Title: The Quantum Approximate Optimization Algorithm and spin chains

Speakers: Glen Mbend

Collection: Machine Learning for Quantum Design

Date: July 09, 2019 - 2:30 PM

URL: http://pirsa.org/19070079

Abstract: Various optimization problems that arise naturally in science are frequently solved by heuristic algorithms. Recently, multiple quantum enhanced algorithms have been proposed to speed up the optimization process, however a quantum speed up on practical problems has yet to be observed. One of the most promising candidates is the Quantum Approximate Optimization Algorithm (QAOA), introduced by Farhi et al. I will then discuss numerical and exact results we have obtained for the quantum Ising chain problem and compare the performance of the QAOA and the Quantum Annealing algorithm. I will also briefly describe the landscape that emerges from the optimization problem and how techniques borrowed from machine learning can be used to improve the optimization process.

Quantum Approximate Optimization Algorithm in spin chains

Glen Bigan Mbeng

Machine learning for quantum design, Waterloo

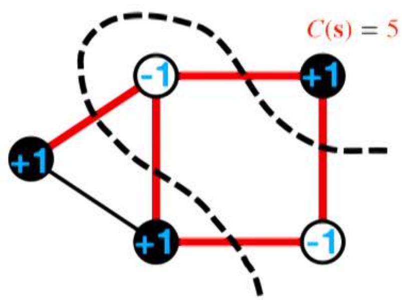
9th July, 2019

SISSA

Classical Optimization

Minimization of a cost function H(**s**): **Single valued** function of **discrete** variables with many local minima

Classical optimization
(MaxCut Problem)



$$H_{cl}(\mathbf{s}) = -C(\mathbf{s}) = -\sum_{\langle i,j \rangle} \frac{1}{2}(1 - s_i s_j)$$

NP-hard problem

Approximation Algorithms

Approximate solution $\mathbf{s}^* = (s_1^*, s_2^*, \ldots)$

Residual energy (or fractional error) $e_{res} \in [0,1]$

$$e_{res}(s_1^*, s_2^*, \ldots) = \frac{H_{cl}(s_1^*, s_2^*, \ldots) - \min_{\mathbf{s}} H_{cl}(\mathbf{s})}{|\min_{\mathbf{s}} H_{cl}(\mathbf{s})|}$$

Best classical result (Goemans and Williamson algorithm)

$$e_{res}^* < 0.13$$

Can Quantum Algorithms do better?

Analog Quantum Annealing (QA)

$s_i \to \hat{\sigma}_i^z$

$$\widehat{H}_z = H_{cl}(\hat{\sigma}_1^z, \hat{\sigma}_2^z, \ldots) = -\sum_{\langle i,j \rangle} \frac{1}{2}(1 - \hat{\sigma}_i^z \hat{\sigma}_j^z)$$

Problem Hamiltonian E_{GS}?

$$\widehat{H}_x = -\sum_i \hat{\sigma}_i^x$$

Driving auxiliary Hamiltonian (quantum fluctuations)

$$\widehat{H}(t) = s(t)\,\widehat{H}_z + (1 - s(t))\,\widehat{H}_x$$

Time dependent Hamiltonian

$$s(t) = \frac{t}{\tau}$$

Linear schedule (simple but not optimal)

annealing time

$|\psi_0\rangle$

$|\rightarrow\rangle$ $|\rightarrow\rangle$ $|\rightarrow\rangle$ $|\rightarrow\rangle$ $|\rightarrow\rangle$

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle$$

$$|\psi^*\rangle = |\psi(\tau)\rangle$$

$$e^*_{res}(\tau)$$

Relies on the **adiabatic theorem**

$$\tau \gg 1/\Delta^2 \implies e_{res} \to 0$$

For hard problems $\Delta \to 0$

[Kadowaki and Nishimori (1998)]

Quantum Approximate Optimization Algorithm

$s_i \to \hat{\sigma}_i^z$

$$\widehat{H}_z = H_{cl}(\hat{\sigma}_1^z, \hat{\sigma}_2^z, \dots) = -\sum_{\langle i,j \rangle} \frac{1}{2}(1 - \hat{\sigma}_i^z \hat{\sigma}_j^z)$$

Problem Hamiltonian E_{GS}?

