Quantum Computing Initiative for High Energy Physics

박명훈

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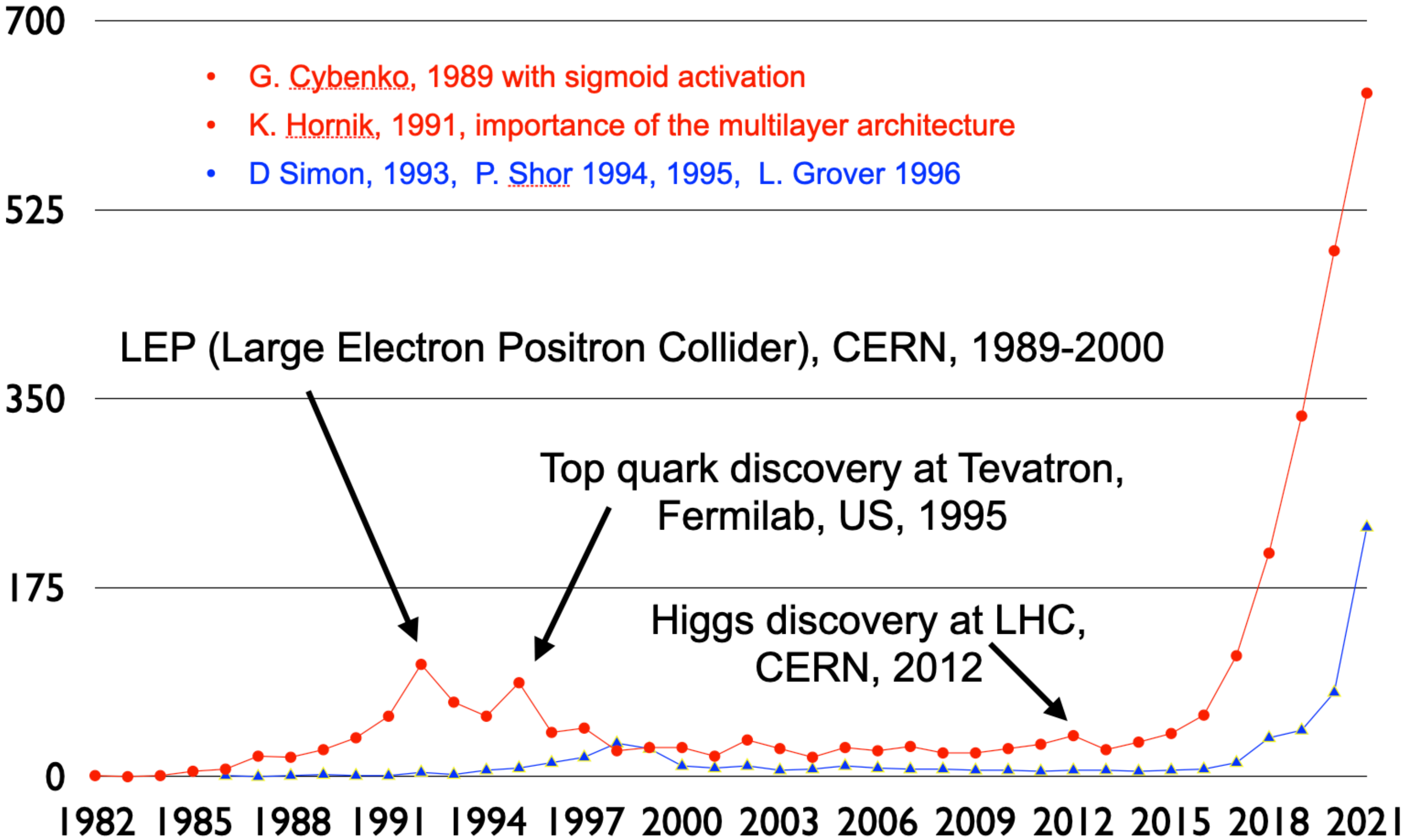
한국 고에너지 물리학회 2023 가을 학술대회

High Energy Physics with new computing methods

High Energy Physics & Computing frontier

Data is obtained via **InspireHEP**

- ● The number of papers (in high energy physics) that has a keyword "Machine Learning", "Deep Learning", "Artificial Intelligence" or "Neural Networks" in their title.
- ▲ The number of papers that has a keyword "Quantum Computer", "Quantum Computing","Quantum Annealing" or "Quantum Machine Learning" in their title.



Now everything is related to

"**Quantum**"

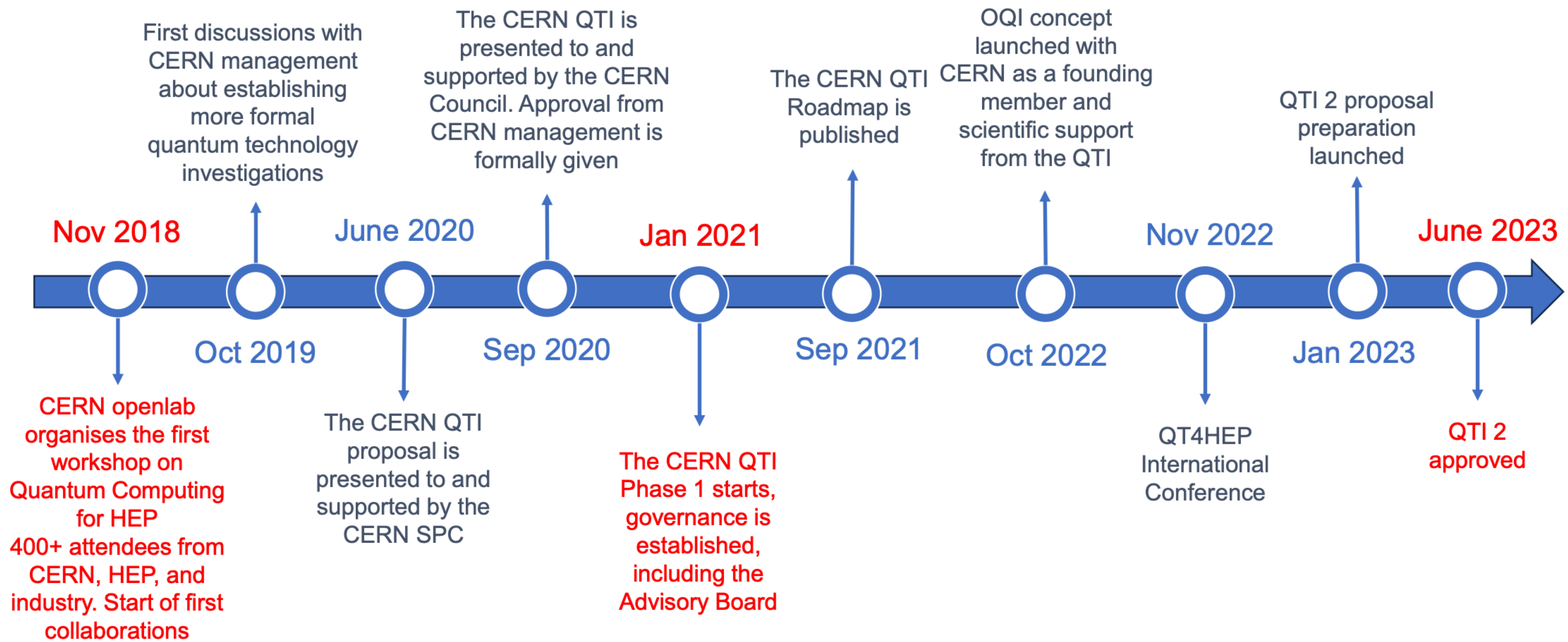
Quantum Innovative

- **CERN**: **Quantum Technology Initiative (2021)**
  - **Quantum Computing and Algorithm**
  - Quantum theory and simulation
  - Quantum Sensing
  - Quantum communication and network

- **Fermilab**: **Quantum Institute (2019)**
  - **Quantum Computing applications and Simulations**
  - Quantum Sensing
  - Quantum communication
  - Electronics and controls for Quantum

more on CERN QTI

CERN and Quantum Technologies



From Alberto Di Meglio's slide (CERN QTI Phase 1 Coordinator)

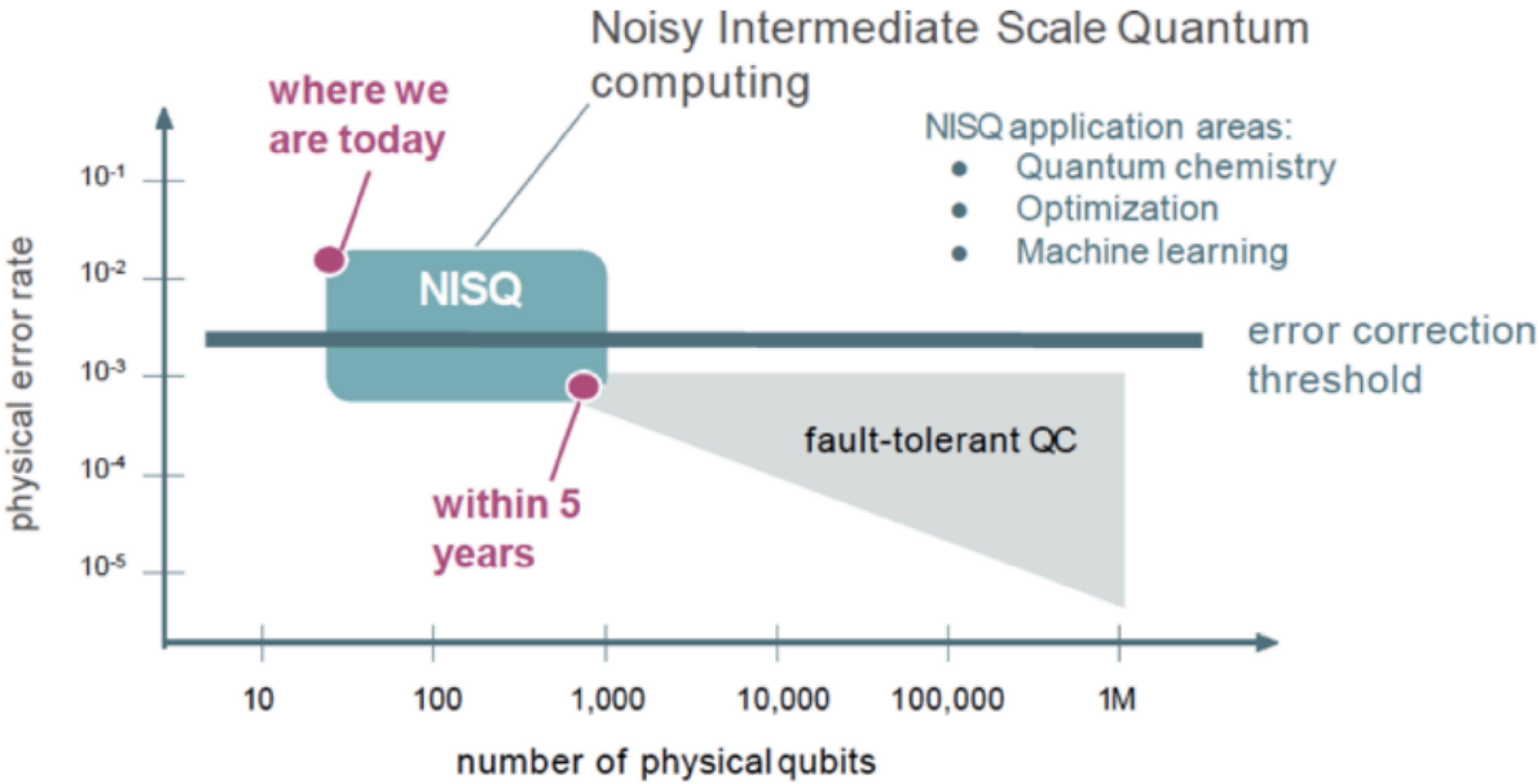
Quantum Hype?
Can we have a good QPU ?

