

# ***Quantum Algorithms for Electronic Structure***

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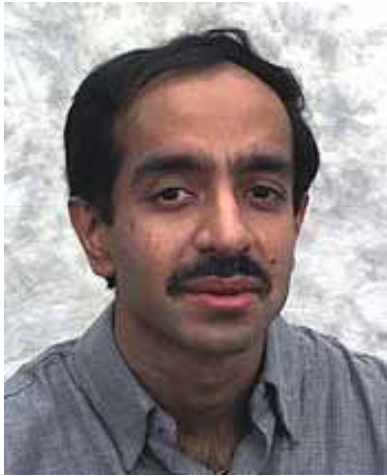
# Quantum Algorithms

Grover

Shor

Deutsch

Feynman



Grover '95

Search unsorted  
databases

**Bell-Labs**



Shor '94

Factoring large  
numbers

**MIT**



Deutsch '92

Constant or  
balanced  
functions

**Oxford**



Feynman '81

Quantum computer  
can be used to  
simulate nature  
exactly in real time

<http://math.nist.gov/quantum/zoo/>

This is a comprehensive catalog of  
quantum algorithms.

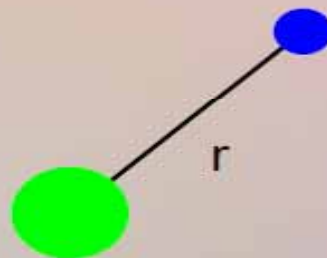
**Solving the Schrodinger  
Equation on a  
Quantum Computer**

$$H \Psi = E \Psi$$

# Hydrogen:

$$N_p = 1$$

$$N_e = 1$$



$$\hat{H} = \hat{T} + \hat{V} = \frac{-\hbar^2}{2m_e} \nabla^2 - \frac{e^2}{4\pi\epsilon_0 r}$$

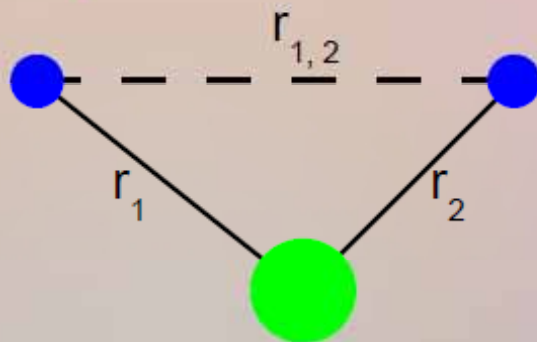
# More than one electron????

$$\hat{H} = \sum_i \hat{T}_i + \sum_i \hat{V}_i + \sum_i \sum_{i+1} R_{i,j}$$

# Hydride:

$$N_p = 1$$

$$N_e = 2$$



$$\hat{H} = \hat{T} + \hat{V} = \frac{-\hbar^2}{2m_e} \left( \nabla_1^2 + \nabla_2^2 \right) - \frac{e^2}{4\pi\epsilon_0} \left( \frac{1}{r_1} + \frac{1}{r_2} \right) + \frac{e^2}{4\pi\epsilon_0 r_{1,2}}$$

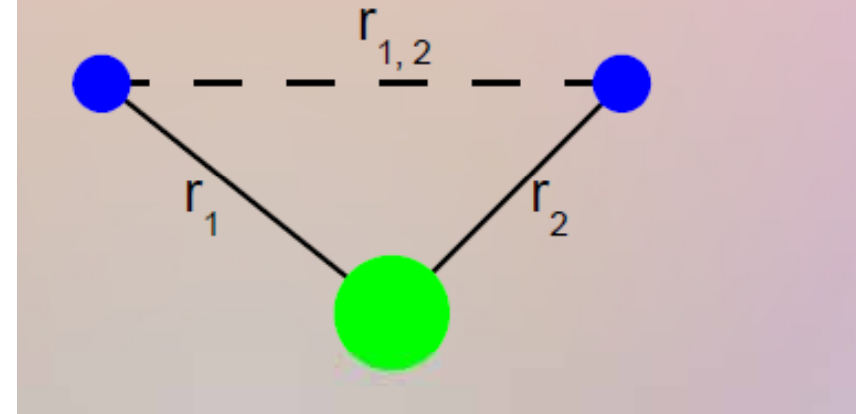
# Modern Quantum Chemistry

$$H\Psi = E\Psi$$

- (A) Ab Initio Methods (Hartree-Fock, Moller-Plesset, Coupled Cluster, Green's Function, ... , and Configuration Interaction).
- (B) Semi-empirical Methods (Extended Huckel, CNDO, INDO, AM1, ..., and PM3).
- (C) Density Functional Methods (LDA, GGA, ..., Hybrid Models). RDM,...
- (D) Algebraic Methods (Lie Groups, Lie Algebras, ..),
- (E) Renormalization Group Methods, Finite Size Scaling, DMRG, ...
- (F) Quantum Monte Carlo Methods (Variational, Diffusion, ..., )
- .....
- .....
- (F) Dimensional Scaling

Accuracy?

Computational Cost?



## II. HOOKE'S LAW MODEL

For the HL atom the Hamiltonian in bohr-hartree atomic units ( $\hbar = m = e = 1$ ) is

$$H = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) + \frac{1}{2}k(r_1^2 + r_2^2) + \frac{1}{r_{12}},$$

$$\Psi(r_1, r_2) = N_0 \left(1 + \frac{1}{2}r_{12}\right) e^{-(1/4)(r_1^2 + r_2^2)}$$

$$\rho(r) = 2N_0^2 e^{-(1/2)r^2} \left\{ \left(\frac{\pi}{2}\right)^{1/2} \left[ \frac{7}{4} + \frac{1}{4}r^2 + \left(r + \frac{1}{r}\right) \text{erf}(2^{-1/2}r) \right] + e^{-(1/2)r^2} \right\},$$

J. Chem. Phys. 91, 7791 (1989); JCP 99, 417 (1993)



ELSEVIER

26 June 1998

**CHEMICAL  
PHYSICS  
LETTERS**

Chemical Physics Letters 290 (1998) 199–204

## Renormalization group approach for electronic excitations in atoms

Ganpathy Murthy <sup>a</sup>, Sabre Kais <sup>b</sup>

Hamiltonian problem and converts it in the standard way to a Grassmann path integral [18]

$$Z = \text{Tr}[\exp - \beta H] = \int D\bar{\eta}_{\alpha,s} D\eta_{\alpha,s} \exp \int_0^\beta d\tau \times \left( \sum_{\alpha,s} \bar{\eta}_{\alpha,s} \frac{\partial}{\partial \tau} \eta_{\alpha,s} - H[\bar{\eta}_{\alpha,s}, \eta_{\alpha,s}] \right) \quad (2)$$



# Dimensional Scaling

## 1. Generalized the Hamiltonian to D-dimensions

$$H_D = -\frac{1}{2} \sum_i^N \sum_j^D \frac{\partial^2}{\partial x_{ij}^2} - Z \sum_i^N \frac{1}{r_{ij}} + \sum_{i,j}^N \frac{1}{r_{ij}}$$

## 2. Scale the distances such that

$$H_D = T/D^2 + U + V$$

## 3. Take the $D \rightarrow \infty$ limit

$$\varepsilon_\infty = \text{minimum}(U + V)$$

## 4. Generate the $1/D$ expansion

$$E_D = \varepsilon_\infty + \varepsilon_1/D + \varepsilon_2/D^2 + \dots$$

## 5. Substitute $D=3$

$$E_D \rightarrow E_3$$

# Exact Calculations

The calculation time for the energy of atoms and molecules scales exponentially with system size on a classical computer

# Examples

## Full CI

electron	orbital	CSFs
4	20	13,300
	30	67,425
	40	213,200
8	20	5,799,465
	30	172,459,665
	40	1,851,013,060

For  $N$  orbitals and  $m$  electrons there are  $\binom{N}{m} \approx \frac{N^m}{m!}$  ways to allocate the electrons among orbitals.

Doing Full CI calculations for  
Methanol (CH<sub>3</sub>OH), using 6-31G\*\*  
(18 electrons and 50 basis functions)  
requires about  $10^{17}$  Configurations

This is an **impossible** task on any current  
computer

The largest FCI  $\sim 10^9$  configurations

Dixon et. al. J.P.C A 103, 152 (1999)

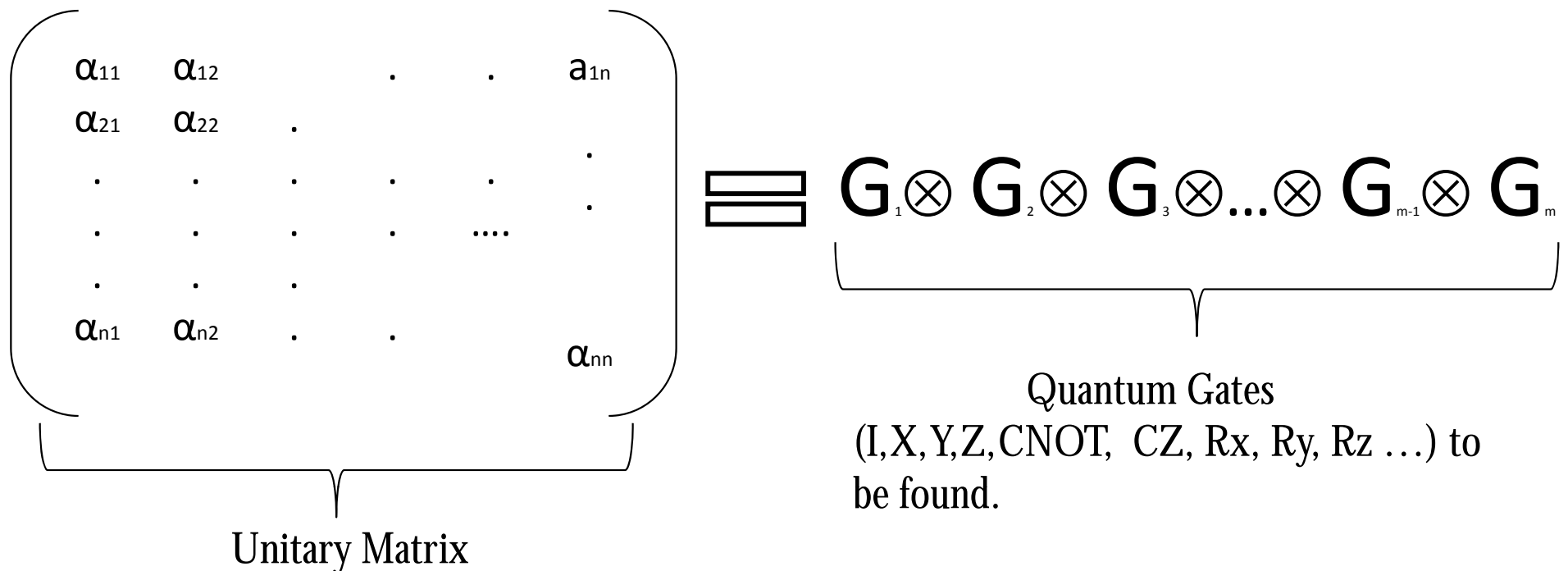
1.3 Billion Configurations for Cr<sub>2</sub> Molecules

# *Schrodinger Equation and Quantum Circuit Model*

The quantum circuit model is the most widely used model of quantum computation. It provides both a framework for formulating quantum algorithms and an architecture for the physical construction of quantum computers

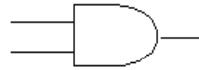
# Quantum Circuit Model

- Decomposition of a given unitary matrix in terms of quantum gates( such as CNOT, X, Y, Z, Control-Z, and Rotation gates)



# Classic Logic Gates

**AND**



A	B	$A \bullet B$
0	0	0
0	1	0
1	0	0
1	1	1

**OR**



A	B	$A + B$
0	0	0
0	1	1
1	0	1
1	1	1

**NOT**



A	$\bar{A}$
0	1
1	0

**NAND**



A	B	$\overline{(A \bullet B)}$
0	0	1
0	1	1
1	0	1
1	1	0

**NOR**



A	B	$\overline{(A + B)}$
0	0	1
0	1	0
1	0	0
1	1	0

**XOR**



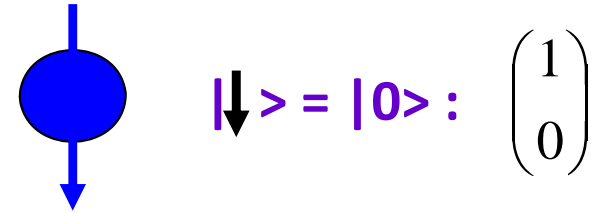
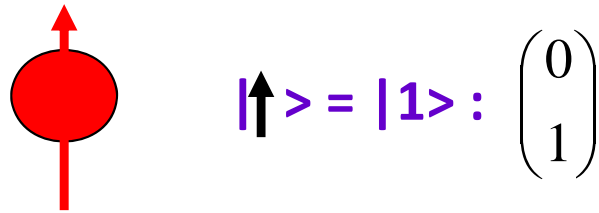
A	B	$A \oplus B$
0	0	0
0	1	1
1	0	1
1	1	0

**XNOR**

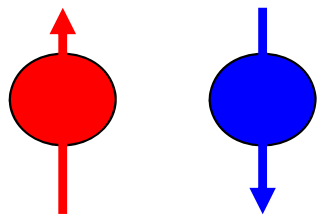


A	B	$\overline{(A \oplus B)}$
0	0	1
0	1	0
1	0	0
1	1	1

# Matrix representation of simple quantum logic gates



A general unitary transformation is a 2x2 matrix:



“ NOT ” gate

$$U_{\theta} = \begin{pmatrix} \cos(\theta/2) & \sin(\theta/2) \\ -\sin(\theta/2) & \cos(\theta/2) \end{pmatrix}$$

$$U_{\pi} |1\rangle = |0\rangle$$



$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\text{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$



