Quantifying expressibility of parameterized quantum circuits for variational quantum algorithms

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DOE CSGF Annual Program Review

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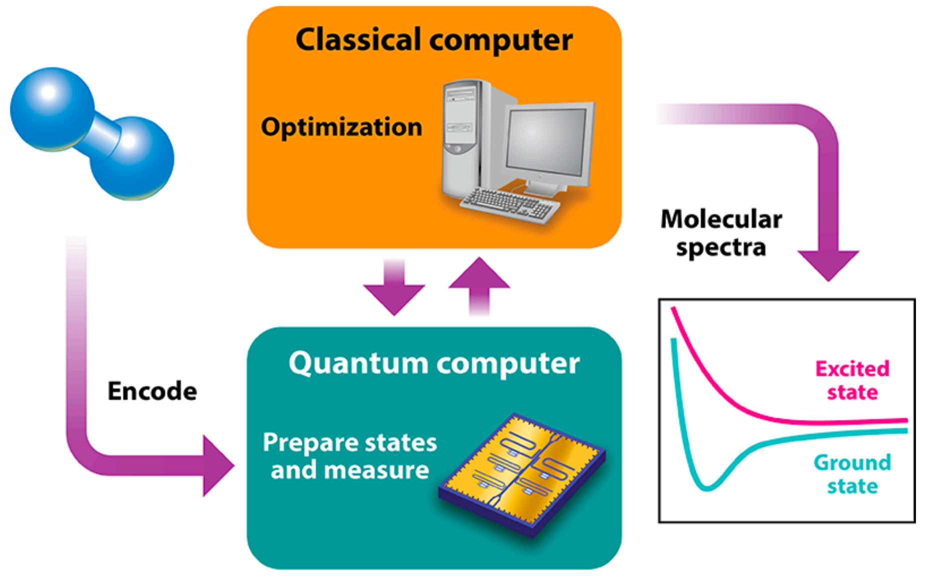
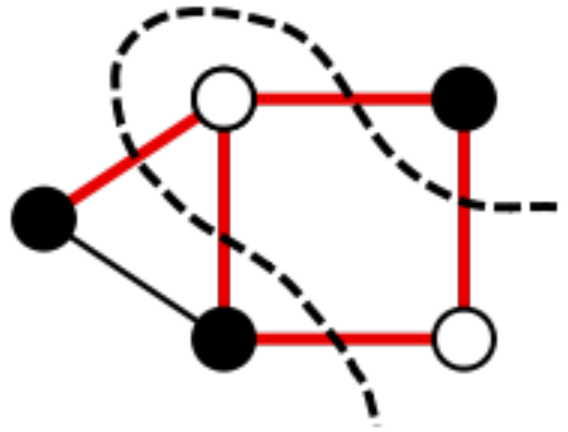
Variational quantum algorithms

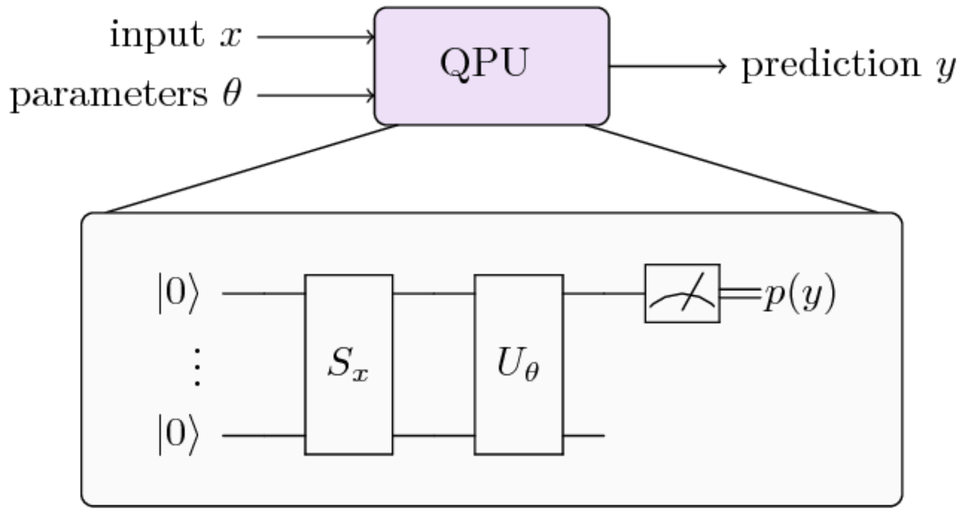
- Near-term quantum computers: ~100 qubits and ~1000 operations



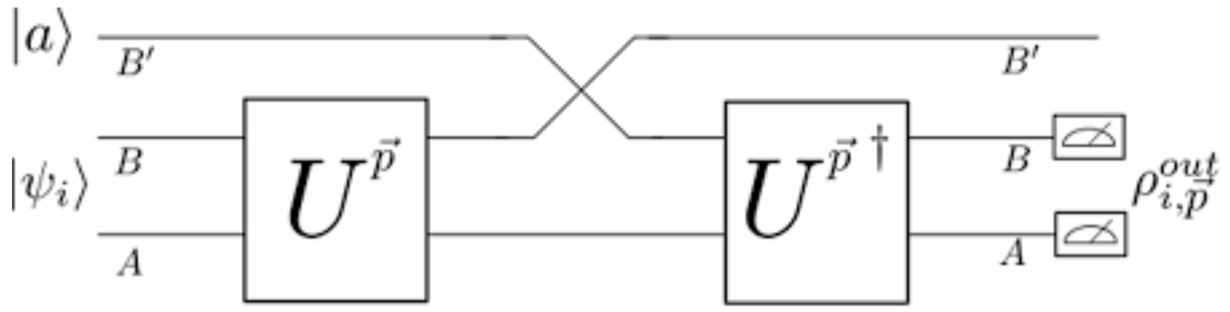
Variational quantum eigensolver (VQE) [1]



Quantum approximate optimization algorithm (QAOA) [2]



Data classification [4, 5]

