Freie Universität Berlin

The quantum sign problem

Dominik Hangleiter

IQC-QuICS Seminar, February 16, 2021

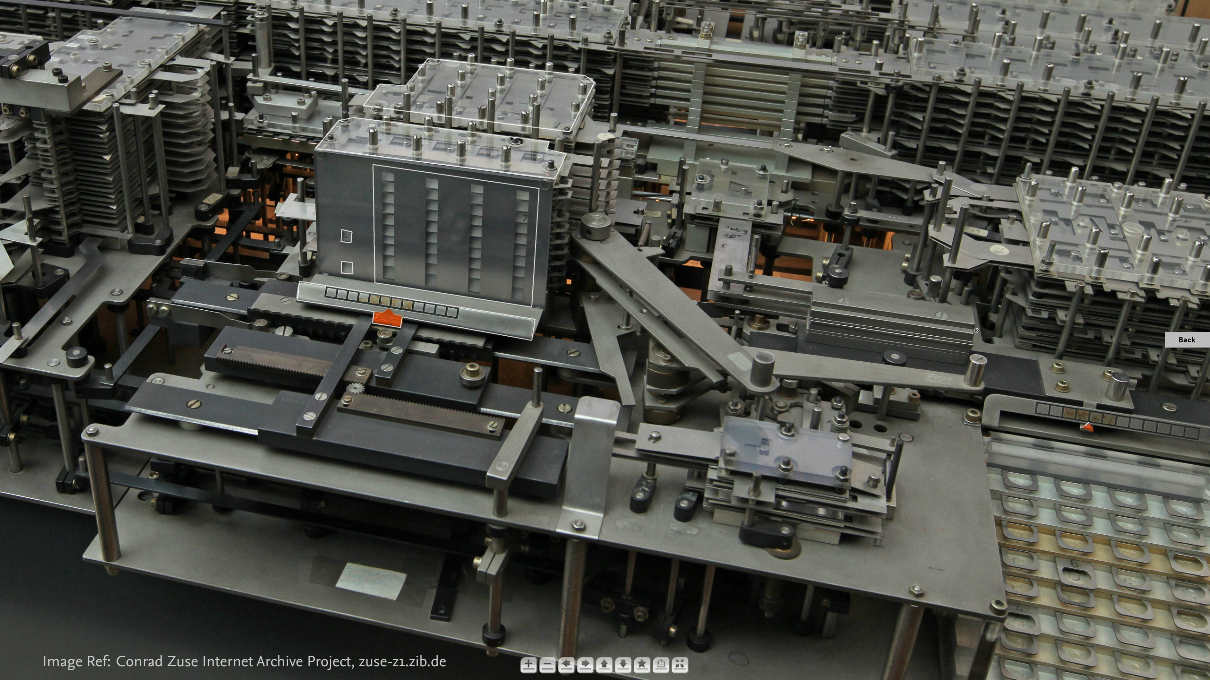
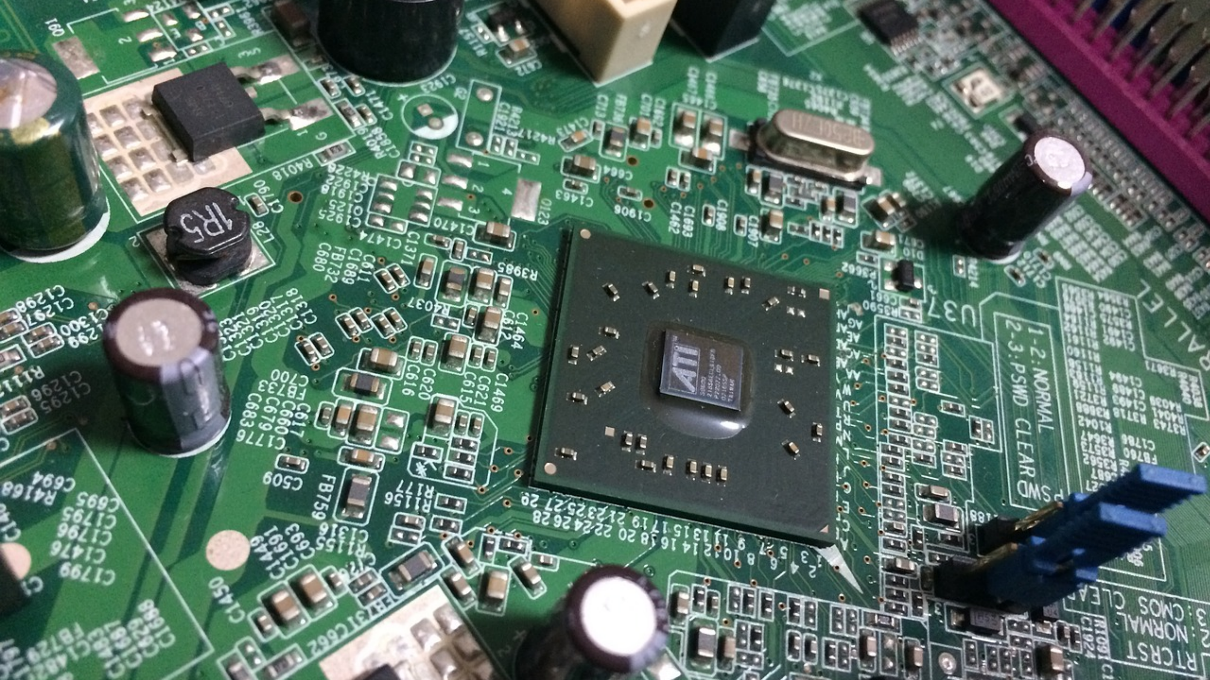


Image Ref: Conrad Zuse Internet Archive Project, zuse-z1.zib.de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circuitOptimizer.py < buffers

```python
        orth = circuit.coreOrths[k]
        newCircuit = copy.deepcopy(circuit)

        P = polynom_order
        # get period and steps
        o  =   np.max(np.abs(np.linalg.eigvalsh(stepDir)))
        t = 2*np.pi/fct_order/o
        mu = np.arange(P+1)*t/P
        # get translations
        r_s = sla.expm(-mu[1]*stepDir)
        R = [np.identity(orth.shape[0], dtype=np.complex128)]
        for i in range(1,P+1):
                R.append(np.dot(R[-1],r_s))
        # get derivatives
        def _derivative(R):
                newCircuit.coreOrths[k] = R.dot(orth)
                return -2*np.real(np.trace(self.calculateEuclideanGradient(newCircuit, k).dot(orth.T.conj()).dot(R.T.conj()).dot(stepDir.T.conj())))
        dervs = list(map(_derivative,R))
        mu_mat_inv = np.linalg.inv(mu[1:,np.newaxis]**np.arange(1,P+1))
        coef = mu_mat_inv.dot(dervs[1:]-dervs[0])
        coef = list(coef[::-1])
        coef.append(dervs[0])
        roots = np.roots(coef)
        pos_real_roots = [np.real(r) for r in roots if np.abs(np.imag(r))<1E-10 and np.real(r)>=0]

        if showPlot is True:
                gridSize = 200
                normPortion = .5
                orth0 = circuit.coreOrths[k]
                newCircuit = copy.deepcopy(circuit)
                gradient = stepDir

                riemGradNormSqrd = .5*np.trace(np.dot(gradient.T,gradient))
                stepSize = normPortion/ riemGradNormSqrd

                xgrid = np.arange(0,gridSize)*stepSize
                objval = np.zeros((gridSize))

                for kk in range(0,len(xgrid)):
                        theOrth = np.dot(sla.expm(-xgrid[kk]*gradient), orth0)
                        newCircuit.coreOrths[0] = theOrth
                        objval[kk] = self.objectiveFunction(newCircuit)
```

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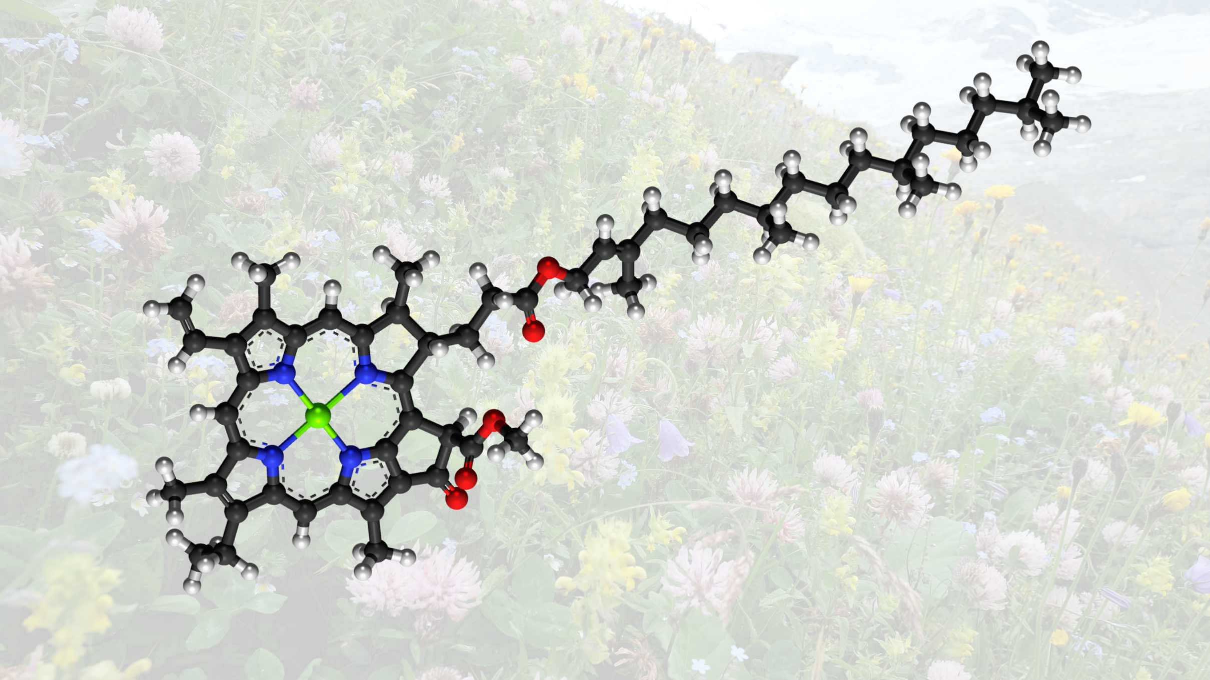


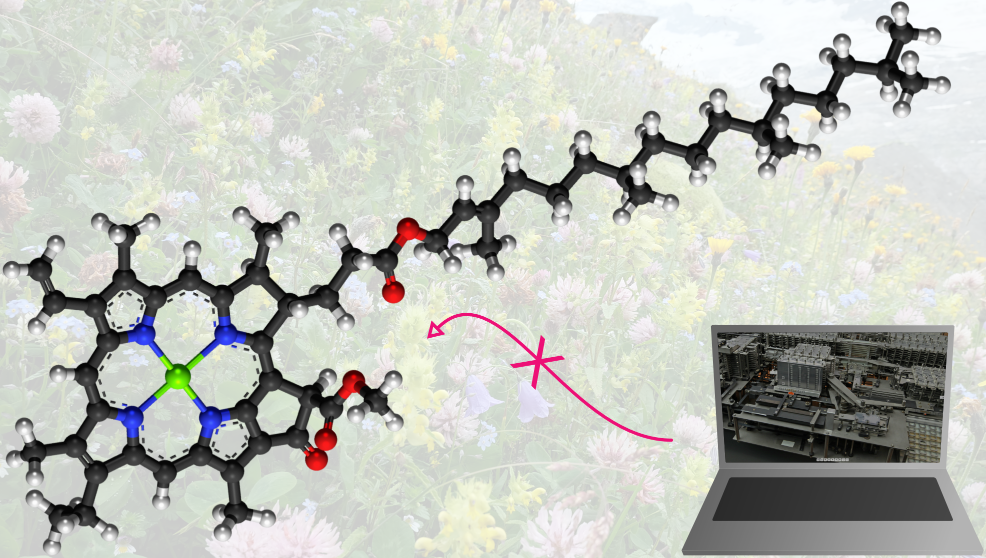
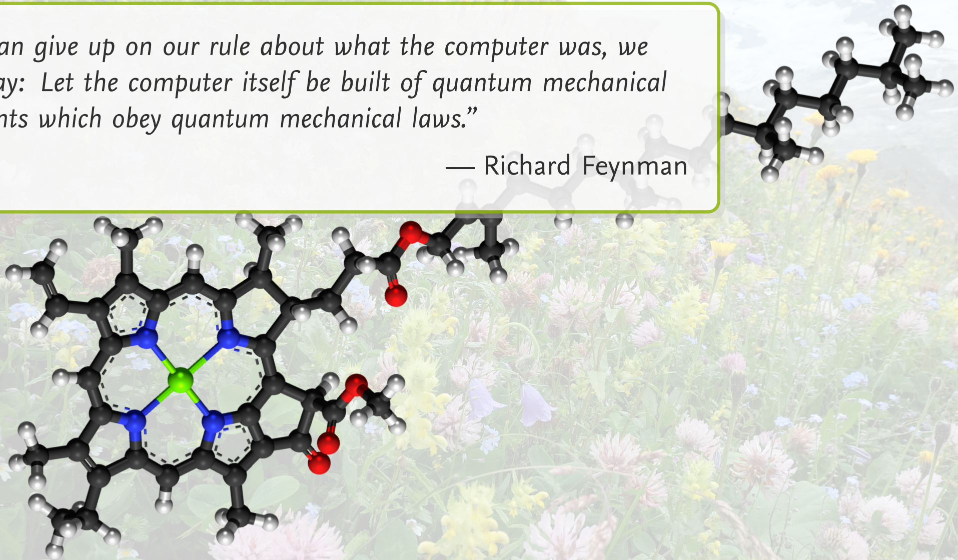


Image Ref.: Jynto, Wikipedia: Chlorophyll & Graham Carlow/IBM

> “We can give up on our rule about what the computer was, we can say: Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws.”
>
> — Richard Feynman



Feynman (1982), p. 474

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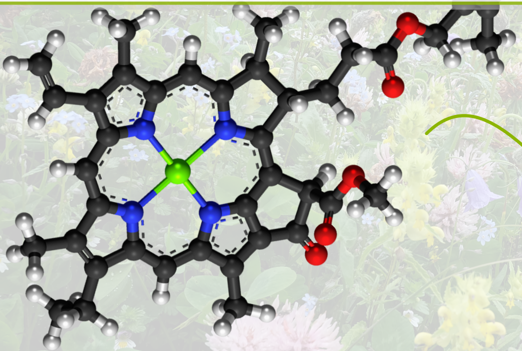

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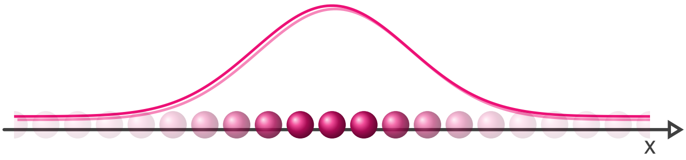
Quantum measurement

Complex-valued wave function:

$$\psi : \mathbb{R} \to \mathbb{C}$$



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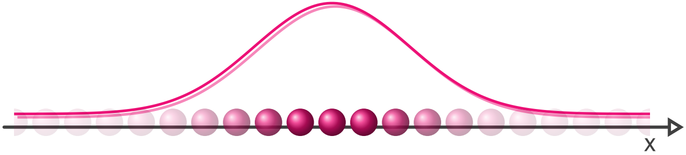

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Wave-function collapse:

$$\Pr[\text{measured at } x] = |\psi(x)|^2$$

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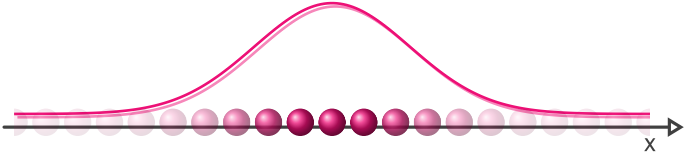

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Probability distribution over possible outcomes .... **Sampling**