# Simple Quantum Gates

$$\mathbf{X} \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

NOT Gate

$$\mathbf{Y} \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\mathbf{Z} \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\mathbf{H} \equiv \sqrt{\text{NOT}} \equiv \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Hadamard Gate

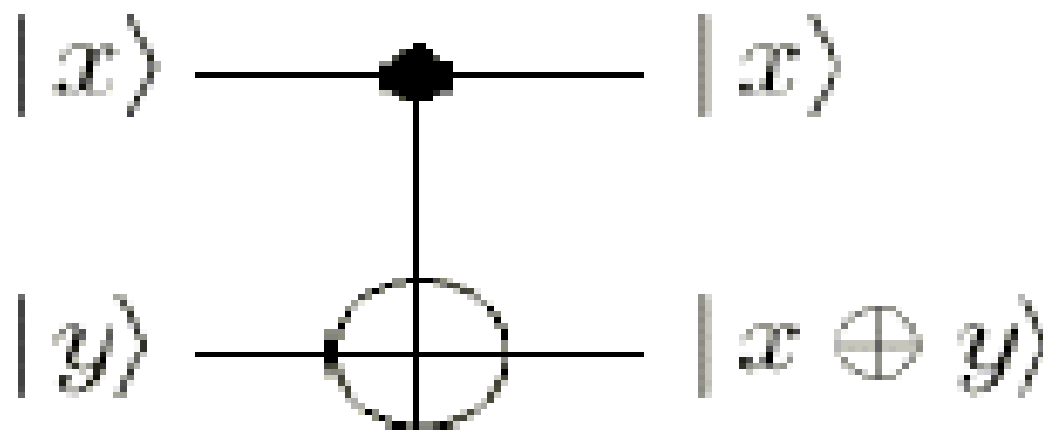
$$\alpha|0\rangle + \beta|1\rangle \longrightarrow \boxed{\mathbf{X}} \longrightarrow \alpha|1\rangle + \beta|0\rangle$$

$$\alpha|0\rangle + \beta|1\rangle \longrightarrow \boxed{\mathbf{Y}} \longrightarrow i \cdot (\alpha|1\rangle - \beta|0\rangle)$$

$$\alpha|0\rangle + \beta|1\rangle \longrightarrow \boxed{\mathbf{Z}} \longrightarrow \alpha|0\rangle - \beta|1\rangle$$

$$\alpha|0\rangle + \beta|1\rangle \longrightarrow \boxed{\mathbf{H}} \longrightarrow \alpha \frac{|0\rangle + |1\rangle}{\sqrt{2}} + \beta \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

# CNOT Gate



$$CN = |00\rangle\langle 00| + |01\rangle\langle 01| + |10\rangle\langle 11| + |11\rangle\langle 10|$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}
 \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}
 =
 \begin{bmatrix} a \\ b \\ d \\ c \end{bmatrix}
 \begin{pmatrix} 00 \\ 01 \\ 10 \\ 11 \end{pmatrix}$$

# Key Challenges

$$H\Psi = E\Psi$$

(1) Isolate qubits in physical systems

(Photonic quantum computer to simulate Hydrogen Molecule.

Logical states  $|0\rangle, |1\rangle$  corresponds to horizontal  $|H\rangle$  and vertical  $|V\rangle$  polarization)

(2) Represent the Hamiltonian  $H$

(Write  $H$  as a sum of Hermitian operators, each to be converted into unitary gates under the exponential map)

(3) Prepare the states,  $\Psi$

(Direct mapping, each qubit represents the fermionic occupation state of a particular orbital, occupied or not. Fock space of the system is mapped onto the Hilbert space of the qubits)

(4) Extract the energy,  $E$

(Using the phase estimation quantum algorithm)

(5) Read out qubit states

# Quantum Fourier Transform

$$\begin{aligned}
 |\omega\rangle &= |x_1 x_2 \dots x_n\rangle \rightarrow \sum_{y=0}^{2^n-1} e^{2\pi i \omega y} |y\rangle \\
 &= \frac{1}{2^{n/2}} \left( |0\rangle + e^{2\pi i (2^{n-1} \omega)} |1\rangle \right) \otimes \left( |0\rangle + e^{2\pi i (2^{n-2} \omega)} |1\rangle \right) \otimes \\
 &\quad \dots \otimes \left( |0\rangle + e^{2\pi i (\omega)} |1\rangle \right) \\
 &= \frac{1}{2^{n/2}} \left( |0\rangle + e^{2\pi i (0.x_n x_{n+1} \dots)} |1\rangle \right) \otimes \left( |0\rangle + e^{2\pi i (0.x_{n-1} x_n x_{n+1} \dots)} |1\rangle \right) \otimes \\
 &\quad \dots \otimes \left( |0\rangle + e^{2\pi i (0.x_1 x_2 \dots)} |1\rangle \right)
 \end{aligned}$$

$$\omega = 0 . x_1 x_2 \cdots x_n$$

*Scaling :*

$$2\omega = x_1 . x_2 x_3 \cdots$$

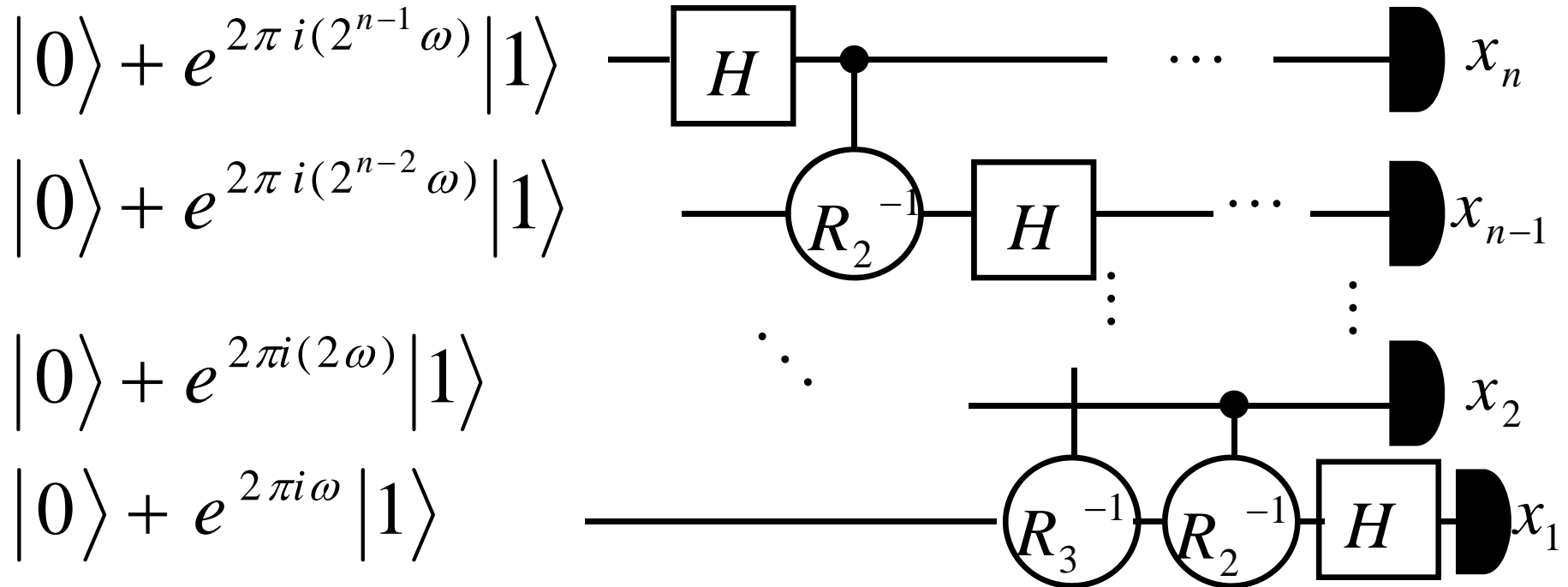
$$QFT : \Theta(n^2)$$

$\vdots$

$$FFT : \Theta(n2^n)$$

$$2^{n-1}\omega = x_1 x_2 x_3 \cdots x_{n-1} . x_n$$

# Implementation of QFT



$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad H|0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle), \quad H|1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$$

# Quantum Phase Estimation

- | To estimate a number  $\omega \in [0,1)$  given unitary operator  $U$  with eigenvector  $|\psi\rangle$ , eigenvalue  $e^{2\pi i\omega}$
- | Prepare two qubit registers: index register and target register
- | Perform the controlled- $U^{2^j}$  on the target register
- | Inverse QFT on the first register, then make a measurement.

Daniel Abrams and Seth Lloyd, PRL 83, 5162 (1999).  
A. Yu. Kitaev, quant-ph/9511026

## Procedures

1.  $|\mathbf{0}\rangle|u\rangle$

**initial state**

2.  $\rightarrow \frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} |j\rangle|u\rangle$

**create superposition**

3.  $\rightarrow \frac{1}{\sqrt{2^t}} \sum_{j=0}^{2^t-1} |j\rangle U^j |u\rangle$

**apply black box**

4.  $\rightarrow |\tilde{\varphi}_u\rangle|u\rangle$

**apply inverse Fourier transform**

5.  $\rightarrow |\tilde{\varphi}_u\rangle$

**measure first register**



# Quantum phase estimation Algorithm

## Inputs:

1. A black box which performs a controlled- $U^j$  operation, for integer  $j$ ,
2. An eigenstate  $|u\rangle$  of  $U$  with eigenvalue  $e^{2\pi i\varphi_u}$ , and
3.  $t = n + \left\lceil \log Q + \frac{1}{2\varepsilon} \right\rceil$  qubits initialized to  $|0\rangle$

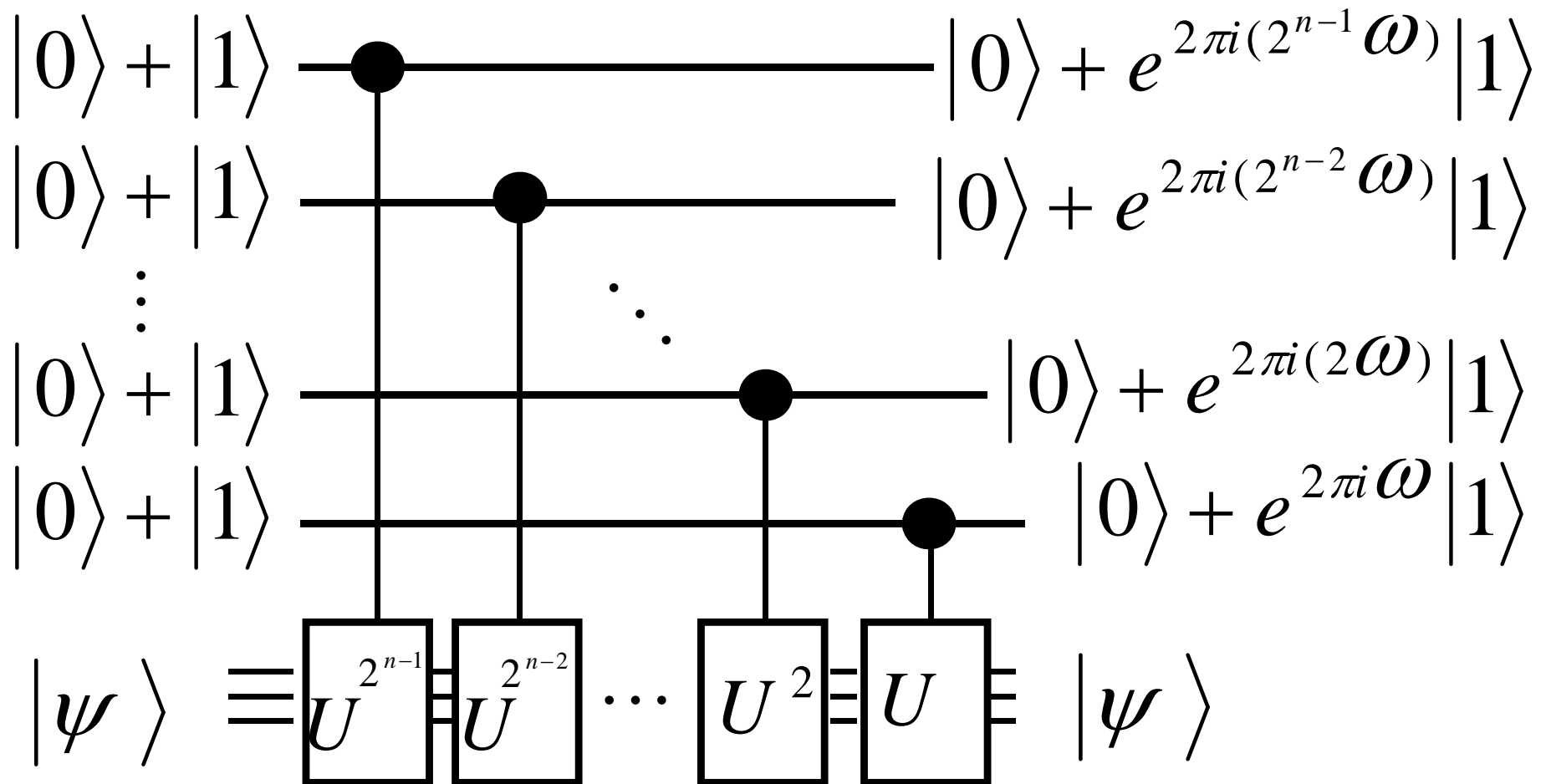
## Outputs:

An  $n$ -bit approximation  $\tilde{\varphi}_u$  to  $\varphi_u$ .

