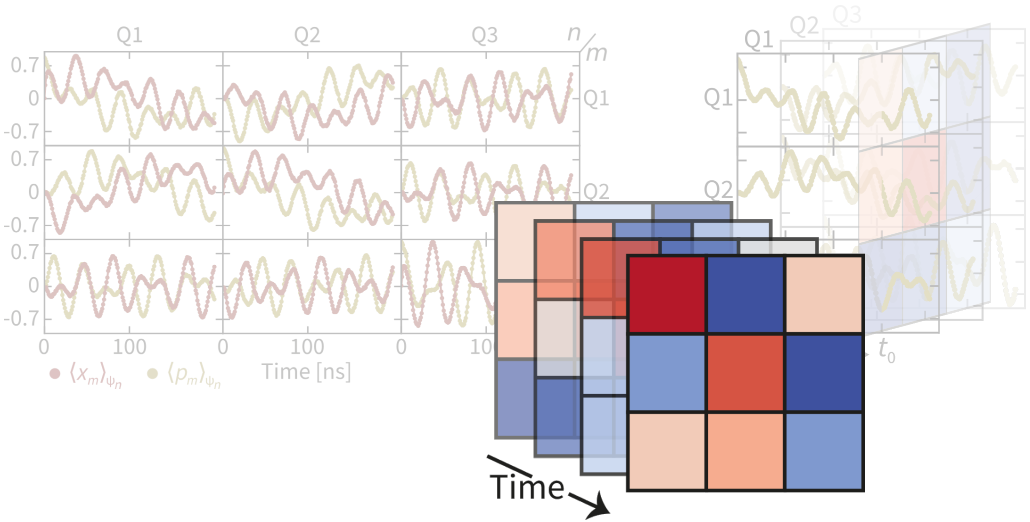
100
0
100
0
100
Time [ns]
$\langle x_m \rangle_{\psi_n}$
$\langle p_m \rangle_{\psi_n}$



Q1
Q2
Q3
Q1
Q2
Q3
Time
t_0

Time slices



Q1
Q2
Q3
n
m
0.7
0
-0.7
Q1
Q2
0
100
Time [ns]
$\langle x_m \rangle_{\psi_n}$
$\langle p_m \rangle_{\psi_n}$
t_0
Time

Identification algorithm

$$e^{-ith} = \sum_{k=1}^{N} e^{-it\lambda_k} \left| \boldsymbol{v}_k \right\rangle \left\langle \boldsymbol{v}_k \right|$$

Identification algorithm

$$e^{-ith} = \sum_{k=1}^{N} e^{-it\lambda_k} |v_k\rangle \langle v_k|$$

1. Extract the eigenfrequencies $\lambda_1, \ldots, \lambda_N$

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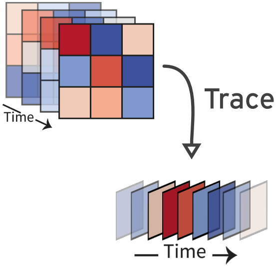
Frequency extraction ła mobile communication: ESPRIT

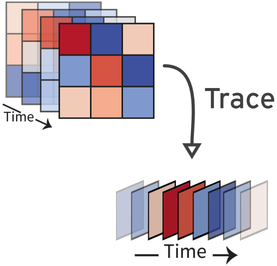
1. Take data at equally spaced times $t_l = l \cdot \Delta t$, $l = 1, \ldots, L$.



2. Prepare data for processing:

$$S[l] = \mathrm{Tr}[e^{-it_l h}] = \sum_{k=1}^{N} e^{-it_l \lambda_k} \longrightarrow \hat{S}[l] = \sum_{k=1}^{N} c_k e^{-i\delta t \lambda_k l} + \eta$$

Frequency extraction ła mobile communication: ESPRIT



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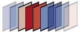
Algorithm ESPRIT(S, n, L)



Input: $S \in \mathbb{C}^L$, $N \in \mathbb{N}$, $M \leq L$.

1: Set $H = \mathrm{Hankel}_M(S)$ $\in \mathbb{C}(M \times L - M + 1)$.

2: Calculate the SVD of $H = (U|U_\perp)\Sigma(V|V_\perp)^\dagger$.

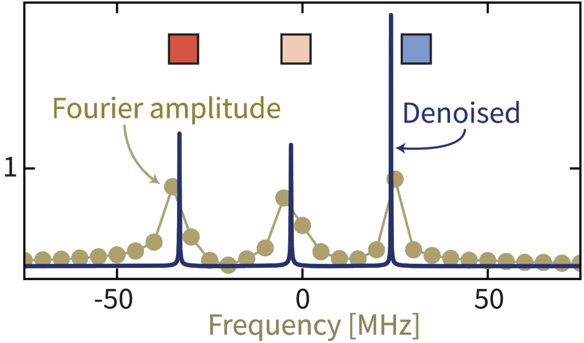
3: Calculate $\Psi = (U^\uparrow)^+ U^\downarrow$, $U^{\uparrow,\downarrow} \in \mathbb{C}(M - 1 \times L)$.

4: Calculate $\mathbf{z} = \mathrm{eigs}(\Psi)$ $\in \mathbb{C}^N$.

