VarQITE for Combinatorial Problem in High Energy Physics

IonQ 2025 Spring Mentoring Program

Quantum Collider / Willie Abourmad

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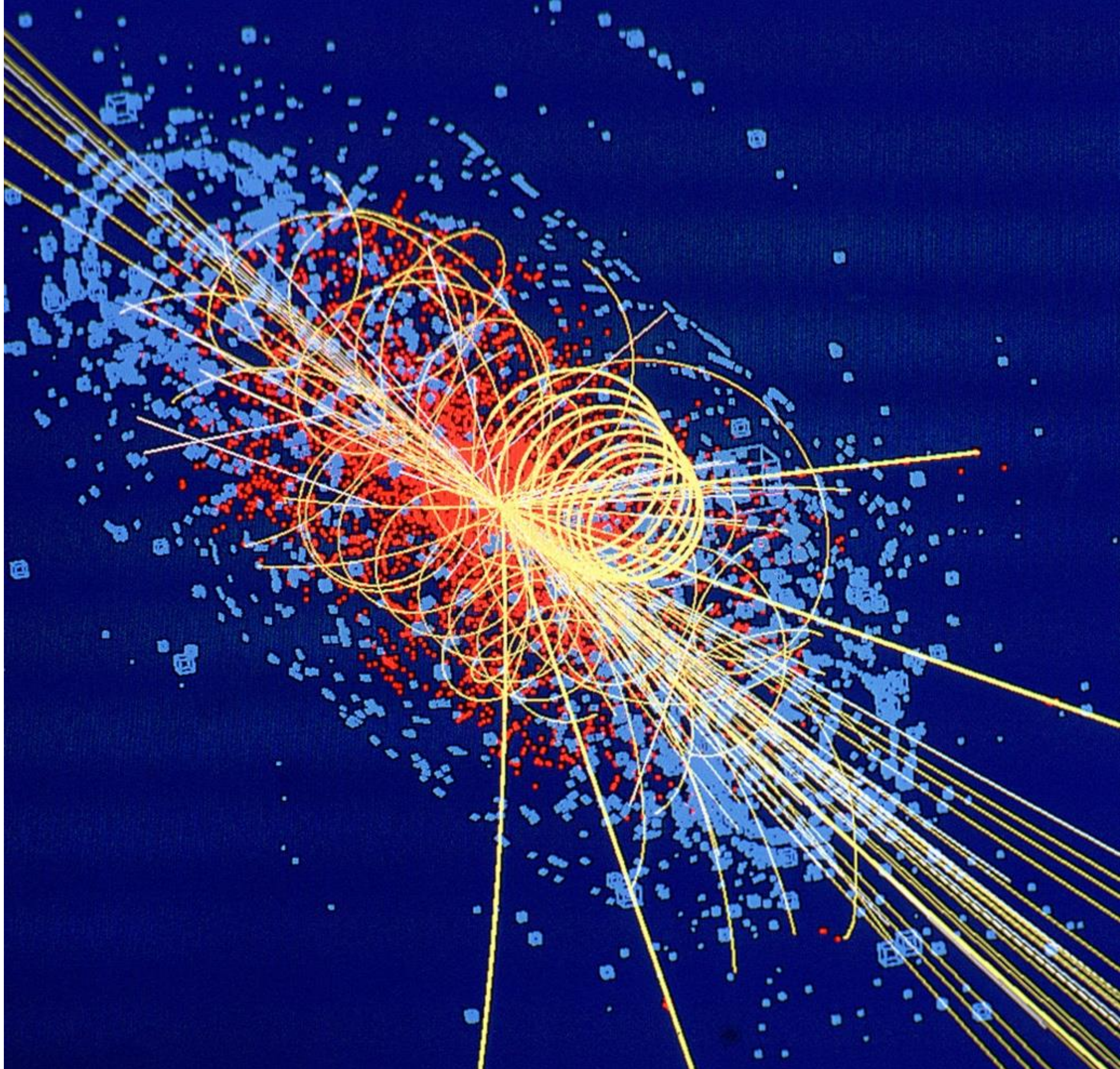
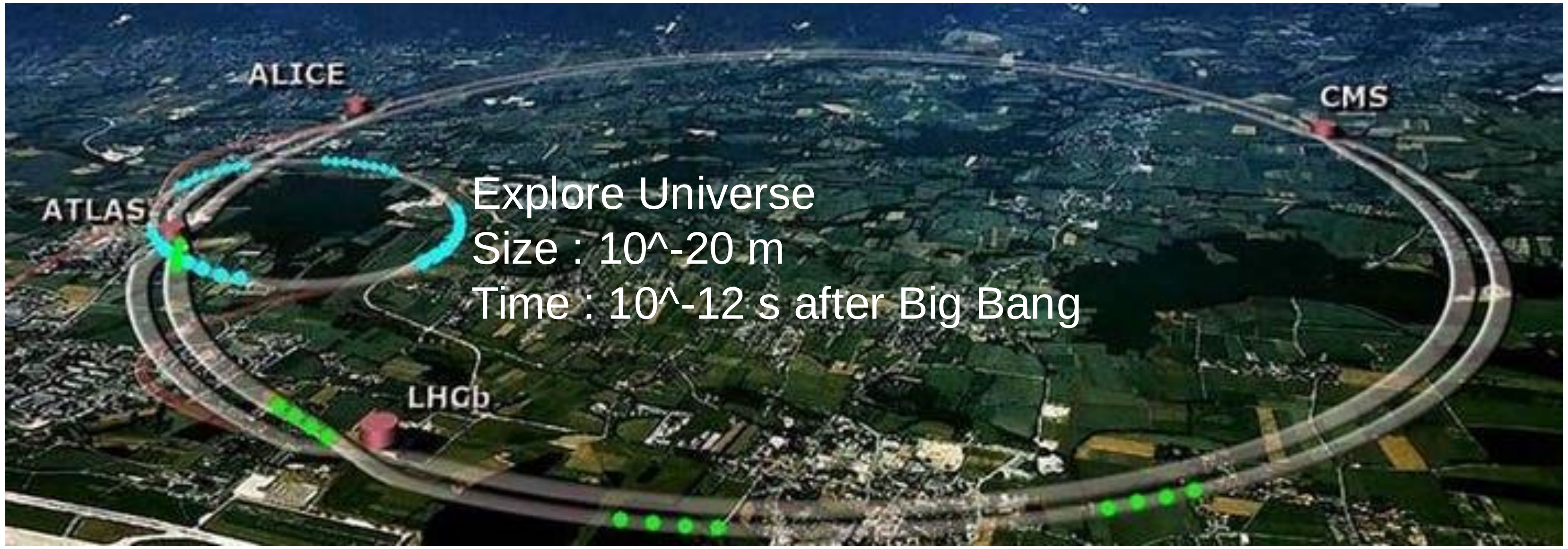
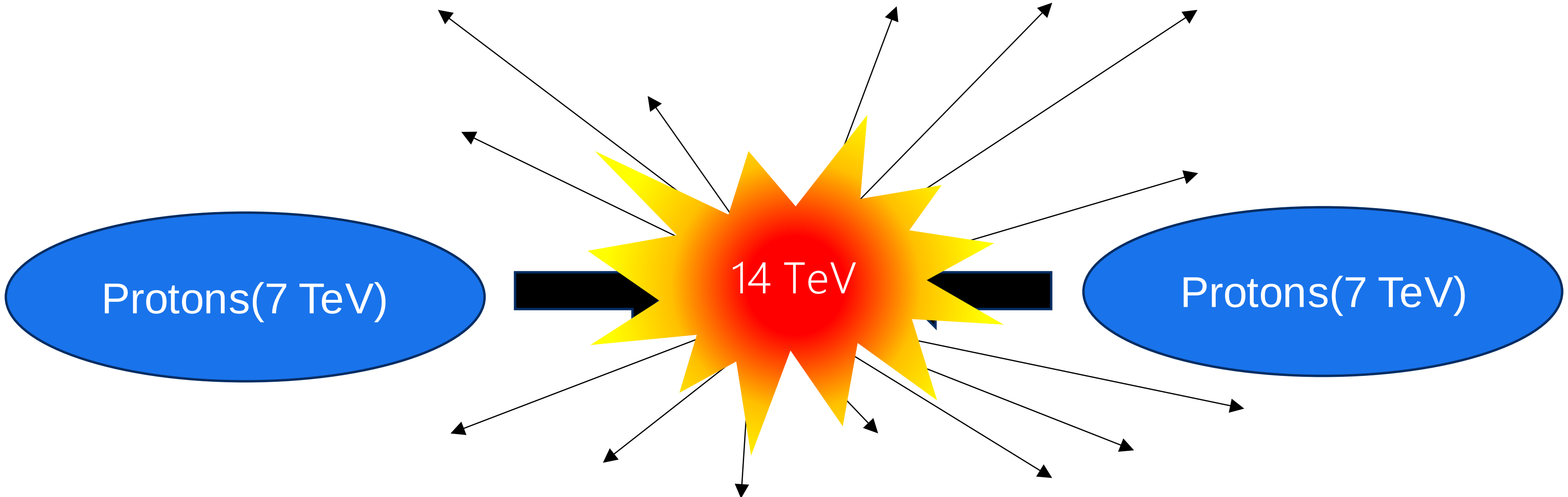


