6. Quantum Algorithms for Applications

Quantum Computing

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DI PARMA

Finding the period of a periodic function

FT: from times to frequencies $\Longrightarrow$ Determine the period of a periodic function $f(x)$!

Classical computer : we need to **evaluate** $f(x)$ **many times**, until we find two identical values

Quantum computer:

$$\frac{1}{\sqrt{N}}\sum_{a=0}^{N-1}|a\rangle\otimes|0\rangle \longrightarrow |\psi_0\rangle = \frac{1}{\sqrt{N}}\sum_{a=0}^{N-1}|a\rangle\otimes|f(a)\rangle$$

This register encodes all the value of $f(a)$, correlated with the inputs a. Hence, the information on the period is present in such a superposition state.

Measure the second register and find $f(a_0)$, i.e.

$$|\mathbb{I}\otimes f(a_0)\rangle\langle\mathbb{I}\otimes f(a_0)|\psi_0\rangle = [|a_0\rangle + |a_0+T\rangle + |a_0+2T\rangle + \cdots]\otimes|f(a_0)\rangle$$

The first register is therefore projected onto the state $|\psi\rangle = \sqrt{\frac{T}{N}}\sum_{m=0}^{\frac{N}{T}-1}|a_0+mT\rangle$ $\quad 0 \le a_0 \le T-1$

$\big\downarrow U_{QFT}$

where $b = lN/T$ $\quad U_{QFT}|\psi\rangle = \sqrt{\frac{T}{N}}\sum_{m=0}^{\frac{N}{T}-1}\frac{1}{\sqrt{N}}\sum_{b=0}^{N-1}e^{i2\pi(a_0+mT)b/N}\,|b\rangle = \frac{1}{\sqrt{T}}\sum_{l=0}^{T-1}e^{i2\pi a_0 l/T}\,|lN/T\rangle$

Finding the period of a periodic function

$$U_{QFT}|\psi\rangle = \sqrt{\frac{T}{N}} \sum_{m=0}^{\frac{N}{T}-1} \frac{1}{\sqrt{N}} \sum_{b=0}^{N-1} e^{i2\pi(a_0+mT)b/N} |b\rangle = \frac{1}{\sqrt{T}} \sum_{l=0}^{T-1} e^{i2\pi a_0 l/T} |lN/T\rangle$$

If we measure the first register, we get one of the values

$$b = \frac{lN}{T} \qquad l = 0, \dots, T-1$$

What happens if we use the QFT to find the period of a periodic function in which a value of f appears twice in a single period?

If l and T are relatively prime, the simplified fraction gives the value of T

$$\frac{b}{N} = \frac{l}{T}$$

Shor's algorithm

Quantum Computing

Problem: finding prime factors of a given number N

We select a random integer $y < N$ relatively prime to N. (If not, we have already found a factor of N). We then define

$$f(a) = y^a \bmod N$$

Note that $f(0) = 1$. We seek the smallest subsequent T such that $f(T) = 1$:

$$f(T) = y^T \bmod N = 1$$

T is the period of f. Having T, with some algebra we determine a factor of N:

$$(y^T - 1) \bmod N = 0$$

$$\left(y^{T/2} + 1\right)\left(y^{T/2} - 1\right) \bmod N = 0$$

$$\left(y^{T/2} + 1\right)\left(y^{T/2} - 1\right) = \lambda N$$

For some integer λ

Ex :

$$2^0 \bmod 15 = 1$$
$$2^1 \bmod 15 = 2$$
$$2^2 \bmod 15 = 4$$
$$2^3 \bmod 15 = 8$$
$$2^4 \bmod 15 = 1$$

$$T = 4$$
$$y^{T/2} + 1 = 5$$
$$y^{T/2} - 1 = 3$$

If T is not even, we must try again with a different value of y

Shor’s algorithm: quantum advantage

Best known classical algorithm for factoring a large n-bit number N is **super-polynomial** in n (i.e. not bounded by any polynomial)

The hard step is the **FT**, which can be performed in a **polynomial (rather than exponential)** time on a quantum computer.

Hence, factoring using a quantum processor can also be done in a polynomial time.

Shor's algorithm: implementation

Use **quantum phase estimation** on the unitary operator $U|y\rangle = |ay \bmod N\rangle$

$a = 3, N = 14$ $\boxed{T = 6}$

Repeated applications of U
(each time we multiply by $a \bmod N$)

$$U|1\rangle = |3\rangle$$
$$U^2|1\rangle = |9\rangle$$
$$U^3|1\rangle = |13\rangle$$
$$U^4|1\rangle = |11\rangle$$
$$U^5|1\rangle = |5\rangle$$
$$U^6|1\rangle = |1\rangle$$

A superposition of the states in this cycle is an eigenstate of U with eigenvalue 1

$$|\xi_0\rangle = \frac{1}{\sqrt{6}}[|1\rangle + |3\rangle + |9\rangle + |13\rangle + |11\rangle + |5\rangle]$$

$$|\xi_0\rangle = \frac{1}{\sqrt{T}}\sum_{k=0}^{T-1}|a^k \bmod N\rangle$$

$$U|\xi_0\rangle = \frac{1}{\sqrt{6}}[|3\rangle + |9\rangle + |13\rangle + |11\rangle + |5\rangle + |1\rangle] = |\xi_0\rangle$$

$$|\xi_1\rangle = \frac{1}{\sqrt{T}}\sum_{k=0}^{T-1}e^{-\frac{2\pi i k}{T}}|a^k \bmod N\rangle$$

$$|\xi_1\rangle = \frac{1}{\sqrt{6}}\left[|1\rangle + e^{-\frac{2\pi i}{6}}|3\rangle + e^{-\frac{4\pi i}{6}}|9\rangle + e^{-\frac{6\pi i}{6}}|13\rangle + e^{-\frac{8\pi i}{6}}|11\rangle + e^{-\frac{10\pi i}{6}}|5\rangle\right]$$

$$U|\xi_1\rangle = e^{\frac{2\pi i}{T}}|\xi_1\rangle$$

$$U|\xi_1\rangle = \frac{1}{\sqrt{6}}\left[|3\rangle + e^{-\frac{2\pi i}{6}}|9\rangle + e^{-\frac{4\pi i}{6}}|13\rangle + e^{-\frac{6\pi i}{6}}|11\rangle + e^{-\frac{8\pi i}{6}}|5\rangle + e^{-\frac{10\pi i}{6}}|1\rangle\right]$$
$$= e^{\frac{2\pi i}{6}}\frac{1}{\sqrt{6}}\left[e^{-\frac{2\pi i}{6}}|3\rangle + e^{-\frac{4\pi i}{6}}|9\rangle + e^{-\frac{6\pi i}{6}}|13\rangle + e^{-\frac{8\pi i}{6}}|11\rangle + e^{-\frac{10\pi i}{6}}|5\rangle + e^{-\frac{12\pi i}{6}}|1\rangle\right] = e^{\frac{2\pi i}{6}}|\xi_1\rangle$$

Quantum Computing

Shor's algorithm: implementation

$$|\xi_s\rangle = \frac{1}{\sqrt{T}}\sum_{k=0}^{T-1} e^{-\frac{2\pi i s k}{T}} |a^k \bmod N\rangle \qquad U|\xi_s\rangle = e^{\frac{2\pi i s}{T}}|\xi_s\rangle$$

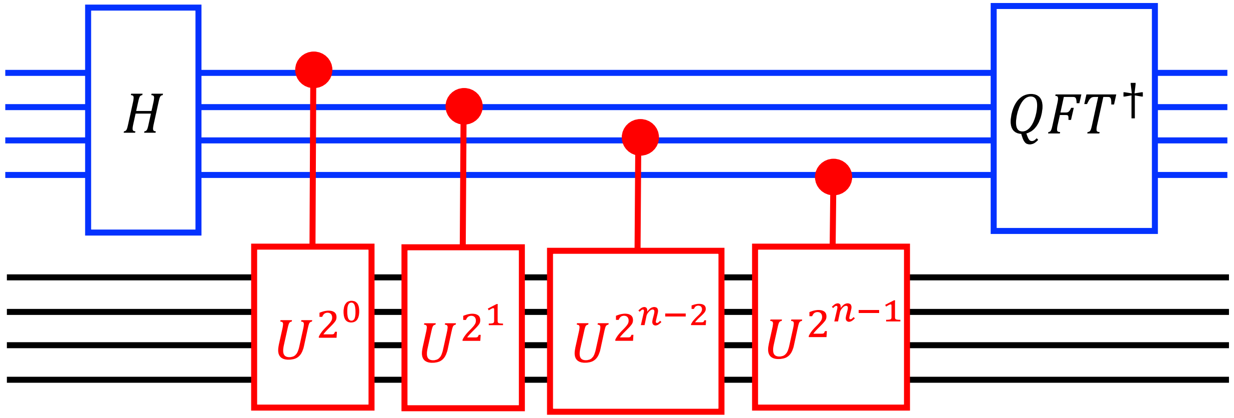
We thus get a unique eigenstate for each ingeter $s \in [0, T-1]$

$$\frac{1}{\sqrt{T}}\sum_{s=0}^{T-1}|\xi_s\rangle = |1\rangle$$

The computational basis state $|1\rangle$ is a superposition of these eigenstates.