NISQ

- Noisy Intermediate-Scale Quantum (NISQ): John Preskill

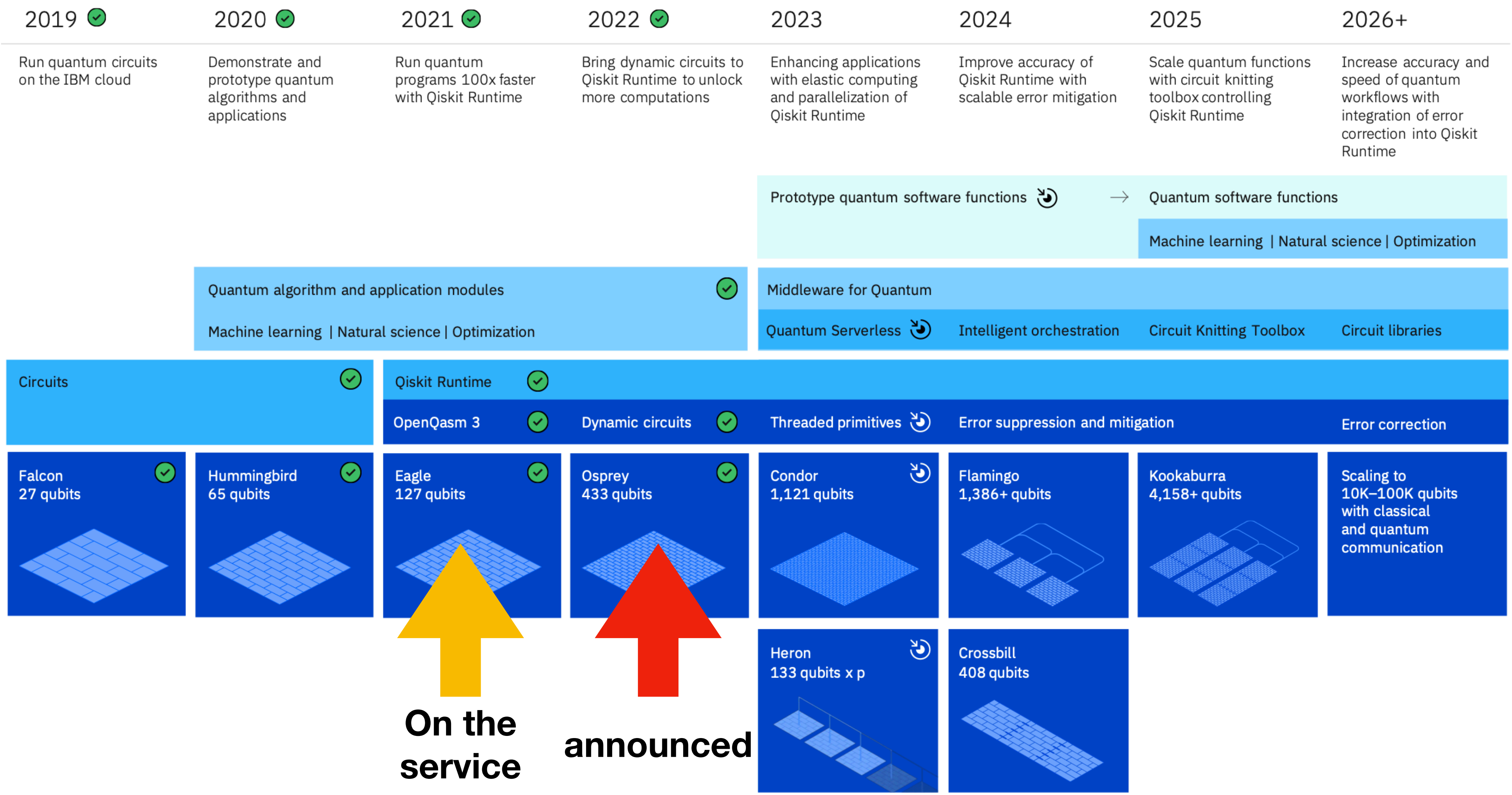
Theoretical physicist
Caltech(Ph.D advisor : Steven Weinberg@Harvard, 1980)

- An advocator of QC/QI area



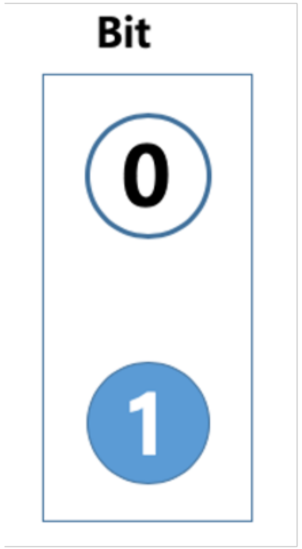
Into the realm of "tech" from science

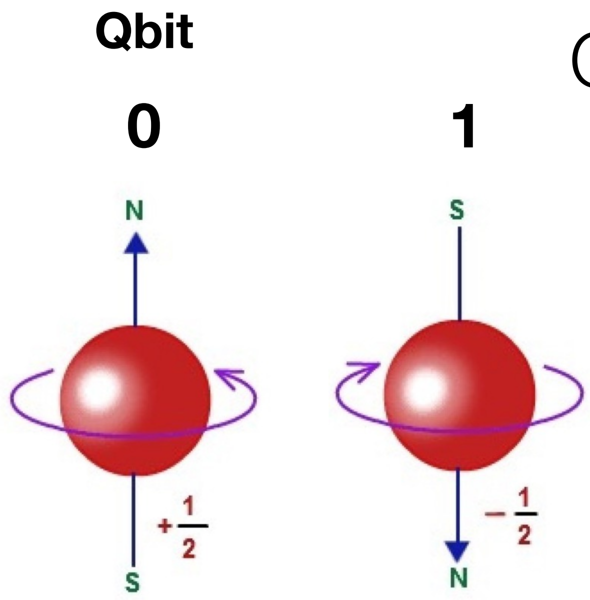
- IBM Development roadmap



What is the magic behind Quantum Computer ?

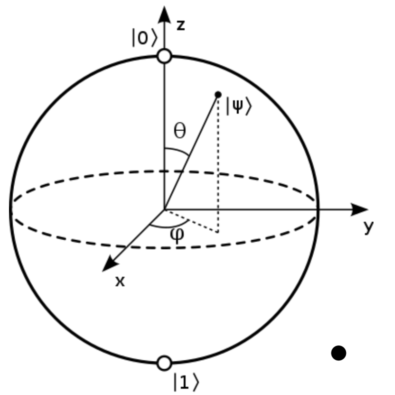
Basic of Qubit





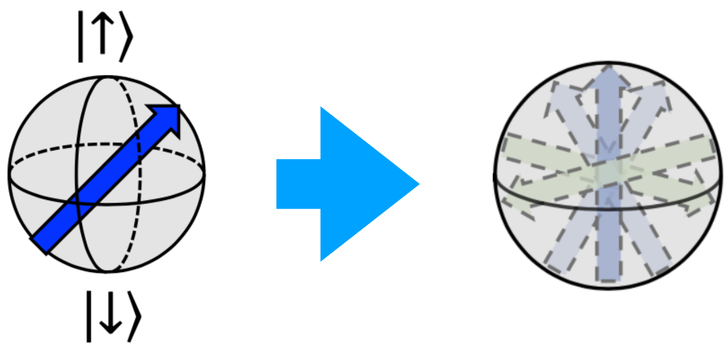
Quantum **Superposition**

$$|\Psi\rangle = a|0\rangle + b|1\rangle$$

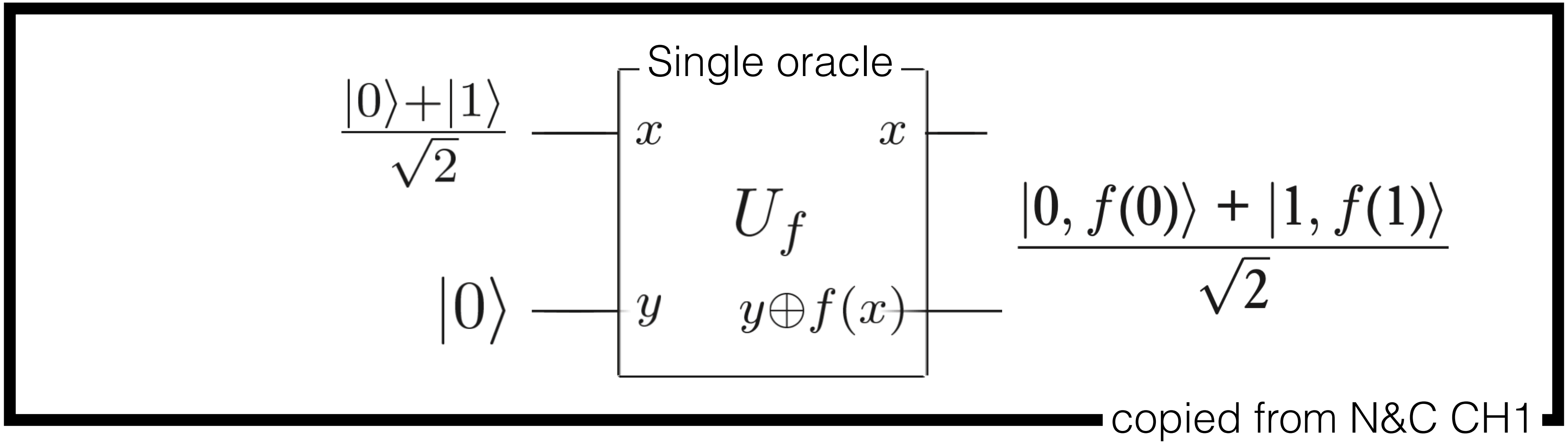


- Bloch sphere

- Classical gate: Two operations (NOT, and Identity) on a bit
- Quantum Gate:**"Infinite" operation**