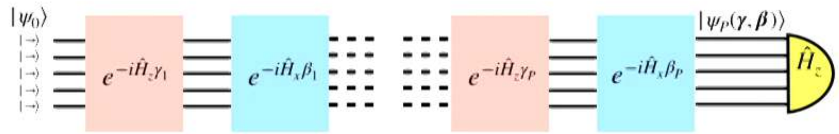
$$\widehat{H}_x = -\sum_i \hat{\sigma}_i^x$$

Driving auxiliary Hamiltonian (quantum fluctuations)

$$e^{-\frac{i}{\hbar}\widehat{H}(s_m)\Delta t_m} \simeq e^{-\frac{i s_m \Delta t_m}{\hbar}\widehat{H}_z} e^{-\frac{i(1-s_m)\Delta t_m}{\hbar}\widehat{H}_x}$$

Digital simulation (Trotter decomposition)

$$\gamma_m = s_m \Delta t_m / \hbar$$
$$\beta_m = (1 - s_m)\Delta t_m / \hbar$$



Perform **classical optimization**
on **2P parmeters**

$$E_P(\boldsymbol{\gamma}, \boldsymbol{\beta}) = \langle \psi_P(\boldsymbol{\gamma}, \boldsymbol{\beta}) | \hat{H}_z | \psi_P(\boldsymbol{\gamma}, \boldsymbol{\beta}) \rangle$$

$$\boldsymbol{\gamma}^*, \boldsymbol{\beta}^*$$
$$|\psi^*\rangle = \psi_P(\boldsymbol{\gamma}^*, \boldsymbol{\beta}^*)\rangle$$

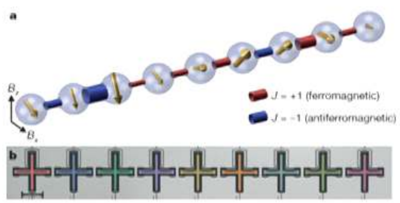
[E. Farhi, *et al*, arXiv:1411.4028 (2014)]
[W. W. Ho and T. H. Hsieh, SciPost Phys. (2019)]

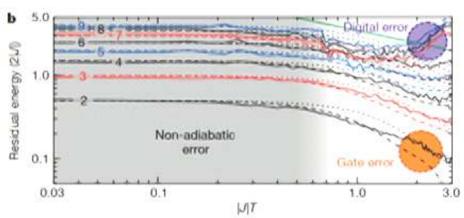
Why QAOA?

- **Low depth QAOA circuits can compete with classical algorithms**
  [E. Farhi et al ,arXiv:1412.6062 (2015)]
  [B. Barak arXiv:1505.03424 (2015)]

- **Experiments**

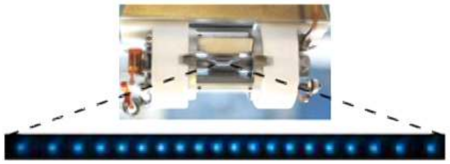
Digital Quantum Annealing

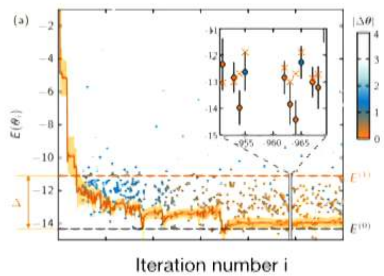




[Barends et al. *Nature*, (2016)]

Variational Quantum Simulation



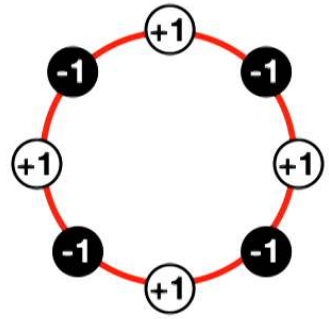


[Kokail, *et al. Nature* (2019)]

MaxCut 2-regular: Ising chain

$$\widehat{H}_z = \sum_{i=1}^{N} \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z$$

