Quantum Chemistry on Near-term Quantum Devices

Matthias Degroote
University of Toronto

CECAM Tel-Aviv 15/09/2019

Hello, my name is Matthias ...

... and I'm a classical quantum chemist.

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CHEMICAL REVIEWS

Review

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Quantum Chemistry in the Age of Quantum Computing

Yudong Cao,[†,‡] Jonathan Romero,[†,‡] Jonathan P. Olson,[†,‡] Matthias Degroote,[†,¶,§] Peter D. Johnson,[†,‡] Mária Kieferová,[∥,⊥,‡] Ian D. Kivlichan,[#,†] Tim Menke,[#,⊗,△] Borja Peropadre,[‡] Nicolas P. D. Sawaya,[▽] Sukin Sim,[†,‡] Libor Veis,[◆] and Alán Aspuru-Guzik[*,†,‡,¶,§,○,□]

[†]Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts 02138, United States
[‡]Zapata Computing Inc., Cambridge, Massachusetts 02139, United States
[¶]Department of Chemistry, University of Toronto, Toronto, Ontario M5G 1Z8, Canada
[§]Department of Computer Science, University of Toronto, Toronto, Ontario M5G 1Z8, Canada
[∥]Department of Physics and Astronomy, Macquarie University, Sydney, NSW 2109, Australia
[⊥]Institute for Quantum Computing and Department of Physics and Astronomy, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada
[#]Department of Physics, Harvard University, Cambridge, Massachusetts 02138, United States
[⊗]Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, United States
[△]Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, United States
[▽]Intel Laboratories, Intel Corporation, Santa Clara, California 95054 United States
[◆]J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic v.v.i., Dolejškova 3, 18223 Prague 8, Czech Republic
[○]Canadian Institute for Advanced Research, Toronto, Ontario M5G 1Z8, Canada

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Quantum computational chemistry

Sam McArdle,[1,*] Suguru Endo,[1] Alán Aspuru-Guzik,[2,3,4] Simon Benjamin,[1] and Xiao Yuan[1,†]

[1]*Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom*
[2]*Department of Chemistry and Department of Computer Science, University of Toronto, Toronto, Ontario M5S 3H6, Canada*
[3]*Vector Institute for Artificial Intelligence, Toronto, Ontario M5S 1M1, Canada*
[4]*Canadian Institute for Advanced Research (CIFAR) Senior Fellow, Toronto, Ontario M5S 1M1, Canada*

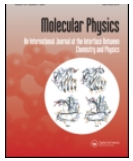
(Dated: August 31, 2018)

One of the most promising applications of quantum computing is solving classically intractable chemistry problems. As a result, quantum computational chemistry is rapidly emerging as an interdisciplinary field requiring knowledge of both quantum information and computational chemistry. This work provides a comprehensive introduction to both fields, bridging the current knowledge gap. We review the key developments in this area, with a focus on near-term quantum computation. We illustrate the methods discussed by explicitly demonstrating how to map chemical problems onto a quantum computer, and solve them. We conclude with an outlook for this nascent field.

nt-ph] 30 Aug 2018

CONTENTS

10.1080/00268976.2011.552441



Molecular Physics

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Simulation of electronic structure Hamiltonians using quantum computers