Output: $\mathbf{z}$

Li *et al.*, arXiv:1905.03782

ESPRIT in action



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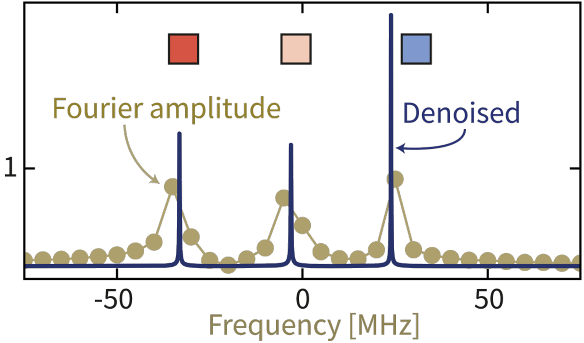
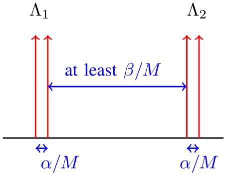


Theory (Li *et al.*, 2019)

For sparse signal $N^2 \leq L$ and
low noise $\|\eta\| \leq \mathrm{SRF}^{-(4|\Lambda|-3)}/L$:

→ $\max_k |\lambda_k - \hat{\lambda}_k| \in O(\mathrm{SRF}^{2|\Lambda|-2}\|\eta\|)$

$\mathrm{SRF} = 1/(L \cdot \min_{i,j} |\lambda_i - \lambda_j|)$



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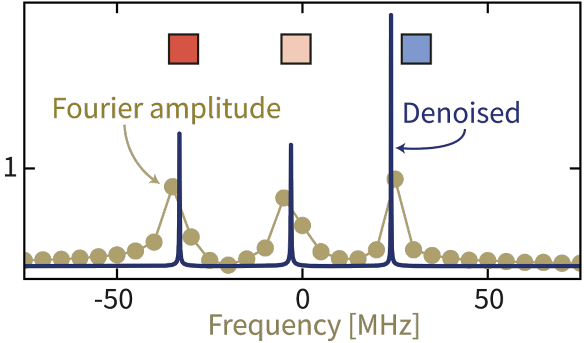

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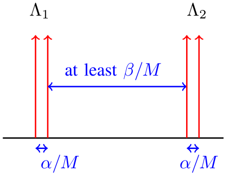

In practice

Roughly $\times$2-4 more accurate than Nyquist resolution $1/(L \cdot \Delta t)$.

Li *et al.*, arXiv:1905.03782

Identification algorithm

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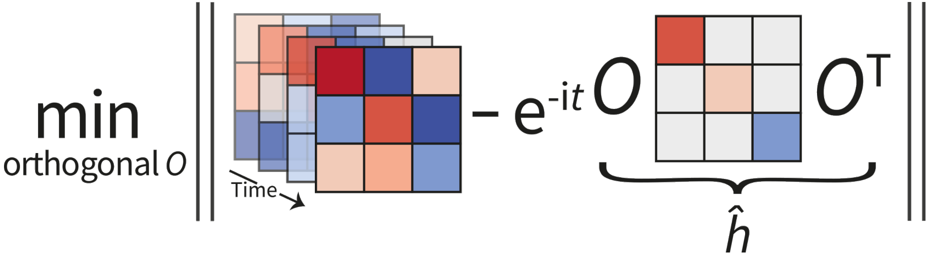
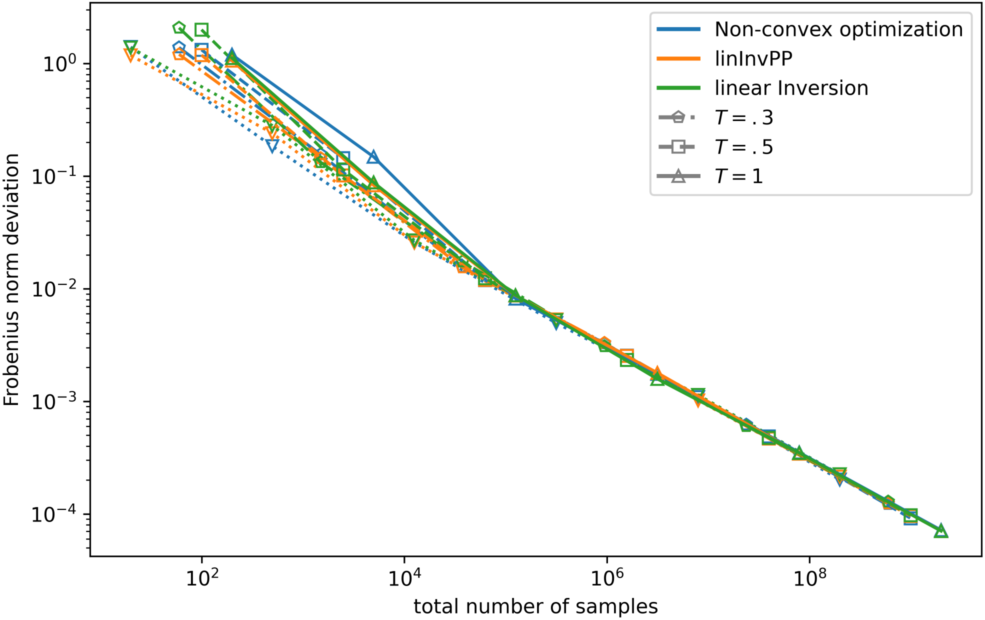
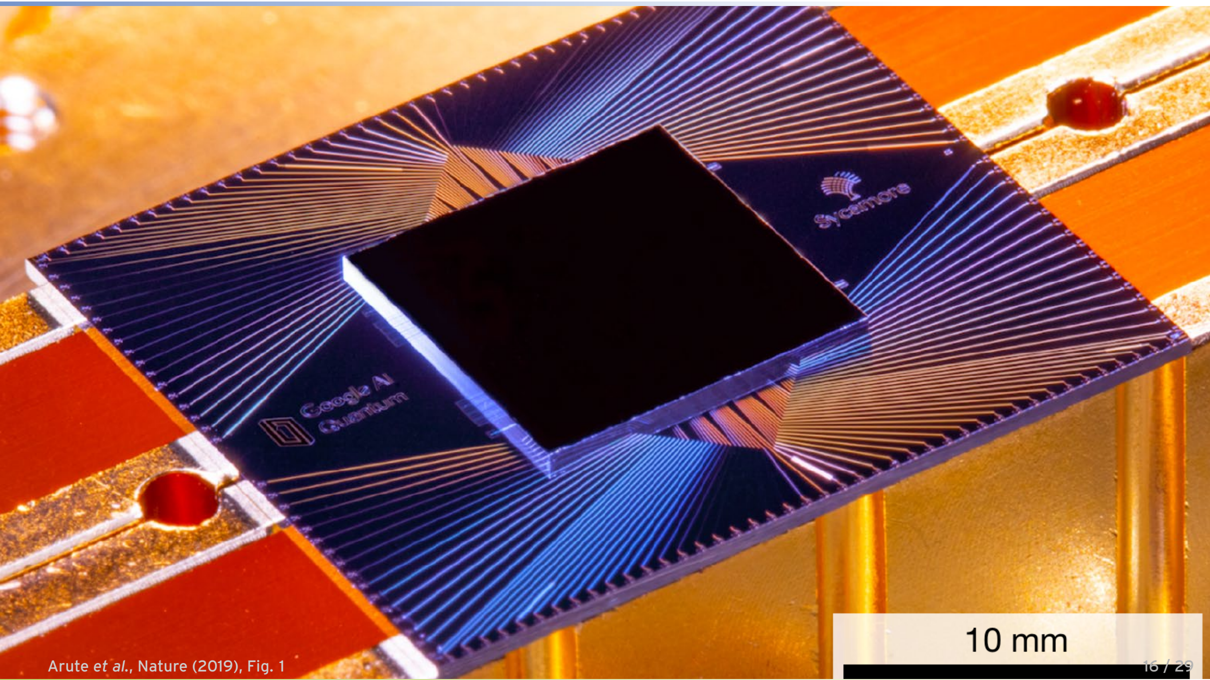