Hence by **QPE** we will measure a phase s/T for a random integer $s \in [0, T-1]$

$$|1\rangle = \frac{1}{\sqrt{T}}[|\xi_0\rangle + |\xi_1\rangle + \cdots + |\xi_{T-1}\rangle]$$



$$\frac{1}{\sqrt{T}}[|2^n 1/T\rangle + |2^n 2/T\rangle + \cdots + |2^n (T-1)/T\rangle]$$

Quantum Computing

Solving linear systems (HHL)

PROBLEM: given $A \in \mathbb{C}^{N\times N}$ $\vec{b} \in \mathbb{C}^N$ **find** $\vec{x} \in \mathbb{C}^N$ $A\vec{x} = \vec{b}$

The system is s-sparse if A has at most s non-zero entries per rows or column.

On a classical computer we can solve an s-sparse system of size N in $O(Nsk\log(1/\epsilon))$ time by the conjugate gradient method, being ϵ the error of the approximation and k the condition number of the system.

HHL [A. W. Harrow, A. Hassidim, S. Lloyd, Phys. Rev. Lett. **103**, 150502 (2009)] algorithm estimates the solution in $O(\log(N)s^2k^2/\epsilon)$ time

- **Exponential advantage**
- We do not find the full solution, but only **approximate** functions of the solution vector
- We assume A Hermitian and efficient oracles for loading the data

Map to quantum states

$\vec{x} \rightarrow |x\rangle$ $\vec{b} \rightarrow |b\rangle$ $\vec{x}, \vec{b}$ must be normalized

$$A|x\rangle = |b\rangle$$

$$A = \sum_{j=0}^{N-1} \lambda_j |u_j\rangle\langle u_j| \qquad \lambda_j \in \mathbb{R}$$

Spectral decomposition

$$A^{-1} = \sum_{j=0}^{N-1} \lambda_j^{-1} |u_j\rangle\langle u_j|$$

$$|b\rangle = \sum_{j=0}^{N-1} b_j |u_j\rangle \qquad b_j \in \mathbb{C}$$

Representation of $|b\rangle$ on A eigenbasis.

$$|x\rangle = A^{-1}|b\rangle = \sum_{j=0}^{N-1} \lambda_j^{-1} b_j |u_j\rangle$$

Implicit normalisation

HHL algorithm

3 registers: $\begin{cases} n_l\text{: Binary representation of the eigenvalues of } A \\ n_b\text{: Vector solution. Hereafter } N = 2^{n_b}. \\ n_a\text{: Ancilla qubit} \end{cases}$

1. Load the data $|b\rangle \in \mathbb{C}^{\mathrm{N}}$ $|0\rangle_{n_b} \to |b\rangle_{n_b}$

2. Apply QPE to $U = e^{-iAt} = \sum_{j=0}^{N-1} \mathrm{e}^{-\mathrm{i}\lambda_j t} |u_j\rangle\langle u_j|$ $\Rightarrow$ $\sum_{j=0}^{N-1} b_j |\lambda_j\rangle_{n_l} |u_j\rangle_{n_b}$

Normalisation constant

3. Add an ancilla qubit and apply a rotation conditioned on $|\lambda_j\rangle$ $\Rightarrow$ $\sum_{j=0}^{N-1} b_j |\lambda_j\rangle_{n_l} |u_j\rangle_{n_b} \left(\sqrt{1 - \frac{c^2}{\lambda_j^2}} |0\rangle + \frac{c}{\lambda_j} |1\rangle \right)$

4. Apply $QPE^\dagger$. Neglecting possible errors in the QPE $\Rightarrow$ $\sum_{j=0}^{N-1} b_j |0\rangle_{n_l} |u_j\rangle_{n_b} \left(\sqrt{1 - \frac{c^2}{\lambda_j^2}} |0\rangle + \frac{c}{\lambda_j} |1\rangle \right)$

5. Measure ancilla. If we find $|1\rangle$ $\Rightarrow$ $\sum_{j=0}^{N-1} \frac{b_j}{\lambda_j} |0\rangle_{n_l} |u_j\rangle_{n_b}$ Apart from a normalization

which corresponds (apart from a factor) to the solution.

QPE within HHL

$$QPE(U, |0\rangle_n, |\psi\rangle_m) = |\tilde{\theta}\rangle_n |\psi\rangle_m \qquad U|\psi\rangle_m = e^{i2\pi\theta}\, |\psi\rangle_m$$

Binary approximation to $2^n\theta$

Within HHL

$$U = e^{iAt} = \sum_{j=0}^{N-1} e^{i\lambda_j t} |u_j\rangle\langle u_j|$$

$$QPE\left(e^{iAt}, |0\rangle_{n_l}, |u_j\rangle_{n_b}\right) = |\tilde{\lambda}_j\rangle_{n_l} |u_j\rangle_{n_b}$$

$\tilde{\lambda}_j$ is a n_l–bit binary approximation to $2^{n_l}\frac{\lambda_j t}{2\pi}$

If λ_j can be represented exactly with n_l bits

$$QPE\left(e^{iA2\pi}, \sum_{j=0}^{N-1} b_j\, |0\rangle_{n_l} |u_j\rangle_{n_b}\right) = \sum_{j=0}^{N-1} b_j\, |\lambda_j\rangle_{n_l}\, |u_j\rangle_{n_b}$$

Otherwise we obtain an approximation

Example: HHL on 4 qubits

$$A = \begin{pmatrix} 1 & -1/3 \\ -1/3 & 1 \end{pmatrix} \qquad |b\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$n_b = 1$ to represent $|b\rangle$ and then the solution
$n_l = 2$ qubits to store the eigenvalues of A
$n_a = 1$ to store if the conditional rotation (and hence the algorithm) was successful

QPE gives a binary approximation (on an n_l-bit string) to $2^{n_l}\frac{\lambda_j t}{2\pi}$. Hence, if we set $t = 2\pi\frac{3}{8}$ we get

$$\lambda_1 = \frac{2}{3} \qquad \lambda_2 = \frac{4}{3}$$

$$\frac{\lambda_1 t}{2\pi} = \frac{1}{4} \downarrow |01\rangle_{n_l} \qquad \frac{\lambda_2 t}{2\pi} = \frac{1}{2} \downarrow |10\rangle_{n_l}$$

Rescaled eigenvalues. We choose this value of t to simplify the problem and get the exact result from QPE.