Sampling

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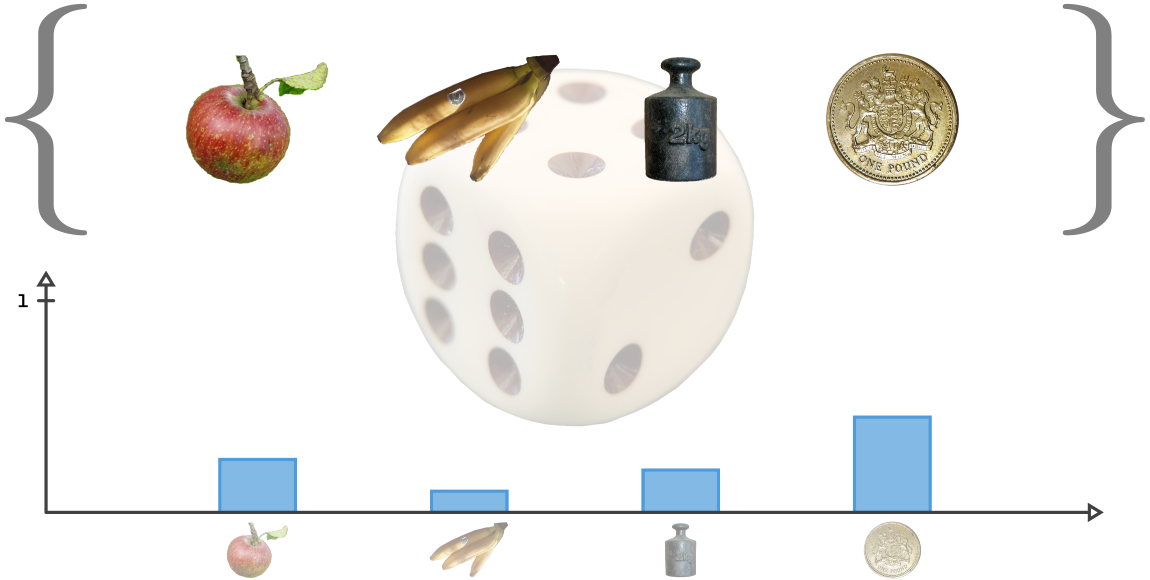

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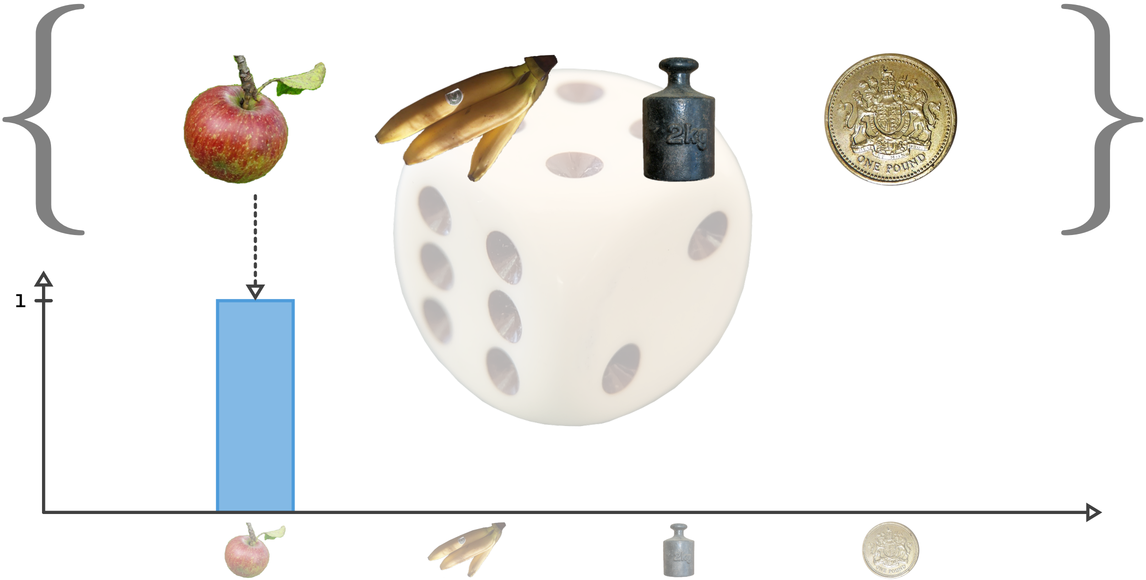

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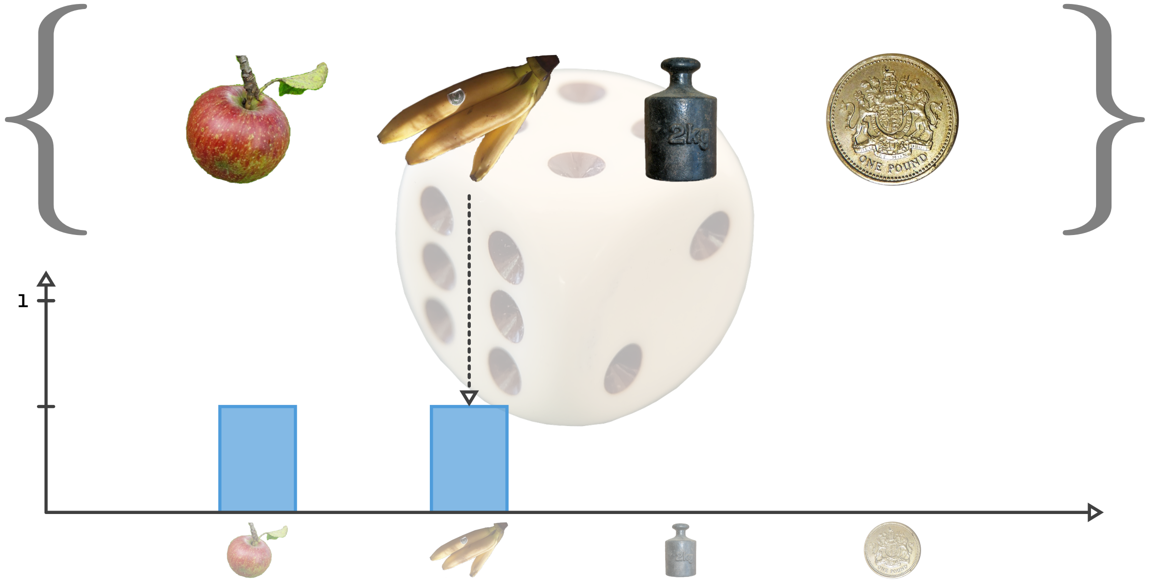

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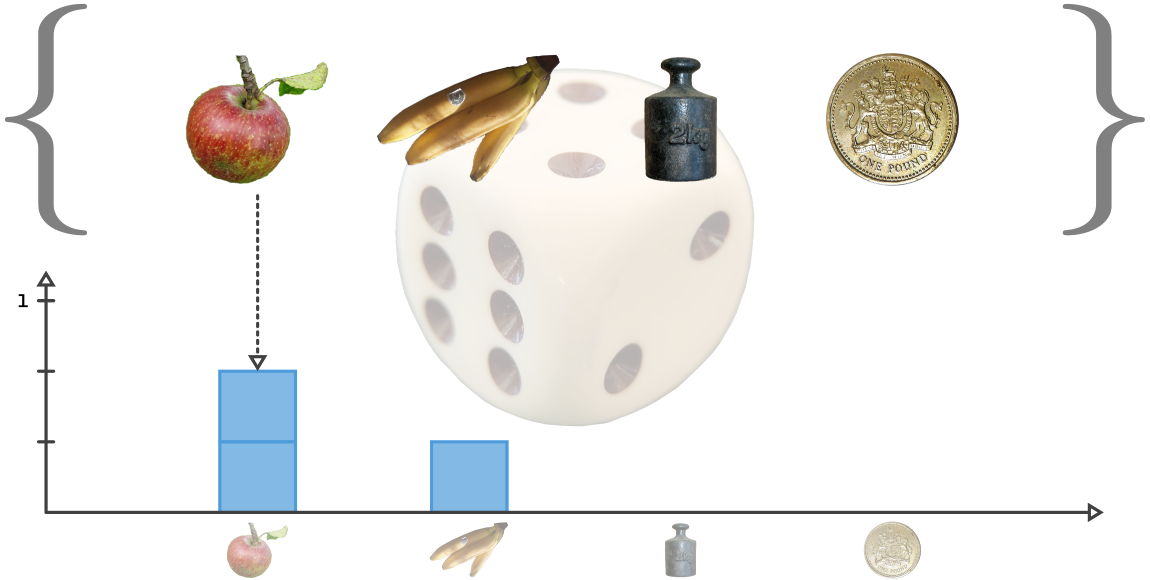

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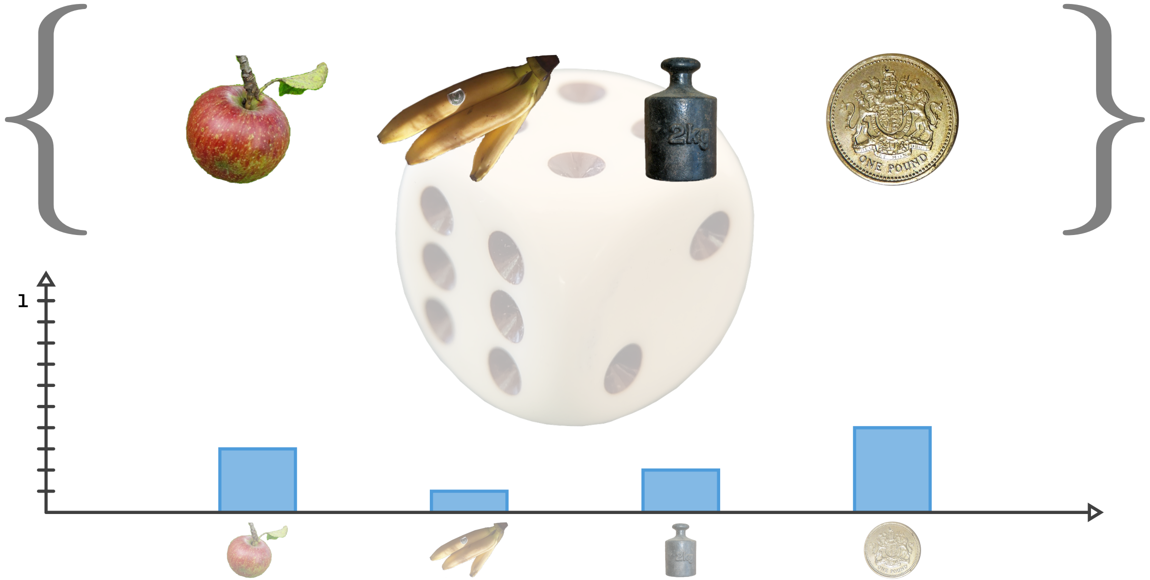

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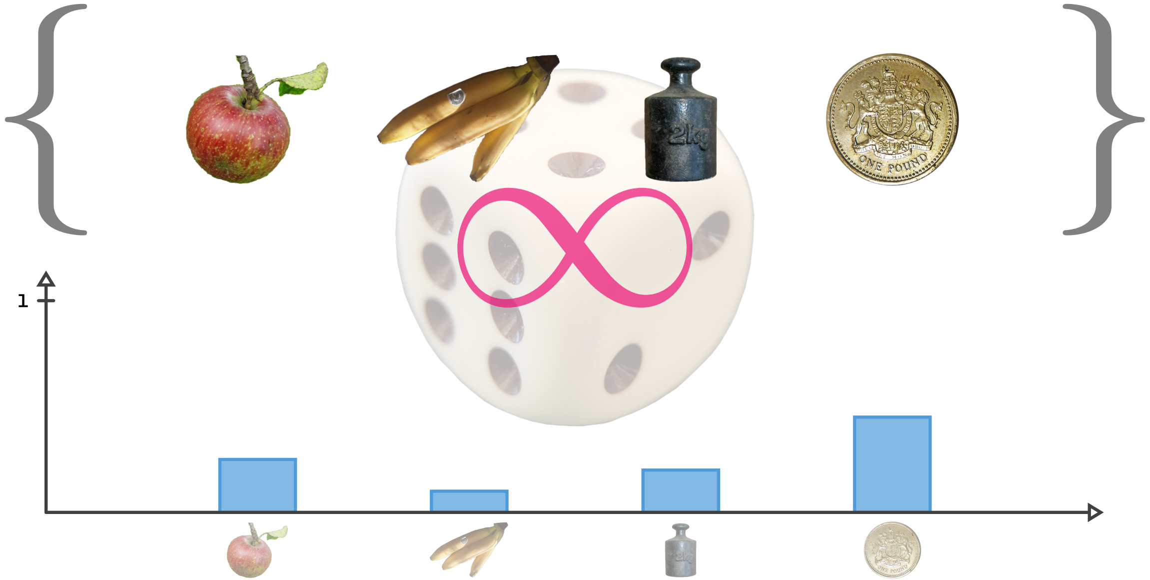

Computational complexity: scaling of runtime

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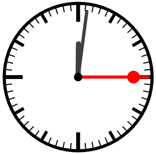

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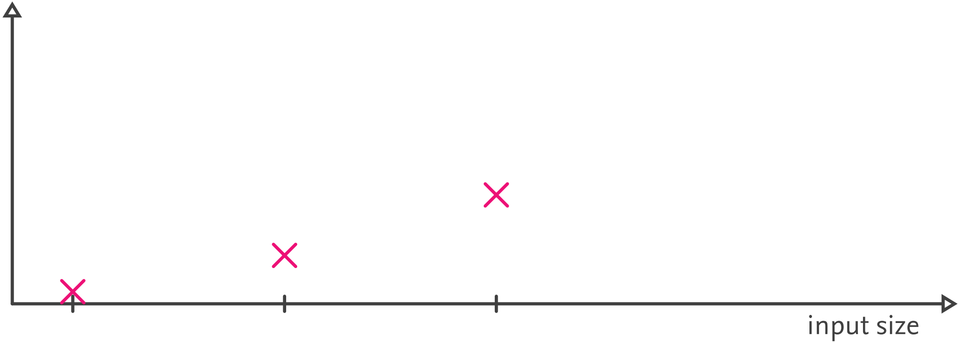

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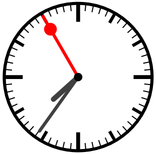

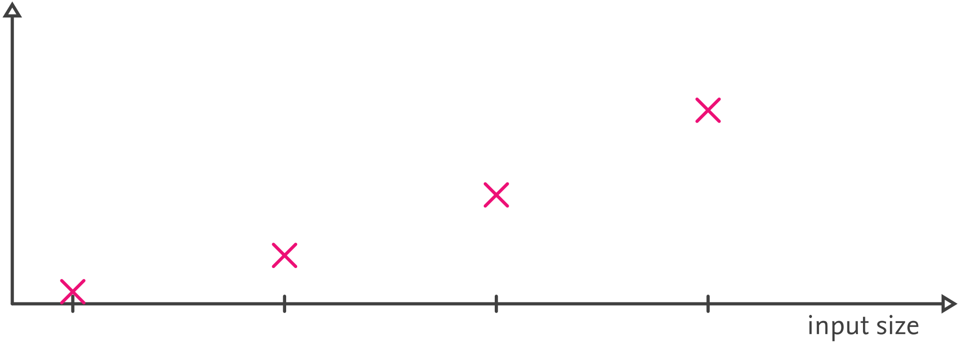

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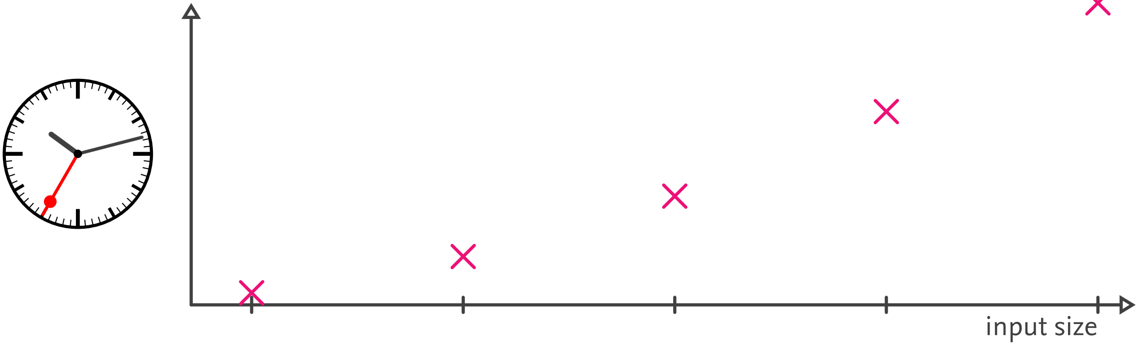

