Quantum Computing (QC)

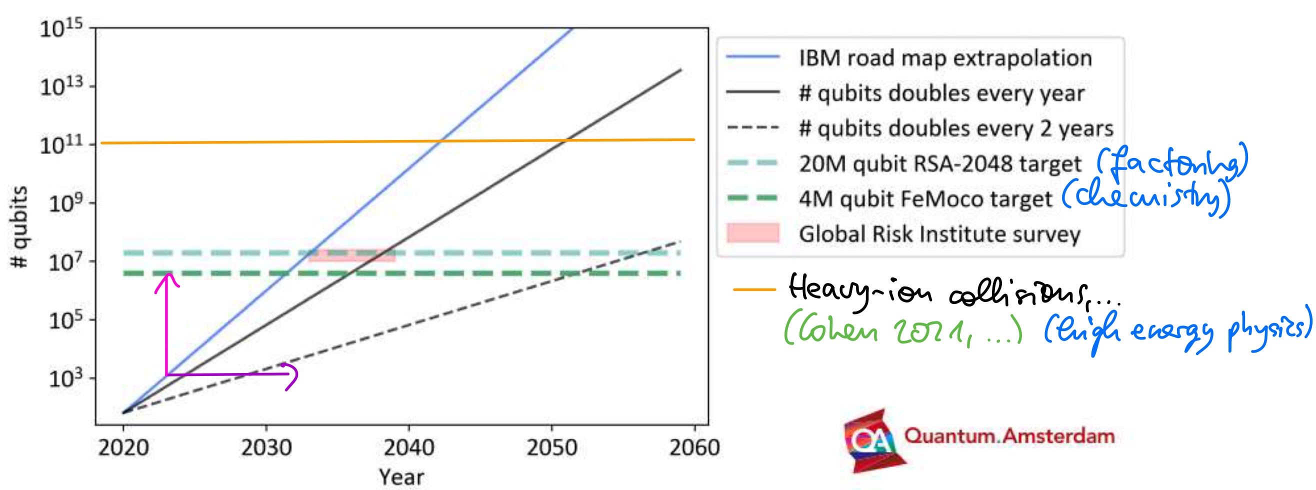
1 Introduction

1.1 Past, present, future of QC

- 1980-82: Concept of QC (Benioff, Feynman, Manin, ...)
- 1985-93: First quantum algorithms (Deutsch, ...) (see Thu.)
- 1994: Quantum algorithm for factoring (Shor)

⋮

- 2019-...: "Quantum supremacy" (Arute et al., Zhong et al., ...)
  - ⇒ exponential speedup of artificial computations, e.g. quantum: 200 s vs. classical: 10,000 y (Arute et al.)
  - ⇒ partially refuted: "Closing the quantum supremacy gap", classical: 2.5 d (2019) → 304 s (2021) (Yong et al.)
- State-of-the-art: Noisy Intermediate-Scale Quantum era
- Rough sketch of the future:

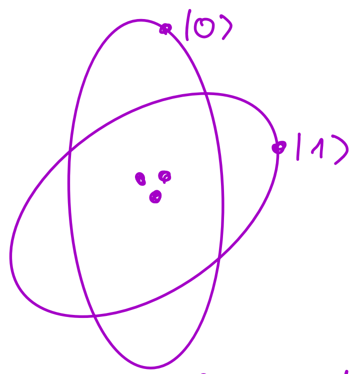


- Biggest challenge: quantum error correction (QEC) (see Thu.)
  - ⇒ need $\mathcal{O}(10^3-10^4)$ qubits to encode one QECed qubit
  - ⇒ still many years away from useful QC applications

1.2 Basics of QC

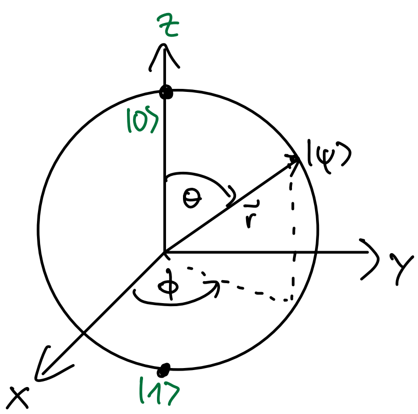
1.2.1 Qubits

- Classical computer: bit takes values 0 or 1
- Quantum computer: qubit is 2-dim. quantum state:
  - ⇒ $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{pmatrix}\alpha \\ \beta\end{pmatrix}$ ⇒ superposition
  - ⇒ basis states: $|0\rangle = \begin{pmatrix}1 \\ 0\end{pmatrix}$, $|1\rangle = \begin{pmatrix}0 \\ 1\end{pmatrix}$ ⇒ "computational basis" = "z basis"
  - ⇒ coefficients: $\alpha, \beta \in \mathbb{C}$, $|\alpha|^2 + |\beta|^2 = 1$
  - ⇒ infinitely many possible states



