Quantum computing zeta regularized vacuum expectation values

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in collaboration with

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- **Zeta regularization of the path integral**
- **Vacuum expectation values with zeta regularization**
- **Quantum computing of vacuum expectation values**
- **Conclusion**

Path integral

- Feynman's trace formula

$$\langle A \rangle = \lim_{T \to \infty + i0^+} \frac{\mathrm{tr}\{U(0,T)A\}}{\mathrm{tr}\{U(0,T)\}}$$

for a Hamiltonian H (T denoting time ordering)

$$U(0,T) = \mathrm{Texp}\left(-\frac{i}{\hbar}\int_0^T H(\tau)d\tau\right)$$

- in general ill defined (trace infinite dimensional)

- solutions
  - regularization through euclidean space-time lattice
  - ζ-regularization

Why zeta-regularization of path integral?

- advantage of ζ-regularization
  - defined in the continuum (although lattice setup included)
  - comprises Minkowski space
  - holds for any metric

- $\Rightarrow$ solves sign problem:
  chemical potential, topological term, real time, curved space, ...

Riemann ζ-function

- Riemann's ζ-function, $\zeta_{\mathrm{R}}(z)$

$$\zeta_{\mathrm{R}}(z) = \sum_{n=1}^{\infty} \frac{1}{n^z} \ , \ z \in \mathbb{C}$$

analytical continuation (through Γ-function)

$\Rightarrow$ well defined for $z \neq 1$

E.g.: choose $z = -1 \rightarrow$ find $\zeta_{\mathrm{R}}(-1) = -\frac{1}{12}$

Example for an operator

- Take the (infinite dimensional) discrete operator $|\partial|$

$$\mathrm{tr}|\partial| \underbrace{=}_{F.T.} \sum_{n=-\infty}^{+\infty} |n| = 2\sum_{n=1}^{\infty} n$$

ill defined

- can we make sense out of the trace?

Let $\varphi(z) := |\partial|^{1+z}$ then for $\mathrm{Re}\, z < -2$:

$$\mathrm{tr}\varphi(z) = 2\sum_{n=1}^{\infty} n^{1+z}$$

- analytical continuation of the trace: *"zeta trace"* $\zeta(\varphi)(z)$

$$\zeta(\varphi)(z) = 2\zeta_{\mathrm{R}}(-z-1) \Rightarrow \mathrm{tr}\,|\partial| := \zeta(\varphi)(0) = 2\zeta_{\mathrm{R}}(-1) = -\tfrac{1}{6}$$

Integral kernel

- time evolution operator

$$U(0,T) = \mathrm{Texp}\left(-\frac{i}{\hbar}\int_0^T H(\tau)d\tau\right)$$

- Fourier integration kernel

$$k(x,y) = \int dr \int d\Omega(\xi) e^{ih_2(x,y,\xi)r^2 + ih_1(x,y,\xi)r} a(x,y,r,\xi)$$

- allows to <u>formally</u> define trace

$$\mathrm{tr}(U(0,T)) = \int dx \int dr \int d\Omega(\xi) e^{ih_2(x,x,\xi)r^2 + ih_1(x,x,\xi)r} a(x,x,r,\xi)$$

Gauged integral kernel

- mathematically well defined trace $\rightarrow$ introduce holomorphic function $\mathfrak{g}(z)$ with $\mathfrak{g}(0) = 1$ and $\mathfrak{g}(z) \propto r^z$ $\rightarrow$ "gauge" kernel

$$k(x,y)(z) = \int dr \int d\Omega(\xi) e^{ih_2(x,y,\xi)r^2 + ih_1(x,y,\xi)r} (a\mathfrak{g}(z)(x,y,r,\xi))$$

- leads to ζ-trace of time evolution operator

$$\boxed{\begin{aligned} \mathrm{tr}_\zeta(U(0,T)) &= \zeta(k(x,y))(z) \\ &= \int dx \int dr \int d\Omega(\xi) e^{ih_2(x,x,\xi)r^2 + ih_1(x,x,\xi)r} (a\mathfrak{g}(z)(x,x,r,\xi)) \end{aligned}}$$