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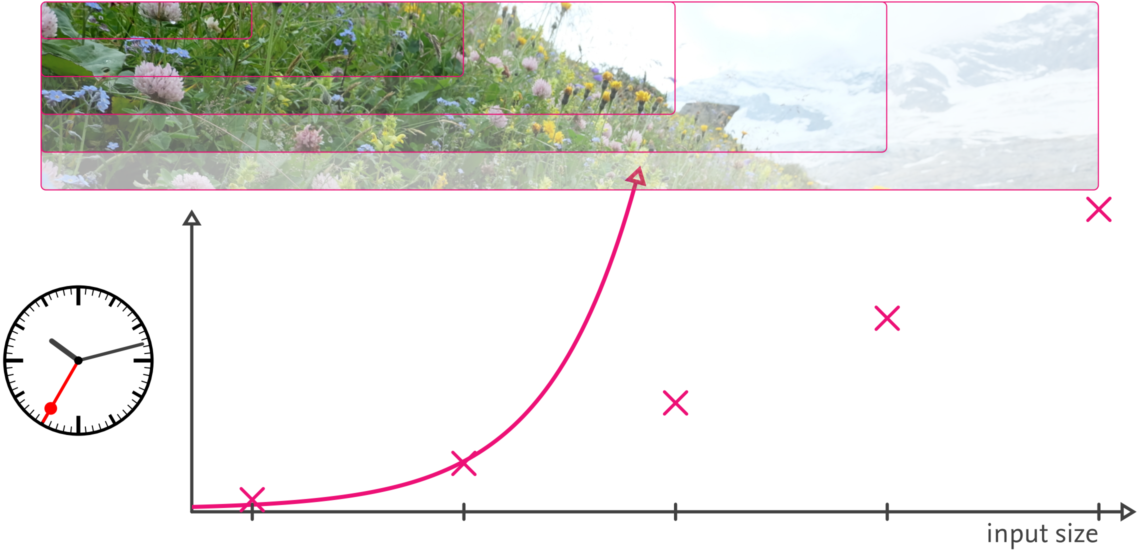
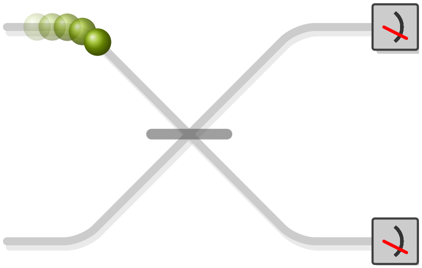


Quantum sampling: The Hong-Ou-Mandel interferometer



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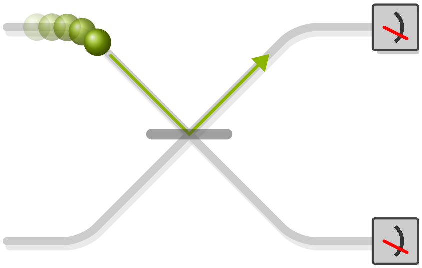

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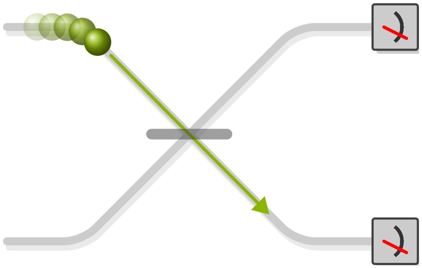

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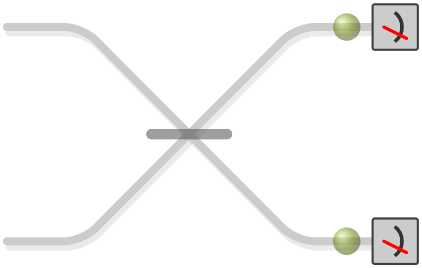

$$\frac{1}{\sqrt{2}}\left(|0,1\rangle + |1,0\rangle\right)$$

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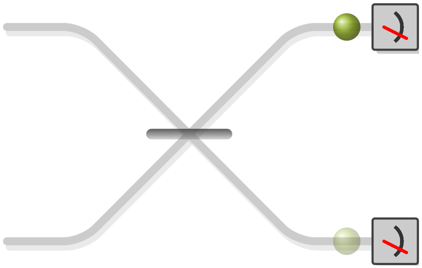

$$\sqrt{\frac{3}{5}}|0,1\rangle + \sqrt{\frac{2}{5}}|1,0\rangle$$

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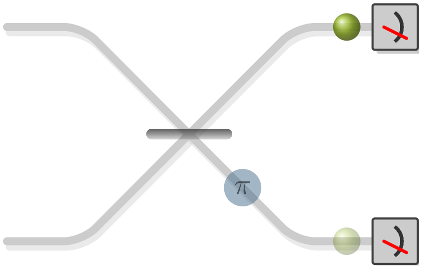

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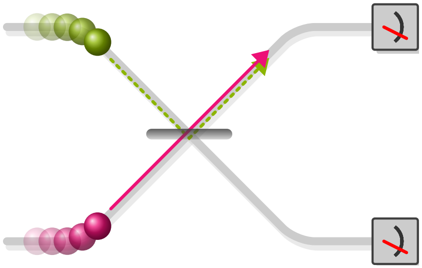
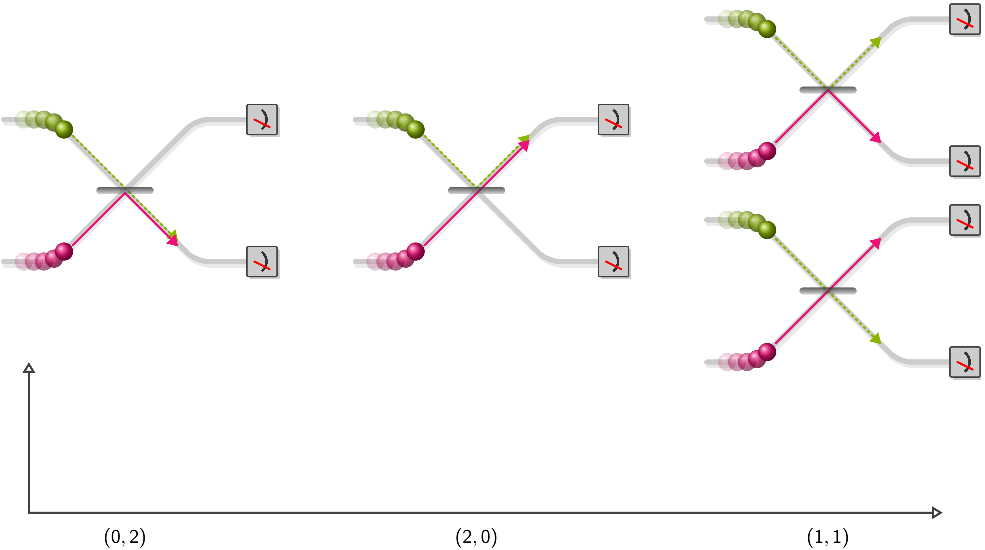


Quantum sampling: The Hong-Ou-Mandel interferometer – two photons



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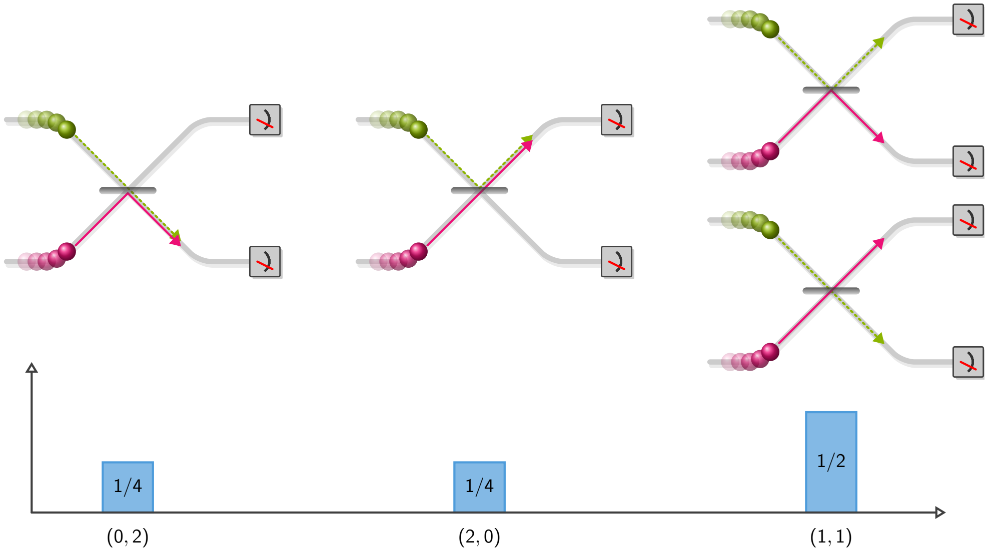

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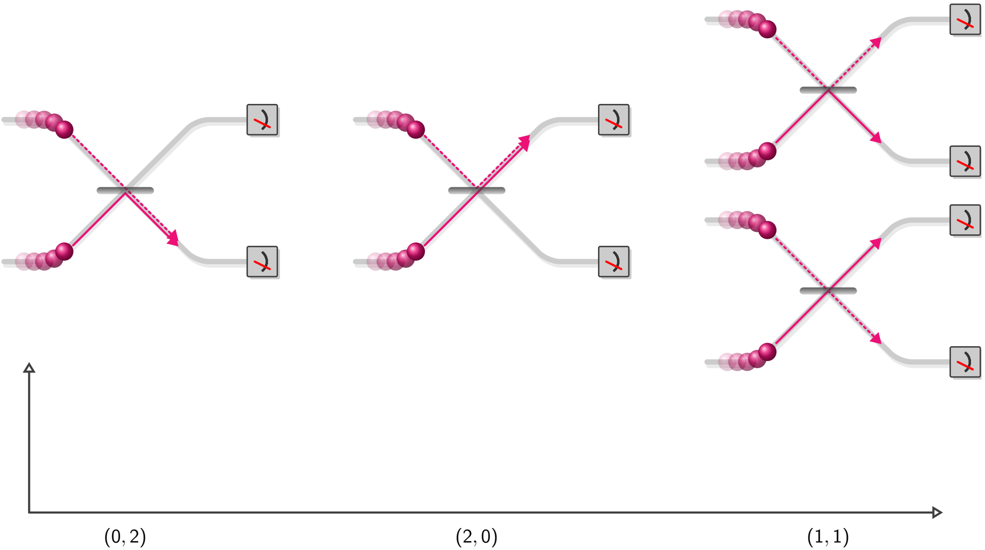

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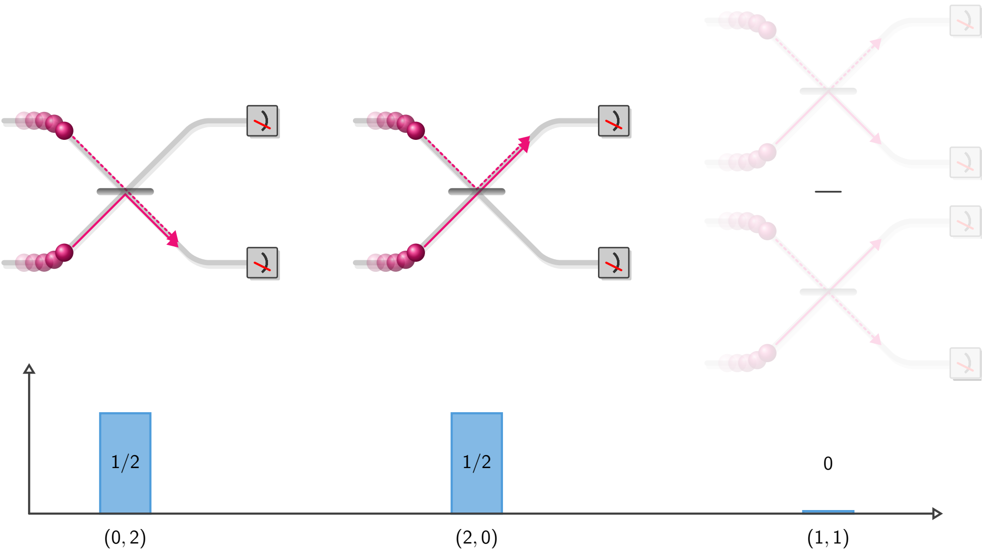

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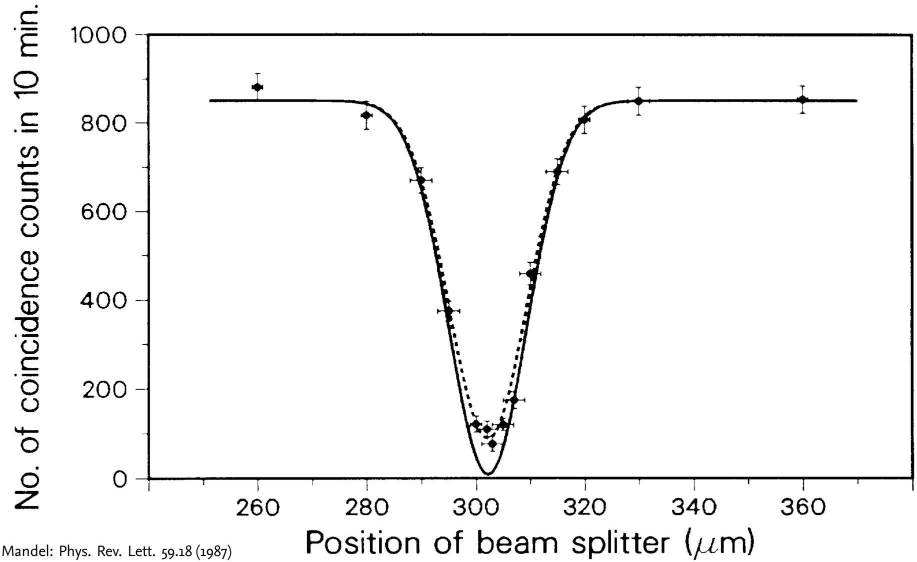
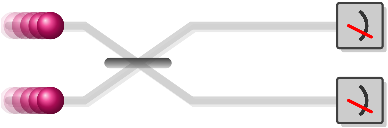


Hong, Ou, Mandel: Phys. Rev. Lett. 59.18 (1987)

Complex quantum sampling: A large network of HOM interferometers



Aaronson and Arkhipov, STOC' (2013)

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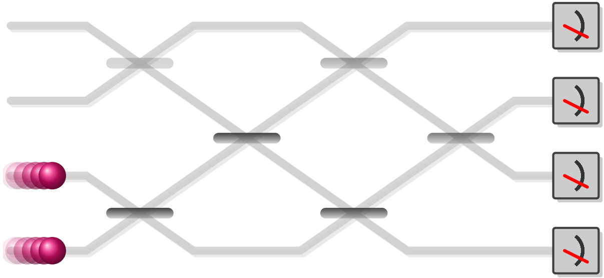

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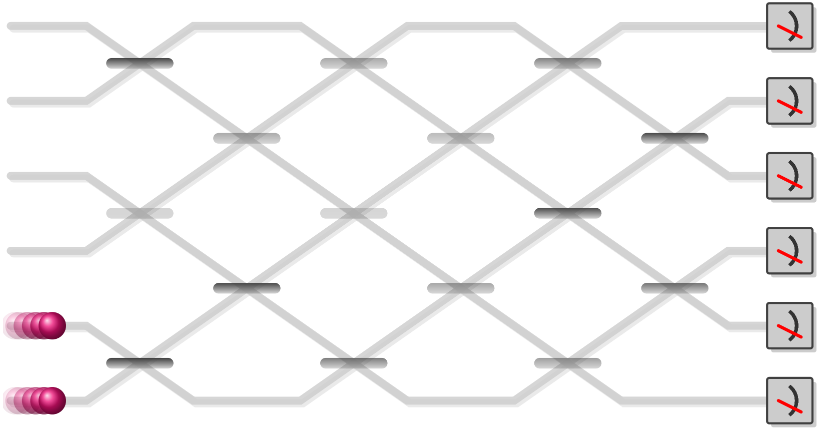