James D. Whitfield , Jacob Biamonte & Alán Aspuru-Guzik

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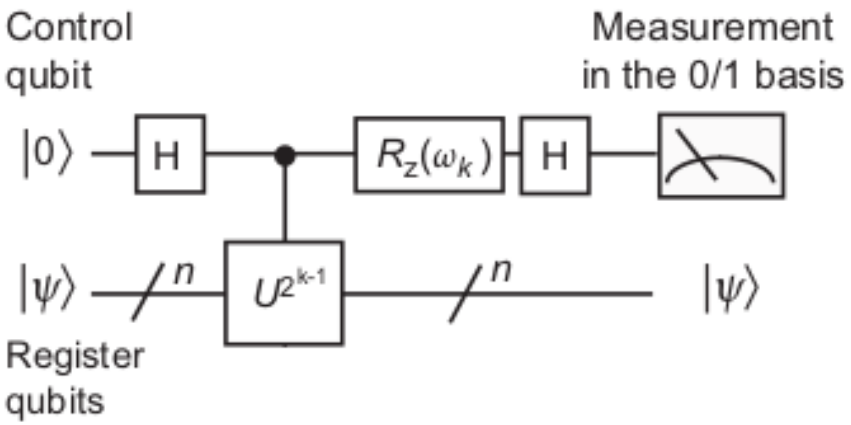
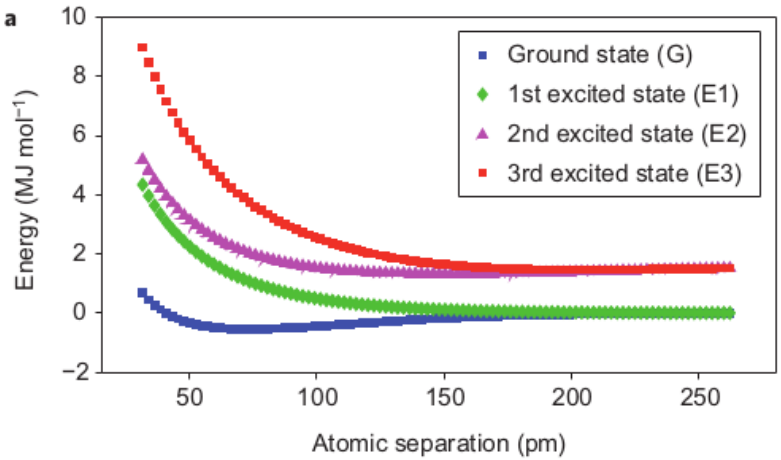
Published online: 03 Mar 2011.

- Constant ancilla overhead of energy register
- Coherence through Hamiltonian evolution and QFT
- Many controlled operations