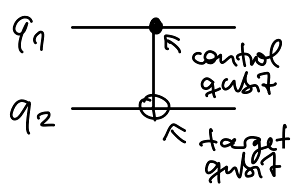
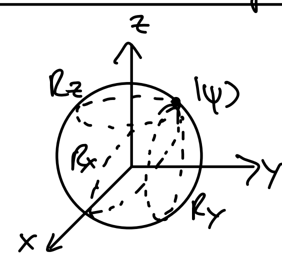
e.g. levels in atom

- Bloch sphere representation:
  - ⇒ $|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle$
  - ⇒ Bloch vector: $\vec{r} = \begin{pmatrix}\sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta\end{pmatrix}$



1.2.2 Quantum gates

- Classical gates: e.g. NOT $\quad 0 \xrightarrow{NOT} 1$, $\; 1 \xrightarrow{NOT} 0$
- Quantum gates: represented by <u>unitary</u> matrices
  $\Rightarrow$ e.g. $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \xrightarrow{NOT} |\psi'\rangle = \alpha|1\rangle + \beta|0\rangle$
- Matrix representation: e.g. $NOT \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = X$ (Pauli σ_x)
  $\Rightarrow |\psi\rangle \xrightarrow{NOT} |\psi'\rangle = X|\psi\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \beta \\ \alpha \end{pmatrix}$
  $\Rightarrow$ unitary: $X^{+}X = XX = 1$
- Common gates:

Name	Circuit rep.	Matrix rep.	Acting on qubit
X	$-\boxed{X}-$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\|0\rangle \to \|1\rangle$, $\|1\rangle \to \|0\rangle$
Y	$-\boxed{Y}-$	$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$	$\|0\rangle \to -i\|1\rangle$, $\|1\rangle \to i\|0\rangle$
Z	$-\boxed{Z}-$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\|0\rangle \to \|0\rangle$, $\|1\rangle \to -\|1\rangle$
Hadamard $\Rightarrow$ superposition	$-\boxed{H}-$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$	$\|0\rangle \to \frac{1}{\sqrt{2}}(\|0\rangle + \|1\rangle)$ $\|1\rangle \to \frac{1}{\sqrt{2}}(\|0\rangle - \|1\rangle)$
CNOT $\Rightarrow$ entanglement		$\begin{pmatrix} \begin{matrix} 1 & 0 \\ 0 & 1 \end{matrix} & 0 \\ 0 & \underbrace{\begin{matrix} 0 & 1 \\ 1 & 0 \end{matrix}}_{X} \end{pmatrix}$	$\|00\rangle \to \|00\rangle$ $\|01\rangle \to \|01\rangle$ $\|10\rangle \to \|11\rangle$ $\|11\rangle \to \|10\rangle$ unchanged = "control" changes iff control is in state $\|1\rangle$ = "target"
$R_X(\theta)$ $R_Y(\theta)$ $R_Z(\theta)$	$-\boxed{R_X(\theta)}-$ $-\boxed{R_Y(\theta)}-$ $-\boxed{R_Z(\theta)}-$	$\exp\left(-i\frac{\theta}{2}X\right)$ $\exp\left(-i\frac{\theta}{2}Y\right)$ $\exp\left(-i\frac{\theta}{2}Z\right)$	

⇒ rotation

⇒ crucial for physics & chemistry applications (see Fri.)

- Remark: N-qubit gates act on N qubits

  ⇒ N qubits can be in superposition of 2^N basis states

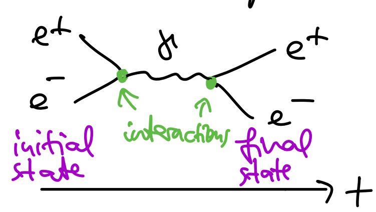
  ⇒ QC efficiently encodes <u>exponentially</u> large Hilbert space