Protons collide forming four muons in this simulation of a collision in the CMS detector (Image: CMS/CERN)

Large Hadron Collider(LHC)





Combinatorial problems at the LHC

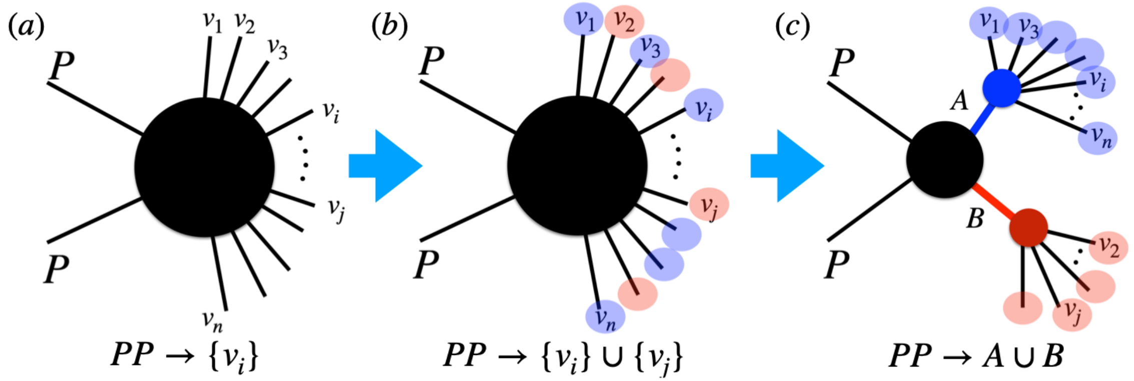


FIG. 1. (a) n-observed particles (b) Dividing n particles into two groups for $2 \to 2$ process (c) Identified event-topology with A and B.

- Assuming $2 \to 2$ production with subsequent decays, identification of a group becomes a binary classification, with 2^n possibilities. Identified groups with A and B.

p_i is the momentum of constituent of A if $x_i = 1$

p_i is the momentum of constituent of B if $x_i = 0$

$$P_1 = \sum_i p_i \, x_i$$

$$P_2 = \sum_i p_i \, (1 - x_i)$$

for all possible combinations of x_i

Combinatorial problems at the LHC

$$P_1 = \sum_{i=1}^{n} p_i \, x_i \,,$$

$$P_2 = \sum_{i=1}^{n} p_i \, (1 - x_i) \,,$$

$$x_i = \frac{1 + s_i}{2}$$

$$H_0 = (P_1^2 - P_2^2)^2 = \sum_{ij} J_{ij} s_i s_j$$

$$H_1 = P_1^2 + P_2^2 = \sum_{ij} P_{ij} s_i s_j$$

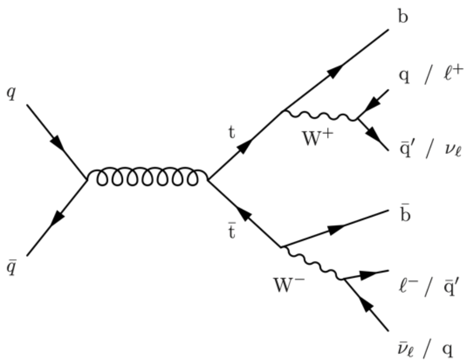
$$P_{ij} = p_i \cdot p_j \qquad J_{ij} = \sum_{k\ell} P_{ik} P_{j\ell},$$

Problem Hamiltonian

$$H_P = H_0 + \lambda H_1$$

Where $\lambda = \min(J_{ij}) / \max(P_{ij})$

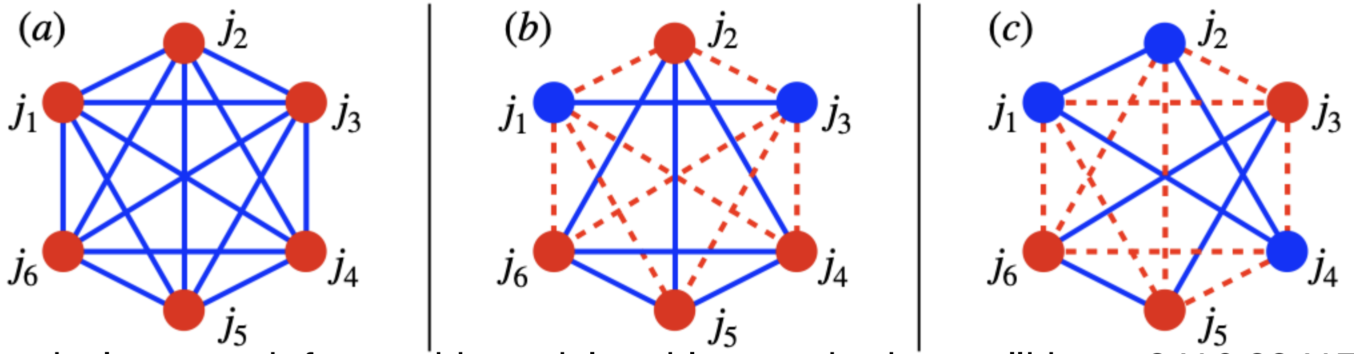
Ex.