Antiferro Ising on an N-ring with PBC



$$E_{\max} = N$$

$$E_{\min} = -N$$

Trivial classical target state

$$\Phi^{\mathrm{cl}}_{\mathrm{target}} = (\uparrow, \downarrow \ldots, \uparrow, \downarrow)$$

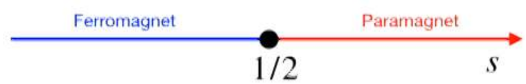
$$\Phi^{\mathrm{cl}}_{\mathrm{target}} = (\downarrow, \uparrow \ldots, \downarrow, \uparrow)$$

Non trivial quantum target state

$$|\psi_{\mathrm{target}}\rangle = \frac{1}{\sqrt{2}}(|\uparrow, \downarrow \ldots, \uparrow, \downarrow\rangle + |\downarrow, \uparrow \ldots, \downarrow, \uparrow\rangle)$$

$$\widehat{H} = s\,\widehat{H}_z + (1-s)\,\widehat{H}_x$$

Quantum phase transition



Variational Bound (preview)

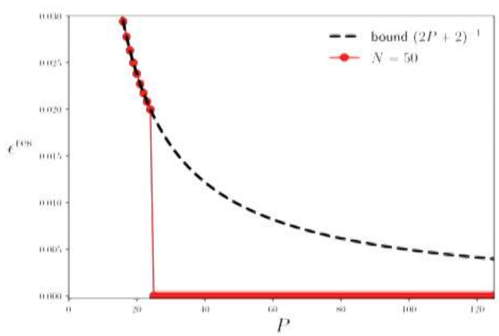
Emergence of the bound

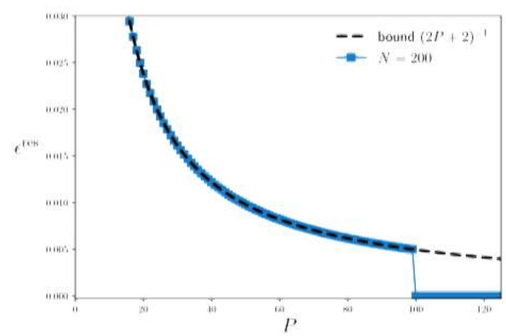
$$e_{\text{res}}(\gamma,\beta) = \frac{E_{\text{P}}(\gamma,\beta) - E_{\min}}{E_{\max} - E_{\min}}$$

$$e_{\text{res}}(\gamma,\beta) \geq \begin{cases} \frac{1}{2\text{P}+2} & 2\text{P} < N \\ 0 & 2\text{P} \geq N \end{cases}$$

- Locality
- Translational invariance

Jordan Wigner results





Variational Bound (preliminaries)

Translational invariance

$$e_{\rm res}(\boldsymbol{\gamma},\boldsymbol{\beta}) = \langle \psi_P(\boldsymbol{\gamma},\boldsymbol{\beta}) \,|\, \frac{\hat{\sigma}^z_{j_s}\hat{\sigma}^z_{j_s} + 1}{2} \,|\, \psi_P(\boldsymbol{\gamma},\boldsymbol{\beta})\rangle$$

Discrete time

$\hat{U}_m = \mathrm{e}^{-i\beta_m \widehat{H}_x}\,\mathrm{e}^{-i\gamma_m \widehat{H}_z}$ m = "*discrete*" time

$$|\,\psi_P(\boldsymbol{\gamma},\boldsymbol{\beta})\rangle = \hat{U}_P\cdots\hat{U}_1\,|\,\psi_0\rangle$$

Heisenberg representation

$$\langle \psi_P(\boldsymbol{\gamma},\boldsymbol{\beta})\,|\,\hat{\sigma}^z_{j_s}\hat{\sigma}^z_{j_s}\,|\,\psi_P(\boldsymbol{\gamma},\boldsymbol{\beta})\rangle = \langle \psi_0\,|\,\hat{U}_1^\dagger\cdots\hat{U}_P^\dagger\;\hat{\sigma}^z_{j_s}\hat{\sigma}^z_{j_s}\;\hat{U}_P\cdots\hat{U}_1\,|\,\psi_0\rangle$$

