Resolving Combinatorial Problems
with Quantum Algorithms

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In collaboration with

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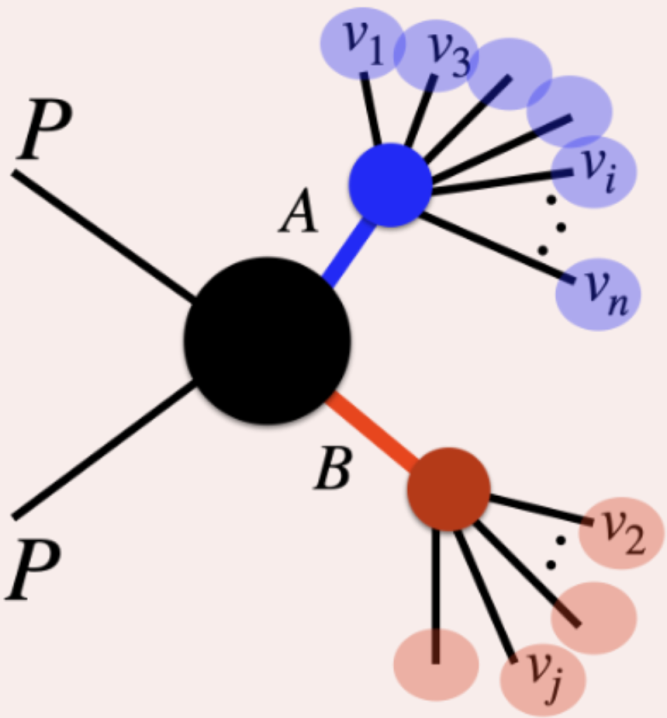
Structure of talk

1. Problem at hand
   - And current alternatives
2. Setting up the problem
3. Quantum algorithms in question (VQAs)
4. Current results

The problem



$2 \to 2 \to n$ collision. From Kim et al. 2021 [2111.07806]

- Binary classification: did particle ν_i come from A or B?
- A QUBO[1] problem: Quadratic Unconstrained Binary Optimization problem:

For an n-bit string x, find x^* such that it minimizes

$$f_w(x) = \sum_{i,j=1}^{n} w_{ij} x_i x_j$$

[1] A rare occurance of a 'Q' *not* standing for 'quantum'

Specific case: $pp \to t\bar{t}$

Two dominant decay modes for t:

- Leptonic: $t \to W^+ b \to \ell \nu_\ell b$
  - Cleaner – only one jet
  - But there's missing momentum
- Hadronic: $t \to W^+ b \to q\bar{q}b$
  - No missing momentum
  - But messier – 3 quarks creating 3 jets

Our focus has been on the latter case:

$$pp \to t\bar{t} \to q\bar{q}q'\bar{q}'b\bar{b} \quad \text{(i.e. 6 jets)}$$

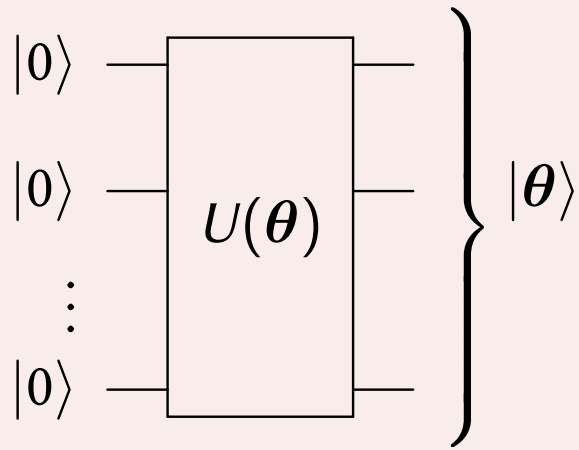
Alternate methods

- Kinematic methods like the hemisphere method [1]
  - Make assertions and assumptions of the kinematics of the system
- Machine learning
  - Great at finding and learning patterns
  - Lot of research that can be applied in HEP, e.g. SPANET (2106.03898, 2012.03542)
  - Classical, so still limited by exponential growth of complexity
- Quantum annealing (2111.07806)
  - Can find the global minimum
  - Smaller energy gaps between eigenvalues requires larger relaxation times
  - Limited with degenerate eigenvalues

