Digitized Counter-Diabatic Quantum Algorithms

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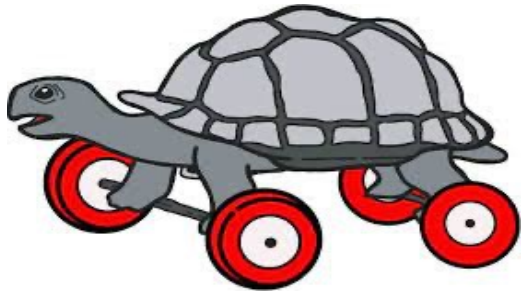
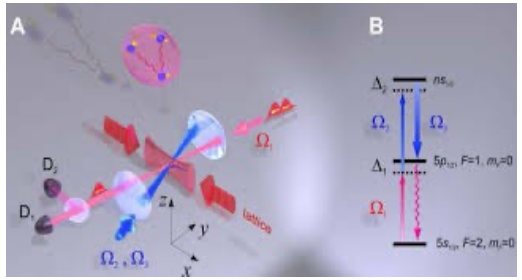


Quantum Information in Spain ICE-8, 29 May - 1 June 2023 @ Santiago de Compostela

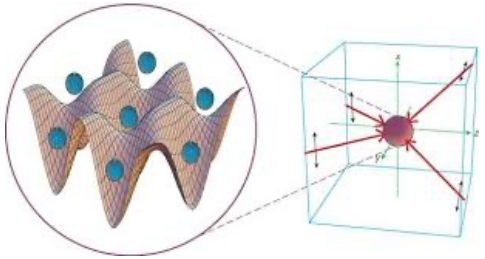
OUTLINE

- Introduction and Background
- Digitalized Adiabatic Computing
- Applications: QAOA & VQE
- Outlook and Conclusion

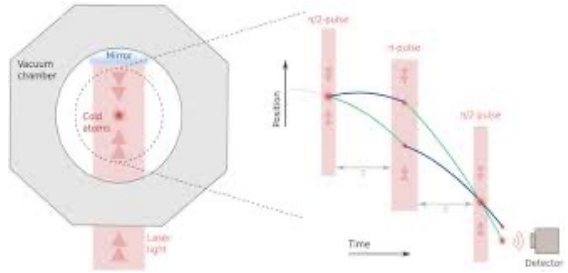
Quantum Information Processing



Quantum Simulation

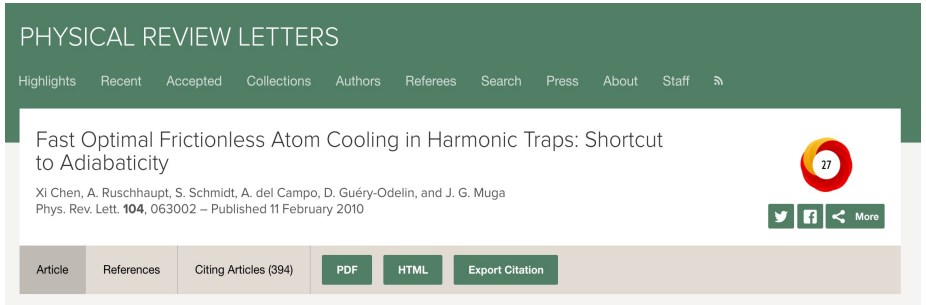


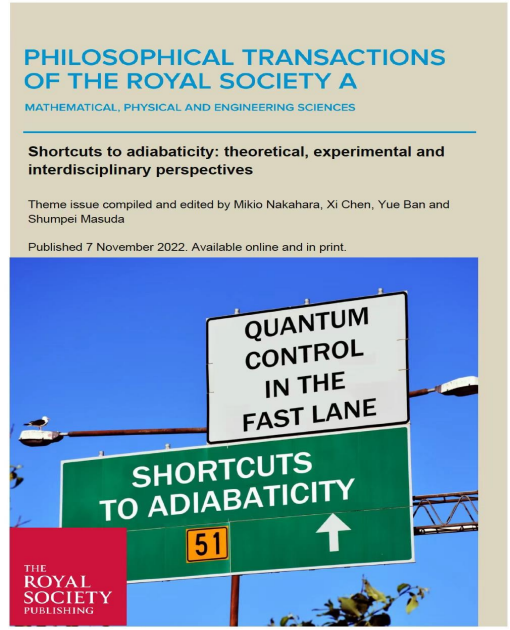
Quantum Metrology



Essential: Preparation, control and manipulation of quantum states with high-fidelity and in a fast and robust way

Shortcuts To Adiabaticity





(a) Inverse engineering

(b) Transitionless quantum driving (counter-diabatic protocols)

(c) Fast-forward scaling approach

Experimental Progress

E. Arimondo & O. Morsch: Nat. Phys. 8, 147 (2012) Accelerated optical lattice

D. Suter: Phys. Rev. Lett. 110, 240501 (2013) Nitrogen-vacancy centers spin

D. D. Awschalom: Nat. Phys. 13, 330 (2017) Nitrogen-vacancy centers spin

G. S. Paraoanu: Science advances 5(2), eaau5999 (2019) Transmon circuit

Dapeng Yu: Phys. Rev. Lett. 122, 080501 (2019) Superconducting qubit

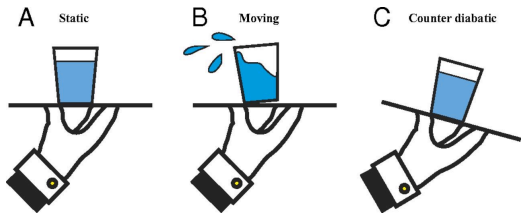
Yi Ying: New J. Phys. 20 065003 (2018)； Phys. Rev. Applied 11, 034030 (2019) Xmon qubit

Xi Chen, Hui Yan and Shiliang Zhu: Nature Commun. 7, 12479 (2016). STIRAP Cold atoms

Xinhua Peng: Phys. Rev. Appl. 13, 044059 (2020) Spin chain

Y. Yan, **Xi Chen**, and S. Kröll, npj Quantum information 7, 138 (2021) rare-earth ion

Counter-diabatic Driving



$$\hat{H}(t) = \hat{H}_0(t) + \dot{\lambda}\hat{A}_\lambda$$

Adiabatic gauge potential
Responsible for transition

First principle: Berry's ' Transitionless quantum driving'

J. Phys. A 42 365303 (2009); PRL 105, 123003 (2010)

$$\hat{H}(t) = \sum_n |n\rangle E_n \langle n| + i\hbar \sum_n (|\partial_t n\rangle\langle n| - \langle n|\partial_t n\rangle |n\rangle\langle n|) \equiv \hat{H}_0(t) + \hat{H}_1(t)$$

CD term

Limitations : priori knowledge of the system's eigen state; hard to implement in the lab.

Consider approximate gauge potential A^*_λ

$$\hat{A}^*_\lambda = \sum_j \alpha_j(t)\sigma_y^j$$

Minimizing the action : $S = \mathrm{Tr}\left[\hat{G}^2_\lambda\right]$

where $\hat{G}_\lambda = \partial_\lambda \hat{H} + i[\hat{A}^*_\lambda, \hat{H}]$

PNAS 114, E3909 (2017)

Consider approximate gauge potential as

$$\hat{A}^{(l)}_\lambda = i\sum_{k=1}^{l} \alpha_k(t)\,\underbrace{[\hat{H},[\hat{H},.....[\hat{H},}_{2k-1}\partial_\lambda \hat{H}]]]$$

First order nested commutator :

$$\hat{A}^{(1)}_\lambda = i\alpha_1(t)[\hat{H}, \partial_\lambda \hat{H}]$$

PRL 123, 090602 (2019)

$$H_{\mathrm{LHZ}}(t) = \sum_{k=1}^{N_p} h_k(t)\sigma_k^x + \sum_{k=1}^{N_p} J_k(t)\sigma_k^z - \sum_{l=1}^{N_c} C_l(t)\sigma_{l,n}^z\sigma_{l,w}^z\sigma_{l,s}^z\sigma_{l,e}^z,$$

LHZ model

quantum annealing of the p-spin model

IOP Publishing New J. Phys. 21 (2019) 043025 https://doi.org/10.1088/1367-2630/ab14a0

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PAPER

Rapid counter-diabatic sweeps in lattice gauge adiabatic quantum computing

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Keywords: quantum computing, adiabatic quantum computing, counter-diabatic driving

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Two-parameter counter-diabatic driving in quantum annealing

Luise Prielinger, Andreas Hartmann, Yu Yamashiro, Kohji Nishimura, Wolfgang Lechner, and Hidetoshi Nishimori
Phys. Rev. Research **3**, 013227 – Published 9 March 2021

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Reinforcement Learning for Many-Body Ground-State Preparation Inspired by Counterdiabatic Driving

Jiahao Yao, Lin Lin, and Marin Bukov
Phys. Rev. X **11**, 031070 – Published 30 September 2021

quantum alternating operator ansatz (QAOA)

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Counterdiabatic driving in the quantum annealing of the p-spin model: A variational approach

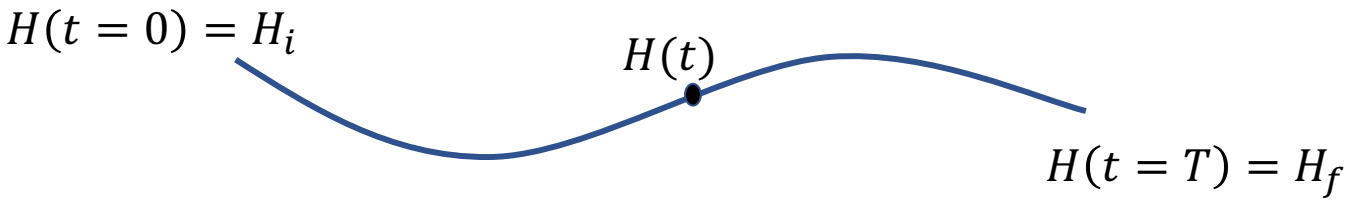
G. Passarelli, V. Cataudella, R. Fazio, and P. Lucignano
Phys. Rev. Research **2**, 013283 – Published 9 March 2020

transverse-field Ising model

Adiabatic Quantum Computation

Adiabatic quantum computation (AQC) is a form of quantum computing which relies on the adiabatic theorem to do calculations and is closely related to quantum annealing

Rev. Mod. Phys. 90, 015002 (2018)



$$H(t) = (1 - \lambda(t))H_i + \lambda(t)H_f$$

- In principle any computational problem can be encoded in this way.
- The total run time depends on the minimum spectral gap (Δ_{min}) of H(t).

LETTER Nature 534, 222 (2016)
doi:10.1038/nature17658

Digitized adiabatic quantum computing with a superconducting circuit

R. Barends[1], A. Shabani[2], L. Lamata[3], J. Kelly[1], A. Mezzacapo[3]†, U. Las Heras[3], R. Babbush[2], A. G. Fowler[1], B. Campbell[4], Yu Chen[1], Z. Chen[4], B. Chiaro[4], A. Dunsworth[4], E. Jeffrey[1], E. Lucero[1], A. Megrant[4], J. Y. Mutus[1], M. Neeley[1], C. Neill[4], P. J. J. O'Malley[4], C. Quintana[4], P. Roushan[1], D. Sank[1], A. Vainsencher[4], J. Wenner[4], T. C. White[4], E. Solano[3,5], H. Neven[2] & John M. Martinis[1,4]

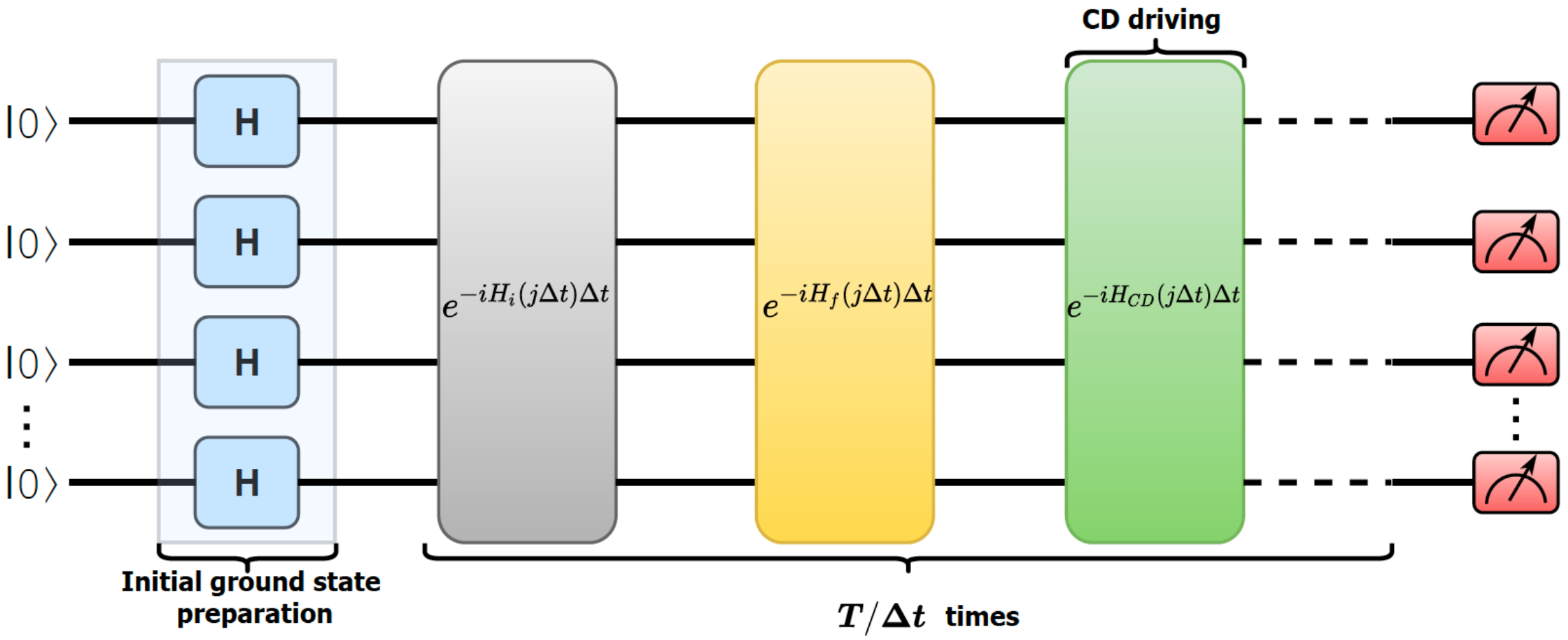
The circuit model can efficiently simulate the adiabatic quantum computing by using the digitization

- Flexibility to construct arbitrary interactions using single and two qubit gates.
- Consistent with error correction.