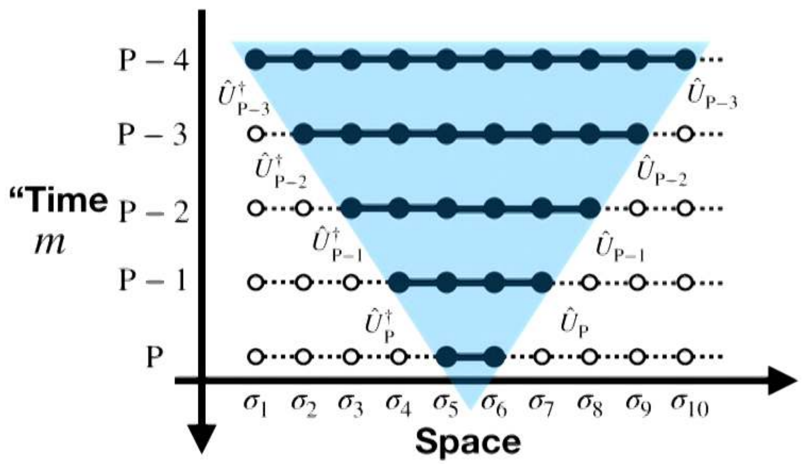
Reduced Chain

$$\langle\psi_0|\widehat{U}_1^\dagger\cdots\widehat{U}_{\mathrm{P}-1}^\dagger\widehat{U}_{\mathrm{P}}^\dagger\;\hat{\sigma}_5^z\hat{\sigma}_6^z\;\widehat{U}_{\mathrm{P}}\widehat{U}_{\mathrm{P}-1}\cdots\widehat{U}_1|\psi_0\rangle$$

$$\cdots\widehat{U}_{\mathrm{P}}^\dagger\;\hat{\sigma}_5^z\hat{\sigma}_6^z\;\widehat{U}_{\mathrm{P}}\cdots$$

$$\cdots\mathrm{e}^{i\gamma_{\mathrm{P}}\widehat{H}_z}\mathrm{e}^{i\beta_{\mathrm{P}}\widehat{H}_x}\;\hat{\sigma}_5^z\hat{\sigma}_6^z\;\mathrm{e}^{-i\beta_{\mathrm{P}}\widehat{H}_x}\mathrm{e}^{-i\gamma_{\mathrm{P}}\widehat{H}_z}\;\ldots$$

$$\cdots\mathrm{e}^{i\gamma_{\mathrm{P}}(\hat{\sigma}_4^z\hat{\sigma}_5^z+\hat{\sigma}_5^z\hat{\sigma}_6^z+\hat{\sigma}_6^z\hat{\sigma}_7^z)}\mathrm{e}^{i\beta_{\mathrm{P}}(\hat{\sigma}_5^x+\hat{\sigma}_6^x)}\;\hat{\sigma}_5^z\hat{\sigma}_6^z\;\mathrm{e}^{-i\beta_{\mathrm{P}}(\hat{\sigma}_5^x+\hat{\sigma}_6^x)}\mathrm{e}^{-i\gamma_{\mathrm{P}}(\hat{\sigma}_4^z\hat{\sigma}_5^z+\hat{\sigma}_5^z\hat{\sigma}_6^z+\hat{\sigma}_6^z\hat{\sigma}_7^z)}\;\ldots$$



