


REAL-TIME SIMULATIONS OF THE QUANTUM APPROXIMATE OPTIMISATION ALGORITHM

With a circuit Hamiltonian model

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JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

The main question of this talk

- What happens if we execute the quantum approximate optimisation algorithm (QAOA) on two and three-qubit virtual quantum information processors or chips?

- Virtual in this context means that we model the processor by means of a circuit Hamiltonian model.

The QAOA a brief introduction:

- The QAOA is a hybrid variational algorithm which was proposed by Farhi, Goldstone and Gutmann (FGG).

- QAOA aims to maximise or minimise a cost function which is given by the expectation value $\langle \gamma, \beta | H_C | \gamma, \beta \rangle$ of a cost Hamiltonian H_C.

- The parameterised trail state $|\gamma, \beta\rangle = \prod_{p=1}^{P} e^{-i\beta_p \hat{H}_M} e^{-i\gamma_p \hat{H}_C} |+\rangle^N$ is obtained by implementing a circuit on a N qubit gate-based quantum computer.

- In total we have $2P$ parameters $\gamma = (\gamma_{p=1}, ..., \gamma_{p=P})$ and $\beta = (\beta_{p=1}, ..., \beta_{p=P})$.

The QAOA a brief introduction:

- For our simulations we use the Ising Hamiltonian $\hat{H}_C = \sum_i h_i \sigma_i^z + \sum_{i<j} J_{i,j} \sigma_i^z \otimes \sigma_j^z$ as our cost Hamiltonian.

- The second Hamiltonian $\hat{H}_M$ in the generator is defined as $\hat{H}_M = \sum_i -\sigma_i^x$.

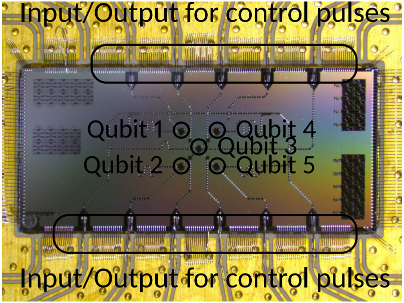
- In this talk, i and j are elements of the set $\{0, ..., N-1\}$.

- Once we have fixed the cost Hamiltonian, we need problems (in terms of parameters h_i and $J_{i,j}$) to solve with the QAOA.

Find the ground state of the Ising Hamiltonian under the following constrains

- (1) The problems have to fit to the hardware.
- (2) The two-qubit gates should be involved $J_{i,j} \neq 0$.
- (3) The problems should have a unique ground state (GS).
- (4) The pen and paper model should find the GS (GS prob. > 0.95).
- (5) The run times have to be reasonable, which means we can do about 50 cost function evaluations.
- (6) We need problems for different circuit depths, i.e. $P \in \{2, 3, 4, 5\}$.
- (7) All previous points should be satisfied for a fixed set of optimisation settings.

How do we model the virtual chips?

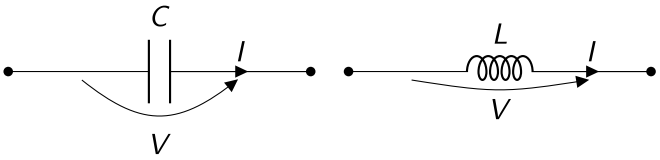


[1]

- We use a lumped-element model to describe the different components of the system and the connection between them.

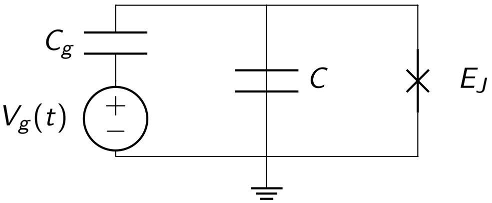
[1] With permission of Jonas Bylander from Chalmers University of Technology

The lumped-element model



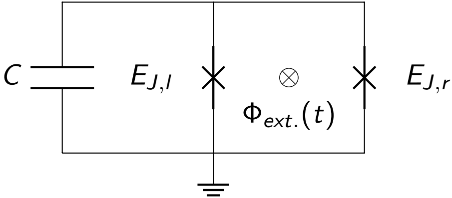
- We assume that all two-terminal elements, i.e. capacitors, inductors and Josephson junctions, can be described by a unique relation.
- This constitutive relation connects the current I flowing through the element and the voltage difference V at its two ports.
- Kirchhoff's laws provide relations which connect the different elements.
- Since we use the Hamiltonian formalism to quantise the circuit, we prefer to work with the flux variable $\hat{\varphi}$ and its conjugate charge variable $\hat{n}$, instead of the voltage V and the current I.