$$p\, p \rightarrow t\, \bar{t} \rightarrow 6\ final\ particles (6\ jets)$$

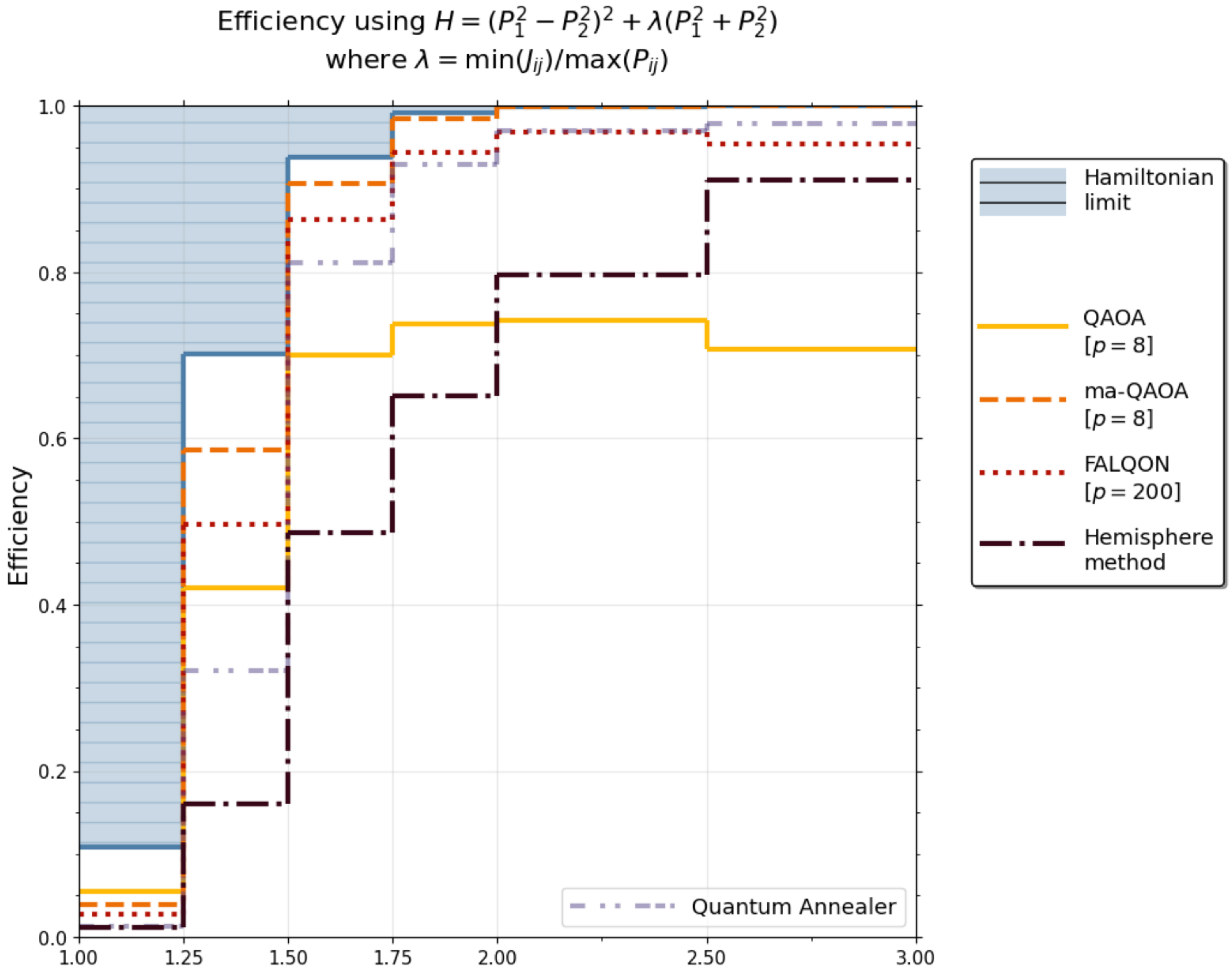
Weighted MAXCUT Problem

- 6 final particles = 6 vertices
- fully connected



Hybrid quantum-classical approach for combinatorial problems at hadron colliders: 2410.22417

Analysis Results Before



$m_{tt}/2m_t$; The speed of the top quark

Quantum Algorithm	Property
QAOA, ma-QAOA	O) Classical Optimizer – Hybrid Algorithm X) Hard to simulate higher order term
FALQON	O) Good Performance X) Needs Large # of gates

<u>VarQITE</u>

- **NO** need of a classical optimizer
- **NOT** need large # of gates
- Possible to simulate **higher order terms**

Hybrid quantum-classical approach for combinatorial problems at hadron colliders: 2410.22417

During the mentoring,

Understanding basic Idea of Variational Quantum Imaginary Time Evolution(VarQITE)

Implement Imaginary Time Evolution with PennyLane

Apply the method to the combinatorial problem at the LHC

Think about different Hamiltonian ansatz including the higher order terms

Run the developed codes on real hardware

Variational Quantum Imaginary Time Evolution(VarQITE)

Quantum imaginary time evolution is governed by the Schrodinger equation

$$|\Psi(\tau)\rangle = \frac{e^{-H\tau}|\Psi(0)\rangle}{\sqrt{\langle\Psi(0)|e^{-2H\tau}|\Psi(0)\rangle}} \sim \sum c_i\, e^{-E_i\tau}|e_i\rangle \qquad \text{where } \hbar = 1, \tau = -it$$

The probability of the energy's eigenstate decays with their energies.

$$\boxed{\lim_{\tau\to\infty}|\Psi(\tau)\rangle = |g\rangle} \quad \text{where} \quad |g\rangle \text{ is the energy ground state}$$

In VarQITE, the time evolution of the state $|\Psi(t)\rangle$ is replaced by the evolution of parameters $\theta(t)$ in a variational quantum circuit ansatz $|\Psi\big(\theta(t)\big)\rangle$

Using McLachlan variational principle, the algorithm updates the parameters by minimizing the distance between the RHS and the LHS of the equation($\underline{\boldsymbol{\frac{\partial}{\partial\tau}|\Psi(\tau)\rangle = (H - E_\tau)|\Psi(\tau)\rangle}}$), that is minimizing

$$\boxed{\left\|\left(\frac{\partial}{\partial\tau} + H - E_\tau\right)|\Psi\big(\theta(\tau)\big)\rangle\right\|} \quad \text{where } E_\tau \text{ is the energy at } \tau$$

The evolution of the parameters is given by,

$$\boxed{\sum_{ij} F_{ij}\dot{\theta}_i = V_j} \quad \text{where } F_{ij} = \Re\left[\frac{\partial\langle\Psi(\theta)|}{\partial\theta_i}\frac{\partial|\Psi(\theta)\rangle}{\partial\theta_j} + \frac{\partial\langle\Psi(\theta)|}{\partial\theta_i}\Big|\Psi(\theta)\Big\rangle\Big\langle\Psi(\theta)\Big|\frac{\partial|\Psi(\theta)\rangle}{\partial\theta_j}\right] \;\&\; V_i = -\Re\Big[\frac{\partial\langle\Psi(\theta)|}{\partial\theta_i}H|\Psi(\theta)\rangle\Big]$$

Variational ansatz-based quantum simulation of imaginary time evolution : 1804.03023

VarQITE for Combinatorial Problem

As the Hamiltonian is constituent of Pauli terms (P_α), they commute with Ising like Problem Hamiltonian H_P

$$\frac{\partial\langle P_\alpha\rangle}{\partial\tau} = \sum_j 2\mathfrak{R}\left(\langle\Psi(\vec{\theta})|P_\alpha\frac{\partial|\Psi(\vec{\theta})\rangle}{\partial\theta_j}\right)\dot{\theta}_j$$
$$= -\langle\Psi(\vec{\theta})|\{P_\alpha, H_c - E_\tau\}|\Psi(\vec{\theta})\rangle\,. \qquad (5)$$

We could make an approximation. It makes the linear equation simpler.

$$\boxed{\sum_{ij} F_{ij}\dot{\theta}_i = V_j} \quad \Longrightarrow \quad \boxed{\sum_{\alpha,j} G_{\alpha,j}\dot{\theta}_j = D_\alpha}$$

$$F_{ij} = \Re\left[\frac{\partial\langle\Psi(\theta)|}{\partial\theta_i}\frac{\partial|\Psi(\theta)\rangle}{\partial\theta_j} + \frac{\partial\langle\Psi(\theta)|}{\partial\theta_i}\Big|\Psi(\theta)\Big\rangle\Big\langle\Psi(\theta)\Big|\frac{\partial|\Psi(\theta)\rangle}{\partial\theta_j}\right]$$
$$V_i = -\Re\left[\frac{\partial\langle\Psi(\theta)|}{\partial\theta_i}H|\Psi(\theta)\rangle\right]$$