1.2.3 Quantum circuits

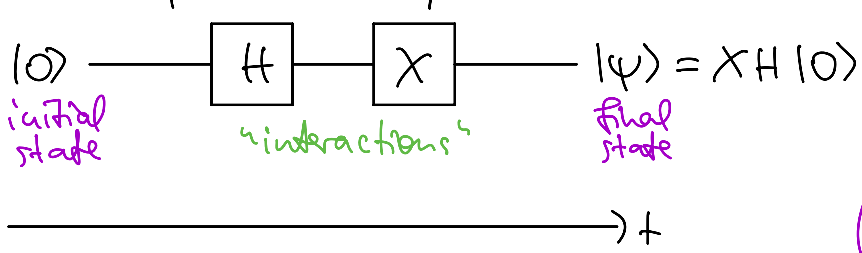
- Three stages of gate-based quantum computations:
  (i) Initialization of all N qubits in $|0\rangle$ state
  (ii) Unitary transformations = quantum gates
  (iii) Measurement of all or some qubits

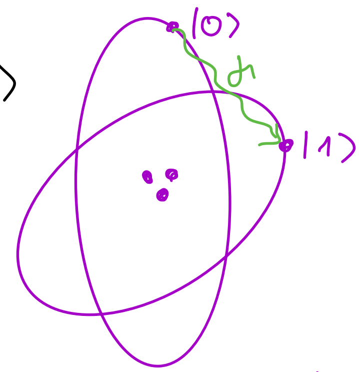
- Quantum circuit diagram:

  ⇒ useful tool to visualize quantum computations, like Feynman diagrams:



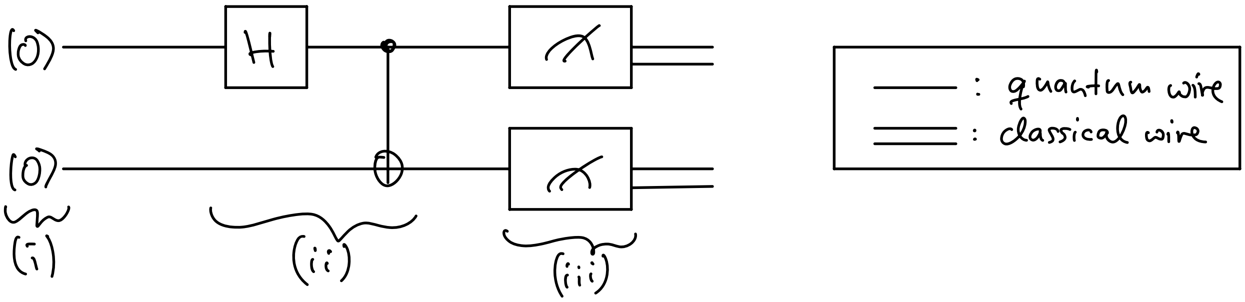
  ⇒ one-qubit example:





e.g. levels in atom
manipulate them by e.g. laser light

- Two-qubit example with measurement:



(i) tensor product: $|0\rangle \otimes |0\rangle \equiv |00\rangle$

(ii) matrix product: $|00\rangle \xrightarrow{H} \frac{1}{\sqrt{2}}\big(|00\rangle + |10\rangle\big)$

$$\xrightarrow{CNOT} \frac{1}{\sqrt{2}}\big(|00\rangle + |11\rangle\big) \equiv |\psi\rangle$$

(iii) —[meter]═ : projective measurement in computational basis

⇒ probability $p_{0,1}$ of measuring $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ in state $|0\rangle, |1\rangle$:

$$p_0 \equiv \langle\psi|M_0|\psi\rangle = \langle\psi|0\rangle\langle 0|\psi\rangle = |\alpha|^2$$

$$p_1 \equiv \langle\psi|M_1|\psi\rangle = \langle\psi|1\rangle\langle 1|\psi\rangle = |\beta|^2$$

⇒ $M_{0,1}$: measurement operators = orthogonal projectors

⇒ Example: $p_{00} \equiv p(|00\rangle) = \frac{1}{2}$, $p_{11} \equiv p(|11\rangle) = \frac{1}{2}$