Eigenspace reconstruction



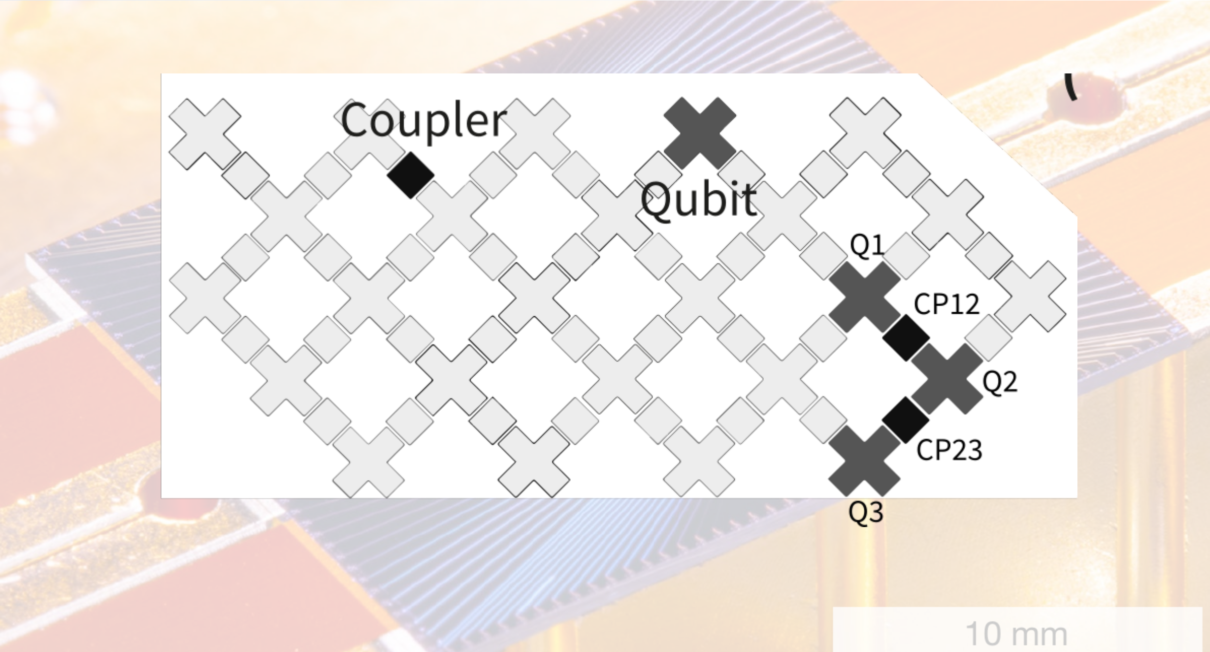
EXPERIMENT

Getting our hands dirty



Arute *et al.*, Nature (2019), Fig. 1

Getting our hands dirty



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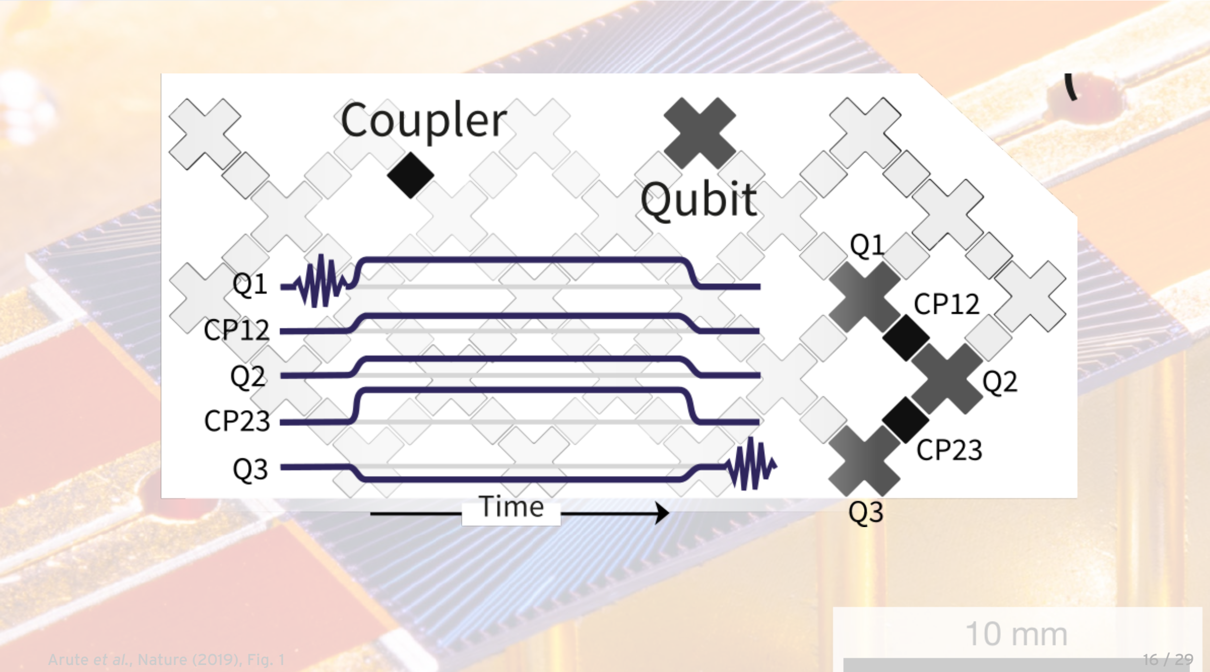