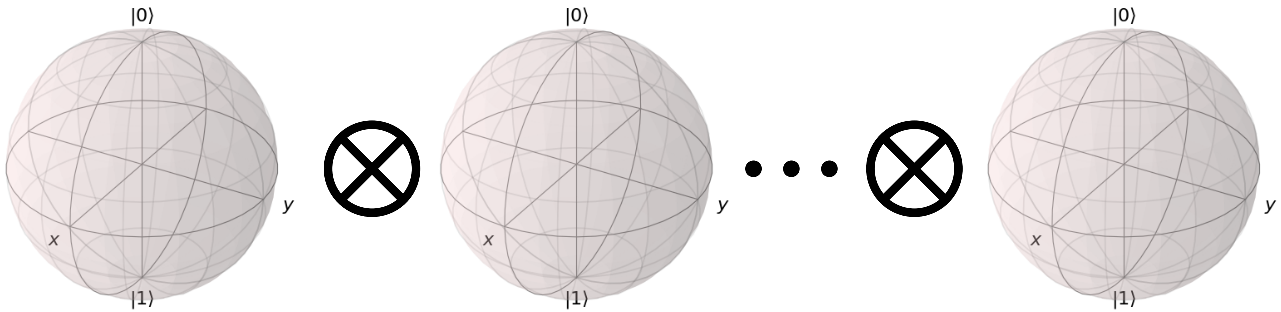
Quantum superposition



- leads to "**quantum parallel**" computing (through Quantum Entanglement)

Quantum Hilbert space

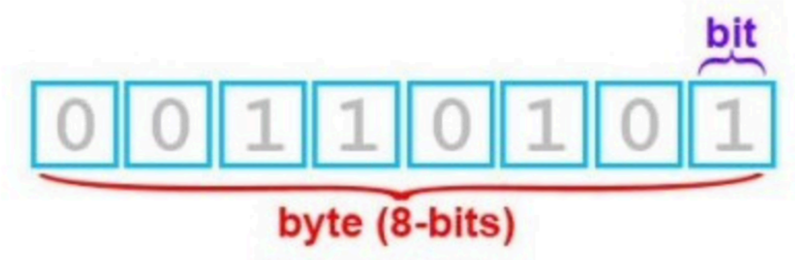
$$|\Psi\rangle = \sum a_{i_1 i_2 \cdots i_n}$$



- Expressing and manipulating input data in an **exponentially large (2^n) and "compact" Quantum Hilbert Space**.

Power of $\mathcal{O}(100)$ logical Qubits

- With quantum superposition, 100 qubits contains 2^{100} bit information



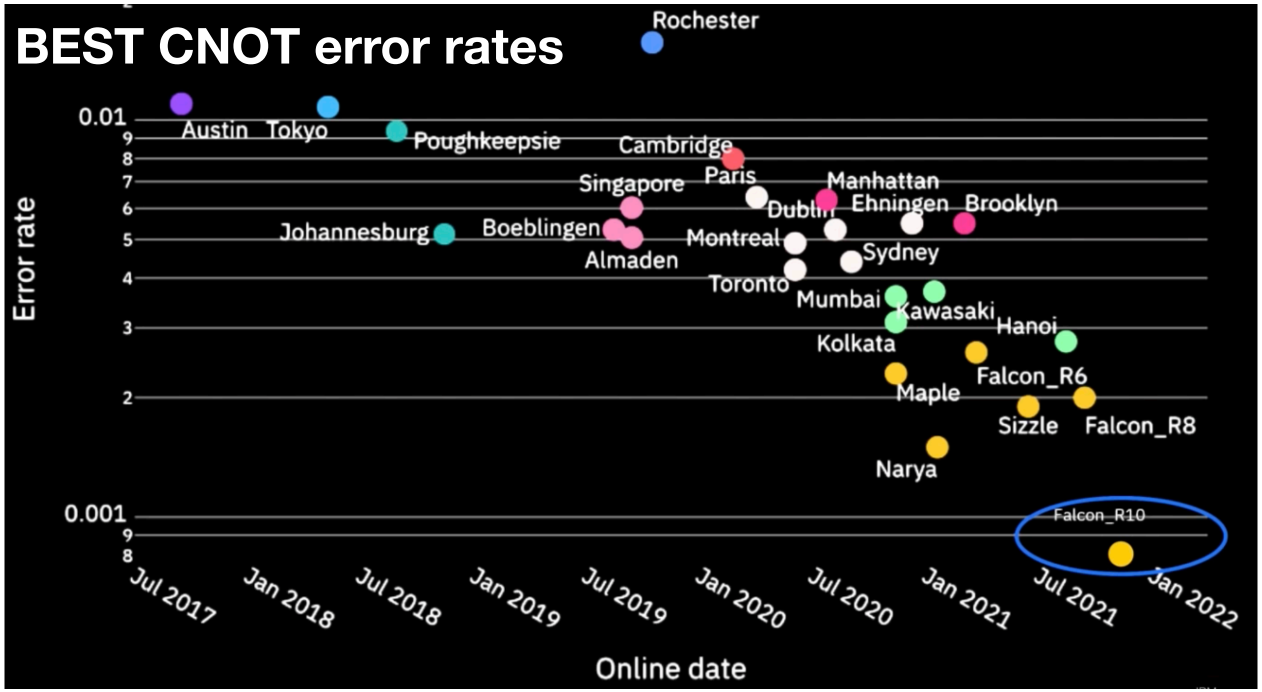
3 qubit= 2^3 bit info. = 8 bit = 1 byte (1B)

43 qubits=2^{43} bit information = $2^{43}/8 = 2^{40}$ byte =

$$\left(2^{10}\times\frac{1\text{KB}}{1\text{Byte}}\right)\times\left(2^{10}\times\frac{1\text{MB}}{1\text{KB}}\right)\times\left(2^{10}\times\frac{1\text{GB}}{1\text{MB}}\right)\left(2^{10}\times\frac{1\text{TB}}{1\text{GB}}\right) = 1\text{TB}$$

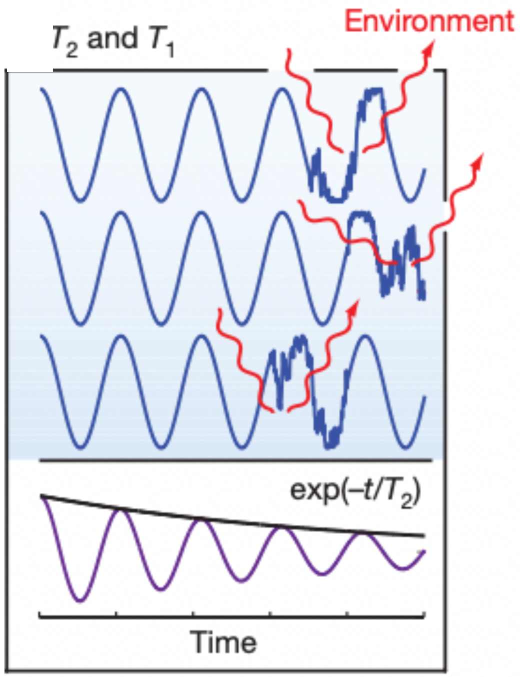
- Thus, **100** qubits :
  2^{100} bit $\simeq 2\times10^{25}\,\text{TB}$

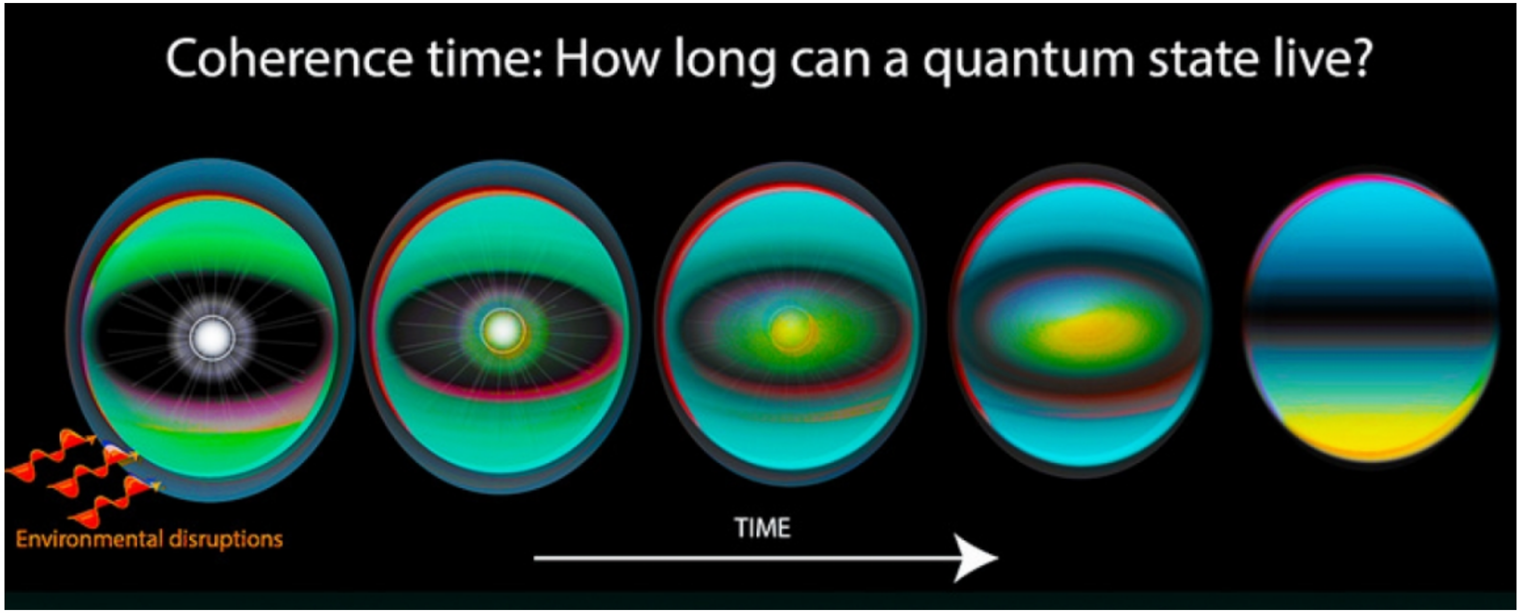
  - Error rate:
    1/ 1000 qubits



Maintain "Quantum-ness"