General definition

(Tobias Hartung, J. Math Phys. 2017)

family of operators $\mathfrak{G}(z)$ with $\mathfrak{G}(0) = 1 \to U(T,0)\mathfrak{G}(z)$

integral kernel of (gauged) time evolution operator $k(z)$ of $U(0,T)\mathfrak{G}(z)$ has form

$$k(x,y)(z) = \int dr \int d\Omega(\xi) e^{ih_2(x,y,\xi)r^2 + ih_1(x,y,\xi)r} (a\mathfrak{g}(z)(x,y,r,\xi))$$

$$\langle \Omega \rangle_{\mathfrak{G}}(z) := \lim_{T \to \infty + i0^+} \frac{\zeta(U(0,T)\mathfrak{G}\Omega)}{\zeta(U(0,T)\mathfrak{G})}(z)$$

$$\langle \Omega \rangle := \langle \Omega \rangle_{\zeta} := \langle \Omega \rangle_{\mathfrak{G}}(0)$$

- path integral well defined
- physical meaning of ζ regulated vacuum expectation value?

Example Dirac operator

- free fermions (in 3+1 dimensions)

$$H = \begin{pmatrix} mc^2 & -i\hbar\sigma_k\partial_k \\ -i\hbar\sigma_k\partial_k & mc^2 \end{pmatrix} \sim \begin{pmatrix} mc^2 & \hbar r\sigma_k\xi_k \\ \hbar r\sigma_k\xi_k & mc^2 \end{pmatrix}$$

- holomorphic extension

$$\mathfrak{g}(z)(x, r, \xi) = r^z$$

- applying the integral kernel

$$\langle H \rangle = \lim_{T\to\infty} \lim_{z\to 0} \frac{\int d\Omega \int dr \left(4mc^2 \cos(Tr) - 4ir \sin(Tr)\right) r^{z+2}}{\int d\Omega \int dr 4 \cos(Tr) r^{z+2}}$$

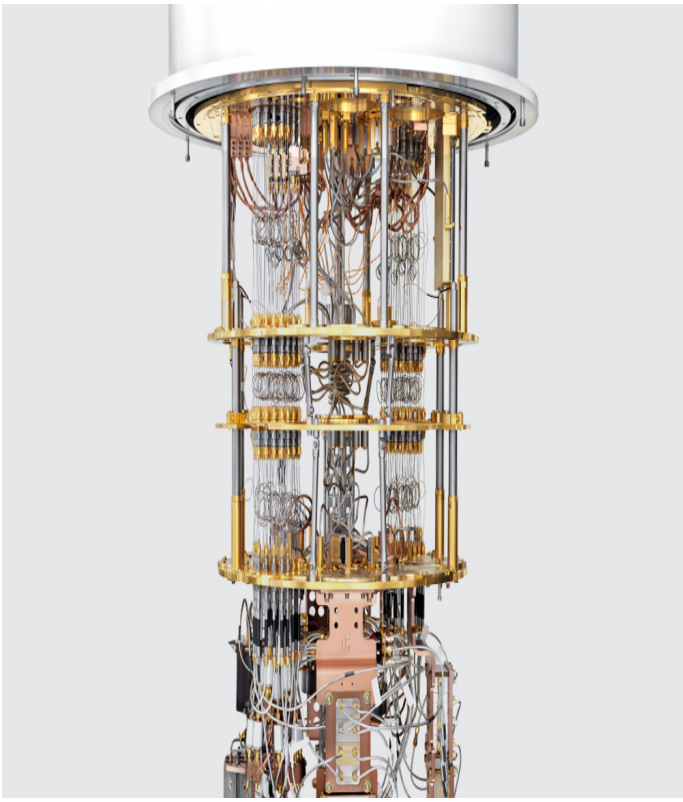
- evaluating the integral (see T. Hartung, K.J., arXiv:1902.09926)

