

\* Typo in the last lecture:  $|0 \dots 0\rangle = \sin\theta |1\rangle + \cos\theta |L\rangle$

$$\begin{aligned} \text{A.A.: } R_0 R_\psi |0 \dots 0\rangle &= \sin(\theta(1+2)) |1\rangle + \cos(\theta(1+2)) |L\rangle \\ (R_0 R_\psi)^n |0 \dots 0\rangle &= \sin(\theta(1+2n)) |1\rangle + \cos(\theta(1+2n)) |L\rangle \end{aligned}$$

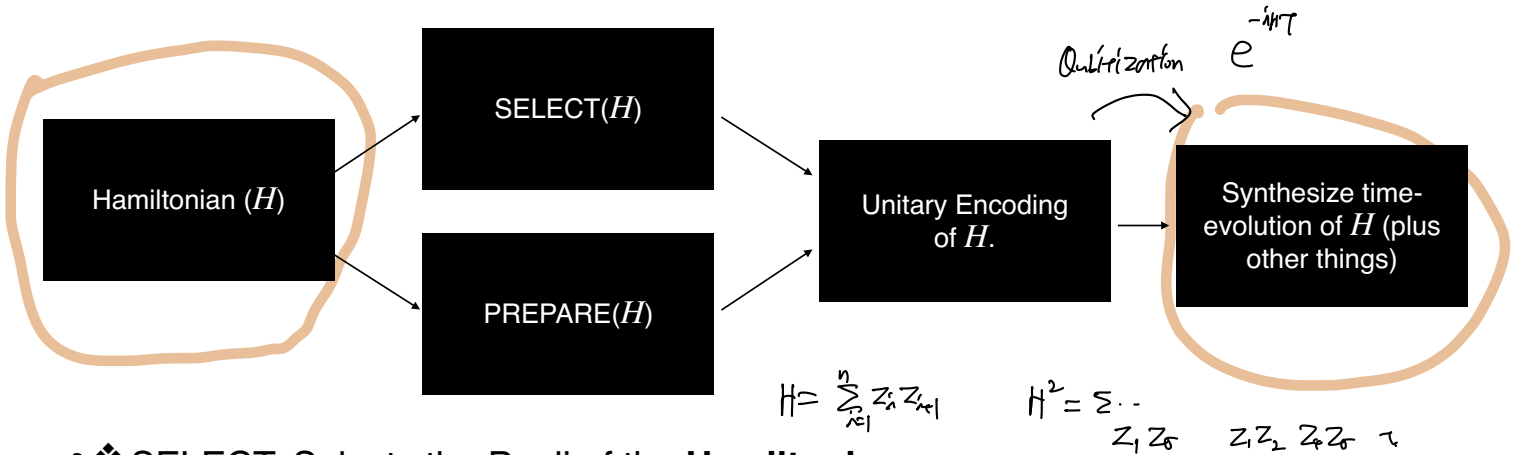
# 7. Qubitization: Quantum Signal Processing

# Overview

$$e^{-iH\tau} = \left( e^{-iH\tau/n} \right)^n \quad \left[ \left| \frac{H\tau}{n} \right| = O(1) \right]$$
$$H = \sum_p \alpha_p P$$

- LCU
  - ❖ Taylor expansion → Linear combination of unitary (Paulis)
  - ❖ SELECT: Selects the Pauli in the Taylor expansion
  - ❖ PREPARE: Encodes coefficients in the Taylor expansion
- Qubitization is an upgraded version of LCU, but it is more flexible and efficient.

# High-level overview of Qubitization



$$H = \sum_{i=1}^n z_i^x z_{i+1}^x$$

$$H^2 = \sum_{z_1, z_2, z_3, z_4} z_1^x z_2^x z_2^x z_3^x z_3^x z_4^x \dots$$

- ❖ SELECT: Selects the Pauli of the **Hamiltonian**.
- ❖ PREPARE: Encodes **coefficients of the Hamiltonian**.