Reduced spin chain:
at depth P, $N_s = 2P+2$

Boundary term is absent

Variational Bound

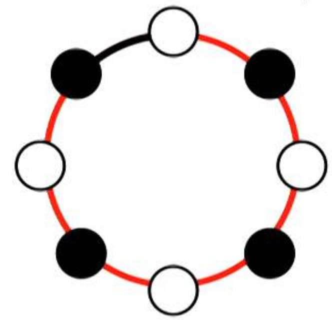
$$\hat{\mathscr{H}}_z = \sum_{j=1}^{N_s-1} \hat{\sigma}^z_j \hat{\sigma}^z_{j+1} \boxed{- \hat{\sigma}^z_1 \hat{\sigma}^z_{N_s}}$$

$$\hat{\mathscr{H}}_x = - \sum_{j=1}^{N_s} \hat{\sigma}^x_j$$

$$|\tilde{\psi}_P(\boldsymbol{\gamma},\boldsymbol{\beta})\rangle = \hat{\mathscr{U}}_P \cdots \hat{\mathscr{U}}_1 |\tilde{\psi}_0\rangle$$

$$e_{\rm res}(\boldsymbol{\gamma},\boldsymbol{\beta}) = \langle \tilde{\psi}_P(\boldsymbol{\gamma},\boldsymbol{\beta}) | \frac{\hat{\sigma}^z_{j_s} \hat{\sigma}^z_{j_s} + 1}{2} | \tilde{\psi}_P(\boldsymbol{\gamma},\boldsymbol{\beta})\rangle$$

ABC $N_s = 2\mathrm{P} + 2$



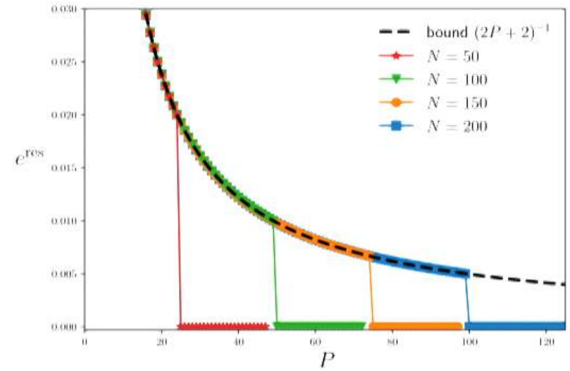
$$\mathscr{E}_{gs} = 2 - N_s$$

Translational invariance $$e_{\rm res}(\boldsymbol{\gamma},\boldsymbol{\beta}) = \langle \tilde{\psi}_P(\boldsymbol{\gamma},\boldsymbol{\beta}) | \frac{\hat{\mathscr{H}}_z}{2N_s} + \frac{1}{2} | \tilde{\psi}_P(\boldsymbol{\gamma},\boldsymbol{\beta})\rangle$$

Variational principle $$\boxed{e_{\rm res}(\boldsymbol{\gamma},\boldsymbol{\beta}) \geq \frac{\mathscr{E}_{gs}}{4\mathrm{P}+4} + \frac{1}{2} = \frac{1}{2\mathrm{P}+2}}$$

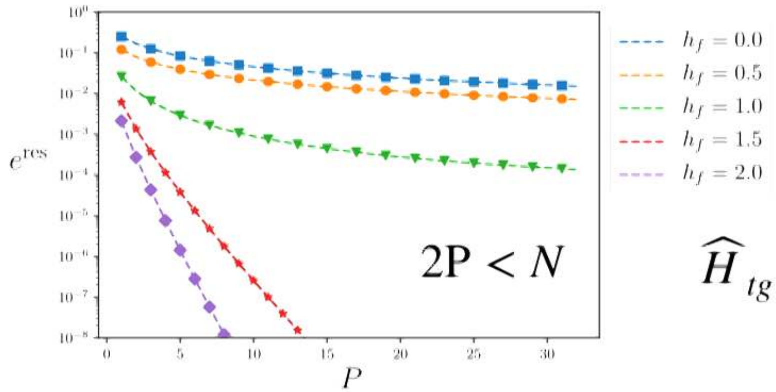
Jordan Wigner Results

$$e_{\text{res}}(\boldsymbol{\gamma},\boldsymbol{\beta}) = \begin{cases} \dfrac{1}{2\text{P}+2} & 2\text{P} < N \\ 0 & 2\text{P} \geq N \end{cases}$$