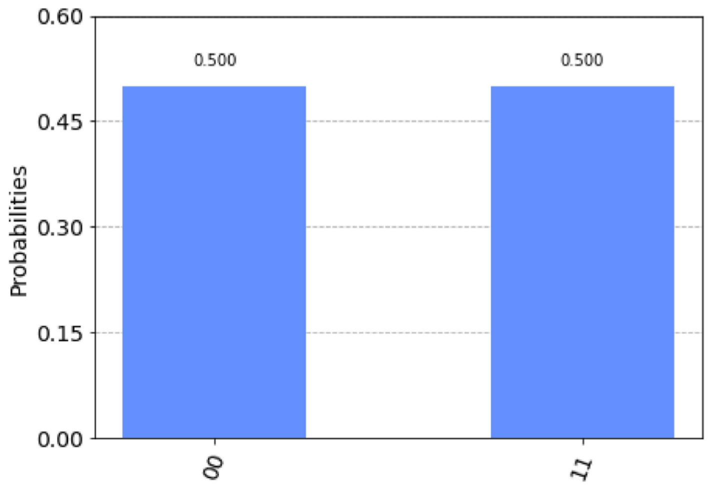
⇒ <u>Bell state</u>: if we measure one qubit, we know state of the other qubit

⇒ <u>Entanglement</u>: key ingredient of quantum parallelism (see Thu.)

2 Quantum errors

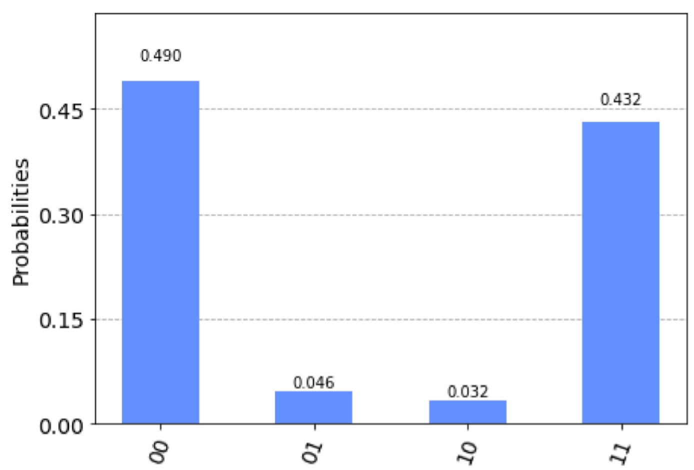
2.1 Example: Bell state

- Classical simulation of noise-free QC:



(see "Quantum Programming Tutorial 1: Bell State" by "Full-Stack Quantum Computation" website)

- Quantum simulation, e.g. on IBM-Q's "Melbourne" device



$\Rightarrow \mathcal{O}(10^{-2})$ errors, but old data (2020, see website above)

$\Rightarrow$ current typical error rates: $\mathcal{O}(10^{-3})$ (Acharya et al. 2408.13687)

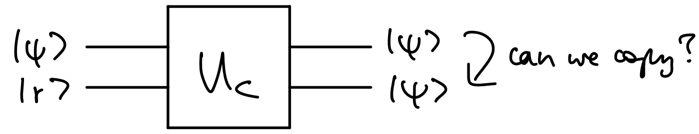
2.2 Quantum error correction (QEC)

- Classically: can copy arbitrary bits

$\Rightarrow$ simple error correction

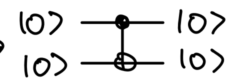
$\Rightarrow$ e.g. repetition code

- Quantum version?

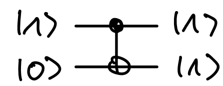


- Aim: find U_c to copy arbitrary state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$
- First: copy basis states ✓

$$U_c|0\rangle \otimes |r\rangle \longrightarrow |0\rangle \otimes |0\rangle \xrightarrow{\text{for } |r\rangle = |0\rangle}$$



$$U_c|1\rangle \otimes |r\rangle \longrightarrow |1\rangle \otimes |1\rangle \xrightarrow{\text{for } |r\rangle = |0\rangle}$$



- Next: try to copy arbitrary state

$$\begin{aligned} U_c|\psi\rangle \otimes |r\rangle &= U_c\,(\alpha|0\rangle + \beta|1\rangle) \otimes |r\rangle \\ &= U_c(\alpha|0\rangle \otimes |r\rangle + \beta|1\rangle \otimes |r\rangle) \\ &= \alpha|0\rangle \otimes |0\rangle + \beta|1\rangle \otimes |1\rangle \\ &\neq |\psi\rangle \otimes |\psi\rangle \end{aligned}$$

- A quantum state cannot be copied with perfect fidelity

  $\Rightarrow$ "no-cloning theorem" (proof: Wootters, Zurek, Nature 299, 802 (1982))

  $\Rightarrow$ no simple QEC!

- QEC requires
  - (i) additional qubits
  - (ii) noise below certain threshold
- Many QEC "codes": Shor's code, GKP code, ...