Variational Quantum Algorithms

If you know neural networks keep that in mind

- We have some operator C whose expectation value, $\langle\boldsymbol{\theta}|C|\boldsymbol{\theta}\rangle$ we want to extremize
  - The state $|\boldsymbol{\theta}\rangle$ is parameterized by parameters $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_n)$
  - e.g. for this talk, think C is a Hamiltonian and we wish to find the ground state energy
- $|\boldsymbol{\theta}\rangle$ can be created with a quantum circuit: $U(\boldsymbol{\theta})\,|0\rangle = |\boldsymbol{\theta}\rangle$
- Use a classical optimizer to update the parameters $\boldsymbol{\theta}_n \to \boldsymbol{\theta}_{n+1}$ and repeat
  - They are *hybrid* algorithms

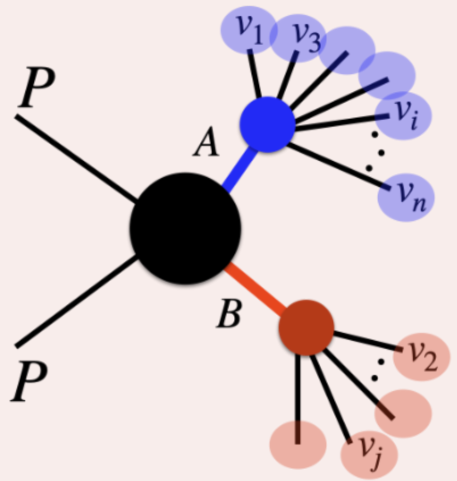


Setup

- With QAOA on our mind, is there a Hamiltonian that we can use?

$$H = (p_A^2 - p_B^2)^2 \quad \text{where} \quad \begin{cases} p_A = \sum x_i p_i \\ p_B = \sum (1 - x_i) p_i \end{cases}$$

and $x_i = 1$ if particle i is associated with A, otherwise 0



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- Change from indicator variables to spin: $x_i = (1 + s_i)/2$,

$$H = \sum_{ij} J_{ij} s_i s_j \quad \text{where} \quad J_{ij} = \sum_{k\ell} (p_i \cdot p_k)(p_j \cdot p_\ell)$$

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- Since $s_i = \pm 1$, we can write our Hamiltonian operator as

$$H_P = \sum_{ij} J_{ij} \sigma_z^i \sigma_z^j.$$

  Eigenvalues are ± 1 and eigenvectors are computation basis vectors

Algorithms [Quantum Approximation Optimization Algorithm]

- **QAOA**: Discretize the adiabatic evolution from **Mixer Hamiltonian** H_M with known ground state/energy to **Problem Hamiltonian** H_P whose ground state solve our problem.

$$H_M \to H_P \quad \Longrightarrow \quad |+\rangle \to |000111\rangle$$

  Each layer of the circuit represents a small time step Δt and has 2 free parameters.

Source: Farhi et al. 2014 [1411.4028]

Algorithms [multiangle-QAOA]

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Source: Herrman et al. 2021 [2109.11455]

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Source: Vijendran et al. 2023 [2302.04479]

Algorithms [Feedback-based ALgorithm for Quantum OptimizatioN]