## Runtime:

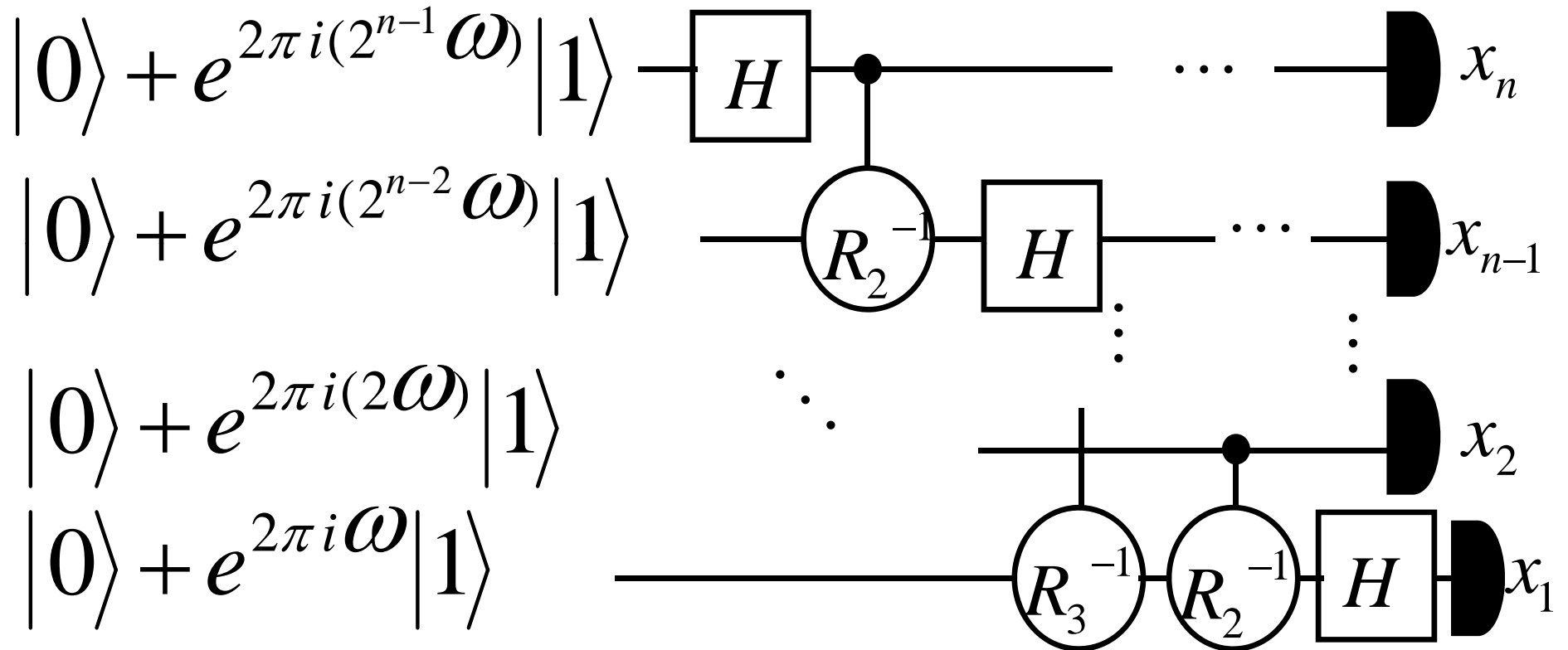
$O(t^2)$  operations and one call to controlled- $U^j$  black box.  
Succeeds with probability at least  $(1 - \varepsilon)$ .

# Circuit for Phase Estimation



# Measurement:

# Inverse QFT



Energy = Binary expansion  $0.x_1.x_2.x_3\dots x_n$

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s.$$

$$a_j \Leftrightarrow \mathbf{1}^{\otimes j-1} \otimes \sigma^+ \otimes \sigma^z \otimes N-j-1$$

$$a_j^\dagger \Leftrightarrow \mathbf{1}^{\otimes j-1} \otimes \sigma^- \otimes \sigma^z \otimes N-j-1$$

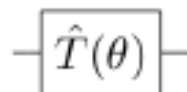
$$\sigma^+ \equiv \frac{\sigma^x + i\sigma^y}{2} = |0\rangle\langle 1| \text{ and } \sigma^- \equiv \frac{\sigma^x - i\sigma^y}{2} = |1\rangle\langle 0|$$

Second quantized operators

Circuit

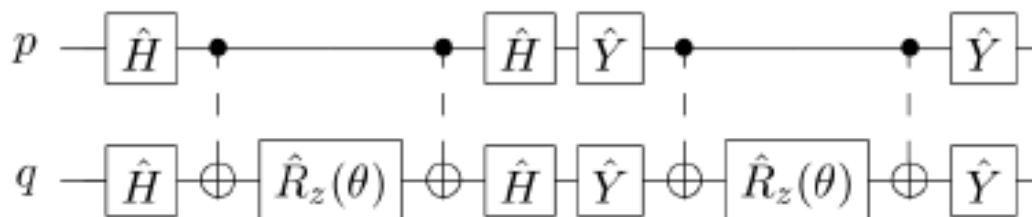
Number operator

$$h_{pp} a_p^\dagger a_p$$



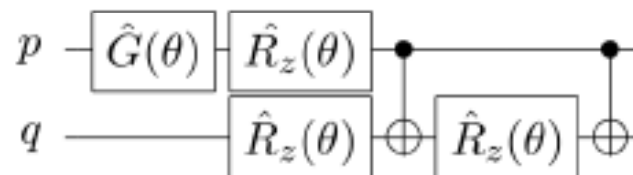
Excitation operator

$$h_{pq} (a_p^\dagger a_q + a_q^\dagger a_p)$$



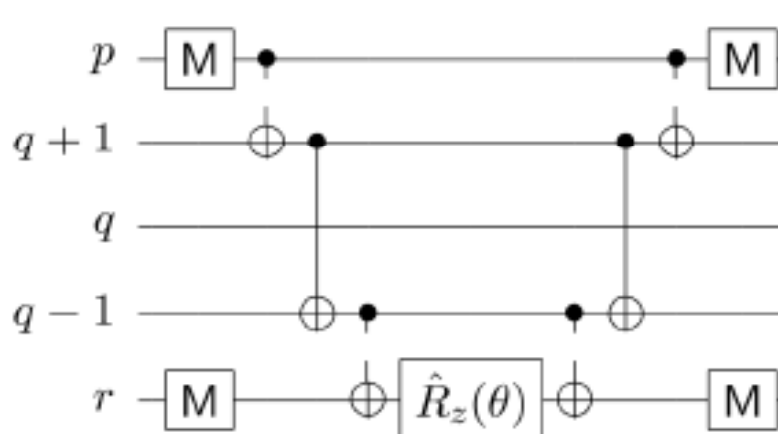
Coulomb and exchange operators

$$h_{pqqp} a_p^\dagger a_q^\dagger a_q a_p$$



Number-excitation<sup>a</sup> operator

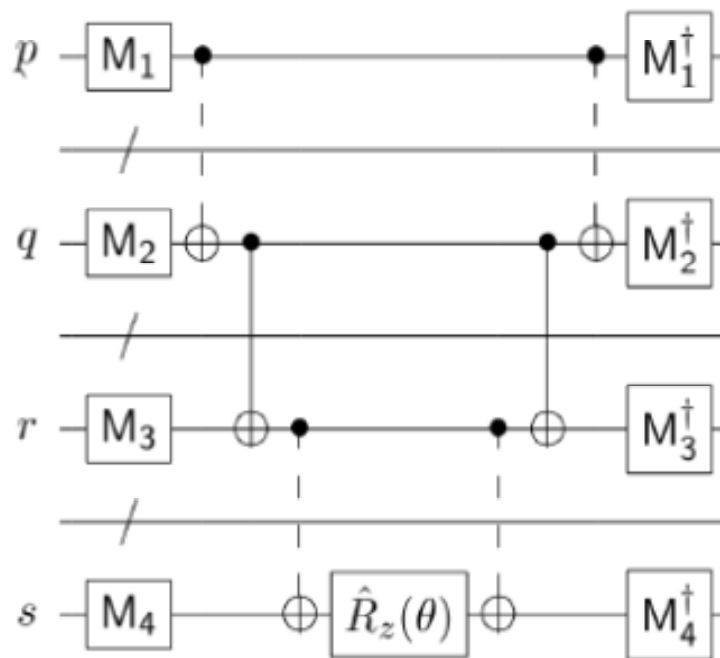
$$h_{pqqr} (a_p^\dagger a_q^\dagger a_q a_r + a_r^\dagger a_q^\dagger a_q a_p)$$



where  $M = \{\hat{H}, \hat{Y}\}$

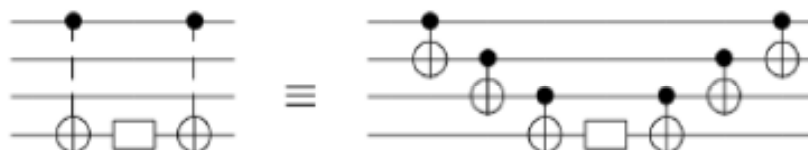
Double excitation operator

$$h_{pqrs} (a_p^+ a_q^+ a_r a_s + a_s^+ a_r^+ a_q a_p)$$



where  $(M_1, M_2, M_3, M_4) = \{(\hat{H}, \hat{H}, \hat{H}, \hat{H}), (\hat{Y}, \hat{Y}, \hat{Y}, \hat{Y}), (\hat{H}, \hat{Y}, \hat{H}, \hat{Y}), (\hat{Y}, \hat{H}, \hat{Y}, \hat{H}), (\hat{Y}, \hat{Y}, \hat{H}, \hat{H}), (\hat{H}, \hat{H}, \hat{Y}, \hat{Y}), (\hat{Y}, \hat{H}, \hat{H}, \hat{Y}), (\hat{H}, \hat{Y}, \hat{Y}, \hat{H})\}$

Notation:

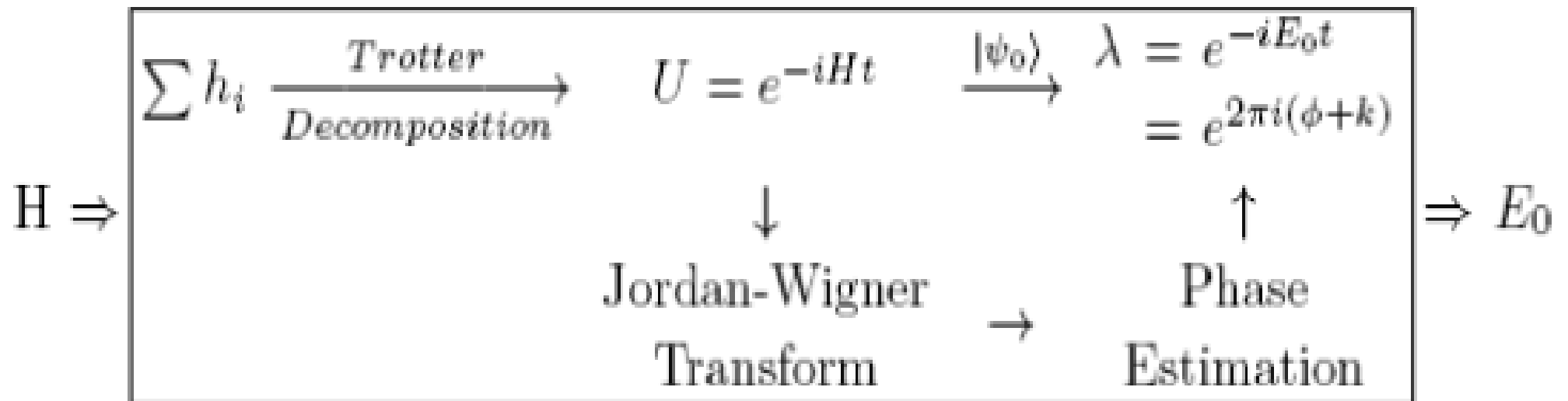


## Simulation of electronic structure Hamiltonians using quantum computers

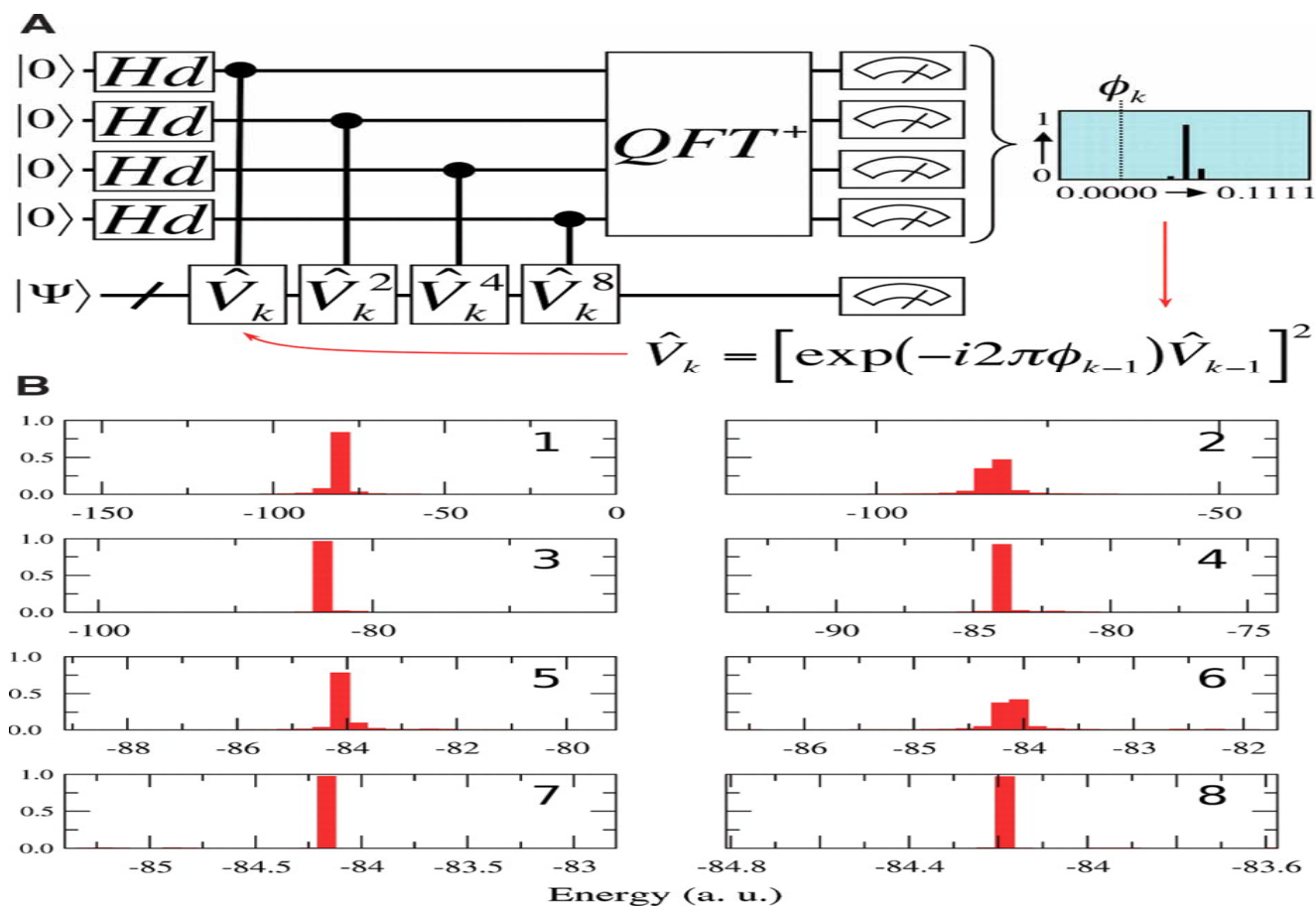
[Whitfield](#); [Biamonte](#); [Aspuru-Guzik](#)