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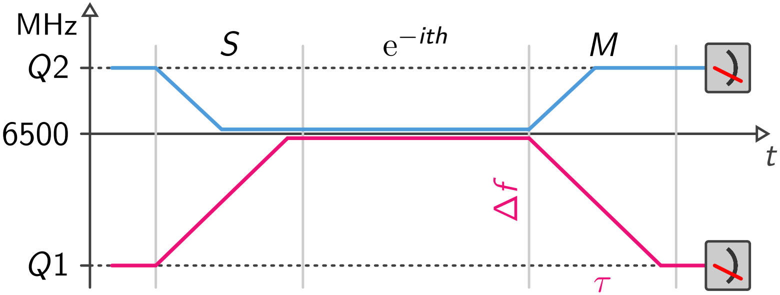
Getting our hands dirty ... and putting the pink glasses back on



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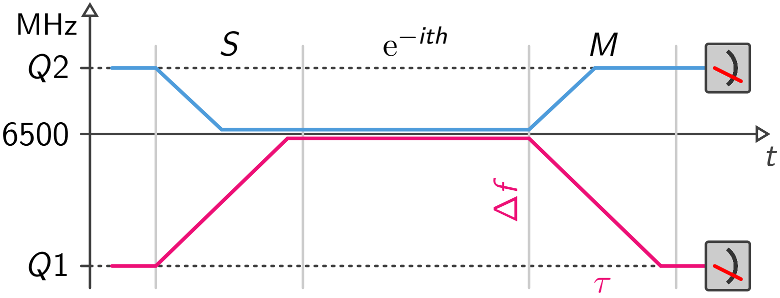
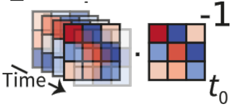


$$y(t) = \frac{1}{2} e^{-ith} \longrightarrow y(t) = \frac{1}{2} M \cdot e^{-ith} \cdot S$$

Getting rid of ramp phases: initial map

$$y(t) = \frac{1}{2} e^{-ith} \cdot S \longrightarrow y^{(t_0)}(t) = \frac{1}{2} y(t) \cdot y(t_0)^{-1}$$



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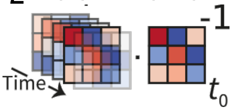

$$\begin{aligned} y^{(l_0)}[l] &= \frac{1}{2} y[l](y[l_0])^{-1} \\ &= \frac{1}{2} e^{-it_l h} S \left(e^{-it_{l_0} h} S\right)^{-1} = \frac{1}{2} e^{-it_l h} S S^{-1} e^{it_{l_0} h} \\ &= \frac{1}{2} e^{-i(t_l - t_{l_0})h} \end{aligned}$$

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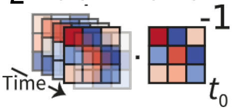

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→ Average over different $y[l_0]$, by concatenating every s data points

$$y_{\text{total},s} = (y^{(0)}, y^{(s)}, y^{(2s)}, \ldots)$$

Getting rid of ramp phases: initial map

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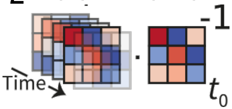


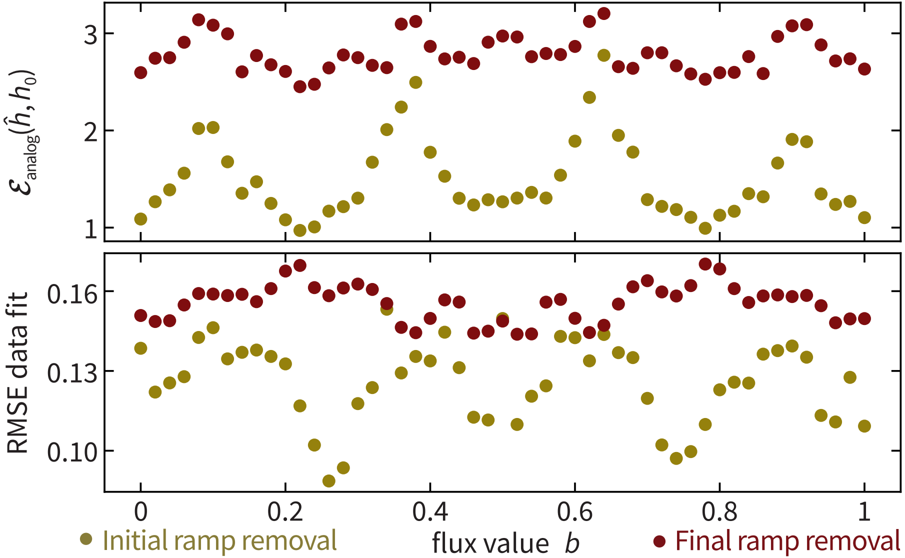
$$\begin{aligned} y^{(l_0)}[l] &= \frac{1}{2} y[l] (y[l_0])^{-1} \\ &= \frac{1}{2} e^{-it_l h} S \left(e^{-it_{l_0} h} S \right)^{-1} = \frac{1}{2} e^{-it_l h} S S^{-1} e^{it_{l_0} h} \\ &= \frac{1}{2} e^{-i(t_l - t_{l_0})h} \end{aligned}$$

→ Average over different $y[l_0]$, by concatenating every s data points

$$y_{\text{total},s} = (y^{(0)}, y^{(s)}, y^{(2s)}, \ldots)$$

Estimate initial map as $\hat{S} = \frac{2}{L} \sum_{l=1}^{L} e^{it_l \hat{h}} y[l]$ given estimate $\hat{h}$ of h.