$$\langle H \rangle = mc^2 - \lim_{T\to\infty} \lim_{z\to 0} \frac{\int dr 4ir \sin(Tr) r^{z+2}}{\int dr \cos(Tr) r^{z+2}} = mc^2$$

zeta-regularized vacuum exptectation values

- give mathematical meaning to Feynman's trace formula
  (Tobias Hartung, J. Math. Phys. 2017)
- provided proof that $\langle\Omega\rangle_\zeta$ *is physical vacuum expectation value*
  (Tobias Hartung, K.J., arXiv:1808.06784, arXiv:1902.09926)
- advantage of ζ-regularization
  - defined in the continuum (although lattice setup included)
  - comprises Minkowski space
  - holds for any metric
- $\Rightarrow$ solves sign problem:
  chemical potential, topological term, real time, curved space, ...
- how to apply this in practice?

An existing quantum computer: Rigetti's Aspen line



- Shielded to 50,000 times less than Earths magnetic field
- In a high vacuum: pressure is 10 billion times lower than atmospheric pressure
- Cooled 180 times colder than interstellar space (0.015 Kelvin)

$\rightarrow$ prevent decoherence

- qubits based based on Josephson junction*
- application of unitary gate operations

$\rightarrow$ generate entanglement

- 200 I/O and control lines from room temperature to the chip
- System consumes less than 25 kW of power

$\star$ *A Josephson junction is formed by two superconducting regions that are separated by a very thin insulating barrier*

Discretization scheme

- projection onto finite dimensional subspaces
  $\rightarrow$ needed for proof and practical application
  - target Hilbert space: $\mathcal{H}$
  - construct Hilbert space $\mathcal{H}_1$: dense in $\mathcal{H}$
    $\leftarrow$ acts in Sobolov-space where $\mathfrak{G}$ is well defined
- use projections on $\mathcal{H}$

$$P_n : \varphi \mapsto \sum_{j=0}^{n-1} \langle e_j, \varphi \rangle_{\mathcal{H}} \, e_j$$

- use projections on $\mathcal{H}_1$
  $\rightarrow$ Q_n: orthogonal projection onto $P_n[\mathcal{H}]$ in $\mathcal{H}_1$
- discretizing observable: $\Omega_n := P_n \Omega Q_n$ same for $(\mathfrak{G}(z)\Omega)_n$
- disretizing time evolution operator

$$U_n := \operatorname{texp}\left(-\frac{i}{\hbar}\int_0^T P_n H(s) Q_n ds\right)$$

  same for $(U\mathfrak{G}(z))_n$

Main result

- obtain physical expectation value

$$
\begin{aligned}
\langle \psi | \Omega | \psi \rangle &= \lim_{n\to\infty} \langle \psi_n, \Omega_n \psi_n \rangle_{\mathcal{H}} \\
&= \lim_{n\to\infty} \frac{\langle (\mathfrak{G}(0)\Omega)_n \rangle}{\langle \mathfrak{G}(0)_n \rangle} \\
&= \lim_{T\to\infty+i0^+} \frac{\zeta(U(0,T)\mathfrak{G}\Omega)}{\zeta(U(0,T)\mathfrak{G})}(0) \\
&= \langle \Omega \rangle_\zeta
\end{aligned}
$$

Example: hydrogen atom

- Hamiltonian

$$H = -\frac{\partial^2}{2m} + U(x)\ , \quad U = \begin{cases} x & ; x \in (0,\pi) \\ 0 & ; x \in (-\pi, 0] \end{cases}$$