MOLECULAR PHYSICS Volume: 109 Issue: 5 Pages: 735-750 (2011)

# Algorithmic overview of the steps taken to simulate a chemical Hamiltonian



# Simulated Quantum Computation of Molecular Energies

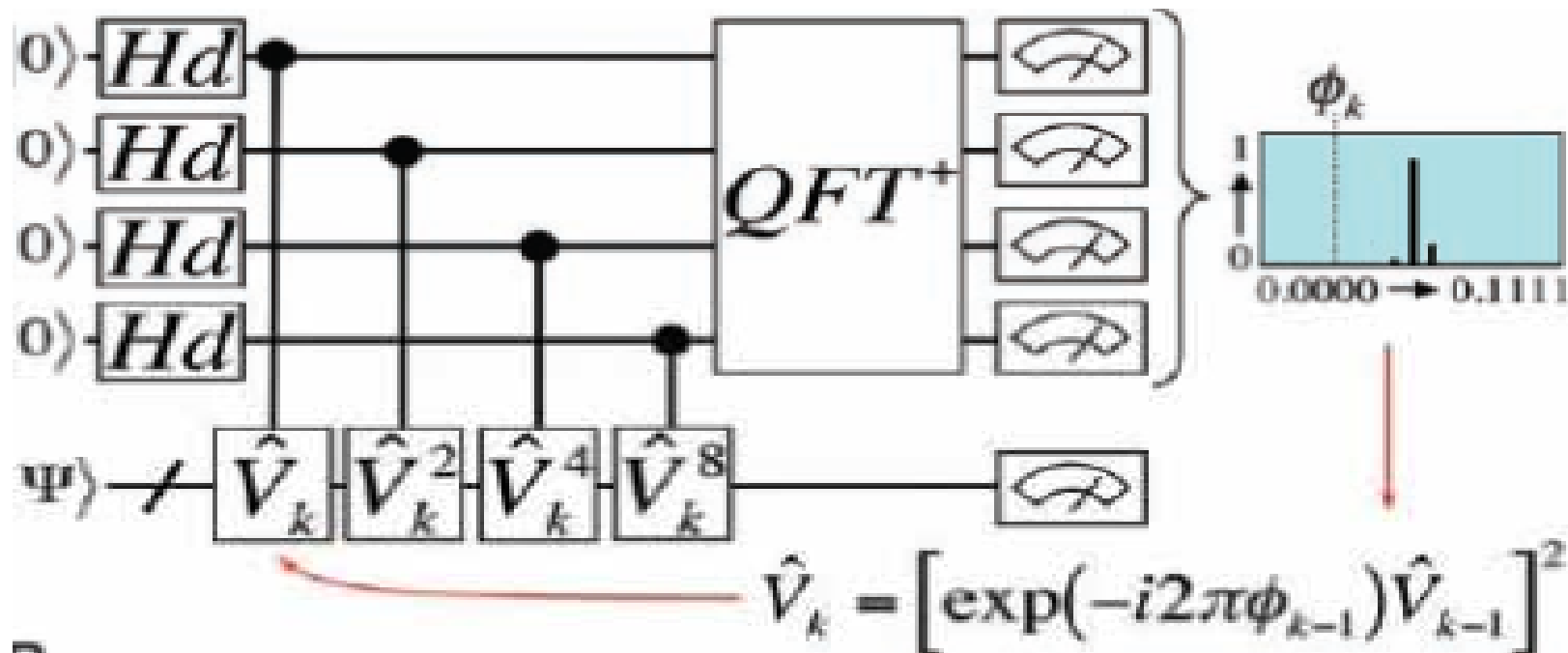


Simulation of the ground state of H<sub>2</sub> and H<sub>2</sub>O Molecules

Alán Aspuru-Guzik, Peter Love,..... Science 309, 1704 (2005).

# Quantum algorithm for obtaining the energy spectrum of molecular systems

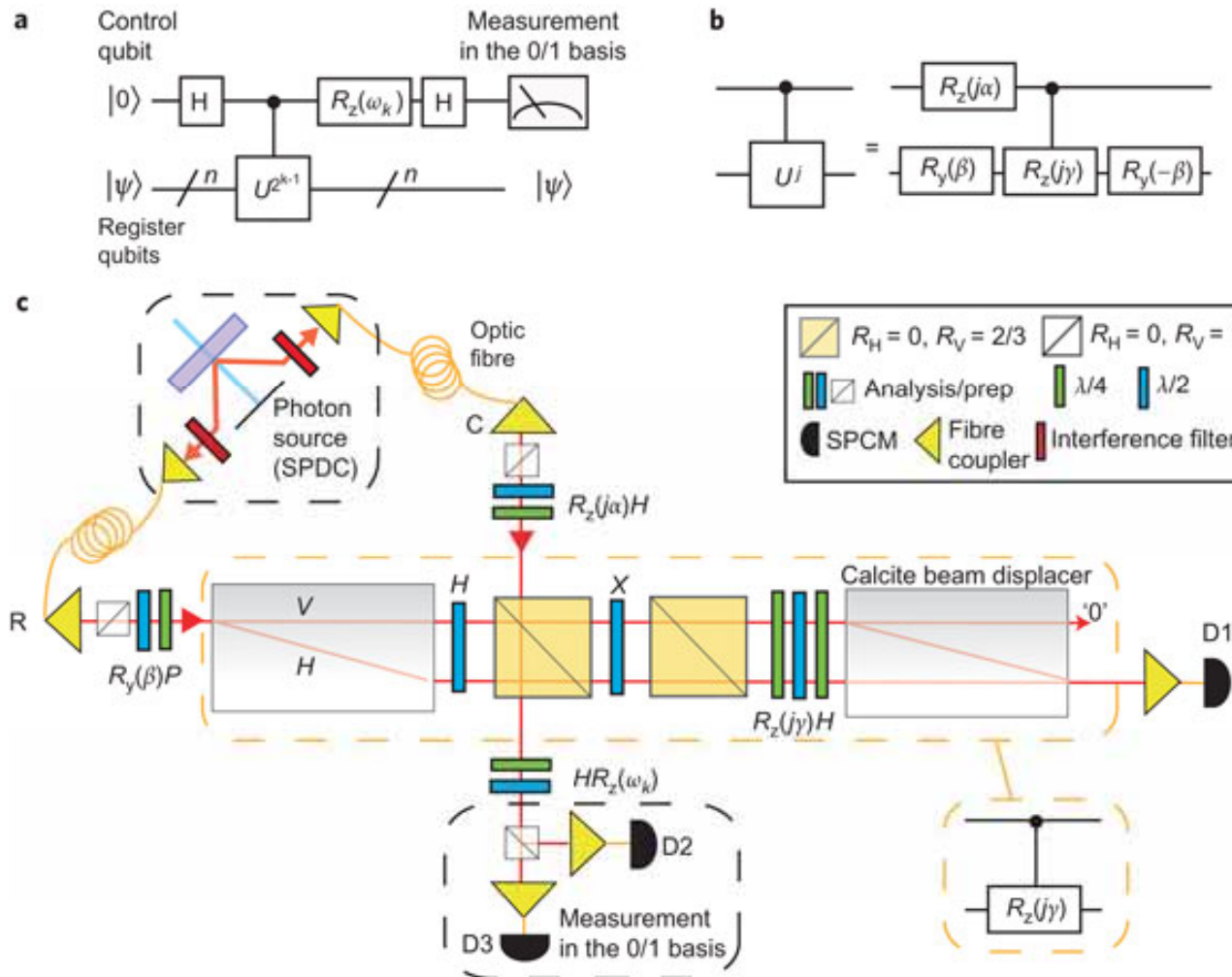
Hefeng Wang, Alán Aspuru-Guzik, and Sabre Kais  
Phys. Chem. Chem. Phys. 10, 5388 (2008)



Simulation of excited states of H<sub>2</sub>O Molecules



# Towards quantum chemistry on a quantum computer



4 qubits and 522 perfect sequential one and two-qubit quantum logic gates.

# Challenges

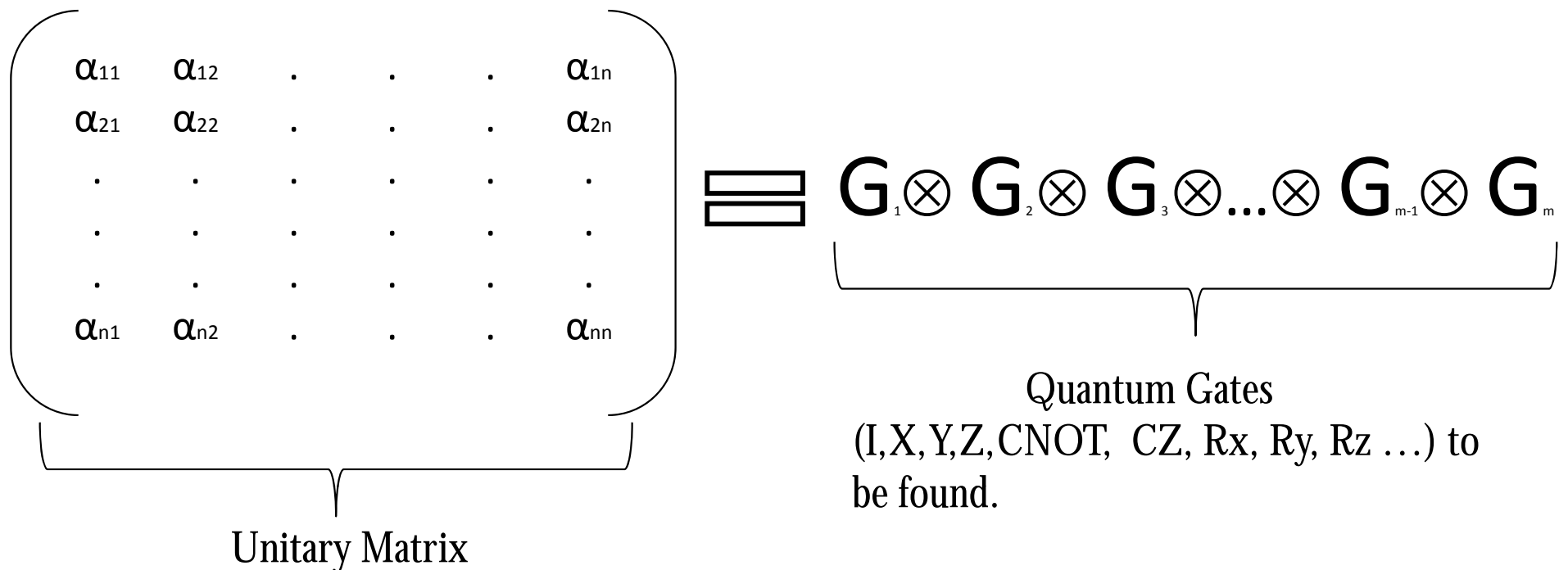
**Open the Black BoX**

$$U = e^{-iH}$$

# Quantum Circuit Design as An Optimization Problem

Anmer Daskin and Sabre Kais

- Decomposition of a given unitary matrix in terms of quantum gates( such as CNOT, X, Y, Z, Control-Z, and Rotation gates)



# Quantum circuit design is not an easy task! I

- Deterministic Methods based on Quantum Shannon Decomposition, Cosine-Sine Decomposition and similar others generate  $O(4^n)$  gates<sup>2</sup>.
- Stochastic methods: Apply Genetic and Evolutionary Algorithms to find efficient quantum circuits.