Removing initial vs. removing final map



Getting rid of ramp phases: final map

$$y^{(t_0)}(t) = \frac{1}{2} M \cdot e^{-ith} \cdot S \longrightarrow y^{(t_0)}(t) = M e^{-i(t-t_0)h} M^{-1}$$

1. Frequencies are unaltered!
2. The eigenbasis of h is constrained to orthogonal

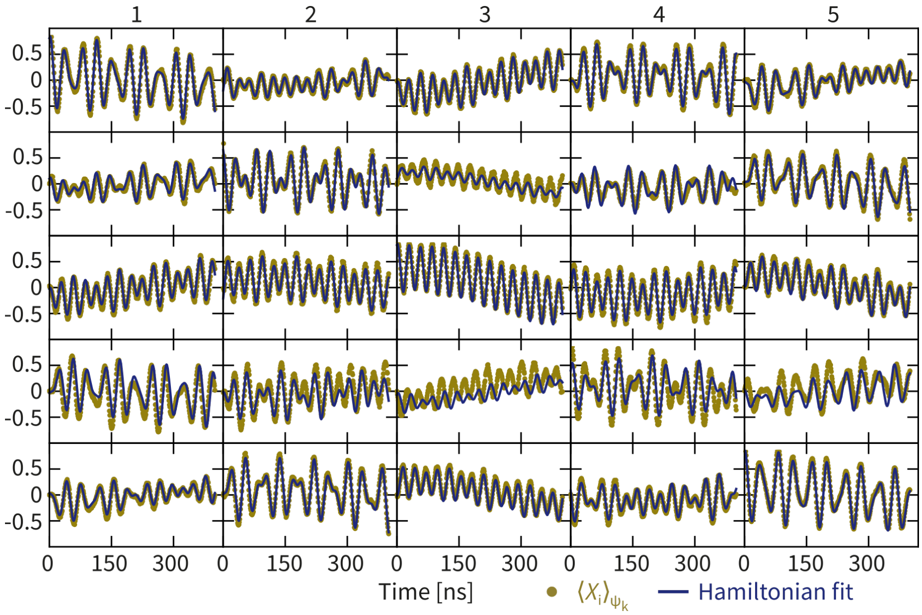
   $\longrightarrow \hat{h} = O_M h O_M^T$ with $O_M = \arg\min_O \|O - M\|_2$

3. For diagonal $M = \mathrm{diag}(e^{i\delta_1}, \ldots, e^{i\delta_N})$: $D_M = \mathrm{diag}(\{+1, -1\}^N)$

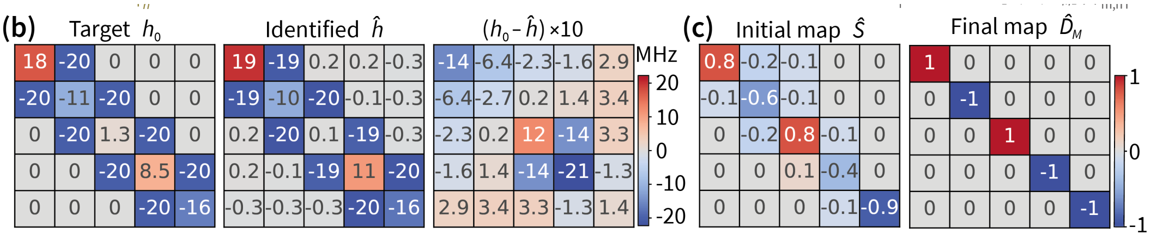
   $\longrightarrow$ We can identify the signs, assuming that Hamiltonian does not deviate by a sign flip in the projectors.

$$\longrightarrow \hat{S} = D_M \hat{S}', \quad \hat{h} = D_M \hat{h}' \hat{D}_M$$