The time evolution operator: $\hat{U}(0,T) = \mathcal{T}\exp\left[-i\int_0^T dt\hat{H}(t)\right]$

digitization

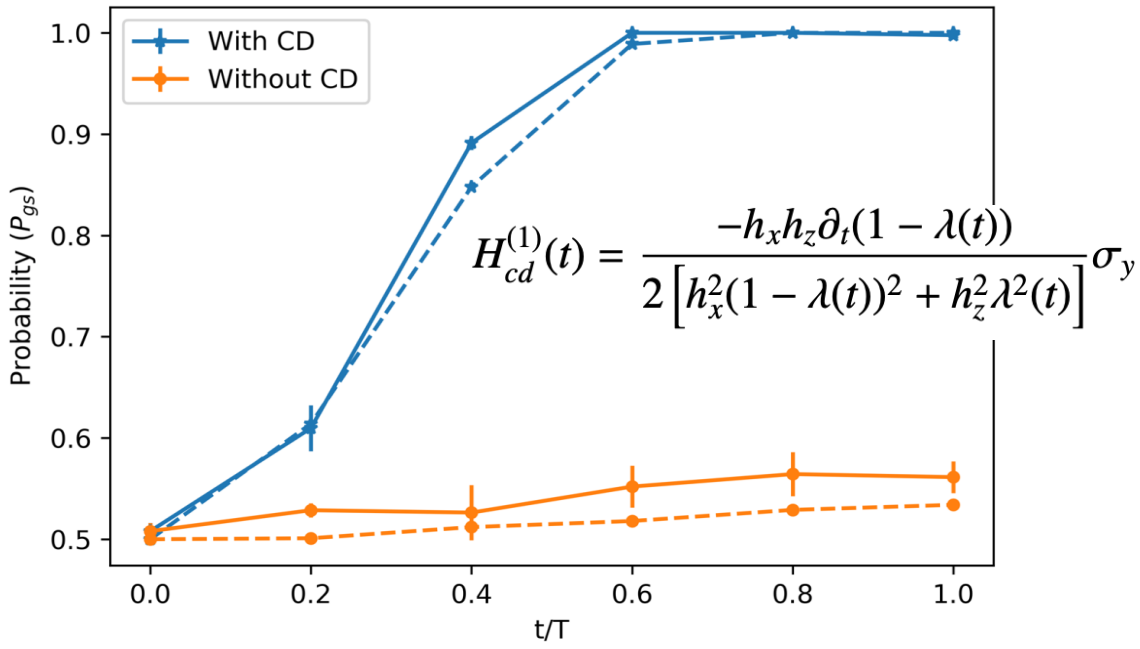
Trotterization -- > $\hat{U}(0,T) \rightarrow \hat{U}(0,T)_{dig} = \prod_{j=1}^{n}\prod_{m=1}^{M}\exp\left\{-i\Delta t C_m(j\Delta t)\hat{H}_m\right\}$

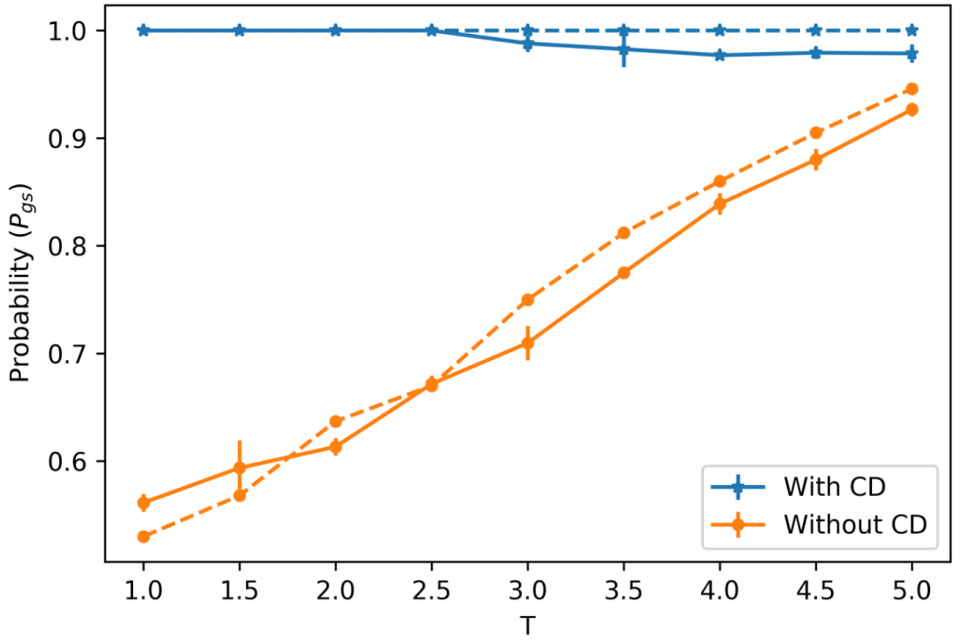


How the CD driving assist the digitalized adiabatic quantum computing?

Single Spin System

$$H^{(1)}(t) = (1 - \lambda(t))h_x\sigma_x + \lambda(t)h_z\sigma_z$$





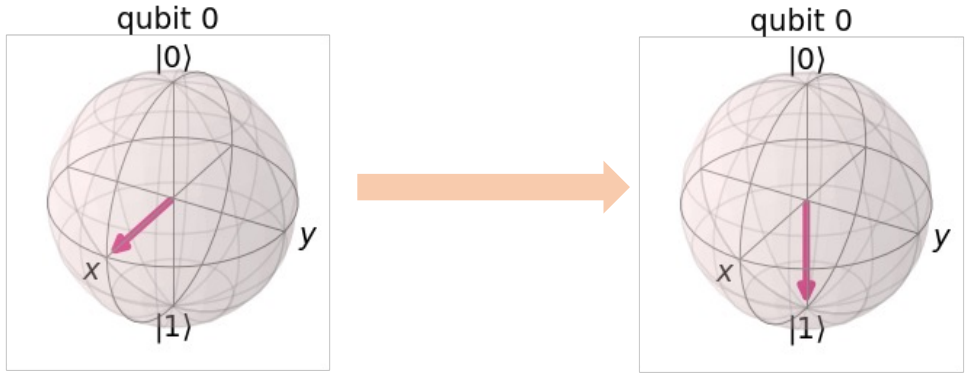
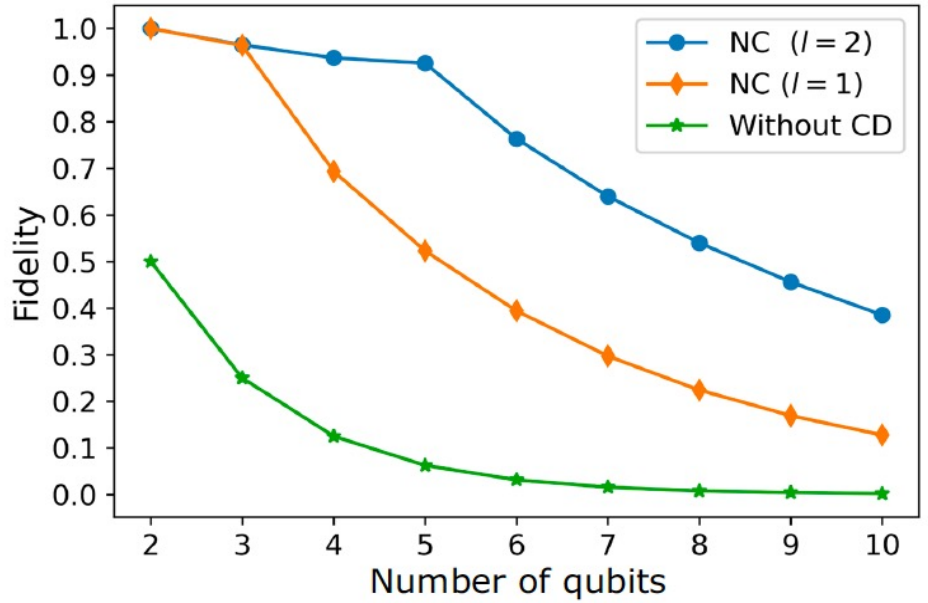


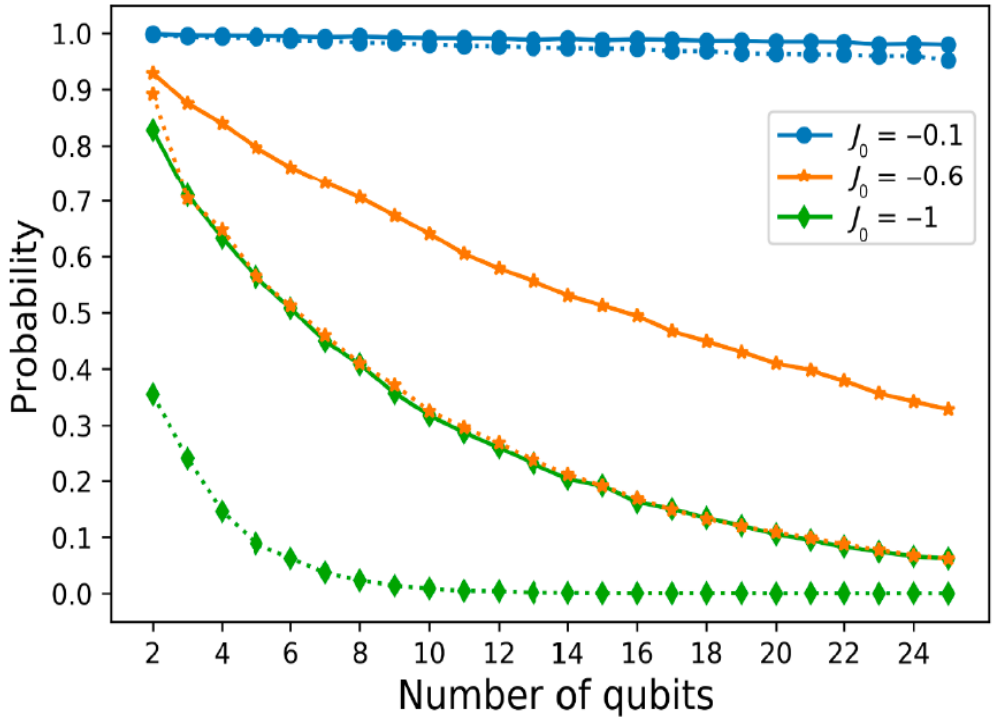
FIG. 2. (a) The final ground state probability $P_{\text{g.s.}}$ versus the simulation time for a single qubit using CD driving on the `ibmq_essex` quantum computer (solid blue line) compared to the ideal simulator (dashed blue line). The simulation without CD driving in the real device (solid orange line) and ideal simulator (dotted orange line). (b) Time evolution using DAQC and STA methods for $T = 1$. The parameters are as follows: $\Delta t = 0.2$, $h_x = -1$, $h_z = 1$, and the number of shots $(N_{\text{shots}}) = 1024$.

STA in Digitized AQC

Phys. Rev. Appl. 15, 024038 (2021)



GHZ: Fidelity to prepare the GHZ state as a function of system size on an ideal digital simulator with CD term from the NC ansatz with different orders and the naive approach without CD term. The parameters are $T = 0.006$ and $\Delta t = 0.001$.