- Hilbert space: $L_2(-\pi,\pi)$ with discretization

$$\varphi_k(x) := \frac{1}{\sqrt{2\pi}} e^{ikx}$$

- orthogonal projection

$$P_n[\mathcal{H}] = \mathrm{lin}\,\{\varphi_k; -n \le k \le n-1\}$$

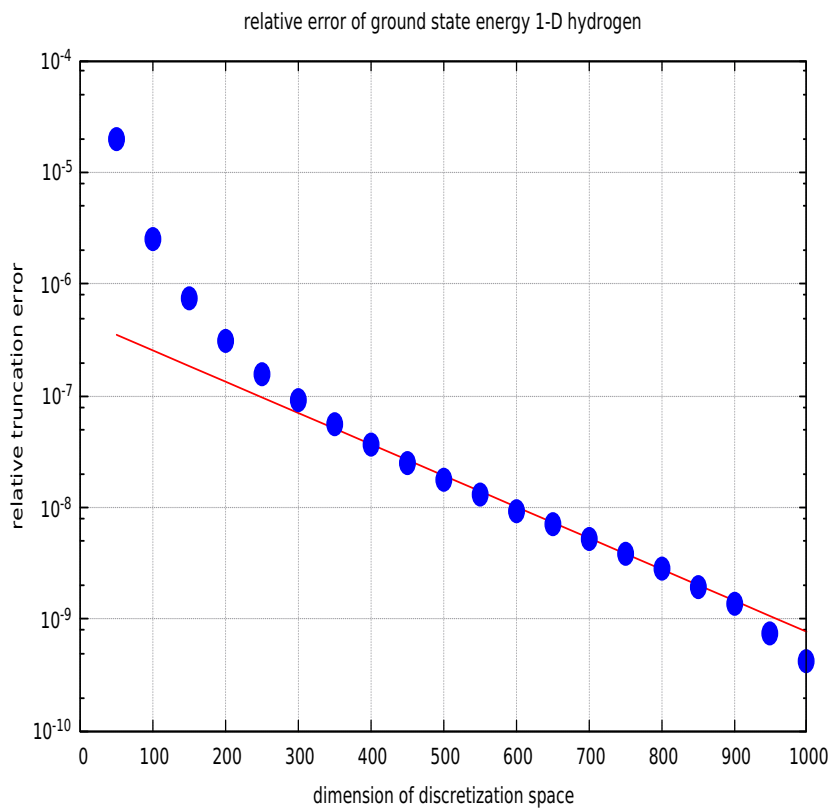
- matrix elements (for $m = 1$)

$$\langle \varphi_l, H\varphi_k \rangle = \frac{\left((-1)^{k-l}(1-i\pi(k-l))-1\right)}{2\pi(k-l)^2}$$

Truncation error

- exact diagonalization of matrix with elements

$$\langle \varphi_l, H\varphi_k \rangle = \frac{\left((-1)^{k-l}(1-i\pi(k-l))-1\right)}{2\pi(k-l)^2}$$



- relative error $\frac{E(j)-E(1024)}{E(1024)}$
- blue points: exact diagonalization
- red line: exponential fit
- find exponentially fast convergence

Hamiltonian for quantum computation

- the qubit Hamiltonian

$$H_q := \langle e_j, H e_k \rangle_{j,k \in 2^Q}$$

- Pauli basis $[(1), \sigma_x, \sigma_y, \sigma_z]$

$$\left\{ S^q = \sigma^{q_{Q-1}} \otimes \sigma^{q_{Q-2}} \otimes \ldots \otimes \sigma^{q_0}; q \in 4^Q \right\}$$

- projecting H_q onto Pauli basis

$$H_Q = \sum_{q \in 4^Q} \frac{\mathrm{tr}\left(H_q S^q\right)}{2^Q} S^q$$

Variational quantum simulation

- start with some initial state $|\Psi_{\text{init}}\rangle$
- apply succesive gate operations $\equiv$ unitary operations $e^{-iS\theta}$
- examples for S: σ_x, σ_y, σ_z, parametric CNOT

$$|\Psi(\vec{\theta})\rangle = e^{-iS_{(n)}\theta_n} \dots e^{-iS_{(1)}\theta_1} |\psi_{\text{init}}\rangle$$