⇒ example: surface code requires

(i) $\Theta(10^4)$ additional qubits per logical qubit

(ii) for physical error rate of $p \leq 10^{-5}$

(see e.g. Campbell et al., 1612.07330)

- Near-future "compromise": quantum error mitigation

⇒ example: zero-noise extrapolation for Schwinger model

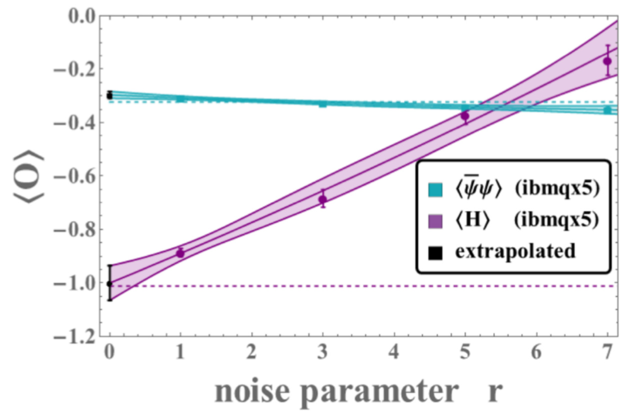


FIG. 2. The $H^{\tilde{\Lambda}=3}_{\mathbf{k}=\mathbf{0},+}$ ground state energy and chiral condensate (purple, blue extrapolated to -1.000(65) and -0.296(13), respectively) expectation values as a function of r, the noise parameter. $r-1$ is the number of additional CNOT gates inserted at each location of a CNOT gate in the original VQE circuit. (1200 IBM allocation units and ∼ 6.4 QPU·s)

(Klco et al., 1803.03326) (algorithm: see Fri.)

3 Quantum algorithms

3.1 Deutsch algorithm

- Simple algorithm that demonstrates concept of quantum parallelism ⇒ inspiration for Shor's algorithm
- Goal: Given a black-box function $f: \{0,1\} \to \{0,1\}$, find out if $f(0) = f(1)$ ⇒ constant 1€ → 1€

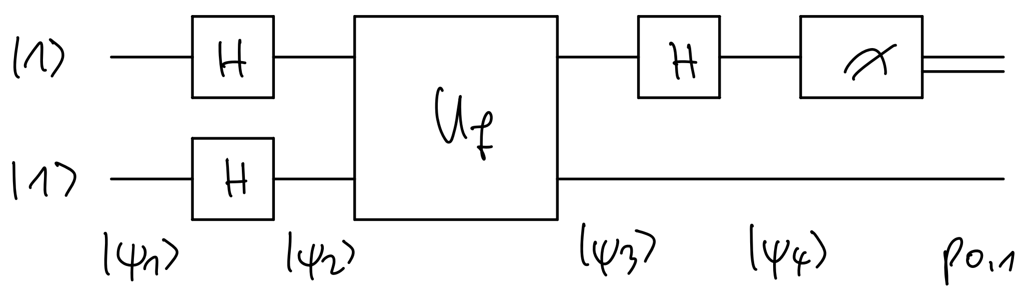
or $f(0) \neq f(1) \Rightarrow$ balanced 1€ $\rightarrow$ ☺

- Generalization: $f: \{0,1\}^n \rightarrow \{0,1\} \Rightarrow$ "Deutsch-Josza"

3.1.1 Quantum circuit

- Define unitary gate: $U_f |x, y\rangle \equiv |x, y \oplus f(x)\rangle$,
  where $|x,y\rangle \equiv |x\rangle \otimes |y\rangle \equiv |xy\rangle$ and $\underbrace{1 \oplus 1}_{\text{addition modulo 2}} = 0$

  $\Rightarrow U_f$ is black box function called "quantum oracle"



- $|\psi_1\rangle = |1\rangle \otimes |1\rangle$
- $|\psi_2\rangle = (H \otimes H)\,|\psi_1\rangle$

$$= \frac{1}{\sqrt{2}}\big(|0\rangle - |1\rangle\big) \otimes \frac{1}{\sqrt{2}}\big(|0\rangle - |1\rangle\big)$$

$$= \frac{1}{\sqrt{2}}\big(|0\rangle \otimes |0\rangle - |1\rangle \otimes |0\rangle - |0\rangle \otimes |1\rangle + |1\rangle \otimes |1\rangle\big)$$