Reconstructing a Hamiltonian



Reconstructing a Hamiltonian



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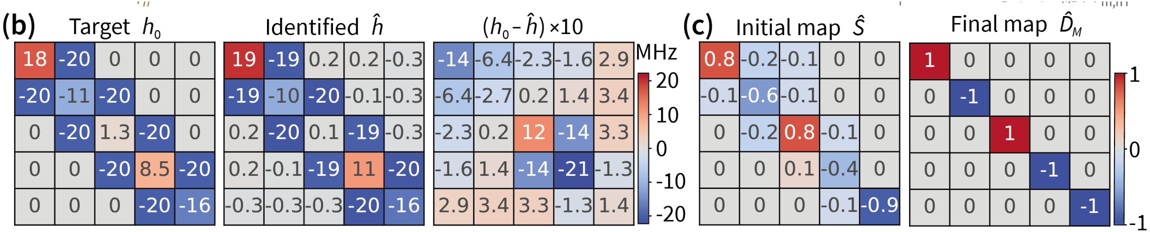
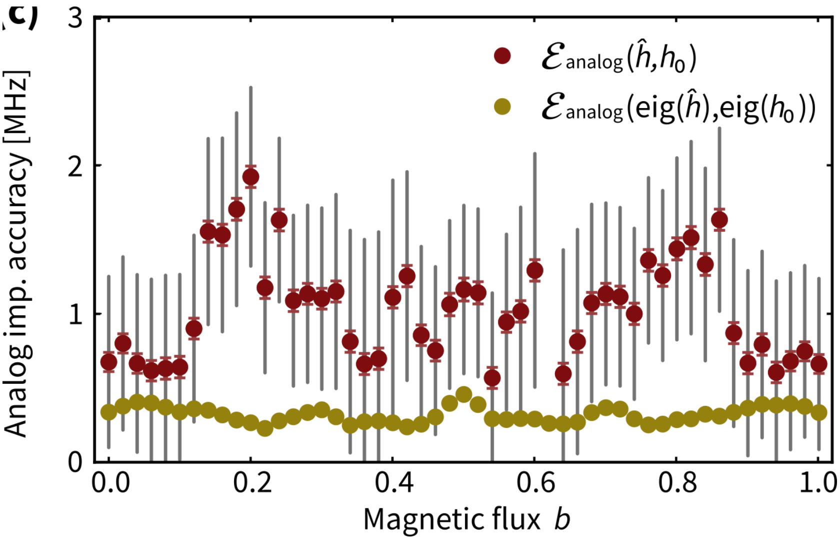
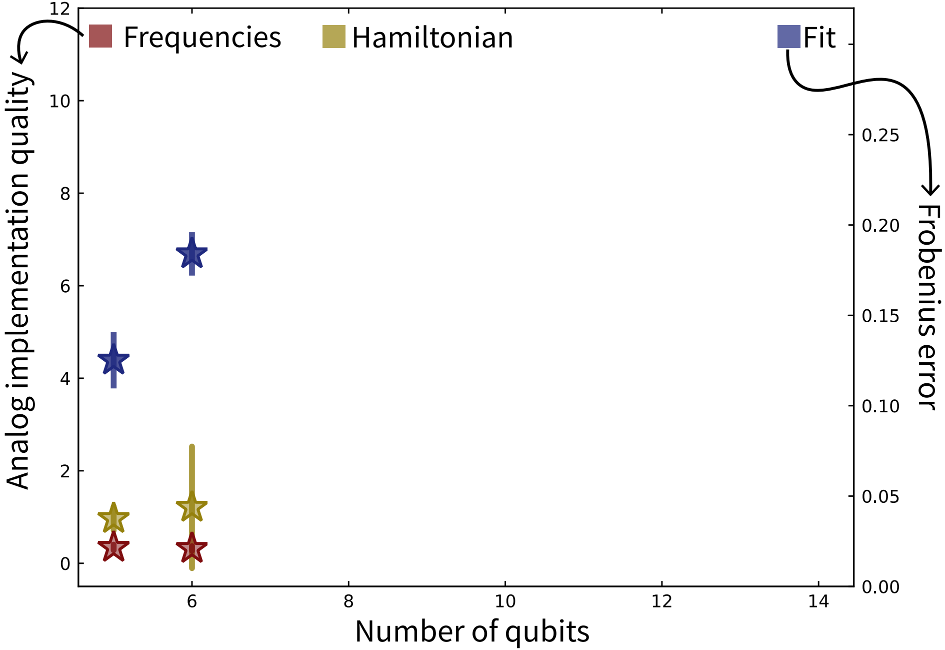


$$\mathcal{E}_{\text{analog}}(\hat{h}, h_0) = \frac{1}{N}\|\hat{h} - h_0\|_2$$

Characterizing the analog performance of an entire chip #1



Characterizing the performance of an entire chip #2



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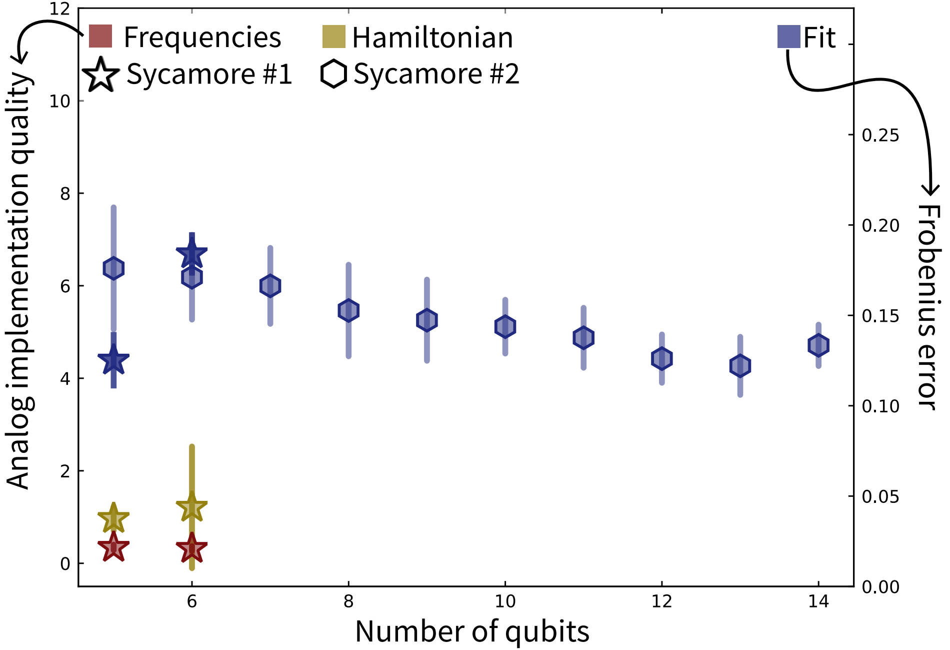