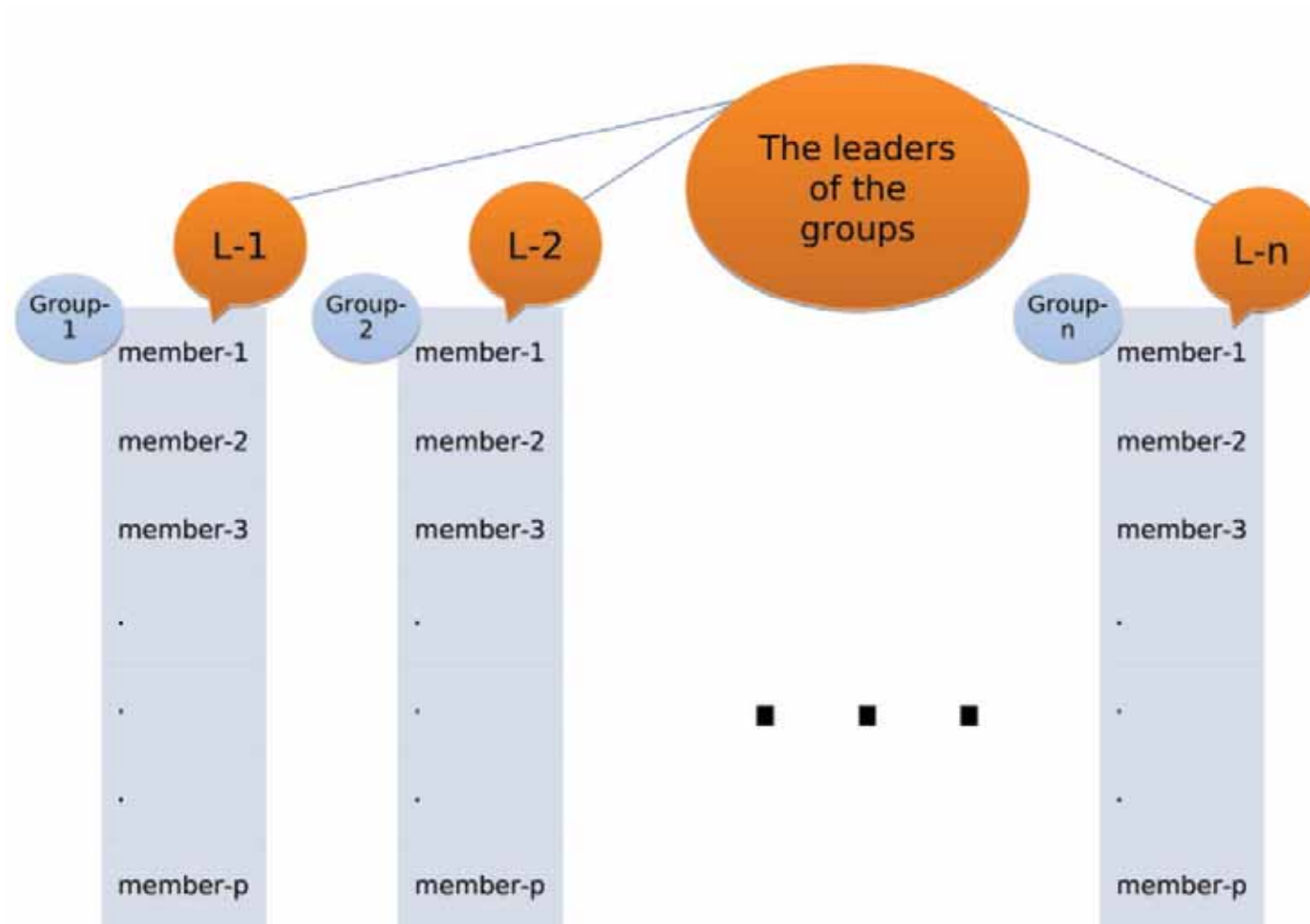
## Cosine-Sine Decomposition

**Cosine-Sine Decomposition** factors a  $2^n \times 2^n$  unitary  $u$ :

$$u = \begin{pmatrix} v_1 & 0 \\ 0 & v_2 \end{pmatrix} \begin{pmatrix} c & s \\ -s & c \end{pmatrix} \begin{pmatrix} v_3 & 0 \\ 0 & v_4 \end{pmatrix}$$

- $v_1, v_2, v_3, v_4$  are  $(2^{n/2}) \times (2^{n/2})$  unitary
- $c = \text{diagonal}(\cos t_0, \cos t_1, \dots, \cos t_{2^{n/2}-1})$
- $s = \text{diagonal}(\sin t_0, \sin t_1, \dots, \sin t_{2^{n/2}-1})$

# Group Leaders Optimization Algorithm



# Group Leaders Optimization Algorithm

- **Step 1**: Generate random-population for each group.
- **Step 2**: Calculate fitness values for the whole population.
- **Step 3**: Determine the leaders for each group by choosing the one from each group, which has the best solution in its group.

- **Step 4:** Recombination and Mutation: Create new member by using the current member, its leader for its group, and some random evaluation. For numerical problems the expression reads:

$$new = r1 * old + r2 * leader + r3 * random.$$

- **Step 5:** One way crossover between different group members: Choose random members starting from the first group, and then transfer some parameters from another random member in a different group

# The fidelity error

- The fidelity error used in the optimization to measure how similar the unitary operators  $U_a$  and  $U_t$  are is defined as:<sup>6</sup>

$$\epsilon = 1 - \mathcal{F}^2,$$

where

$$\mathcal{F} = \frac{1}{N} \left| \text{Tr} \left( U_a U_t^\dagger \right) \right|,$$

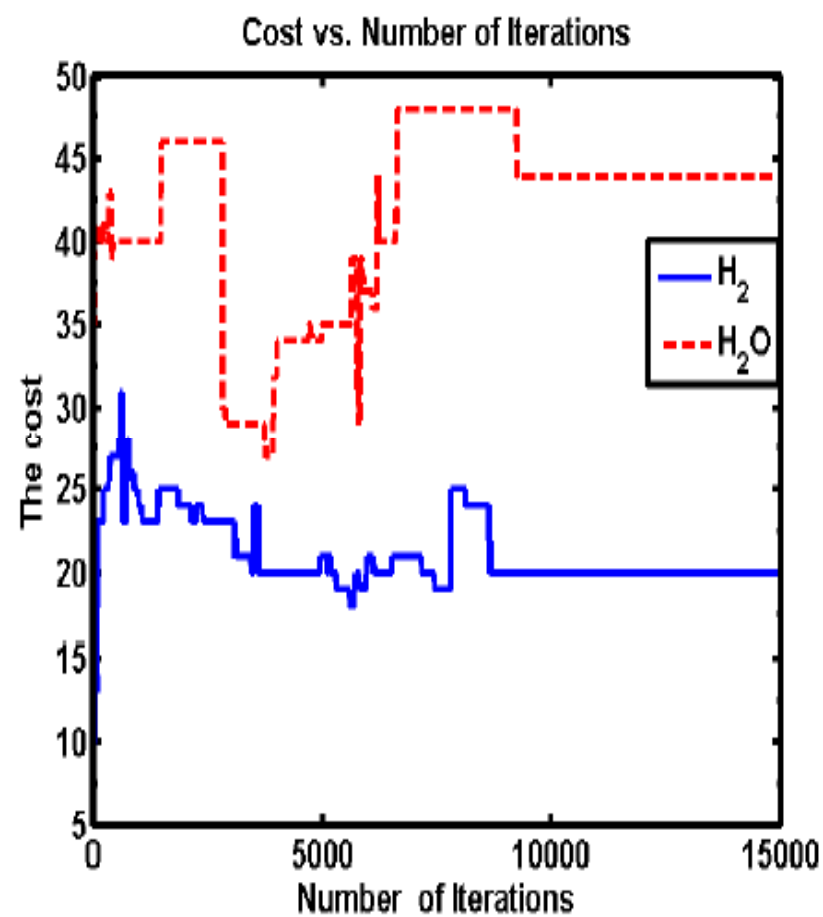
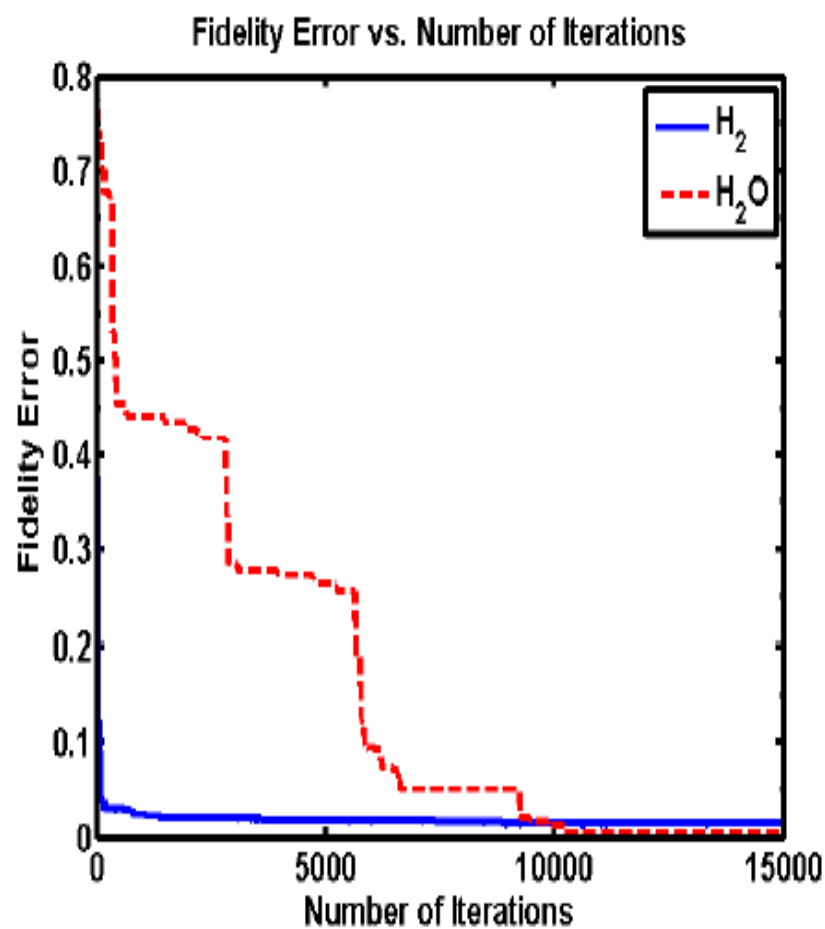
where  $N = 2^n$  ( $n$  is the number of qubits).

- $\mathcal{F}$  is always in the range  $[0, 1]$  and is equal to 1 when  $U_a = U_t$ :
  - Product of two unitary matrices is another unitary matrix all eigenvalues of which have absolute value 1.

.....



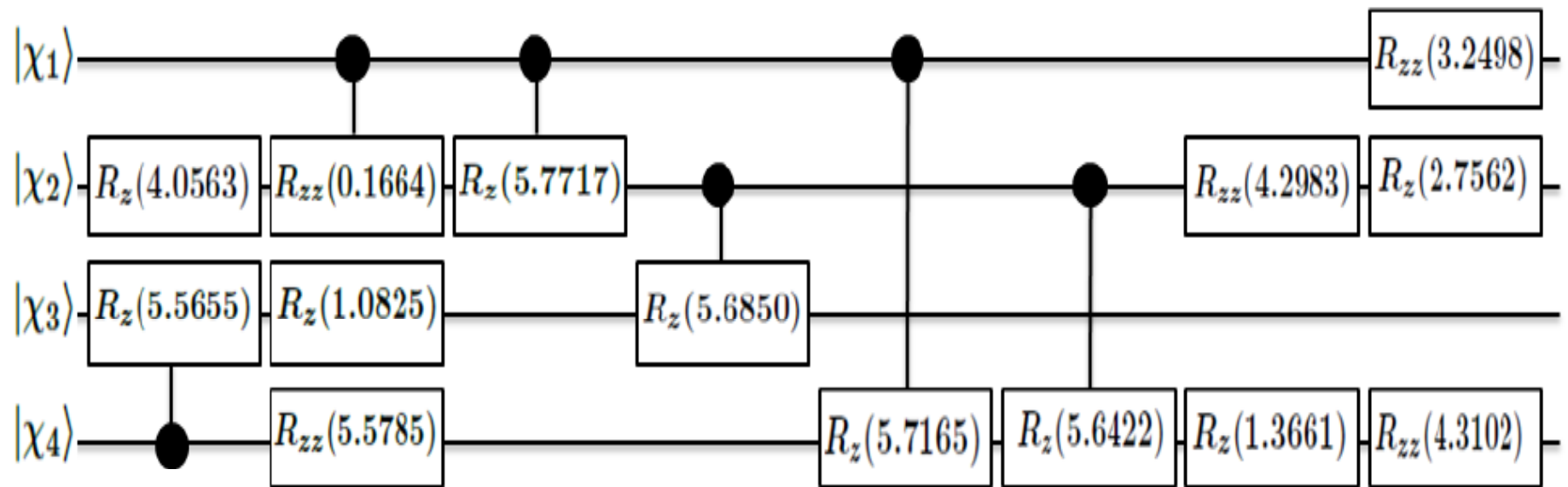
- The evolution of the error and the cost in the optimization:



(a) The evolution of the fidelity error.

(b) The evolution of the cost.

- The found circuit design for the hydrogen molecule ( $U = e^{-i\mathcal{H}t}$ ):



**Figure:** The circuit design for the unitary propagator of the Hamiltonian of hydrogen molecule.

- The found circuit design for the complex exponential of the water molecule ( $\hat{U}_{H_2O} = e^{i\tau(E_{max}-\mathcal{H})t}$ ).