Ground state preparation

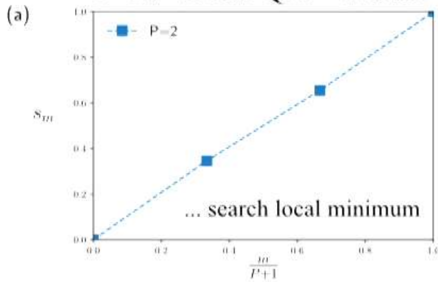
[W. W. Ho and T. H. Hsieh, SciPost Phys. (2019)]



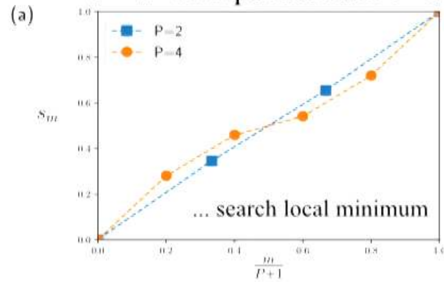
$$\widehat{H}_{tg} = \sum_{i=1}^{N} \hat{\sigma}^z_i \hat{\sigma}^z_{i+1} - h \sum_{i=1}^{N} \hat{\sigma}^x_i$$

Smooth solution learns to slow down

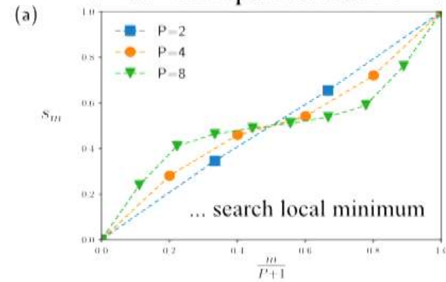
P=2: linear-QA + Trotter



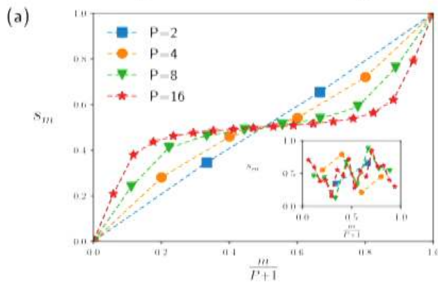
P=4: interpolate from P=2

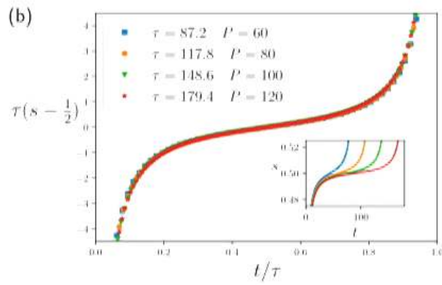


P=8: interpolate from P=4



... procede iteratively ....

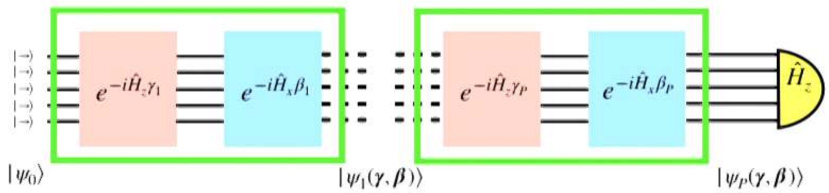




$$\begin{cases} \gamma_m = s_m \dfrac{\Delta t_m}{\hbar} \\ \beta_m = (1 - s_m) \dfrac{\Delta t_m}{\hbar} \end{cases}$$

Smooth ``*optimal solutions*'' can be constructed
No ``*spectral information*'' needed, it is learned from the data

Adiabatic nature of s(t)



$$|\psi_{m+1}(\boldsymbol{\gamma},\boldsymbol{\beta})\rangle = \widehat{U}_m|\psi_m(\boldsymbol{\gamma},\boldsymbol{\beta})\rangle$$

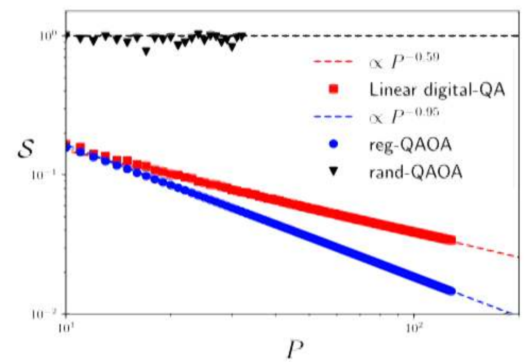
$$\widehat{U}_m|\theta_m\rangle = \mathrm{e}^{-i\theta_m}|\theta_m\rangle$$