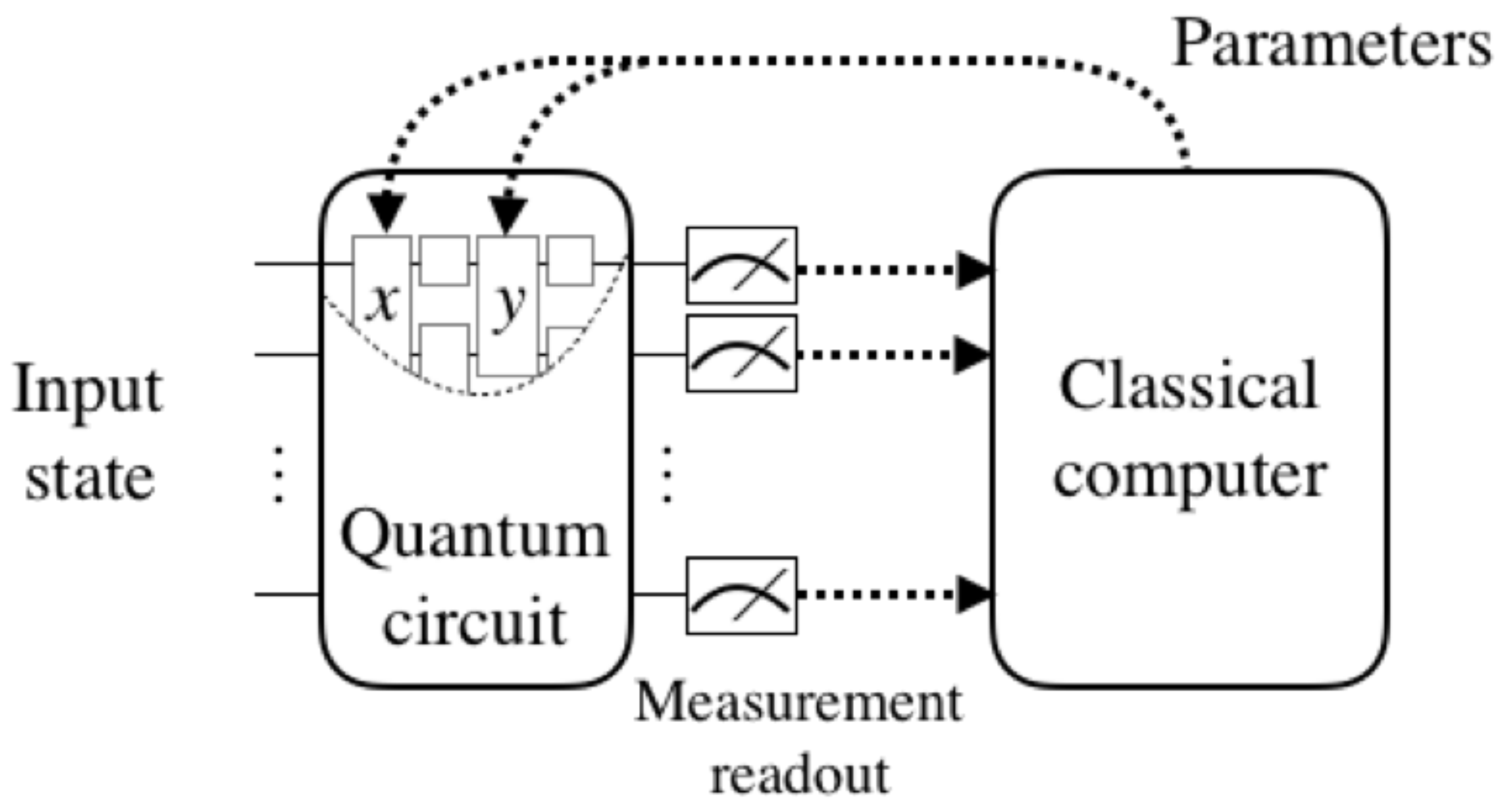


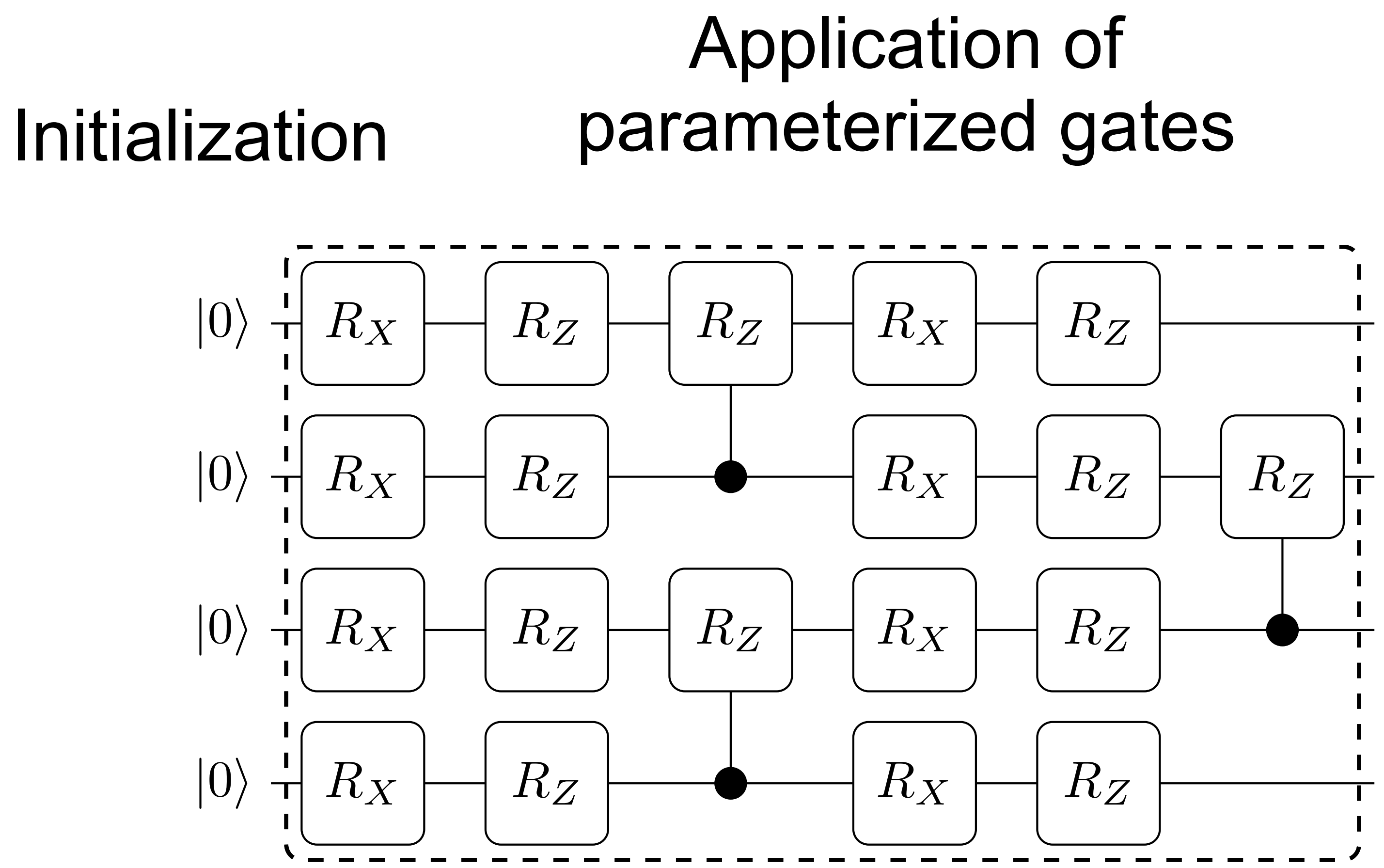
Quantum autoencoder [3]

… and more!
(e.g. generative modeling, variational factoring)

[1] Peruzzo, Alberto, et al. *Nature Commun.* 5 (2014).
[2] Farhi, Edward, et al. arxiv:1411.4028 (2014).
[3] Romero, Jonathan, et al. *Quantum Sci. Technol.* 2 045001 (2017).
[4] Schuld, Maria, et al. arxiv:1804.00633 (2018).
[5] Havlicek, Vojtech, et al. *Nature* 567 (2019).

A common ingredient:
Parameterized quantum circuits (PQCs)





$$R_X(\theta) = \begin{bmatrix} \cos\frac{\theta}{2} & -i\,\sin\frac{\theta}{2} \\ -i\,\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$

$$R_Z(\theta) = \begin{bmatrix} \mathrm{e}^{-i\theta/2} & 0 \\ 0 & \mathrm{e}^{i\theta/2} \end{bmatrix}$$

- **Point-of-contact** for quantum and classical resources
- Crucial to algorithm performance (e.g. VQE)
- What makes a parameterized quantum circuit “good” or “effective?”

Image: courtesy of Yudong Cao

Effective parameterized quantum circuits

What makes an effective PQC?

A difficult question!

1. Can we distinguish/compare among circuit structures?
2. Can we rule out PQCs with limited capabilities?
3. What is a good circuit choice for a particular application?

Effective parameterized quantum circuits

What makes an effective PQC?

A difficult question!

1. **Can we distinguish/compare among circuit structures?**
2. **Can we rule out PQCs with limited capabilities?**
3. What is a good circuit choice for a particular application?

Approach:

Can we develop easily-computable and problem-independent *descriptors* that can help characterize and distinguish among PQCs?

Expressibility

Expressibility: How well can a PQC generate states from the Hilbert space?

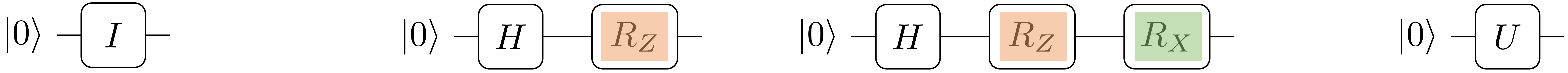
Low expressibility | High expressibility

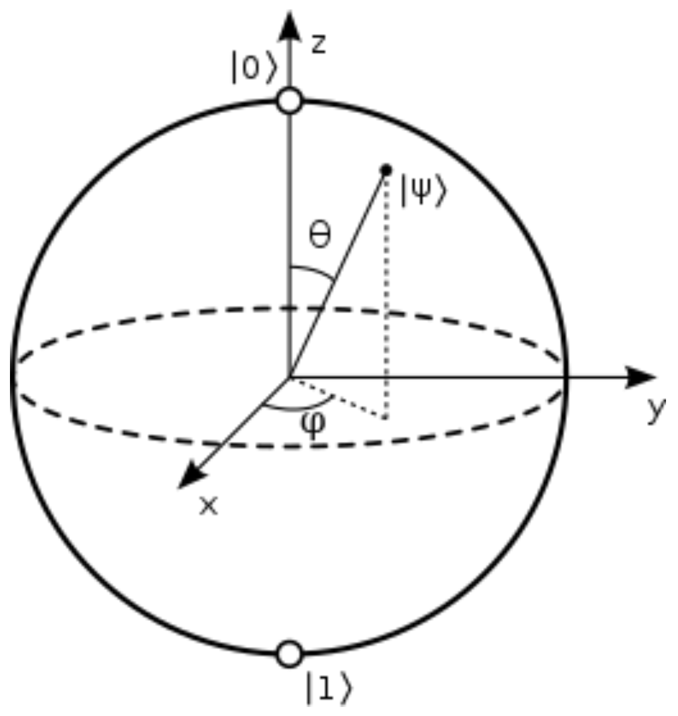
Expressibility demo

Expressibility: How well can a PQC generate states from the Hilbert space?

Low expressibility ⟷ High expressibility

Idle circuit | Circuit A | Circuit B | Arbitrary unitary





How much “coverage” on the Bloch sphere?

Expressibility demo

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Low expressibility ⟷ High expressibility

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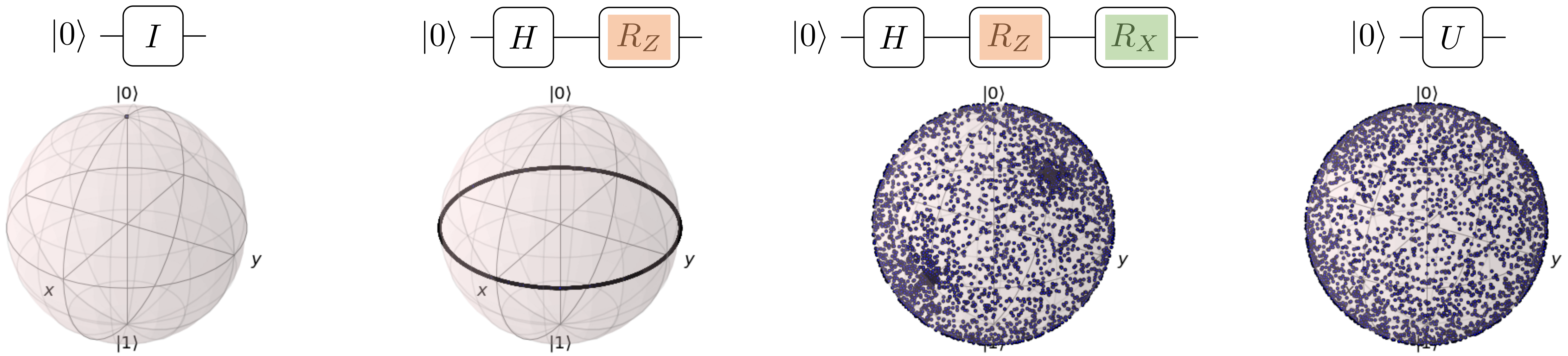
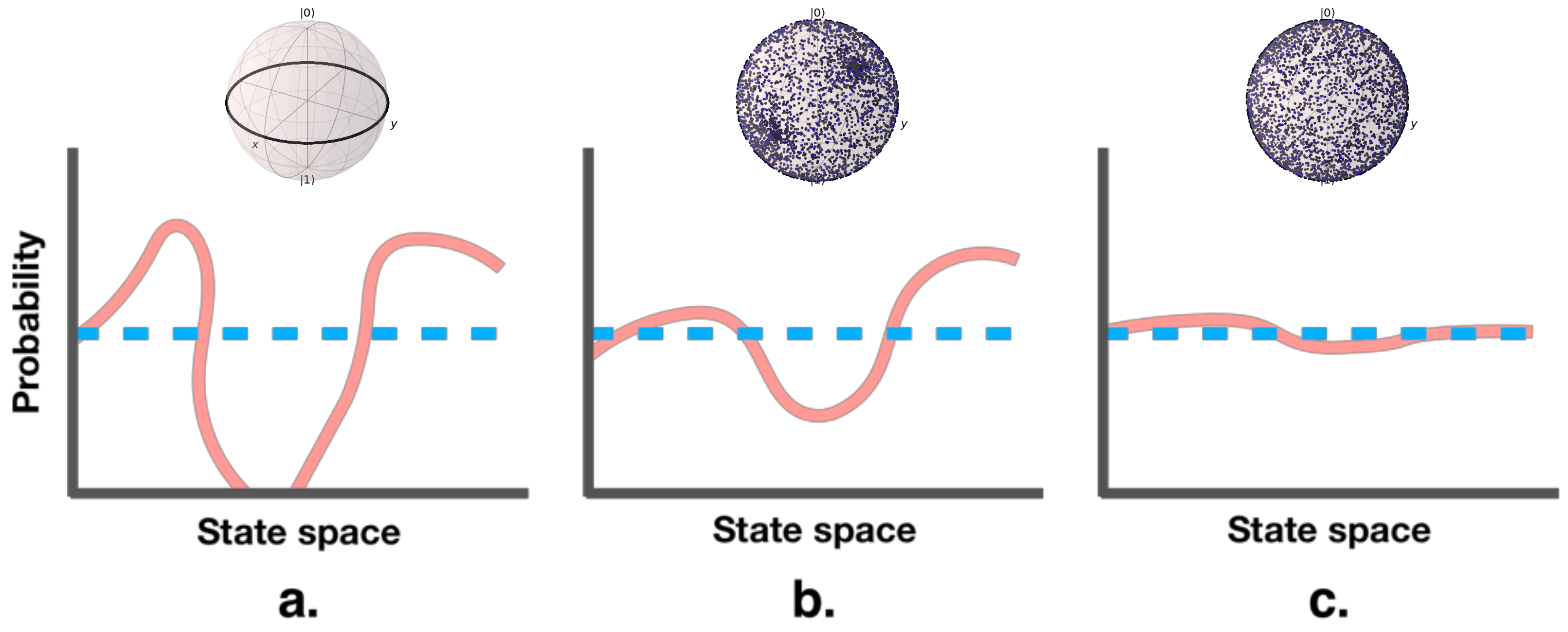


Can we quantify this?