- "Coherence time" sets a limit on the calculation time



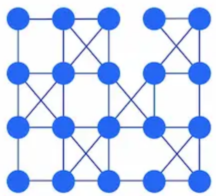
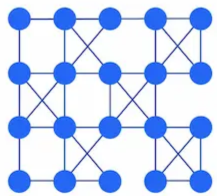
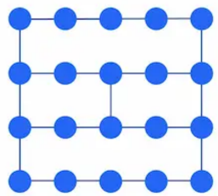
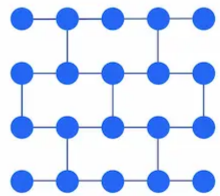
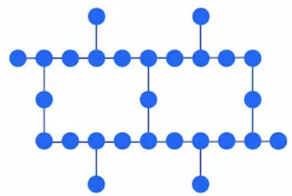


Type of qubit	T_2
Infrared photon	0.1 ms
Trapped ion	15 s
Trapped neutral atom	3 s
Liquid molecule nuclear spins	2 s
e^- spin in GaAs quantum dot	3 μs
e^- spins bound to ^{31}P:^{28}Si	0.6 s
^{29}Si nuclear spins in ^{28}Si	25 s
NV centre in diamond	2 ms
Superconducting circuit	4 μs

- This provides limits not only the operation time but also the connectivity among qubits.

More than Logical Qubits

- We need a "connection" to operate between arbitrary two qubits (e.g. controlled-gate)

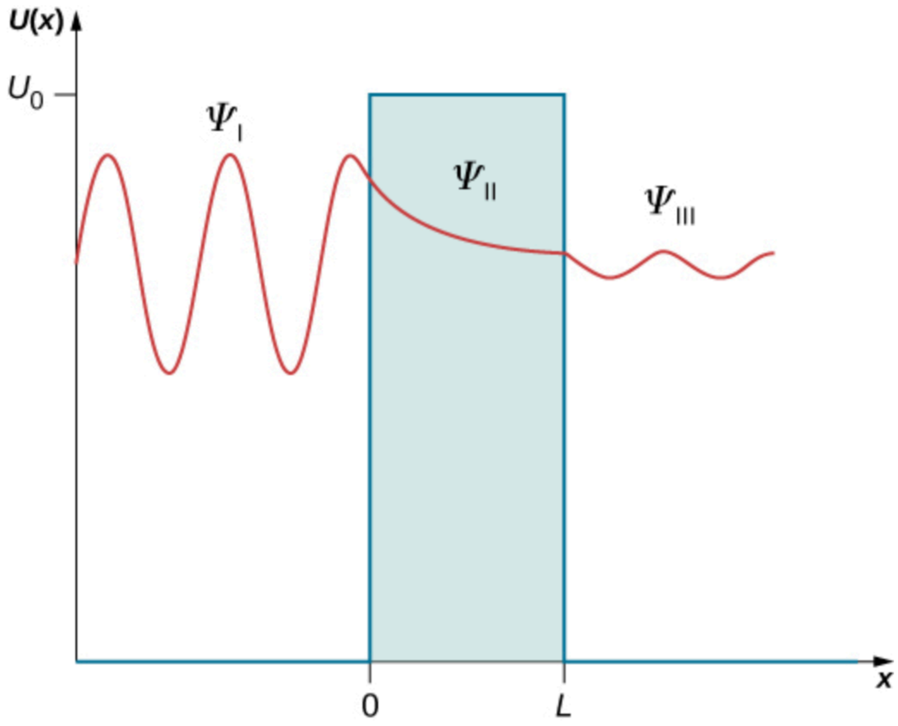
Processor	Penguin v1	Penguin v2	Penguin v3	Penguin v4	Falcon r4
					
Avg. qubit connectivity	3.9	3.7	2.3	2.3	2.1

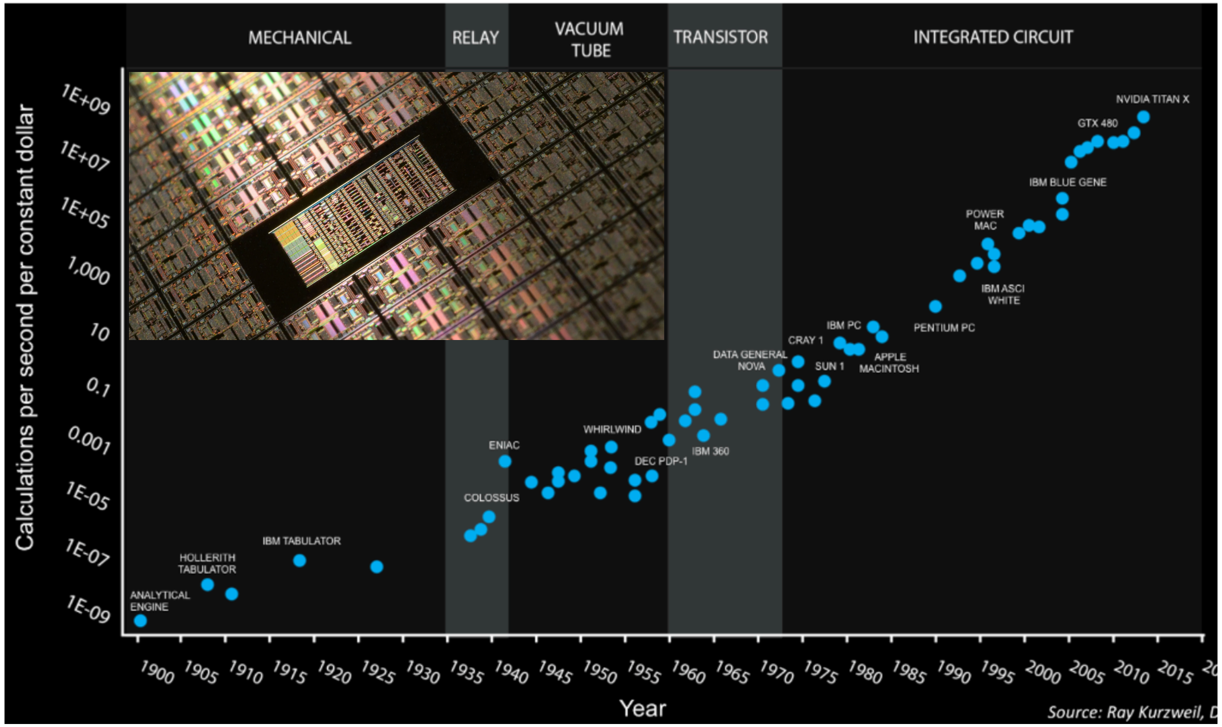
- Due to "error-propagation", Gated-QC reduces the connectivity

= # of required qubits to program > # of (logical) qubits in an algorithm

Another "Quantum"

Quantum tunneling



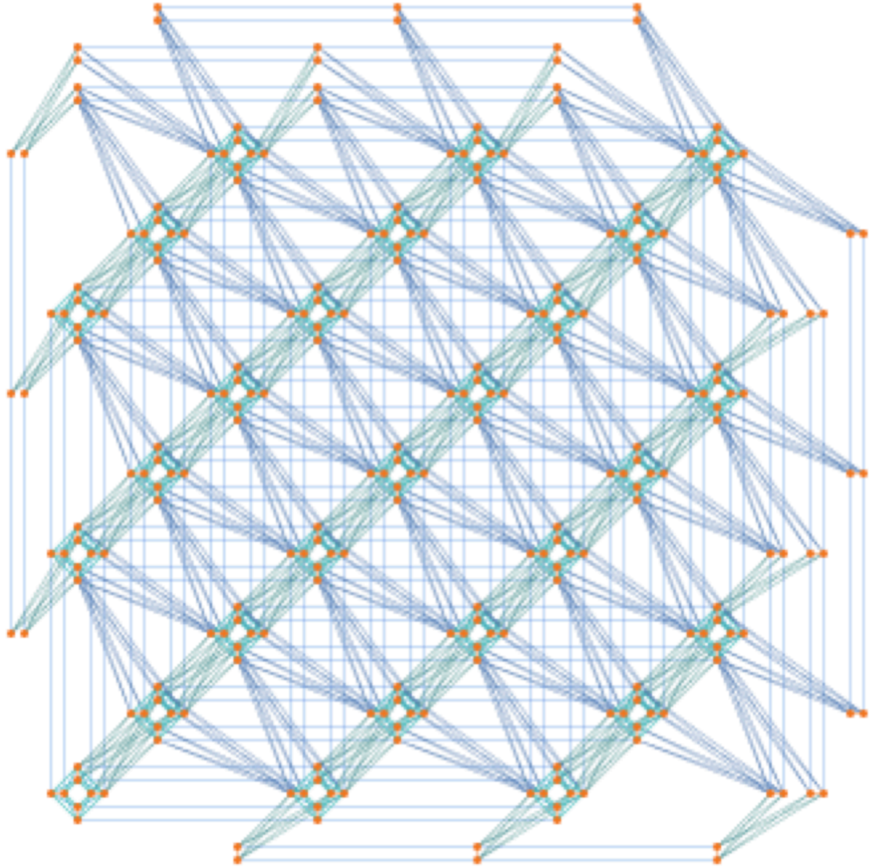


- which is the big "barrier" to make very tiny chip,

  There would be the end of Moore's law
  - uncontrolled leakage from Quantum tunneling gives the errors in computing

"Quantum" annealer

	2000Q	Advantage
Graph topology	Chimera	Pegasus
Graph size	C16	P16
Number of qubits	> 2000	> 5000
Number of couplers	> 6000	$> 35,000$
Couplers per qubit	6	15