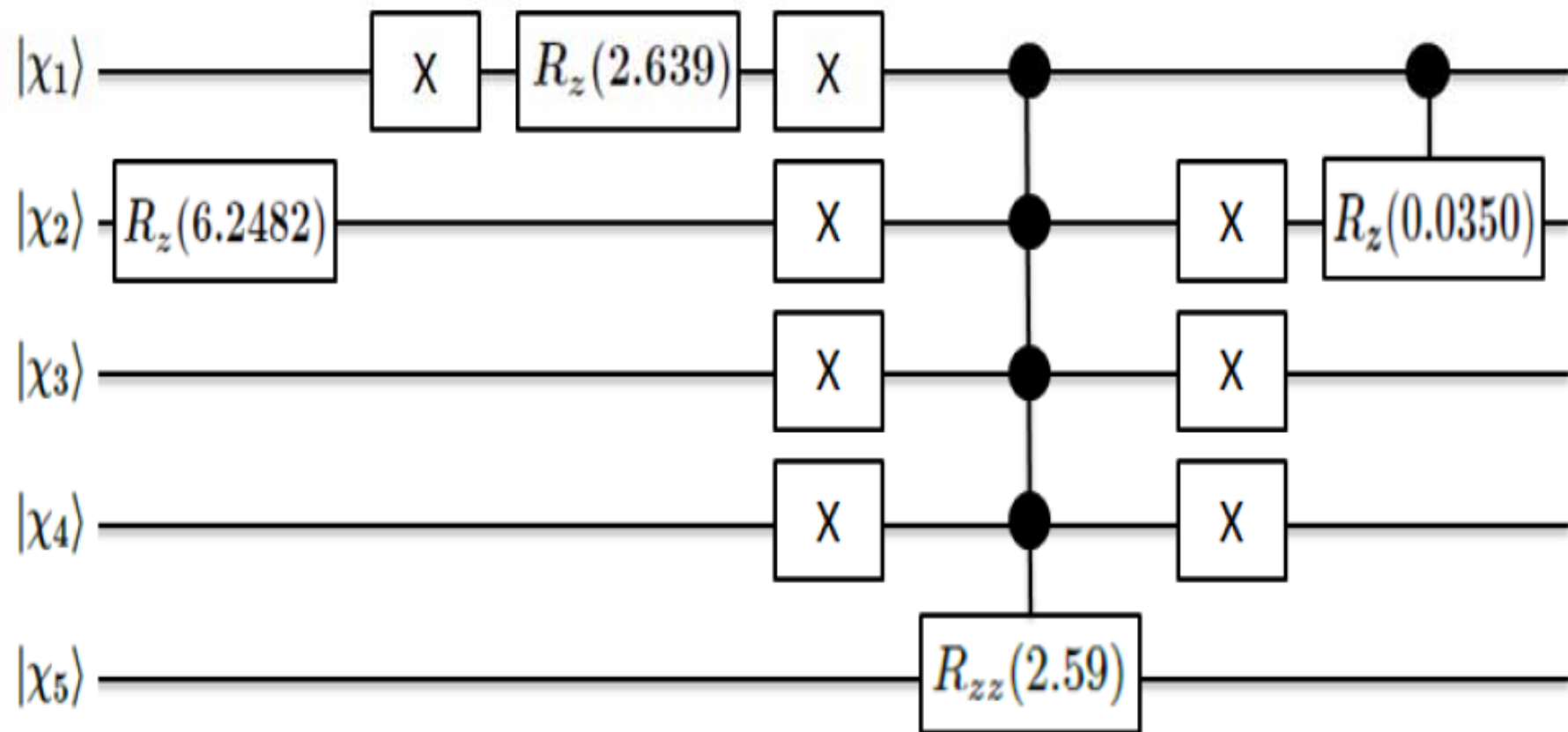


Figure: The circuit design for the unitary propagator of the Hamiltonian of water molecule.

**Constructing appropriate unitary matrix operators for electronic structure quantum algorithms and finding the minimum cost gate sequences for the implementation of these unitary operators is of fundamental importance in the field of quantum chemistry**

**Evolution of quantum circuits faces two major challenges:**

complex and huge search space and the  
high costs of simulating quantum  
circuits on classical computers

**We Need to Design Efficient Programmable Quantum Circuits for Atomic and Molecular Hamiltonians**

# Universal Programmable Quantum Circuits

# The General Circuit Design

- The relationship between input and output for quantum circuits is given as:

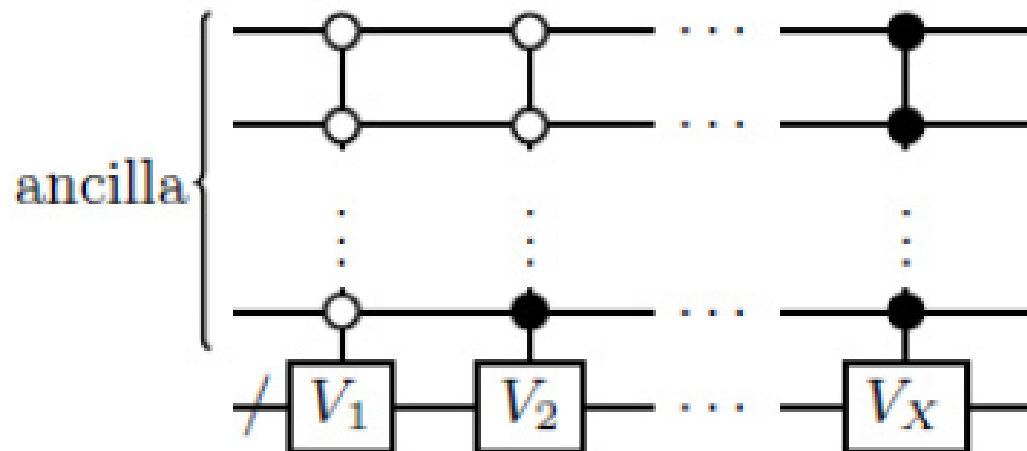
$$U|\psi\rangle = \begin{pmatrix} u_{11} & \dots & u_{1N} \\ \vdots & & \vdots \\ u_{N1} & \dots & u_{NN} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_N \end{pmatrix} = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_N \end{pmatrix}$$

- Using a large system where the block matrices on the diagonal has a row of U as their leading row, we can get the same input-output relationship on predetermined states:

$$V|\tilde{\psi}\rangle = \begin{pmatrix} V_1 & & & \\ & V_2 & & \\ & & \ddots & \\ & & & V_X \end{pmatrix} |\tilde{\psi}\rangle = \begin{pmatrix} \kappa\beta_1 \\ \vdots \\ \kappa\beta_2 \\ \vdots \\ \kappa\beta_N \\ \vdots \end{pmatrix},$$

$$V|\tilde{\psi}\rangle = \begin{pmatrix} V_1 & & & \\ & V_2 & & \\ & & \ddots & \\ & & & V_X \end{pmatrix} |\tilde{\psi}\rangle = \begin{pmatrix} \kappa\beta_1 \\ \vdots \\ \kappa\beta_2 \\ \vdots \\ \kappa\beta_N \\ \vdots \end{pmatrix},$$

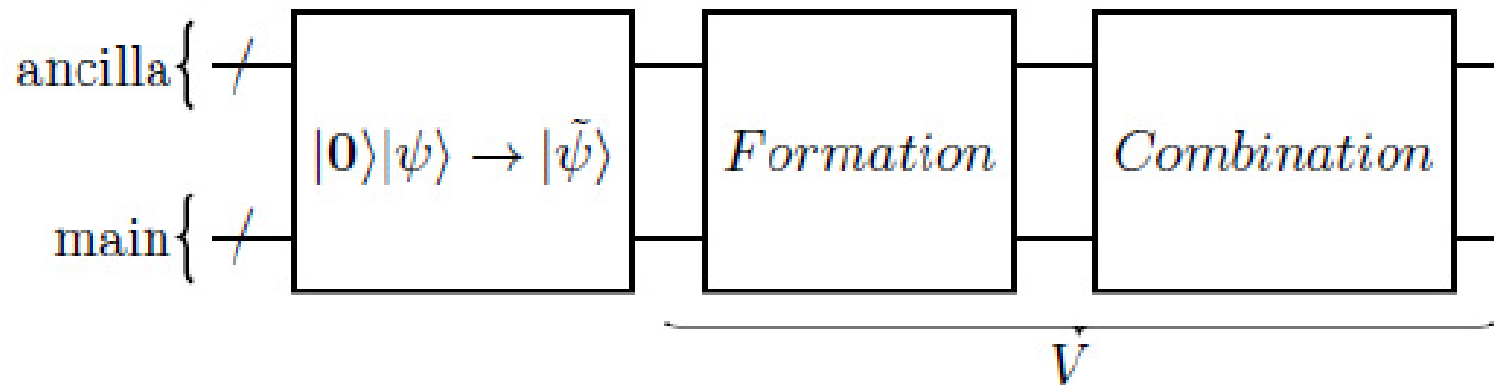
- The matrix  $V$  can be generated by using the following circuit where each  $V_i$  produces one row of  $U$ :



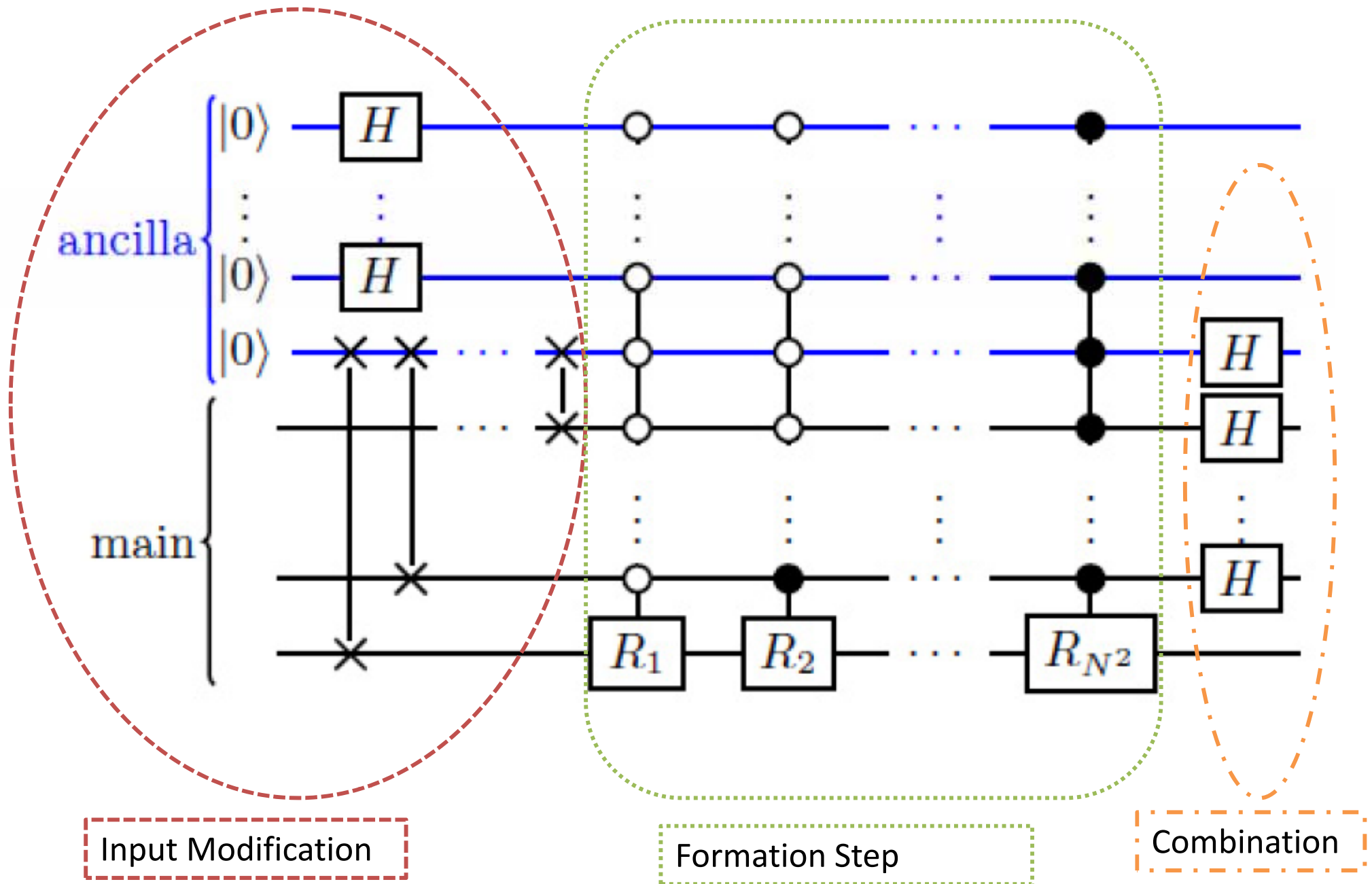


# Generation of $V$ and $|\psi\rangle \rightarrow |\tilde{\psi}\rangle$

- We will get to the final circuit in three steps:



# The Final Circuit



# The advantages of circuit

- The angles are computed from the matrix elements directly  $R(\arccos(u_{ij}))$ .
  - Generation of angles very efficient on classical computers  $O(N^2)$ .
- Fixed design
  - The same design for any type of operator
  - can be used to design microprocessors
- Non-unitary matrices can be simulated
- For sparse or structured matrices more efficient designs can be found:
  - More efficient application specific designs
  - Example: Hydrogen molecule

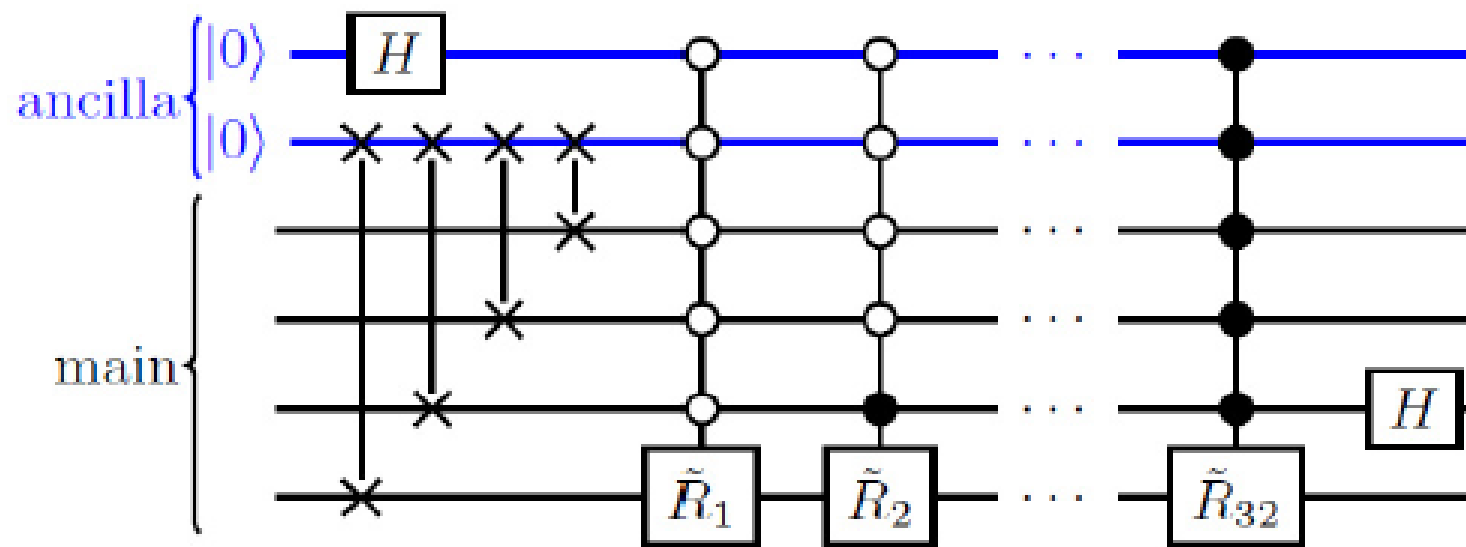


# Example: Hydrogen Molecule

- Apply a permutation matrix  $P$  to reduce the bandwidth of the matrix.
  - For  $PxU$ , where  $U=e^{-iHt}$ , in each row we have maximum two non-zero elements.
    - only four rows have two non-zeros
    - The rest is diagonal
  - The blocks  $V_i$  s in  $V$  are to be 4 by 4.
  - We will need two ancilla qubits.