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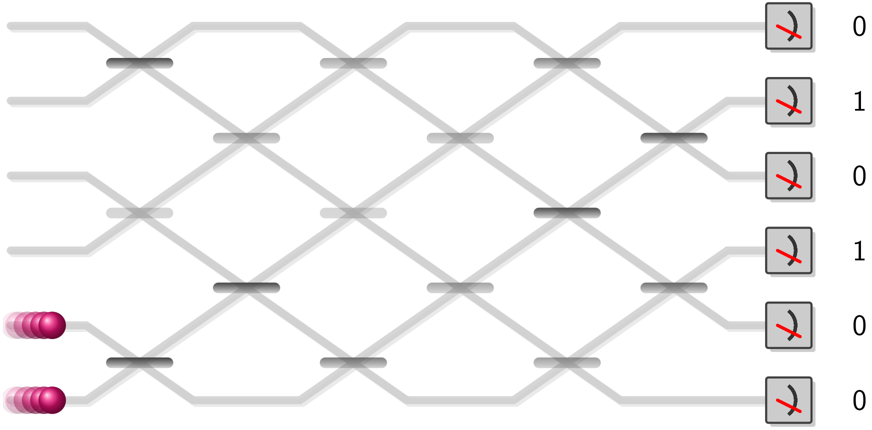

$$|\Phi_{m,n}| \sim m^n$$

Aaronson and Arkhipov, STOC' (2013)

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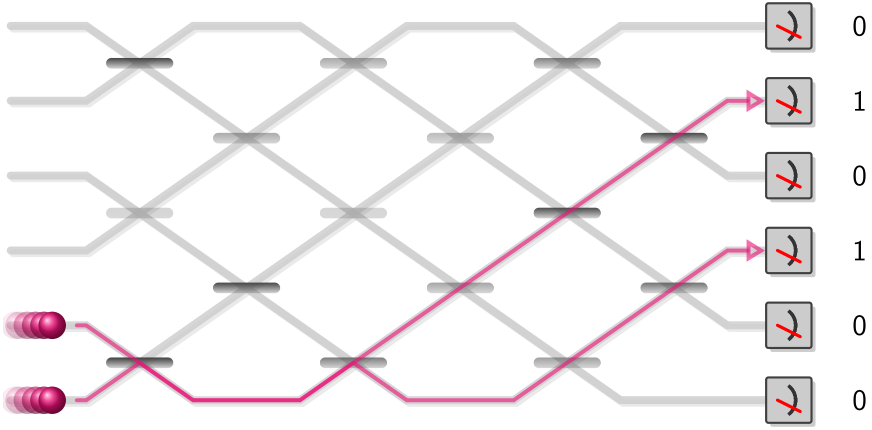

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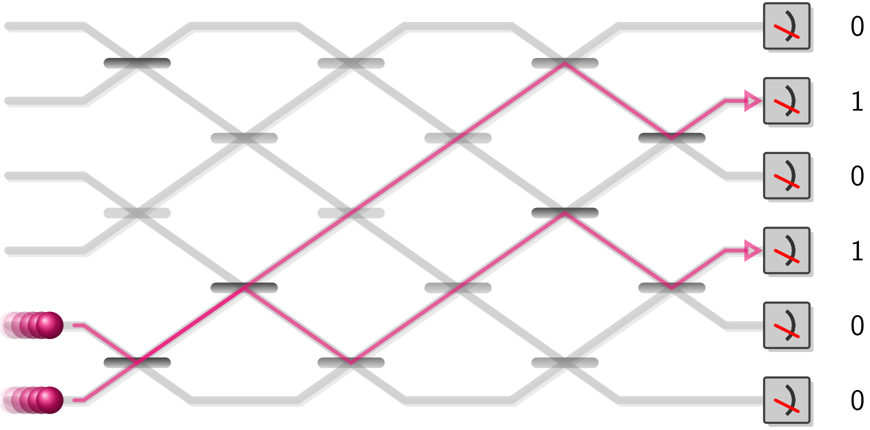

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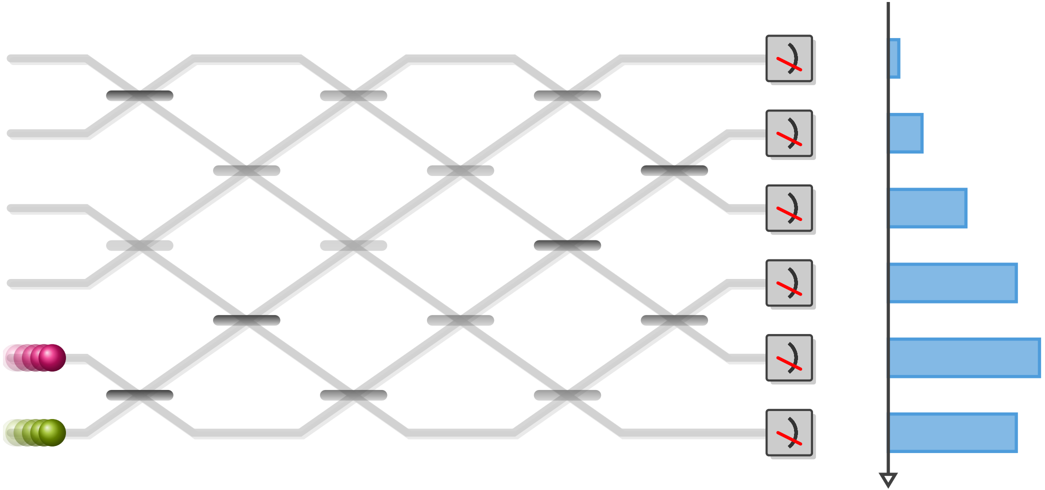

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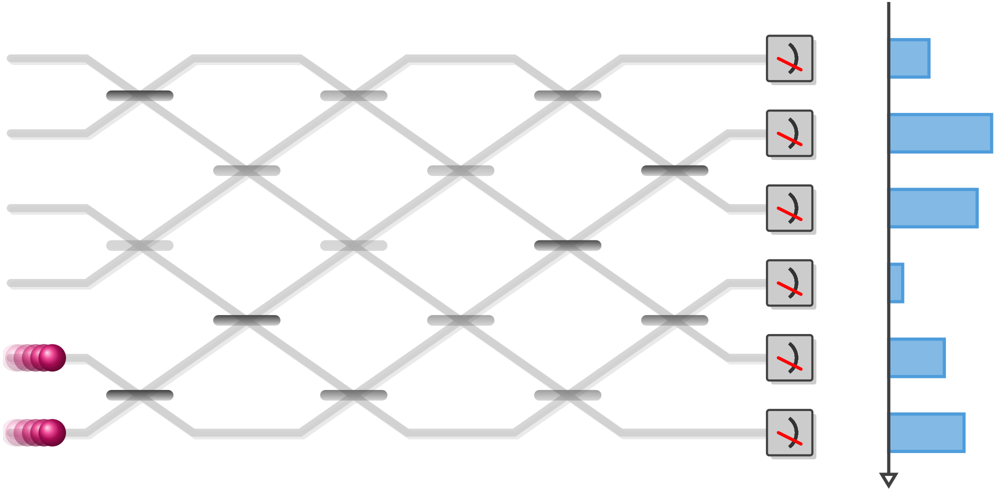

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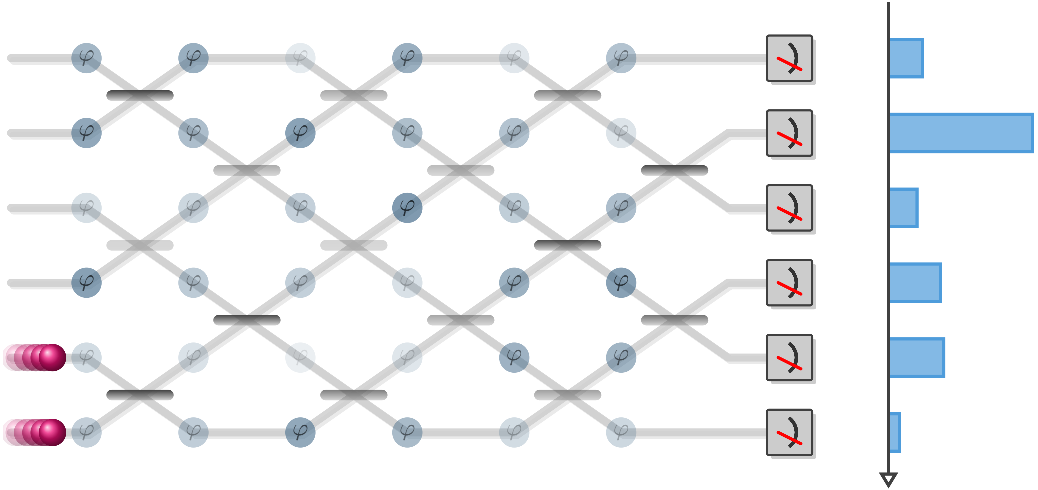

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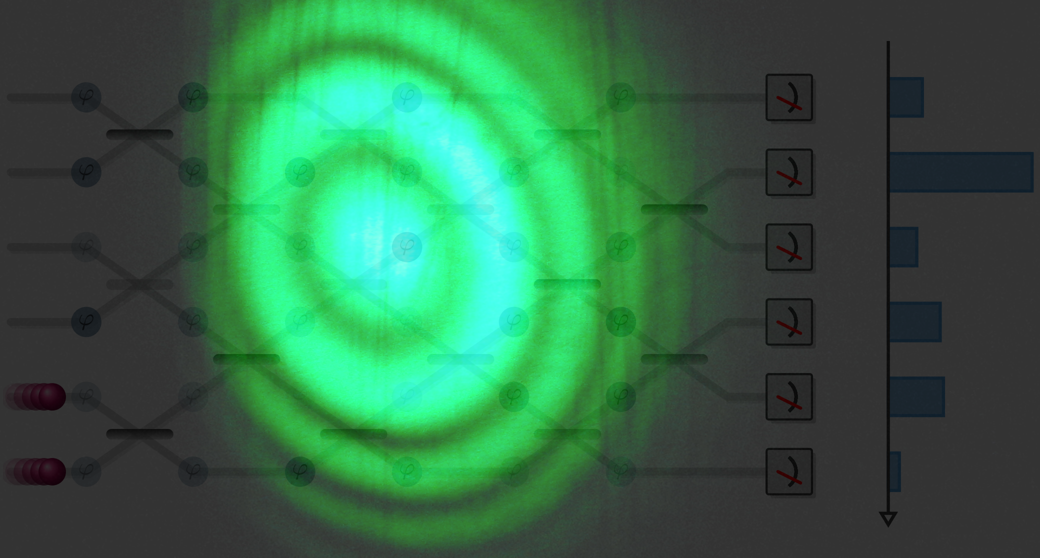

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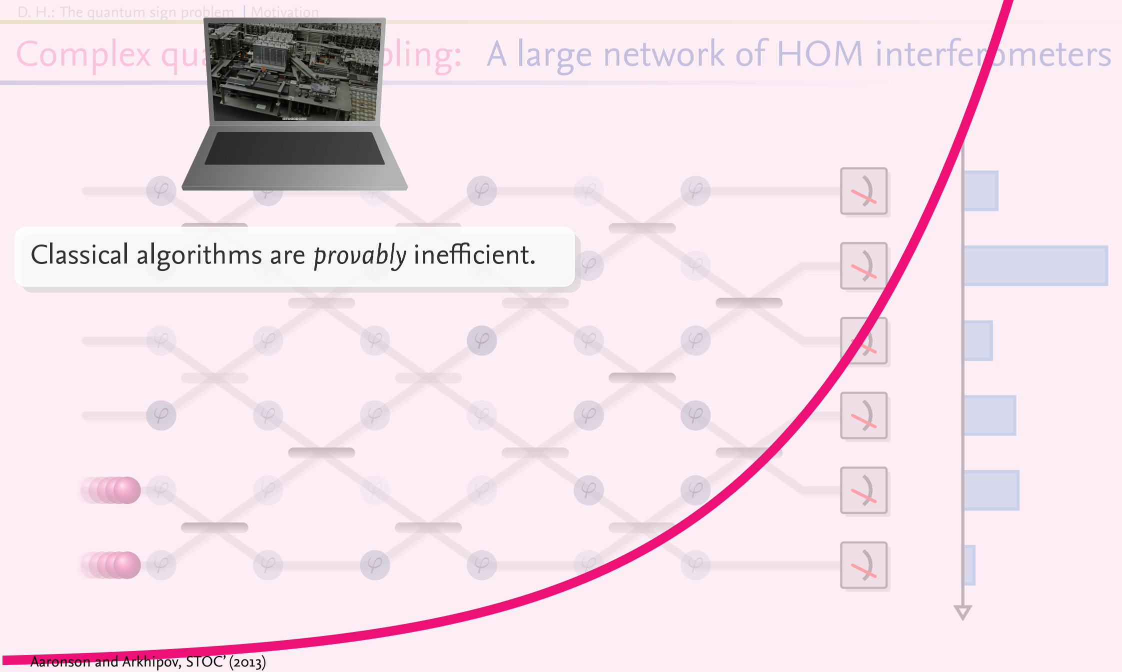
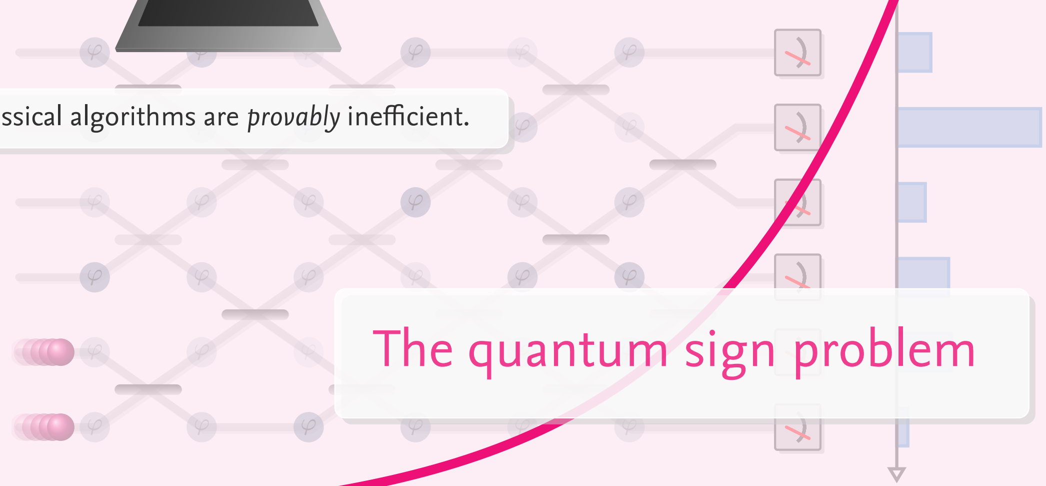


Classical algorithms are *provably* inefficient.