- Iterative QPEA partly solves this problem

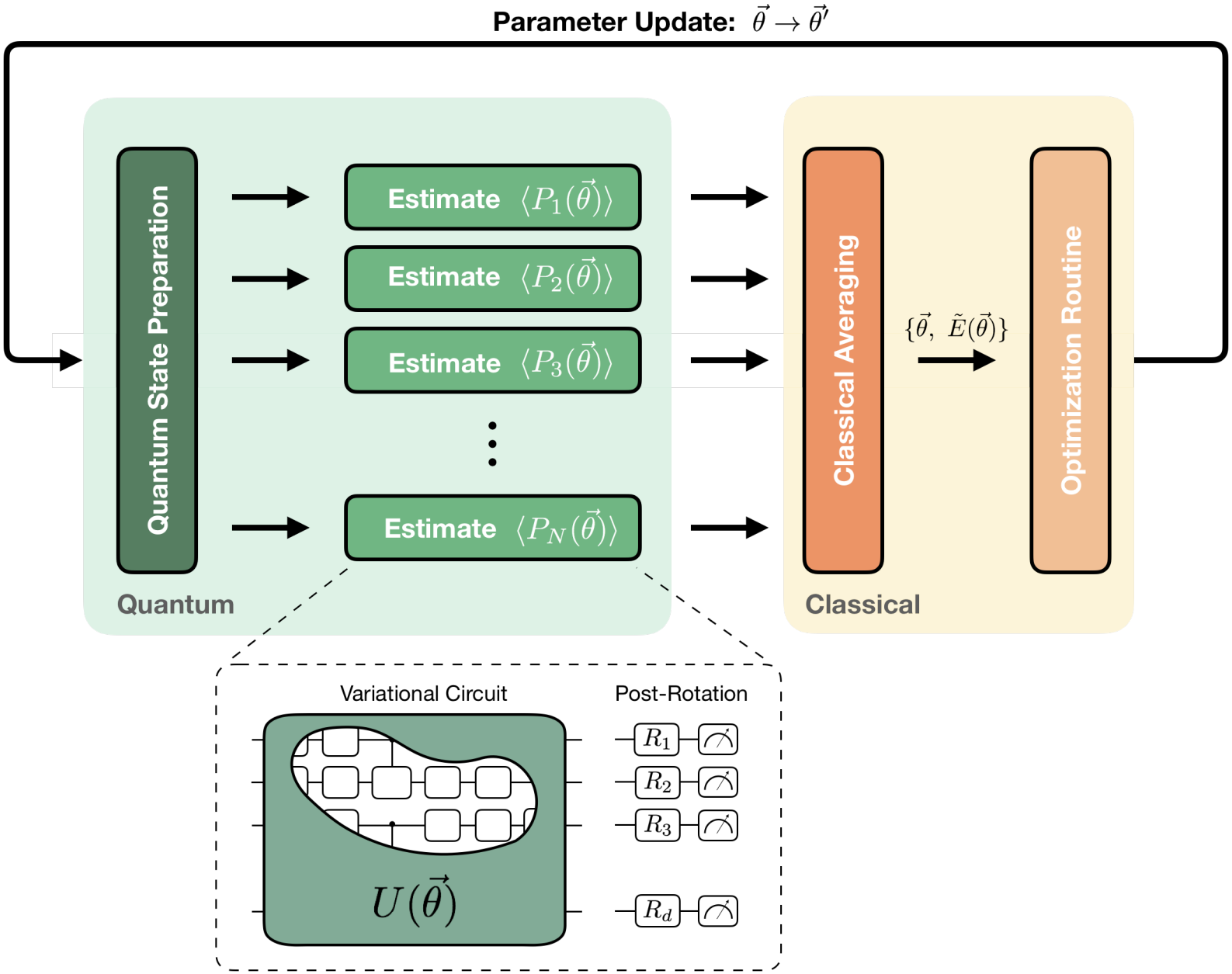




10.1038/nchem.483


HERZLIYA

Do something in the current available quantum volume


Parameter Update: $\vec{\theta} \rightarrow \vec{\theta'}$
Quantum State Preparation
Estimate $\langle P_1(\vec{\theta})\rangle$
Estimate $\langle P_2(\vec{\theta})\rangle$
Estimate $\langle P_3(\vec{\theta})\rangle$
Estimate $\langle P_N(\vec{\theta})\rangle$
Quantum
Classical Averaging
$\{\vec{\theta},\ \tilde{E}(\vec{\theta})\}$
Optimization Routine
Classical
Variational Circuit
Post-Rotation
$U(\vec{\theta})$
R_1
R_2
R_3
R_d

Start point

- gate based quantum computer
- Quantum chemical first principles hamiltonian in second quantization

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

- Time independent Schrödinger equation

$$H |\Psi_0\rangle = E_0 |\Psi_0\rangle$$

Energy

$$E\left(\vec{\theta}\right) = \frac{\left\langle \psi\left(\vec{\theta}\right) \middle| H \middle| \psi\left(\vec{\theta}\right) \right\rangle}{\left\langle \psi\left(\vec{\theta}\right) \middle| \psi\left(\vec{\theta}\right) \right\rangle}$$

$$E\left(\vec{\theta}\right) \geq E_0$$

- Equality holds when the ground state is reached

QPEA

- ☹ Many ancilla qubits
- ☹ Long circuits
- ☺☹ Measurements to build statistics with same circuit
- ☺☹ Guaranteed ground state
- ☺ No optimization

VQE

- ☺ No ancilla qubits
- ☺ Short circuits
- ☺☹ Lots of measurements with different circuit
- ☺☹ As good as the ansatz
- ☹ Iterative noisy optimization

Short circuits make the difference

1. State preparation
    1. Reference state
    2. Ansatz
2. Measurement
3. Optimization

Classical

Starting from empty vacuum

$$a_i \left|-\right\rangle = 0, \forall i$$

Add particles by acting with $a_i^\dagger$
For instance Hartree-Fock state

$$\begin{aligned} \left|\phi_0\right\rangle &= \prod_{i=0}^{M} a_i^\dagger \left|-\right\rangle \\ &= \left|\underbrace{0\ldots0}_{N-M}\underbrace{1\ldots1}_{M}\right\rangle \end{aligned}$$

for the M lowest energy orbitals

Quantum Computer

Initialized to all 0's

$$\left|\psi_0\right\rangle = \left|0\right\rangle^{\otimes N}$$

Particles can be added by working with $Q_i^\dagger$:

$$\begin{aligned} Q_i^\dagger &= \left|1\right\rangle\left\langle 0\right|_i \\ &= \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}_i \\ &= \frac{1}{2}\left(X_i - iY_i\right) \end{aligned}$$

How do we map states on electrons to a state of qubits?