The fixed-frequency transmon



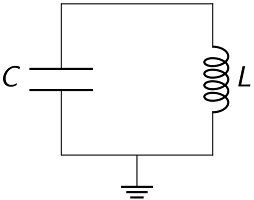
$$\hat{H}_{\text{Fix.}} = E_C \left(\hat{n} - n_g(t)\right)^2 - E_J \cos\left(\hat{\varphi}\right)$$

The flux-tunable transmon



$$\hat{H}_{\text{Tun.}} = E_C \hat{n}^2 - E_{J,l}\cos(\hat{\varphi}) - E_{J,r}\cos(\hat{\varphi} - \varphi(t))$$
$$\varphi(t) = \Phi_{ext.}(t)/\phi_0$$

The LC resonator



$$\hat{H}_{\text{Res.}} = \omega^R \hat{a}^\dagger \hat{a}$$

The complete model Hamiltonian

$$\hat{H}_{\text{Circuit}} = \hat{H}_{\text{Fix.},\Sigma} + \hat{H}_{\text{Tun.},\Sigma} + \hat{H}_{\text{Res.},\Sigma} + \hat{V}_{\text{Int.}}$$

$$\hat{H}_{\text{Fix.},\Sigma} = \sum_{i \in I} E_{C_i} \left(\hat{n}_i - n_{g,i}(t) \right)^2 - E_{J_i} \cos\left(\hat{\varphi}_i \right),$$

$$\hat{H}_{\text{Tun.},\Sigma} = \sum_{j \in J} E_{C_j} \left(\hat{n}_j - n_{g,j}(t) \right)^2 - E_{J_{l,j}} \cos\left(\hat{\varphi}_j \right) - E_{J_{r,j}} \cos\left(\hat{\varphi}_j - \varphi_j(t) \right),$$

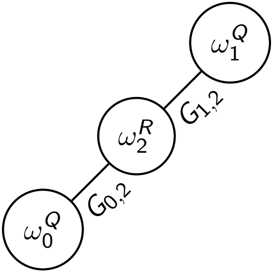
$$\hat{H}_{\text{Res.},\Sigma} = \sum_{k \in K} \omega_k^R \hat{a}_k^\dagger \hat{a}_k,$$

$$\hat{V}_{\text{Int.}} = \sum_{(i,i') \in I \times I'} G^{(0)}_{i,i'} \left(\hat{n}_i \otimes \hat{n}_{i'} \right) + \sum_{(j,i) \in J \times I} G^{(1)}_{j,i} \left(\hat{n}_j \otimes \hat{n}_i \right)$$

$$+ \sum_{(j,j') \in J \times J'} G^{(2)}_{j,j'} \left(\hat{n}_j \otimes \hat{n}_{j'} \right) + \sum_{(k,i) \in K \times I} G^{(3)}_{k,i} \left(\hat{a}_k + \hat{a}_k^\dagger \right) \otimes \hat{n}_i$$

$$+ \sum_{(k,j) \in K \times J} G^{(4)}_{k,j} \left(\hat{a}_k + \hat{a}_k^\dagger \right) \otimes \hat{n}_j + \sum_{(k,k') \in K \times K'} G^{(5)}_{k,k'} \left(\hat{a}_k + \hat{a}_k^\dagger \right) \otimes \left(\hat{a}_{k'} + \hat{a}_{k'}^\dagger \right)$$

The two-qubit system



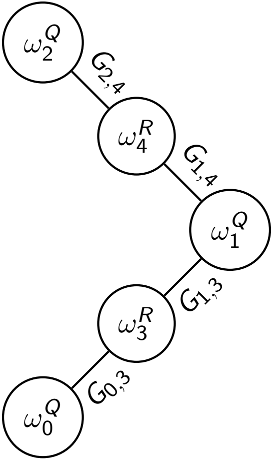
The two-qubit device parameters in GHz

i	$\omega_i^R/2\pi$	$\omega_i^Q/2\pi$	$\alpha_i/2\pi$	$E_{C_i}/2\pi$	$E_{J_i,l}/2\pi$	$E_{J_i,r}/2\pi$	$\varphi_{0,i}/2\pi$
0	n/a	4.200	-0.320	1.068	2.355	7.064	0
1	n/a	5.200	-0.295	1.037	3.612	10.837	0
2	45.000	n/a	n/a	n/a	n/a	n/a	n/a

$G_{0,2}/2\pi$	$G_{1,2}/2\pi$
0.300	0.300

- Note that throughout this talk all flux offsets $\varphi_{0,i}$ are given in units of the flux quantum ϕ_0.

The three-qubit system



The three-qubit device parameters in GHz

i	$\omega_i^R/2\pi$	$\omega_i^Q/2\pi$	$\alpha_i/2\pi$	$E_{C_i}/2\pi$	$E_{J_i,l}/2\pi$	$E_{J_i,r}/2\pi$	$\varphi_i/2\pi$
0	n/a	4.200	-0.320	1.068	2.355	7.064	0
1	n/a	5.200	-0.295	1.037	3.612	10.837	0
2	n/a	5.700	-0.285	1.017	4.374	13.122	0
3	45.000	n/a	n/a	n/a	n/a	n/a	n/a
4	45.000	n/a	n/a	n/a	n/a	n/a	n/a