1000 state samples

Quantifying expressibility

- **Proposal:** compare the distribution of states generated by PQC with the (expressive) uniform distribution of states, i.e. Haar random states.



- Compute deviation from the Haar integral (comparing statistical moments)

$$A = \int_{\text{Haar}} (|\psi\rangle\langle\psi|)^{\otimes t} d\psi - \int_{\Theta} (|\psi_\theta\rangle\langle\psi_\theta|)^{\otimes t} \, d\theta \qquad |\psi_\theta\rangle = U(\theta)\,|0\rangle^{\otimes n}$$

Compute the Hilbert-Schmidt norm of A.

Quantifying expressibility

- Can express terms in $\|A\|_{\mathrm{HS}}^2$ to *frame potentials* (“probes of randomness” [1]):

$$\|A\|_{\mathrm{HS}}^2 = -\mathcal{F}_{\mathrm{Haar}}^{(t)} + \mathcal{F}^{(t)}$$

$$\mathcal{F}^{(t)} = \int_{\boldsymbol{\Theta}} \int_{\boldsymbol{\Phi}} |\langle \psi_\theta | \psi_\phi \rangle|^{2t} \, d\theta \, d\phi$$

- Property: The *t*-th frame potential is minimized *if and only if* the ensemble is a state *t*-design.

- Interpretation: *t*-th frame potentials = *t*-th moment of **distribution of fidelities**

$$\mathbb{E}[X^t] = \int_{\Theta} \int_{\Phi} |\langle \psi_\theta | \psi_\phi \rangle|^{2t} \, d\theta \, d\phi, \quad \text{where } X = \boxed{|\langle \psi_\theta | \psi_\phi \rangle|^2}$$

Comparing moments?

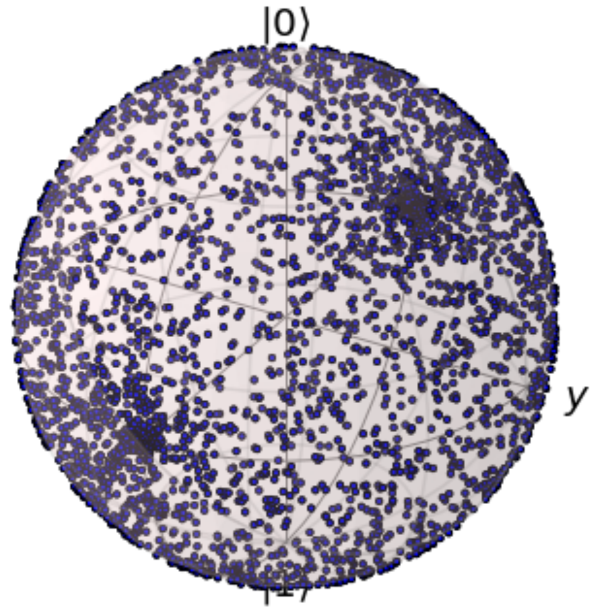
[1] Roberts, Daniel A, et al. *High Energ. Phys*, (2017).

Quantifying expressibility using classical simulations

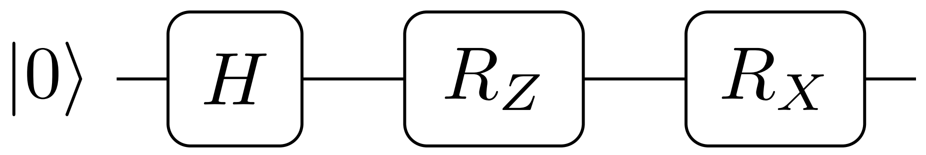
- In practice:
  1.) Select a circuit parameterized by $\boldsymbol{\theta}$
  2.) Uniformly sample pairs of parameters $\boldsymbol{\theta}_i$ and $\boldsymbol{\theta}_j$ and obtain their corresponding states
  3.) Compute the fidelities between the two pure states
  4.) Repeat to collect *M* samples of fidelities

- Compute **KL divergence** between distributions of state fidelities, *F* (sampled vs. Haar)

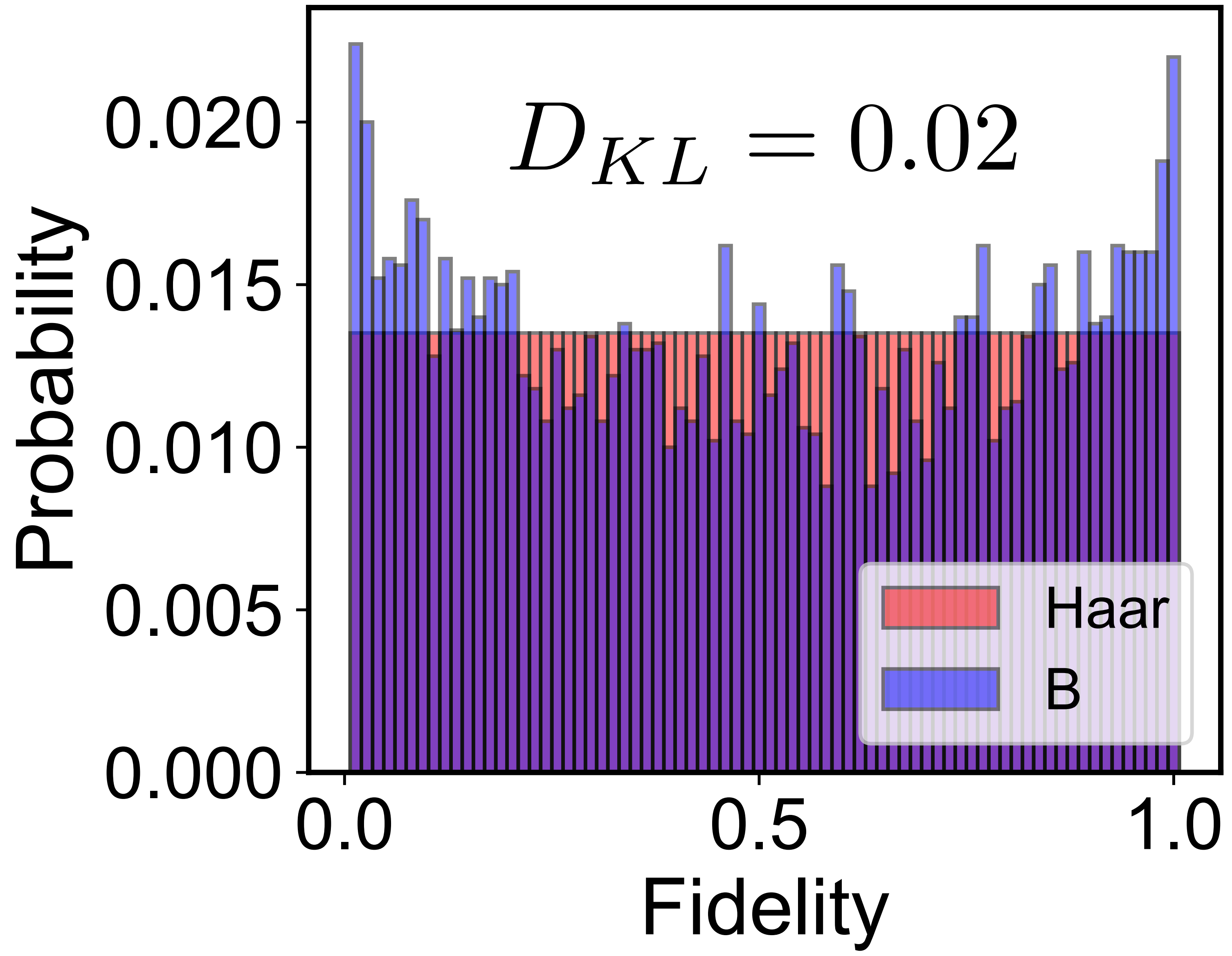
$$P(F) = (d-1)(1-F)^{d-2}$$ [1]



Circuit B



$\boldsymbol{\theta} = [\theta_z, \theta_x]$

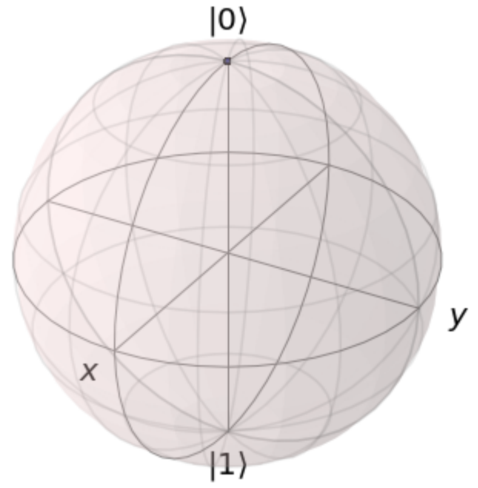


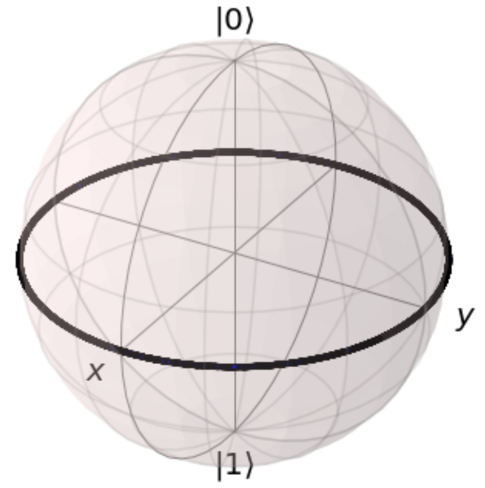
[1] Zyczkowski, Karol, et al. *Phys. Rev. A*, (2005).