Aaronson and Arkhipov, STOC' (2013)

Complex qua… pling: A large network of HOM interferometers



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The quantum sign problem

Aaronson and Arkhipov, STOC' (2013)

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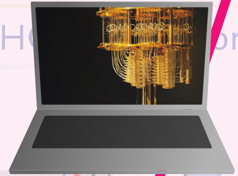

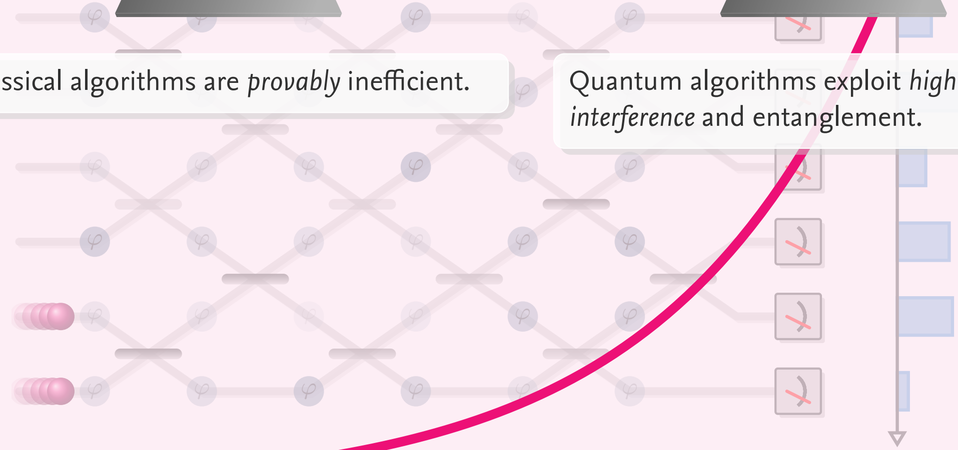

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Quantum algorithms exploit *high-dimensional interference* and entanglement.

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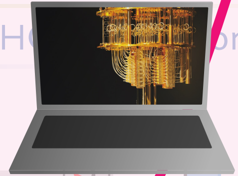

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How is the quantum sign problem reflected in the computational complexity of different sampling-related tasks?

Aaronson and Arkhipov, STOC' (2013)

Delineating the quantum-classical boundary

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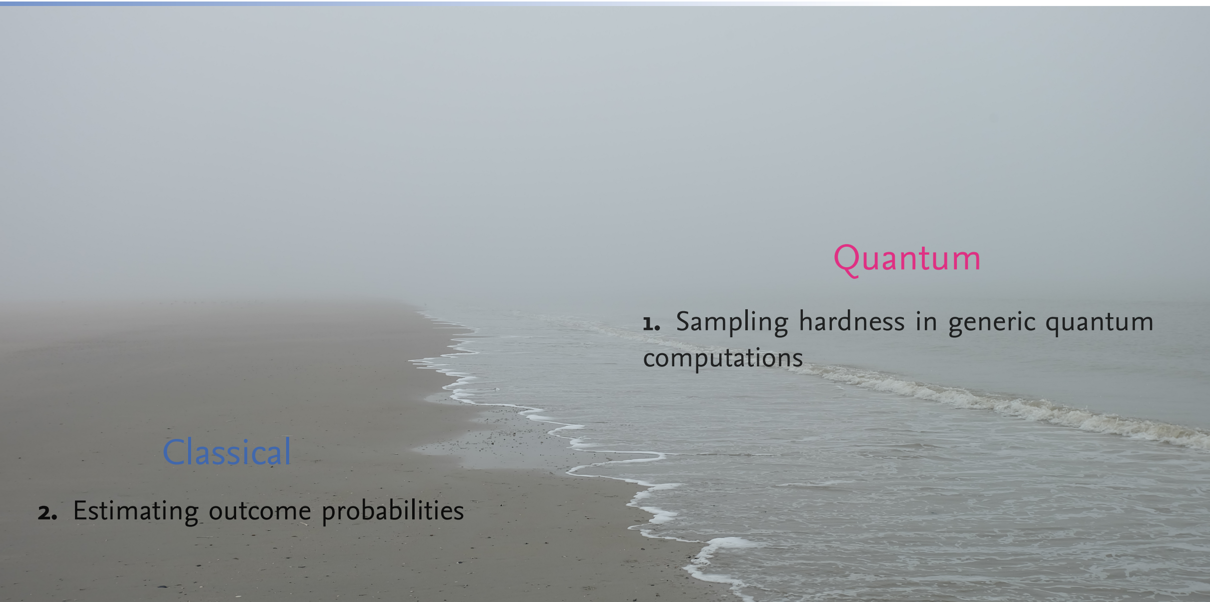
Quantum

1. Sampling hardness in generic quantum computations

Classical

Delineating the quantum-classical boundary



Perspective 1
The sign problem in complexity theory

The sign problem in complexity theory: the basics

3-SAT formula

$$f(x) = (x_1 \vee \bar{x}_7 \vee x_{137}) \wedge (x_5 \vee x_{12} \vee \bar{x}_{17}) \wedge (\bar{x}_{32} \vee \bar{x}_7 \vee x_{17}) \wedge \cdots \wedge (\bar{x}_3 \vee \bar{x}_2 \vee \bar{x}_1)$$

NP: Decide whether $\exists x : f(x) = 1$.

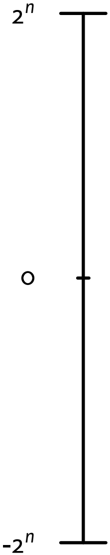
#P: Compute $acc(f) := |\{x : f(x) = 1\}| \in \{0, \ldots, 2^n\}$.

GapP: Compute $gap(f) := acc(f) - rej(f) \in \{-2^n, \ldots, 2^n\}$.

PP: Decide whether $gap(f) > 0$ or ≤ 0.

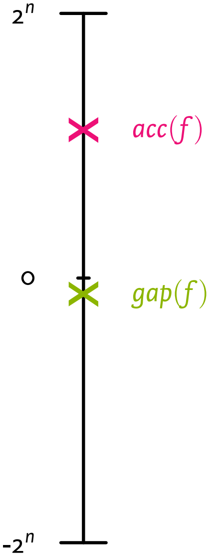
$$P^{\#P} = P^{\mathrm{GapP}} = P^{\mathrm{PP}}$$

The sign problem in complexity theory: approximations



Relative error r: $(1-r)X \leq \tilde{X} \leq (1+r)X$

The sign problem in complexity theory: approximations



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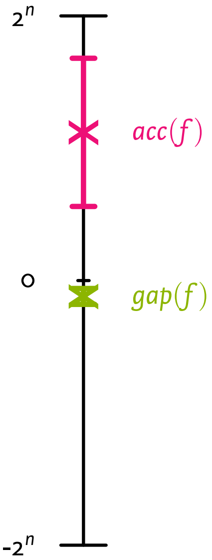

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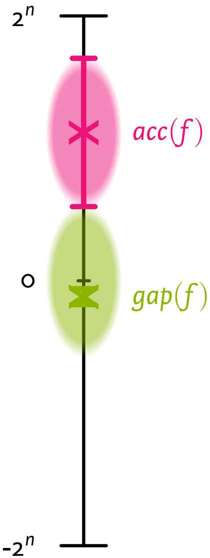

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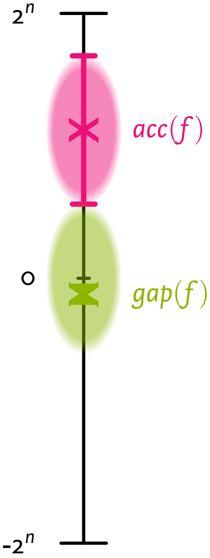
The sign problem in complexity theory: approximations



Relative error r: $(1-r)X \leq \tilde{X} \leq (1+r)X$

$$P^{\mathrm{Apx}_r\mathrm{GapP}} = P^{\mathrm{GapP}} = P^{\mathrm{PP}}$$

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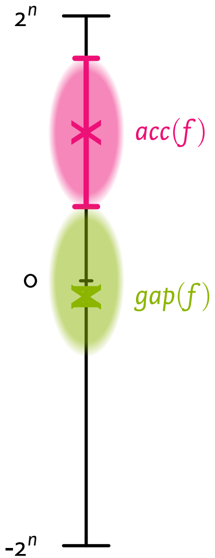

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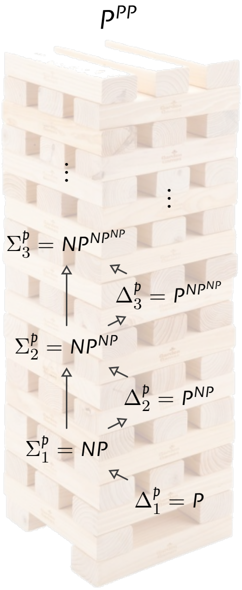

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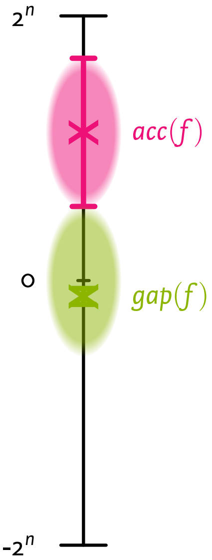

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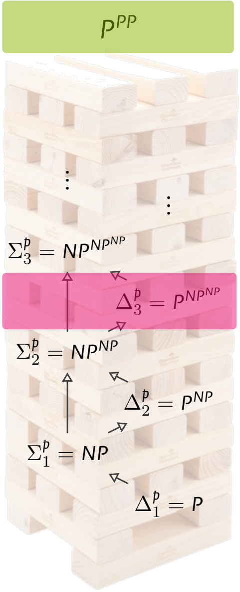
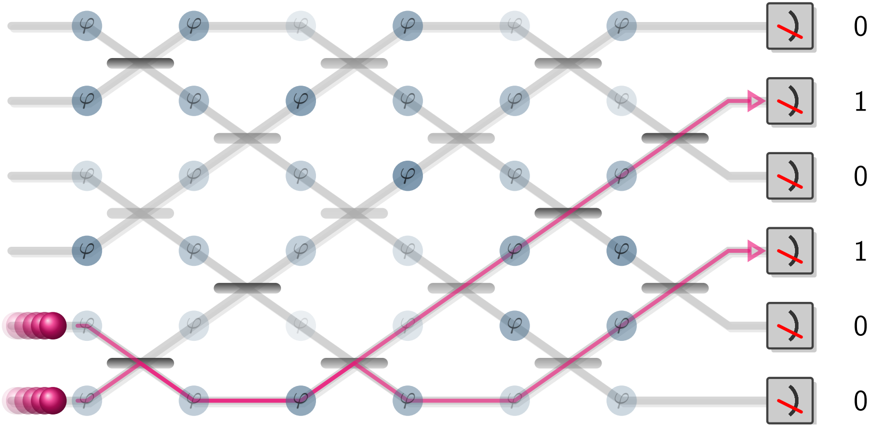


Success probabilities of quantum and classical circuits



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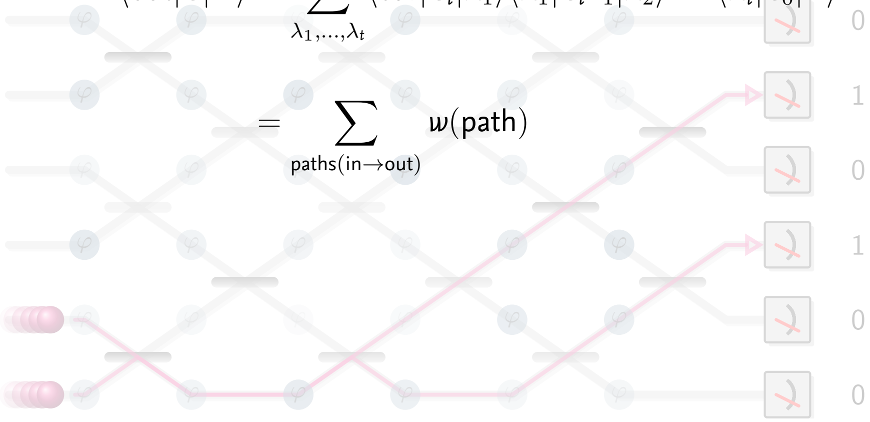

$$\langle \text{out}|C|\text{in}\rangle = \sum_{\lambda_1,\ldots,\lambda_t} \langle out|C_t|\lambda_1\rangle\langle\lambda_1|C_{t-1}|\lambda_2\rangle\cdots\langle\lambda_t|C_0|in\rangle$$

$$= \sum_{\text{paths(in}\to\text{out)}} w(\text{path})$$

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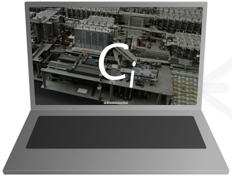
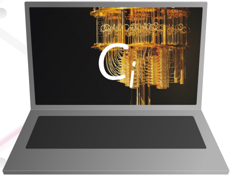
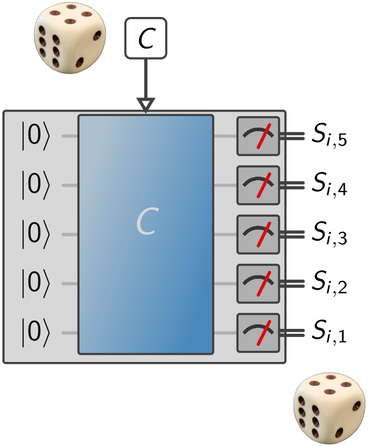


$w(\text{path}) \in C\cdot\{0,1\}$ → #P



$w(\text{path}) \in C'\cdot\{-1,0,1\}$ → GapP

Leveraging hardness of estimation to hardness of sampling



Consider

- n qubits
- $\mathcal{U}$ family of quantum circuits, e.g.
  - $\mathcal{U}$ = Universal circuits (e.g. using Clifford + T-gates) [Boi18]
  - $\mathcal{U}$ = Diagonal (IQP) circuits [BMS16]
- $p_U(x) := |\langle x|U|0\rangle^{\otimes n}|^2$

TASK: Given $U \in_R \mathcal{U}$, sample from p_U.

[BMS16] Bremner, Montanaro, Shepherd, PRL (2016)

[Boi18] Boixo *et al.*, Nature Physics (2018)

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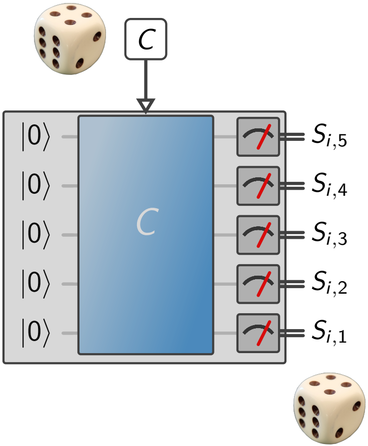

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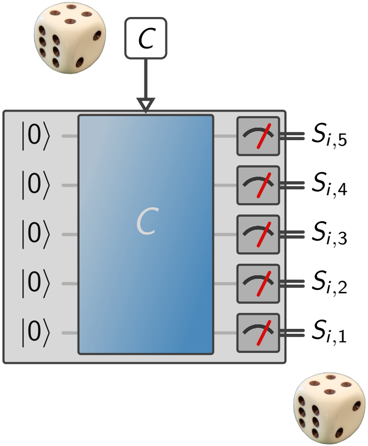

CLASSICAL DERANDOMIZABLE SAMPLING

Given $U \in \mathcal{U}$, uniformly random r, output y s.t.

$$\Pr_x[y] \propto \sum_r f_U(r) = p_U(0^n),$$

for $f_U : \{0,1\}^m \to \{0,1\}$ a #P function.

[BMS16] Bremner, Montanaro, Shepherd, PRL (2016)

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Approximate quantum sampling is classically hard

Assume there exists a *classical polynomial-time, derandomizable algorithm* $\mathcal{A}$ that samples from a distribution p'_U such that $\|p'_U - p_U\|_{\ell_1} \leq \epsilon$.