``**Instantaneous**'' eigenvectors

Adiabaticity
only for *digital*-QA

$$p_{\boldsymbol{\gamma},\boldsymbol{\beta}}(\theta_m) = |\langle\theta_m|\psi_m(\boldsymbol{\gamma},\boldsymbol{\beta})\rangle|^2$$

$$\mathcal{S}_{\boldsymbol{\gamma},\boldsymbol{\beta}}(\mathrm{P}) = -\frac{1}{\mathrm{P}}\sum_{m=1}^{\mathrm{P}}\sum_{\theta_m} p_{\boldsymbol{\gamma},\boldsymbol{\beta}}(\theta_m)\log[p_{\boldsymbol{\gamma},\boldsymbol{\beta}}(\theta_m)]$$



Quantum Approximate Optimization Algorithm in spin chains

Glen Bigan Mbeng

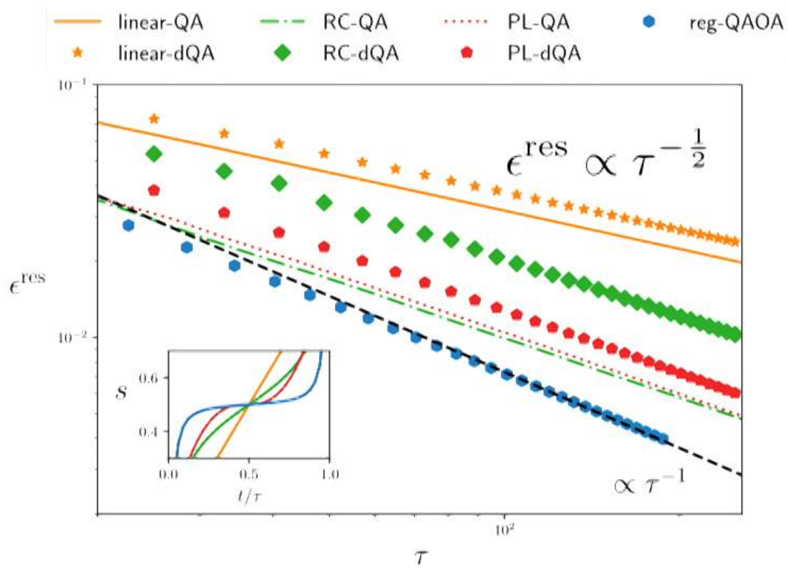
SISSA

Comparison to other adiabatic schedules s(t)

Quadratic speedup!
Optimal digital-QA

! Fully recursive: No spectral information needed

Dziarmaga, PRL **95**, 245701 (2005)
Roland & Cerf, PRA **65**, 042308 (2002)
Zurek, Dorner, and Zoller, PRL **95**, 105701 (2005)
Barankov & Polkovnikov, PRL **101**, 076801 (2008)

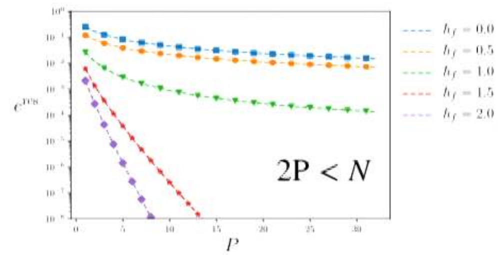


Open issues / ongoing work

- How special?
  - Higher dimensions? Non integrable models?
- Role of noise and disorder?
- Role of locality (Lieb-Robinson bound)?
  - Fully connected p-spin models

Summary

- Variational bound
  (Locality & playing with Boundary Conditions)



- Optimal digital-QA solutions can be constructed in the QAOA Ansatz

- No spectral info needed & speedup
  (even when cost for optimization is accounted)