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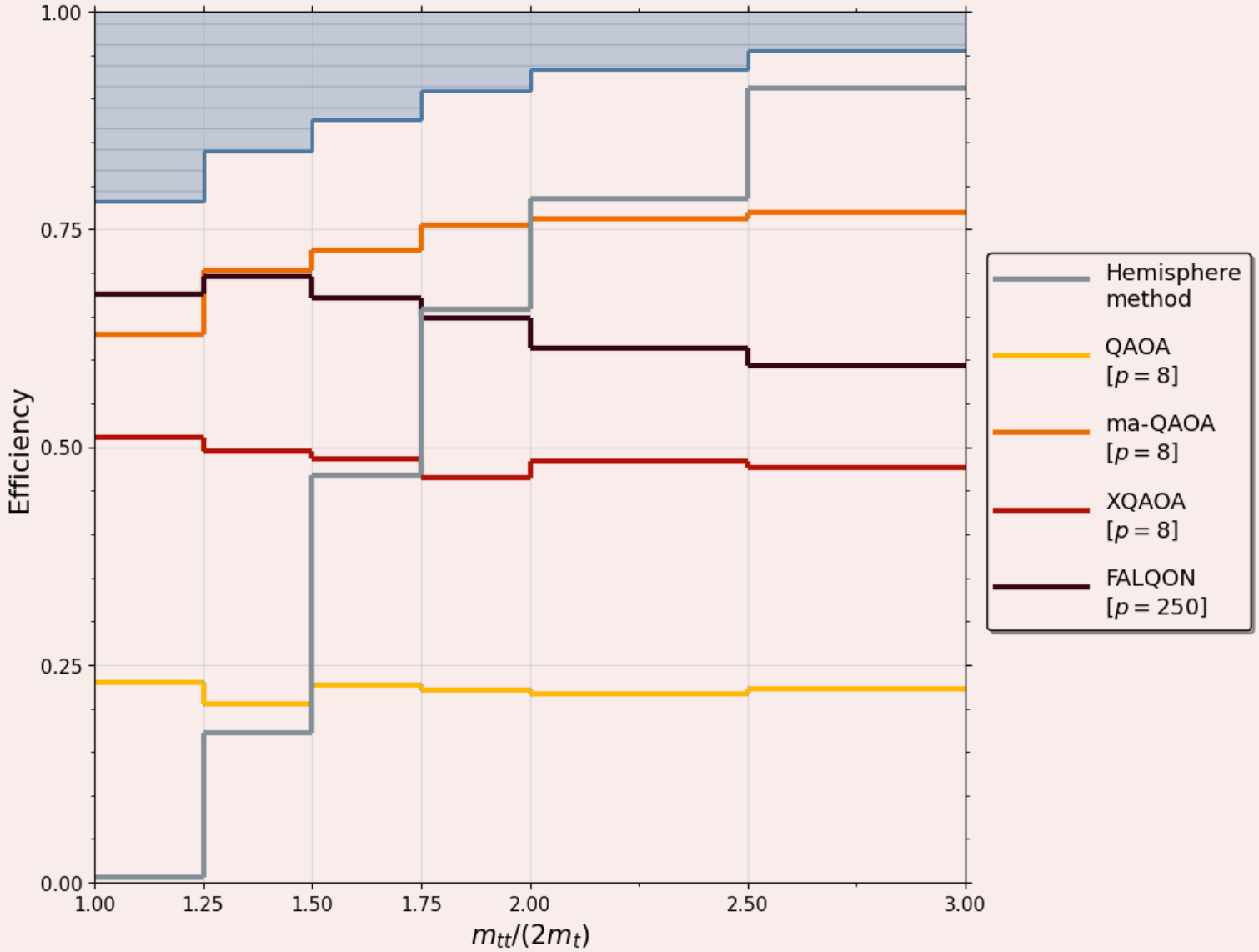
- **ma-QAOA**: What if each *qubit* has it's own free parameter?
- **XQAOA**: What if there is also another Mixer Hamiltonian, H_X?