Preparing GHZ State - Nested Commutator

$$\hat{H}(\lambda(t)) = (1-\lambda(t))\sum_{j}^{N} h_x \sigma_x^j + \lambda(t) J_0 \sum_{j}^{N} \sigma_z^j \sigma_z^{j+1}$$

Non-Integrable Ising Model - Local CD driving

$$\hat{H}_0^{(N)}(t) = (1-\lambda(t))\sum_{j=1}^{N} h_x \sigma_x^j + \lambda(t)\sum_{j=1}^{N}(h_z^j \sigma_z^j + J_0 \sigma_z^j \sigma_z^{j+1})$$

SPSA Algorithm and Optimization

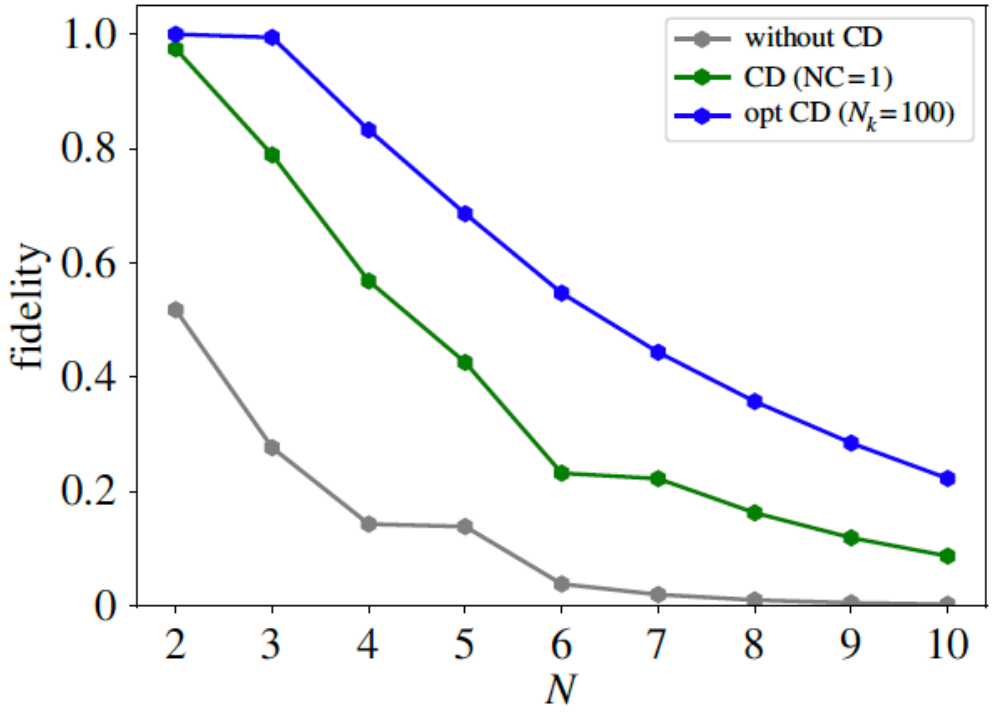


Figure 3. Fidelity of the prepared GHZ state in Ising spin systems with various sizes ranging from 2 to 10 qubits, where the approximate CD NC ($\ell = 1$) and its optimization by SPSA are included, and for completeness, the case without CD terms is also compared. The parameters: $J = -1$, $\Delta t = 0.2$, $T = 1$ and $N_{\text{shots}} = 1000$ are implemented on the ideal quantum simulator Qiskit. (Online version in colour.)

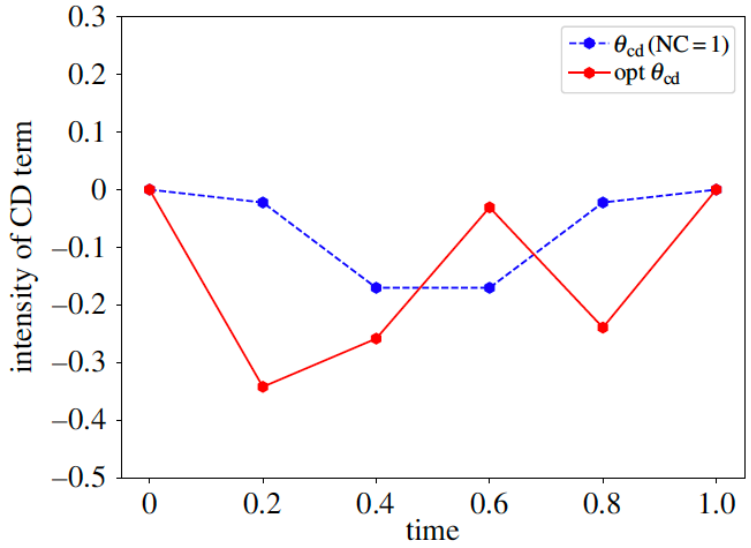


Table 1. Table on the fidelity comparison between two methods of optimal CD driving and QAOA at $T' = T = 1$.

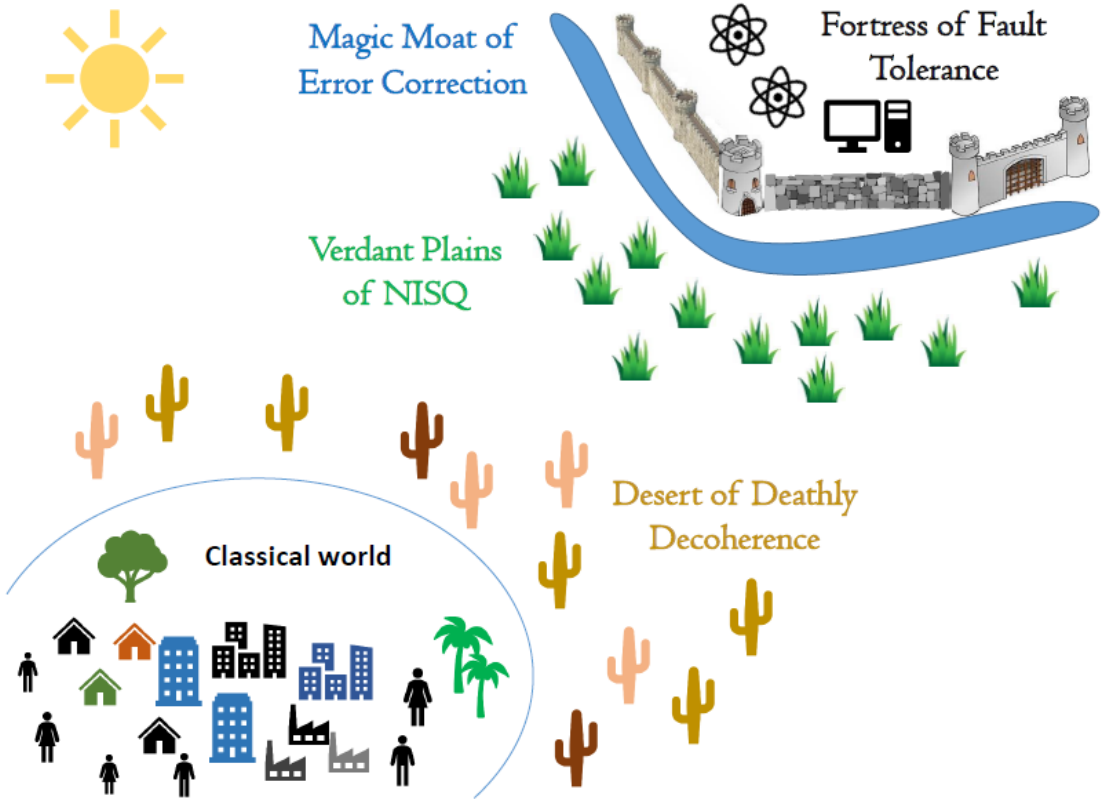
qubit number	optimal CD	QAOA ($p = 1$)	QAOA ($p = 2$)
4	0.77	0.46	0.62
6	0.49	0.25	0.37
8	0.30	0.10	0.19
10	0.18	0.04	0.10

Phil. Trans. R. Soc. A 380: 20210282 (2022)

Nearest-neighbour Ising model and GHZ state preparation

Noisy Intermediate-Scale Quantum (NISQ)

NISQ era



NISQ devices

- No fault-tolerant quantum error correction
- Noise-mitigation techniques
- Circuit depth determined by gate fidelity

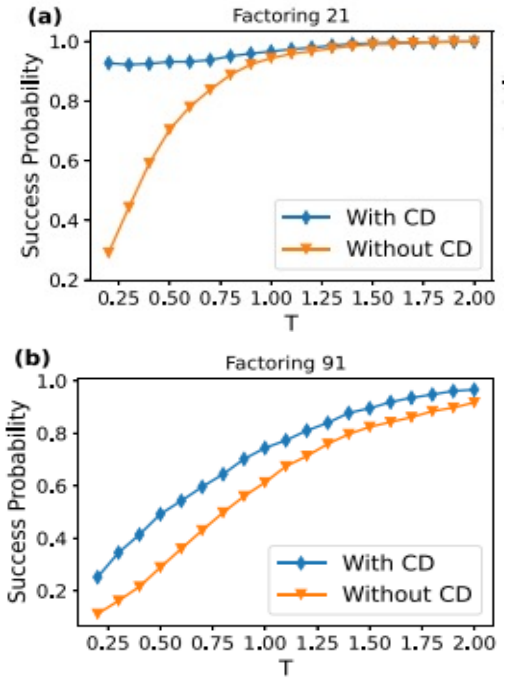
NISQ algorithms

- Performance analyzed mostly heuristically
- Quantum-classical feedback loops
- Paradigm: prepare, reset, repeat

Digitalized Counter-Diabatic Quantum Computing （DCQC）-> Quantum Advantage

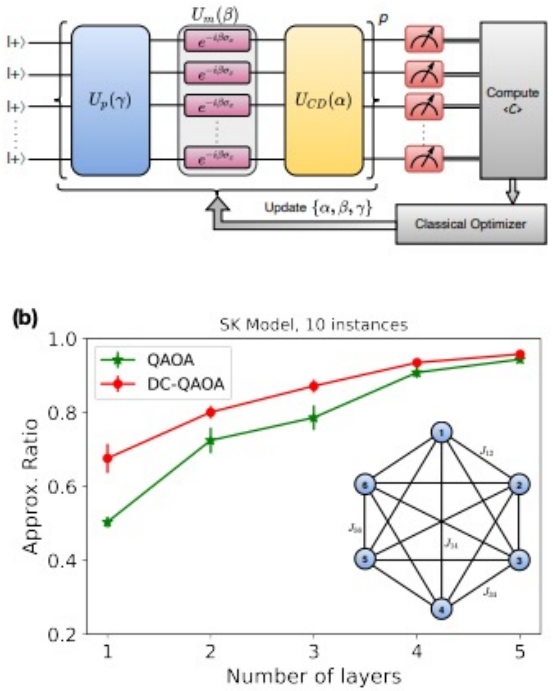
Applications & Extensions

Factorization



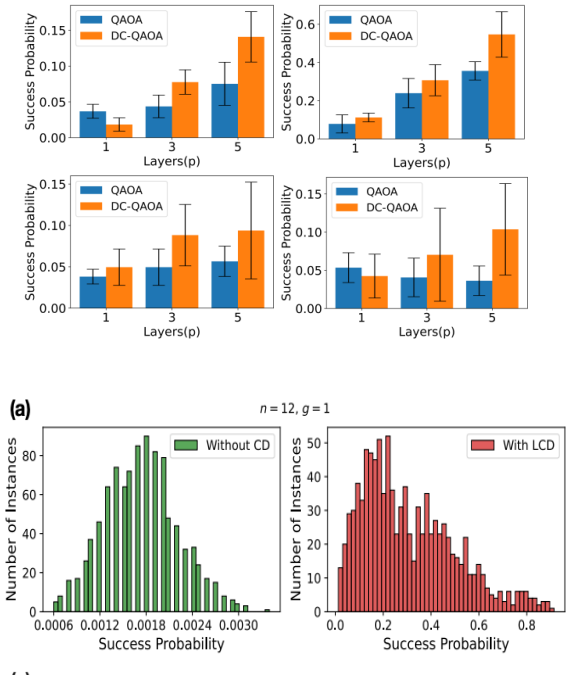
PRA 104, L050403 (2021)

QAOA



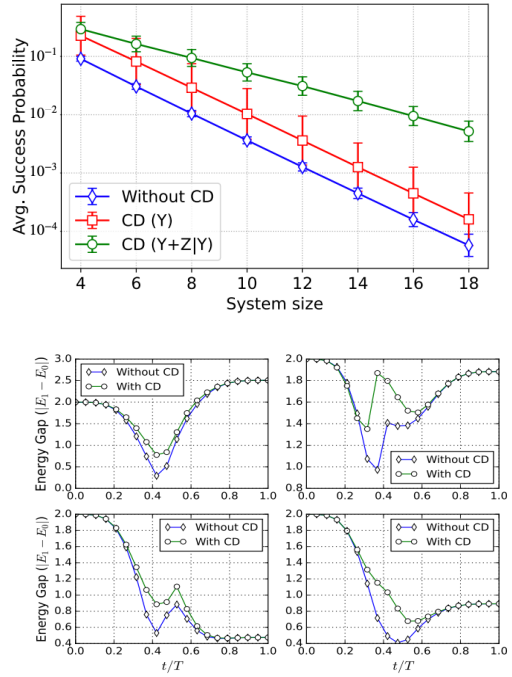
PRR 4, 013141 (2022)

Portfolio



PRR 4, 043204 (2022)

QUBO



PRR 4, L042030 (2022)

Non-stoquastic Catalyst

Adiabatic Quantum Factorization

Let **N** be the number we want to factorize, **p** and **q** are the prime factors satisfying the equation **N-pq = 0**.