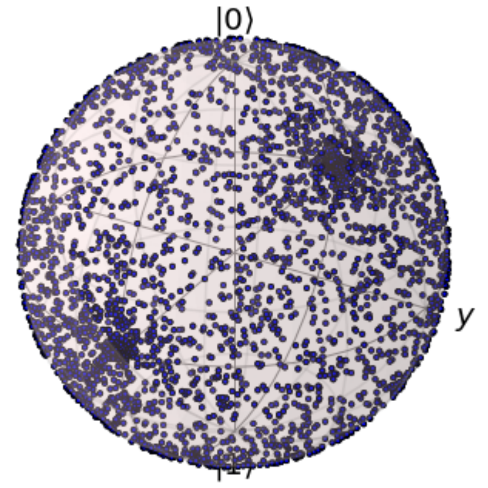
Back to demo: KL divergence

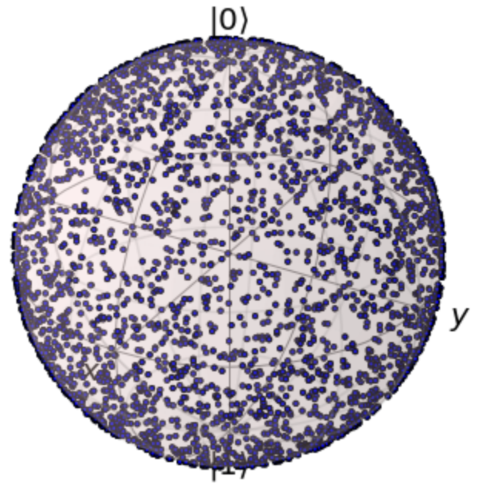
Low expressibility ⟷ High expressibility

Idle circuit	Circuit A	Circuit B	Uniformly sampled unitary
$\|0\rangle - I -$	$\|0\rangle - H - R_Z -$	$\|0\rangle - H - R_Z - R_X -$	$\|0\rangle - U -$