- **FALQON**: Purely quantum. What if we iteratively build the circuit where the next free parameter depends on an expectation value of the current circuit?

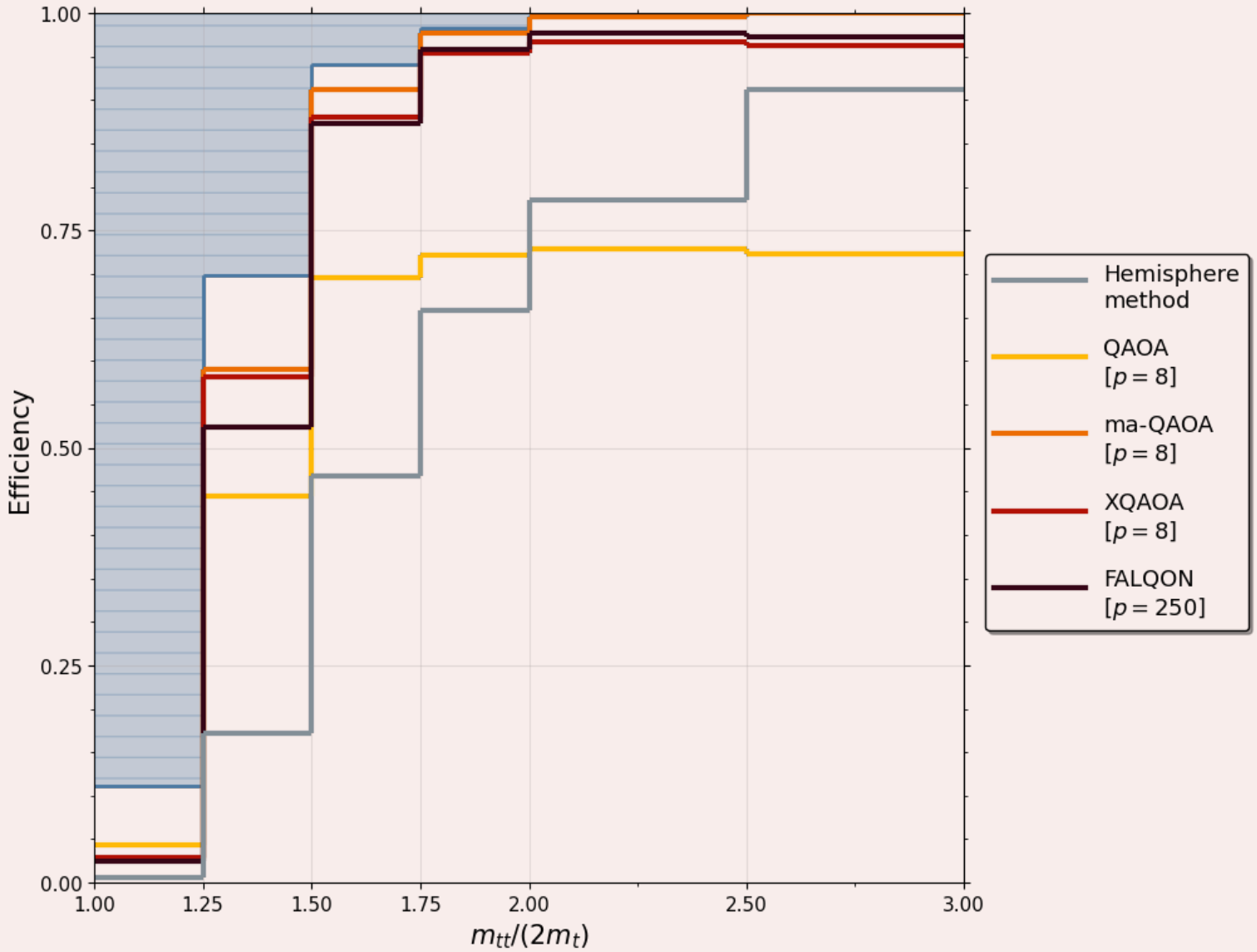
(unmentioned: ADAPT-QAOA, WSQAOA)