$G_{0,3}/2\pi$	$G_{1,3}/2\pi$	$G_{1,4}/2\pi$	$G_{2,4}/2\pi$
0.300	0.300	0.300	0.300

The control pulses

- Two-qubit CZ gates are implemented with unimodal flux control pulses

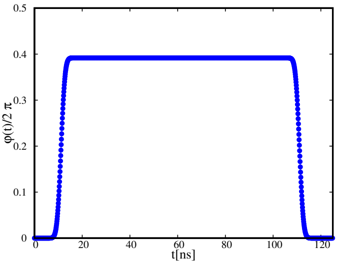
$$\varphi_j(t) = \frac{\delta}{2}\left(\operatorname{erf}\left(\frac{t}{\sqrt{2}\sigma}\right) - \operatorname{erf}\left(\frac{tT_p}{\sqrt{2}\sigma}\right)\right).$$

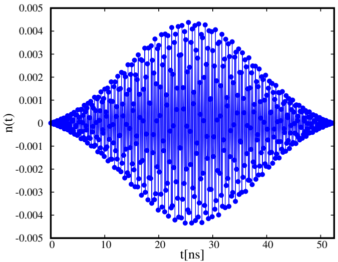
- Note that throughout this talk all pulse amplitudes δ are given in units of the flux quantum ϕ_0.
- Single-qubit $R_X(\pi/2)$ rotations are implemented with charge control pulses

$$n_{i/j}(t) = a\frac{\exp\left(\frac{(2t-T_d)^2}{8\sigma^2}\right) - \exp\left(\frac{T_d^2}{8\sigma^2}\right)}{1-\exp\left(\frac{T_d^2}{8\sigma^2}\right)}\cos\left(\tilde{\omega}t-\gamma\right).$$

- The DRAG component is not shown here (the corresponding pulse parameter is refered to as β).

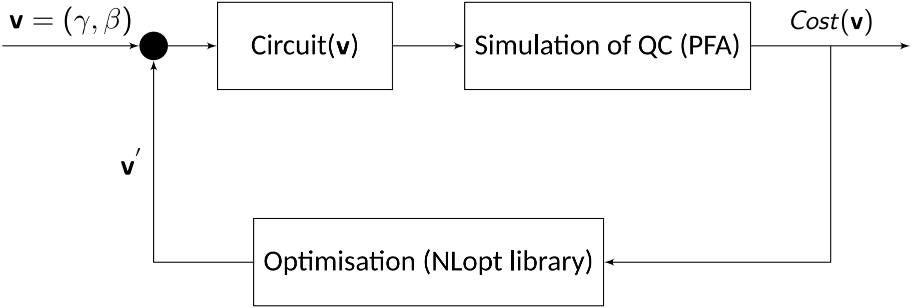
The control pulses





- Flux control pulse (left panel) and charge control pulse (right panel).

QAOA program structure



- PFA = Product Formula Algorithm (solves the TDSE for $\hat{H}_{\text{Circuit}}$)

The classical optimisation algorithms

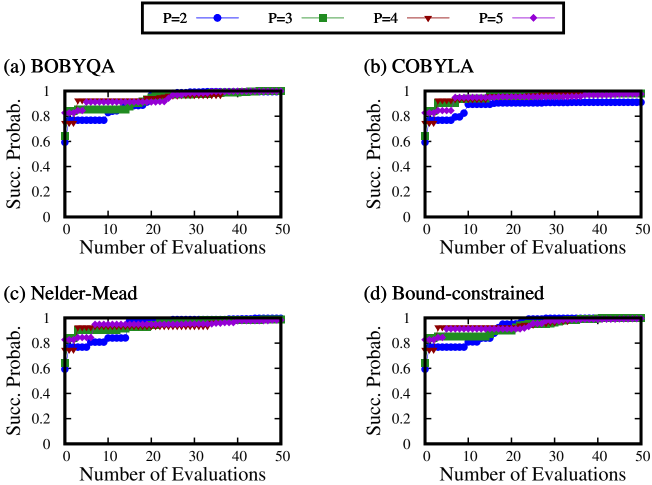
- For our simulations we use the NLopt library which contains more then ten gradient-free optimisation algorithms.
- BOBYQA = Bound Optimisation By Quadratic Approximation.
- COBYLA = Constrained Optimisation By Linear Approximations.
- Nelder-Mead = Simplex Method (considered good for noisy problems).
- Bound-constrained = Predecessor of BOBYQA.