- with $R_j := e^{-iS_{(j)}\theta_j}$ we obtain cost function

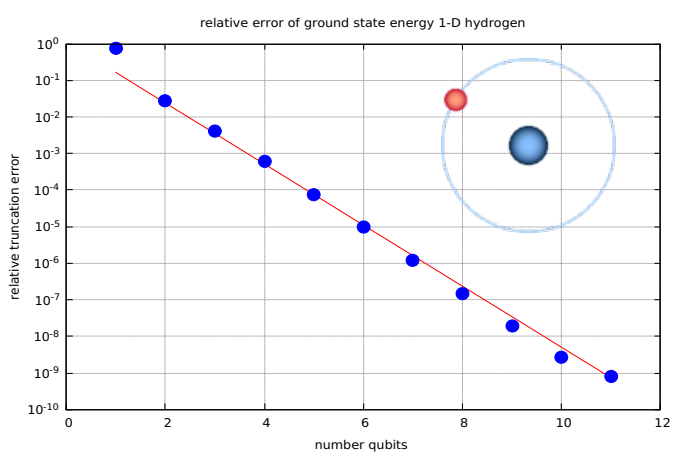
$$C := \left\langle \psi_{\text{init}} \middle| \left(\prod_{j=1}^n R_j\right)^\dagger H \prod_{j=1}^n R_j \middle| \psi_{\text{init}} \right\rangle$$

- goal: minimize C over the angles $\vec{\theta}$
  $\rightarrow$ obtain minimal energy, i.e. ground state
- in original paper:
  - minimization on classical computer
  - minimize over one angle at a time
  - loop several times over the complete set of angle

Simulation

- noise free simulation on Rigetti's QVM

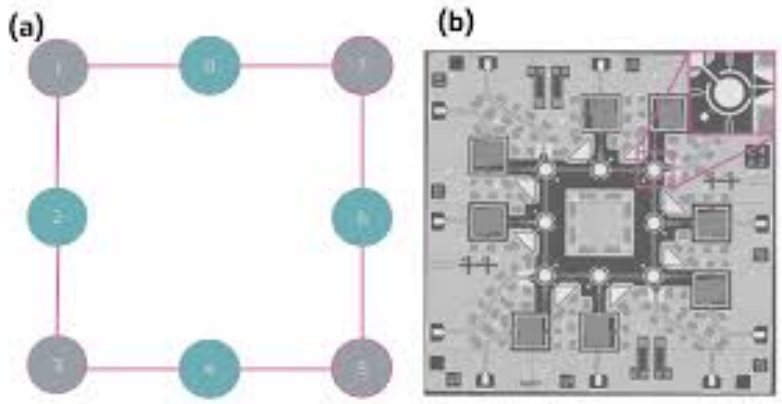
Q qubits	min. eig. H_Q	$\langle \psi_{2^Q}, H_Q \psi_{2^Q} \rangle$
1	.392108816647	.392108816647
2	.229395425745	.229395425968
3	.224258841712	.224258841747
4	.223452200306	.223452200445
5	.223336689755	.223336690423



- relatice error $\Delta E = \frac{E(q) - E(q{=}12)}{E(q{=}12)}$
- blue points: quantum simulator results
- find exponentially fast convergence
- line: fit $\Delta E(q) \approx 1.14 \cdot e^{-1.92q}$

Running on the Rigetti hardware

- Practical example: compute ground state energy of 1-dimensional hydrogen atom on Rigetti's 8-qubit Agave chip
  - performed variational quantum simulation



Agave chip

- hardware performance
  - select the qubit of the day
  - found gate fidelity $F_{1Q} = 0.982$, readout fidelity $F_{RO} = 0.94$
  - ground state energy with 4.9% error
  - more qubits: no significant result

Implement better algorithm

(T. Hartung, P. Stornati, KJ)

- new algorithm: quantum gradient descent
  - example for 2 unitaries, cost function:

$$C := \left\langle \psi_{\text{init}} \middle| \left(e^{i\sigma_x\theta_1} e^{i\sigma_y\theta_2}\right)^\dagger H e^{i\sigma_x\theta_1} e^{i\sigma_y\theta_2} \middle| \psi_{\text{init}} \right\rangle$$