# Example: Hydrogen Molecule

- The circuit includes 32 gates:
  - only 19 of them are the rotations,
  - the rest are X gates for the zero elements



# Example: Hydrogen Molecule

TABLE I: Parameters for the Rotation Gates

State of Control Qubits	Matrix Elements	Angle for $R_z$	Angle for $R_y$
00000	0.9788-0.2049i	-0.4127	0
00010	0.3987+0.9171i	2.3214	0
00100	0.3987+0.9171i	2.3214	0
00110	-0.2607+0.9517i	3.6763	0.3253
00111	0.1401-0.0817i	-1.0559	2.8158
01000	0.1401-0.0817i	-1.0559	2.8158
01001	-0.2607+0.9517i	3.6763	0.3253
01011	0.9354+0.3535i	0.7226	0
01101	0.3189+0.9478i	2.4925	0
01110	0.4766+0.8604i	2.1299	0.3629
01111	-0.1577+0.0874i	5.271	2.779
10000	-0.1577+0.0874i	5.271	2.779
10001	0.4766+0.8604i	2.1299	0.3629
10011	0.3130+0.9498i	2.5049	0
10101	0.3189+0.9478i	2.4925	0
10111	0.3130+0.9498i	2.5049	0
11001	0.9569+0.2410i	0.4934	0
11011	0.8889+0.4582i	0.9519	0
11101	0.8889+0.4582i	0.9519	0
11111	1	0	0

***Schrodinger Equation***

***and***

***Variational Calculations***



# Quantum algorithm for solving linear systems $A\vec{x} = \vec{b}$

---

**The problem:** Given a unit vector  $\vec{b} = (b_1, b_2, \dots, b_N)^T$  and an  $N \times N$  sparse Hermitian matrix  $A$  with condition number  $\kappa$ , find  $\vec{x}$  up to an error  $\varepsilon$

**Best classical algorithm:** Conjugate gradient method<sup>1</sup>. Runtime scaling  $O(N\sqrt{\kappa} \log(1/\varepsilon))$ .

**Quantum algorithm**<sup>2</sup>: Runtime scaling  $O(\kappa^2 \log N / \varepsilon)$ .

→ **Exponential speedup with respect to system size  $N$**

<sup>1</sup> Jonathan R. Shewchuk. *An introduction to the conjugate gradient method without the agonizing pain*. Technical report CMU-CS-94-125, School of Computer Science, Carnegie Mellon University, Pittsburgh, Pennsylvania, March 1994.

<sup>2</sup> Aram W. Harrow, Avinatan Hassidim, and Seth Lloyd. Quantum Algorithm for Linear Systems of Equations. *Phys. Rev. Lett.* 103(15) 150502 (2009).

# Quantum algorithm outline

---

**Input:** Quantum state  $|b\rangle = \sum b_i |i\rangle$  and ancilla qubit initialized to  $|0\rangle$ . Here indices  $i$  label the computational basis state vectors.

**Output:** Quantum state  $|x\rangle$  which encodes the solution to the linear system that is normalized to 1:  $|x\rangle = \tilde{C}^{-1} \sum_i x_i |i\rangle$

where  $\tilde{C} = (x_1^2 + x_2^2 + \dots + x_N^2)^{1/2}$  is a normalization constant.

## Summary:

1. Initial state  $|b\rangle|0\rangle$  where  $|0\rangle$  represents the all-zero state of the ancilla qubits.
2. Consider the expansion  $|b\rangle = \sum_j \beta_j |u_j\rangle$  in the eigenspace of  $e^{-iAt}$  with the  $j$ -th eigenpair being  $|u_j\rangle$  and  $\lambda_j$ . Applying phase estimation on the initial state transforms the system to approximately  $\sum_j \beta_j |u_j\rangle |\lambda_j\rangle$ .
3. Add an ancilla qubit and use the register that holds  $\lambda_j$  as the control register to apply a controlled rotation on the ancilla  $R_y|0\rangle = \sqrt{1 - C^2 / \lambda_j^2} |0\rangle + C / \lambda_j |1\rangle$ . The final state is  $\sum_j \left( \sqrt{1 - C^2 / \lambda_j^2} |0\rangle + C / \lambda_j |1\rangle \right) \beta_j |u_j\rangle |\lambda_j\rangle$ .
4. Uncompute step 2 such that all  $|\lambda_j\rangle$  states return to  $|0\rangle$ .

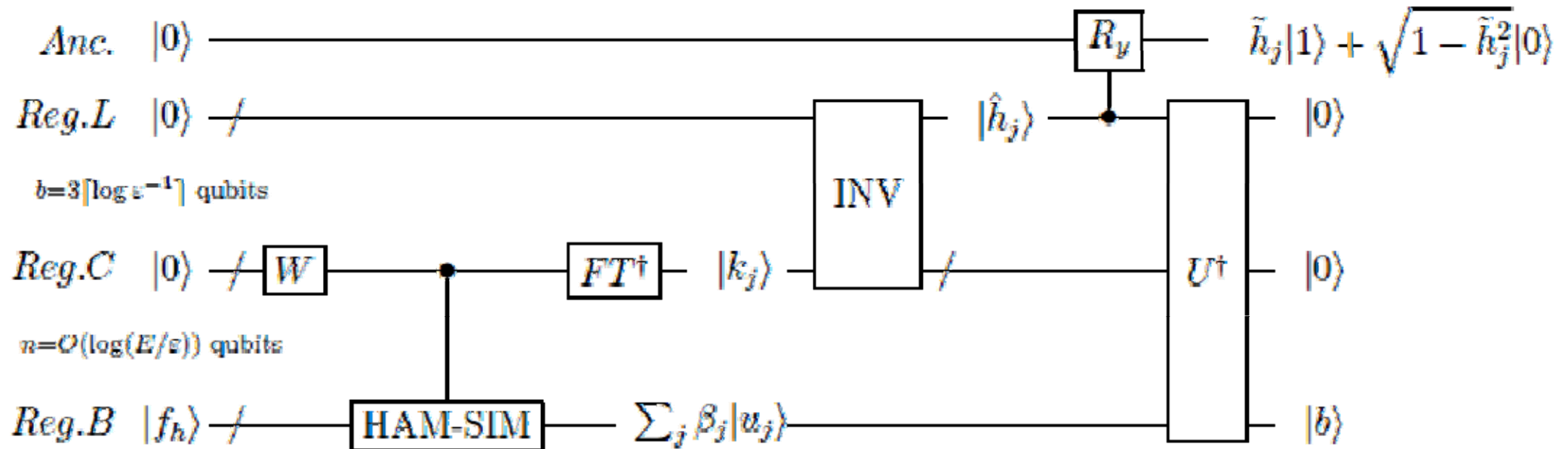
**The final state of the system is:**

$$|\psi_f\rangle = \sum_j \beta_j \left( \sqrt{1 - \frac{C^2}{\lambda_j^2}} |0\rangle + \frac{C}{\lambda_j} |1\rangle \right) |u_j\rangle |0\rangle$$

**Measure the ancilla qubit:**

1. If measure  $|1\rangle \rightarrow C' \sum_j \beta_j \lambda_j^{-1} |u_j\rangle |0\rangle = |x\rangle |0\rangle$  where  $C'$  is a constant.
2. If measure  $|0\rangle \rightarrow$  the algorithm has failed and needs to be repeated.

# Quantum circuit for general linear systems



**HAM-SIM:** Hamiltonian simulation  $U = e^{-iAt}$

**INV:** Subroutine for computing  $\lambda_j^{-1}$

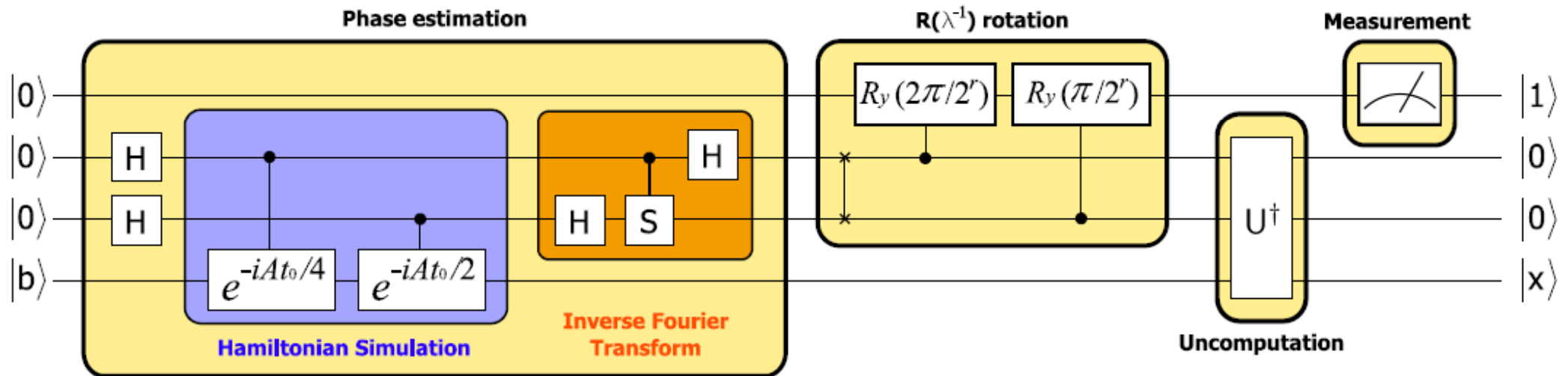
For the purpose of experimental implementation using currently available resources, quantum circuits for small linear systems have been found<sup>6</sup>.

<sup>6</sup>Yudong Cao, Anmer Daskin, Steven Frankel and Sabre Kais. Quantum circuit design for solving linear systems of equations. *Mole. Phys.* 110(15-16): 1675-1680. (2012)

# Experimental implementation: quantum circuit

To experimentally implement the algorithm using NMR<sup>7</sup>, we choose the following linear system:

$$A = \frac{1}{2} \begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix} \quad \vec{b} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$



The four-qubit quantum circuit for the algorithm.

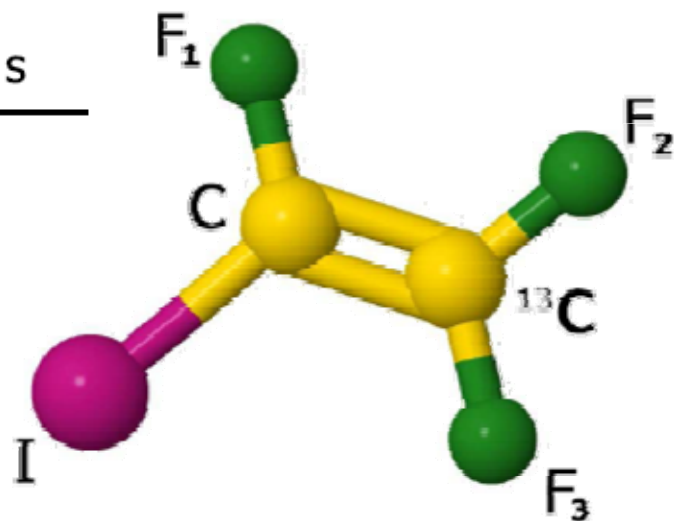
Numerical solution  $\vec{x} = \frac{1}{4} \begin{pmatrix} 3 & -1 \end{pmatrix}^T$

Quantum solution  $|x\rangle = \frac{1}{\sqrt{10}} (3|0\rangle - |1\rangle)$

<sup>7</sup>Jian Pan, Yudong Cao, Xiwei Yao, Zhaokai Li, Chenyong Ju, Xinhua Peng, Sabre Kais, and Jiangfeng Du. Unpublished.