Last time

$$e^{-iHt} = \sum_p \alpha_p |p\rangle$$

$$\text{SELECT}(|p\rangle|\psi\rangle) = |p\rangle P|p\rangle \quad (\text{for } p \text{ s.t. } \alpha_p \neq 0)$$

$$\text{PREPARE}(|0\dots 0\rangle) = \sum_p \sqrt{\alpha_p} |p\rangle$$

This lecture

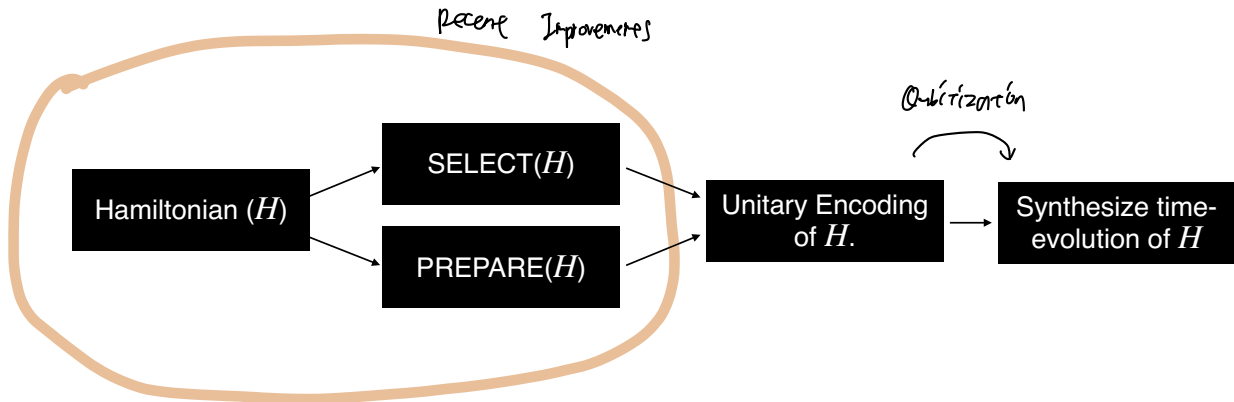
$$H = \sum_p \alpha_p |p\rangle$$

$$\text{SELECT}(H) |p\rangle|\psi\rangle = |p\rangle P|p\rangle \quad (\text{for } p \text{ s.t. } \alpha_p \neq 0)$$

$$\text{PREPARE}(H) |0\dots 0\rangle = \sum_p \sqrt{\alpha_p} |p\rangle$$

# Why Qubitization?

- The best state-of-the-art quantum algorithms for quantum chemistry is based on qubitization, in one form or another.
- Improvements are made in more efficient constructions of SELECT and PREPARE, but the framework of qubitization lives on.
- If you view SELECT and PREPARE as black boxes, qubitization is optimal, and even the constants are reasonable.