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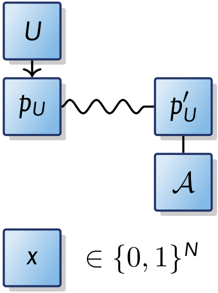

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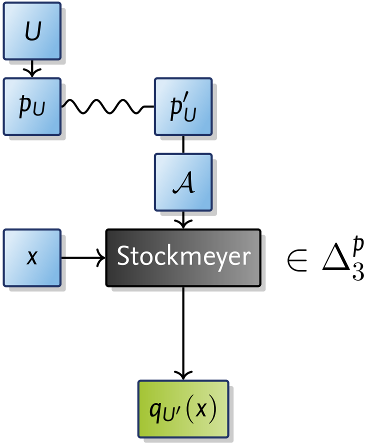

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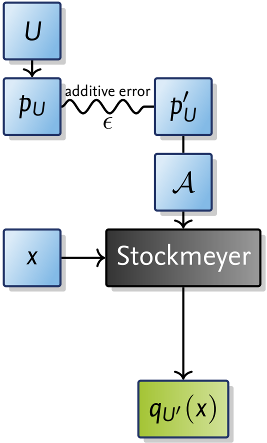

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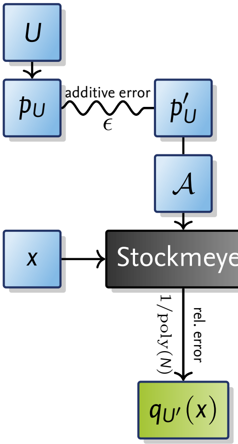

Approximate sampling: $\|p_U - p'_U\|_{\ell_1} \leq \epsilon$

Stockmeyer error: $|q_U(x) - p'_U(x)| \leq \frac{p'_U(x)}{\mathrm{poly}(n)}$

With probability $1-\delta$ over $U \in_R \mathcal{U}$

$$|q_U(x) - p_U(x)| \leq \frac{p_U(x)}{\mathrm{poly}(n)} + \frac{\epsilon}{2^n \delta}\left(1 + \frac{1}{\mathrm{poly}(n)}\right)$$

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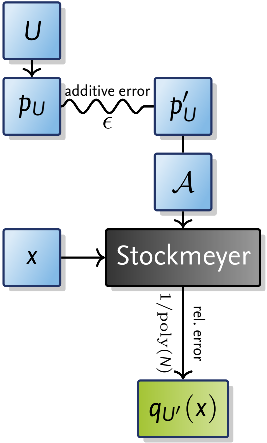

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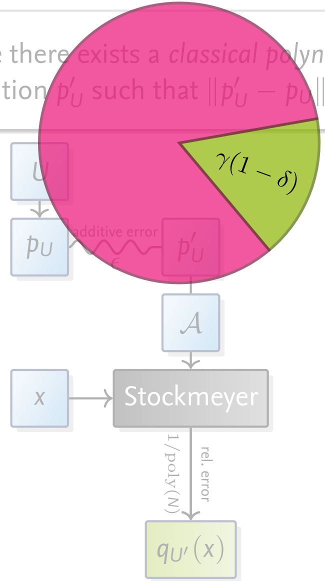

$$|q_U(x) - p_U(x)| \leq \text{const.} \cdot p_U(x)$$

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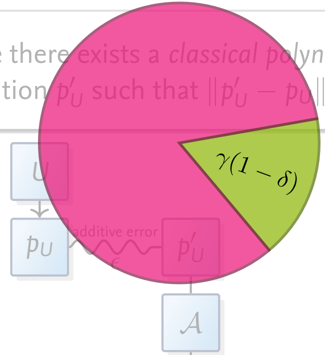

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$q_{U'}(x)$

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$|q_U(x) - \ldots x)|$

Approximate sampling: …

Stockmeyer error: $|q_U(x) \ldots$

With probability $1-\delta$ ove…

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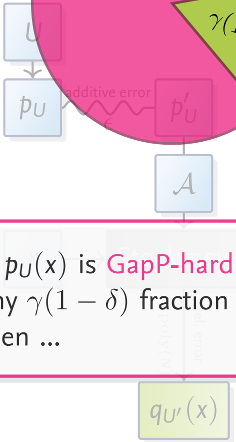

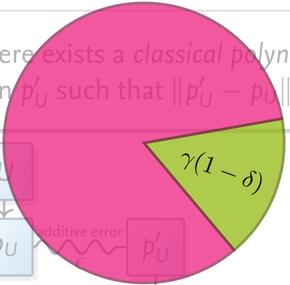

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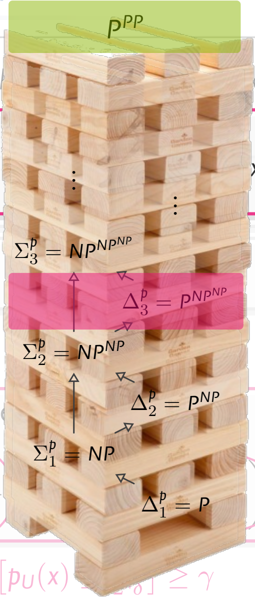

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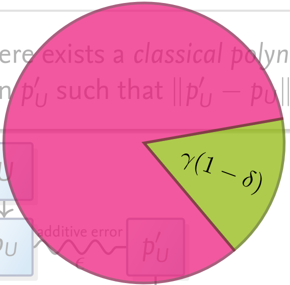

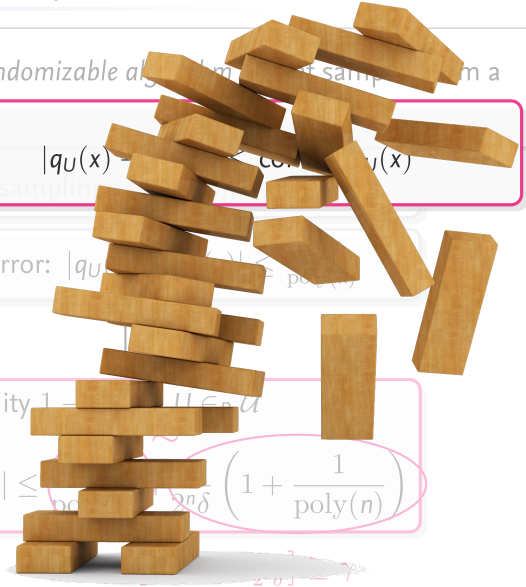

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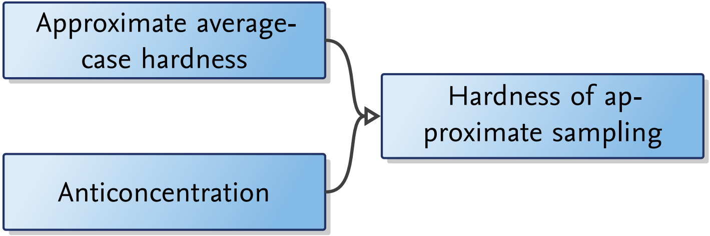
Closing loopholes: the complexity-theoretic argument



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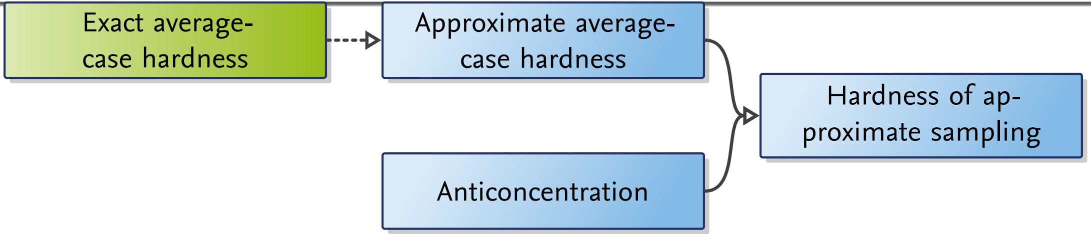
Theorem (Approximate worst-case hardness)

It is #P-hard to approximate the output probabilities of the RQIS scheme to within relative error 1/4.

Theorem (Exact average-case hardness)

It is #P-hard to exactly compute any $3/4 + 1/\mathrm{poly}(n)$ fraction of the output probabilities of the RQIS scheme.



D.H., Bermejo-Vega *et al.* Quantum (2018). Haferkamp, **D.H.** *et al.*, PRL (2020). Brandao, Harrow, Horodecki, CMP (2016). Bouland, Fefferman *et al.* Nat. Phys. (2019).

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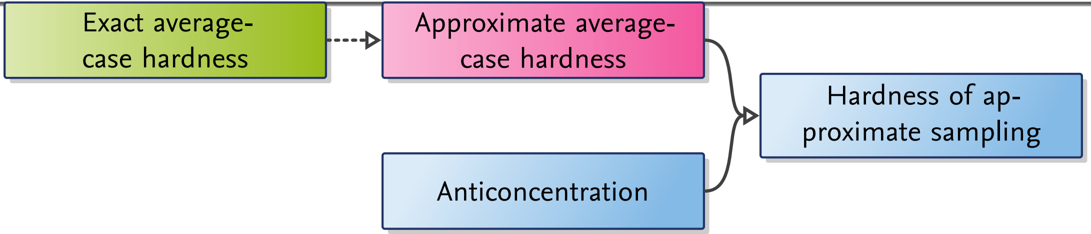

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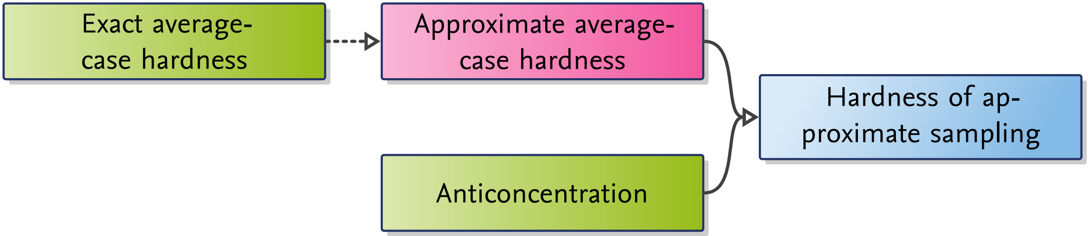
If a circuit family $\mathcal{U}$ satisfies a second moment bound, then its output probabilities $|\langle x|U|0\rangle|^2$ anticoncentrate in the following sense: There exist constants $\alpha, \gamma(\alpha)$ such that

$$\Pr_{U \in_{rand} \mathcal{U}} \left[|\langle x|U|0\rangle|^2 > \frac{\alpha}{2^n} \right] \geq \gamma(\alpha)$$



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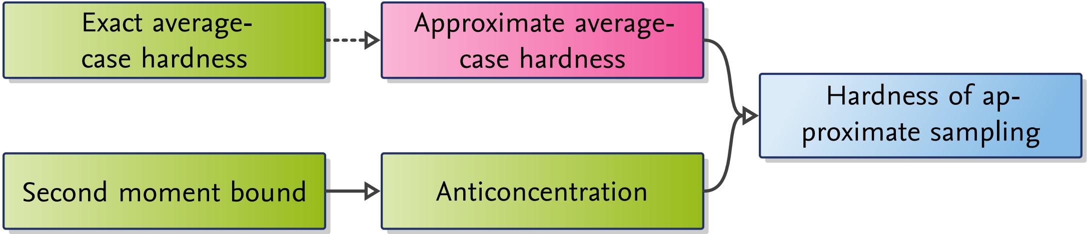

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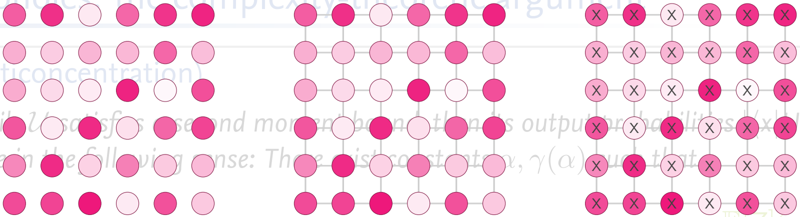
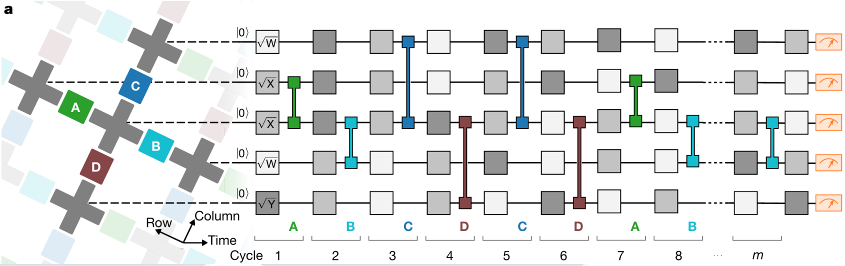


E1: Prepare $|\psi_\beta\rangle$ E2: Quench with H E3: Measure in X



Arute *et al.* Nat. Phys. (2020), Fig. 3a.

D.H., Bermejo-Vega *et al.* Quantum (2018). Haferkamp, **D.H.** *et al.*, PRL (2020). Brandao, Harrow, Horodecki, CMP (2016). Bouland, Fefferman *et al.* Nat. Phys. (2019).

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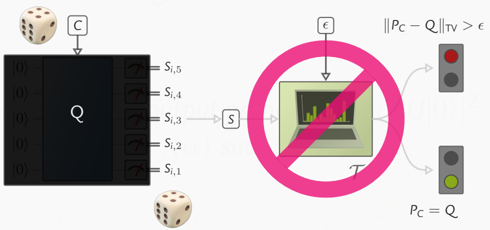


D.H., Kliesch, *et al.*, PRL (2019).

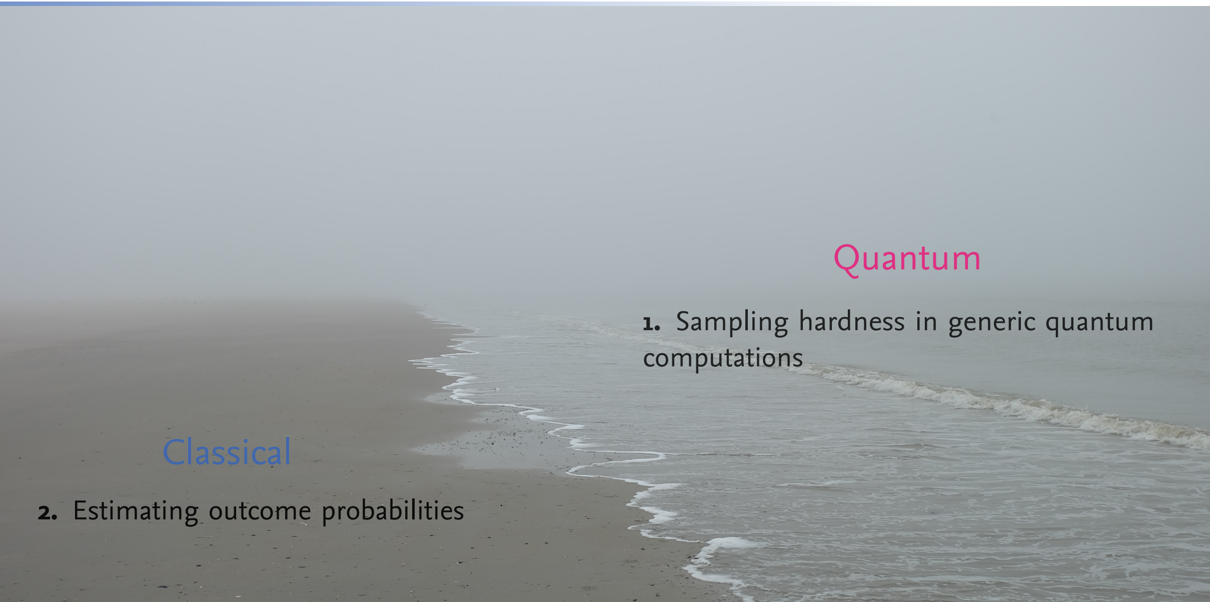
Exact average-case hardness → Approximate average-case hardness

Second moment bound → Anticoncentration

Approximate average-case hardness + Anticoncentration → Hardness of approximate sampling

D.H., Bermejo-Vega *et al.* Quantum (2018). Haferkamp, **D.H.** *et al.*, PRL (2020). Brandao, Harrow, Horodecki, CMP (2016). Bouland, Fefferman *et al.* Nat. Phys. (2019).