Quality assessment of two-qubit chip

- The Frobenius square norm μ_{F^2}.
- The diamond norm $\mu_{\diamond}$
- The average infidelity $\mu_{\mathrm{IF_{avg}}}$
- A leakage measure μ_{Leak}

Pulse	μ_{F^2}	$\mu_{\diamond}$	$\mu_{\mathrm{IF_{avg}}}$	μ_{Leak}
$\mathrm{RX}(\pi/2)_0$	0.0002	0.0084	0.0004	0.0004
$\mathrm{RX}(\pi/2)_1$	0.0003	0.0108	0.0004	0.0004
$\mathrm{CZ}_{0,1}^{1}$	0.0008	0.0193	0.0014	0.0012

Results for the two-qubit chip



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Initialisation of γ and β with a linear annealing schedule

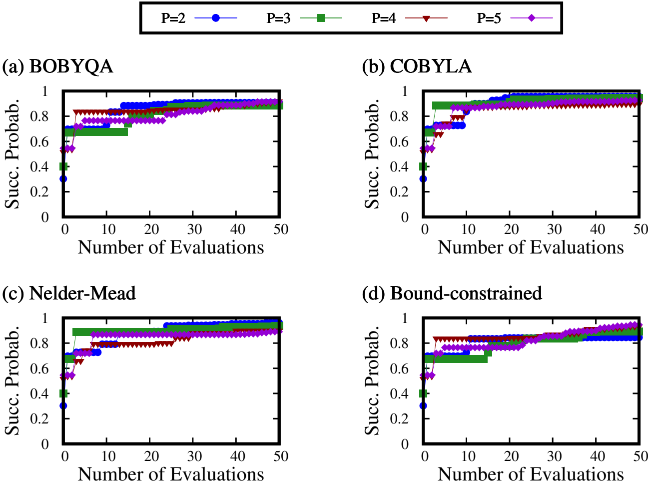
- Note that the initial success probability is quite high and grows with P.
- FGG's paper contains a section with the title: relation to the quantum adiabatic algorithm.
- We use the line of reasoning presented in this section to initialise the γ and β parameters with a linear annealing schedule.
- We expect to see that the initial success probability grows with the discrete variable P.

Quality assessment of the three-qubit chip

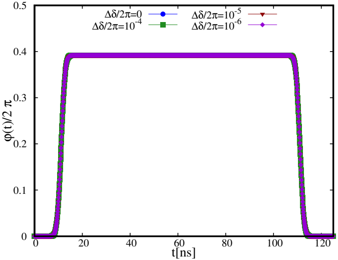
- The Frobenius square norm μ_{F^2}.
- The diamond norm $\mu_\diamond$
- The average infidelity $\mu_{\mathrm{IF_{avg}}}$
- A leakage measure μ_{Leak}

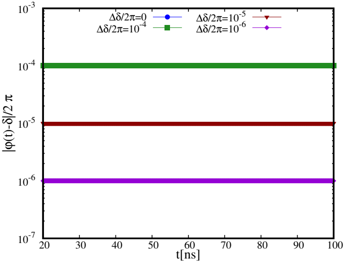
Pulse	μ_{F^2}	$\mu_\diamond$	$\mu_{\mathrm{IF_{avg}}}$	μ_{Leak}
$\mathrm{RX}(\pi/2)_0$	0.010	0.015	0.003	0.002
$\mathrm{RX}(\pi/2)_1$	0.006	0.013	0.002	0.001
$\mathrm{RX}(\pi/2)_2$	0.007	0.014	0.002	0.001
$\mathrm{CZ}_{0,1}^1$	0.008	0.049	0.010	0.010
$\mathrm{CZ}_{1,2}^2$	0.001	0.014	0.002	0.002

Results for the three-qubit chip



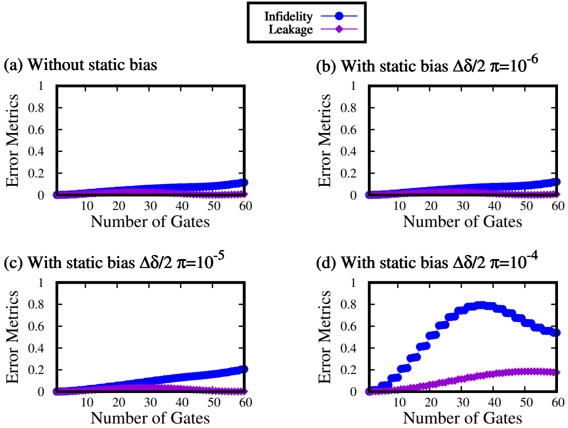
CZ gate flux control pulse for four different static biases $\Delta\delta$





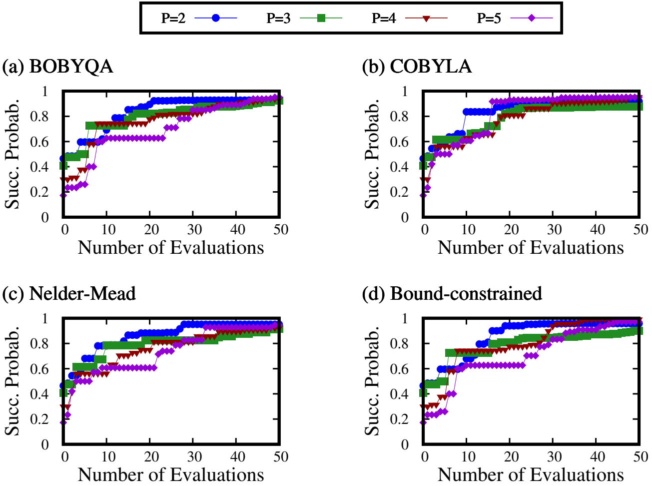
$$\varphi(t) = \frac{\delta + \Delta\delta}{2}\left(\mathrm{erf}\left(\frac{t}{\sqrt{2}\sigma}\right) - \mathrm{erf}\left(\frac{tT_p}{\sqrt{2}\sigma}\right)\right).$$

Twenty CNOT repetitions with the two-qubit chip for different static biases of the pulse amplitude δ



- The initial $CZ_{0,1}$ gate infidelity increases roughly from 0.001 without bias to 0.01 with bias $\Delta\delta/2\pi = 10^{-4}$.