Then, we can define the cost function as,

$$f(x,y) = (N - xy)^2$$

It's possible to encode the solution of a minimization problem in the ground state of a Hamiltonian,

$$\hat{H}_f = \left[NI - \left(\sum_{l=1}^{X} 2^l \hat{x}_l + I \right) \left(\sum_{m=1}^{Y} 2^m \hat{y}_m + I \right) \right]^2$$

where $\hat{x}_l = \frac{I-\sigma_l^z}{2}$ and $\hat{y}_m = \frac{I-\sigma_m^z}{2}$. This Hamiltonian can be written as,

$$\hat{H}_f = \sum_i h_i \sigma_i^z + \sum_{i<j} J_{ij} \sigma_i^z \sigma_j^z + \sum_{i<j<k} K_{ijk} \sigma_i^z \sigma_j^z \sigma_k^z + \sum_{i<j<k<l} L_{ijkl} \sigma_i^z \sigma_j^z \sigma_k^z \sigma_l^z$$

Multiplication Table Method - Factoring 2479

TABLE I: Multiplication table for $67 \times 37 = 2479$ in binary.

	2^{11}	2^{10}	2^9	2^8	2^7	2^6	2^5	2^4	2^3	2^2	2^1	2^0
x						1	x_5	x_4	x_3	x_2	x_1	1
y							1	y_4	y_3	y_2	y_1	1
						1	x_5	x_4	x_3	x_2	x_1	1
					y_1	y_1x_5	y_1x_4	y_1x_3	y_1x_2	y_1x_1	y_1	
				y_2	y_2x_5	y_2x_4	y_2x_3	y_2x_2	y_2x_1	y_2		
			y_3	y_3x_5	y_3x_4	y_3x_3	y_3x_2	y_3x_1	y_3			
		y_4	y_4x_5	y_4x_4	y_4x_3	y_4x_2	y_4x_1	y_4				
	1	x_5	x_4	x_3	x_2	x_1	1					
carries	$c_{10,11}$	$c_{9,10}$	$c_{8,9}$	$c_{7,8}$	$c_{6,7}$	$c_{5,6}$	$c_{4,5}$	$c_{3,4}$	$c_{2,3}$	$c_{1,2}$		
	$c_{9,11}$	$c_{8,10}$	$c_{7,9}$	$c_{6,8}$	$c_{5,7}$	$c_{4,6}$	$c_{3,5}$	$c_{2,4}$				
$x \times y = 2479$	1	0	0	1	1	0	1	0	1	1	1	1

Factorization equations after classical pre-processing

$$
\begin{aligned}
x_3y_1 - y_1 &= 0 \\
x_3y_2 - y_1 &= 0 \\
x_3 + y_2 + c_{7,8} - 1 &= 0 \\
y_1 - y_2 - 2c_{7,8} + 1 &= 0 \\
x_3 - 2y_1y_2 - y_1 + y_2 - 1 &= 0.
\end{aligned}
$$

By squaring and summing all the equations, we get the cost function as

$$
\begin{aligned}
f(x,y,c) =& (x_3y_1 - y_1)^2 + (x_3y_2 - y_1)^2 + (x_3 + y_2 + c_{7,8} - 1)^2 \\
&+ (y_1 - y_2 - 2c_{7,8} + 1)^2 + (x_3 - 2y_1y_2 - y_1 + y_2 - 1)^2
\end{aligned}
$$

$$
\begin{aligned}
xy - 1 = 0 &\implies x = y = 1, \\
x + y - 1 = 0 &\implies xy = 0, \\
a - bx = 0 &\implies x = 1, \\
\sum_i x_i = 0 &\implies x_i = 0, \\
\sum_{i=1}^{a} x_i - a = 0 &\implies x_i = 1.
\end{aligned}
$$

Factoring 2479 using approximate CD driving

By mapping the binary variables to the qubit operator, the final Hamiltonian corresponding to factoring 2479 is obtained

$$H_f = -2.5\sigma_1^z - 1.5\sigma_z^z + 0.75\sigma_3^z - 0.5\sigma_4^z + 0.25\sigma_1^z\sigma_2^z - 1.5\sigma_1^z\sigma_3^z - \sigma_1^z\sigma_4^z + 0.5\sigma_2^z\sigma_3^z + 1.5\sigma_2^z\sigma_4^z + 0.5\sigma_3^z\sigma_4^z + 0.75\sigma_1^z\sigma_2^z\sigma_3^z + 5.75\mathbb{I}$$

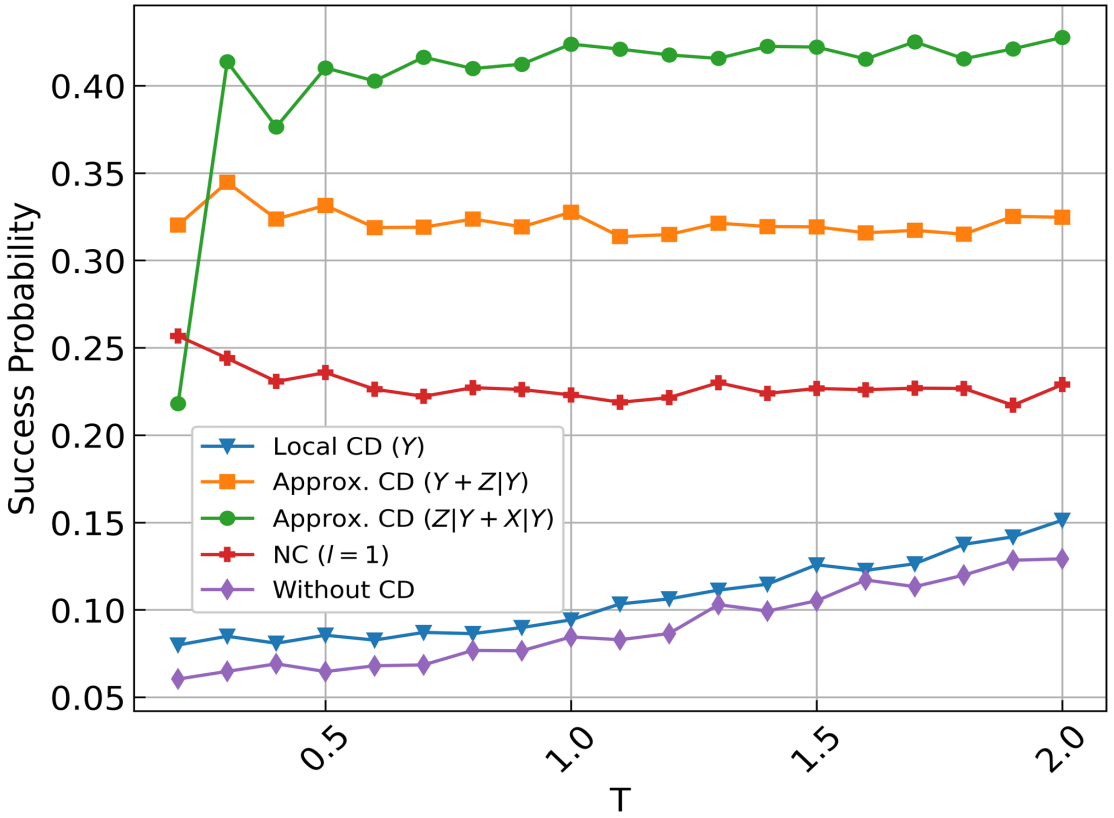
The approximate CD term calculated from 1st order nested-commutator ansatz takes the form,

$$A_\lambda^{(1)} = 2\alpha_1(t)\tilde{h}_x\left[\sum_i \tilde{h}_i^z\sigma_y^i + \sum_{i<j}\tilde{J}_{ij}\left(\sigma_z^i\sigma_y^j + \sigma_y^i\sigma_z^j\right) + \sum_{i<j<k}\tilde{K}_{ijk}\left(\sigma_z^i\sigma_z^j\sigma_y^k + \sigma_z^i\sigma_y^j\sigma_z^k + +\sigma_y^i\sigma_z^j\sigma_z^k\right)\right].$$

where $\alpha_1(t) = 0.0830/[h_x^2(1-\lambda)^2 + 5.0112\lambda^2]$, calculated using the variational method.

Using Approximate CD driving

PRA 104, L050403 (2021)



The CD terms are chosen from the operator pool, restricted to only one and two spin terms.

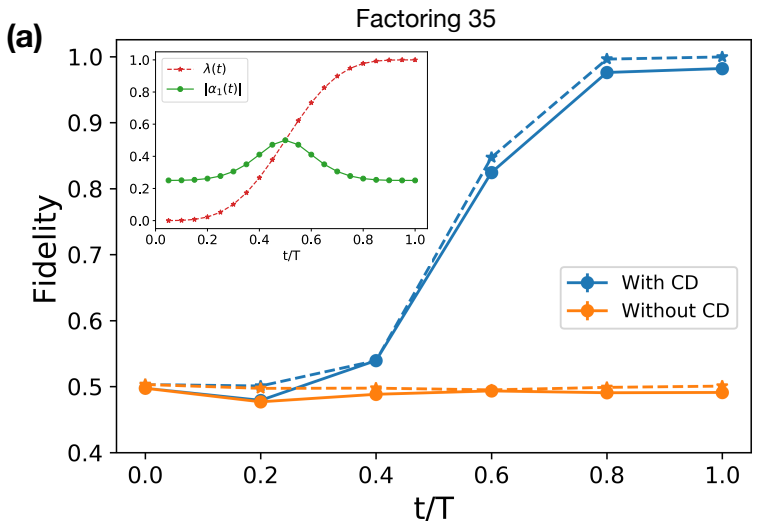
$$A_\lambda^* = \{Y,\ Z|Y,\ X|Y\},\ \text{where } Y = \sum_i \alpha_i(t)\sigma_i^y\ ,$$

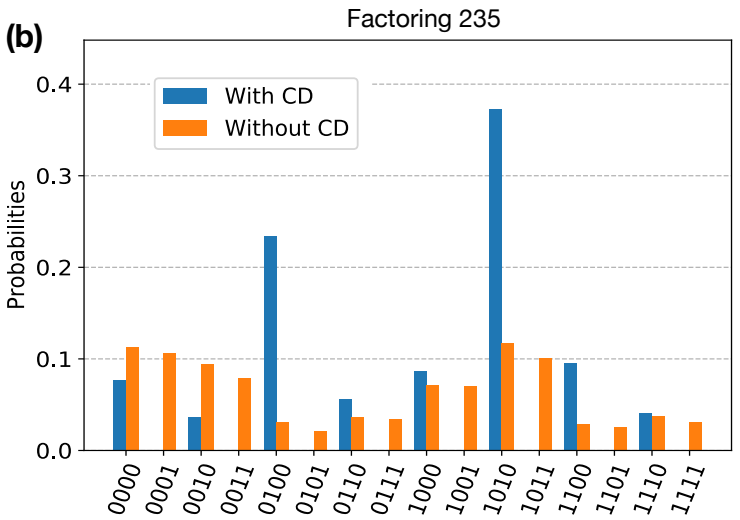
$$Z|Y = \sum_{i<j} \beta_i(t)(\sigma_i^z\sigma_j^y + \sigma_i^y\sigma_j^z)\ ,$$

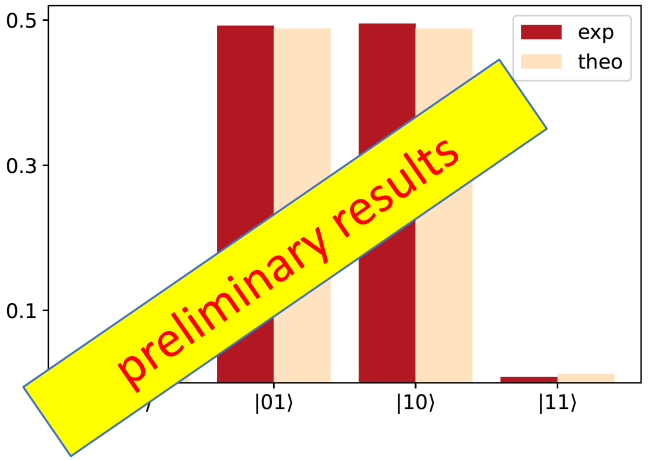
$$X|Y = \sum_{i<j} \gamma_i(t)(\sigma_i^x\sigma_j^y + \sigma_i^y\sigma_j^x).$$

The success probability of obtaining the ground state $|0100\rangle$ for the Hamiltonian corresponding to the factorization of 2479 as a function of total evolution time is shown. The performance of different CD terms chosen from the operator pool is compared.