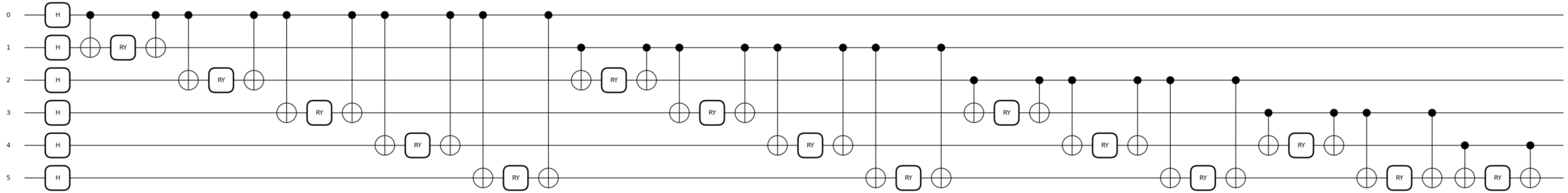
$$G_{\alpha j} = \Re\left[\langle\Psi(\theta)|P_\alpha\frac{\partial|\Psi(\theta)\rangle}{\partial\theta_j}\right]$$
$$D_\alpha = -\frac{1}{2}\langle\Psi(\theta)|\{P_\alpha, H - E_\tau\}|\Psi(\theta)\rangle$$

$\theta \to \theta - \delta\dot{\theta}$ where δ is a learning rate

Performant near-term quantum combinatorial optimization : 2404.16135

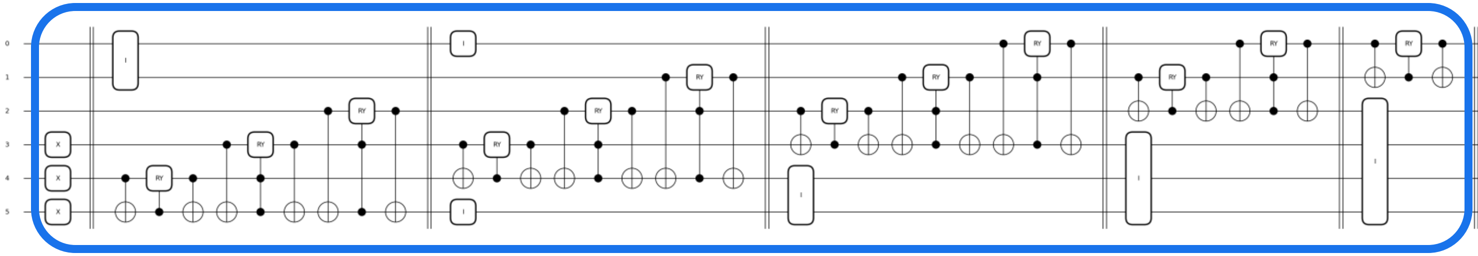
VarQITE Ansatz

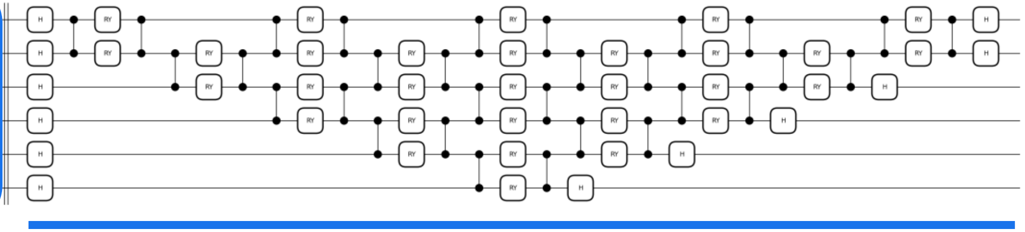
Ansatz 1 (Fully Connected / # of training parameters = 15)



Performant near-term quantum combinatorial optimization : 2404.16135

Ansatz 2 (With assumption : Symmetric Allocation & Reconfigurable Beam Splitter(RBS) Gate / # of training parameters = 15)





Dicke state (1904.07358)

$$|D_6^3 > = \frac{1}{\sqrt{20}}(|000111 > + |001011 > + |001101 > + \cdots + |111000 >)$$