# Experimental implementation: physical system

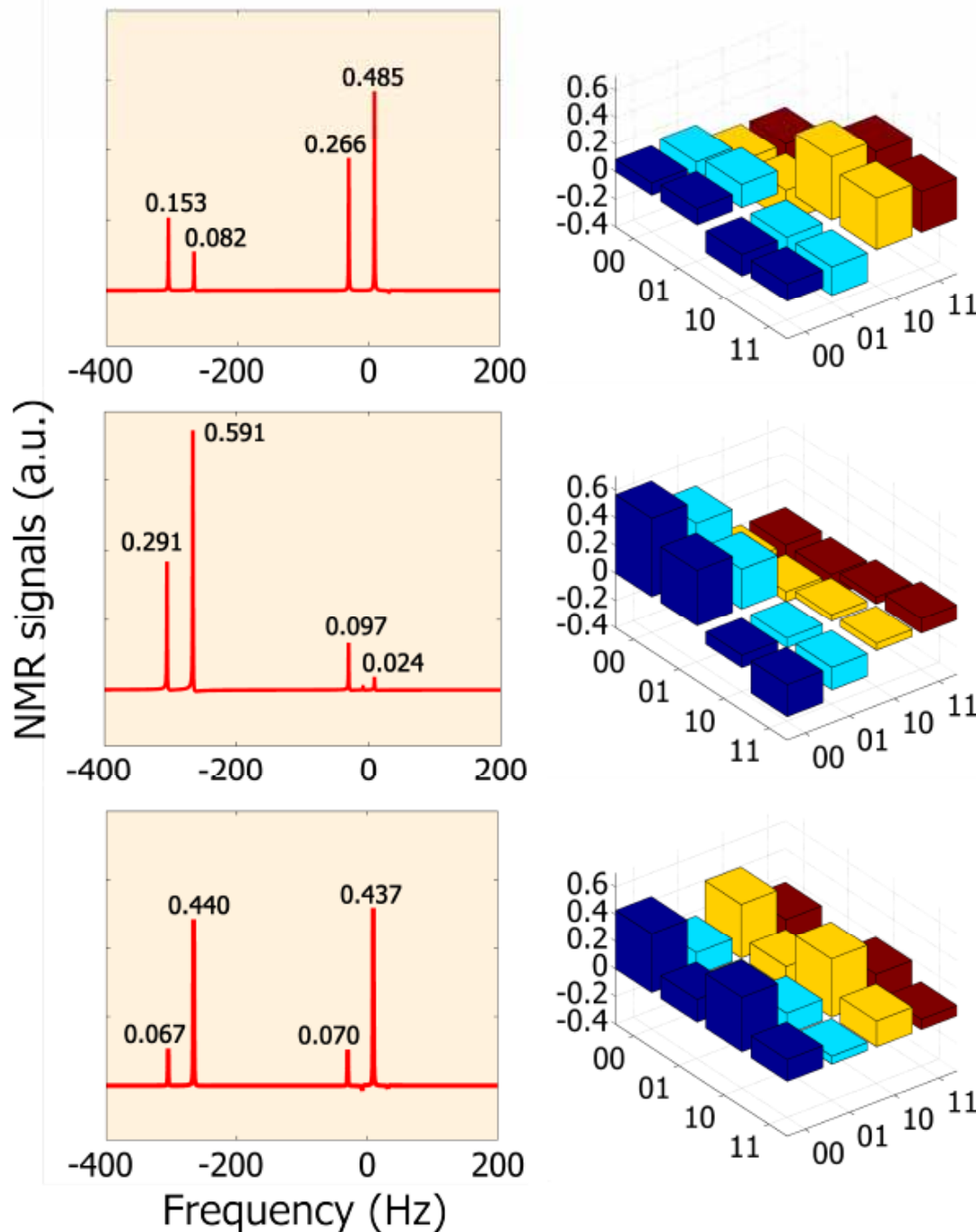
	$^{13}\text{C}$	$F_1$	$F_2$	$F_3$
$^{13}\text{C}$	15479.7 Hz			
$F_1$	-297.7 Hz	-33122.4 Hz		
$F_2$	-275.7 Hz	64.6 Hz	-42677.7 Hz	
$F_3$	39.1 Hz	51.5 Hz	129.0 Hz	-56445.8 Hz
$T_2^*$	1.22 s	0.66 s	0.63 s	0.61 s
$T_2$	7.9 s	4.4 s	6.8 s	4.8 s



$^{13}\text{C}$ -labelled  
iodotrifluoroethylene

Properties of the molecular iodotrifluoroethylene.

# Experimental results



Experimental spectra of  $\mathcal{C}$  and the reconstructed density matrix of the final state in the subspace where the first and the second qubits both are  $|0\rangle$ .

(a), (b), (c) are the final state spectra in experiment 1, 2, 3.

(d), (e), (f) are the real part of the reconstructed density matrices of the final states for experiment 1, 2, 3.

Exp. No.	$\vartheta$ (rad)	$ b\rangle$	$ x\rangle_{\text{theory}}$	$ x\rangle_{\text{exp}}$	$ \Delta x_i/x_i _{\text{max}}$	$\langle x_{\text{theory}} x_{\text{exp}}\rangle$
1	-2.23	$\begin{pmatrix} 0.4393 \\ -0.8983 \end{pmatrix}$	$\begin{pmatrix} 0.5541 \\ -0.7836 \end{pmatrix}$	$\begin{pmatrix} 0.5561 \\ -0.7366 \end{pmatrix}$	0.06	96.4%
2	-0.57	$\begin{pmatrix} 0.9572 \\ -0.2894 \end{pmatrix}$	$\begin{pmatrix} 0.7903 \\ -0.4564 \end{pmatrix}$	$\begin{pmatrix} 0.7308 \\ -0.4424 \end{pmatrix}$	0.08	96.6%
3	-1.57	$\begin{pmatrix} 0.7071 \\ 0.7071 \end{pmatrix}$	$\begin{pmatrix} 0.3535 \\ 0.3535 \end{pmatrix}$	$\begin{pmatrix} 0.3299 \\ 0.3690 \end{pmatrix}$	0.07	96.7%

***Schrodinger Equation***

***and***

***Adiabatic Quantum  
Computing***



# AQC based on spin Hamiltonians

---

$$H(s) = (1 - s)H_B + sH_P$$

**Beginning Hamiltonian  $H_B$ :** Usually a Hamiltonian that

- 1) is easily implementable experimentally
- 2) has a ground state that is simple to calculate

e.g. Hamiltonian of  $N$  spins<sup>3</sup>

$$H_B = \sum_{i=1}^N X_i$$

**Final Hamiltonian (or problem Hamiltonian)  $H_P$ :**

- 1) is easily implementable experimentally
- 2) has its ground state representing the solution to the problem

e.g. 2-local Hamiltonian of  $N$  spins<sup>4</sup>

$$H_P = \sum_{i=1}^N h_i Z_i + \sum_{\{i,j\}} J_{ij} Z_i Z_j$$

<sup>3</sup> In this presentation, the Pauli matrices are written as  $X$ ,  $Y$ , and  $Z$ . In particular,  $X_i$  means a tensor product of  $N$  operators where the  $i$ -th term is  $X$  and the rest are identities.

<sup>4</sup>  $k$ -local means the Hamiltonian contains at most  $k$ -body interaction terms.

# Spin Hamiltonians and Optimization problems

---

**Spin Hamiltonian:**

$$H_P = \sum_{i=1}^N h_i Z_i + \sum_{\substack{\{i,j|i \neq j \\ 1 \leq i,j \leq N\}}} J_{ij} Z_i Z_j$$

Since each spin  $Z$  has eigenstates  $|\uparrow\rangle$  with energy  $+1$   
 $|\downarrow\rangle$  with energy  $-1$  ;

The ground state of  $H_P$  therefore is the spin configuration that minimizes the function

$$E(s_1, s_2, \dots, s_N) = \sum_{i=1}^N h_i s_i + \sum_{\substack{\{i,j|i \neq j \\ 1 \leq i,j \leq N\}}} J_{ij} s_i s_j$$

where  $s_j = 1$  if the  $j$ -th spin is up and  $-1$  if down.

**Optimization:**

This is useful for solving two fundamental types of optimization problems:

1. Ising model  $E(\mathbf{s}) = \min_{\mathbf{s}} (\mathbf{s}^T \mathbf{J} \mathbf{s} + \mathbf{w}^T \mathbf{s})$  ,  $\mathbf{s} = (s_1, s_2, \dots, s_N)^T$  ,  $\mathbf{J}$  and  $\mathbf{w}$  are respectively a real symmetric matrix and a real vector. Each  $s_i \in \{-1, 1\}$  .

2. Quadratic Unconstrained Binary Optimization (QUBO)

$$F(\mathbf{x}) = \min_{\mathbf{x}} (\mathbf{x}^T \mathbf{J} \mathbf{x} + \mathbf{w}^T \mathbf{x}) , \mathbf{x} = (x_1, x_2, \dots, x_N)^T \quad x_i \in \{-1, 1\}$$

$\mathbf{J}$  and  $\mathbf{w}$  are respectively a real symmetric matrix and a real vector.

# Application on quantum simulation: Finite Element

---

In quantum chemistry it is common to solve Schrodinger's equation using Finite Element method, which essentially reduces Schrodinger's equation to a linear system.

Any linear system  $\mathbf{Ax} = \mathbf{b}$  can be reduced to an optimization problem:

$$\min_{\mathbf{x}} (\mathbf{x}^T \mathbf{A}^T \mathbf{Ax} - 2\mathbf{b}^T \mathbf{Ax})$$

Important open issues that remain to be resolved: for what type(s) of linear system could AQC outperform classical algorithms in terms of runtime scaling?

# QMA-complete spin Hamiltonians

---

$$H_P = \sum_{i=1}^N h_i Z_i + \sum_{\substack{\{i,j\} \\ 1 \leq i,j \leq N \\ i \neq j}} J_{ij} Z_i Z_j$$

The spin Hamiltonian  $H_P$  is experimentally feasible and scalable (for an example of 81-spin AQC implementation see Ref. <sup>5</sup>). However, it is unlikely that a Hamiltonian of this form is universal for quantum computation <sup>6</sup>.

With slight deviation from  $H_P$  defined above, the following Hamiltonians are QMA-complete <sup>7</sup>:

$$H_{ZZXX} = \sum_i h_i Z_i + \sum_i \Delta_i X_i + \sum_{\{i,j\}} J_{ij} Z_i Z_j + \sum_{\{i,j\}} K_{ij} X_i X_j$$
$$H_{ZX} = \sum_i h_i Z_i + \sum_i \Delta_i X_i + \sum_{i < j} J_{ij} X_i Z_j + \sum_{i < j} K_{ij} Z_i X_j$$

<sup>5</sup> Alejandro Perdomo-Ortiz, Neil Dickson, Marshall Drew-Brook, Geordie Rose, Alán Aspuru-Guzik, Finding low-energy conformations of lattice protein models by quantum annealing, *Nature Scientific Reports*, DOI: 10.1038/srep00571. (2012)

<sup>6</sup> Sergey Bravyi, David P. DiVincenzo, Roberto I. Oliveira, Barbara M. Terhal. The Complexity of Stoquastic Local Hamiltonian Problems. *Quant. Inf. Comp.* 8(5):0361-0385 (2008).

<sup>7</sup> Jacob D. Biamonte, Peter J. Love. Realizable Hamiltonians for Universal Adiabatic Quantum Computers. *Phys. Rev. A* 78, 012352 (2008).

# Application: Electronic Structure

The electronic Hamiltonian in the second quantization form is expressed as

$$H = \sum_{pq} h_{pq} a_p^+ a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^+ a_q^+ a_s a_r$$

where the matrix elements  $h_{pq}$  and  $h_{pqrs}$  are the set of one- and two-electron integrals. Each of the raising and lowering operators can be expressed in terms of Pauli matrices. For hydrogen molecule, the Hamiltonian is

$$H = H^{(1)} + H^{(2)}$$

$$H^{(1)} = \frac{1}{2} [h_{11}(I + Z_1) + h_{22}(I + Z_2) + h_{33}(I + Z_3) + h_{44}(I + Z_4)]$$

$$H^{(2)} = \frac{1}{4} [h_{1221}(I + Z_1 + Z_2 + Z_1 Z_2) + h_{3443}(I + Z_3 + Z_4 + Z_3 Z_4)$$

$$+ h_{1441}(I + Z_1 + Z_4 + Z_1 Z_4) + h_{2332}(I + Z_2 + Z_3 + Z_2 Z_3)$$

$$+ (h_{1331} - h_{1313})(I + Z_1 + Z_3 + Z_1 Z_3) + (h_{2442} - h_{2424})(I + Z_2 + Z_4 + Z_2 Z_4)$$

$$+ 4h_{1423} X_1 X_2 X_3 X_4 (-I + Z_1 + Z_2 + Z_3 - Z_4 - Z_1 Z_2 + Z_1 Z_3 + Z_1 Z_4 - Z_2 Z_3$$

$$+ Z_2 Z_4 + Z_3 Z_4 - 3Z_1 Z_2 Z_3 - Z_1 Z_2 Z_4 + 3Z_1 Z_3 Z_4 - Z_2 Z_3 Z_4 - Z_1 Z_2 Z_3 Z_4)$$

$$+ 4h_{1243} X_1 X_2 X_3 X_4 (-2I + 2Z_1 Z_3 - 2Z_1 Z_2 + 2Z_1 Z_4 + 2Z_2 Z_3 + 2Z_2 Z_4$$

$$- 2Z_3 Z_4 - 2Z_1 Z_2 Z_3 Z_4)]$$

High order terms

Using the technique of perturbative gadgets<sup>10</sup> one can in principle reduce the high order terms in the Hamiltonian to 2-local.

Although certain forms of 2-local Hamiltonians are implementable in lab, the main issue with the perturbative gadget approach is that the magnitude of coupling strengths (the coefficients of the Pauli terms in  $H$ ) scales unrealistically as the order of the gadget increases<sup>1</sup>.

<sup>1</sup>Sergey Bravyi, David P. DiVincenzo, Daniel Loss, and Barbara M. Terhal. Quantum simulation of many-body Hamiltonians using perturbation theory with bounded-strength interactions. *Phys. Rev. Lett.*, 101:070503 (2008)

# Simulating H2 molecule using 8-local spin Hamiltonian

The **generalized k-local gadget** formulation would require much more insights to be reduced **to 2-local**, possibly related to Feynman diagram for perturbation theory of spins. **This problem has not been solved yet.**

# NSF Center for Quantum Information and Computation for Chemistry

## CCI Phase I



<http://web.ics.purdue.edu/~kais/qc/>



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