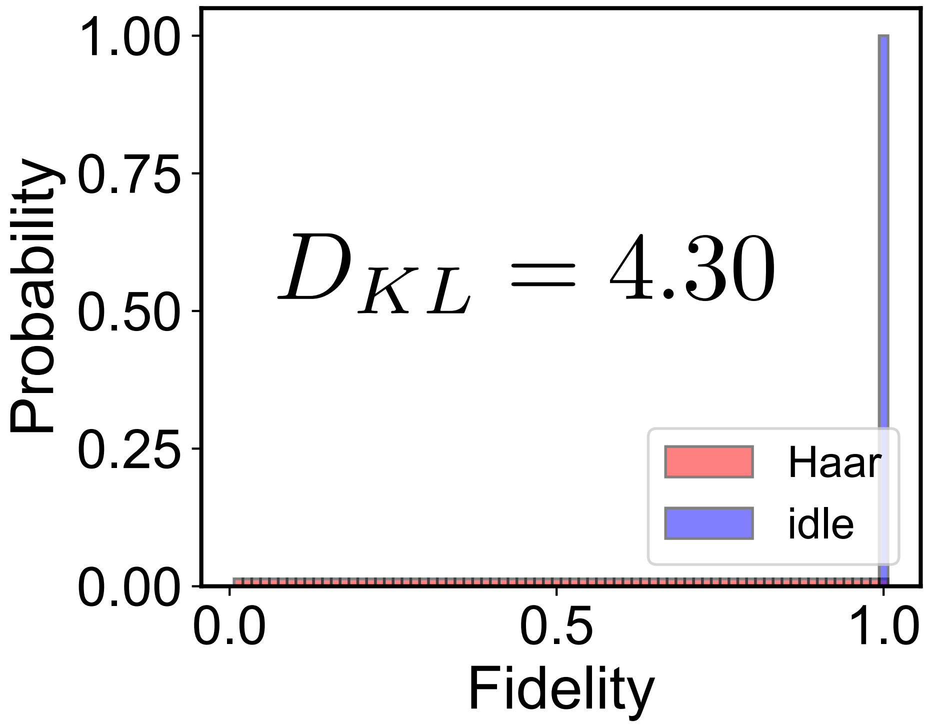


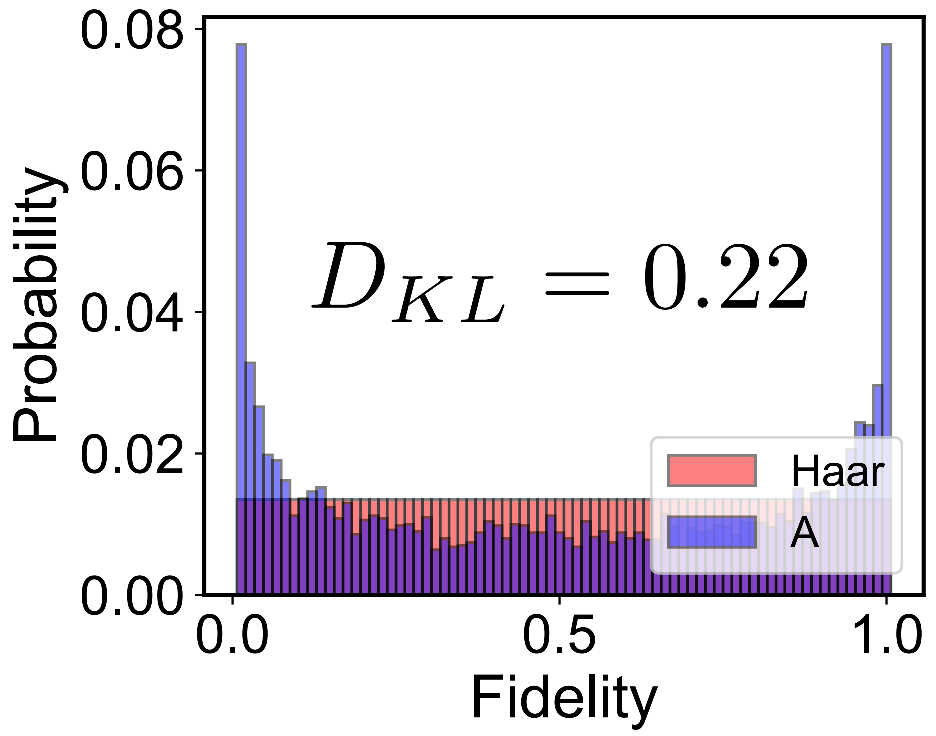


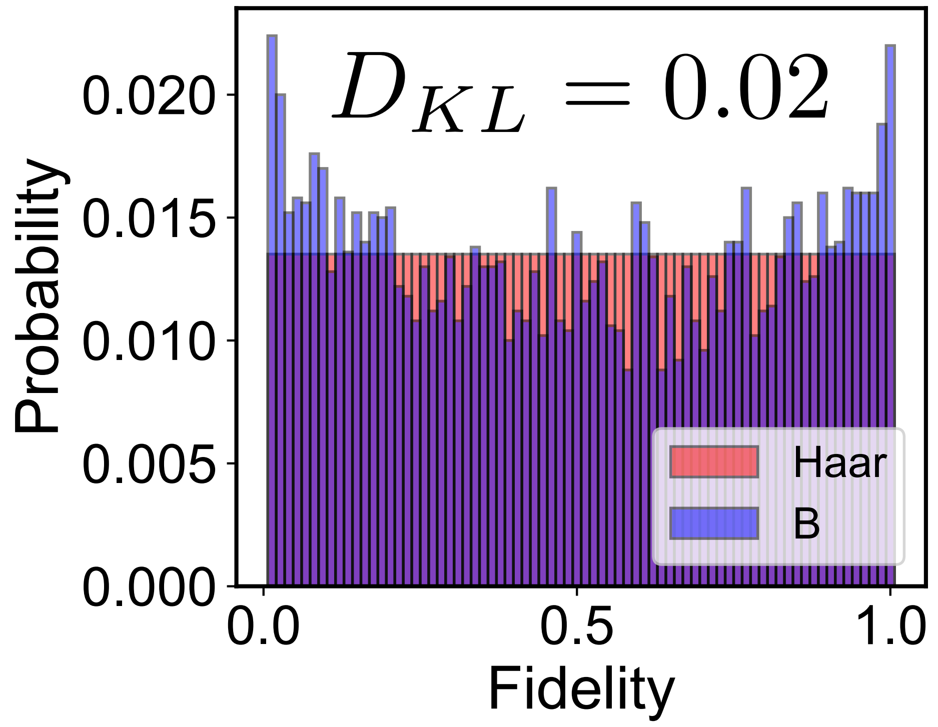


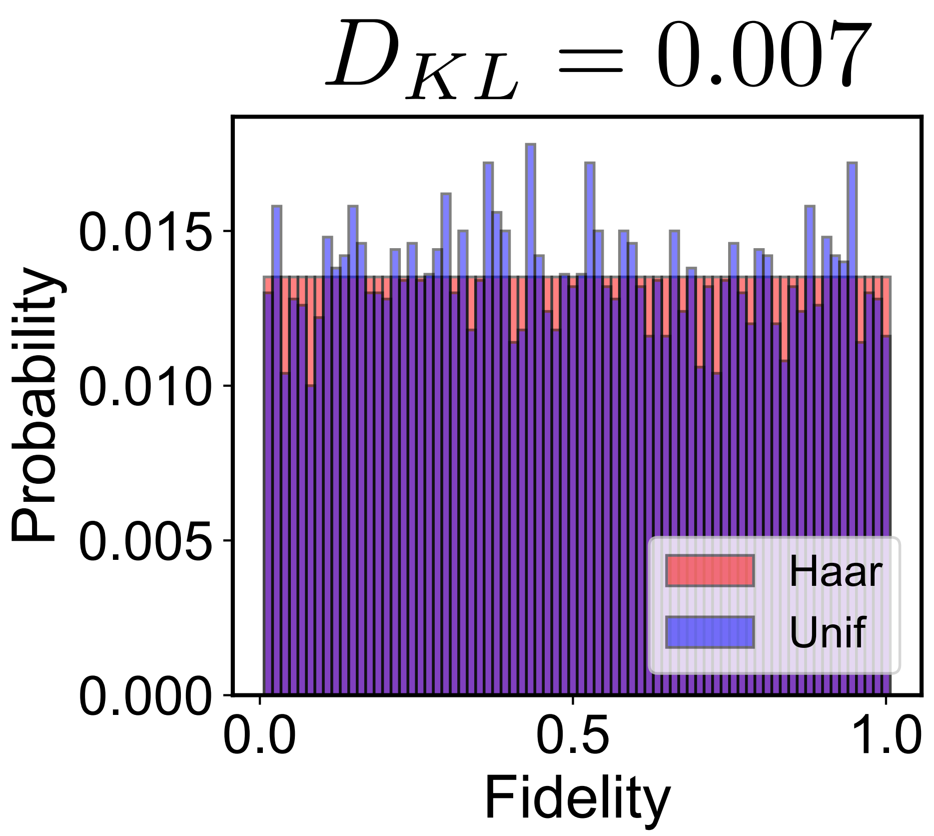


Smaller KL divergence ⟶ **closer** to Haar



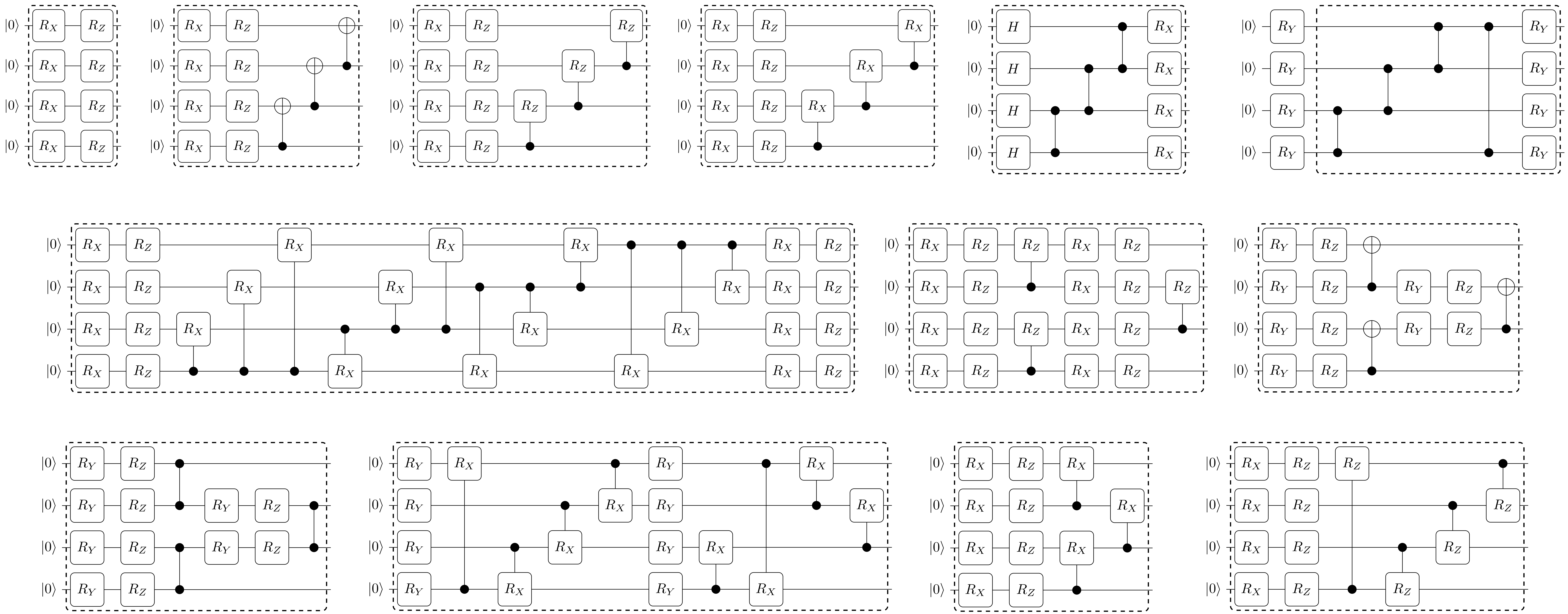






75 bins 5000 samples

Test circuits (multi-layer circuit designs)



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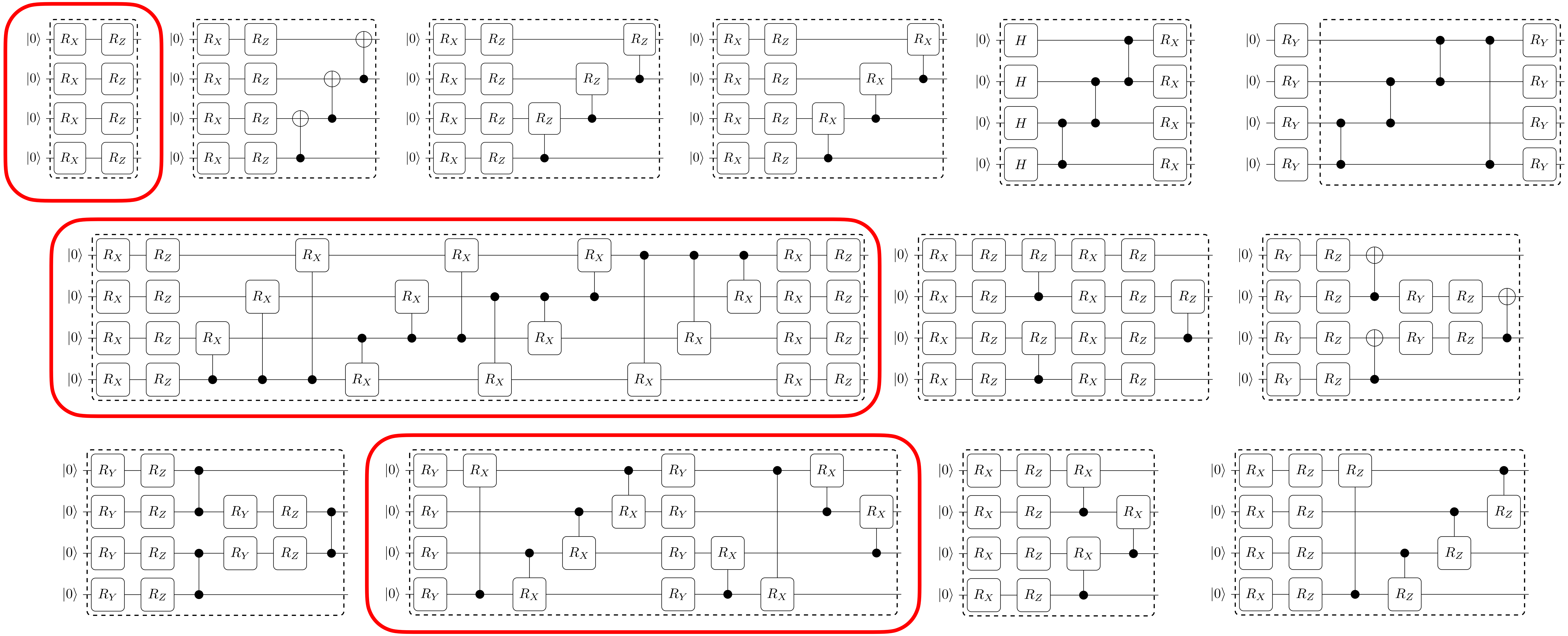
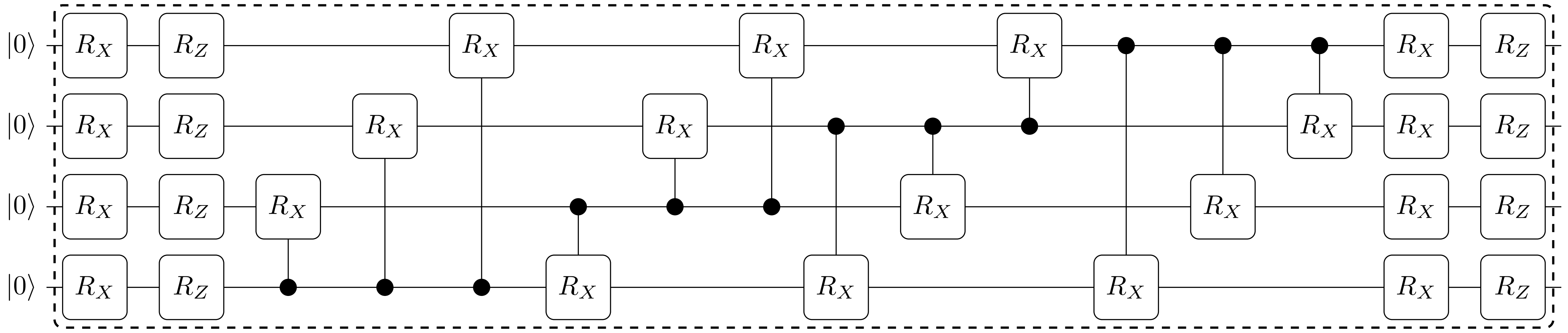


Numerical results

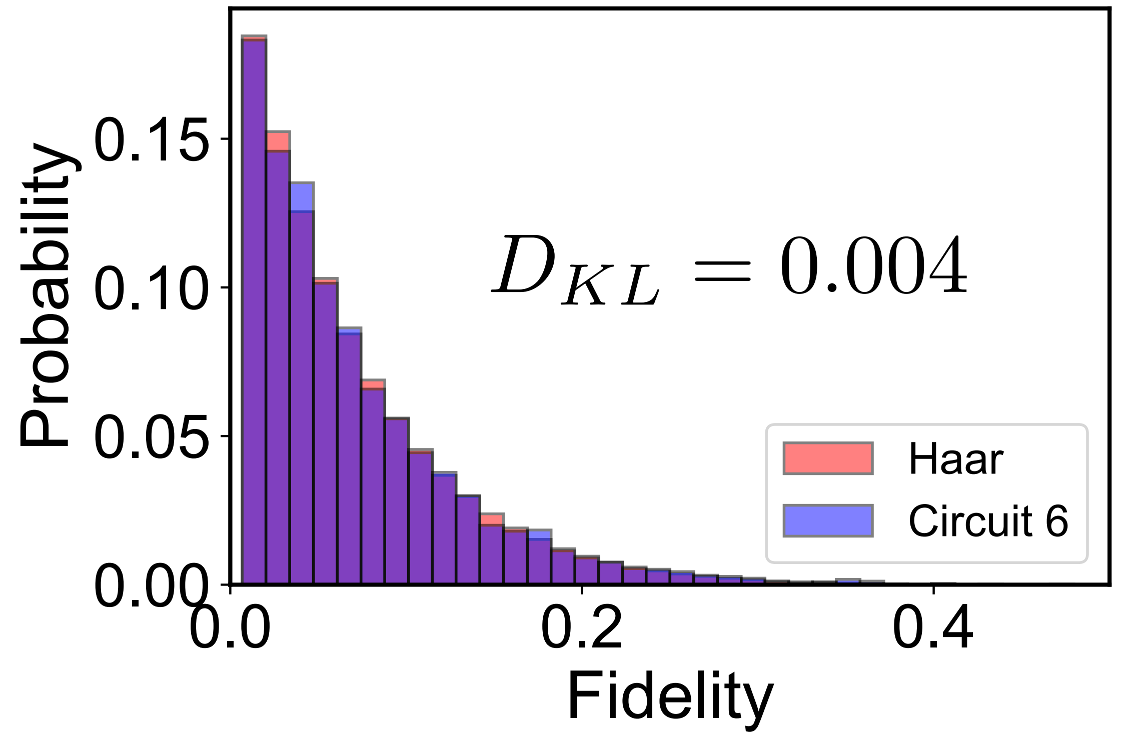
Circuits with high expressibility

Programmable circuit (used for autoencoder) [1,2]

Costly!