Eigenvectors of A: $\quad |u_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad |u_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

$$|b\rangle = |0\rangle = \frac{1}{\sqrt{2}}(|u_1\rangle + |u_2\rangle)$$

Note that we do not need to know eigenvalues and eigenvectors [$\mathcal{O}(N)$ problem]

Example: HHL on 4 qubits

Initial state $$|\psi\rangle = |0\rangle_{n_l}|0\rangle_{n_b}|0\rangle_a = |0\rangle_{n_l}\frac{1}{\sqrt{2}}(|u_1\rangle_{n_b} + |u_2\rangle_{n_b})|0\rangle_a$$

$$\Big\downarrow QPE$$

$$\frac{1}{\sqrt{2}}(|01\rangle_{n_l}|u_1\rangle_{n_b} + |10\rangle_{n_l}|u_2\rangle_{n_b})|0\rangle_a$$

$\Big\downarrow$ Conditioned rotation of the ancilla ($c = 3/8$ to compensate rescaling of the eigenvalues)

$$\frac{1}{\sqrt{2}}|01\rangle_{n_l}|u_1\rangle_{n_b}\left(\sqrt{1-\frac{(3/8)^2}{(1/4)^2}}|0\rangle_a + \frac{(3/8)}{(1/4)}|1\rangle_a\right) + \frac{1}{\sqrt{2}}|10\rangle_{n_l}|u_2\rangle_{n_b}\left(\sqrt{1-\frac{(3/8)^2}{(1/2)^2}}|0\rangle_a + \frac{(3/8)}{(1/2)}|1\rangle_a\right)$$

$$\Big\downarrow QPE^\dagger$$

$$\frac{1}{\sqrt{2}}|00\rangle_{n_l}|u_1\rangle_{n_b}\left(\sqrt{1-\frac{9}{4}}|0\rangle_a + \frac{3}{2}|1\rangle_a\right) + \frac{1}{\sqrt{2}}|00\rangle_{n_l}|u_2\rangle_{n_b}\left(\sqrt{1-\frac{9}{16}}|0\rangle_a + \frac{3}{4}|1\rangle_a\right)$$

$\Big\downarrow$ Project onto $|1\rangle_a$

$$\propto |00\rangle_{n_l}(2|u_1\rangle_{n_b} + |u_2\rangle_{n_b})|1\rangle_a = |00\rangle_{n_l}(3|0\rangle_{n_b} + |1\rangle_{n_b})|1\rangle_a$$

Which is the correct solution

Hybrid algorithms: VQE

Quantum Computing

Findind the **minimum or maximum eigenvalue** is important in many problems: e.g. determine the results of internet search engines, designing new materials and drugs, calculating physical properties.

This problem is very hard for a classical computer.

QPE: exponential speed-up, but to estimate the eigenvalue with precision ϵ it requires $\mathcal{O}(1/\epsilon)$ noiseless operations, during which the QC must remain **coherent**.

The hybrid algorithm Variational Quantum Eigensolver (VQE) provides an interesting alternative, offering an exponential speedup in evaluating the expectation value of a given Hamiltonian, compared to classical exact diagonalization.

The algorithm is **hybrid** because it combines a quantum and a classical part. This **reduces the coherence requirements** and allows us to implement it efficiently on NISQs.

Variational theorem

We consider a Hamiltonian H and its spectral decomposition:

$$H = \sum_k E_k |\phi_k\rangle\langle\phi_k|$$

The expectation value of H on an arbitrary state $|\psi\rangle$ is given by $\langle H\rangle_\psi = \langle\psi|H|\psi\rangle$

Which can be re-written as $$\langle H\rangle_\psi = \langle\psi|H|\psi\rangle = \sum_k E_k \langle\psi|\phi_k\rangle\langle\phi_k|\psi\rangle = \sum_k E_k |\langle\phi_k|\psi\rangle|^2$$

Hence, the expectation value of H on a given state $|\psi\rangle$ is a linear combination of its eigenvalues with **POSITIVE** weights.

$$\boxed{E_{min} \leq \langle H\rangle_\psi = \sum_k E_k |\langle\phi_k|\psi\rangle|^2}$$

We can use this result to obtain an **approximation** of the **ground state** of a given Hamiltonian

And this value is minimized by $|\psi_{min}\rangle$ such that $H|\psi_{min}\rangle = E_{min}|\psi_{min}\rangle$

Variational Quantum Eigensolver

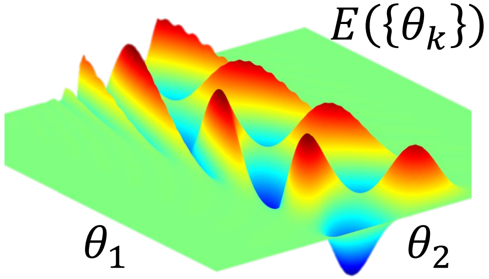
QUANTUM HARDWARE

1. Generate a variational ansatz depending on a set of parameters $|\psi(\{\theta_k\})\rangle$

2. Evaluate the expectation value of the Hamiltonian as a linear combination of Pauli products (local measurements)

CLASSICAL

3. Combine measurement results and optimize using a classical algorithm to explore the energy surface



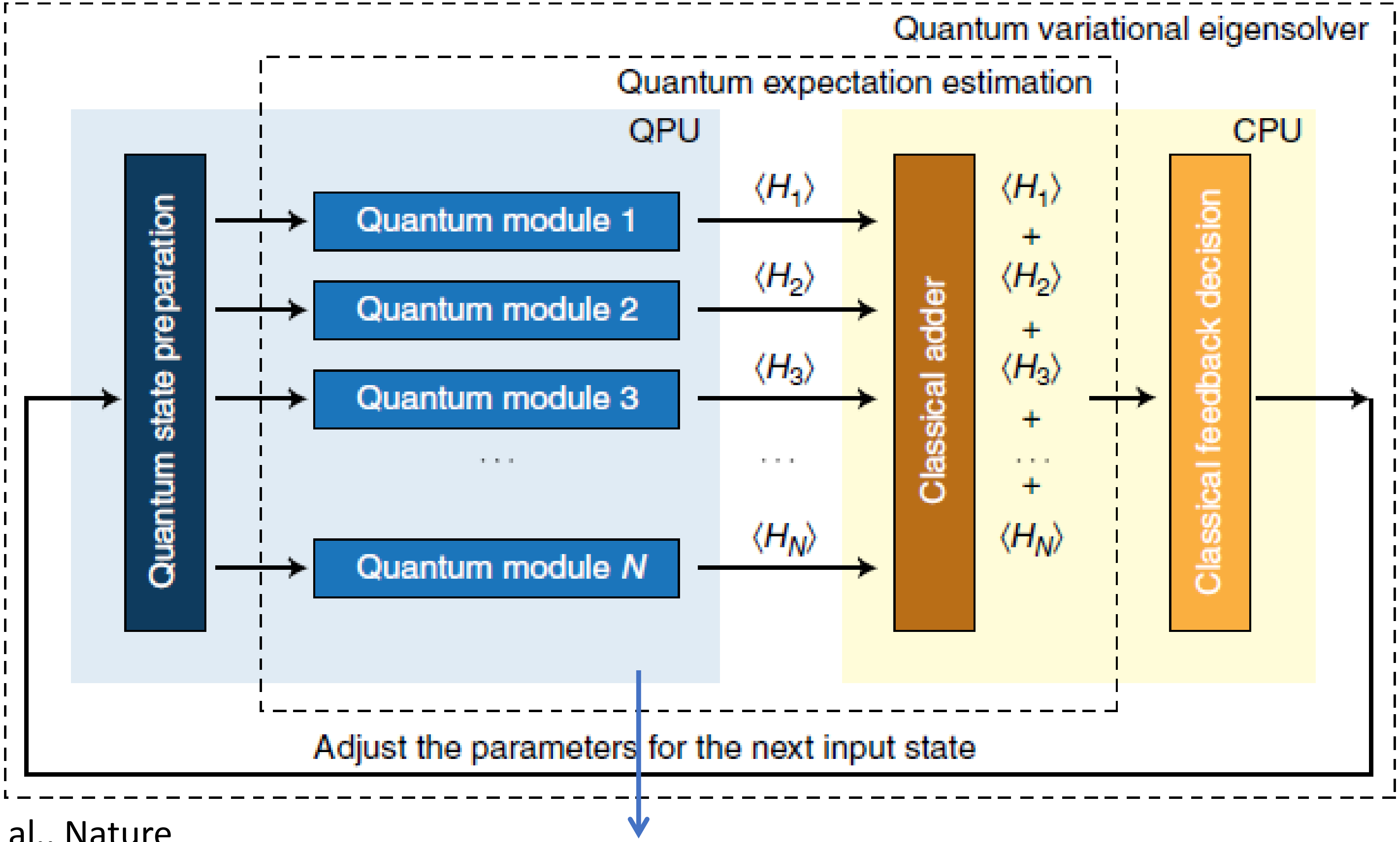
Repeat until convergence (energy variation below a threshold)

$$E(\{\theta_k\}) = \frac{\langle\psi(\{\theta_k\})|H|\psi(\{\theta_k\})\rangle}{\langle\psi(\{\theta_k\})|\psi(\{\theta_k\})\rangle} = \sum_j \frac{\langle\psi(\{\theta_k\})|H_j|\psi(\{\theta_k\})\rangle}{\langle\psi(\{\theta_k\})|\psi(\{\theta_k\})\rangle}$$

Any hermitian Hamiltonian can be expressed as a **combination of tensor products of Paulis**.