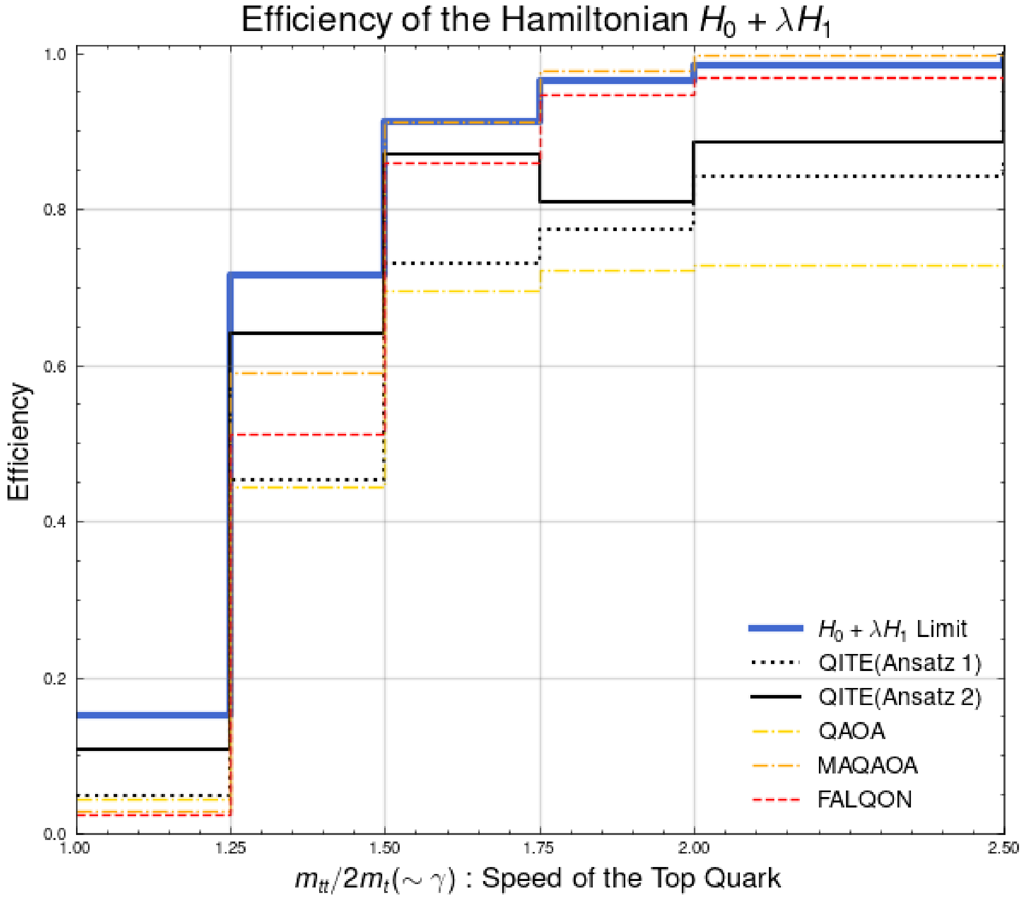
RBS Gate Operation

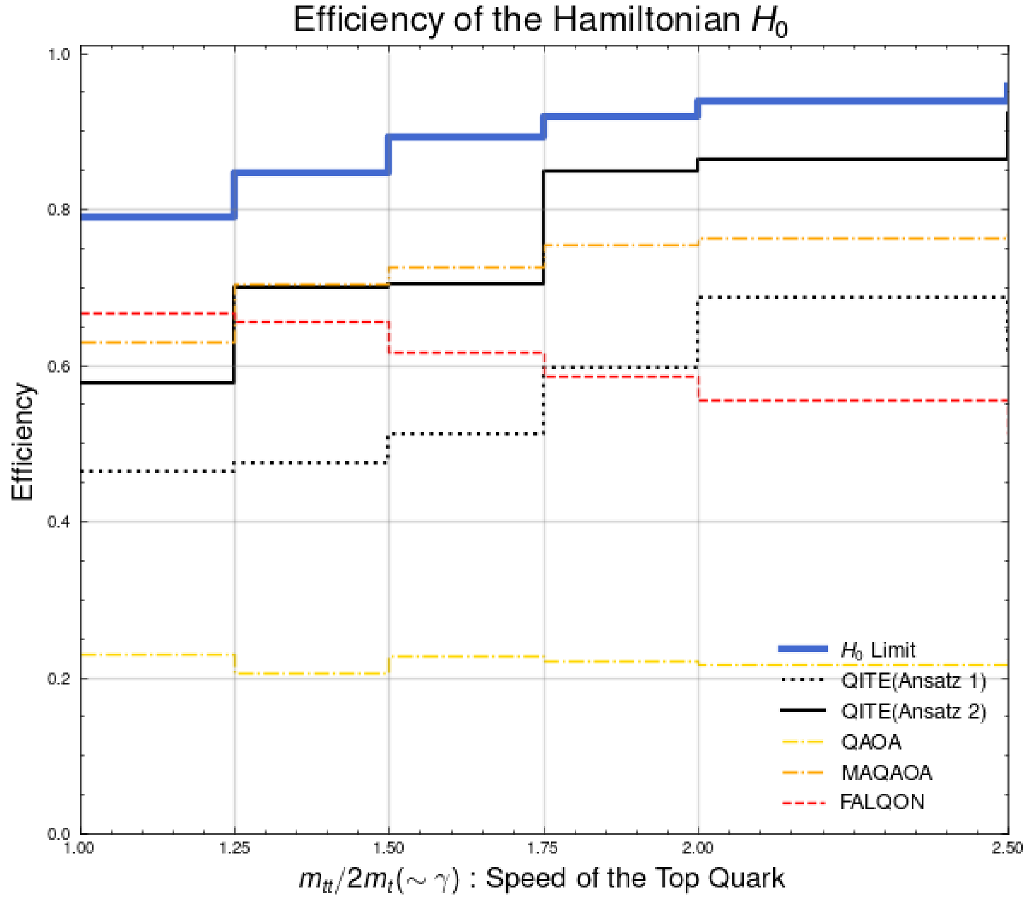
Classical and Quantum Algorithms for Orthogonal Neural Networks : 2106.07198

QITE Result for the Problem $(p\, p \to t\, \bar{t} \to 6\ jets)$

$$H_0 + \lambda H_1 = \sum_{ii} (J_{ij} + \lambda P_{ij})\, s_i s_j$$

$$H_0 = \sum J_{ij} s_i s_j$$





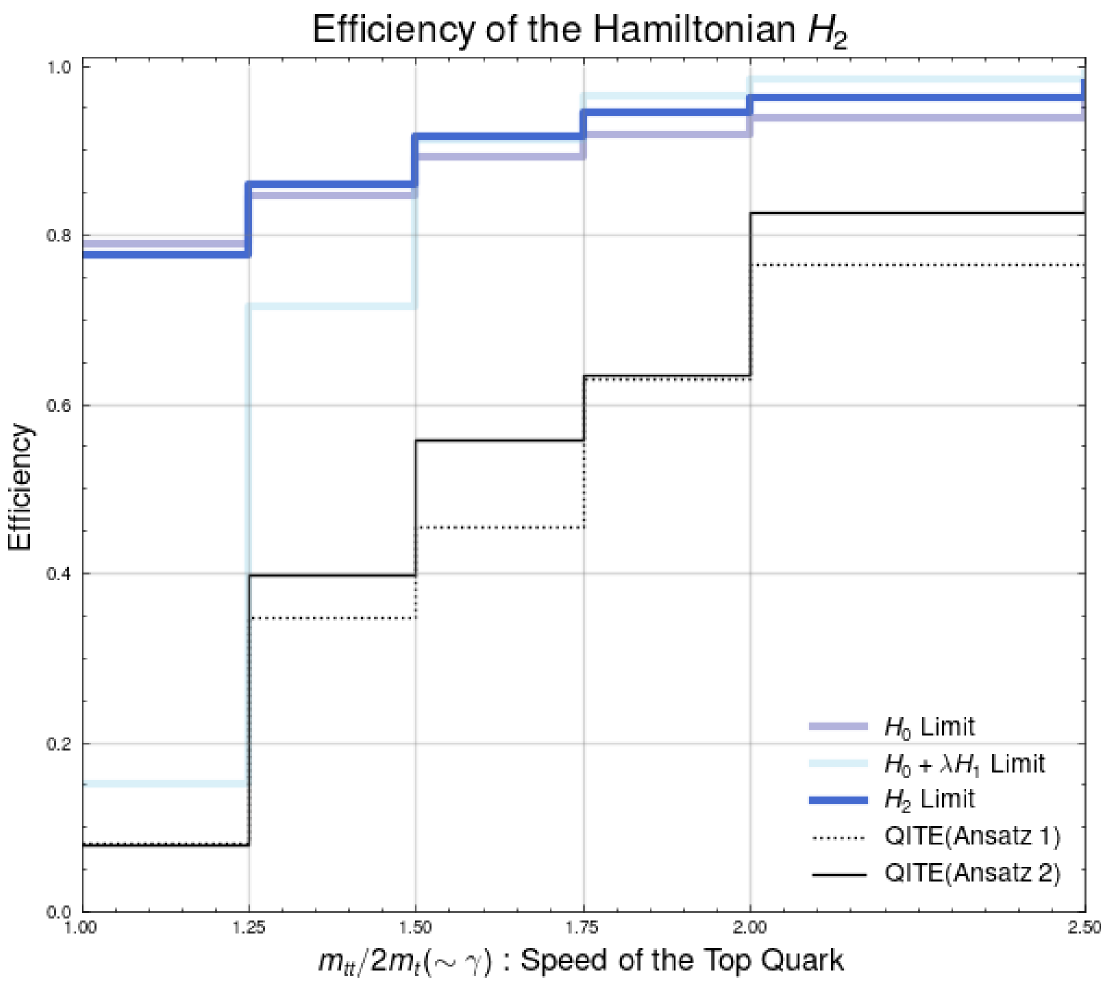
New Hamiltonian Candidate $H_2 = H_0 H_1$

$$H_2 = H_0 H_1$$

$$= (P_1^2 - P_2^2)^2 \cdot (P_1^2 + P_2^2)$$

$$= \frac{1}{2}\left[\left(\sum_{kl} P_{kl}\right) \sum_{ij} J_{ij} s_i s_j + \sum_{ijkl} J_{ij} P_{kl} s_i s_j s_k s_l\right]$$

- It is extended to a problem with higher order (quartic) terms.
- 85% of the time, the ground state of H2 resolves the combinatorial problem
- QAOA is not an efficient algorithm due to many combination of quartic terms.



Conclusion – Back to Our Plan

Understanding basic Idea of Variational Quantum Imaginary Time Evolution

Implement Imaginary Time Evolution with PennyLane

Apply the method to the combinatorial problem at the LHC,

Think about different Hamiltonian ansatz including the higher order terms

Run the developed codes on real hardware

Conclusion - Summary

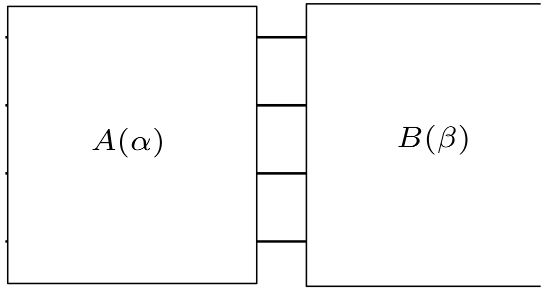
VarQITE for HEP

Merits
- Better than QAOA to solve our problem
- Get some freedom to use Hamiltonian with higher order term