Source: Magann et al. 2022 [2103.08619]

Results: $H = H_0 =$ difference^2



Results: $H = H_0 + \lambda H_1 = \mathbf{difference}^2 + \lambda \mathbf{sum}$

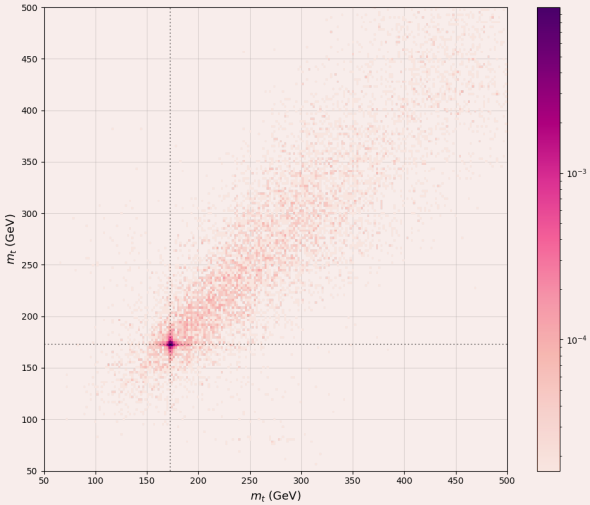


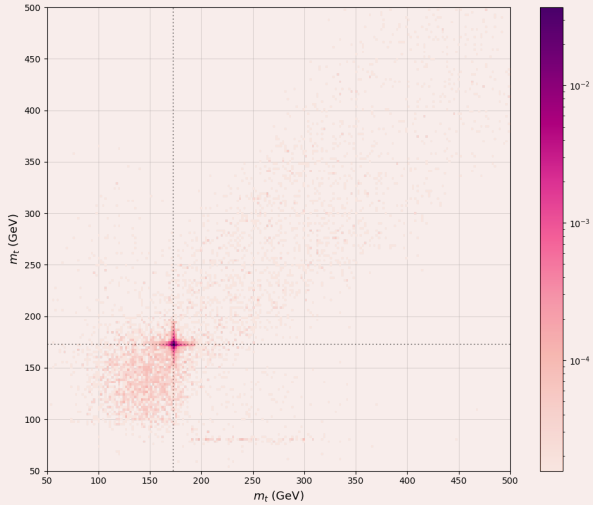
Results: Mass Distribution

H_0

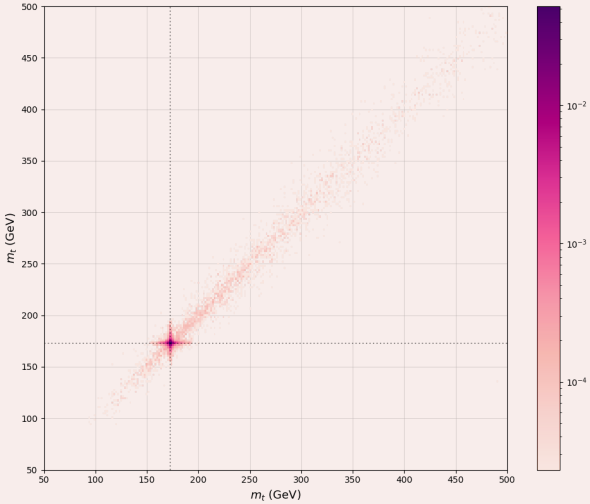
$H_0 + \lambda H_1$

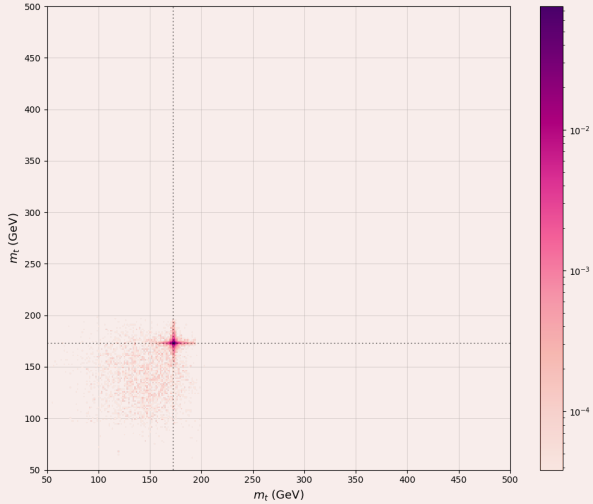
QAOA





maQAOA





Conclusion

To Sum Up:

- VQAs can be effective in finding the ground state of a Hamiltonian
- Choice of Hamiltonian is essential for solving the combinatorial problem
- Issues can arise navigating the parameter space:
  - Low expressibility
  - Barren plateaus

Other Routes:

- Look at asymmetric production via tW
- Look at effects of noisy circuits
- Look at choice of λ and other potential Hamiltonians

References

[1] G. L. Bayatian et al. "CMS technical design report, volume II: Physics performance". In: *J. Phys. G* 34.6 (2007), pp. 995–1579. DOI: 10.1088/0954-3899/34/6/S01.

[2] Edward Farhi, Jeffrey Goldstone, and Sam Gutmann. *A Quantum Approximate Optimization Algorithm.* 2014. arXiv: 1411.4028 [quant-ph].

[3] Rebekah Herrman et al. *Multi-angle Quantum Approximate Optimization Algorithm.* 2021. arXiv: 2109.11455 [quant-ph].

[4] Minho Kim et al. *Leveraging Quantum Annealer to identify an Event-topology at High Energy Colliders.* 2021. arXiv: 2111.07806 [hep-ph].

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[6] Alicia B. Magann et al. "Feedback-Based Quantum Optimization". In: *Physical Review Letters* 129.25 (2022). DOI: 10.1103/physrevlett.129.250502. eprint: 2103.08619. URL: https://doi.org/10.1103%2Fphysrevlett.129.250502.