Since the expectation value is linear, we can evaluate all these terms separately, by **local measurements** on each qubit performed in parallel.

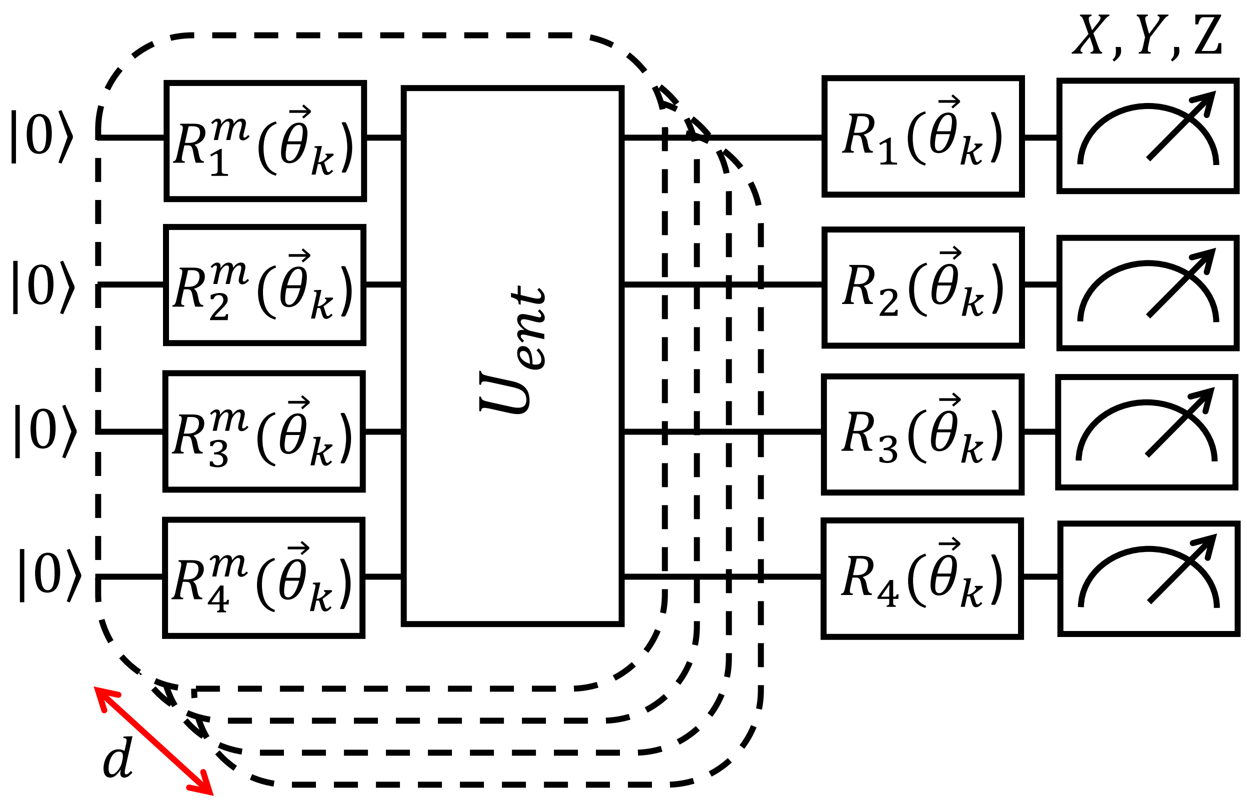
Variational Quantum Eigensolver



A. Peruzzo et al., Nature Commun. **5**, 4213 (2014)

$$H = H_1 + H_2 + \cdots H_N \Rightarrow \langle H \rangle = \langle H_1 \rangle + \langle H_2 \rangle + \cdots \langle H_N \rangle$$

Preparation of the variational ansatz



Generate ansatz $|\psi(\{\theta_k\})\rangle$

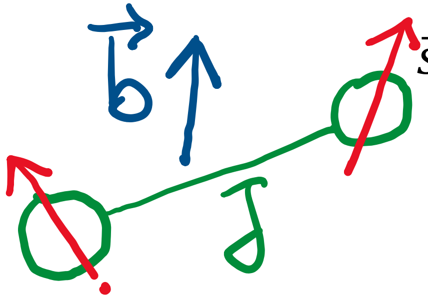
Uses layers of rotations (depending on some parameters) and entangling gates to generate the variational ansatz

A. Kandala et al., Nature **242**, 549 (2017)

Example: VQE on a spin dimer

Spin systems are an **ideal test-bed** for a quantum hardware

$$H = J_x X_1 X_2 + J_y Y_1 Y_2 + J_z Z_1 Z_2 + b(Z_1 + Z_2)$$



$$\vec{s}_2 = {(X_2, Y_2, Z_2)}/_{2}$$

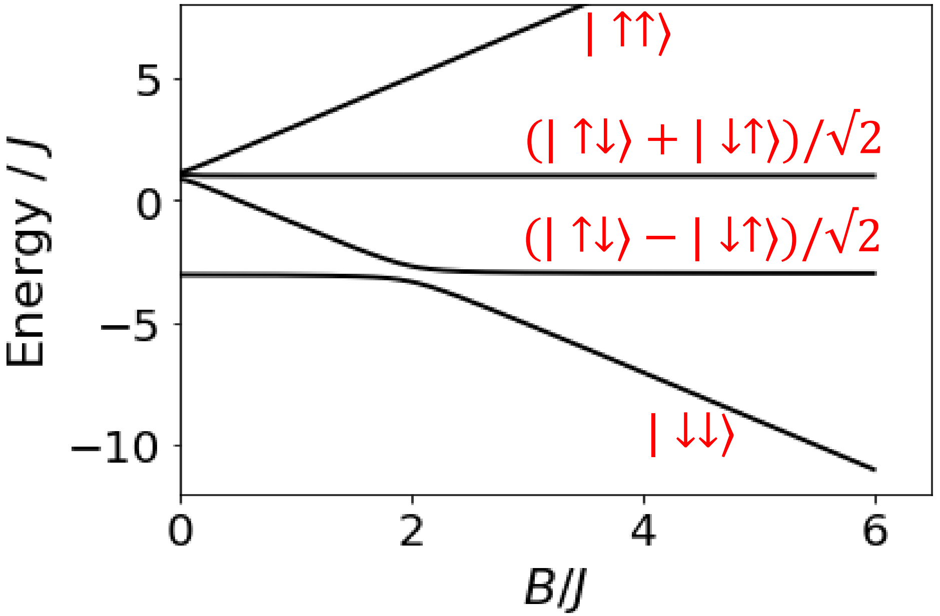
$$\vec{s}_1 = {(X_1, Y_1, Z_1)}/_{2}$$

The Hamiltonian (and hence its expectation value) is already a sum of products of Paulis

$$\langle\psi|H|\psi\rangle$$
$$= J_x\langle\psi|X_1X_2|\psi\rangle + J_y\langle\psi|Y_1Y_2|\psi\rangle + J_z\langle\psi|Z_1Z_2|\psi\rangle$$
$$+ b\langle\psi|Z_1|\psi\rangle + b\langle\psi|Z_2|\psi\rangle$$

In this simple example we can compare the solution by exact diagonalization with that found using the VQE algorithm and calculate the final **fidelity** (i.e. ‘closeness’ of two states)

$$\mathcal{F} = \left|\left\langle\psi_0\middle|\psi(\{\tilde{\theta}_k\})\right\rangle\right|$$



We can also compute some **observables** (e.g. magnetization) on the **final ground state**

$$\langle\psi(\{\tilde{\theta}_k\})|M_z|\psi(\{\tilde{\theta}_k\})\rangle = \langle\psi(\{\tilde{\theta}_k\})|(Z_1 + Z_2)|\psi(\{\tilde{\theta}_k\})\rangle/2$$