Factoring 35 & 235 experimentally: Using 1st order NC method in IBMQ

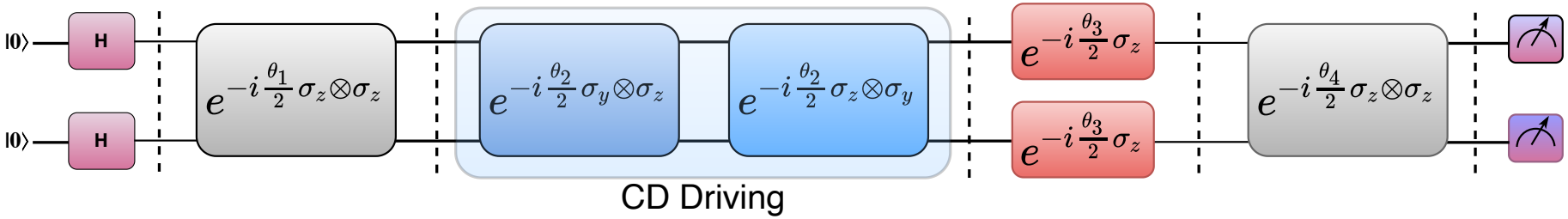






Target ground state $\rightarrow \frac{1}{\sqrt{2}}(\,|10\rangle + |01\rangle\,)$

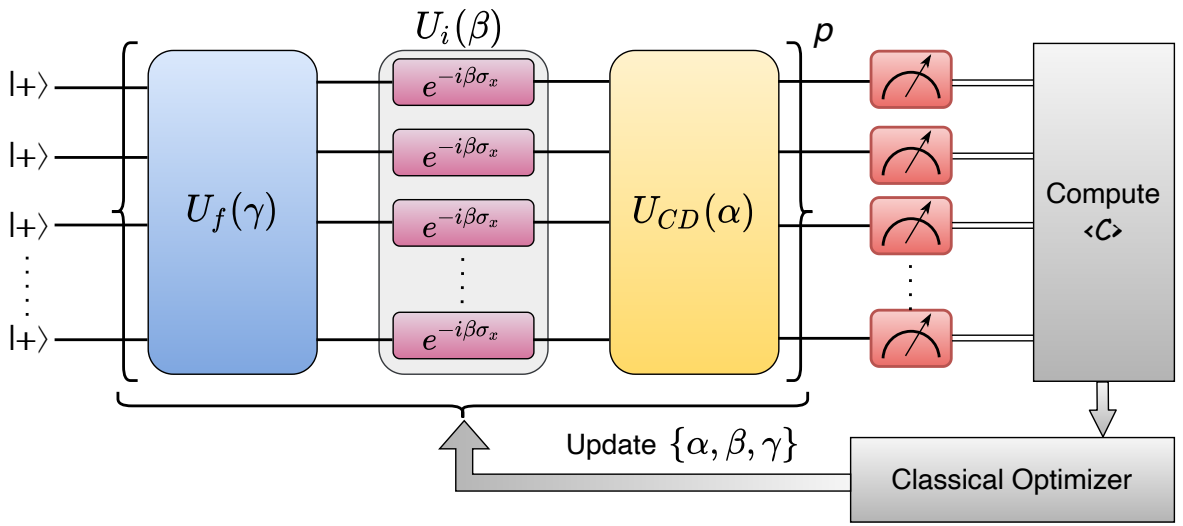
Target ground state $\rightarrow |0101\rangle$



Circuit implementation for the time evolution of the Hamiltonian to factorize

35 = 7 × 5 using CD driving (two trotter steps).

DC-QAOA



Variational wavefunction, generalized by **3p** parameters

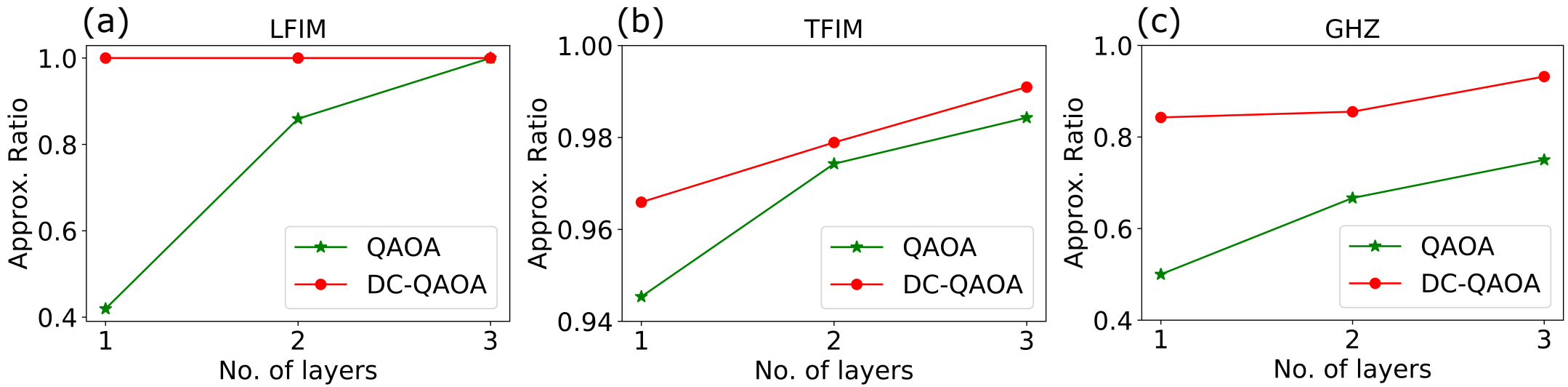
$$\left|\psi_p(\vec{\alpha},\vec{\beta},\vec{\gamma})\right\rangle = e^{-i\beta_p H_i} e^{-i\gamma_p H_f} e^{-i\alpha_{p-1} H_{CD}} \ldots e^{-i\alpha_1 H_{CD}} e^{-i\beta_1 H_i} e^{-i\gamma_1 H_f} |+\rangle^{\otimes N}$$

The expectation value is calculated by repeated measurements in the computational basis

$$F_p(\vec{\alpha},\vec{\beta},\vec{\gamma}) = \left\langle \psi_p(\vec{\alpha},\vec{\beta},\vec{\gamma}) \left| H_f \right| \psi_p(\vec{\alpha},\vec{\beta},\vec{\gamma}) \right\rangle$$

The optimal parameters (α,β,γ) are found by using the classic computer.

Ising Spin Models

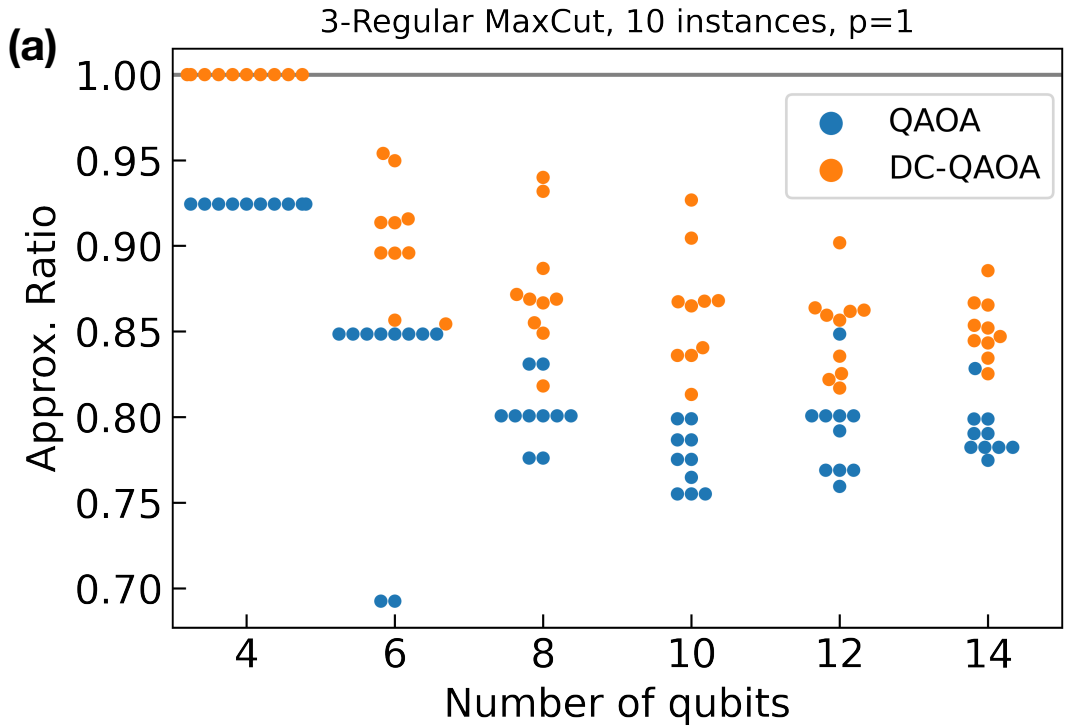


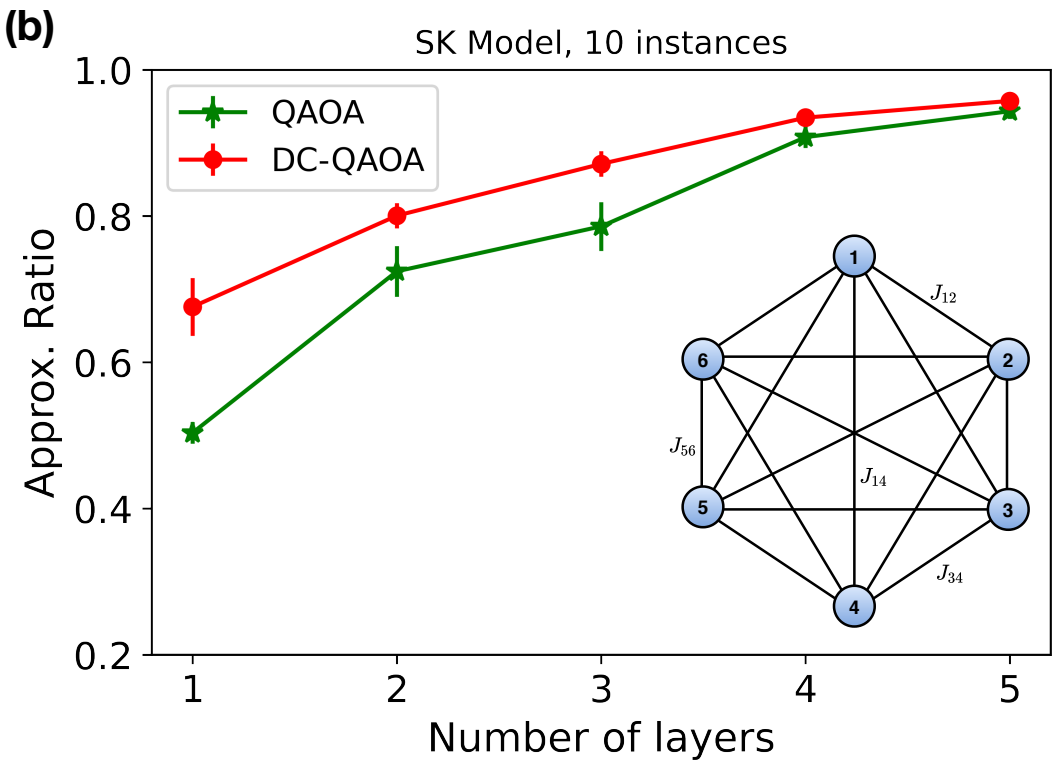
$$H_{prob}(\sigma) = -\sum_{<i,j>} J_{ij}\sigma_i^z\sigma_j^z - \sum_i h_i\sigma_i^z - \sum_i k_i\sigma_i^x$$

$$A = \{\sigma^y, \sigma^z\sigma^y, \sigma^y\sigma^z, \sigma^x\sigma^y, \sigma^y\sigma^x\}$$

PR Research 4, 013141 (2022); Phys. Rev. X 11, 031070 (2021)

Classical Optimization Problems





$$C(z) = \frac{1}{2} \sum_{(i,j)\in E} w_{ij}(1 - z_i z_j)$$

$$H(\sigma) = -\sum_{(i,j)\in E} J_{ij}\sigma_i^z \sigma_j^z$$

$$A_t = \{\sigma^z\sigma^y, \sigma^y\sigma^z\}$$

Sherrington-Kirkpatrick (SK)

Comparing Powell and Adagrad Optimizers

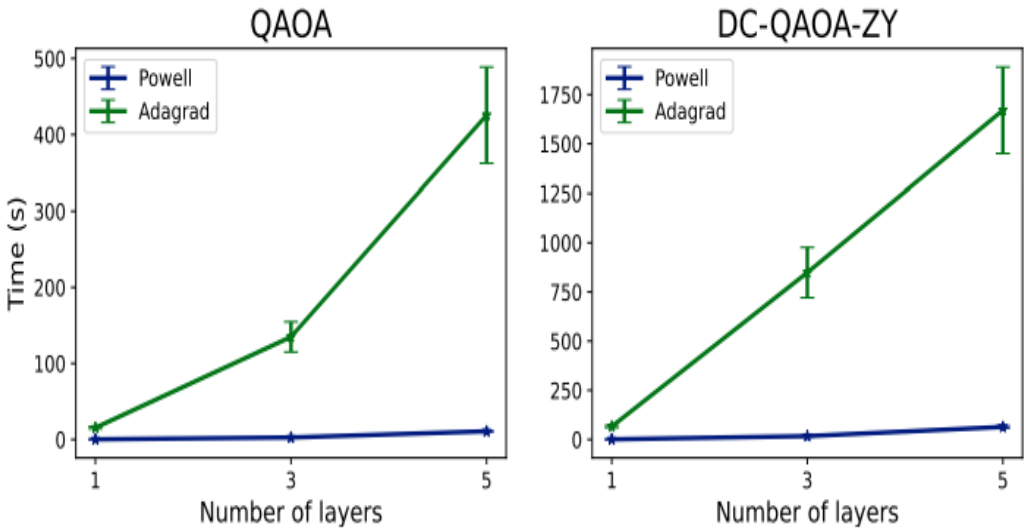
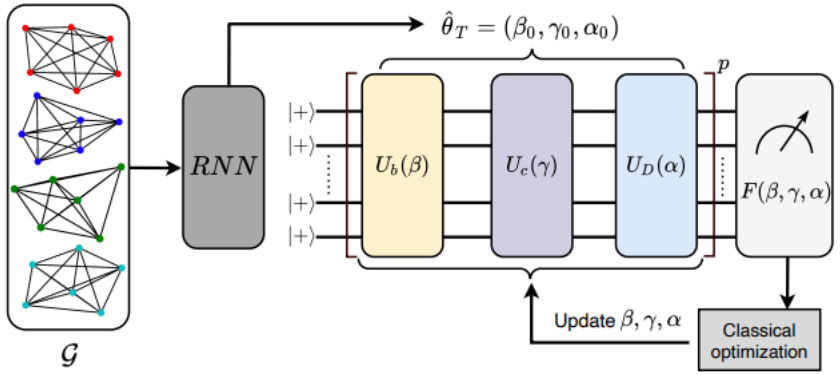


Figure 6.2: Mean computation times (in seconds) for the problem studied in this section for Powell and Adagrad with 0.1 learning rate. It can be seen how Powell optimization takes much less time.