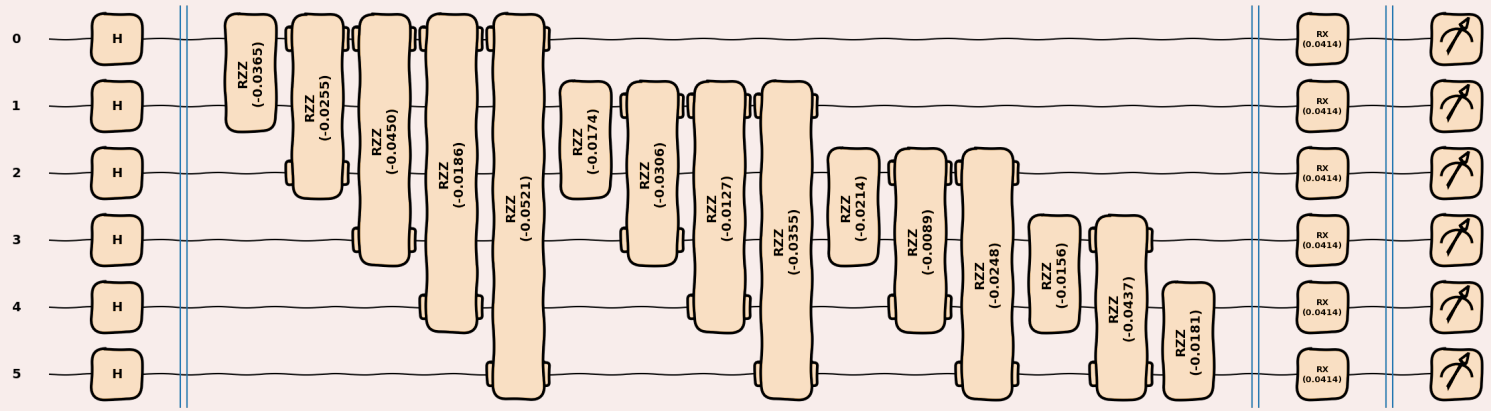
[7] Alexander Shmakov et al. "SPANet: Generalized permutationless set assignment for particle physics using symmetry preserving attention". In: *SciPost Physics* 12.5 (May 2022). DOI: 10.21468/scipostphys.12.5.178. eprint: 2106.03898. URL: https://doi.org/10.21468%2Fscipostphys.12.5.178.

[8] V. Vijendran et al. *An Expressive Ansatz for Low-Depth Quantum Optimisation.* 2023. arXiv: 2302.04479 [quant-ph].

[9] Linghua Zhu et al. *An adaptive quantum approximate optimization algorithm for solving combinatorial problems on a quantum computer.* 2022. arXiv: 2005.10258 [quant-ph].

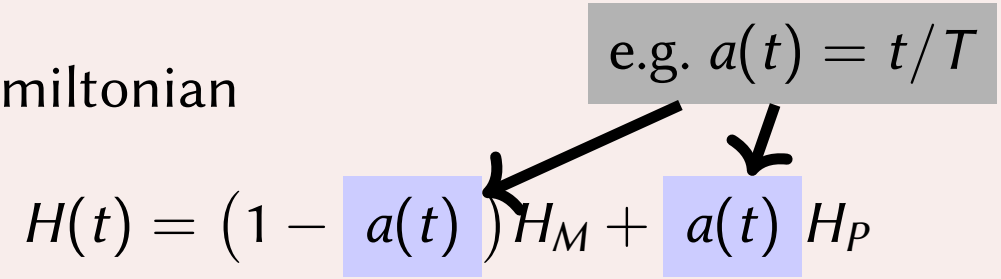
QAOA Circuit

- One qubit for each final state particle
  - $n = 6$ qubits in the $t\bar{t}$ decay
- The mixer layer consists of 6 1-qubit R_X gates with rotation β_k
- The problem layer consists of $\binom{6}{2} = 15$ R_{ZZ} gates with rotation $J_{ij}\gamma_k$ between the i and j qubit



Quantum Approximation Optimization Algorithm (QAOA)

- Start with Hamiltonian



  such that $a(0) = 0$ and $a(T) = 1$
  - Means that we start in system H_M and, if T is large, slowly evolve into state H_P
  - **Mixer Hamiltonian**: H_M, an easily solvable system with easily initializable eigenstates, usually $H_M = \sum \sigma_x^k$
  - **Problem Hamiltonian**: H_P, Hamiltonian whose minimum energy state is the answer we wish to find
- Exploit the adiabatic theorem: start in ground state of H_M, evolve slowly into ground state of H_P

Original paper: Farhi et al. 2014 [1411.4028]

Quantum Approximation Optimization Algorithm (QAOA)

Remember from our quantum mechanics courses:

$$H|\psi\rangle = i\frac{\partial}{\partial t}|\psi\rangle \Longrightarrow |\psi\rangle = e^{-iHt}|\psi_0\rangle$$

In our case, $|\psi\rangle = |\boldsymbol{\theta}\rangle$. What do we choose for $|\psi_0\rangle$? How do we do time-evolution on a circuit?