Example: VQE on a spin dimer

$$\langle\psi(\{\tilde{\theta}_k\})|M_z|\psi(\{\tilde{\theta}_k\})\rangle = \langle\psi(\{\tilde{\theta}_k\})|(Z_1 + Z_2)|\psi(\{\tilde{\theta}_k\})\rangle/2$$

$$|\psi(\{\tilde{\theta}_k\})\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

$$\begin{aligned}
\langle\psi(\{\tilde{\theta}_k\})|(Z_1 + Z_2)|\psi(\{\tilde{\theta}_k\})\rangle &= \langle\psi(\{\tilde{\theta}_k\})|Z_1|\psi(\{\tilde{\theta}_k\})\rangle + \langle\psi(\{\tilde{\theta}_k\})|Z_2|\psi(\{\tilde{\theta}_k\})\rangle \\
&= |\alpha_{00}|^2\langle 00|Z_1|00\rangle + |\alpha_{01}|^2\langle 01|Z_1|01\rangle + |\alpha_{10}|^2\langle 10|Z_1|10\rangle + |\alpha_{11}|^2\langle 11|Z_1|11\rangle \\
&+ |\alpha_{00}|^2\langle 00|Z_2|00\rangle + |\alpha_{01}|^2\langle 01|Z_2|01\rangle + |\alpha_{10}|^2\langle 10|Z_2|10\rangle + |\alpha_{11}|^2\langle 11|Z_2|11\rangle
\end{aligned}$$

$$\begin{aligned}
&= |\alpha_{00}|^2\langle 0|Z_1|0\rangle + |\alpha_{01}|^2\langle 0|Z_1|0\rangle + |\alpha_{10}|^2\langle 1|Z_1|1\rangle + |\alpha_{11}|^2\langle 1|Z_1|1\rangle \\
&+ |\alpha_{00}|^2\langle 0|Z_2|0\rangle + |\alpha_{01}|^2\langle 1|Z_2|1\rangle + |\alpha_{10}|^2\langle 0|Z_2|0\rangle + |\alpha_{11}|^2\langle 1|Z_2|1\rangle \\
&= |\alpha_{00}|^2 + |\alpha_{01}|^2 - |\alpha_{10}|^2 - |\alpha_{11}|^2 + |\alpha_{00}|^2 - |\alpha_{01}|^2 + |\alpha_{10}|^2 - |\alpha_{11}|^2 \\
&= 2(|\alpha_{00}|^2 - |\alpha_{11}|^2)
\end{aligned}$$

Example: spin dimer

If $J_x = J_y = J_z = J$ (isotropic exchange interaction) the solution is analytic, but it requires a bit of Quantum Mechanics.

$$\vec{S} = \vec{s}_1 + \vec{s}_2$$

$$s_1 = s_2 = 1/2$$

$$S = |s_1 - s_2|, \ldots, s_1 + s_2$$

$$M = -S, \ldots, S$$

We can rewrite $H = H_1 + H_2$, with

$$H_1 = J(X_1X_2 + Y_1Y_2 + Z_1Z_2) = 2J\, 2\vec{s}_1 \cdot \vec{s}_2 = 2J(S^2 - s_1^2 - s_2^2)$$

$$H_2 = b(Z_1 + Z_2) = 2b\, S_z$$

$$[H_1, H_2] = 0 \qquad S^2|S,M\rangle = S(S+1)|S,M\rangle$$

$$S_z|S,M\rangle = M|S,M\rangle$$

$$H_1|S,M\rangle = 2J[S(S+1) - s_1(s_1+1) - s_2(s_2+1)]|S,M\rangle = 2J[S(S+1) - 3/2]|S,M\rangle$$

$$H_2|S,M\rangle = 2bM\,|S,M\rangle$$

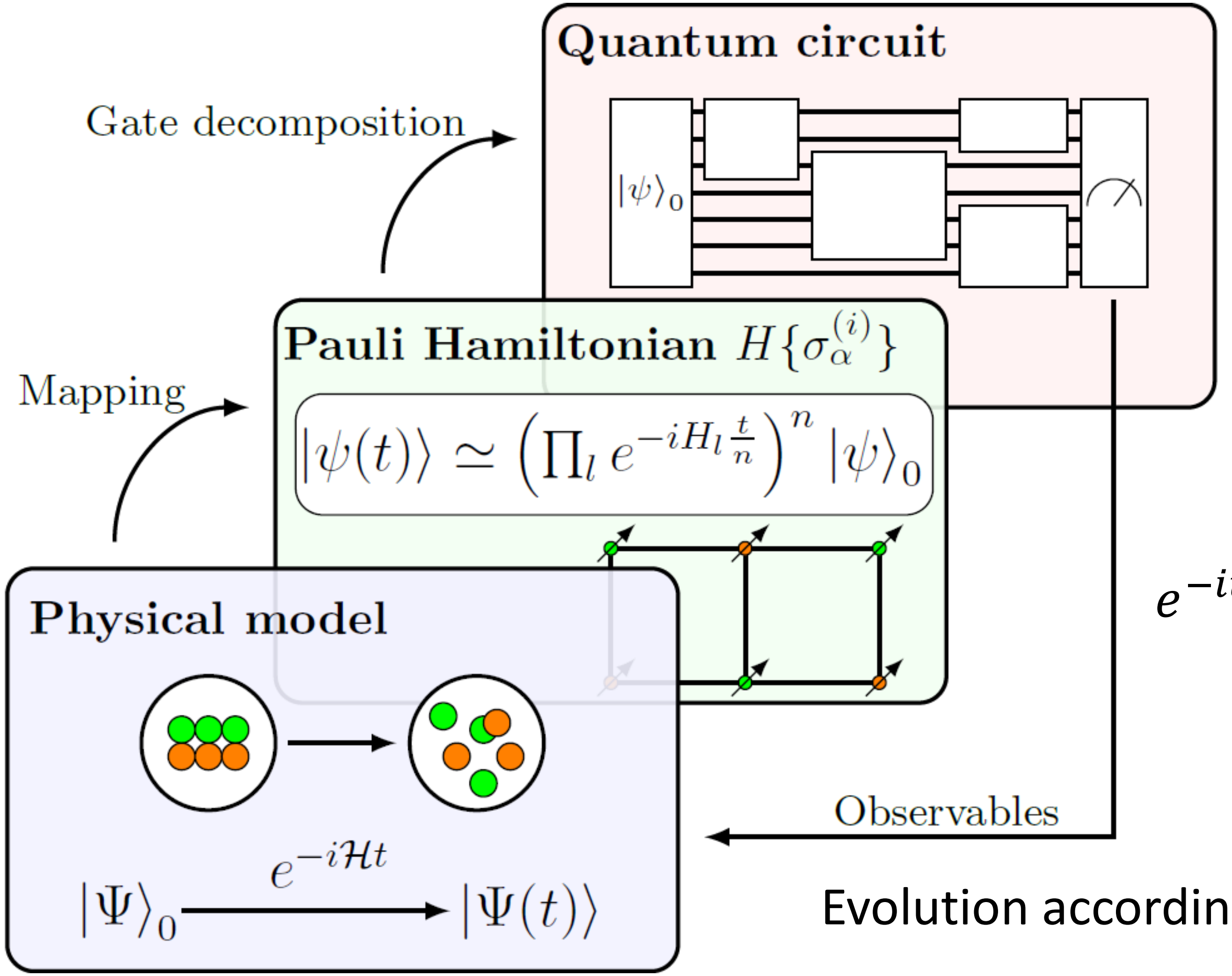
$$(H_1+H_2)|S,M\rangle = [2bM + 2JS(S+1) - 3J]|S,M\rangle$$

$$\left\{\begin{array}{ll} |S=1, M=1\rangle & J+2b \\ |S=1, M=0\rangle & J \\ |S=1, M=-1\rangle & J-2b \\ |S=0\rangle & -3J \end{array}\right.$$

$S = 1$ split by b

Two multiplets separated by $4J$

Quantum Simulation



Compute **observables**

$$A(t) = \langle \psi(t)|A|\psi(t)\rangle$$

Suzuki-Trotter approximation

$$e^{-it/\hbar \sum_l H_l}|\psi(0)\rangle \approx \left(\prod_l e^{-\frac{iH_l t}{\hbar n}}\right)^n |\psi(0)\rangle$$

$$\mathcal{H} = \sum_l H_l \qquad [H_l, H_k] \neq 0$$

Evolution according to target Hamiltonian $\mathcal{H}$

S. Lloyd, Science **273**, 1073 (1996)

F. Tacchino et al., https://arxiv.org/pdf/1907.03505.pdf Adv. Quant. Technol. 1900052 (2019)

Optimizing the digitalization

In the **NISQ** (noisy-intermediate scale quantum computing) era each operation is error-prone

By increasing the circuit depth we increase the error probability.