Results for the two-qubit chip with static bias $\Delta\delta/2\pi = 10^{-4}$



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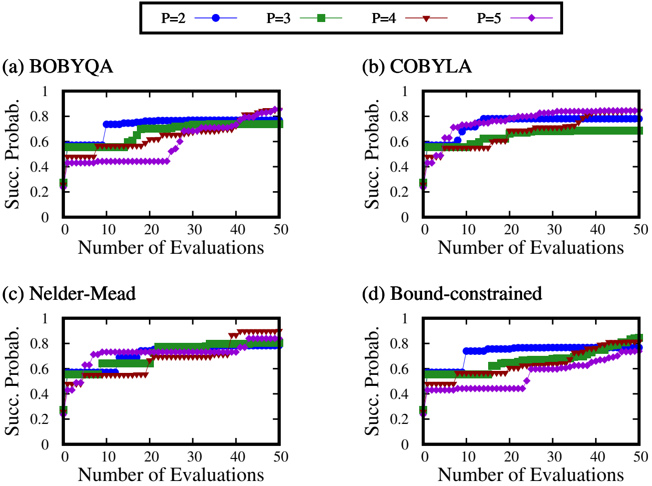
Results for the two-qubit chip with static bias $\Delta\delta/2\pi = 10^{-4}$

- Note that the initial success probability for $P = 5$ is now the lowest while the one for $P = 2$ is the highest.
- The carefully crafted parameter initialisation has lost its value.
- However, the overall performance for the given Ising problems and the optimisation settings is still quite good.

Results for the three-qubit chip with static bias $\Delta\delta/2\pi = 10^{-4}$



Final remarks regarding the results

- The results are only valid for the virtual chips we discussed and the circuit model!
- We performed simulations (data not shown) with other models, i.e. simpler models and/or different device architectures.
- The results can vary a lot for the same Ising problems and the same optimisation settings.
- This makes it very difficult to judge the QAOA.

Summary and conclusions

- We find that for the given problems and simulation settings the QAOA yields reasonably good results.
- We saw an example where QAOA was able to compensate for low-quality two-qubit gates.
- We deal with highly parameterised models which are difficult to understand.
- Therefore, we should not compare different devices by means of this algorithm.

Outlook

- Simulate different types of variational problems, i.e. different problem Hamiltonians (the software can do this already).

- Repeat the simulations with different types of circuit architectures and larger chips (these are already calibrated).

- Run the problems on the devices in the Jülich laboratory.

- Test different noise spectra for different devices.

The end

- Many thanks to the QIP group and Daniel Zeuch for useful comments regarding the talk!
- Thank you for your attention!

The problem at hand

- We would like to solve the TDSE numerically

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle .$$

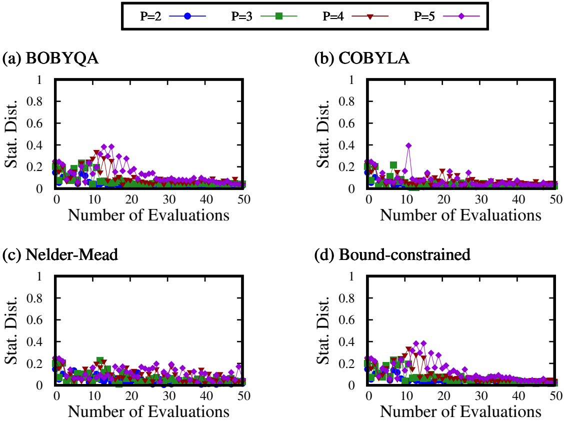
- The well known, formal solution to this problem reads

$$\hat{\mathcal{U}} = \mathcal{T}exp(-i\int_t^{t+\tau}\hat{H}(t^{'})dt^{'}).$$

- If we assume that $\tau \ll 1$ and $\hat{H}(t)$ is piecewise constant between two time steps t and $t+\tau$, we have