$\Rightarrow$ superposition

- $|\psi_3\rangle = U_f |\psi_2\rangle$

$$= \frac{1}{2}\Big(|0\rangle \otimes |f(0)\rangle - |1\rangle \otimes |f(1)\rangle - |0\rangle \otimes |1 \oplus f(0)\rangle + |1\rangle \otimes |1 \oplus f(1)\rangle\Big)$$

- Two cases:

	$f(0)=f(1)$	$f(0)=1\oplus f(1)\neq f(1)$
$\lvert\psi_3\rangle$	$\frac{1}{\sqrt{2}}(\lvert 0\rangle-\lvert 1\rangle) \otimes \frac{1}{\sqrt{2}}(\lvert f(0)\rangle-\lvert 1\oplus f(0)\rangle)$	$\frac{1}{\sqrt{2}}(\lvert 0\rangle+\lvert 1\rangle) \otimes \frac{1}{\sqrt{2}}(\lvert f(0)\rangle-\lvert 1\oplus f(0)\rangle)$
$\lvert\psi_4\rangle$ (*)	$\lvert 1\rangle \otimes \ldots$	$\lvert 0\rangle \otimes \ldots$
p_0	0	1
p_1	1	0

3.1.2 Quantum parallism

- with a single measurement of the first qubit in the state $\lvert\psi_4\rangle$, we find out if 1€ ↗ 1€ or 1€ ↗ ☺
- 1 instead of 2 function calls, only 1 application of U_f
  $\Rightarrow$ "quantum parallelism"
- Note: quantum parallelism alone yields no advantage
  $\Rightarrow$ interference : $H(\lvert 0\rangle \mp \lvert 1\rangle) \overset{(*)}{=} \frac{1}{\sqrt{2}}\left[(\lvert 0\rangle+\lvert 1\rangle) \mp (\lvert 0\rangle-\lvert 1\rangle)\right]$
- without interference: QC can enable parallel computation but either no useful output or sequential measurement

3.2 Quantum simulation of quantum systems

- Motivation: "curse of dimensionality" (see Wed.)

  $\Rightarrow$ state space grows <u>exponentially</u> with system size

3.2.1 Time evolution

Perspective

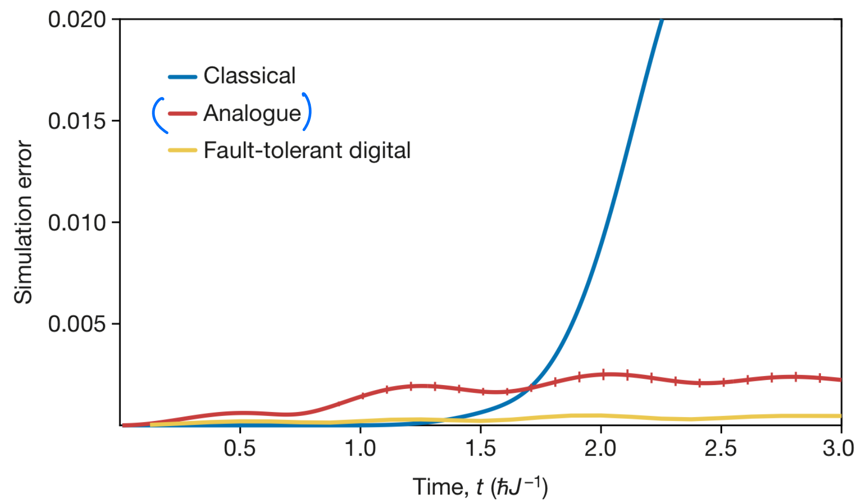


Fig. 2 | Quantum advantage of quantum simulators over classical simulation. A future fault-tolerant digital quantum simulation will be able to

(Daley et al., Nature 607, 667 (2022))

- Schrödinger equation: $i\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle$, $\hbar = 1$
- Time evolution: $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$

  $\Rightarrow$ problem: H is large!

- Solution: For most quantum systems, H can be written as sum over <u>local</u> interactions: $H = \sum_e H_e$

  $\Rightarrow$ example: Ising model, $H = -\sum_i (J_i Z_i Z_{i+1} + h_i X_i)$

- **Trotter formula**: for $H = A + B$

$$e^{-iHt} = e^{-i(A+B)t} = \lim_{n\to\infty} \left(e^{-iAt/n} \, e^{-iBt/n} \right)^n$$

- Discretized time evolution: approximate e^{-iHt} using n time steps $\delta t = \frac{t}{n}$ ("Trotter steps"), exact for $n \to \infty$

  ⇒ example: SU(3) lattice gauge theory in 1+1D:

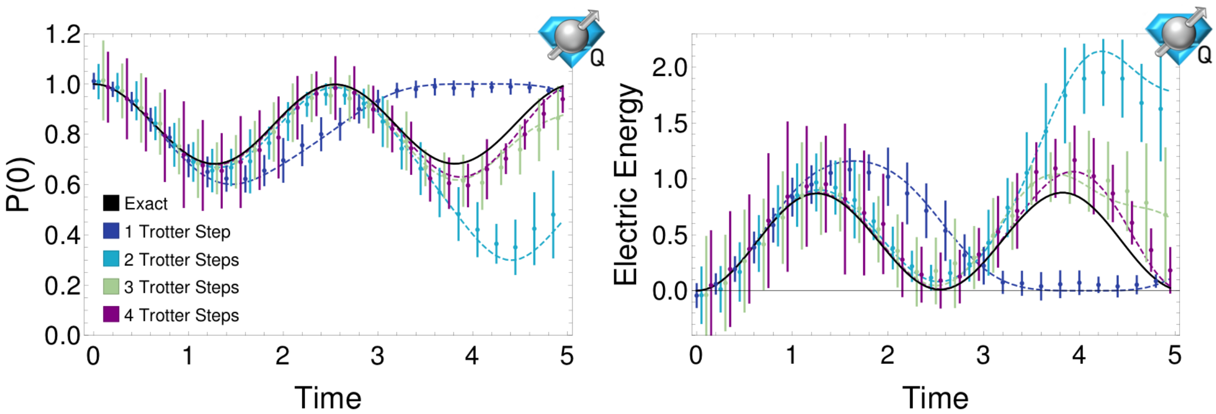


FIG. 6. The (trivial-) vacuum-to-vacuum persistence probability $|\langle 00| \hat{U}(t) |00\rangle|^2$ (left panel) and the energy in the electric field (right panel) of the one-plaquette system derived from the Hamiltonian given in Eq. (14) for color irreps $\mathbf{1}, \mathbf{3}, \overline{\mathbf{3}}, \mathbf{8}$. Dashed lines correspond to the exact results for 2nd-order Trotterization given in Eq. (20) with $\Delta t = t, t/2, t/3, t/4, 0$. Points correspond to quadratic extrapolations of results obtained from IBM's `Athens` quantum processor, with systematic and statistical uncertainties combined in quadrature.

(Chiavarell et al., 2101.10227)

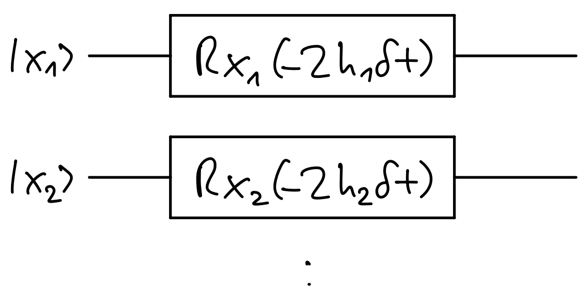
- **Quantum circuit**: map discrete time evolution steps to gates

  ⇒ e.g. Ising model: $B_i = -h_i X_i$ ⇒ $e^{-iB_i \delta t} = e^{+ih_i X_i \delta t}$

  ⇒ corresponds to rotation: $R_{X_i}(\theta_i) = e^{-i\frac{\theta_i}{2} X_i}$ for $\theta_i = -2h_i\delta t$

  ⇒ quantum circuit:

  (see Wed.)

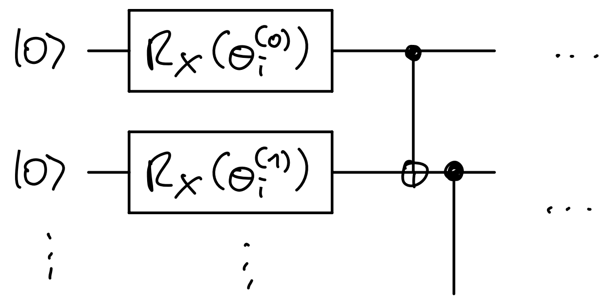


$|x_n\rangle$ — $\boxed{Rx(-2h_n\delta t)}$ —

- Map spins to qubits: identify spin i with qubit i
  $\Rightarrow |x_i\rangle, \; x_i \in \{0,1\} \quad \Rightarrow |0\rangle \to |\downarrow\rangle, \; |1\rangle \to |\uparrow\rangle$