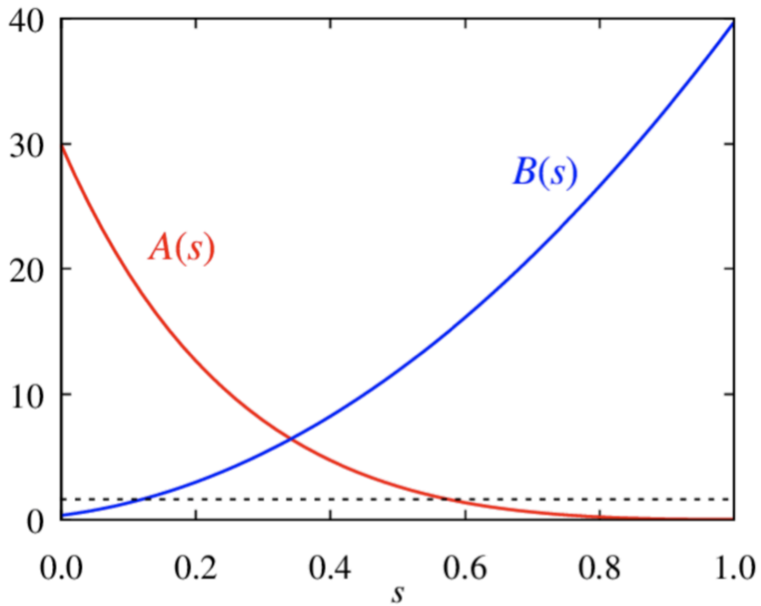
- Current "Advantage" machine has **5000+ qubits** (though limited couplers ~ 35,000 $\ll {}_{5000}C_2 \simeq 10^7$

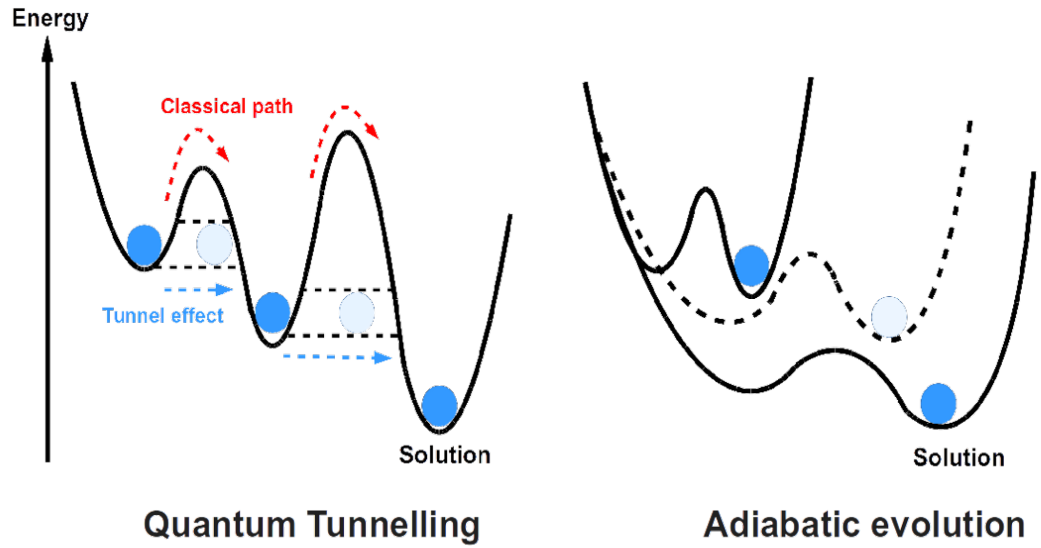
Quantum Annealing

- With adiabatic theorem, we can find the ground state of a complicate hamiltonian H_{QUBO} starting from simple H_0.

$$H_{\text{QA}} = A(s)\,H_0 + B(s)\,H_{\text{QUBO}} \text{ with } H_0 = \sum \sigma_i^x \text{ and } H_{\text{QUBO}} = \sum J_{ij}\sigma_i^z\sigma_j^z + \sum h_i\sigma_i^z$$

(T. Kadowaki and H. Nishimori, Quantum annealing in the transverse ising model, 1998)





- Annealing time $< 2000\mu s$, (mostly) $\mathcal{O}(10)\mu s$

"Quantum annealing"

- claims to utilize "quantum tunneling" to find the minimum of the hamiltonian

$$H_{\mathrm{QUBO}} = \sum J_{ij}\sigma_i\sigma_j + \sum h_i\sigma_i$$

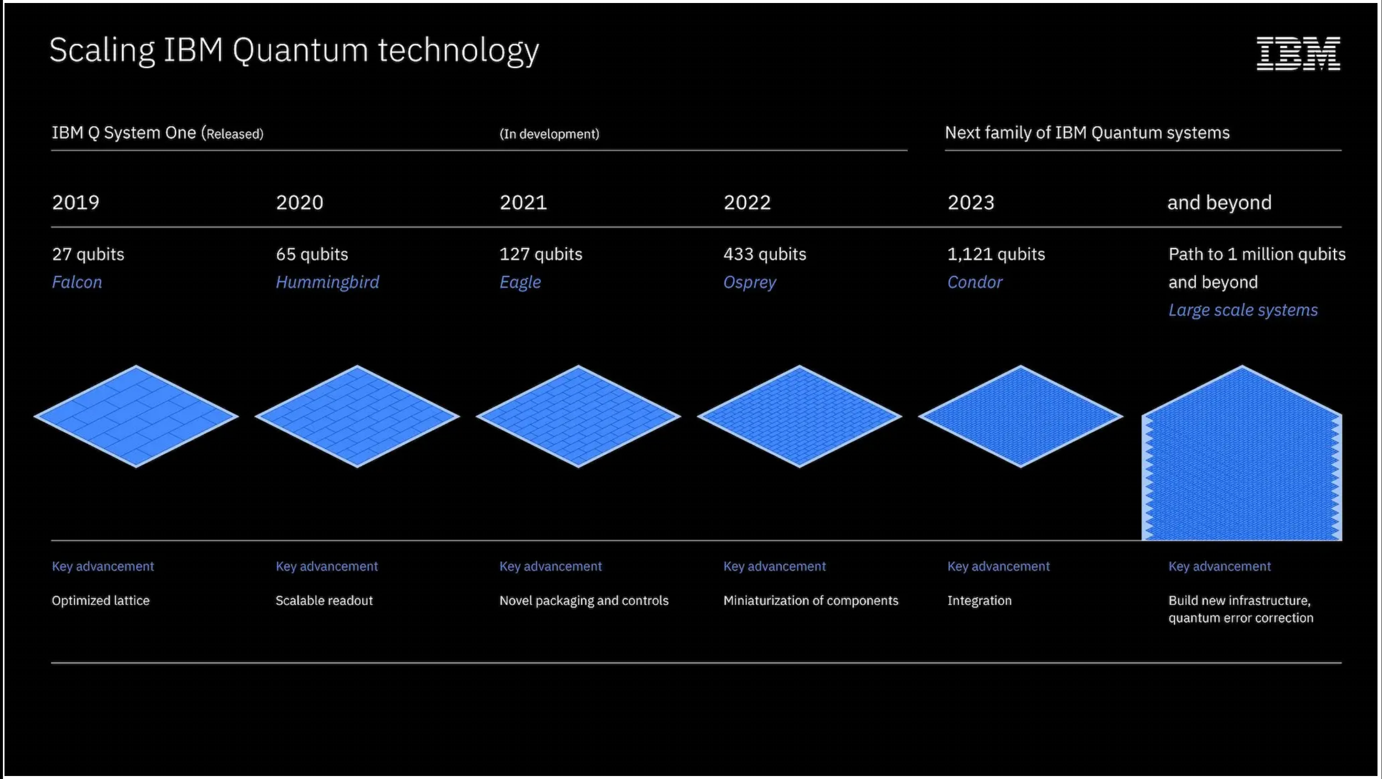
for **Q**uadratic **U**nconstrained **B**inary **O**ptimization problems. (to attack various NP - hard problems)

In short, Digital and Analog QC

- Gate type QC: Programable Quantum Computer

- Annealing type QC: "Optimizing" Hamiltonian

currently 433 Qubits (IBM Ospery)



Quantum Annealer

Temperature: below 1.5×10^{-2}K
dimension: $3\text{m} \times 2.1\text{m} \times 3\text{m}$
Weight: 3800kg
Power: (max) 25kW

The virtue of Quantum-ness

- Superposition principle : $|\Psi\rangle = a_0|0\rangle + a_1|1\rangle$

- Quantum entanglement : $|\Psi\rangle = |\Psi_0\Psi_1\cdots\Psi_N\rangle$
  - obtaining "large" data space
  - so called "Quantum parallelism"

Quantum Gate Machine

- Quantum tunneling

Quantum Annealing Machine

Computer which utilizes full "Quantum-ness"

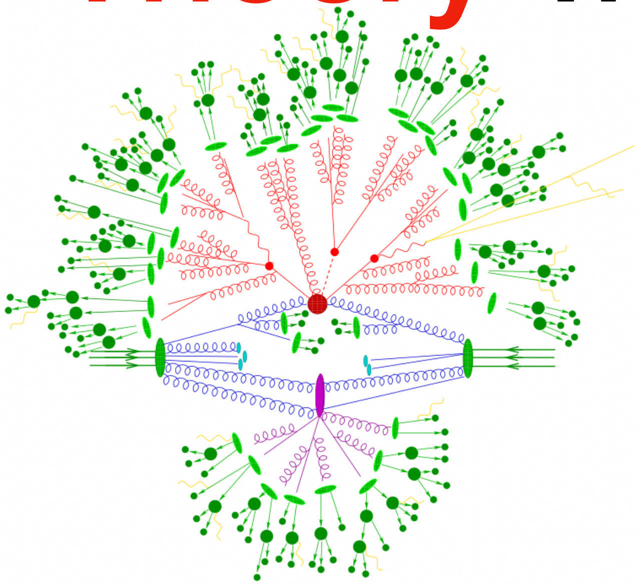
- R. Feynman: You need **more than** a classical computer.