Trade-off **Targeted error mitigation strategies**

N Trotter steps

$\tau = t/N$

$\tau' < \tau$

$N' > N$

$\tau'' < \tau'$

$N'' > N'$

Too many noisy gates

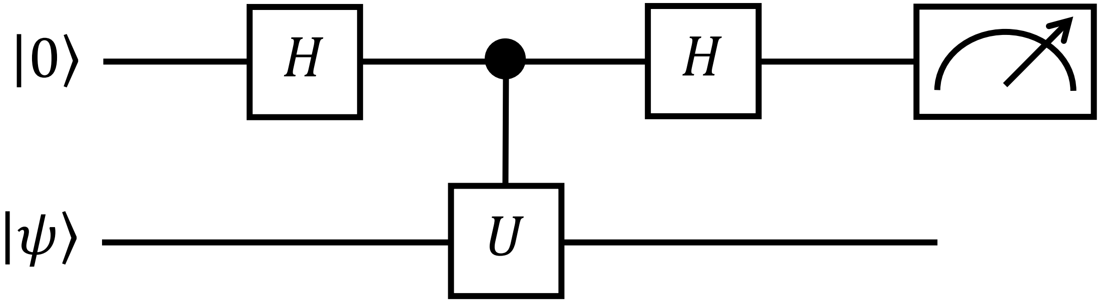
Coarse discretization

Good simulation

Simulator fails

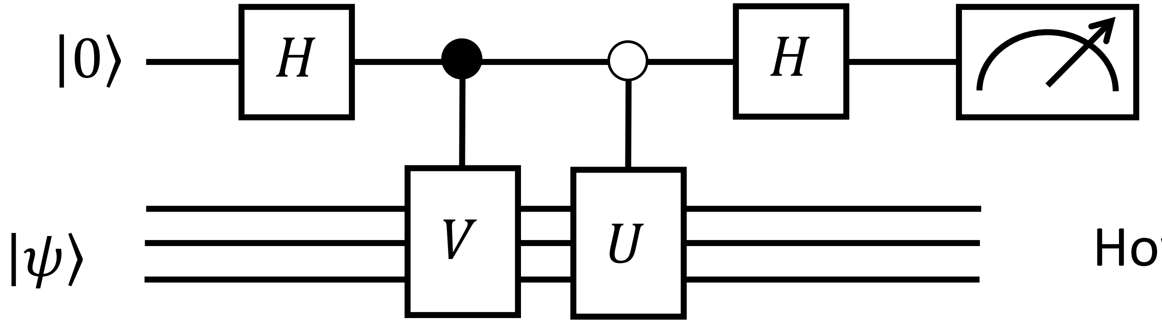
Quantum Simulation: Hadamard test

Compute observables and/or correlation functions using an ancilla for the Hadamard test:



$$P_0 - P_1 = \mathrm{Re}\langle U \rangle_\psi$$

Check this identity



$$P_0 - P_1 = \mathrm{Re}\left\langle U^\dagger V \right\rangle_\psi$$

How can you compute the imaginary part $\mathrm{Im}\langle U \rangle_\psi$?

R. Somma et al., Phys. Rev A **65**, 042323 (2002).

Quantum Simulation: correlation functions

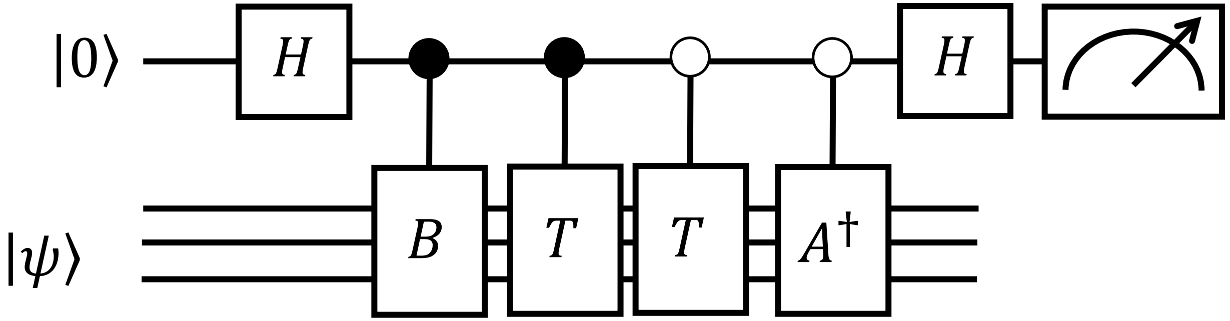
Quantum Computing

It is often useful in Physics to compute dynamical **correlation functions,** i.e.

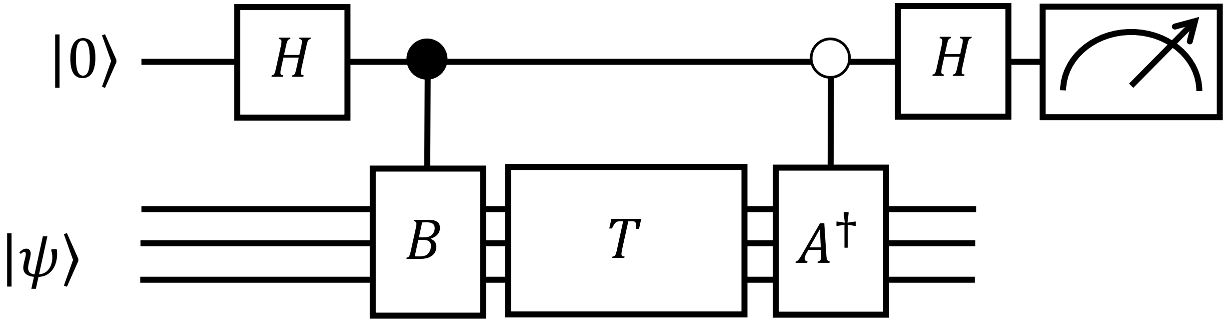
$$\langle\psi|A(t)B(0)|\psi\rangle = \langle\psi|T^\dagger A T B|\psi\rangle$$

As before, with $U^\dagger = T^\dagger A$ and $V = TB$

$$T = e^{-i\mathcal{H}t}$$



$$P_0 - P_1 = \mathrm{Re}\langle A(t)B\rangle_\psi$$



R. Somma et al., Phys. Rev A **65**, 042323 (2002).
A. Chiesa et al., Nature Phys. **15**, 455 (2019).

Quantum Approximate Optimization

Goal: minimize or maximize a function $C(x)$ subject to $x \in S$

Cost, distance, length of a trip, weight, processing time, energy consumption, number of objects

Profit, yield, efficiency, utility, capacity, number of results

Binary combinatorial problems

$$C(x) = \sum_{(Q,\bar{Q})\subset[n]} w_{(Q,\bar{Q})} \prod_{i\in Q} x_i \prod_{j\in\bar{Q}} (1 - x_j)$$

n bit strings $x \in \{0,1\}^n$

$x_i \in \{0,1\}$ $\qquad$ $w_{(Q,\bar{Q})} \in \mathbb{R}$

Map to diagonal Hamiltonian in the computational basis $H = \sum_{x\in\{0,1\}^n} C(x)\,|x\rangle\langle x|$ $\qquad |x\rangle \in \mathbb{C}^{2^n}$

If $C(x)$ only has at most weight k terms (terms with at most k bits), this diagonal Hamiltonian is the sum of weight k Z operators.