  - derivative D of $R = e^{i\sigma_x\theta_1} e^{i\sigma_y\theta_2}$

    $D = (\frac{\partial R}{\partial \theta_1}, \frac{\partial R}{\partial \theta_2})$
  - obtain gradient of cost function

$$\partial/\partial\theta_1 C = \left\langle \psi_{\text{init}} \middle| \left(e^{i\sigma_x\theta_1} e^{i\sigma_y\theta_2}\right)^\dagger \left[H i\sigma_x^\dagger + i\sigma_x H\right] e^{i\sigma_x\theta_1} e^{i\sigma_y\theta_2} \middle| \psi_{\text{init}} \right\rangle$$

- can re-use generated state vector, measure $H i\sigma_x^\dagger + i\sigma_x H$
- obtain new vector of angles: $\vec{\theta}^{\text{new}} := \vec{\theta}^{\text{old}} - \eta \nabla C \left(\vec{\theta}^{\text{old}}\right)$
- tune "learning rate" η

Generalization

- general form of the quantum gradient descent algorithm
  - cost function, $R_j = e^{iS_{(j)}\theta_j}$

$$C := \left\langle \psi_{\text{init}} \middle| \left(\prod_{j=1}^{n} R_j\right)^{\dagger} H \prod_{j=1}^{n} R_j \middle| \psi_{\text{init}} \right\rangle$$

  - define derivative operator

$$D_k := \left(\prod_{j=k+1}^{n} R_j\right) R_k' \left(\prod_{j=k+1}^{n} R_j\right)^{\dagger}$$

  - express CNOT gate in Pauli matrices

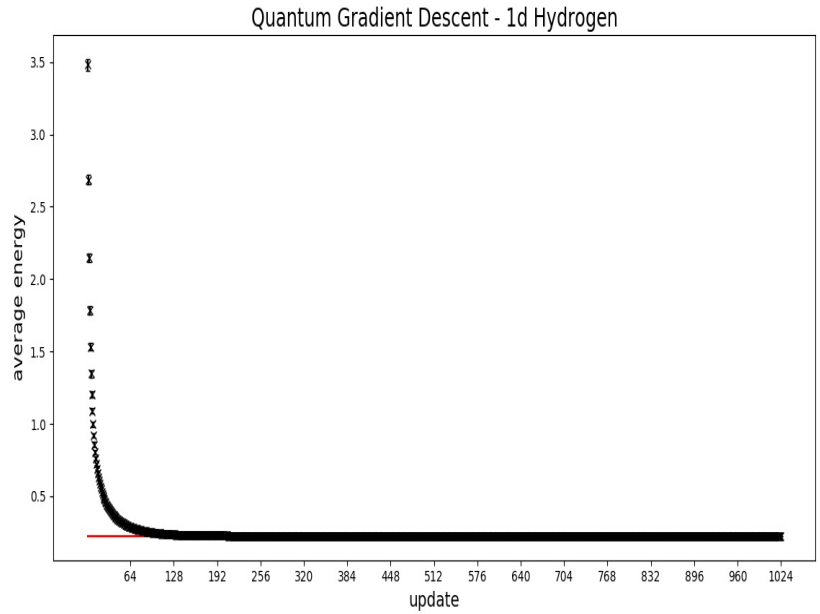
$$CNOT_{1\to 2} = \frac{\mathbb{1}_1 + \sigma_1^z}{2} \otimes \mathbb{1}_2 + \frac{\mathbb{1}_1 - \sigma_1^z}{2} \otimes \sigma_2^x$$