3.2.2 Computing ground and excited states

- So far, discussed time evolution of $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$, but not how to prepare state $|\psi(0)\rangle$
- In many physics and chemistry applications, aim to compute and lower excited states of quantum systems
- Limitation of classical algorithms?
  $\Rightarrow$ e.g. Lattice QCD: sign problem (no θ-term, baryon asymm.)
  $\Rightarrow$ e.g. tensor networks: no highly entangled states
- Quantum algorithms? One possibility: variational approach
- Variational Quantum Eigensolver (VQE): originally developed for quantum chemistry (Peruzzo et al., 1304.3061)
- Goal: minimize energy E (often called cost function C)
  $$C(\vec{\theta}_i) = E(\vec{\theta}_i) = \langle \psi(\vec{\theta}_i) | H | \psi(\vec{\theta}_i) \rangle$$
  for given Hamiltonian H and set of parameters $\vec{\theta}_i$
- Method: hybrid quantum-classical algorithm:
  (i) realize $|\psi(\vec{\theta}_i)\rangle$ by parametric quantum circuit,

e.g. $|\psi(\vec{\theta}_i)\rangle =$ 

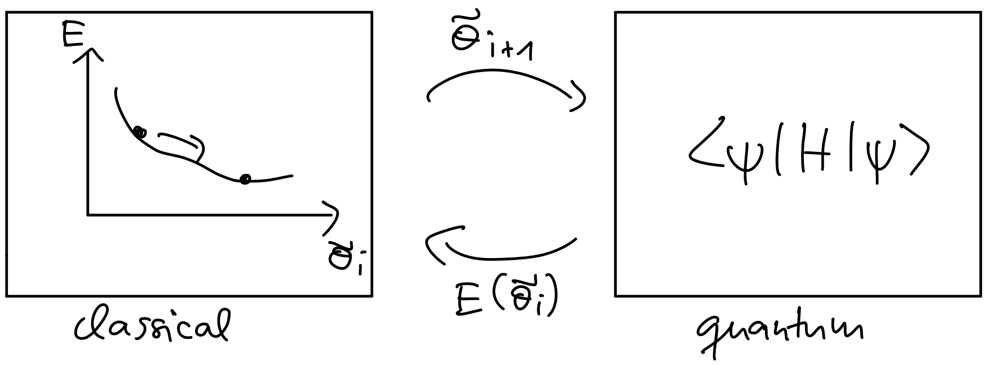
(ii) measure $E(\vec{\theta}_i)$ on QC

(iii) use classical non-linear optimizer (e.g. Nelder-Mead) to find new parameters $\vec{\theta}_{i+1}$ that decrease E

$\Rightarrow$ or use machine learning (Kim et al., 2406.06150)

(iv) iterate until converging to ground state

$\Rightarrow$ quantum-classical feedback loop



$\Rightarrow$ "quantum coprocessor unit" (QPU) for classically hard part of computation

- Examples: VQE for
  - 1+1D Schwinger model (see Thu.)
  - 1+1D SU(2) "proton" mass

- Problems of VQE:
  - local minima
  - Barren plateaus
  - ...

(Anschuetz, Kiani, 2205.05786)

- Review on QC for lattice field theory (Funcke et al., 2302.00467)

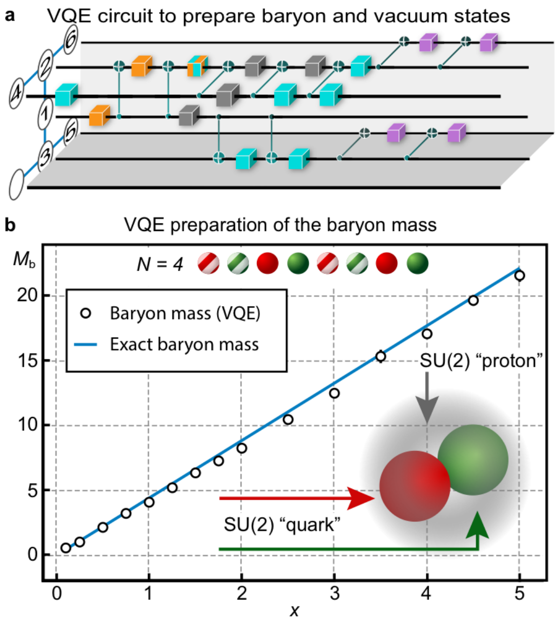


FIG. 2. **VQE calculation of a baryon.** We variationally...

(Atas at el., 2102.08920)