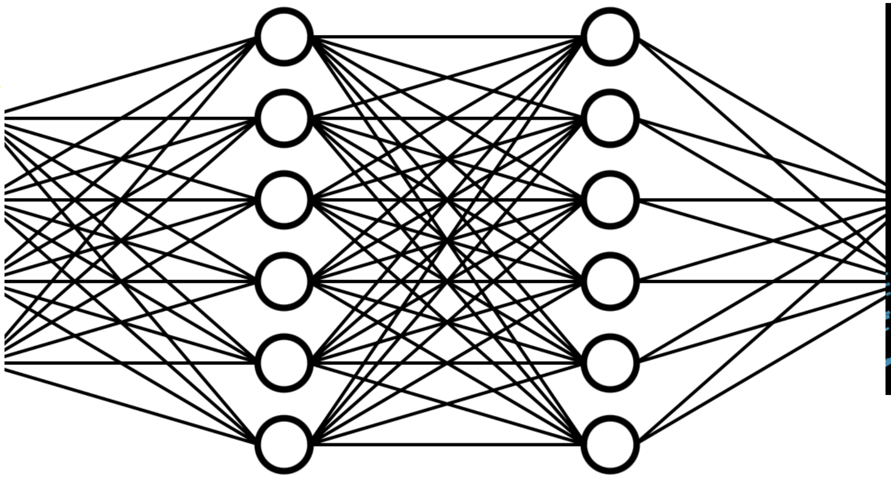
. . . trying to find a computer simulation of physics seems to me to be an excellent program to follow out. . . . the real use of it would be with quantum mechanics. . . . Nature isn't classical . . . and if you want to make a simulation of Nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.
—1981

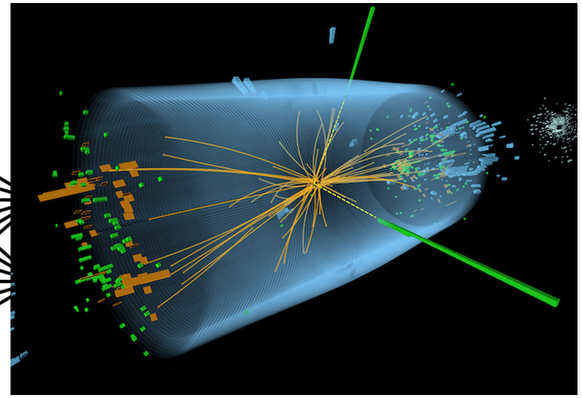
Example @ Collider

Collider experiments

Theory-Machine Learning-Data







- With a **fundamental theory** of particle interactions

  1) Get **expectations** from **MC simulations**

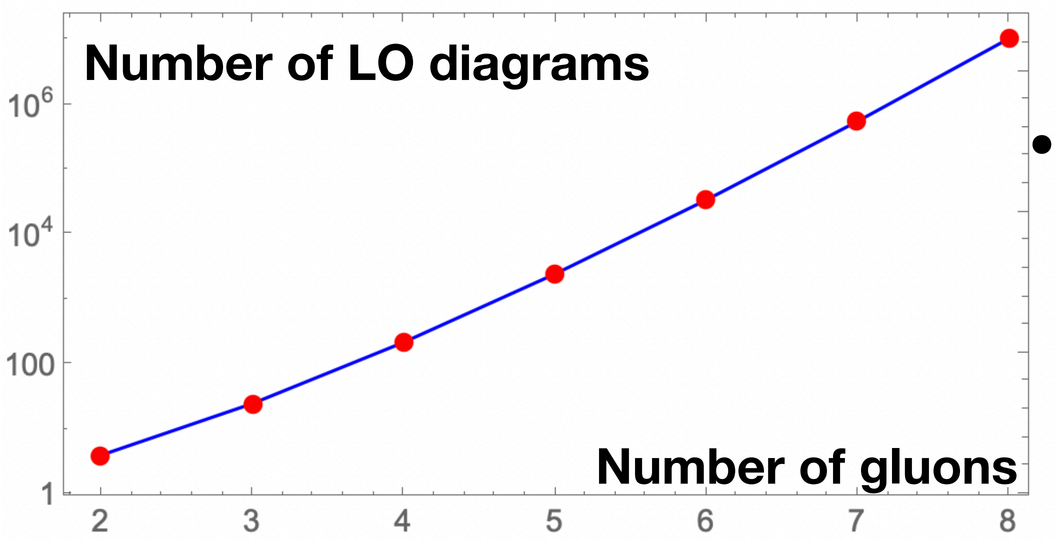
  2) Get **data** from **experiments** (LHC)

  3) Compare our expectation to data with sophisticated computer **algorithms (ML)**

1) Exponential Growth in # of diagrams

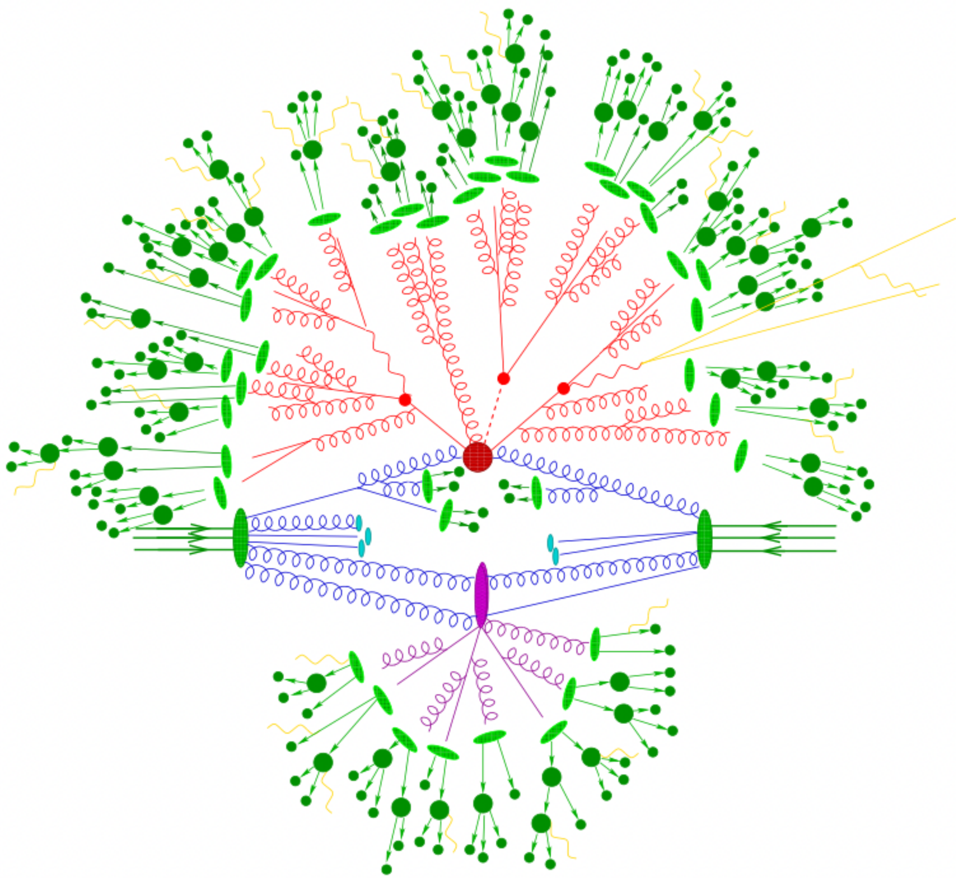
- Calculating an amplitude with multi-jet (gluon) is always challenging

	$gg \to 2g$	$gg \to 3g$	$gg \to 4g$	$gg \to 5g$	$gg \to 6g$	$gg \to 7g$	$gg \to 8g$
Number of LO diagrams	4	25	220	2,485	34,300	559,405	10,525,900



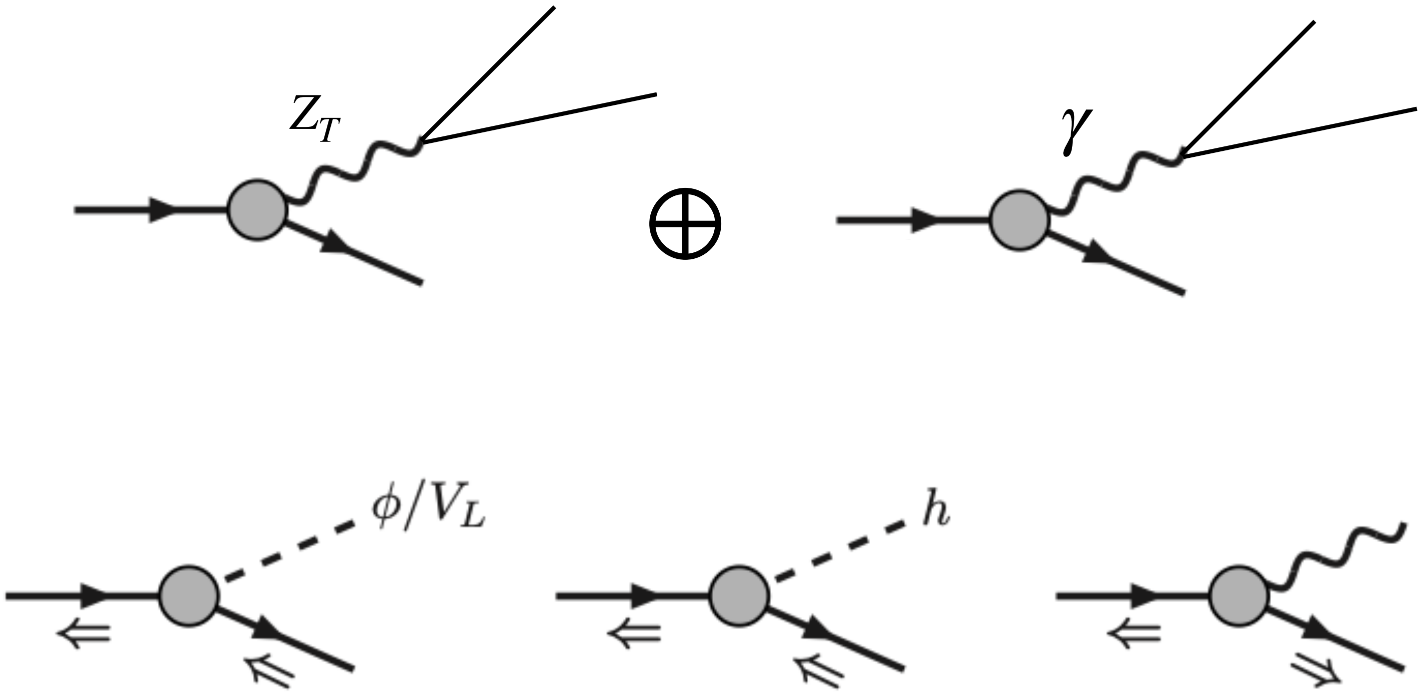
- The number of Feynman diagrams explodes ! This would become a serious issue for FCC, the next level of High Energy Collider.