  - obtain kth-component of gradient

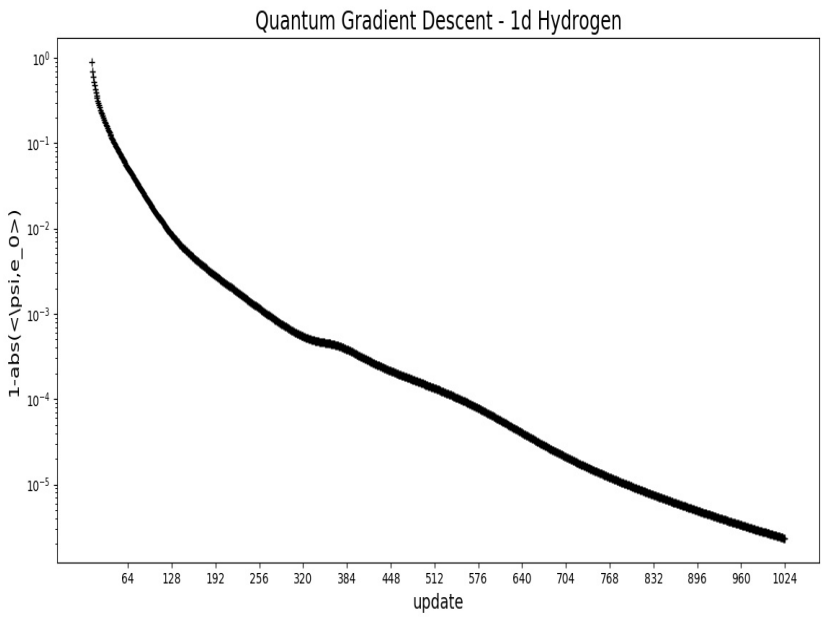
$$\partial_k C = \left\langle \prod_{j=1}^{n} R_j \psi_{\text{init}} \middle| HD_k + (HD_k)^{\dagger} \middle| \prod_{j=1}^{n} R_j \psi_{\text{init}} \right\rangle$$

- can re-use generated state vector, measure $HD_k + (HD_k)^{\dagger}$
- obtained new vector of angles: $\vec{\theta}^{new} := \vec{\theta}^{old} - \eta \nabla C \left(\vec{\theta}^{old}\right)$

Testing the algorithm



- average energy
  - simulator
  - no noise
  - 3 qubits
  - red line: exact result

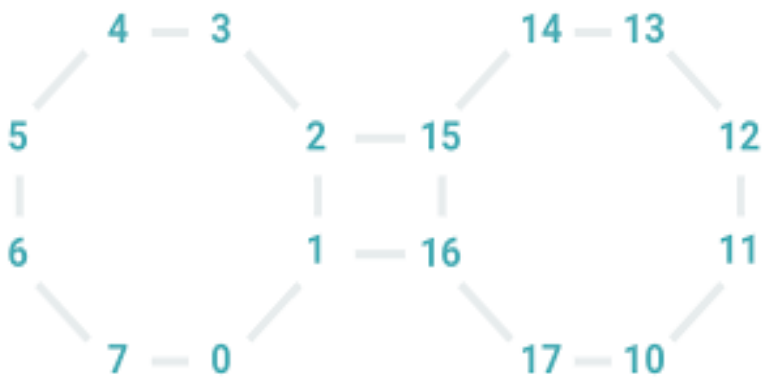


- distance to groundstate
- $|1 - \langle \Psi(j) | \Psi_0 \rangle|$

  Ψ_0 ground state wave function

New hardware

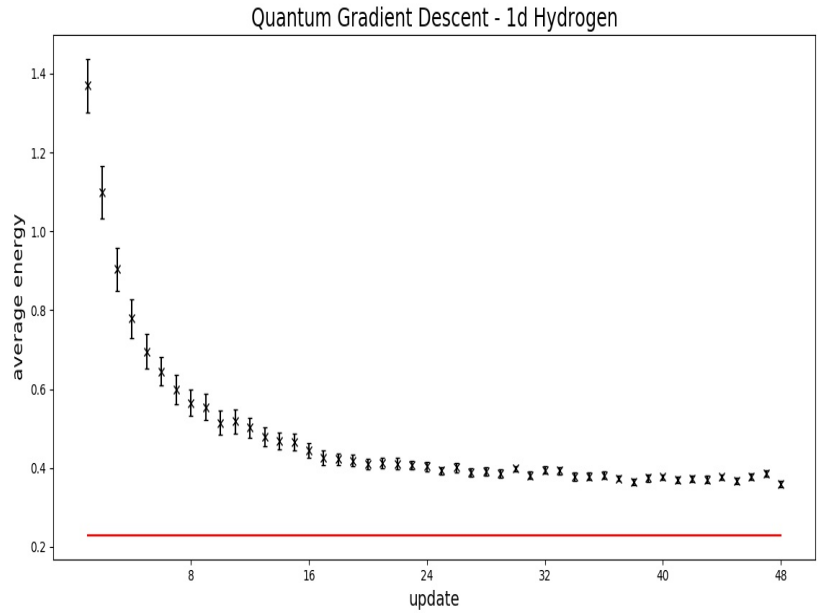
- new hardware: Aspen line (up to 128 qubits)