Intel Core i5-7200 U 2.50 GHz

Meta-Learning



arXiv > quant-ph > arXiv:2206.09966

Quantum Physics

[Submitted on 20 Jun 2022]

Meta-Learning Digitized-Counterdiabatic Quantum Optimization

Pranav Chandarana, Pablo S. Vieites, Narendra N. Hegade, Enrique Solano, Yue Ban, Xi Chen

Solving optimization tasks using variational quantum algorithms has emerged as a crucial application of the current noisy intermediate-scale quantum devices. However, these algorithms face several difficulties like finding suitable ansatz and appropriate initial parameters, among others. In this work, we tackle the problem of finding suitable initial parameters for variational optimization by employing a meta-learning technique using recurrent neural networks. We investigate this technique with the recently proposed digitized-counterdiabatic quantum approximate optimization algorithm (DC-QAOA) that utilizes counterdiabatic protocols to improve the state-of-the-art QAOA. The combination of meta learning and DC-QAOA enables us to find optimal initial parameters for different models, such as MaxCut problem and the Sherrington-Kirkpatrick model. Decreasing the number of iterations of optimization as well as enhancing the performance, our protocol designs short depth circuit ansatz with optimal initial parameters by incorporating shortcuts-to-adiabaticity principles into machine learning methods for the near-term devices.

Protein Folding

PHYSICAL REVIEW APPLIED

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Accepted Paper

Digitized counterdiabatic quantum algorithm for protein folding

Phys. Rev. Applied

Pranav Chandarana, Narendra N. Hegade, Iraitz Montalban, Enrique Solano, and Xi Chen

Accepted 25 May 2023

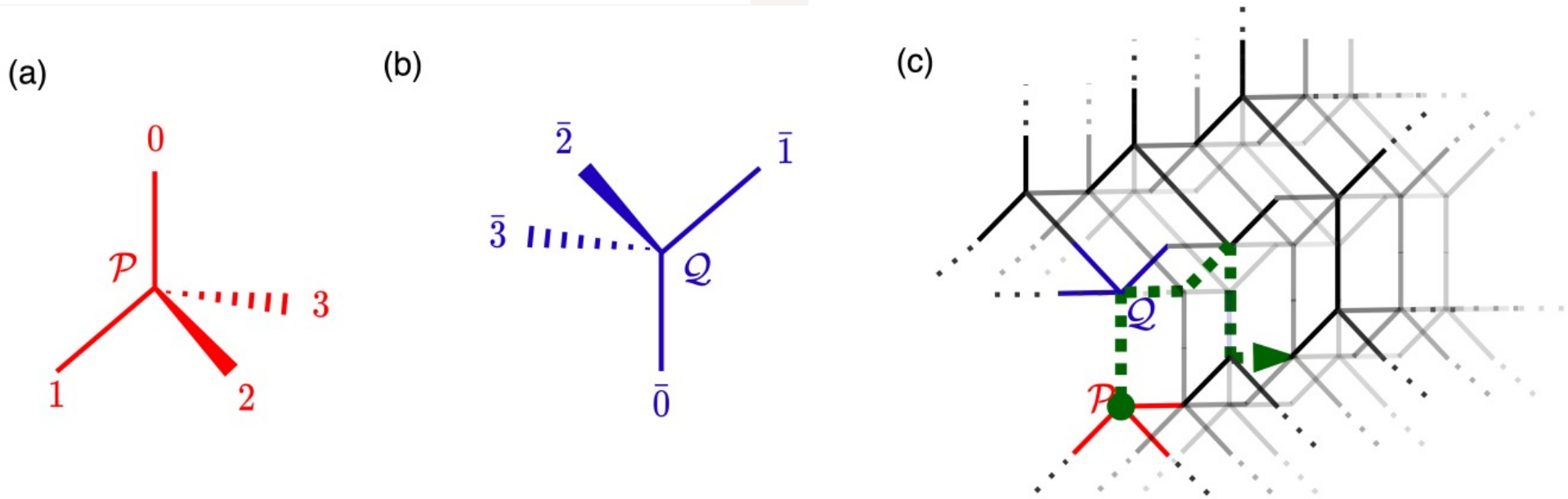

FIG. 8. Schematic diagram showing the tetrahedral lattice structures. (a) shows the lattice $\mathcal{P}$ and (b) shows the inverted lattice $\mathcal{Q}$. The turns taken by the amino acids will be one of the four directions ($t = 0, 1, 2, 3$ or $\bar{0}, \bar{1}, \bar{2}, \bar{3}$) and both lattices are switched at each turn. (c) shows the mesh made of $\mathcal{P}$ (shown in red) and $\mathcal{Q}$ (shown in blue), while the green line shows a schematic of the turns taken by an arbitrary protein in 3D.

Quantinuum Trapped-ions

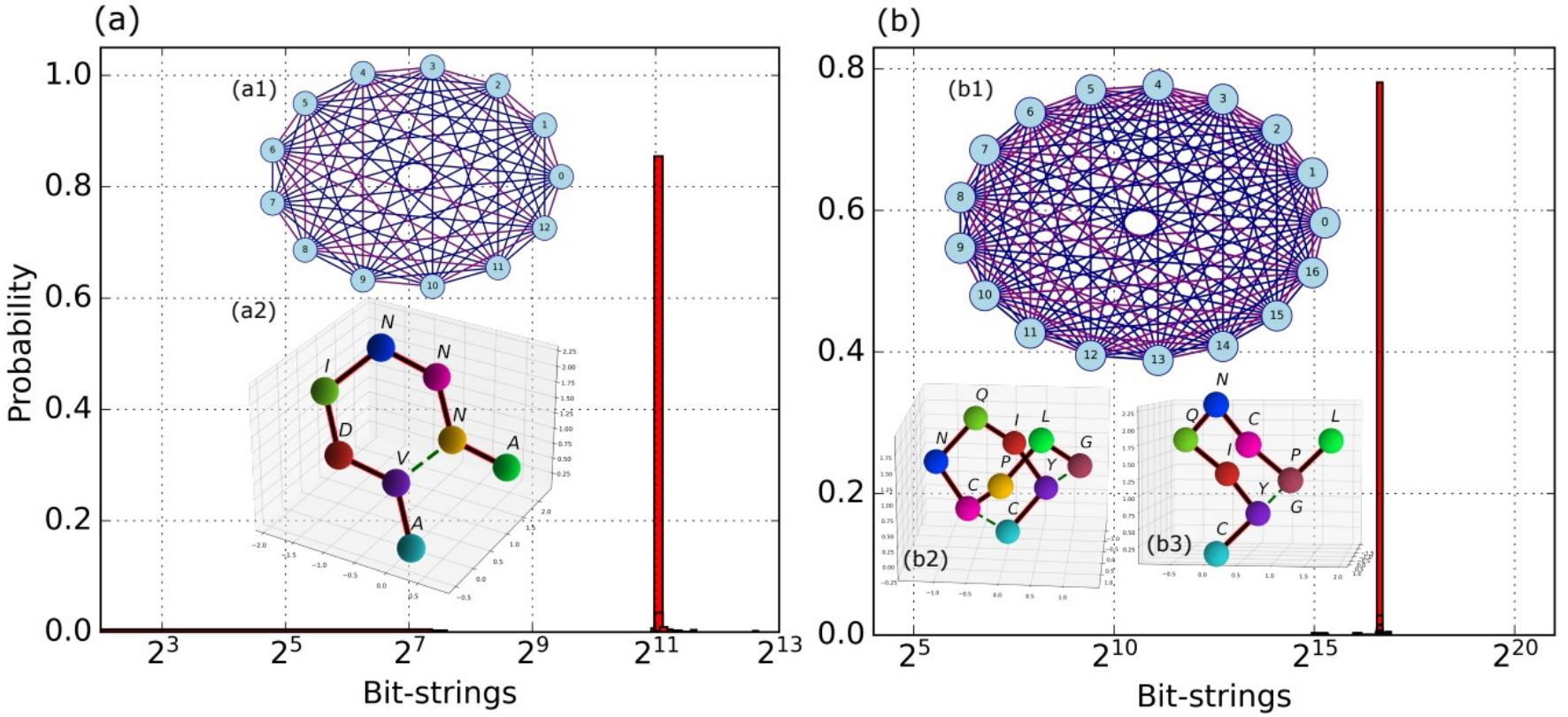

FIG. 6. Output probability distribution of $N = 13$ AVDINNNA protein and $N = 17$ CYIQNCPLG protein on a trapped-ion system: Quantinuum system H1 with 1000 shots. (a) show the $N = 13$ case and (b) show the $N = 17$ case. (a1) and (b1) show the graph corresponding to two-body interactions implemented in the CD-inspired ansatz. Blue edges show the present two-body connections while the purple edges show the connections that are absent. (a2) shows the optimal protein configuration with a dotted green line depicting the connection of the nearest-neighbor interaction. (b2) show the optimal configuration of protein obtained from exactly solving the problem whereas (b3) shows the protein configuration obtained in the experiment. In (b3) amino acids 'P' and 'G' are overlapping.

IBM Superconducting chip

Google QVM

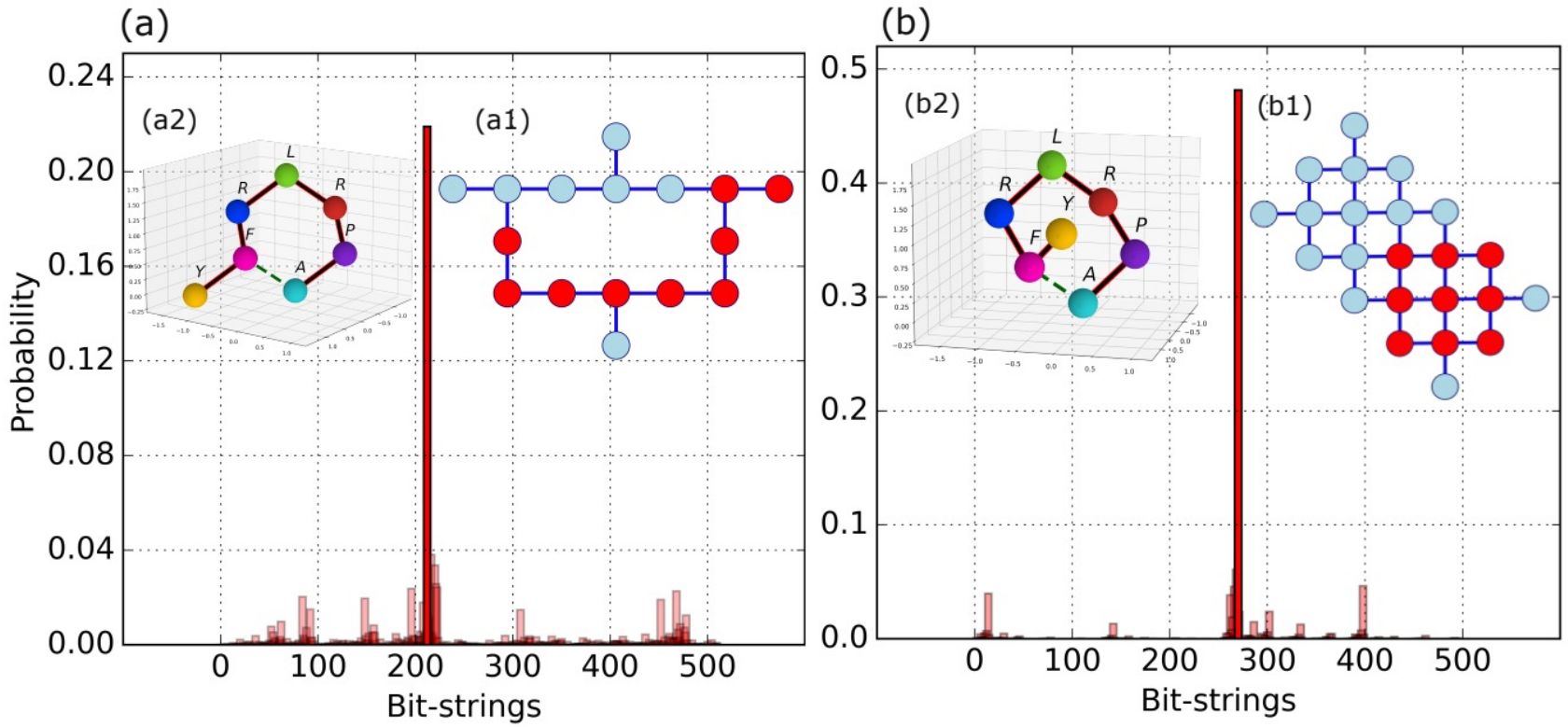

FIG. 7. Output probability distribution of $N = 9$ qubits by implementing the optimal circuit on (a) IBM *ibmq_guadalupe* where the experiment was performed with 8192 shots and (b) Google's quantum virtual machine *rainbow* [49] where the experiment was performed with 10000 shots. Dark-colored bars show the ground-state probability of the physical qubits whereas light-colored bars show the rest of the distribution (a1) and (b1) show the hardware topology and selected qubits are shown using red color. (a2) and (b2) both show the optimal protein configurations with the nearest neighbor connection between 'A' and 'F' shown by a dotted green line.