# Why Qubitization?

Year	Reference	Primary algorithmic innovation	Space complexity	Toffoli/T complexity
2005	Aspuru-Guzik <i>et al.</i> [4]	First algorithm (no compilation or bounds)	$\mathcal{O}(N)$	$\mathcal{O}(\text{poly}(N/\epsilon))$
2010	Whitfield <i>et al.</i> [11]	First compilation (no Trotter bounds)	$\mathcal{O}(N)$	$\mathcal{O}(\text{poly}(N/\epsilon))$
2012	Seeley <i>et al.</i> [41]	Use of Bravyi-Kitaev transformation	$\mathcal{O}(N)$	$\mathcal{O}(\text{poly}(N/\epsilon))$
2013	Wecker <i>et al.</i> [42]	First chemistry specific Trotter bounds	$\mathcal{O}(N)$	$\tilde{\mathcal{O}}(N^{10}/\epsilon^{3/2})$
2013	Toloui <i>et al.</i> [43]	Use of first quantization	$\mathcal{O}(\eta \log N)$	$\tilde{\mathcal{O}}(\eta^2 N^8/\epsilon^{3/2})$
2014	Hastings <i>et al.</i> [44]	Better compilation and multi-resolution Trotter	$\mathcal{O}(N)$	$\tilde{\mathcal{O}}(N^8/\epsilon^{3/2})$
2014	Poulin <i>et al.</i> [45]	Tighter Trotter bounds and ordering	$\mathcal{O}(N)$	$\tilde{\mathcal{O}}(N^6/\epsilon^{3/2})$
2014	McClean <i>et al.</i> [25]	Exploiting Hamiltonian sparsity with Trotter	$\mathcal{O}(N)$	$\tilde{\mathcal{O}}(N^4 S/\epsilon^{3/2})$
2014	Babbush <i>et al.</i> [46]	Tighter system specific Trotter bounds	$\mathcal{O}(N)$	$\tilde{\mathcal{O}}(N^2 S/\epsilon^{3/2})$
2015	Babbush <i>et al.</i> [47]	Use of Taylor series (database method)	$\mathcal{O}(N)$	$\tilde{\mathcal{O}}(N^4 \lambda_V/\epsilon)$
2015	Babbush <i>et al.</i> [47]	Use of Taylor series (on-the-fly method)	$\mathcal{O}(N)$	$\tilde{\mathcal{O}}(N^5/\epsilon)$
2015	Babbush <i>et al.</i> [48]	Use of Taylor series with first quantization	$\mathcal{O}(\eta \log N)$	$\tilde{\mathcal{O}}(\eta^2 N^3/\epsilon)$
2016	Reiher <i>et al.</i> [23]	First T count and tighter Trotter bounds	$\mathcal{O}(N)$	$\tilde{\mathcal{O}}(N^2 S/\epsilon^{3/2})$
2018	Motta <i>et al.</i> [29]	Use of low rank factorization with Trotter	$\mathcal{O}(N)$	$\tilde{\mathcal{O}}(N^4 \Xi/\epsilon^{3/2})$
2018	Campbell [49]	Use of randomized compiling with Trotter	$\mathcal{O}(N)$	$\tilde{\mathcal{O}}(\lambda_V^2/\epsilon^2)$
2019	Berry <i>et al.</i> [9]	Use of qubitization (sparse method)	$\tilde{\mathcal{O}}(N + \sqrt{S})$	$\tilde{\mathcal{O}}((N + \sqrt{S}) \lambda_V/\epsilon)$
2019	Berry <i>et al.</i> [9]	Use of qubitization (single factorization)	$\tilde{\mathcal{O}}(N^{3/2})$	$\tilde{\mathcal{O}}(N^{3/2} \lambda_{\text{SF}}/\epsilon)$
2019	Kivlichan <i>et al.</i> [50]	Better randomized compiled phase estimation	$\mathcal{O}(N)$	$\tilde{\mathcal{O}}(\lambda_V^2/\epsilon^2)$
2020	von Burg <i>et al.</i> [10]	Use of qubitization (double factorization)	$\tilde{\mathcal{O}}(N\sqrt{\Xi})$	$\tilde{\mathcal{O}}(N \lambda_{\text{DF}} \sqrt{\Xi}/\epsilon)$
2020	Present work	Use of tensor hypercontraction	$\tilde{\mathcal{O}}(N)$	$\tilde{\mathcal{O}}(N \lambda_C/\epsilon)$

↳ qubitization

- From Lee *et al.*, PRX Quantum 2, 030305 (2021).

# Why Qubitization?

$$e^{-iHT}$$

- Qubitization is also **flexible**. While Hamiltonian simulation is one of its most important applications, it can also do other things.
- For instance, you can apply  $e^{i \cos^{-1}(H/\|H\|)}$ . This may seem very obscure, but this is actually a very useful thing to do. (We'll talk about that next week.)

# Quantum Signal Processing

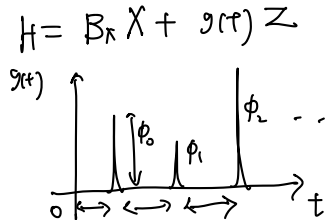
- The precursor to qubitization is Quantum Signal Processing (QSP) [Low, Yoder, and Chuang (2016), Low and Chuang (2016)]
- Physical model: Always-on magnetic field in one direction + instantaneous pulses

$$e^{i\phi_0 Z} e^{i\theta X} e^{i\phi_1 Z} \dots e^{i\theta X} e^{i\phi_d Z}$$

$|0\rangle, |1\rangle$

$$\chi = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \gamma = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\chi\gamma = iZ \quad \gamma z = i\chi \quad z\chi = i\gamma$$



# Quantum Signal Processing

- The precursor to qubitization is Quantum Signal Processing (QSP)
- Physical model: Always-on magnetic field in one direction + instantaneous pulses