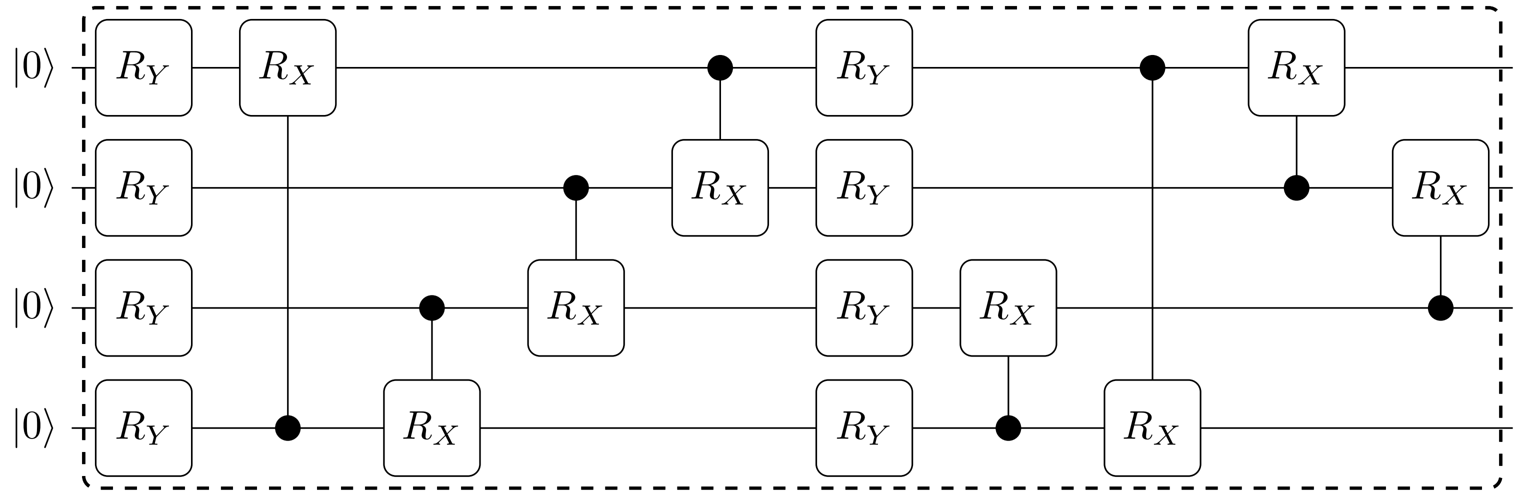


Circuit 6

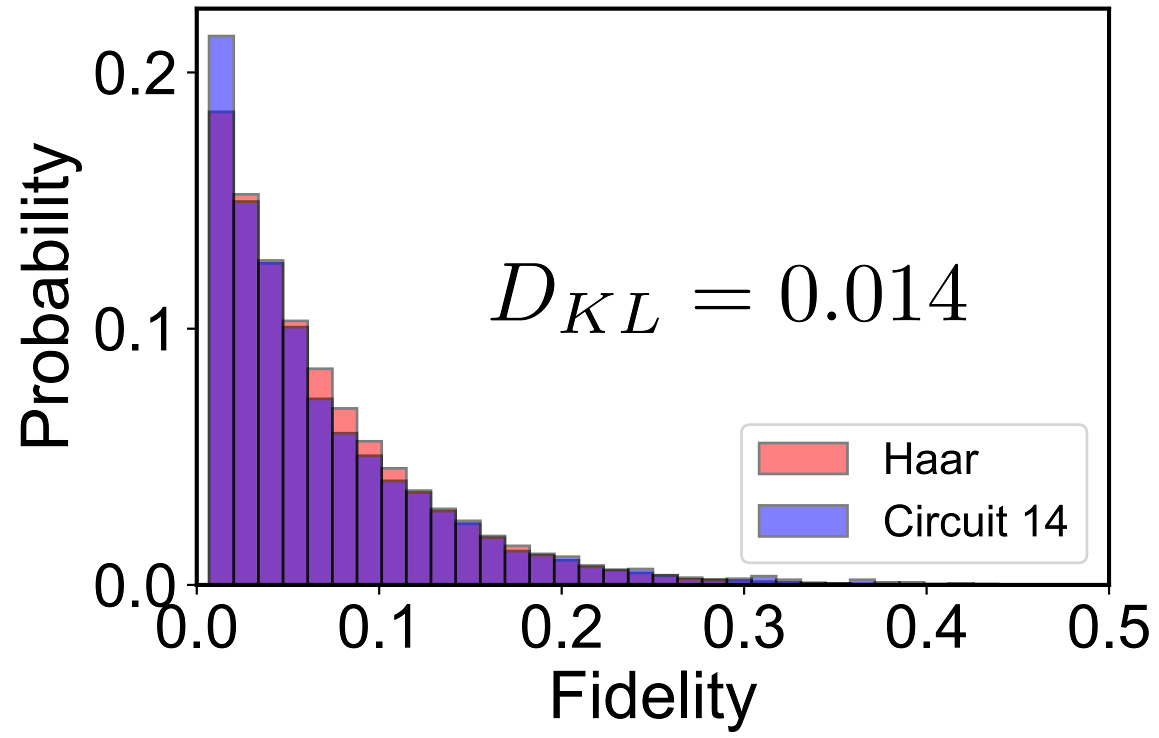


Block-based circuits (used for classifiers) [3]

Cheaper alternative?



Circuit 14



Histogram: 75 bins

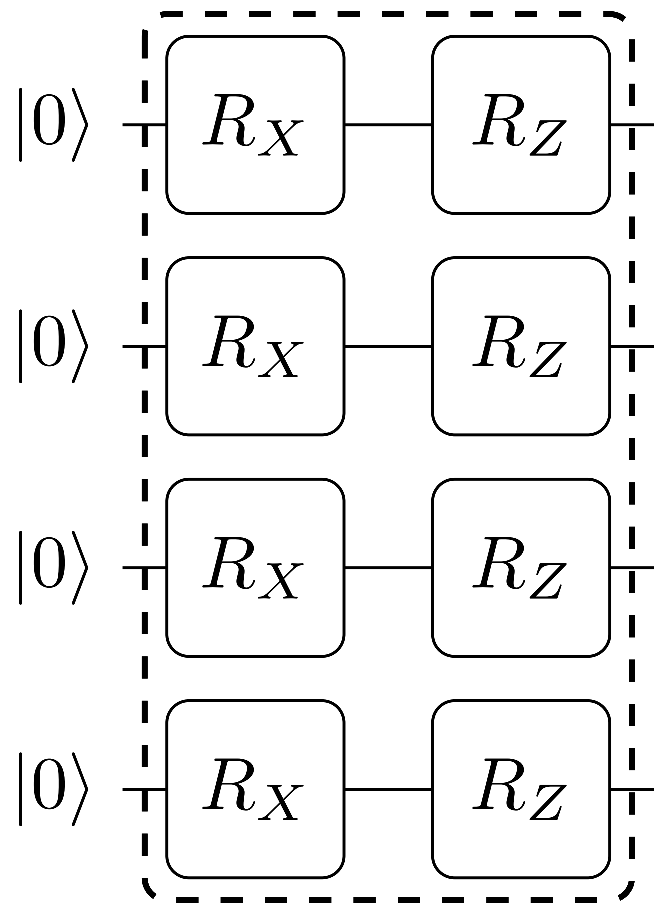
[1] Sousa, P. B., et al. arxiv:quant-ph/0602174.

[2] Romero, Jonathan, et al. *Quantum Sci. Technol.* 2 045001 (2017).

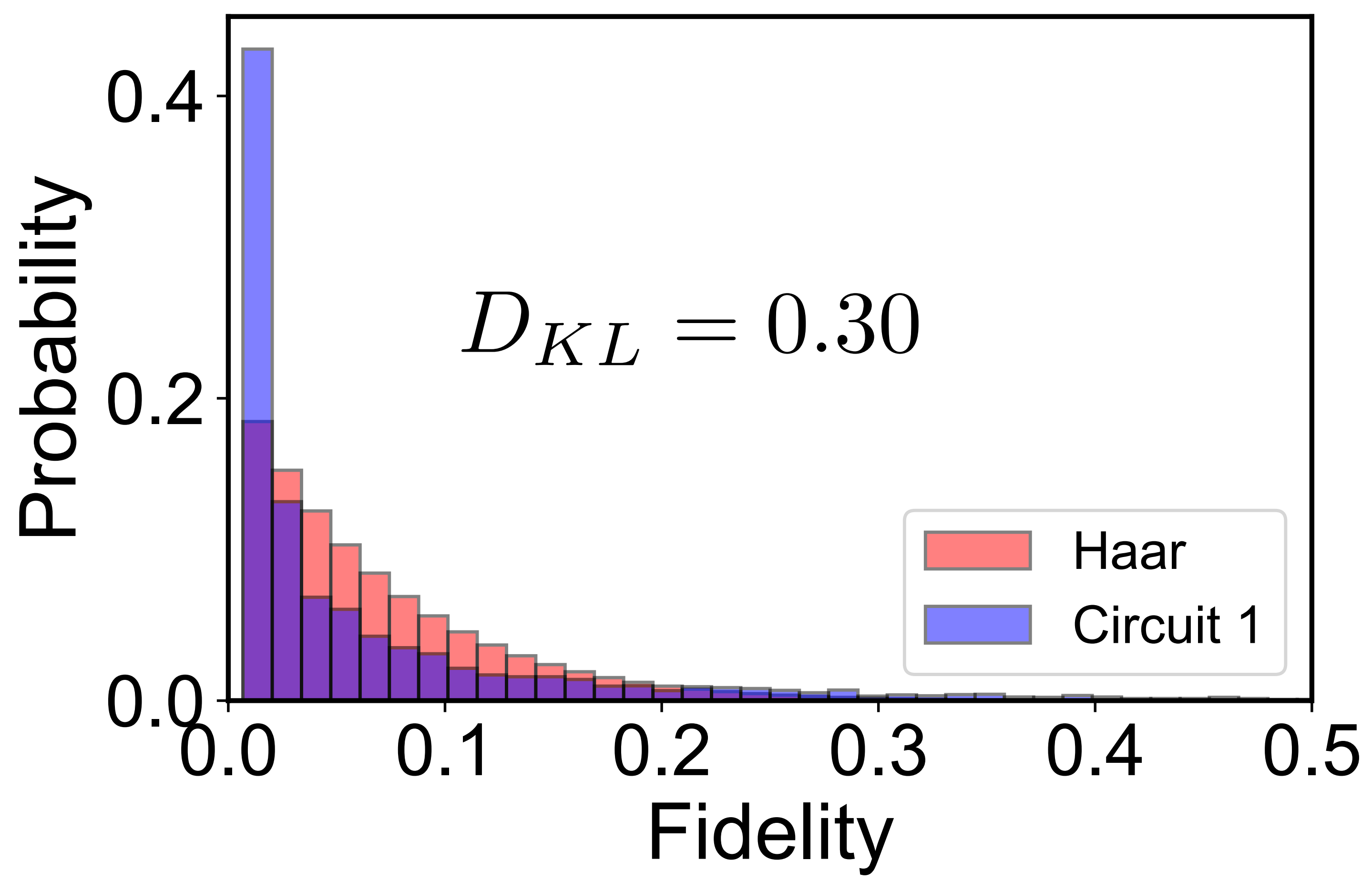
[3] Schuld, Maria, et al. arxiv:1804.00633 (2018).