- Equal number of qubits as spin-orbitals
  $|f_0 \dots f_{N-1}\rangle \rightarrow |q_0 \dots q_{N-1}\rangle$ with $f_i, q_i \in \{0, 1\}$

But:

- Fermions are indistinguishable and anti-symmetric under exchange
  $a_i^\dagger a_j^\dagger |\psi\rangle = -a_j^\dagger a_i^\dagger |\psi\rangle$
- Qubits are distinguishable and have orthogonal Hilbert spaces
  $\frac{1}{2}(X_i - iY_i)\frac{1}{2}(X_j - iY_j)|\psi_q\rangle = \frac{1}{2}(X_j - iY_j)\frac{1}{2}(X_i - iY_i)|\psi_q\rangle$

$\Rightarrow$ different statistics, we need a one to one mapping between states in fermionic Fock space and qubit Hilbert space

Jordan-Wigner (JW)

- uses occupation encoding

$$q_i = f_i, \forall p$$

- sign gets counted by strings of Z's from qubit 0 or $N-1$

$$a_i^\dagger = Q_i^\dagger \otimes \underbrace{Z_{i-1} \otimes \cdots \otimes Z_0}_{i \text{ times}}$$

- density operators stay local

$$\begin{aligned} n_i &= a_i^\dagger a_i \\ &= \frac{1}{2}\left(\mathbb{1}_i - Z_i\right) \end{aligned}$$

- $\mathcal{O}(N)$

Bravyi-Kitaev (BK)

- Recursive procedure

$$q_i = \sum_{j=0}^{i} \beta_{ij}^{(N)} f_j \,(\text{mod} 2)$$

$$\beta^{(1)} = \begin{bmatrix} 1 \end{bmatrix}$$

$$\beta^{(2)} = \begin{bmatrix} \beta^{(1)} & 0 \\ 1 & \beta^{(1)} \end{bmatrix}$$

$$\beta^{(2^{q+1})} = \begin{bmatrix} \beta^{(2^q)} & \mathbf{0} \\ \mathbf{A} & \beta^{(2^q)} \end{bmatrix}$$

- densities no longer local
- $\mathcal{O}(\log N)$

There is always a unitary that describes the exact ground-state wave function

$\exists U : U |\phi_0\rangle = |\Psi_0\rangle$

- a general unitary has $2^N - 1$ real parameters
- implementing this in a circuit is costly
- finding the parameters would be hard

$\Rightarrow$ Not realistic

We will have to approximate the general unitary

- Physically motivated ansatz
- Hardware heuristic ansatz

$$
\begin{aligned}
|\Psi\rangle &= \exp(T)\,|\phi_0\rangle \\
&= |\phi_0\rangle + T_1\,|\phi_0\rangle + \left(\frac{T_1 T_1}{2} + T_2\right)|\phi_0\rangle + \dots \\
T &= \sum_{p=1}^{M} T_p \\
T_p &= \frac{1}{(p!)^2} \sum_{a_0 \dots a_p, i_0 \dots i_p} t_{i_0 \dots i_p}^{a_0 \dots a_p}\, a_{a_p}^\dagger \dots a_{a_0}^\dagger\, a_{i_0} \dots a_{i_p}
\end{aligned}
$$

- Only excitations from occupied to virtual
  $T_1\,|\phi_0\rangle = \sum_{a,i} t_i^a |\ \underbrace{0\dots0}_{N-M-a-1}\ 1\underbrace{0\dots0}_{a-1}\underbrace{1\dots1}_{M-i-1}0\underbrace{1\dots1}_{i-1}\rangle$
- Number of parameters rises exponentially with p

$\Rightarrow$ Truncation to only singles and doubles

- Not a unitary operator

$\Rightarrow$ Needs adjustment for a quantum computer

$$
\begin{aligned}
|\Psi\rangle &= \exp\left(T - T^\dagger\right)|\phi_0\rangle \\
&= \left(1 - T_1^\dagger T_1 + \ldots\right)|\phi_0\rangle + \left(T_1 - T_1^\dagger T_2 + \ldots\right)|\phi_0\rangle \\
&\quad + \left(\frac{T_1 T_1}{2} + T_2 + \ldots\right)|\phi_0\rangle + \ldots
\end{aligned}
$$

- Generally impossible on a classical computer
- Transform with JW or BK $\exp\left(T - T^\dagger\right) = \exp\left(\sum_i \theta_i P_i\right)$
- Exponential of sum of non-commuting terms