*d+1 variable angles*

$$\underbrace{e^{i\phi_0 Z} e^{i\theta X} e^{i\phi_1 Z} \dots e^{i\theta X} e^{i\phi_d Z}} = \begin{bmatrix} P(a) & iQ(a)\sqrt{1-a^2} \\ iQ^*(a)\sqrt{1-a^2} & P^*(a) \end{bmatrix},$$

*Handwritten annotations:  $P(a)$  and  $P^*(a)$  are circled in red.  $iQ(a)\sqrt{1-a^2}$  and  $iQ^*(a)\sqrt{1-a^2}$  are circled in black. A handwritten  $\approx \sin \theta$  is above the top-right element.*

where  $\theta = \cos^{-1}(a)$  and  $a = \cos \theta$

1. Degrees of P and Q are at most d and d-1, respectively.
2. P, Q has parity d and (d-1) mod 2.
3.  $|P|^2 + (1 - a^2)|Q|^2 = 1$ .

$$\begin{pmatrix} a e^{i(\phi_0 + \phi_1)} & i\sqrt{1-a^2} e^{i(\phi_0 - \phi_1)} \\ i\sqrt{1-a^2} e^{i(\phi_1 - \phi_0)} & a e^{-i(\phi_0 + \phi_1)} \end{pmatrix}$$



# Quantum Signal Processing

$$* e^{i\theta X} = I \cos \theta + i S \sin \theta X$$

- The precursor to qubitization is Quantum Signal Processing (QSP)
- Physical model: Always-on magnetic field in one direction + instantaneous pulses

$$e^{i\phi_0 Z} e^{i\theta X} e^{i\phi_1 Z} = \begin{pmatrix} e^{i\phi_0} & 0 \\ 0 & e^{-i\phi_0} \end{pmatrix} \begin{pmatrix} a & i\sqrt{1-a^2} \\ i\sqrt{1-a^2} & a \end{pmatrix} \begin{pmatrix} e^{i\phi_1} & 0 \\ 0 & e^{-i\phi_1} \end{pmatrix}$$

$$= \begin{pmatrix} a e^{i(\phi_0 + \phi_1)} & i\sqrt{1-a^2} e^{i(\phi_0 - \phi_1)} \\ i\sqrt{1-a^2} e^{i(\phi_1 - \phi_0)} & a e^{-i(\phi_0 + \phi_1)} \end{pmatrix}$$

where  $\theta = \cos^{-1}(a)$ .

1. Degrees of P and Q are at most d and d-1, respectively.
2. P, Q has parity d and (d-1) mod 2.
3.  $|P|^2 + (1 - a^2)|Q|^2 = 1$ .

# Quantum Signal Processing

- The precursor to qubitization is Quantum Signal Processing (QSP)
- Physical model: Always-on magnetic field in one direction + instantaneous pulses

$$P_1 = P_1(\alpha)$$

$$Q_1 = Q_1(\alpha)$$

where  $\theta = \cos^{-1}(a)$ .

$$= \begin{pmatrix} P_1 & i\sqrt{1-a^2} Q_1 \\ i\sqrt{1-a^2} Q_1^* & P_1^* \end{pmatrix} \begin{pmatrix} P_2 & i\sqrt{1-a^2} Q_2 \\ i\sqrt{1-a^2} Q_2^* & P_2^* \end{pmatrix} = \begin{pmatrix} P_1 P_2 - (1-a^2) Q_1 Q_2 & i\sqrt{1-a^2} (P_1 Q_2 + Q_1 P_2^*) \\ - & - \end{pmatrix}$$

1. Degrees of P and Q are at most d and d-1, respectively.
2. P, Q has parity d and (d-1) mod 2.
3.  $|P|^2 + (1 - a^2) |Q|^2 = 1$ .

$$\begin{pmatrix} a e^{i(\phi_0 + \phi_1)} & i\sqrt{1-a^2} e^{i(\phi_0 - \phi_1)} \\ i\sqrt{1-a^2} e^{i(\phi_1 - \phi_0)} & a e^{-i(\phi_0 + \phi_1)} \end{pmatrix}$$

	degree	even/odd
$P_1$	1	odd
$Q_1$	0	even
$P_2$	1	odd
$Q_2$	0	even

# Recursion

$$e^{i\phi_0 Z} e^{i\theta X} e^{i\phi_1 Z} \dots e^{i\theta X} e^{i\phi_d Z} = \begin{bmatrix} P(a) & iQ(a)\sqrt{1-a^2} \\ iQ^*(a)\sqrt{1-a^2} & P^*(a) \end{bmatrix},$$

where  $\theta = \cos^{-1}(a)$  and

1. Degrees of P and Q are at most d and d-1, respectively.

2. P, Q has parity d and (d-1) mod 2.

3.  $|P|^2 + (1-a^2)|Q|^2 = 1$ .