Quantum Chemistry

Molecular Physics
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Taylor & Francis
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RESEARCH ARTICLE

Simulation of electronic structure Hamiltonians using quantum computers

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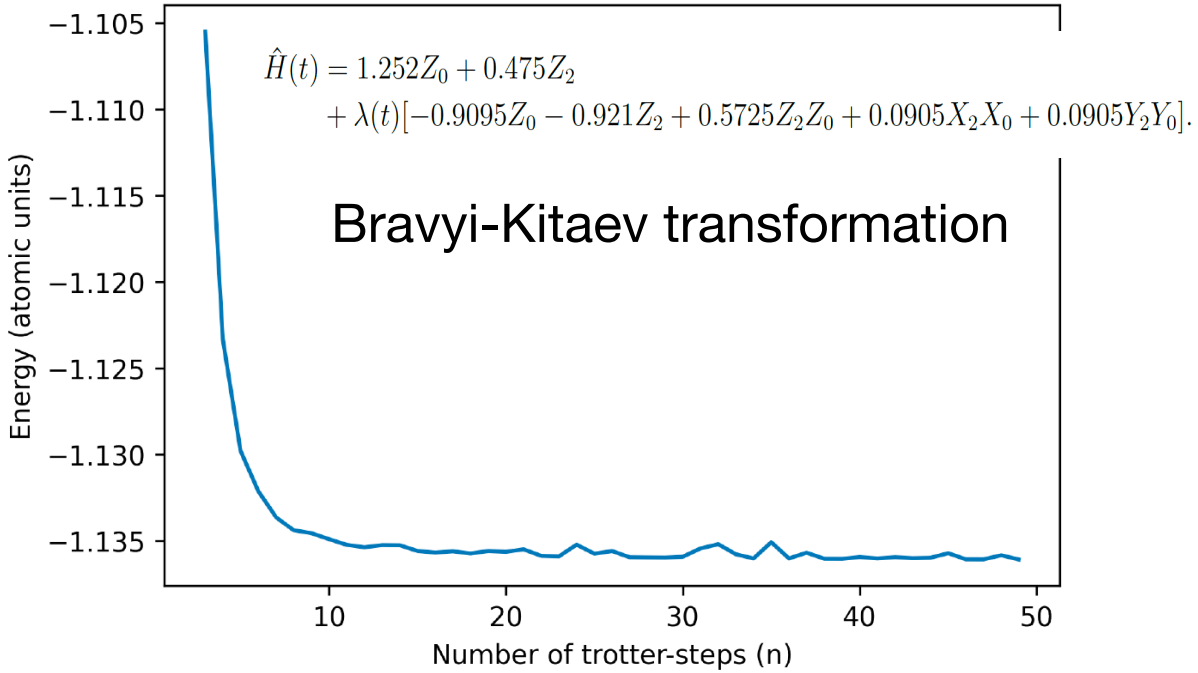
(*Received 8 October 2010; final version received 18 December 2010*)

Over the last century, a large number of physical and mathematical developments paired with rapidly advancing technology have allowed the field of quantum chemistry to advance dramatically. However, the lack of computationally efficient methods for the exact simulation of quantum systems on classical computers presents a limitation of current computational approaches. We report, in detail, how a set of pre-computed molecular integrals can be used to explicitly create a quantum circuit, i.e. a sequence of elementary quantum operations, that, when run on a quantum computer, obtains the energy of a molecular system with fixed nuclear geometry using the quantum phase estimation algorithm. We extend several known results related to this idea and discuss the adiabatic state preparation procedure for preparing the input states used in the algorithm. With current and near future quantum devices in mind, we provide a complete example using the hydrogen molecule of how a chemical Hamiltonian can be simulated using a quantum computer.

Keywords: electronic structure; quantum computing



nature COMMUNICATIONS

ARTICLE

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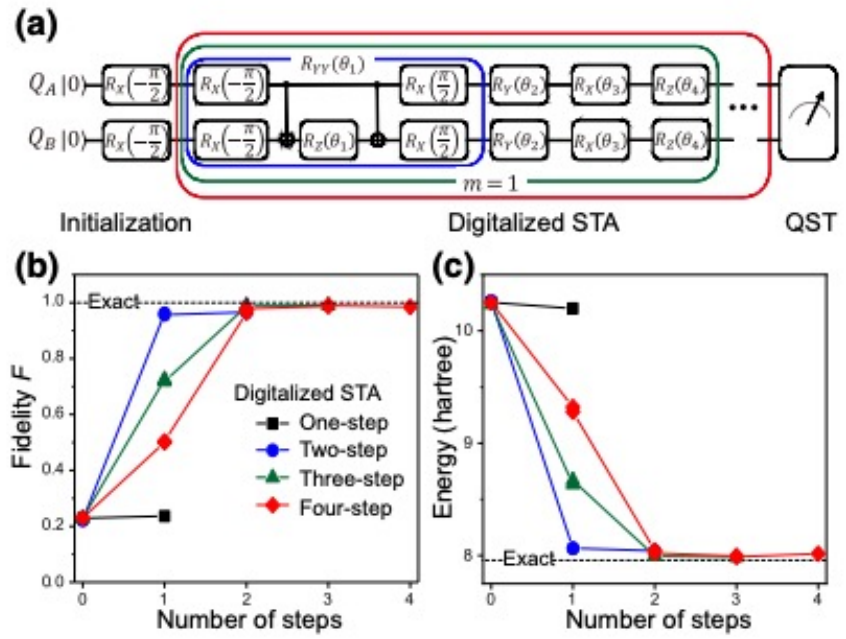
A variational eigenvalue solver on a photonic quantum processor

Alberto Peruzzo[1,*,†], Jarrod McClean[2,*], Peter Shadbolt[1], Man-Hong Yung[2,3], Xiao-Qi Zhou[1], Peter J. Love[4], Alán Aspuru-Guzik[2] & Jeremy L. O'Brien[1]



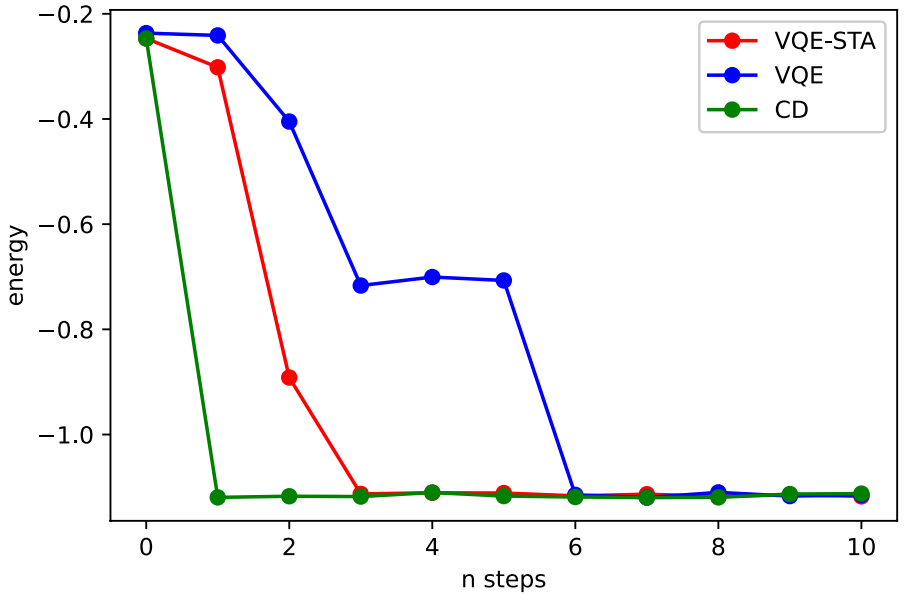
VQE-STA

$$U(\theta_i) = e^{T(\theta_i) - T(\theta_i)^\dagger}$$

$$T(\theta_i) = T_1(\theta_i) + T_2(\theta_i) + \ldots + T_{CD}(\theta_i)$$

$$T_1 = \sum_{pr} t_p^r \hat{a}_p^\dagger \hat{a}_r$$

$$T_2 = \sum_{pqrs} t_{pq}^{rs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$



STA in Quantum Chemistry

STA Design (H_2)

Starting from the Hartree hamiltonian, we design the problem hamiltonian.

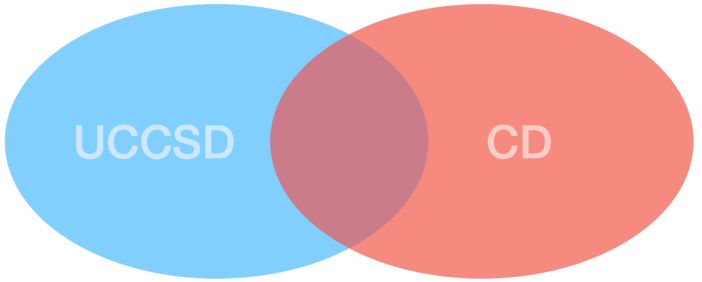
$$H_{ad} = H_0 + \lambda(t)(H_f - H_0) \longrightarrow H_{ad} = 1.252Z_0 + 0.475Z_2 + \lambda(t)[0.9095Z_0 + -0.921Z_2 + 0.5725Z_2Z_0 + 0.0905(X_2X_0 + Y_2Y_0)]$$

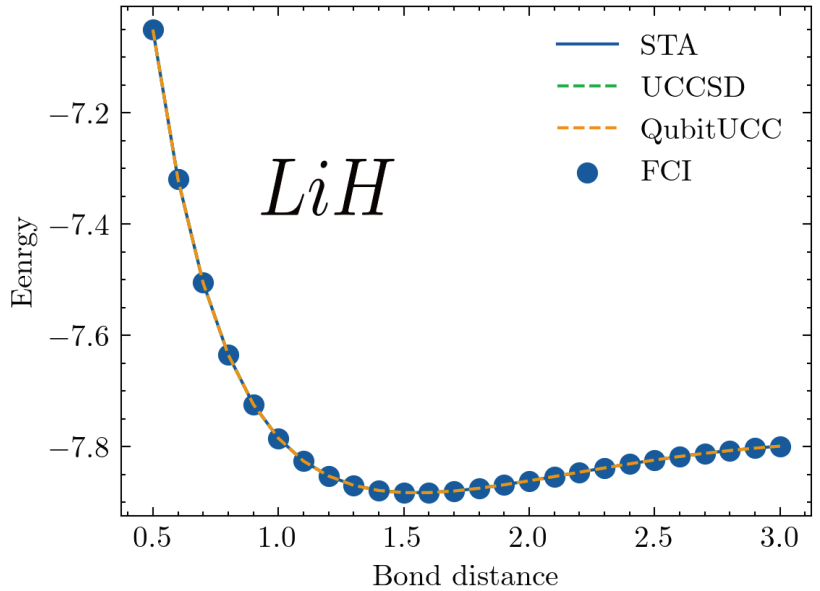
Once we have the hamiltonian structure, we calculate the CD term using the nested commutator

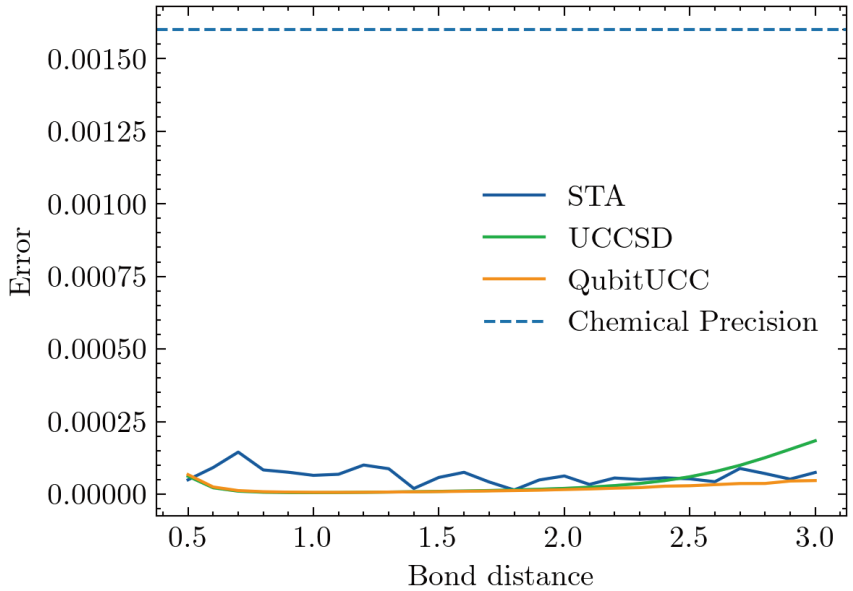
$$A_\lambda^{(n)} = i \sum_{k=1}^{n} \alpha_k [H, [H, \ldots [H, \partial_\lambda H]]] \longrightarrow H_{cd} = g_{cd}(t)(X_0Y_2 - Y_0X_2)$$