Result:

Ground state of H_M

- Our state is: $|\boldsymbol{\beta}, \boldsymbol{\gamma}\rangle = \prod_{j=1}^{p} U(\beta_j, H_M)U(\gamma_j, H_P)\ |+\rangle^{\otimes n}$

where $U(\beta_j, H_M) = \exp\left[-i\beta_j H_M\right]$,
$U(\gamma_j, H_P) = \exp\left[-i\gamma_j H_P\right]$
and p is the **depth** of the circuit

Original paper: Farhi et al. 2014 [1411.4028]

Quantum Approximation Optimization Algorithm (QAOA)

Continuous time-evolution approximated by small discrete steps alternating applications of the Hamiltonians

- **Circuit**: $|\boldsymbol{\beta}, \boldsymbol{\gamma}\rangle = \prod_{j=1}^{p} U(\beta_j, H_M) U(\gamma_j, H_P) \; |+\rangle^{\otimes n}$
  - This approximation is exact when $p \to \infty$
- **Mixer Hamiltonian**: $H_M = \sum_{k=1}^{n} \sigma_x^k$
  - As quantum gates:

    $$\exp\left[-i\beta_j \sum_{k=1}^{n} \sigma_x^k\right] = \prod_{k=1}^{n} e^{-i\beta_j \sigma_x^k} = \prod_{k=1}^{n} R_X(\beta_j)$$

Just X rotations on every qubit

- **Problem Hamiltonian**: H_P depends on problem
  - Can we write it as Pauli matrices?
- **Goal**: minimize $\langle \boldsymbol{\beta}, \boldsymbol{\gamma} | H_P | \boldsymbol{\beta}, \boldsymbol{\gamma} \rangle$

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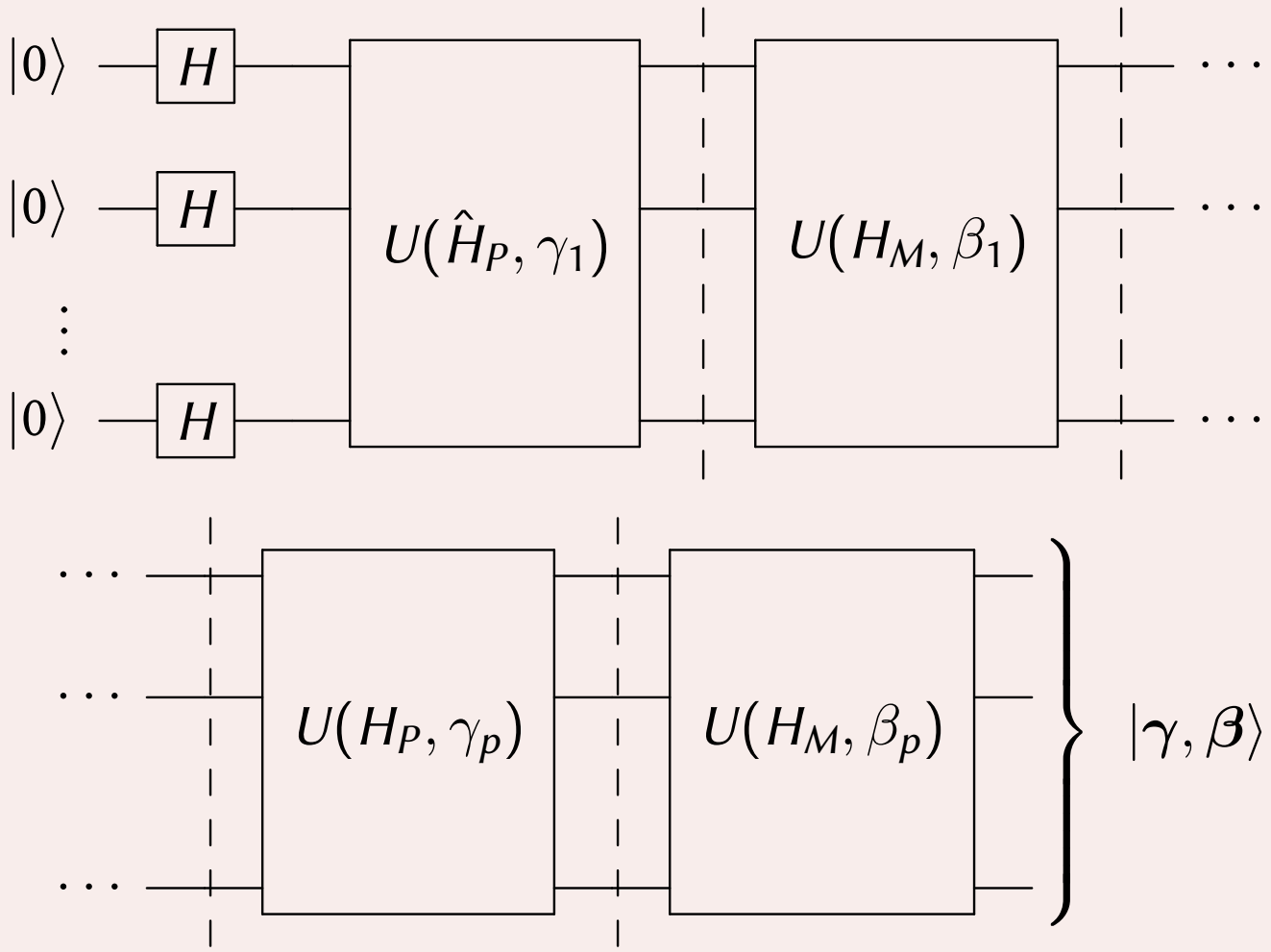
Quantum Approximation Optimization Algorithm (QAOA)