Numerical results

Circuit with low expressibility

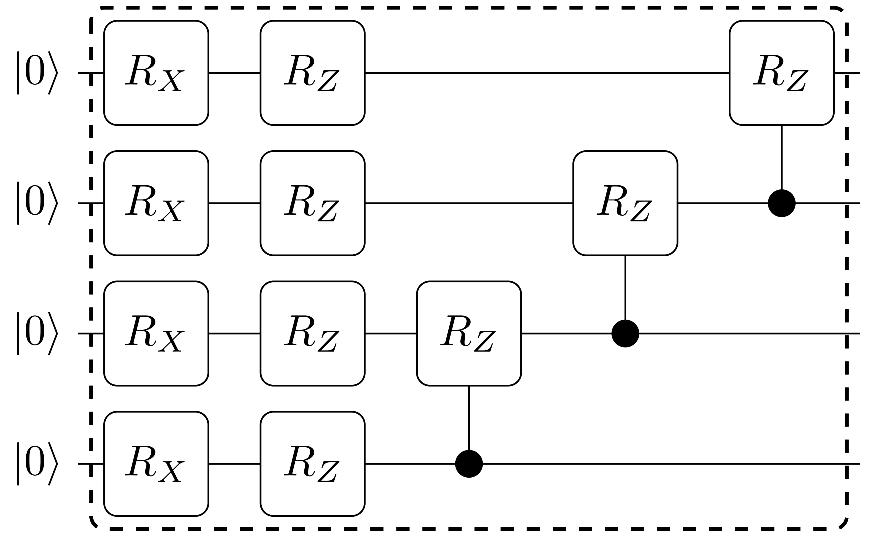


Circuit 1



Histogram: 75 bins

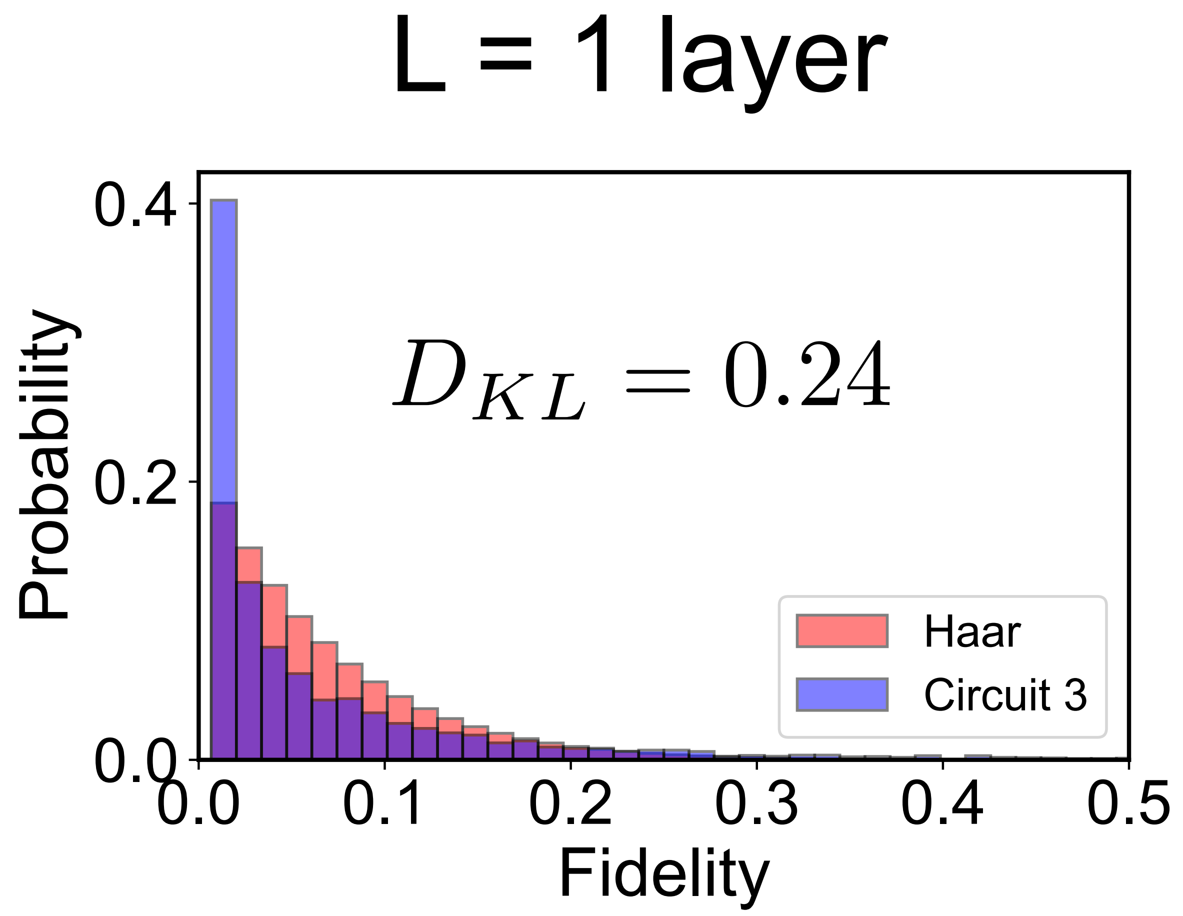
Numerical results

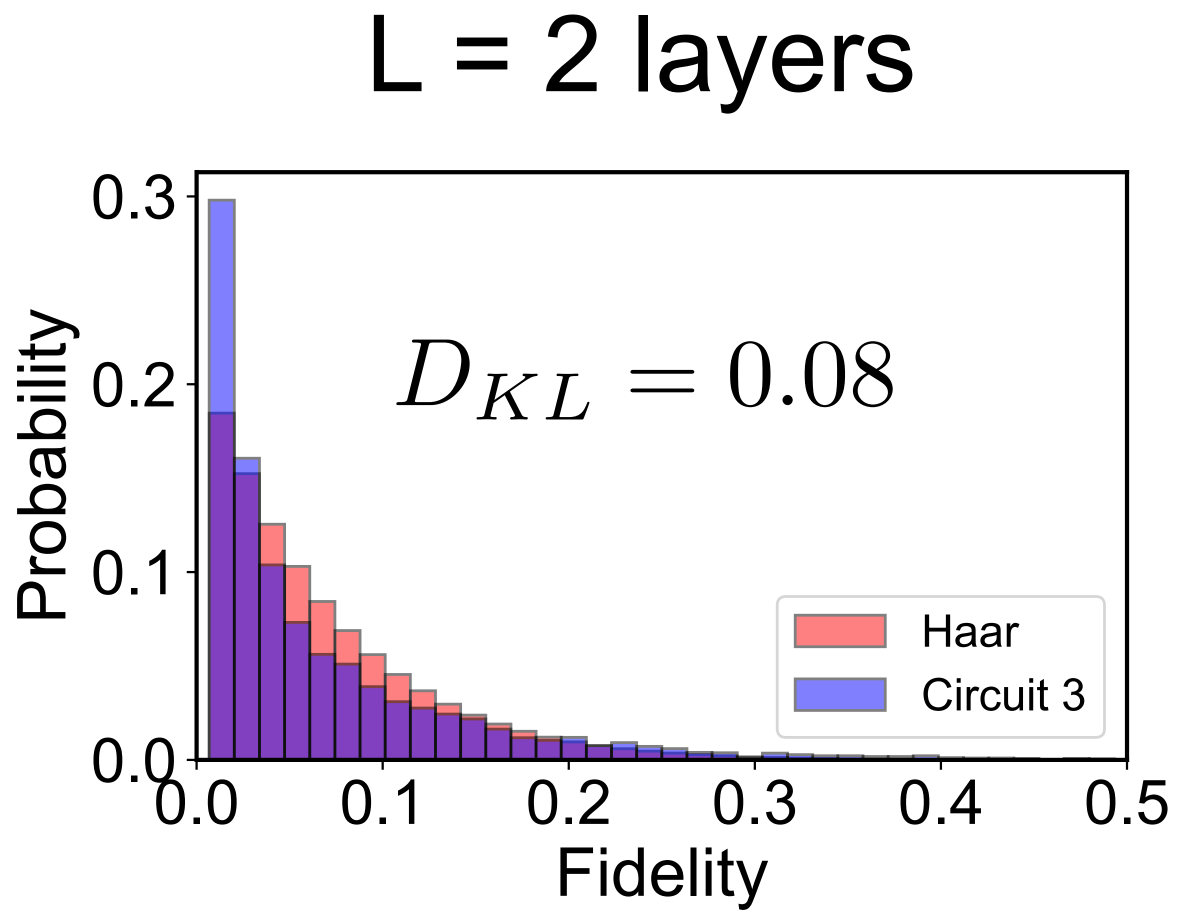


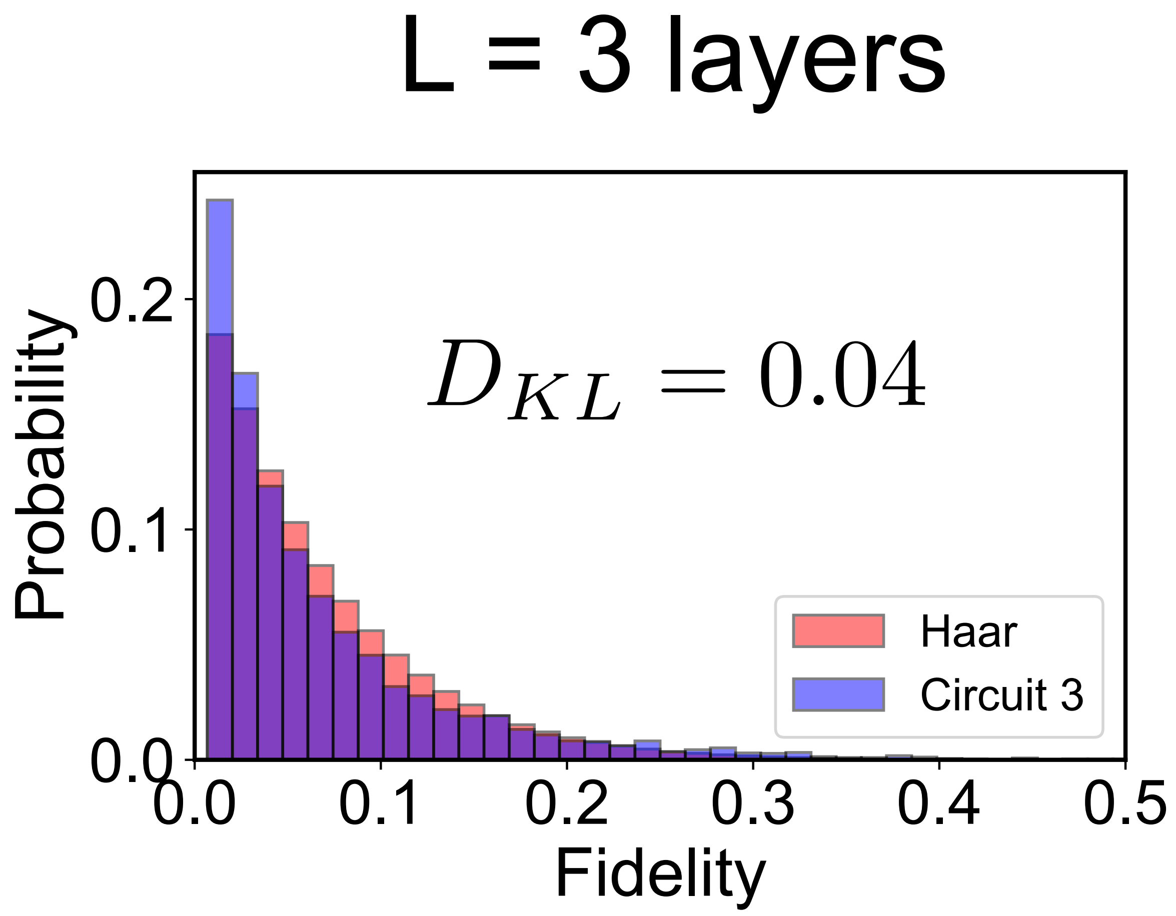
Circuit 3

Increase in expressibility as you add more layers

(Decrease in KL divergence)

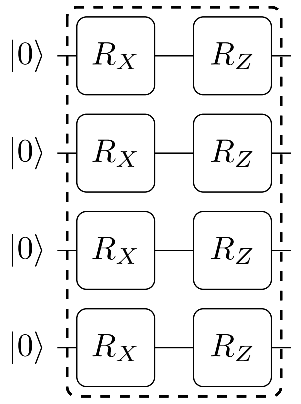




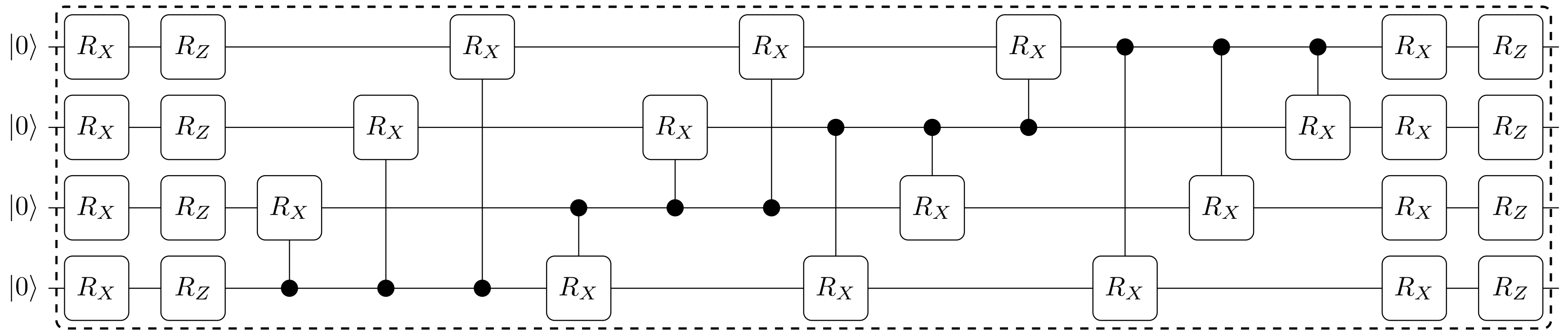


Histogram: 75 bins

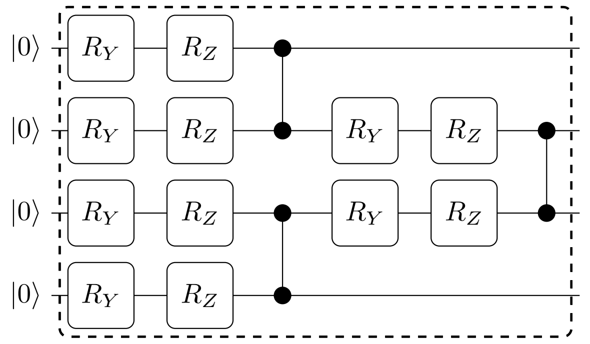
Expressibility saturation



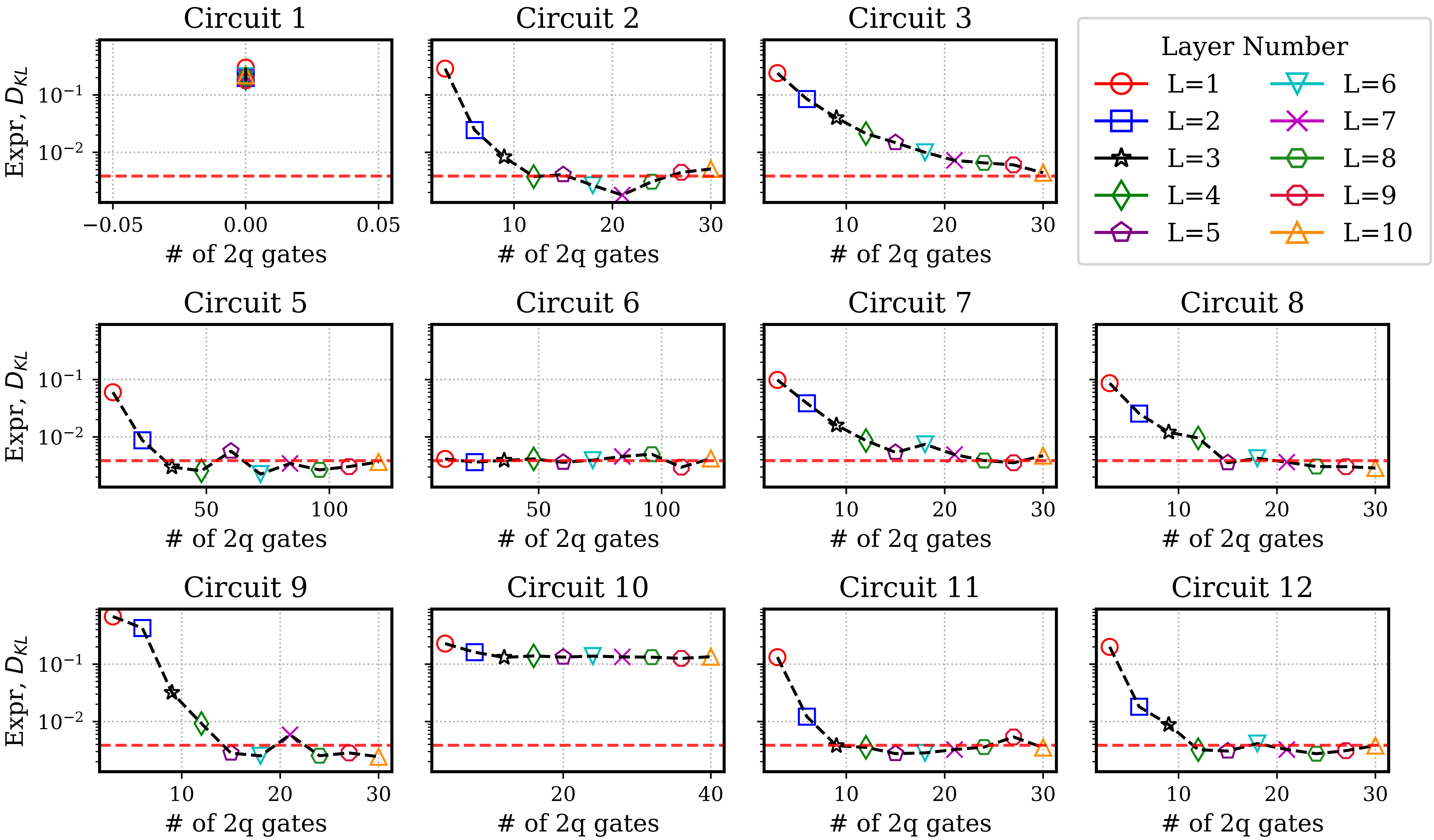
Circuit 1



Circuit 6



Circuit 12



Expressibility “saturates” with increased circuit depth.

4 qubits
5000 samples

Why Haar as a reference?

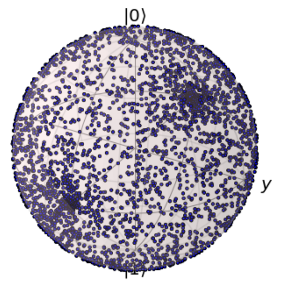
1. The Haar ensemble has properties and analytical expressions we can leverage.

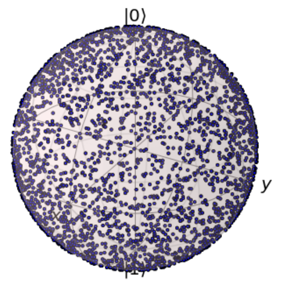
$$P(F) = (d-1)(1-F)^{d-2}$$

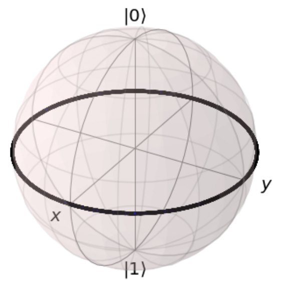
2. Satisfies the two criteria we posed on descriptors: ease of computation, problem independence.

3. Lack of expressibility may be unfavorable for some problem instances.

Example: single-qubit VQE. Circuits B and C generally more effective ansatze than circuit A.







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Might be worth testing first with expressible circuits for modest-sized problem instances when the structure of the solution is not well-understood!

Future directions

- Benchmark existing circuit structures
- Explore relation between expressibility and algorithm performance

For which applications is expressibility a *figure-of-merit*?

Evaluation of Parameterized Quantum Circuits: on the design, and the relation between classification accuracy, expressibility and entangling capability

Thomas Hubregtsen [1,2] · Josef Pichlmeier [1] · Koen Bertels [1]

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ZAPATA

Reference: Sim, S. , Johnson, P. D. and Aspuru‐Guzik, A. (2019), Adv. Quantum Technol. doi:10.1002/qute.201900070