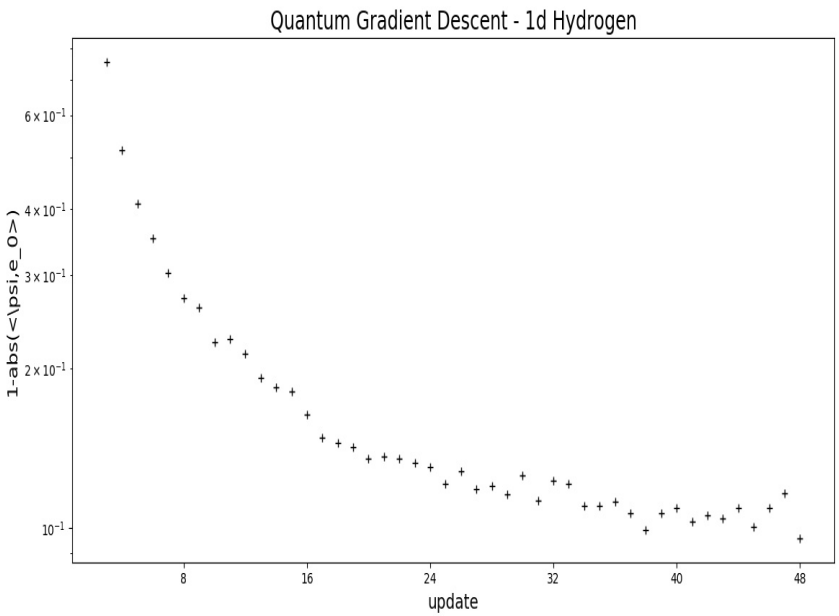
Aspen layout

- Rigetti's setup
  - Quantum Cloud Service
  - Pyquil (Python based) program enviroment
  - mean single qubit fidelity 95.5%

Running on Rigetti's Aspen hardware



- average energy
  - 2 qubits
  - red line: exact result
  - 60% fidelity



- distance to groundstate
- 90% fidelity
- reaching machine precision

Remarks

- with new hardware and better algorithm
  from impossible (2 qubits) $\rightarrow$ 90% fidelity for ground state

- still, 3 qubits: no significant result

- quantum gradient descent very expensive
  - justified for 1-d hydrogen atom (expensive itself)
  - for local Hamiltonians (e.g. Heisenberg)
    $\rightarrow$ need better algorithm (... and we are working on this)
    $\rightarrow$ can reach O(10) qubits

- quantum simulations of Schwinger model on real hardware
  - E.A. Martinez et.al., Nature 534 (2016) 516 (trapped ions)
  - N. Klco et.al., Phys.Rev. A98 (2018) no.3, 032331 (IBMQ)
  - C. Kokail et.al., Nature 569 (2019) no.7756, 355 (trapped ions, > 10 qubits)

Summary

- have a mathematically rigorous formulation of Feynman's path integral
  - in the continuum
  - in a Lorentzian background
  - non-perturbatively
  - providing physical vacuum expectation values
- have discretization schemes
  - that converge to physical vacuum expectation value
  - can be implemented on a quantum computer
- gave example of 1-d hydrogen atom on Rigetti's hardware
- this is fascinating, but there is a lot to do
  - need better hybrid classical-quantum algorithms
  - need better hardware
- need to explore better the ζ-regularization framework
  $\rightarrow$ more applications