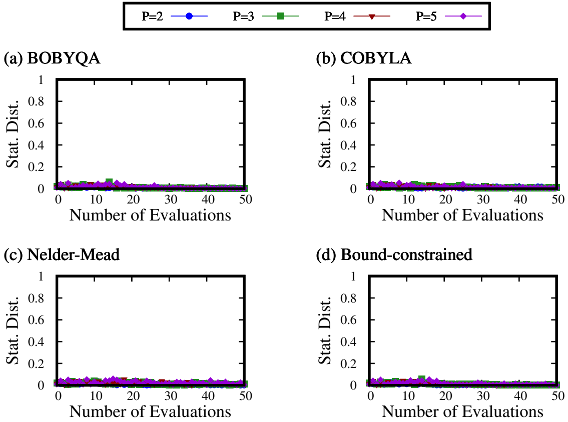
$$|\psi(t+\tau)\rangle = exp(-i\tau\hat{H}(t+\tau/2))|\psi(t)\rangle .$$

Results for the three-qubit chip



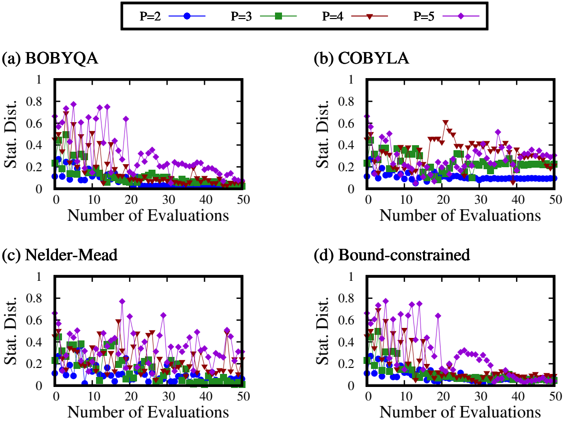
$$\text{Stat. Dist.} = \frac{1}{2} \sum_{\mathbf{z} \in \{0,1\}^N} \left| p_{\mathbf{z}}^{\text{PFA}} - p_{\mathbf{z}}^{\text{PAP}} \right|$$

Results for the two-qubit chip



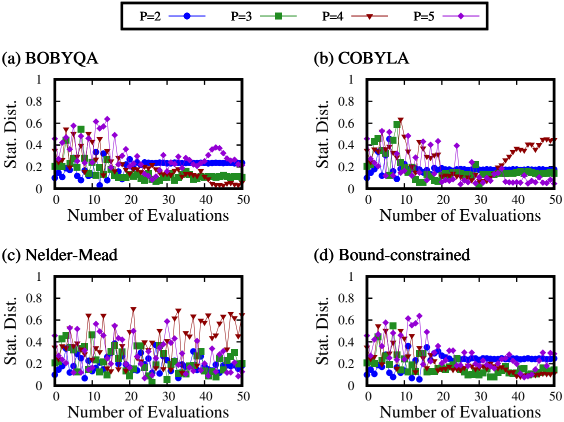
$$\text{Stat. Dist.} = \frac{1}{2} \sum_{\mathbf{z} \in \{0,1\}^N} \left| p_{\mathbf{z}}^{\text{PFA}} - p_{\mathbf{z}}^{\text{PAP}} \right|$$

Results for the two-qubit chip with static bias $\Delta\delta/2\pi = 10^{-4}$



$$\text{Stat. Dist.} = \frac{1}{2} \sum_{\mathbf{z}\in\{0,1\}^N} \left| p_{\mathbf{z}}^{\text{PFA}} - p_{\mathbf{z}}^{\text{PAP}} \right|$$

Results for the three-qubit chip with static bias $\Delta\delta/2\pi = 10^{-4}$



$$\text{Stat. Dist.} = \frac{1}{2} \sum_{\mathbf{z} \in \{0,1\}^N} \left| p_{\mathbf{z}}^{\mathrm{PFA}} - p_{\mathbf{z}}^{\mathrm{PAP}} \right|$$

How to determine the action of $\exp(-i\tau\hat{H}(t+\tau/2))$ efficiently with respect to $|\psi(t)\rangle$?

- Make use of the Lie-Trotter-Suzuki product formula

$$\exp\left(\sum_{i\in\mathcal{I}}\hat{A}_i\right) = \lim_{n\to\infty}\left(\prod_{i\in\mathcal{I}}\exp\left(\hat{A}_i/n\right)\right)^n ,$$

and decompose $\hat{H} = \sum_{i\in\mathcal{I}}\hat{K}_i$ into Hermitian operators $\hat{K}_i$.

- For the first-order approximation we have

$$\hat{\mathcal{U}}_1 := \prod_{i\in\mathcal{I}}\exp(-i\tau\hat{K}_i).$$

- One can formally show that the first-order local error is given by

$$\|\hat{\mathcal{U}} - \hat{\mathcal{U}}_1\| \leq c_1\tau^2.$$

How to determine the action of exp$(-i\tau\hat{H}(t+\tau/2))$ efficiently with respect to $|\psi(t)\rangle$?