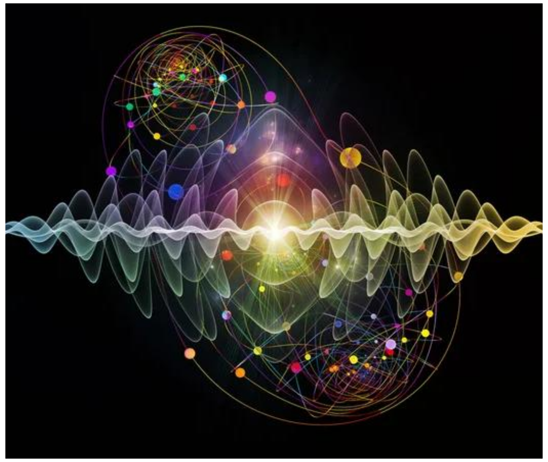
More Applications
- Apply the method to another examples
  - more particles, anti-symmetric energy group …

Hardness
- Hard to efficiently solve the Hamiltonian with non-constant coefficients
- Convergence Problem : Struggle in a local minimum

Conclusion - Future Developments & Works



Explore Different Ansatz



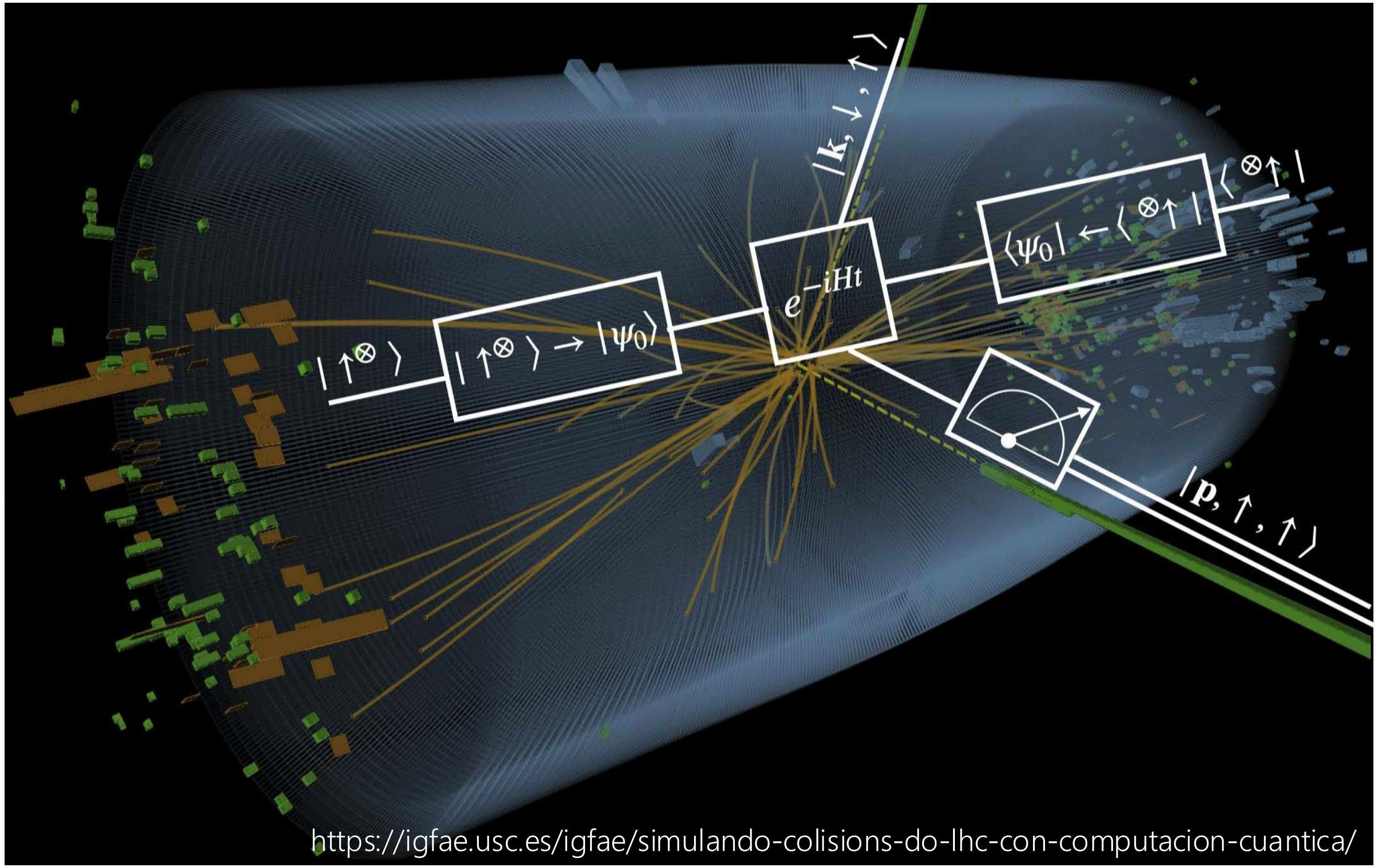
Investigate Impact of Noise

Run VarQITE on Real Quantum Hardware

Thank you

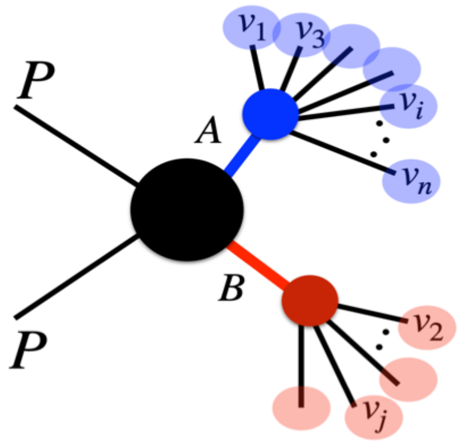
Code & Data Availability
https://github.com/HeechanYi/VarQITE_for_HEP

Appendix



https://igfae.usc.es/igfae/simulando-colisions-do-lhc-con-computacion-cuantica/

Designing a Hamiltonian for the Combinatorial Problem



$$P_1 = \sum_{i=1}^{n} p_i \, x_i \,,$$

$$P_2 = \sum_{i=1}^{n} p_i \, (1 - x_i) \,,$$

$$H_0 = (P_1^2 - P_2^2)^2$$

$$\begin{aligned} H_0 &= \left(\sum_{ij} P_{ij} x_i x_j - \sum_{ij} P_{ij} (1 - x_i)(1 - x_j) \right)^2 \\ &= \left(\frac{1}{4} \sum_{ij} P_{ij} \left[(1 + s_i)(1 + s_j) - (1 - s_i)(1 - s_j) \right] \right)^2 \\ &= \left(\sum_{ij} P_{ij} s_i \right)^2 = \sum_{ij} J_{ij} s_i s_j \,, \end{aligned} \tag{4}$$

$$\begin{aligned} H_1 &= (P_1^2 + P_2^2) \\ &= \frac{1}{4} \sum_{ij} P_{ij} \left[(1 + s_i)(1 + s_j) + (1 - s_i)(1 - s_j) \right] \\ &\to \frac{1}{2} \sum_{ij} P_{ij} s_i s_j \,, \end{aligned} \tag{5}$$