$$\begin{pmatrix} P_1 & i\sqrt{1-a^2} Q_1 \\ i\sqrt{1-a^2} Q_1^* & P_1^* \end{pmatrix} \begin{pmatrix} P_2 & i\sqrt{1-a^2} Q_2 \\ i\sqrt{1-a^2} Q_2^* & P_2^* \end{pmatrix} = \begin{pmatrix} P_1 P_2 - (1-a^2) Q_1 Q_2 & i\sqrt{1-a^2} (P_1 Q_2 + Q_1 P_2^*) \\ - & - \end{pmatrix}$$

$P_1$   $d_1$   
 $Q_1$   $d_1-1$   
 $P_2$   $d_2$   
 $Q_2$   $d_2-1$

$$\deg(P_1 P_2 - (1-a^2) Q_1 Q_2) = d_1 + d_2$$

$$\deg(P_1 Q_2 + Q_1 P_2^*) = d_1 + d_2 - 1$$

	degree	even/odd
$P_1$ :	1	odd
$Q_1$ :	0	even
$P_2$ :	1	odd
$Q_2$ :	0	even

# A remarkable fact: Converse is true!

- For any

$$\begin{bmatrix} P(a) & iQ(a)\sqrt{1-a^2} \\ iQ^*(a)\sqrt{1-a^2} & P^*(a) \end{bmatrix},$$

where  $\theta = \cos^{-1}(a)$  and

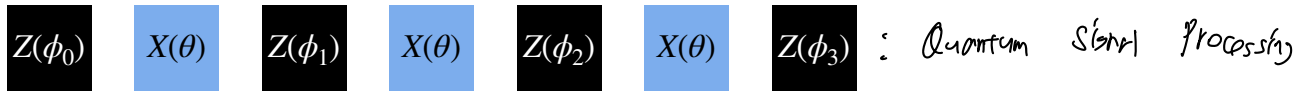
1. Degrees of P and Q are at most d and d-1, respectively.
2. P, Q has parity d and (d-1) mod 2.
3.  $|P|^2 + (1-a^2)|Q|^2 = 1$ .

There is a set of angles  $\phi_0, \dots, \phi_d$  such that  $e^{i\phi_0 Z} e^{i\theta X} e^{i\phi_1 Z} \dots e^{i\theta X} e^{i\phi_d Z} =$

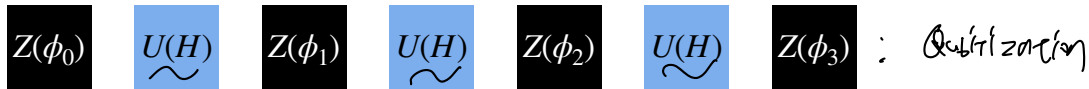
$$\begin{bmatrix} P(a) & iQ(a)\sqrt{1-a^2} \\ iQ^*(a)\sqrt{1-a^2} & P^*(a) \end{bmatrix}.$$

# An analogy

$$e^{-i\lambda z \phi_0}$$



$$e^{-i\lambda z \phi_0}$$



$$U(H) = \begin{pmatrix} \overset{N}{\cdot} & & \\ \cdot & \cdot & \\ \cdot & & \cdot \end{pmatrix} \begin{matrix} \cdot \\ \cdot \\ \cdot \end{matrix} \begin{matrix} \cdot \\ \cdot \\ \cdot \end{matrix}$$

(Note: The top-left element of the matrix is circled and labeled  $H_{\text{Hilb}}$ )

$$\|U(H)\| = 1$$

# Recap

- Quantum Signal Processing: A flexible framework to synthesize an arbitrary element of  $SU(2)$  by an always-on magnetic field and a sequence of variable “pulses.”
- This is just about a qubit, but the lesson extends more generally. Let’s talk about that in the next lecture.