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Quantum Approximation Optimization Algorithm (QAOA)

But there are problems!

- How quickly does it converge?
  - We don't have the technology for a circuit of $\mathcal{O}(10)$ depth, let alone ∞ depth
- How easy is it to navigate the parameter space?
  - Are there many local minima to get stuck in?
  - Barren plateaus?
- "...short-depth QAOA is not really the digitized version of the adiabatic problem, but rather an ad hoc ansatz, and as a result should not be expected to perform optimally, or even well."
  - From Zhu et al. 2022 [2005.10258]

So we say good riddance to the justification of this approximate adiabaticity and consider other ansatzes

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Original paper: Farhi et al. 2014 [1411.4028]

Multi-Angle QAOA (ma-QAOA)

- **Expressibility** is a circuit's ability to explore its Hilbert space
  - Or, for a single qubit, to traverse the Bloch sphere
- Idea: give *every* gate its own free parameter:

$$U(\beta_j, H_M) = \exp\left[-i\beta_j \sum_{k=1}^{n} \sigma_x^k\right]$$

$$\Downarrow$$

$$U(\boldsymbol{\beta}_j, H_M) = \exp\left[-i \sum_{k=1}^{n} \beta_{jk} \sigma_x^k\right]$$

- This allows for lower depth circuits that are more accessible with current quantum computers, i.e. NISQ era
- Tradeoff between the quantum and classical computers

Original paper: Herrman et al. 2021 [2109.11455]

Feedback-based ALgorithm for Quantum OptimizatioN (FALQON)

- A purely quantum algorithm – no optimization
- Considers the Hamiltonian: $H(t) = H_P + \beta(t)H_M$
- Want

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)|H_P|\psi(t)\rangle \leq 0 \Longrightarrow A(t)\beta(t) \leq 0$$

  where $A(t) = \langle\psi(t)|i[H_M, H_P]|\psi(t)\rangle$
- Choose $\beta(t) = -A(t - 2\Delta t)$ and descritize: $\beta_{k+1} = -A_k$
- Our state is: $|\boldsymbol{\beta}\rangle = \prod_{j=1}^{p} U(\beta_j, H_M)U(H_P)$
  - where $U(\beta_j, H_M) = e^{-i\beta_j H_M \Delta t}$ and $U(H_P) = e^{-iH_P\Delta t}$

eXpressive QAOA (XQAOA)

Sacrifice away adiabaticity for even more expressibility

- Add another mixer Hamiltonian to ma-QAOA: $H_X = \sum_{k=1}^{n} \sigma_y^k$
- Our quantum state is now

$$|\boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\gamma}\rangle = \prod_{j=1}^{p} U(\boldsymbol{\alpha}_j, H_X) U(\boldsymbol{\beta}_j, H_M) U(\boldsymbol{\gamma}_j, H_P) \, |+\rangle^{\otimes n}$$

- ma-QAOA is just XQAOA when $\boldsymbol{\alpha} = \mathbf{0}$

Original paper: Vijendran et al. 2023 [2302.04479]

Adaptive Derivative Assembled Problem Tailored QAOA (ADAPT-QAOA)

The kitchen sink emporium

- The choice of mixer Hamiltonian is not fixed but rather chosen from a *pool*, $\mathcal{A}$, in an iterative fashion
- Choice made by whichever maximizes energy gradient. Calculate

$$\Delta E_k(A_j) = \frac{\partial}{\partial \beta_k} \langle \psi_k | H_P | \psi_k \rangle \Big|_{\beta_k = 0}$$

  for each A_j then choose $A_k = \underset{A_j \in \mathcal{A}}{\operatorname{argmax}} \Delta E_k(A_j)$ as the mixer Hamiltonian for layer k.
- Optimize circuit as with normal QAOA and repeat for next layer

Original paper: Zhu et al. 2022 [2005.10258]