2) Radiations from "charged" particles



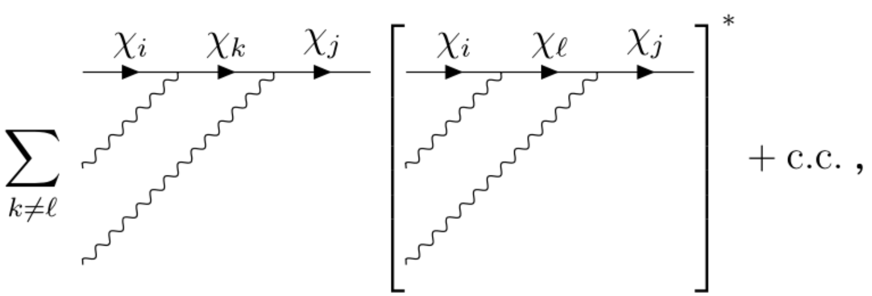
- Electroweak Radiations !

- Problems of **EW Radiation**
  - One needs to consider **Quantum Interference**



- Quantum algorithm for HEP simulations **(Toy example)**
  - So Chigusa et.al, (2022)

$$\mathcal{L}_{\rm dark} = \bar{\chi}(i\not\partial - m_\chi + ig\not A')\chi - \frac{1}{4}F'_{\mu\nu}F'^{\mu\nu} + \frac{1}{2}m^2_{A'}A'_\mu A'^\mu$$



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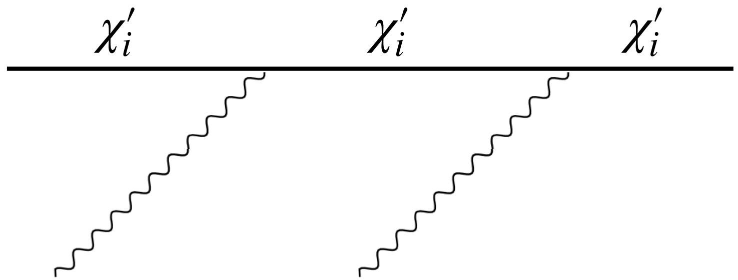
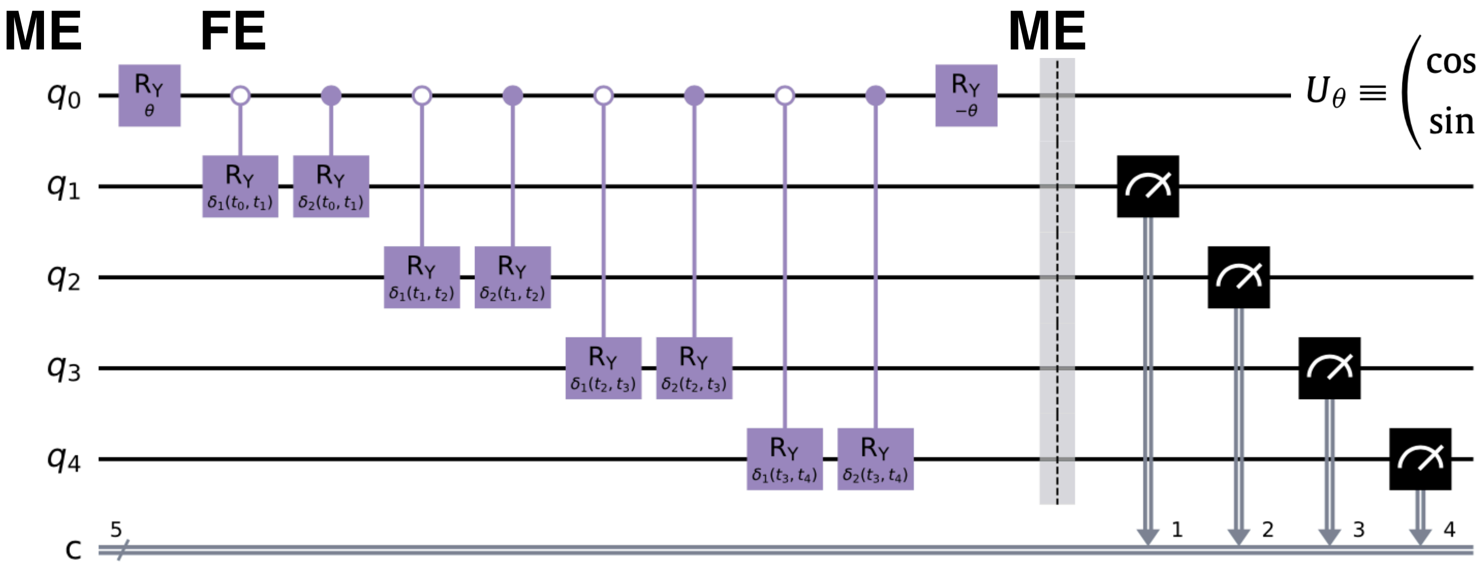


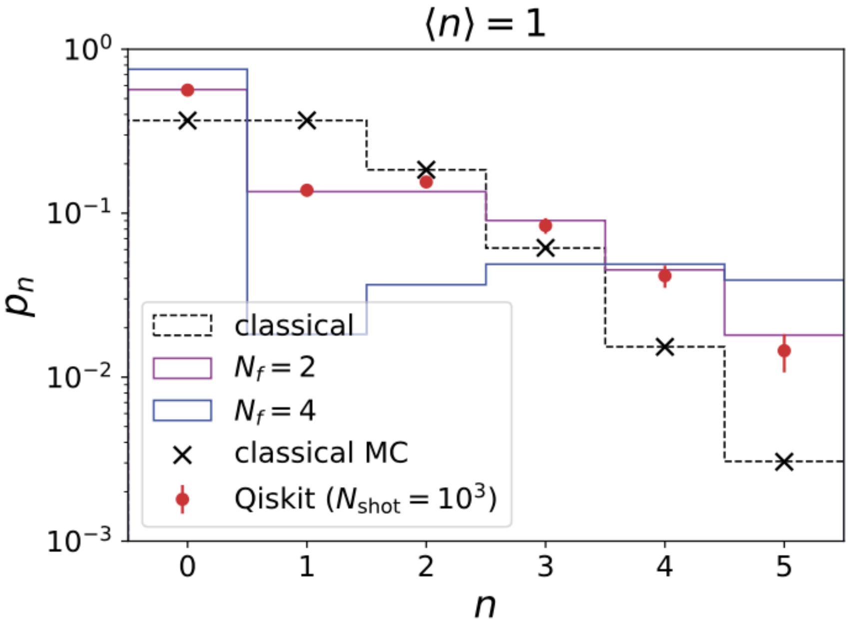
mass eigenstate χ_i

flavour eigenstate χ'_i

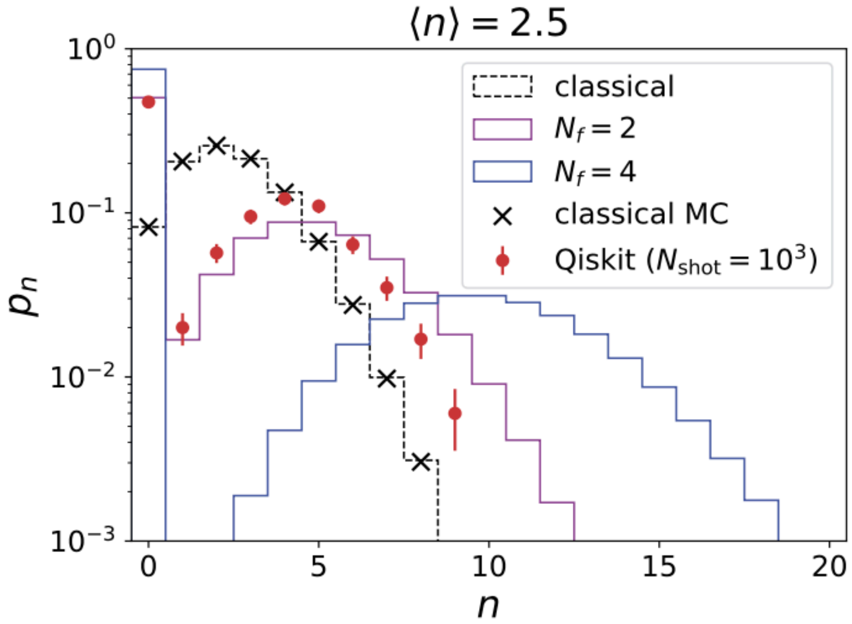


$$U_\theta \equiv \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \; ; \; G \equiv \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix}$$

$$U_\theta G U_\theta^\dagger = \begin{pmatrix} g'_1 & 0 \\ 0 & g'_2 \end{pmatrix}$$