$\Rightarrow$ No straighforward protocol

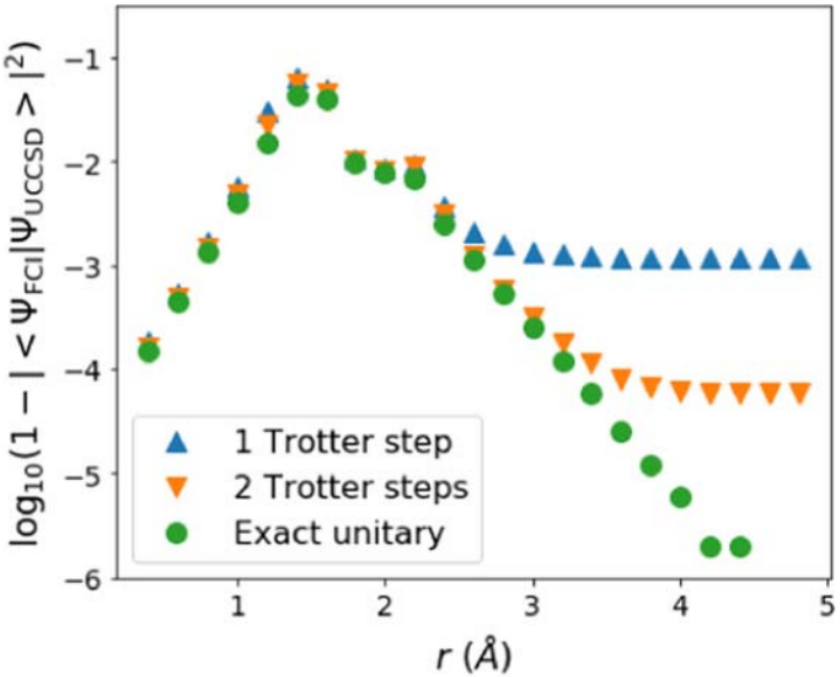
- Zassenhaus formula

$$\exp(A+B) \quad = \quad \exp(A)\exp(B)\exp(-[A,B])\ldots$$

- Trotter-Suzuki formula

$$\begin{aligned}
\exp\left(\sum_i \theta_i P_i\right) &\approx \left(\prod_i \exp\left(\frac{\theta_i}{r} P_i\right)\right)^r \\
&\approx \underbrace{\exp\left(\frac{\theta_0}{r} P_0\right)\ldots\exp\left(\frac{\theta_{L-1}}{r} P_{L-1}\right)\times \exp\left(\frac{\theta_0}{r} P_0\right)\ldots\exp\left(\frac{\theta_{L-1}}{r} P_{L-1}\right)\times\ldots}_{r \text{ times}}
\end{aligned}$$

- most of the time $r = 1$ is sufficient

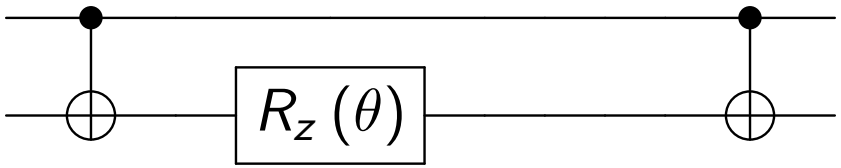


10.1088/2058-9565/aad3e4

- optimization compensates for different ansatz

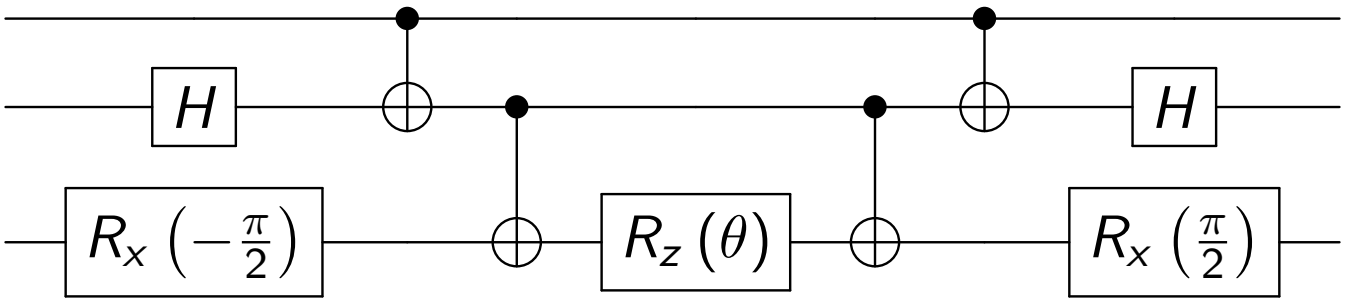
$$\vec{\theta}_{r=1} \neq \vec{\theta}_{exact}$$
$$E_{r=1} \approx E_{exact}$$