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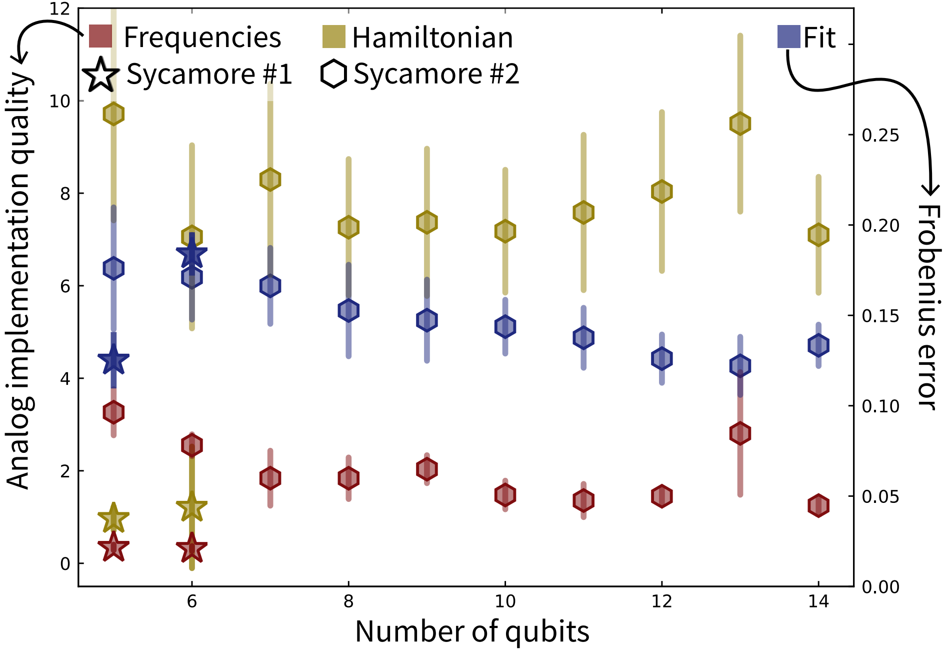
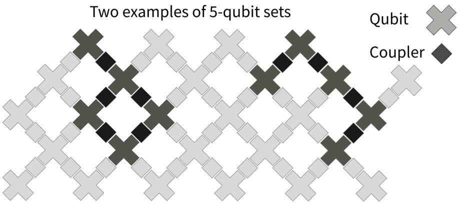
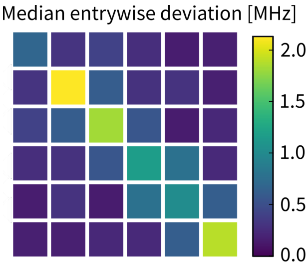


Characterizing the analog performance of an entire chip #3





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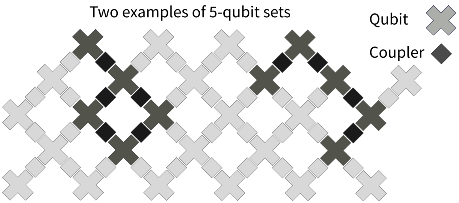

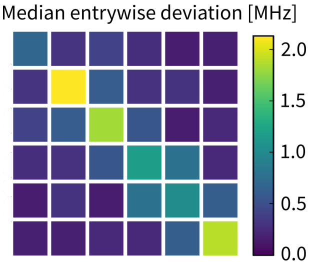

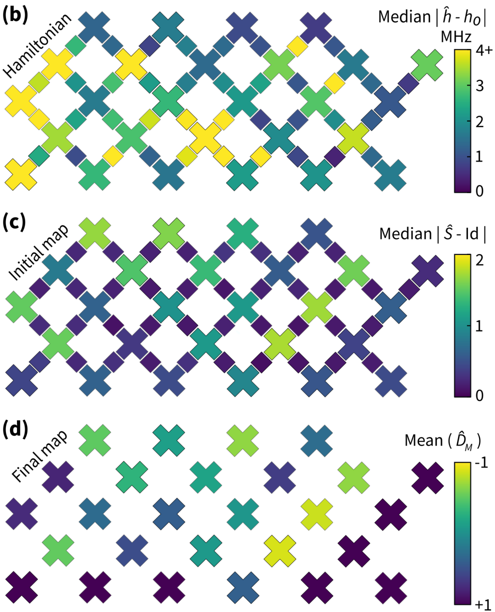

Summary

So how did we solve the Hamiltonian identification problem?

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STRUCTURE, STRUCTURE, STRUCTURE!!

1. **Sparsity** of the frequency spectrum.
2. **Orthogonality** of the eigenbasis.
3. **Sparsity** of the Hamiltonian support.
4. **SPERROR** removal.

Summary

So how did we solve the Hamiltonian identification problem?

→ STRUCTURE, STRUCTURE, STRUCTURE!!

ROBUSTNESS TO NOISE

- → does not respect structure
  - → particle loss
  - → shot noise
  - → diagonal phases

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Outlook #1: Interactions

Two-body interactions ongoing with Jonas Fuksa, Ingo Roth

$$H(h, V) = \sum_{ij} h_{i,j} a_i^\dagger a_j + \sum_{ij,kl} V_{ij,kl} a_i^\dagger a_j^\dagger a_k a_l.$$

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Identification

$$|\psi_{kl}\rangle = \begin{cases} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle_k \otimes |1_l\rangle), & k \neq l \\ \frac{1}{\sqrt{2}}(|0\rangle + |2\rangle_k), & k = l \end{cases}$$

$$\langle a_m a_n \rangle_{kl}(t) = \frac{1}{2} \exp\{-i(h \otimes 1 + 1 \otimes h + 2V)\}_{mn,kl}$$

- Need to measure correlators $\langle x_m x_n \rangle_{kl}$, $\langle x_m p_n \rangle_{kl}$, $\langle p_m x_n \rangle_{kl}$, $\langle p_m p_n \rangle_{kl}$.
- V symmetric and diagonalizable by $O \otimes O$.