$$x_i = \frac{1 + s_i}{2}$$

$$P_{ij} = p_i \cdot p_j$$

$$J_{ij} = \sum_{k\ell} P_{ik} P_{j\ell},$$

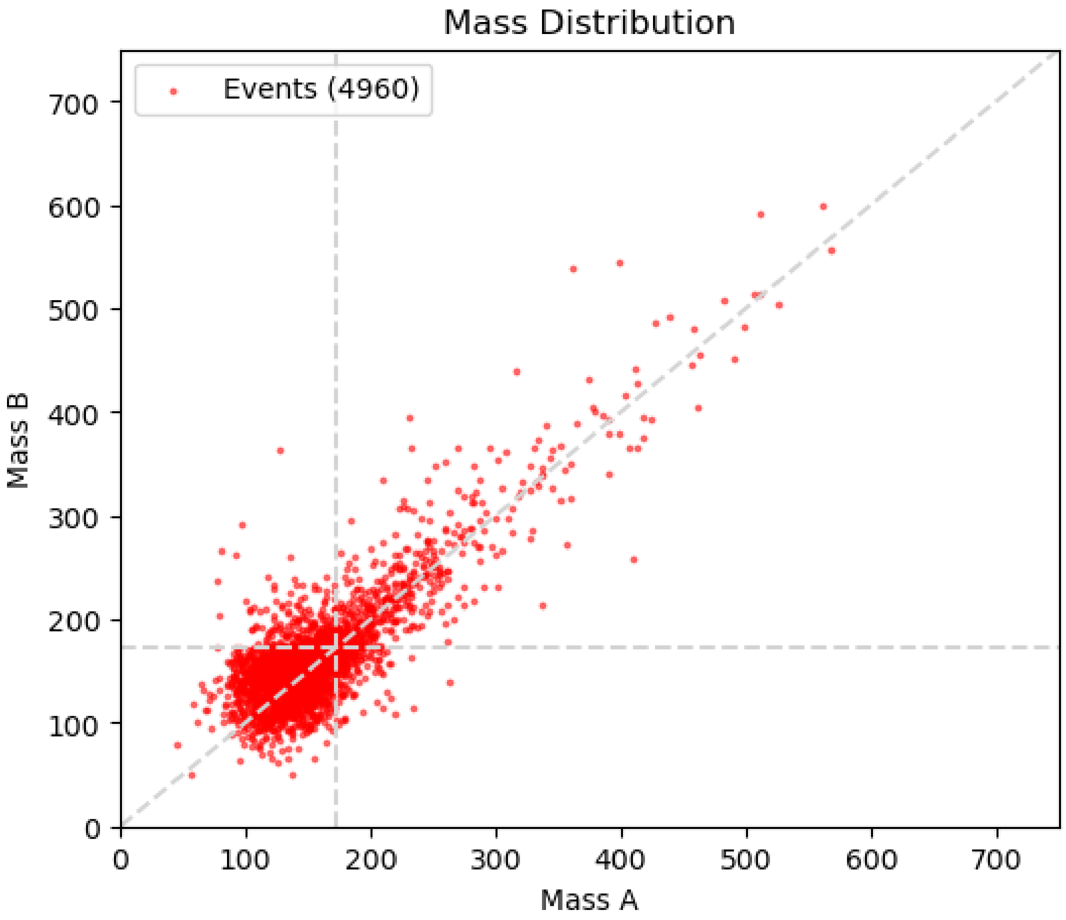
Problem Hamiltonian Candidate

$$H_P = H_0 + \lambda H_1$$

Where $\lambda = \min(J_{ij}) / \max(P_{ij})$

Hybrid quantum-classical approach for combinatorial problems at hadron colliders: 2410.22417