e.g. $\exp\left(-i\theta Z_1 Z_0\right)$



$\lvert 00\rangle$	$\lvert 00\rangle$	$\exp\left(-i\theta\right)\lvert 00\rangle$	$\exp\left(-i\theta\right)\lvert 00\rangle$
$\lvert 01\rangle$	$\lvert 11\rangle$	$\exp\left(i\theta\right)\lvert 11\rangle$	$\exp\left(i\theta\right)\lvert 01\rangle$
$\lvert 10\rangle$	$\lvert 10\rangle$	$\exp\left(i\theta\right)\lvert 10\rangle$	$\exp\left(i\theta\right)\lvert 10\rangle$
$\lvert 11\rangle$	$\lvert 01\rangle$	$\exp\left(-i\theta\right)\lvert 01\rangle$	$\exp\left(-i\theta\right)\lvert 11\rangle$

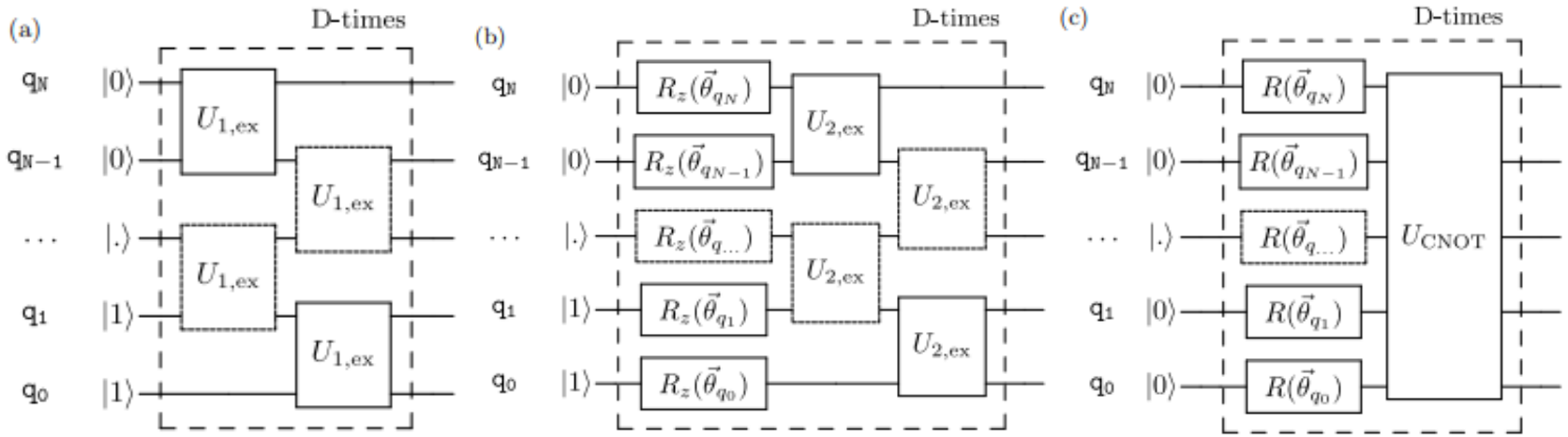
e.g. $\exp\left(-i\theta Y_2 X_1 Z_0\right)$



- D layers of rotations and entangling gates

$$\left|\Psi\left(\vec{\theta}\right)\right\rangle = U^{(D-1)}\left(\vec{\theta}^{(D-1)}\right)\ldots U^{(0)}\left(\vec{\theta}^{(0)}\right)|\phi\rangle$$

- as D increases, approximates full unitary
- either machine efficient or middle ground



10.1103/PhysRevA.98.022322

- transform with JW or BK $H = \sum_p h_p P_p$
- hamiltonian averaging $\langle H \rangle = \sum_p h_p \langle P \rangle$