Outlook #2: Specific systems

Solid-state simulators ongoing with Noah Berthusen, Ingo Roth, Michael Gullans

- Measure n_i
- Initial states $|1\rangle_k + |1\rangle_l$ and $|1\rangle_k + i|1\rangle_l$

→ $y_{i,kl} = U(t)_{ik} U(t)^{\dagger}_{li}$

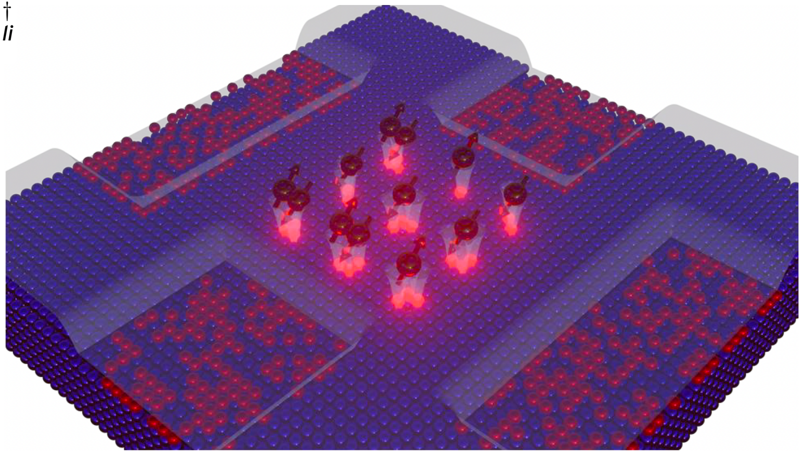

Image Ref.: Wang, Khatami, *et al.* 2110.08982

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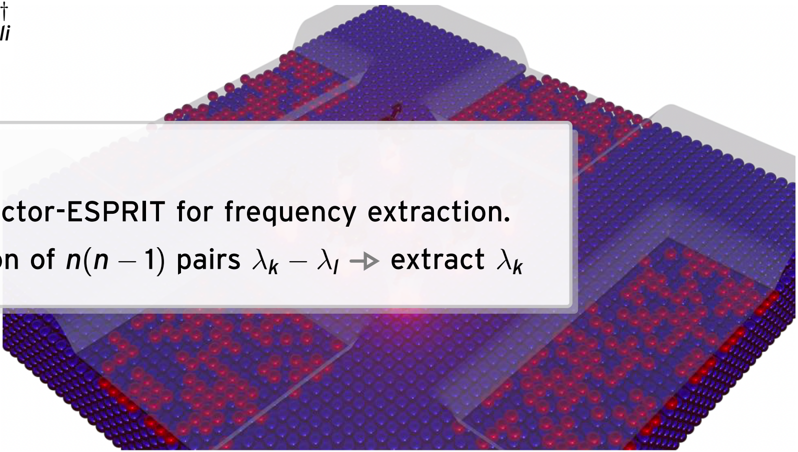

Challenges

- Requires vector-ESPRIT for frequency extraction.
- Identification of $n(n-1)$ pairs $\lambda_k - \lambda_l \rightarrow$ extract λ_k

Image Ref.: Wang, Khatami, *et al.* 2110.08982

Outlook #3: Improving scalability

- **System size scaling**
  Frequency resolution scales as $1/T$, but the number of detected frequencies scales as $\mathrm{poly}(N)$
  ⟶ $T \in \mathrm{poly}(N)$ ...
- **Data type**
  Scalar version of ESPRIT does not work on photon-number data.

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  $\longrightarrow$ $T \in \mathrm{poly}(N)$ ...
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Vectorizing ESPRIT — with Jonas Fuksa and Ingo Roth

- Recover frequencies jointly from the entries of

$$U(t) = \sum_{\lambda,i,j} e^{-i\lambda t} \underbrace{\langle i|\lambda\rangle\langle\lambda|j\rangle}_{a_{\lambda,i,j}} |i\rangle\langle j|$$

Outlook #4: Theory questions

Recovery guarantees for

- variants of ESPRIT
- conjugate-gradient method

Application to spin systems

→ hopping + single excitations

Measurement errors

[YSHY22] ← [HYF21]

+ RB of the measurements

- short-time evolution

More

→ ??????????

Comparison to other methods

→ Generalized energy conservation [LZH20]

[YSHY22] Yu *et al.*, 2201.00190 [HYF21] PRX Quantum (2021) [LZH20] Lie, Zhu, Hsieh, PRL (2020)

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Frequency extraction à la mobile communication: ESPRIT

Algorithm ESPRIT(S, n, L)

Input: $S \in \mathbb{C}^L$, $N \in \mathbb{N}$, $M \leq L$.

1: Set $H = \text{Hankel}_M(S)$.
2: Calculate the SVD of $H = (U|U_\perp)\Sigma(V|V_\perp)^\dagger$.
3: Calculate $\Psi = (U^\uparrow)^+ U^\downarrow$.
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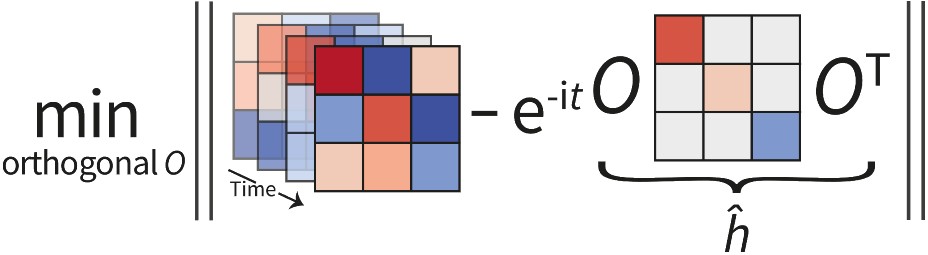
Eigenspace reconstruction



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$$\min_{\{|v_k\rangle\}} \sum_{l=1}^{L} \left\| y[l] - \sum_{k=1}^{N} e^{-i\lambda_k t_l} |v_k\rangle\langle v_k| \right\|_2^2$$

subject to

1. $\langle v_m | v_n \rangle = \delta_{m,n}$
2. $\left(\sum_k \lambda_k |v_k\rangle\langle v_k| \right)_{\overline{\Omega}} = 0$
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Solution:

Algorithm Conjugate gradient descent

Input: Objective function $f : O(N) \rightarrow \mathbb{R}$

1: Calculate Euclidean gradient $E_k = \nabla f(Q_k)$

2: Calculate Riemannian gradient $R_k(E_k, Q_k)$.

3: Parallel transport R_{k-1} to Q_k and calculate conjugate search direction $H_k(R_k, \hat{R}_{k-1})$.

4: Perform line search with H_k to obtain t_k.

5: Set $Q_{k+1} = \exp(H_k t_k) Q_k$.

Output: Q_{final}