- For the second-order approximation we have

$$\hat{\mathcal{U}}_2 := \left(\prod_{i=|\mathcal{I}|-1}^{1} e^{-i\tau\hat{K}_i/2}\right) e^{-i\tau\hat{K}_0} \left(\prod_{i=1}^{|\mathcal{I}|-1} e^{-i\tau\hat{K}_i/2}\right).$$

- One can show that the second-order local error is given by

$$\|\hat{\mathcal{U}} - \hat{\mathcal{U}}_2\| \leq c_2\tau^3.$$

A simple model Hamiltonian in the harmonic bias

$$\hat{H} = \hat{H}_{\text{Transmon},\Sigma} + \hat{H}_{\text{Resonator},\Sigma} + \hat{V}_{\text{Interaction}}$$

$$\hat{H}_{\text{Transmon},\Sigma} = \sum_{i\in I} \omega_i^Q(t)\hat{b}_i^\dagger \hat{b}_i + \frac{\alpha_i^Q(t)}{2}\hat{b}_i^\dagger \hat{b}_i \left(\hat{b}_i^\dagger \hat{b}_i - \hat{I}\right),$$

$$\hat{H}_{\text{Resonator},\Sigma} = \sum_{j\in J} \omega_j^R \hat{a}_j^\dagger \hat{a}_j,$$

$$\begin{aligned}\hat{V}_{\text{Interaction}} = & \sum_{(i,i')\in I\times I'} g^{(0)}_{i,i'}(t)\left(\hat{b}_i + \hat{b}_i^\dagger\right)\otimes\left(\hat{b}_{i'} + \hat{b}_{i'}^\dagger\right) \\ & + \sum_{(j,j')\in J\times J'} g^{(1)}_{j,j'}\left(\hat{a}_j + \hat{a}_j^\dagger\right)\otimes\left(\hat{a}_{j'} + \hat{a}_{j'}^\dagger\right) \\ & + \sum_{(j,i)\in J\times I} g^{(2)}_{j,i'}(t)\left(\hat{a}_j + \hat{a}_j^\dagger\right)\otimes\left(\hat{b}_{i'} + \hat{b}_{i'}^\dagger\right)\end{aligned}$$

The adiabatic algorithm makes use of the fact that

$$\hat{H}(t) = (1 - s(t))\hat{H}_{\text{Start}} + s(t)\hat{H}_{\text{Final}}$$

$$\hat{H}_{\text{Start}} = \sum_i -\sigma_i^x$$

$$\hat{H}_{\text{Final}} = \sum_i h_i \sigma_i^z + \sum_{i<j} J_{i,j} \sigma_i^z \otimes \sigma_j^z$$

- If initialise a system $\hat{H}(t)$ in its ground state and vary $s(t) \in [0, 1]$ slow enough, the system will remain in its instantaneous ground state.
- Note that $|+\rangle$ is the ground state of $\hat{H}_{\text{Start}}$.

Trotterisation of the time-evolution operator $\hat{\mathcal{U}}(T)$

$$\hat{\mathcal{U}}(T) = \mathcal{T} e^{-i \int_0^T \hat{H}(t) dt}$$

$$\hat{\mathcal{U}}(T) \simeq \prod_{p=0}^{P} e^{-i \hat{H}(t_p) \tau}$$

$$\hat{\mathcal{U}}(T) \simeq \prod_{p=0}^{P} e^{-i(1-s(t_p))\hat{H}_{\text{Start}} \tau} e^{-is(t_p)\hat{H}_{\text{Final}} \tau}$$

$$\hat{\mathcal{U}}(T) \simeq \prod_{p=0}^{P} e^{-i\beta_p \hat{H}_{\text{Start}}} e^{-i\gamma_p \hat{H}_{\text{Final}}}$$

- Such that $\beta_p = (1 - s(t_p))\tau$ and $\gamma_p = s(t_p)\tau$.

Recasting the operator $\hat{\mathcal{U}}(T) \to \hat{U}(\gamma_p, \beta_p)$

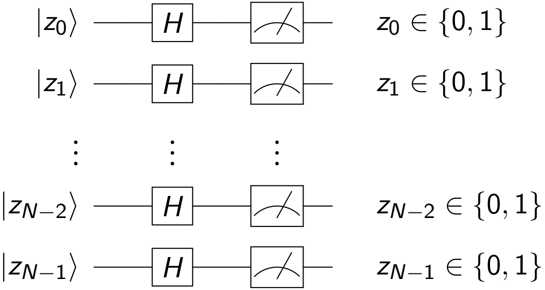
- The previous steps enable us to make use of the diagonal structure of $\hat{H}_{\text{Start}}$ and $\hat{H}_{\text{Final}}$ (in their respective bias).