QITE Clustering and Mass Distribution



Problem Hamiltonian

$$H_P = H_0 + \lambda H_1$$

Where $\lambda = \min(J_{ij}) / \max(P_{ij})$

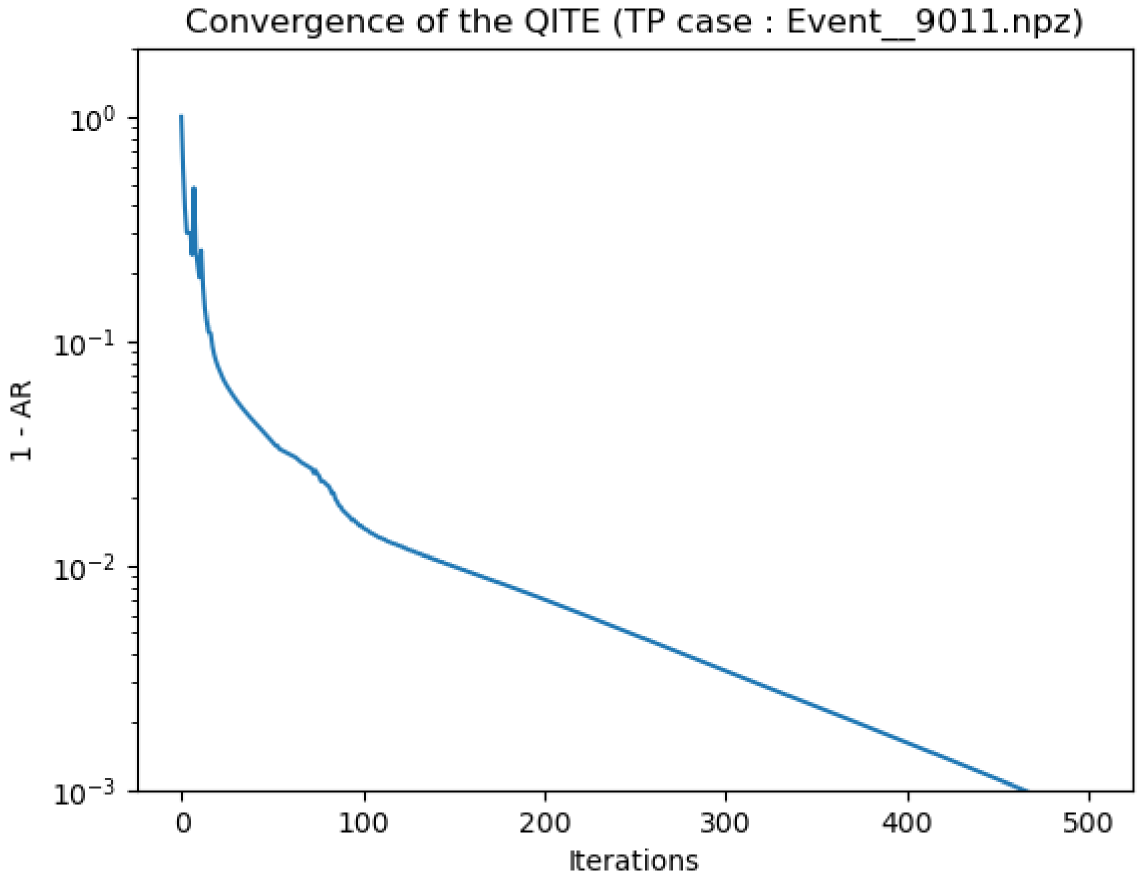
★ Confusion matrix

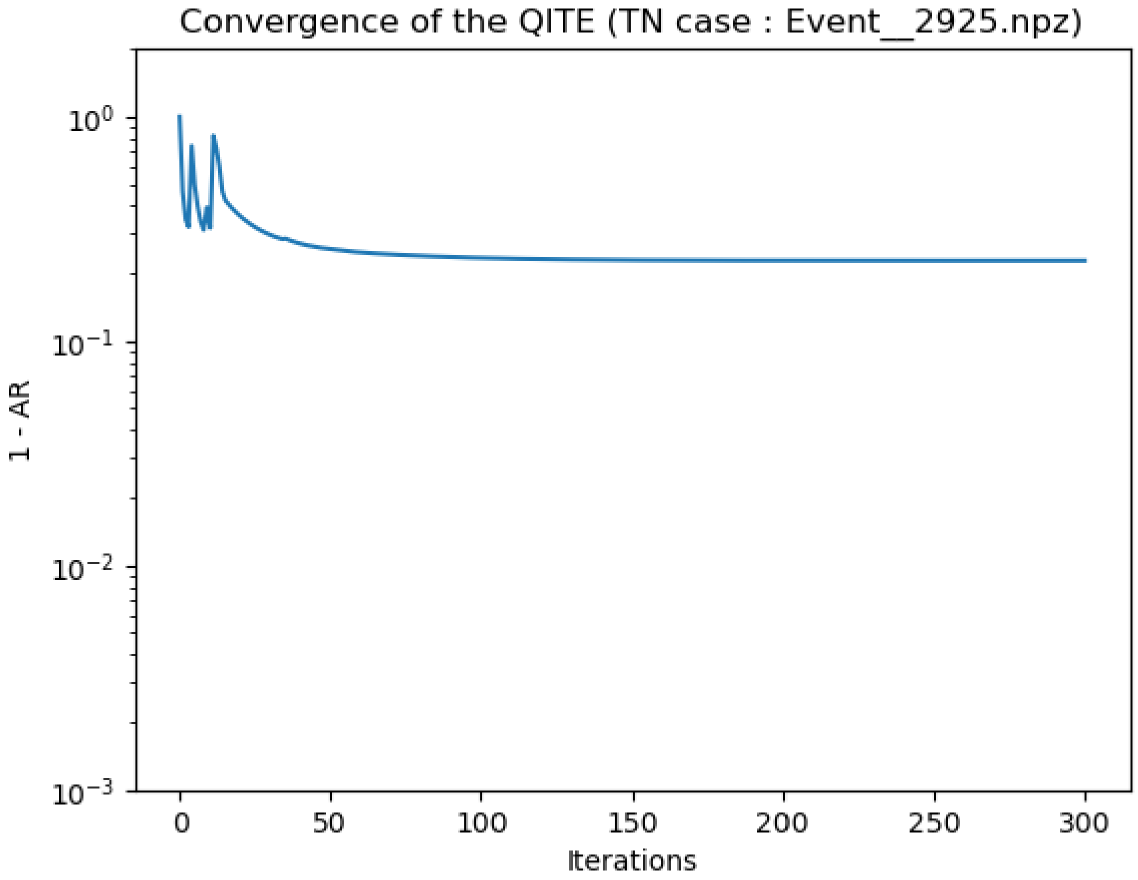
```
True Positive Convergence : 2163 / 4960 (43.608870967741936 %)
False Positive Convergence : 1888 / 4960 (38.064516129032256 %)
Ground Sate Converging Rate : 81.67338709677419 %
---------------------------------------------------------------------
True Negative Convergence : 720 / 4960 (14.516129032258066 %)
False Negative Convergence : 189 / 4960 (3.8104838709677415 %)
Non Ground Sate Converging Rate : 18.326612903225808 %
---------------------------------------------------------------------
```

True : The Hamiltonian resolves the combinatorial problem

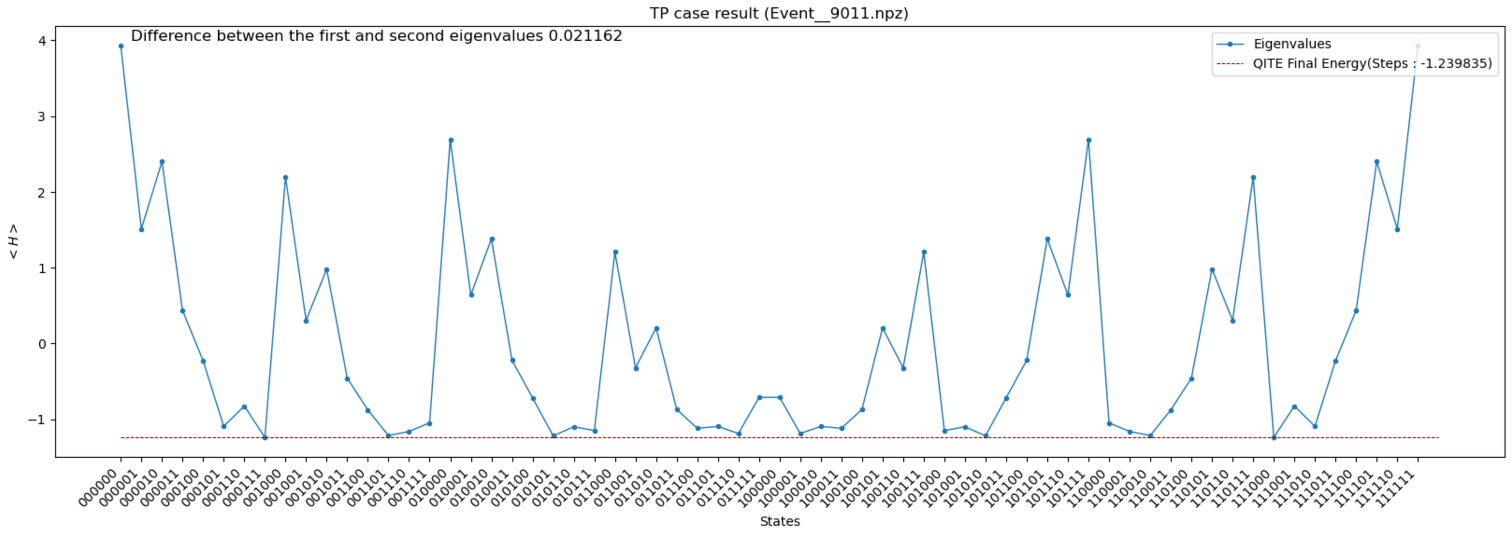
Positive : QITE reaches to the Hamiltonian ground state

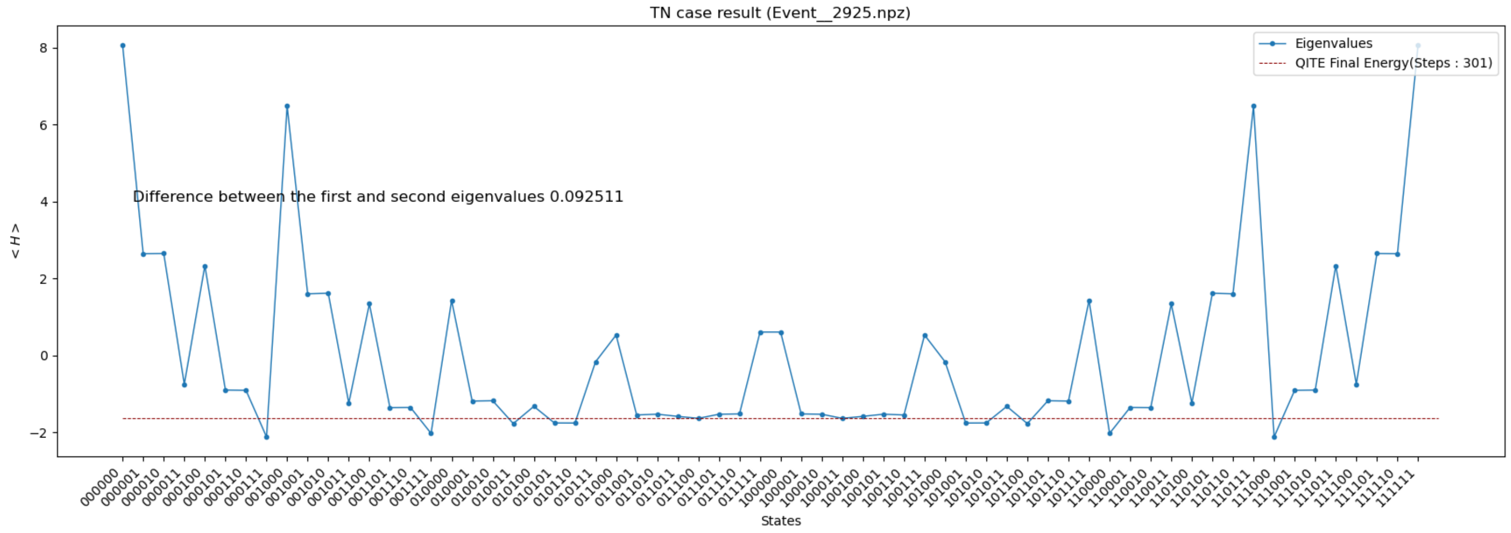
Convergence of QITE





Problem Hamiltonian's$(H_0 + \lambda H_1)$ Energies





Problem Hamiltonian's$(H_0 + \lambda H_1)$ Energies