Delineating the quantum-classical boundary

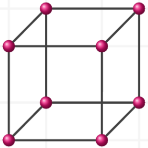


Quantum

1. Sampling hardness in generic quantum computations

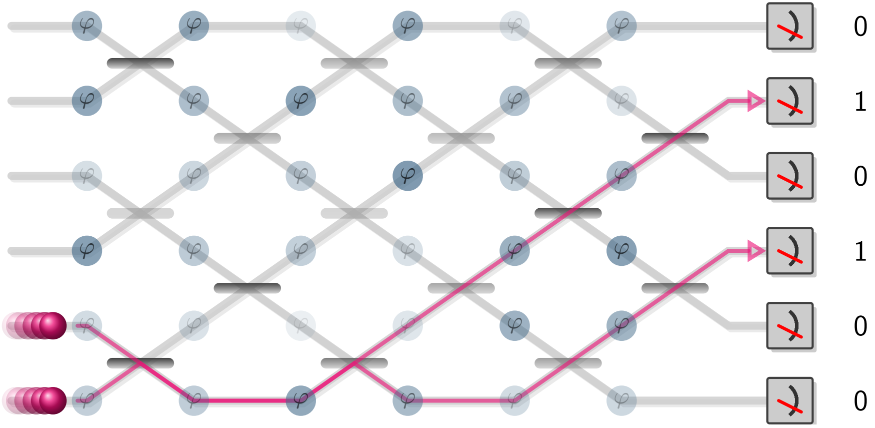
Classical

2. Estimating outcome probabilities



Perspective 2
Estimating quantum properties via classical sampling

The quantum sign problem



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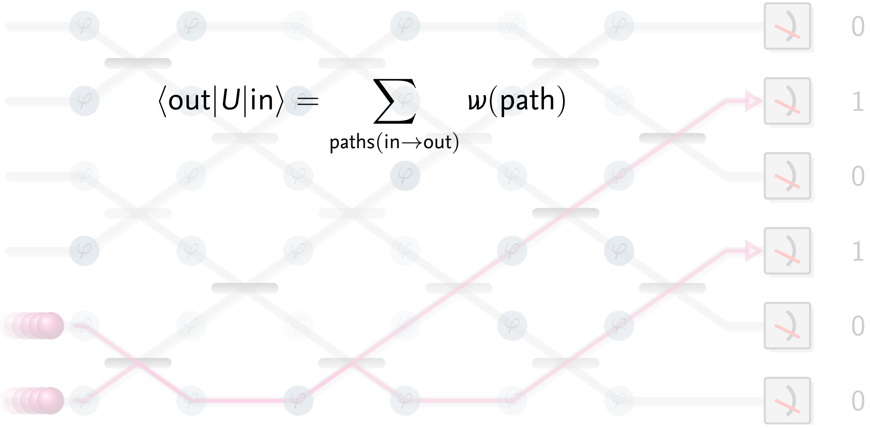
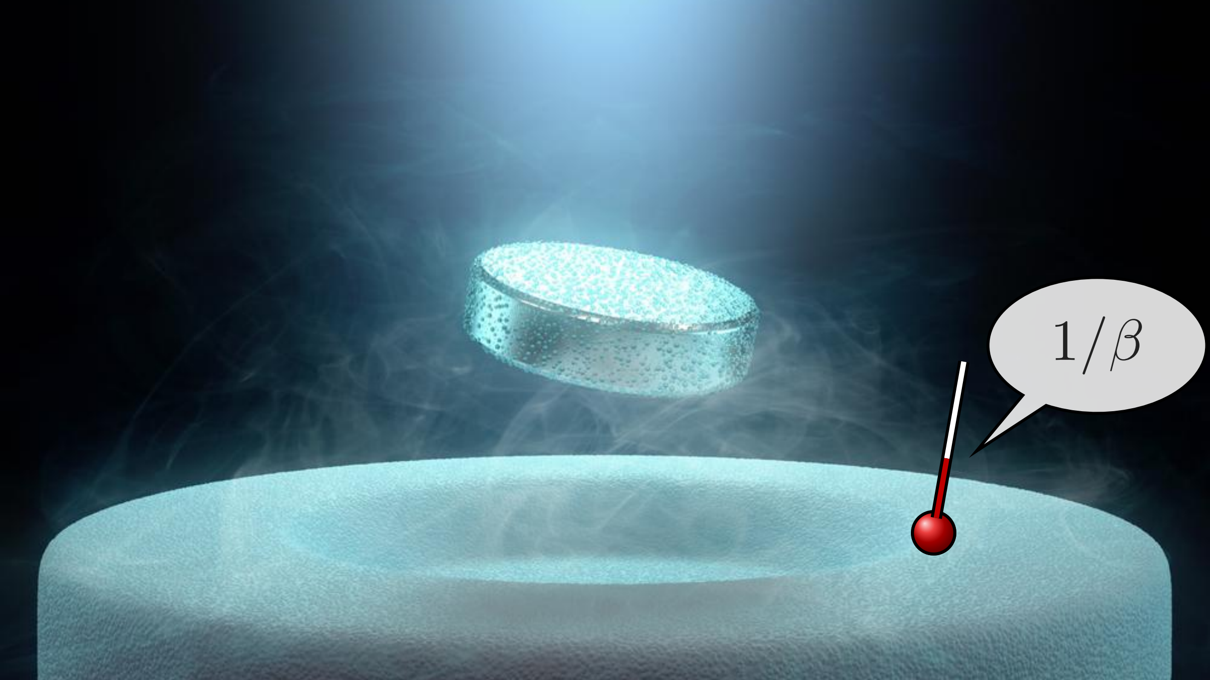


$$\langle \text{out} | U | \text{in} \rangle = \sum_{\text{paths(in}\to\text{out)}} w(\text{path})$$

D.H., Roth *et al.*, Science Adv. (2020).

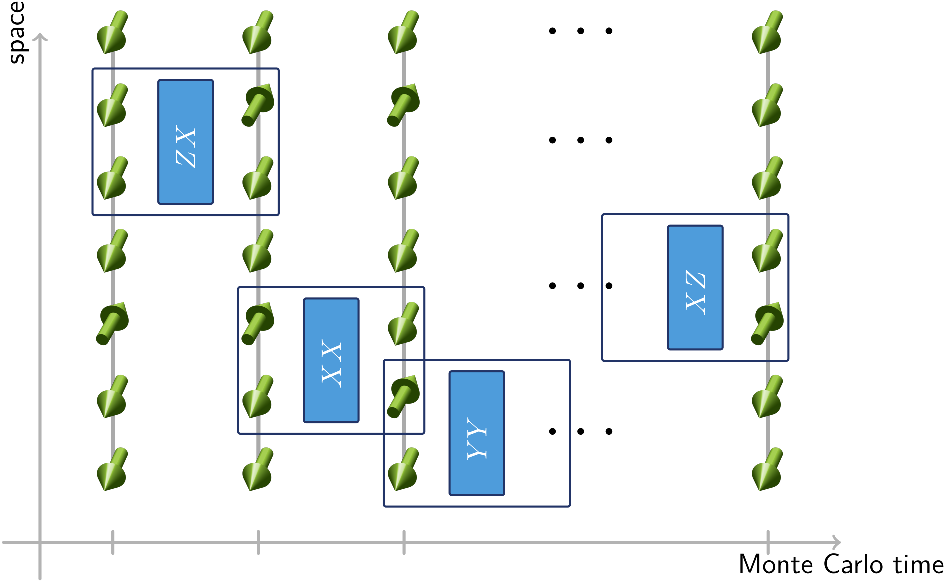
Quantum Monte Carlo


$1/\beta$


$1/\beta$


MC sign problem
$1/\beta$

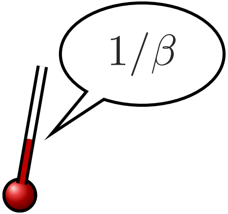
Quantum Monte Carlo



Quantum Monte Carlo

Calculating expectation values via expectation values

$$\langle O \rangle_{\beta,H} = \frac{1}{Z}\,\mathrm{Tr}[\mathrm{e}^{-\beta H} O] = \sum_{\lambda} q(\lambda) O(\lambda) = \langle O \rangle_q$$



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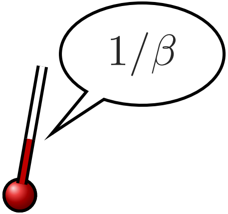
$$\mathrm{e}^{-\beta H} = \left(\mathrm{e}^{-\beta H/m}\right)^m \approx \left(1-\frac{\beta}{m}H\right)^m =: (T_m)^m$$



Quantum Monte Carlo

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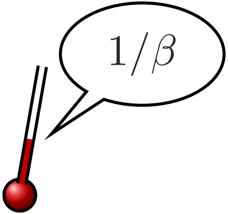
$$\downarrow \qquad \downarrow \qquad \downarrow$$

$$\langle O\rangle_{\beta,H} = \frac{1}{Z}\,\mathrm{Tr}[\mathrm{e}^{-\beta H}O] \approx \frac{1}{Z}\,\mathrm{Tr}[T_m^m O]$$

$$= \frac{1}{Z}\sum_{\lambda} T_m(\lambda_1|\lambda_2)T_m(\lambda_2|\lambda_3)\cdots T_m(\lambda_m|\lambda_{m+1})O(\lambda_{m+1}|\lambda_1)$$

$$\equiv \frac{1}{Z}\sum_{\lambda} a(\lambda)O(\lambda)$$



Quantum Monte Carlo

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$$e^{-\beta H} = \left(e^{-\beta H/m}\right)^m \approx \left(1 - \frac{\beta}{m}H\right)^m =: (T_m)^m$$

$1/\beta$

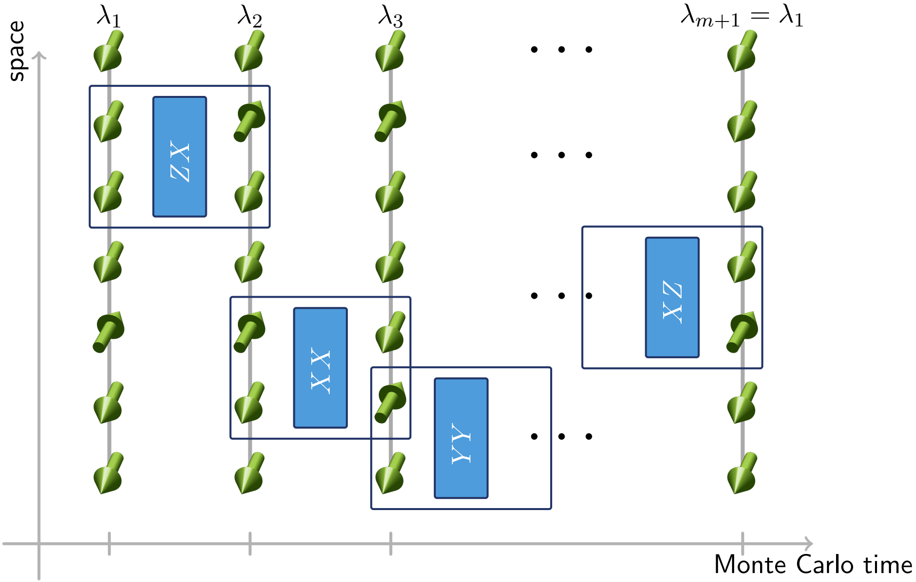
$\langle O\rangle_\beta$

Monte Carlo sampling

Draw λ with probability $q(\lambda) = \frac{a(\lambda)}{\sum_\lambda a(\lambda)}$.

- Metropolis sampling with transition rate $W_{\lambda\to\lambda'} = q(\lambda')/q(\lambda)$:
- Markov chain: $\lambda^{(1)} \to \lambda^{(2)} \to \cdots \to \lambda^{(s)}$

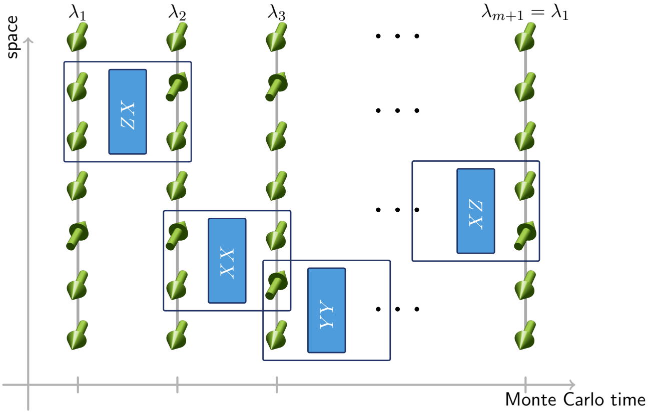
$$\equiv \frac{1}{Z}\sum_\lambda a(\lambda)O(\lambda)$$



$$a(\lambda) = \quad T_m(\lambda_1|\lambda_2) \cdot T_m(\lambda_2|\lambda_3) \cdot T_m(\lambda_3|\lambda_4) \cdot \;\cdots\; \cdot T_m(\lambda_m|\lambda_1)$$

The Monte Carlo sign problem

$$\langle O \rangle_{\beta,H} = \langle O \rangle_q$$



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$$\langle O \rangle_{\beta,H} = \langle O \rangle_q = \sum_{\lambda} p(\lambda) O'(\lambda)$$

The best Monte Carlo estimator: Absolute value

The variance-optimal estimator

$$q(\lambda) \to p(\lambda) = |q(\lambda)| / \|q(\lambda)\|_{\ell_1}$$
$$O(\lambda) \to O'(\lambda) = \mathrm{sign}(q(\lambda)) \|q(\lambda)\|_{\ell_1} O(\lambda)$$

The Monte Carlo sign problem

$$\langle O\rangle_{\beta,H} = \langle O\rangle_q = \sum_{\lambda} p(\lambda) O'(\lambda) \approx \frac{1}{M}\frac{1}{\langle \mathrm{sign}\rangle} \sum_{\lambda_1,\ldots,\lambda_M} \mathrm{sign}(q(\lambda_i))$$

$\lambda_i \sim_{\mathrm{rand}} p$

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Pashayan, Wallman, Bartlett: PRL, 2015.

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has sample complexity

$$s \sim \|q\|_{\ell_1}^2 - 1 \equiv \frac{1}{\langle\mathrm{sign}\rangle_q^2} - 1 \qquad \text{with} \qquad \langle\mathrm{sign}\rangle_q = \frac{\sum_\lambda |q(\lambda)|\,\mathrm{sign}(q(\lambda))}{\sum_\lambda |q(\lambda)|}.$$

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The Monte Carlo sign problem

The Monte Carlo sign problem

- $T_m = (1 - \beta H/m)$
- $a(\lambda) = T_m(\lambda_1|\lambda_2)T_m(\lambda_2|\lambda_3)\cdots T_m(\lambda_m|\lambda_1)$

  $\Rightarrow q(\lambda) = a(\lambda)/\sum_\lambda a(\lambda)$
- Sign problem: $q(\lambda) < 0$

  $\Rightarrow p(\lambda) = |q(\lambda)|/\sum_\lambda |q(\lambda)|$
- Exponential increase in sample complexity!

has sample complexity

$$s \sim \|q\|_{\ell_1}^2 - 1 \equiv \frac{1}{\langle \mathrm{sign} \rangle_q^2} - 1 \in \exp(n) \quad \text{with} \quad \langle \mathrm{sign} \rangle_q = \frac{\sum_\lambda |q(\lambda)|\, \mathrm{sign}(q(\lambda))}{\sum_\lambda |q(\lambda)|}.$$

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Easing the sign problem

Sign problem 2: Invariance under basis transformations

$$\mathrm{Tr}[\mathrm{e}^{-\beta H} O] = \mathrm{Tr}[Z \mathrm{e}^{-\beta H} O Z^{-1}] = \mathrm{Tr}[(Z T_m Z^{-1})^m Z O Z^{-1}].$$

→→ The sign problem is a basis-dependent property. ←←

Bravyi, DiVincenzo, Oliveira, Terhal: arXiv:quant-ph/0606140.
Bravyi, Terhal: arXiv:0806.1746.
Cubitt, Montanaro: arXiv:1311.3161.
Troyer and Wiese, PRL, 2008.
Hastings, J. Math. Phys (2015)
Marvian, Hen, Lidar, arXiv:1802.03408.
Klassen and Terhal, arXiv:1806.05405.
Klassen, Marvian *et al.*, arXiv:1906.08800.