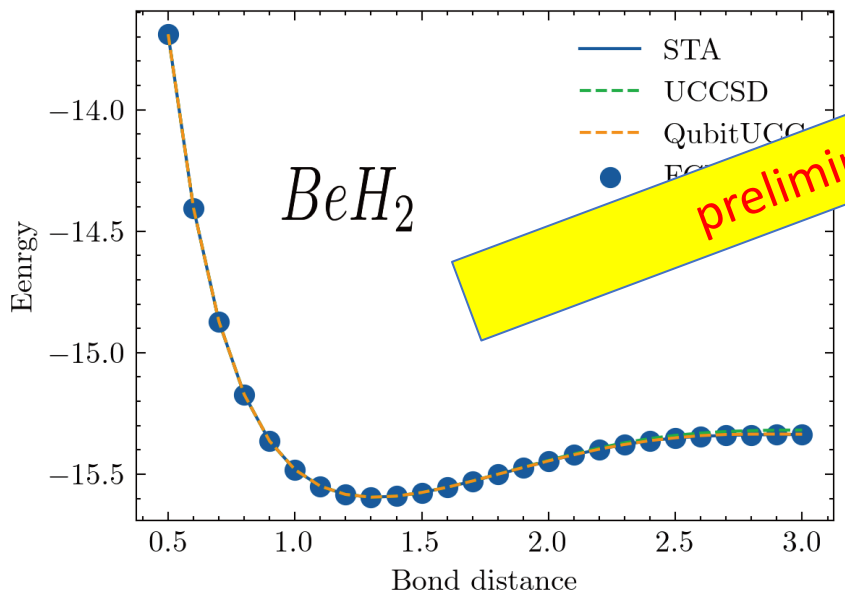
Finally we choose the new hamiltonian $H(t) = H_0(t) + H_{CD}(t)$ as the Ansatz to optimise

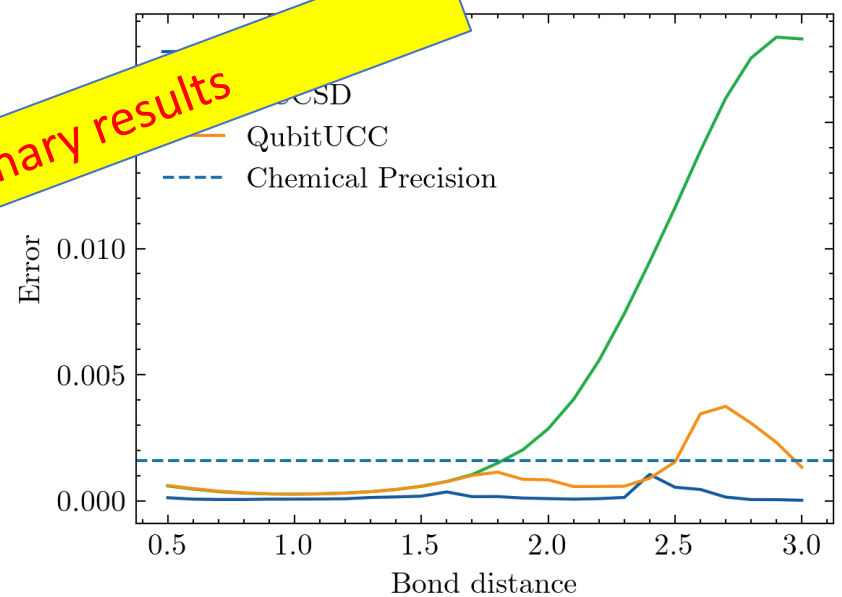
$$T(\theta_i) = \theta_1 Z_0 + \theta_2 Z_2 + \theta_3 Z_0 Z_2 + \theta_4 X_0 X_2 + \theta_5 Y_0 Y_2 + \theta_6 (X_0 Y_2 - Y_0 X_2)$$











preliminary results

	UCCSD	AGA	AGAR
H_2	4 (14)	2	2
LiH	20 (130)	56	9
BeH_2	77 (574)	30*	10*

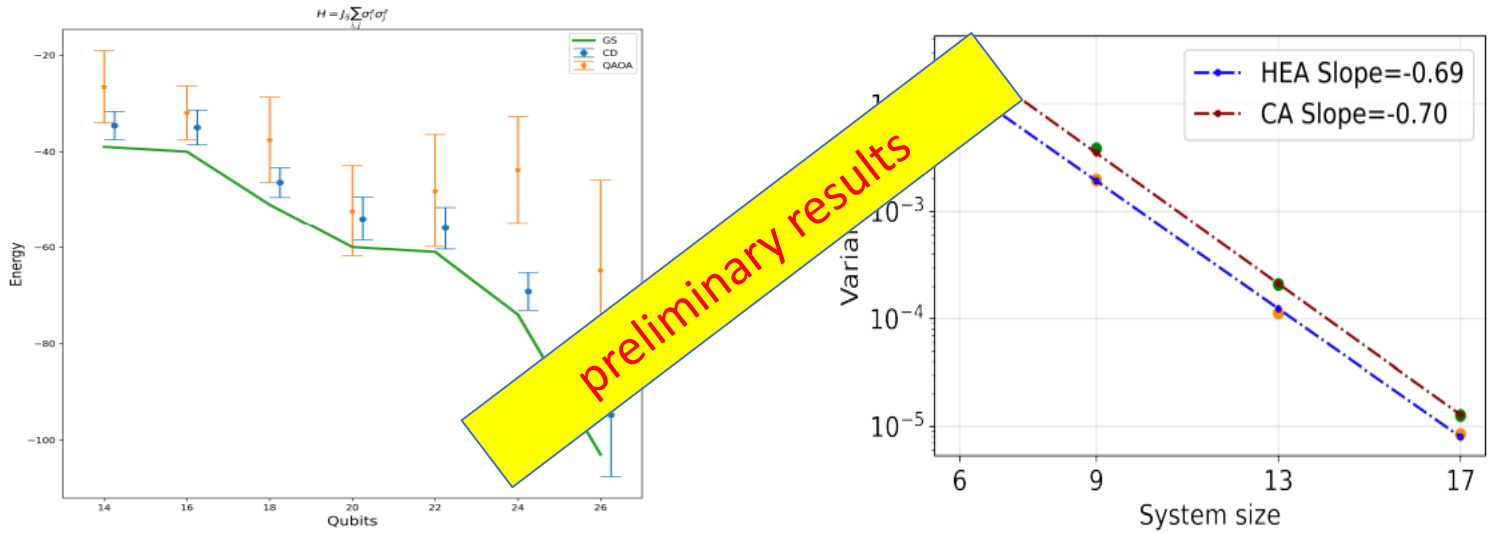
See Poster by Julian and Inaki

Conclusion

- **Digitized-adiabatic Quantum Computation:**
  - Flexibility to introduce arbitrary interactions: Non-stoquastic Hamiltonian's can be easily implemented. Any k-local Hamiltonian can be easily encoded without reducing it to QUBO form.
  - Consistent with error correction. Error mitigation techniques are being developed for NISQ devices
- **Shortcuts to adiabaticity for AQC:**
  - Substantial improvement in the fidelities in a very short time: Achieving the desired computation results within the coherence time of the device. Reduced gate counts on a circuit model.
  - Approximate CD term calculation does not require knowledge of the spectrum of the Hamiltonian. Both variational and algebraic methods have been developed for the efficient calculation of the CD coefficient.
- **Digitized-Counterdiabatic QAOA & VQE:**
  - Counterdiabatic driving term to design a better ansatz for fast convergence.

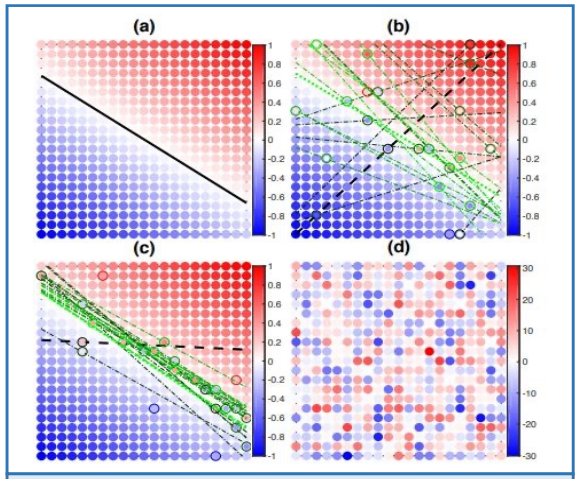
Outlook

- **Scalability**
- **Complexity**
- **Cost of STA**
- **Trotter Error**

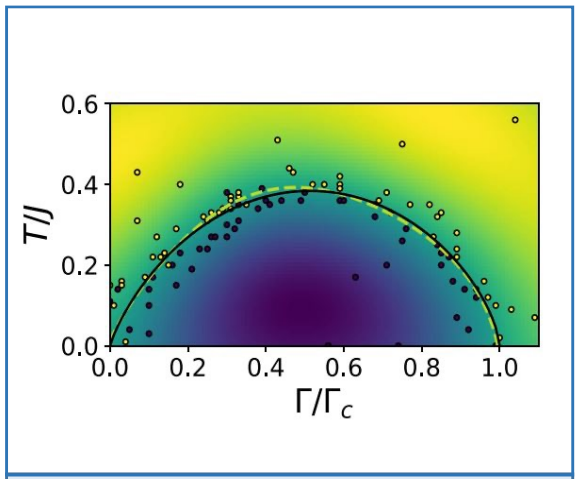


Extend the results to higher qubits \ Optimial Compliation (two-body intetaction)

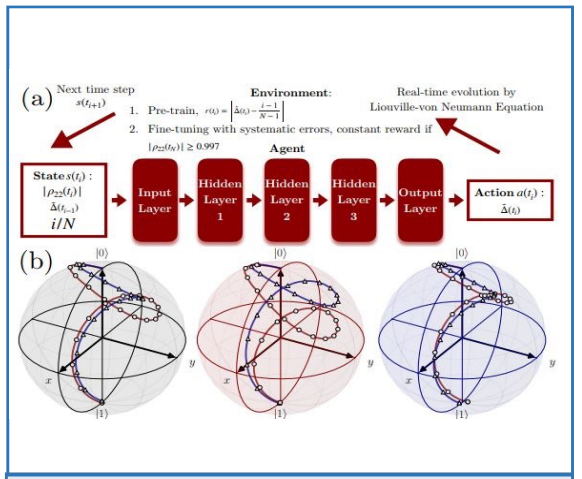
Different optimizers \ Trotter error & adiabatic error \Barren plateau



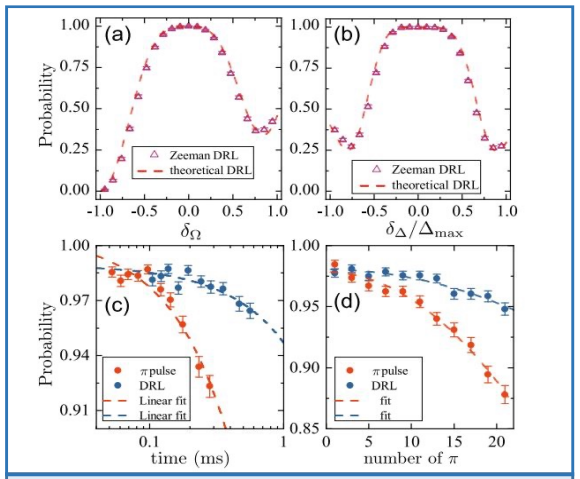
PRL 124, 140504 (2020)



PRR 4, 013213 (2022)



PRA 101, L040401 (2021)



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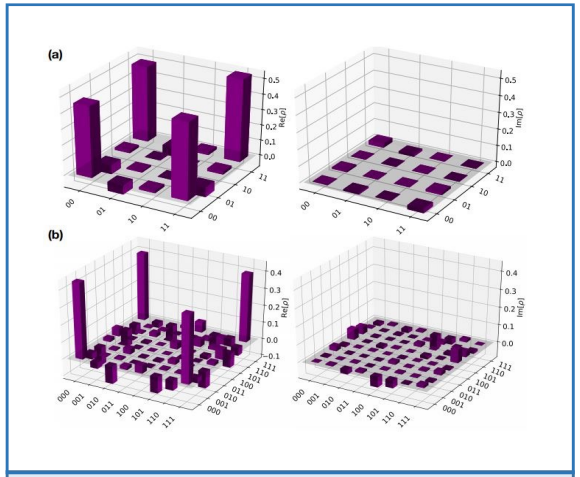
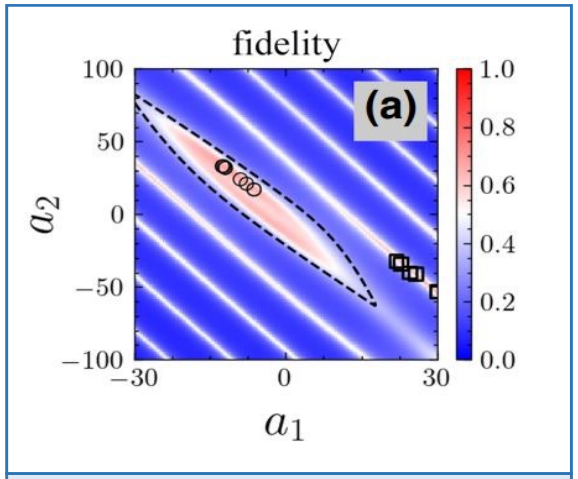


PR Applied 15, 024038 (2021)



PR Applied 17, 024040 (2022)

Thank You for Your Attention!

N. N. Hegade & E. Solano @ Kipu Quantum

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