- Rearranging the exponential operators yields

$$
\begin{aligned}
\hat{U}(\gamma_p, \beta_p) &= e^{-i\beta_p \hat{H}_{\text{Start}}} e^{-i\gamma_p \hat{H}_{\text{Final}}}, \\
e^{-i\gamma_p \hat{H}_{\text{Final}}} &= \prod_i e^{(2\gamma_p h_i) - i\sigma_i^z/2} \prod_{i<j} e^{(\gamma_p J_{i,j}) - i\sigma_i^z \otimes \sigma_j^z}, \\
e^{-i\beta_p \hat{H}_{\text{Start}}} &= \prod_i e^{(-2\beta_p) - i\sigma_i^x/2}, \\
\hat{U}(\gamma_p, \beta_p) &= \prod_i e^{i\beta_p \sigma_i^x} \prod_i e^{-i\gamma_p h_i \sigma_i^z} \prod_{i<j} e^{-i\gamma_p J_{i,j} \sigma_i^z \otimes \sigma_j^z}.
\end{aligned}
$$

Implementation of $|\gamma, \beta\rangle = \prod_{p=1}^{P} e^{-i\beta_p \hat{H}_M} e^{-i\gamma_p \hat{H}_C} |+\rangle^N$

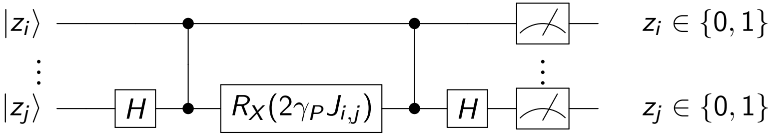
- First move the system into the state $|+\rangle^N$.



- Since $\sum_i h_i \sigma_i^z$ and $\sum_{i<j} J_{i,j} \sigma_i^z \otimes \sigma_j^z$ commute, we can implement the corresponding exponential operators individually one after another.

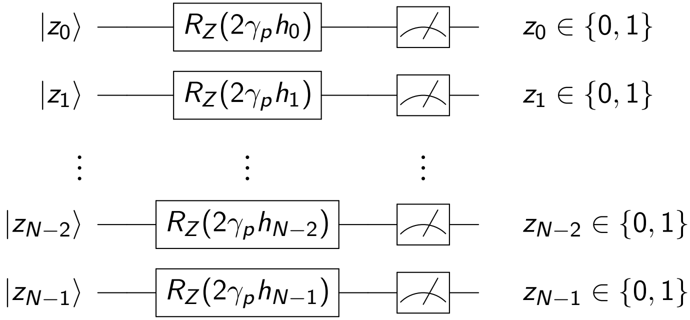
Step 0: implement $\prod_{i<j} e^{-i\gamma_p J_{i,j}\sigma_i^z \otimes \sigma_j^z}$

- A single term in the product $\prod_{i<j} e^{-i\gamma_p J_{i,j}\sigma_i^z \otimes \sigma_j^z}$ can be implement as:

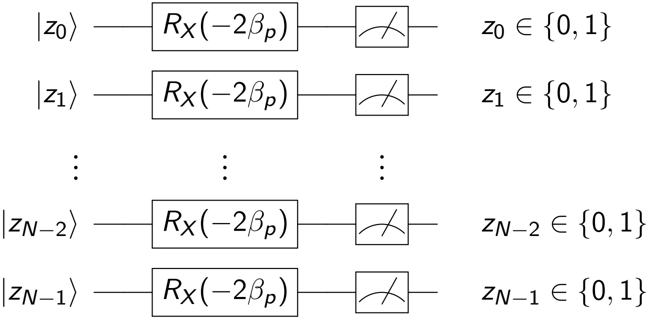


- Note that one can interchange the qubits without changing the results.

Step 1: implement $\prod_i e^{-i\gamma_p h_i \sigma_i^z}$



Step 2: implement $e^{-i\beta_p \hat{H}_M} = \prod_i e^{i\beta_p \sigma_i^x}$



- Once we have the circuit, we need problems to solve with the QAOA.

Various error measures for the target operator $\hat{U}$

- If $\hat{M}$ denotes the projected state vector operator, we can define $\hat{V} = \hat{U}\hat{M}^\dagger$ such that the error measures can be expressed as

$$
\begin{aligned}
\mu_{F^2} &= \|\hat{M} - u\hat{U}\|_F, \\
\mu_{\mathrm{F_{Avg}}} &= \frac{\|\mathrm{Tr.}(\hat{V})\|_1^2 + \mathrm{Tr.}(\hat{M}\hat{M}^\dagger)}{D\,(D+1)}, \\
\mu_\diamond &= \frac{1}{2} \sup_{|\psi\rangle \in \mathcal{H}_D} \left(\| \left(\hat{V}^\dagger \otimes \hat{I}\right) |\psi\rangle\langle\psi| \left(\hat{V}^\dagger \otimes \hat{I}\right)^\dagger - |\psi\rangle\langle\psi| \, \|_{\mathrm{Tr.}} \right), \\
\mu_{\mathrm{Leak}} &= 1 - \left(\frac{\mathrm{Tr.}(\hat{M}\hat{M}^\dagger)}{D} \right),
\end{aligned}
$$

- where $u = \pm\sqrt{\mathrm{Tr.}(\hat{V}^\dagger)/\mathrm{Tr.}(\hat{V}^\dagger)^*}$, $D = \dim(\mathcal{H}_D)$ and $\mathcal{H}_D \subseteq \mathbb{C}^D$.