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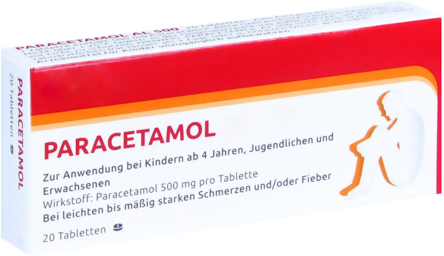

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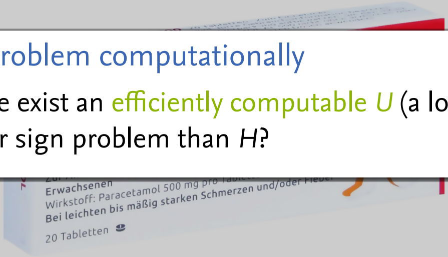

Easing the sign problem computationally

Given H, does there exist an efficiently computable U (a local circuit) such that $UHU^\dagger$ has a smaller sign problem than H?

Bravyi, DiVincenzo, Oliveira, Terhal: arXiv:quant-ph/0606140.
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What is the optimal basis?

Recall the sample complexity of QMC: $s \sim \langle \mathrm{sign} \rangle_p^{-2} - 1$.

Chandrasekharan, Wiese: PRL, 1999.

Shinaoka *et al.*: PRB, 2015.

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$$\arg\min_{U \in \mathcal{U}} \frac{1}{\langle \mathrm{sign} \rangle_p} = \arg\min_{U \in \mathcal{U}} \mathrm{Tr}\left[|U T_m U^\dagger|^m - (U T_m U^\dagger)^m \right]$$

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Computing the average sign via Monte Carlo

$$\frac{\mathrm{Var}[\langle \mathrm{sign} \rangle_q]}{\langle \mathrm{sign} \rangle^2} = \frac{1}{\langle \mathrm{sign} \rangle^2} - 1$$

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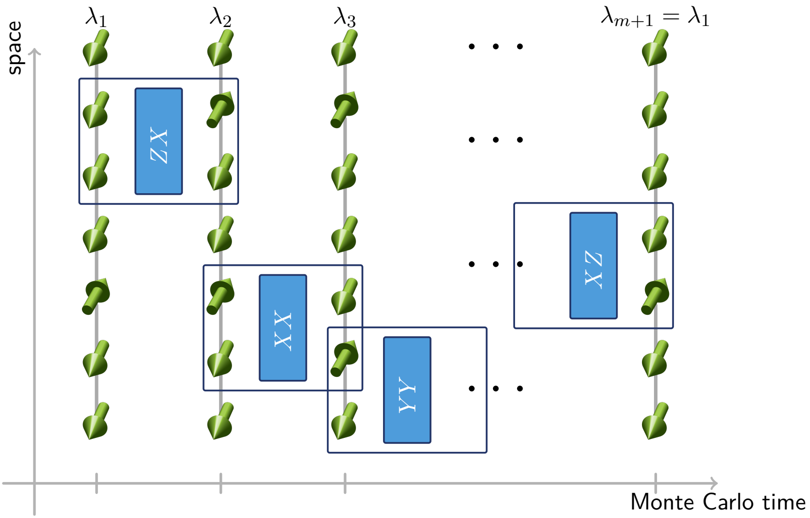

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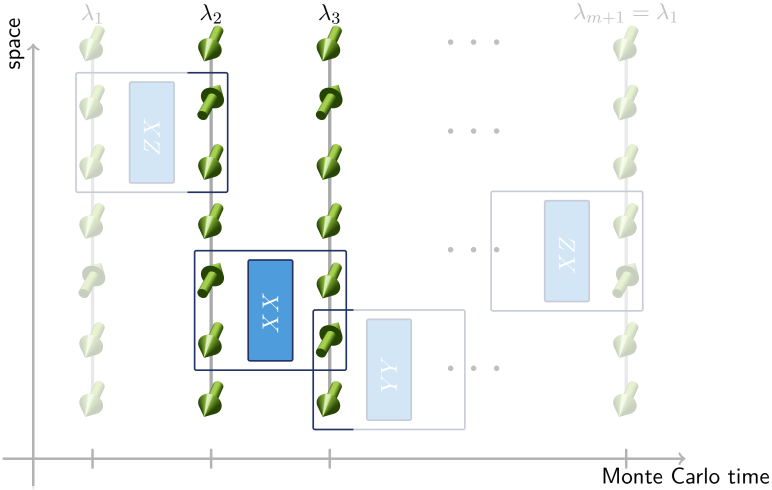

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Non-stoquasticity

$$\begin{pmatrix} - & + & + & 0 \\ + & + & 0 & - \\ + & 0 & - & 0 \\ 0 & - & 0 & 0 \end{pmatrix}$$

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Non-stoquasticity

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Easing the sign problem: average sign vs. non-stoquasticity

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The non-stoquasticity

$$\nu_1(UHU^\dagger) := \| |UT_mU^\dagger| - UT_mU^\dagger \|_{\ell_1} = \| (UHU^\dagger)_{\text{non-stoq.}} \|_{\ell_1}$$

can be *computed efficiently* for 2-*local* Hamiltonians

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Average sign vs. non-stoquasticty: Analytical evidence

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To first order in the *non-stoquastic matrix entries*:

$$S(U) \approx 2m \| |UT_mU^\dagger| - UT_mU^\dagger \|_{\ell_1} \cdot \| (|UT_mU^\dagger| + UT_mU^\dagger)^{m-1} \|_{\ell_\infty}$$

$$\propto d\, \nu_1(H).$$

Average sign vs. non-stoquastiсty: Analytical evidence

For generic instances, we expect

$$1/\langle \mathrm{sign} \rangle \propto \exp\left(d\nu_1(H)\right)$$

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SPARSITY

ℓ_1-norm

NEGATIVITY

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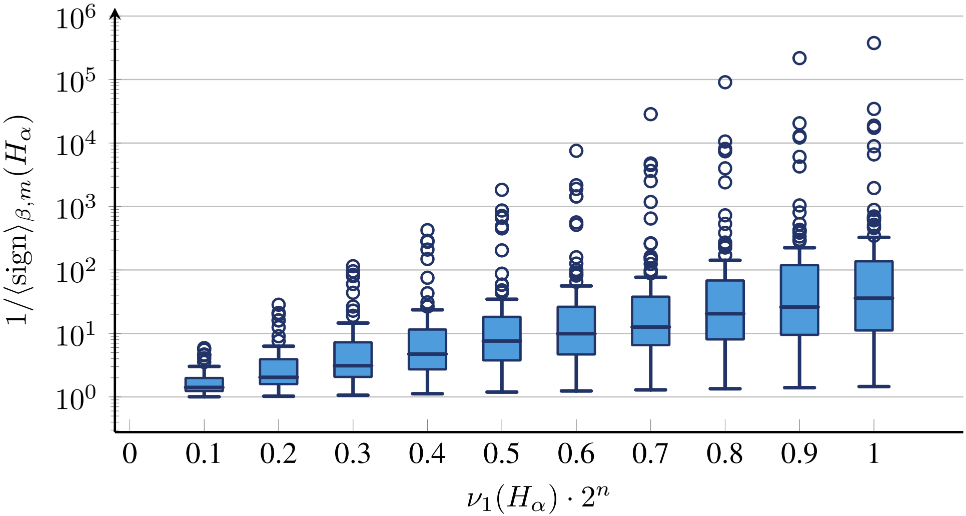
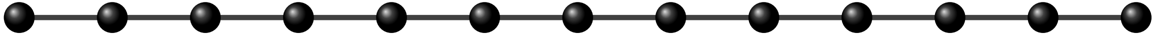
Average sign vs. non-stoquasticty: Numerical evidence



$$H_\alpha = \frac{H - H_{\text{non-stoq.}} + \alpha H_{\text{non-stoq.}}}{\|H_{\text{non-stoq.}}\|_{\ell_1}}.$$



Easing in practice: Translation-invariant problems

Translation-invariant non-stoquasticity

$$H = \sum_{i=1}^{n} T_i(h)$$

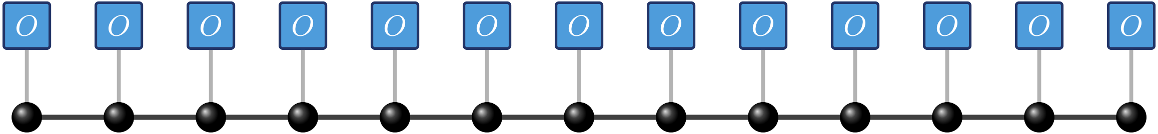
$$\longrightarrow \quad \nu_1(H) \propto \tilde{\nu}_1(h)$$

Easing in practice: Translation-invariant problems

Translation-invariant non-stoquasticity

$$O^{\otimes n} H (O^T)^{\otimes n} = \sum_{i=1}^{n} T_i((O \otimes O) h (O^T \otimes O^T))$$

$$\longrightarrow \quad \nu_1(H) \propto \tilde{\nu}_1((O \otimes O) h (O^T \otimes O^T))$$



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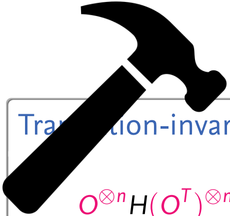

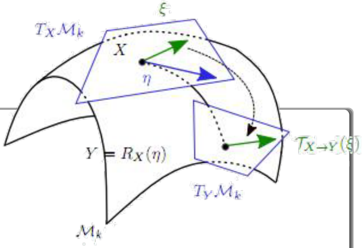

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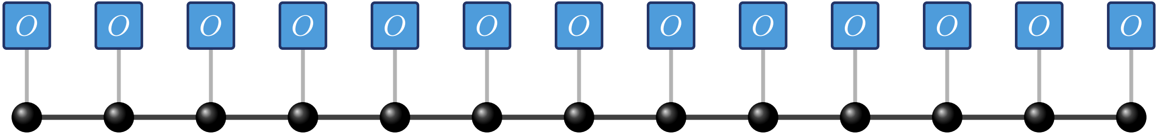
GitLab



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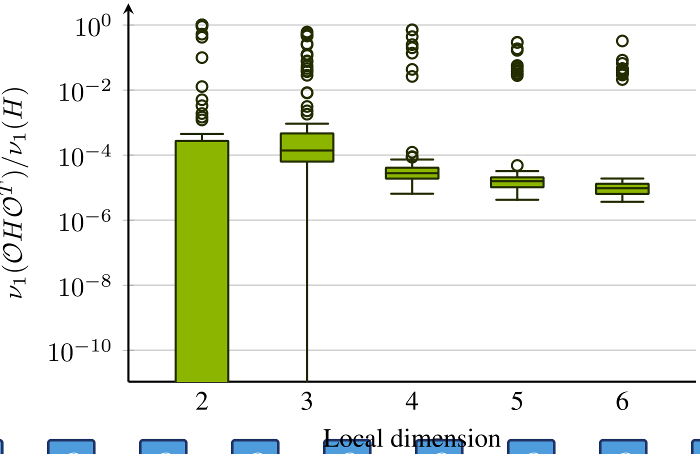
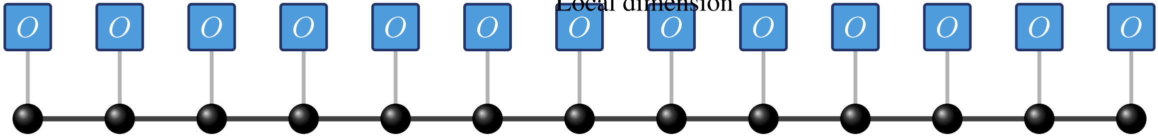


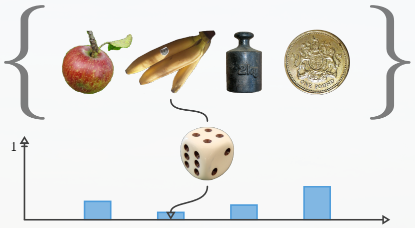



Quantum
Classical


Quantum
Classical


Classical
Quantum

Outlook



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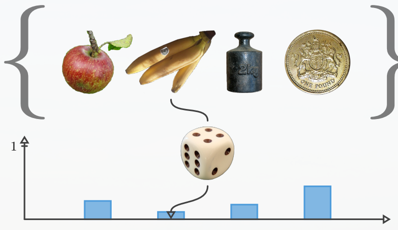

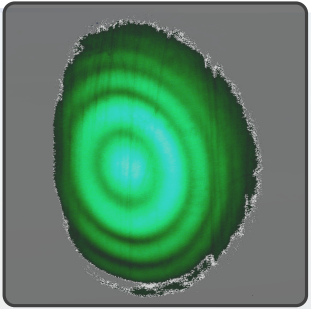

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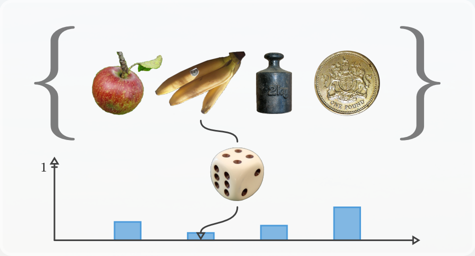
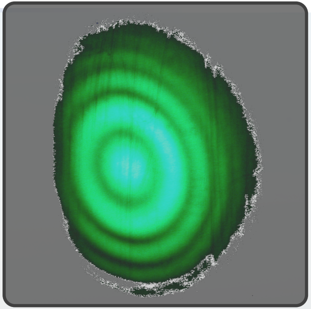
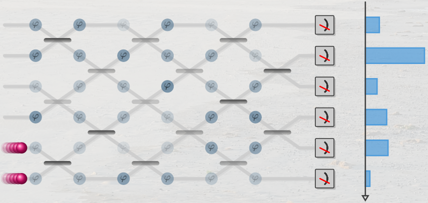
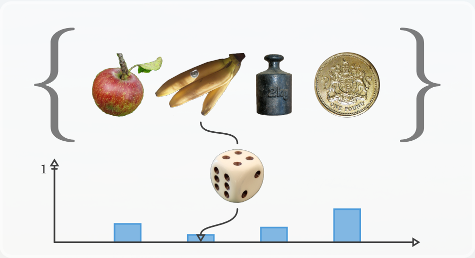
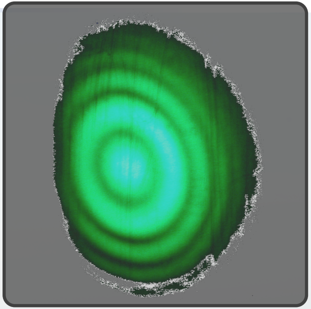


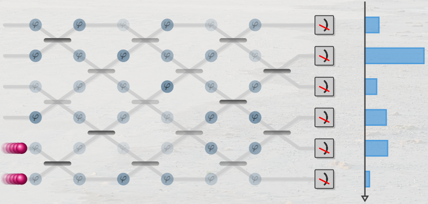


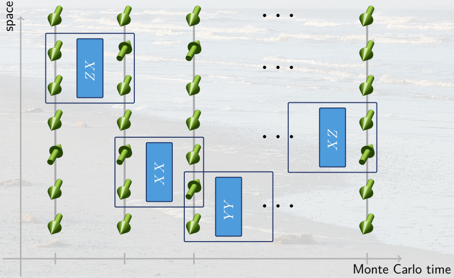


Outlook









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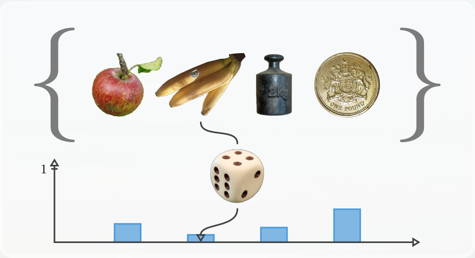

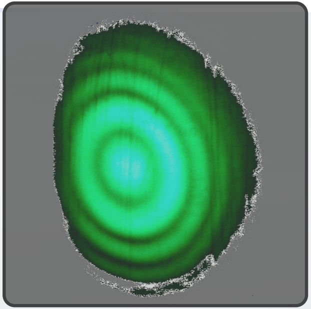

Is the quantum sign problem intrinsic or artificial? [ZOR20]

[ZOR20] Zurel, Okay, Raussendorf, PRL (2020).