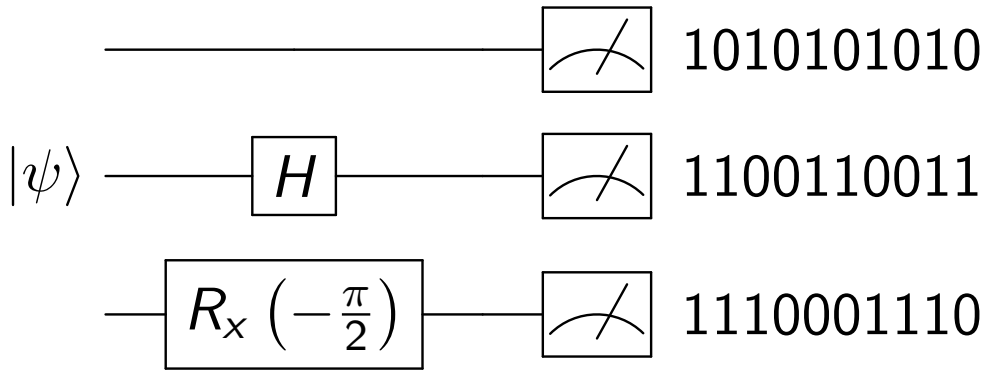
$\Rightarrow$ reduced to measure single operator at a time

- Transform into eigenbasis with $\mathbb{1}$, H, or $R_x\left(-\frac{\pi}{2}\right)$

$$\begin{aligned} \langle H \rangle &= \sum_p h_p \left[P\left(P_p = 0\right) - P\left(P_p = 1\right) \right] \\ &= \sum_p h_p \frac{\#P_0 - \#P_p = 1}{\#P_p = 0 + \#P_p = 1} \end{aligned}$$

- not all measurements can be made simultaneously

$$H = Z_0 + 2X_1Y_2 + 3Z_0X_1Y_2 + X_0X_1X_2$$



$$\langle H \rangle = \frac{5-5}{10} + 2\frac{7-3}{10} + 3\frac{8-2}{10} + ?$$

Naively $m = \mathcal{O}\left(\frac{N^8}{\epsilon^2}\right)$

- different representation
- finding commuting groups, or more advanced
- apply a cut-off on Hamiltonian matrix elements
- constraints on RDMS that link measurements

Goal:

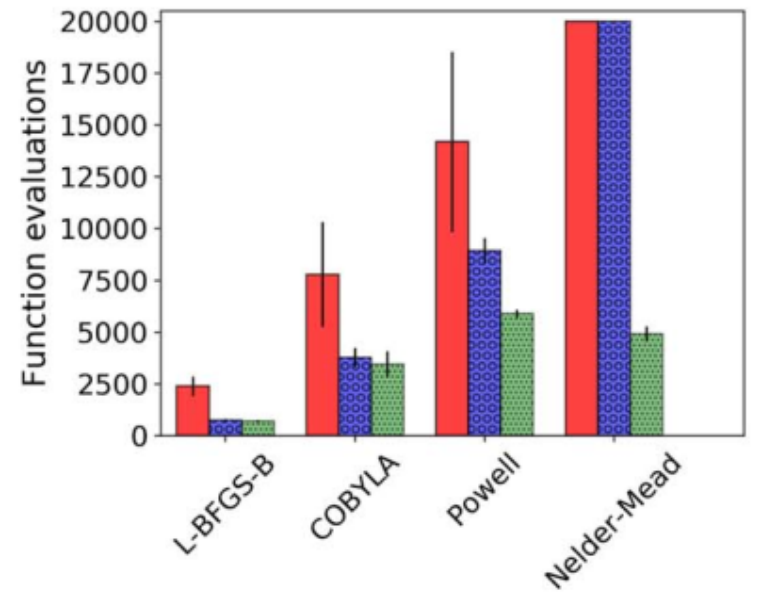
- $\vec{\theta}^{(k+1)} = f\left(\vec{\theta}^{(k)}\right)$
- or stop