Quantum Computing

Quantum Approximate Optimization

$$H = \sum_{(Q,\bar{Q})\subset[n]} w_{(Q,\bar{Q})} \frac{1}{2^{|Q|+|\bar{Q}|}} \prod_{i\in Q}(1-Z_i) \prod_{j\in\bar{Q}}(1-Z_j)$$

$$H = \sum_{k=0}^{m} C_k$$

We assume only a m (polynomial in n) w are non-zero

$$B = \sum_{i=1}^{n} X_i$$

$$\left|\psi_p\left(\vec{\gamma},\vec{\beta}\right)\right\rangle = e^{-i\beta_p B} e^{-i\gamma_p H} \cdots e^{-i\beta_1 B} e^{-i\gamma_1 H} |+\rangle^n$$

Ansatz obtained by combining p alternating evolutions of H and B

$$F_p\left(\vec{\gamma},\vec{\beta}\right) = \left\langle\psi_p\left(\vec{\gamma},\vec{\beta}\right)\right|H\left|\psi_p\left(\vec{\gamma},\vec{\beta}\right)\right\rangle = \sum_k \left\langle\psi_p\left(\vec{\gamma},\vec{\beta}\right)\right|C_k\left|\psi_p\left(\vec{\gamma},\vec{\beta}\right)\right\rangle$$

To be minimized, as in VQE

E. Farhi, J. Goldstone, and S. Gutmann, arXiv:1411.4028 (2014)

Quantum Image Processing

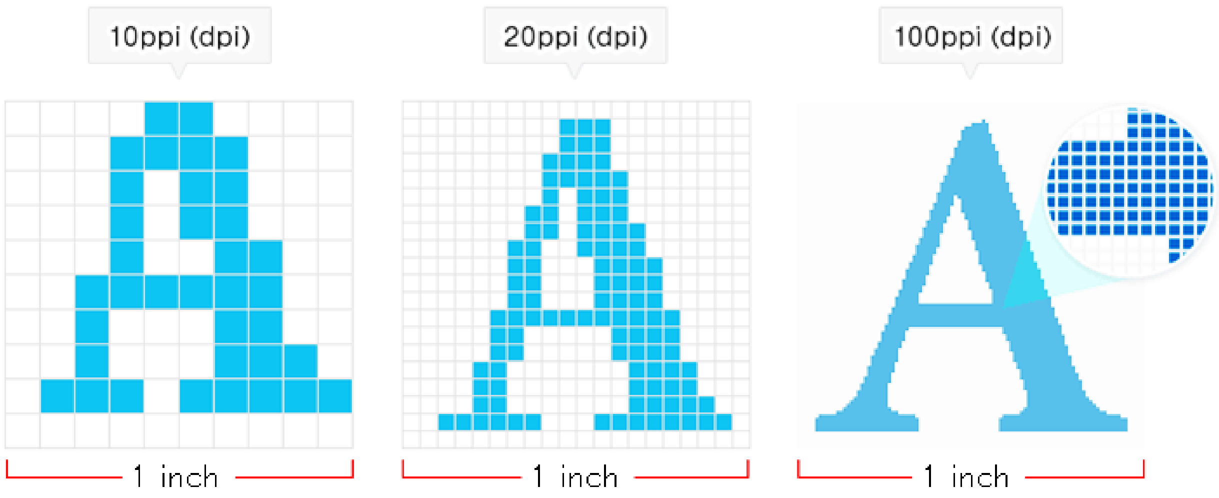
Various applications:

- Visual recognition
- Video analysis
- Optical character recognition (OCR)
- Movement detection

We focus on:

- Image encoding
- Edge detection

- Efficiency decreases by:
  - Increasing image size
  - Increasing image resolution (dpi: dots per inch, ppi: pixels per inch)



Flexible Representation of Quantum Images

$$|I(\theta)\rangle = \frac{1}{2^n}\sum_{i=0}^{2^{2n}-1}(\cos\theta_i\,|0\rangle + \sin\theta_i\,|1\rangle)\otimes|i\rangle$$

$$\theta_i \in \left[0,\frac{\pi}{2}\right], i = 0,1,\cdots,2^{2n}-1$$

- Created for black and white images is easily generalised for color images.

Requirements:
$2n+1$ qubits are needed to encode a square $2^n \times 2^n$ gray tones image. Gray tones must be encoded from 0 to $\frac{\pi}{2}$.

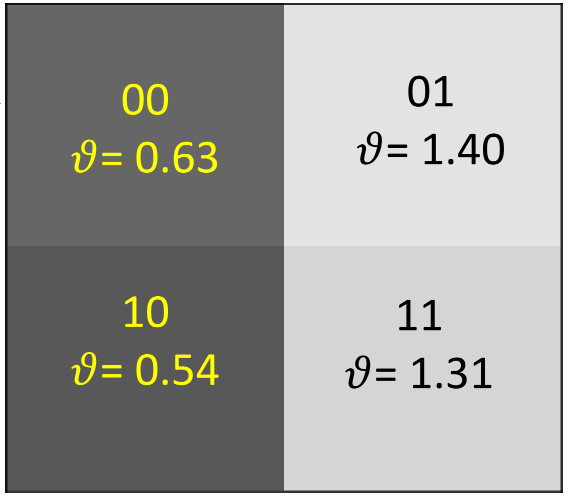
Superposition state:

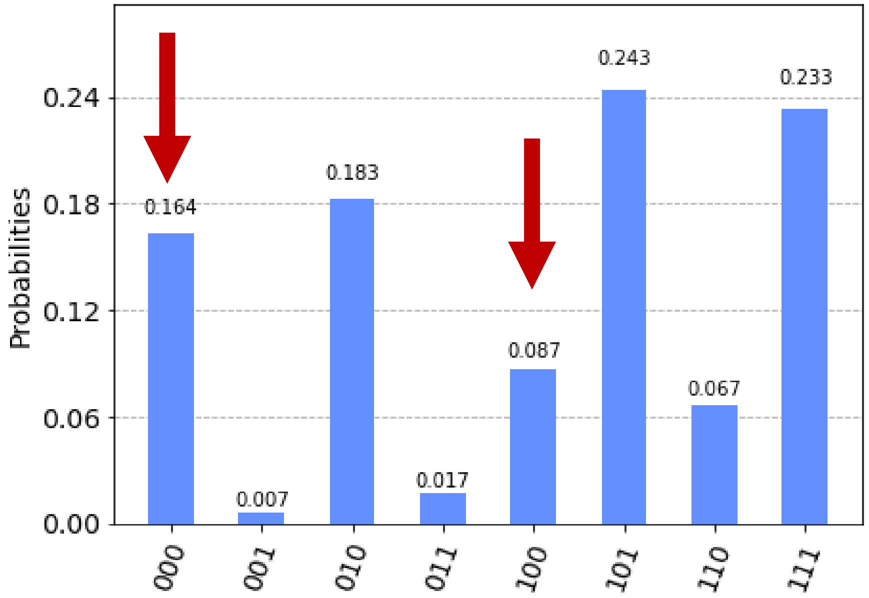
$$|H\rangle = \frac{1}{2^n}\,|0\rangle \otimes H^{\otimes 2n}|0\rangle$$

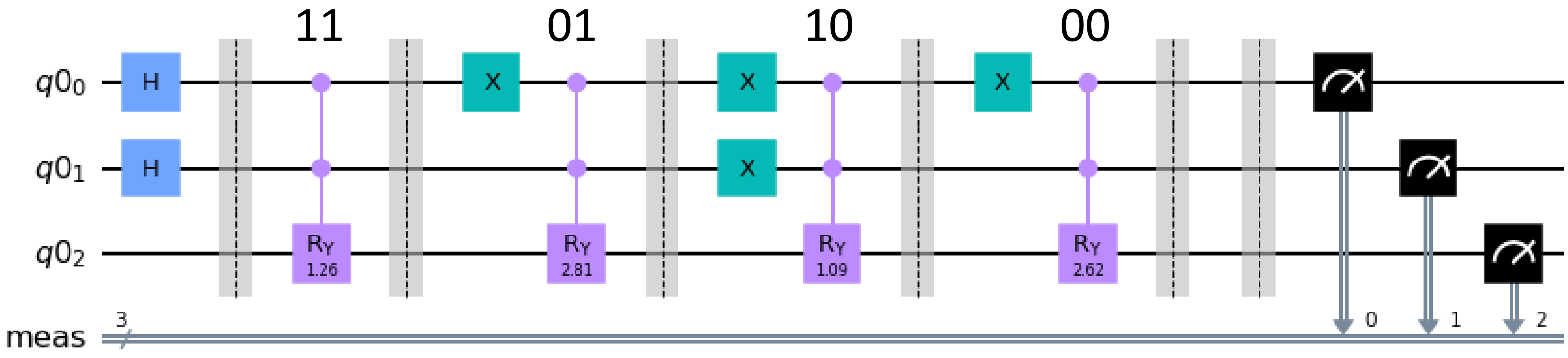
Encoding gray tones: Applying Multi Control Ry gates (MCRY)

$$C^{2n}\left(R_y(2\theta_i)\right)\,|H\rangle = |I(\theta)\rangle$$

Flexible Representation of Quantum Images







Novel Enhanced Quantum Representation

$$|I\rangle = \frac{1}{2^n} \sum_{Y=0}^{2^{2n}-1} \sum_{X=0}^{2^{2n}-1} | \otimes_{i=0}^{q-1} \rangle |C_{XY}^i\rangle |YX\rangle$$

$$i = 0,1,\cdots,7$$

- Quadradic speedup of the time complexity to prepare the NEQR quantum image with respect to FRQI.
- Accurate image retrieval after measurement, as opposed to probabilistic as for FRQI
- Complex operations can be achieved

Requirements:
$2n + m$ qubits are needed to encode a square $2^n \times 2^n$ image. The various shades of gray intensity must be encoded in m bits.

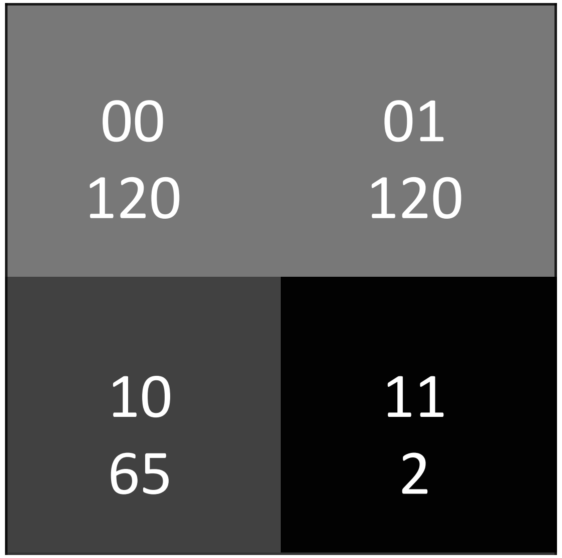
Superposition state:

$$|H\rangle = \frac{1}{2^n} |0\rangle \otimes H^{\otimes 2n} |0\rangle$$

Encoding gray tones: Applying Multi Control X gates (MCX)

$$C^{2n}(X)\,|H\rangle = |I\rangle$$

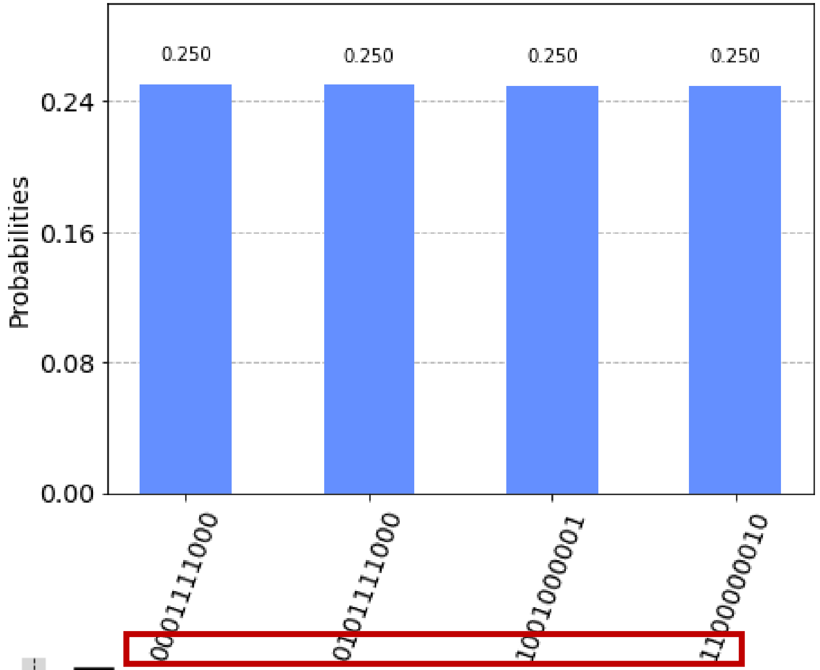
Quantum Computing

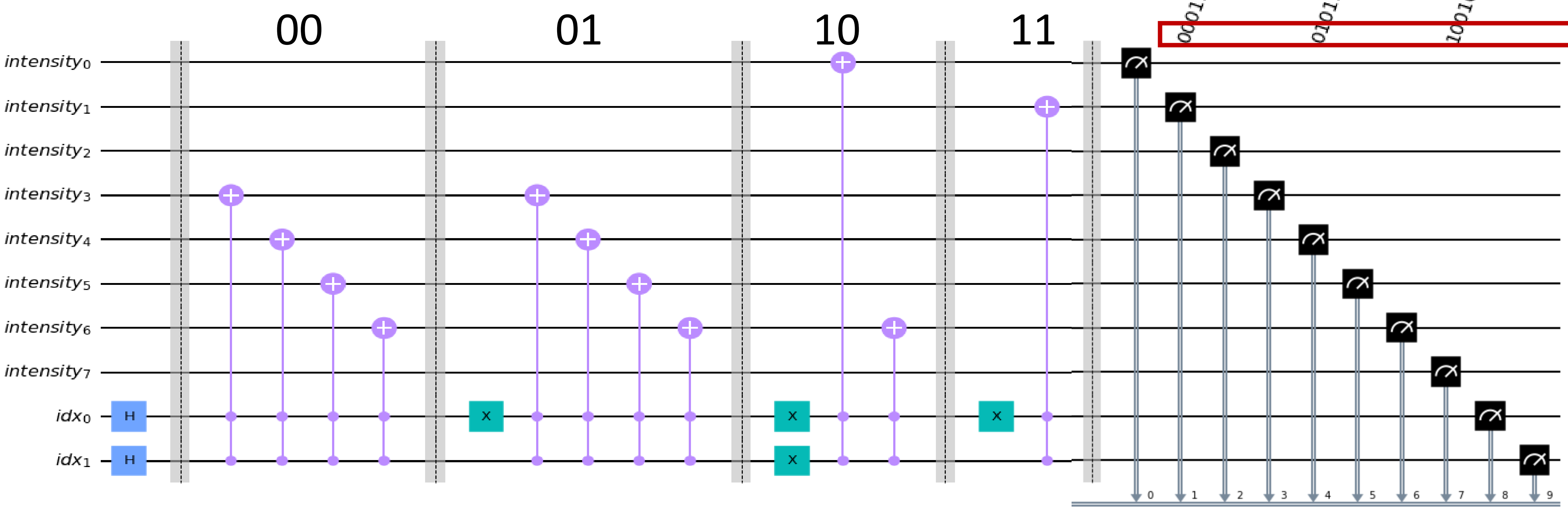


$$120 = 2^6 + 2^5 + 2^4 + 2^3$$

$$65 = 2^6 + 2^0$$

$$2 = 2^1$$

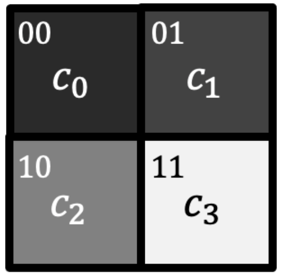




Edge detection

An edge is a change on image intensity, and it is usually gradual on a certain number of pixels

$$|\mathrm{Img}\rangle = \sum_{i=0}^{2^n-1} c_i\,|i\rangle$$



$$|\mathrm{Img}\rangle \otimes \frac{(|0\rangle + |1\rangle)}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{bmatrix} c_0 \\ c_0 \\ c_1 \\ c_1 \\ c_2 \\ c_2 \\ \vdots \\ c_{N-2} \\ c_{N-2} \\ c_{N-1} \\ c_{N-1} \end{bmatrix}$$

Add an ancilla

$$D_{2^{n+1}} = \begin{bmatrix} 0 & 1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & 1 & \dots & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & 0 & 0 & \dots & 0 & 0 \end{bmatrix}$$

Decrement gate

$$(I_{2^n} \otimes H) \cdot \begin{bmatrix} c_0 \\ c_1 \\ c_1 \\ c_2 \\ c_2 \\ c_3 \\ \vdots \\ c_{N-2} \\ c_{N-1} \\ c_{N-1} \\ c_0 \end{bmatrix} \rightarrow \begin{bmatrix} c_0 + c_1 \\ c_0 - c_1 \\ c_1 + c_2 \\ c_1 - c_2 \\ c_2 + c_3 \\ c_2 - c_3 \\ \vdots \\ c_{N-2} + c_{N-1} \\ c_{N-2} - c_{N-1} \\ c_{N-1} + c_0 \\ c_{N-1} - c_0 \end{bmatrix}$$

Gradient

Phys. Rev. X **7**, 031041 (2017)

https://journals.aps.org/prx/abstract/10.1103/PhysRevX.7.031041