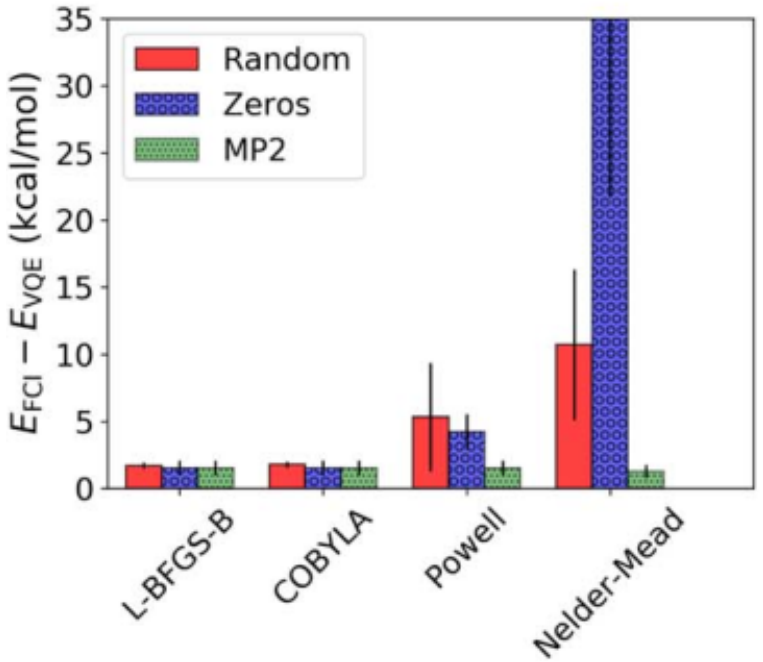
Slow optimization is costly: every optmization cycle adds measurements

- gradient-free: only based on function evaluations
  e.g. simplex methods, COBYLA, Powell, particle-swarm optimization
- gradient-based: also use derivatives
  e.g. L-BFGS-B, SPSA
  - numerical gradient
  - analytical gradient

Performance and hyper-parameters highly depend on the situation

- noise
- size of the system
- local minima
- required accuracy
- number of measurements





Now you have an approximation of the ground state, you can

- construct potential energy surfaces
- calculate properties

$$\langle O_1 \rangle = \sum_{pq} O_{pq} \left\langle a_p^\dagger a_q \right\rangle$$

$$\langle O_2 \rangle = \sum_{pqrs} O_{pqrs} \left\langle a_p^\dagger a_q^\dagger a_s a_r \right\rangle$$

- Improve the accuracy of advanced quantum chemical methods

Frank Boys

Year	Calculation	Citation	Number of qubits
1933	H_2	[74]	1
1950	Be	[76]	3, 4
1952	He	[77]	2
1955	He	[78]	2, 3
1956	BH	[41]	5
1956	H_2O	[41]	7
1957	LiH	[79]	3, 4, 5
1957	BeH^+	[79]	3, 4, 5
1960	Be	[82]	6
1960	CH_2	[83]	19
1963	H_2	[84]	3, 4, 5, 6
1966	HeH	[85]	3
1966	Li_2	[85]	3
1967	H_2O	[86]	10
1967	H_2O	[87]	24
1967	H_2O	[88, 89]	38, 39
1968	H_2O	[90]	39, 46
1968	Be	[91]	11
1969	Li, Be^+, B^{++}	[92]	9, 10
1969	BH, FH	[93]	12, 14
1970	H_2O	[94]	23

arXiv:1208.5524

VQE experimental applications

Architecture/ Platform	**System-of-interest**	**Number of physical qubits**	**Year**
Photonic chip	HeH^+	2	2014
Single trapped ion	HeH^+		2017
Superconducting processor (transmon qubits)	H_2	2	2016
Superconducting processor (transmon qubits)	H_2	2	2017
	LiH	4	2017
	BeH_2	6	2017
Ion trap processor (Ca^+ ions)	H_2	2	2018
	LiH	3	2018
Superconducting processor (transmon qubits)	H_2	2	2018
Silicon photonic chip	Two chlorophyll units in 18-mer ring of LHII complex	2	2018
Superconducting processor (transmon qubits) via Cloud	Deuteron	2-3	2018
Ion trap processor ($^{171}Yb^+$ ions)	H_2O	2-3	2019

10.1021/acs.chemrev.8b00803

https://www.bbc.com/news/technology-12181153

https://www.research.ibm.com/ibm-q/

https://en.wikipedia.org/wiki/Summit_(supercomputer)

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Thank you for your attention!

Questions are welcome

Slides: `https://mfdgroot.github.io/`