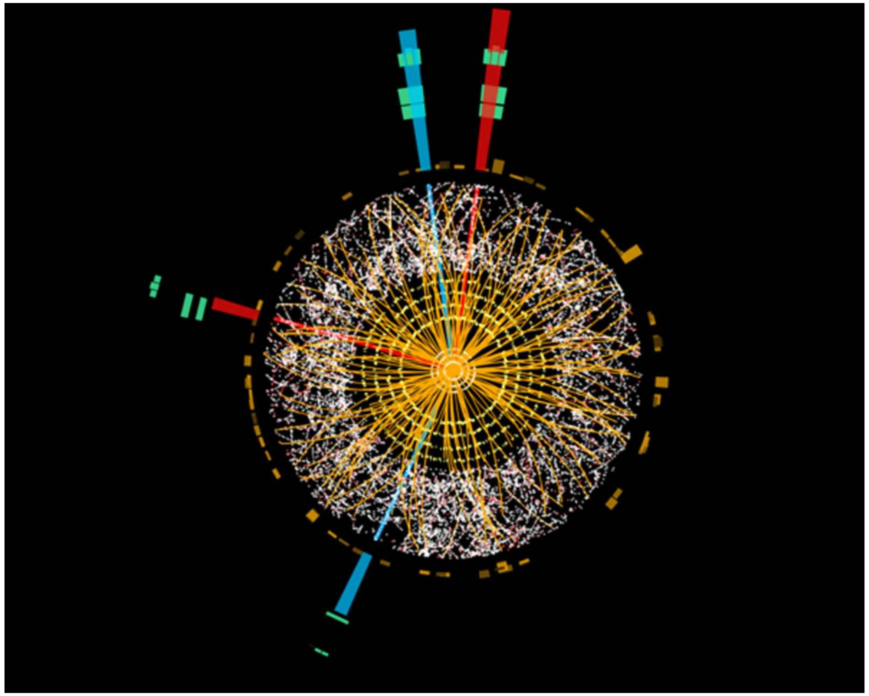
small coupling $\alpha \simeq 0.14$

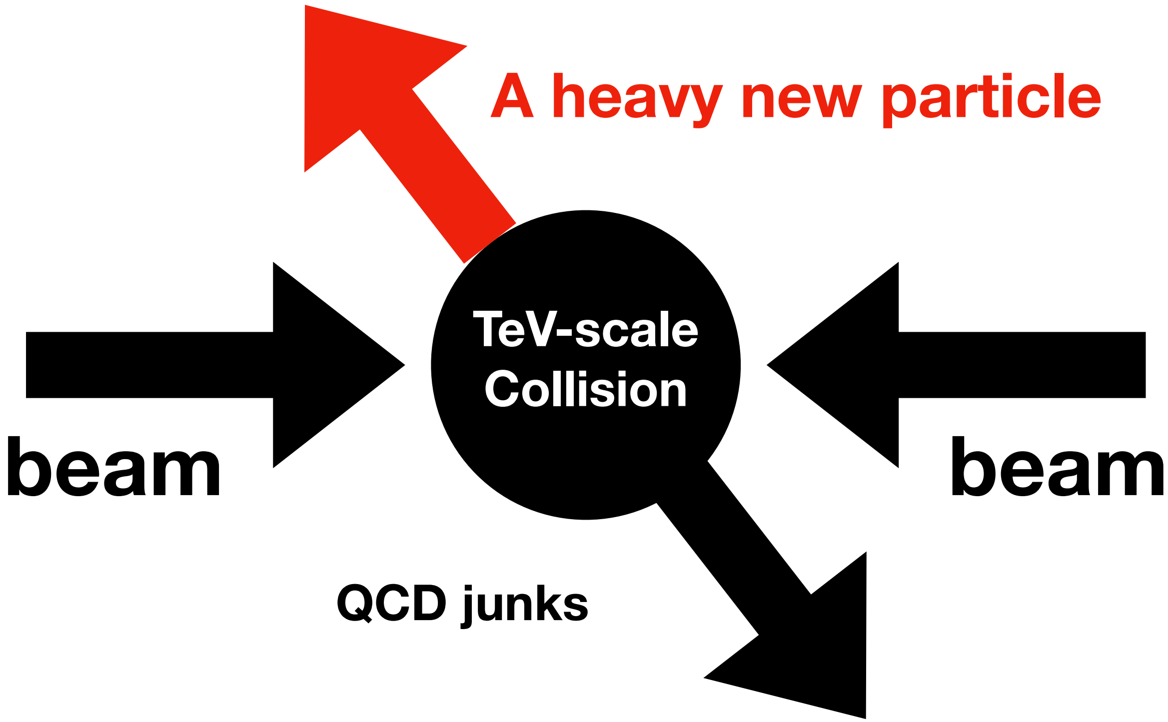


Moderate coupling $\alpha \simeq 0.35$

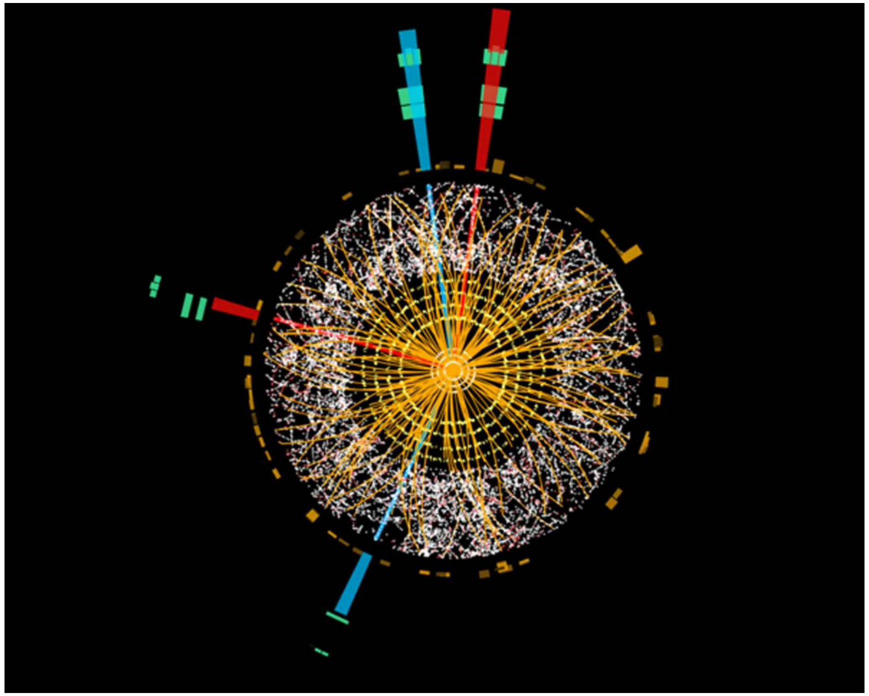
- Even in the simplest case, we observe the **difference**
- We are **limited** by number of qubits, circuit length of QC

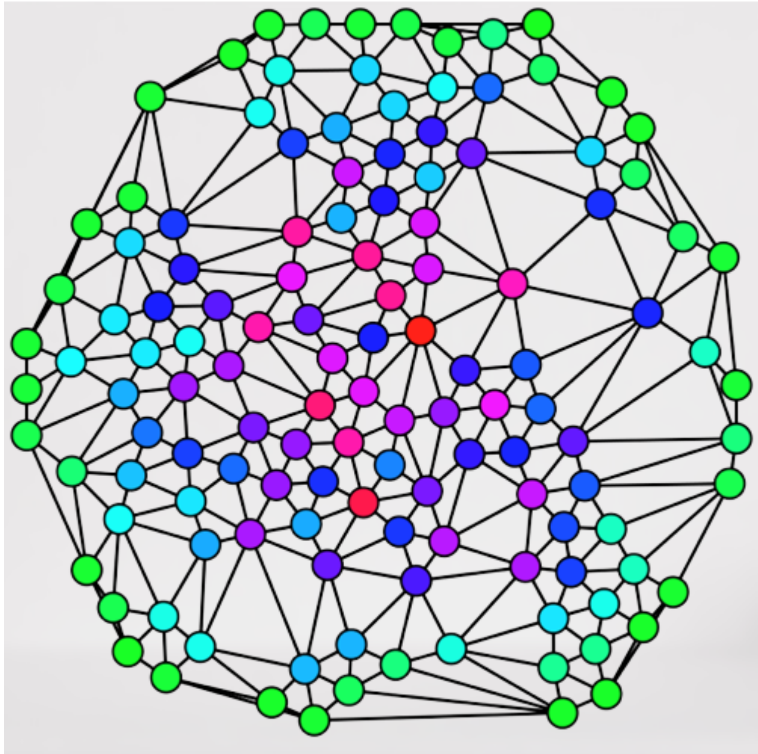
3) Combinatorics in reconstructions



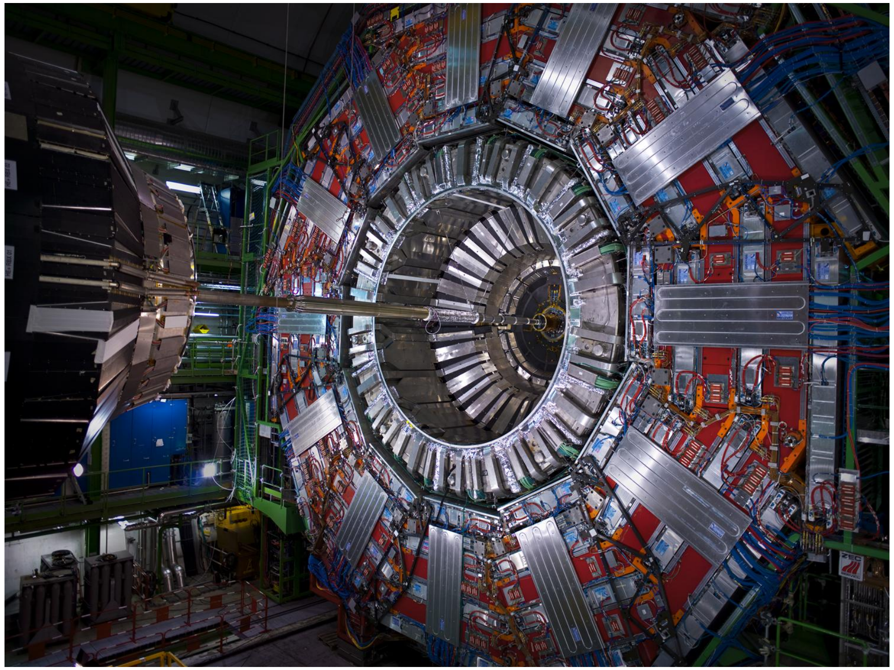


- In a High energy collision, there would be huge number of QCD particles (activities) more than particles from a signal process

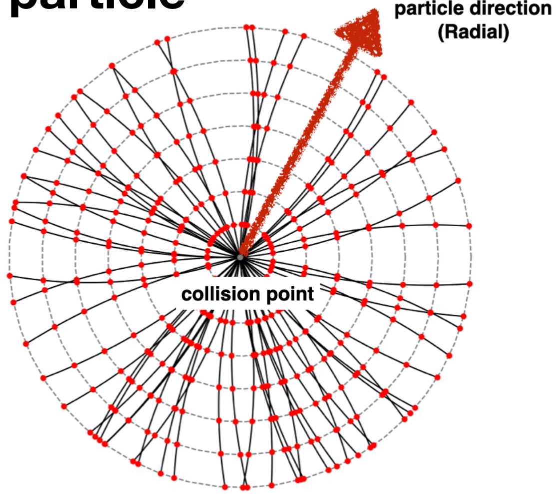


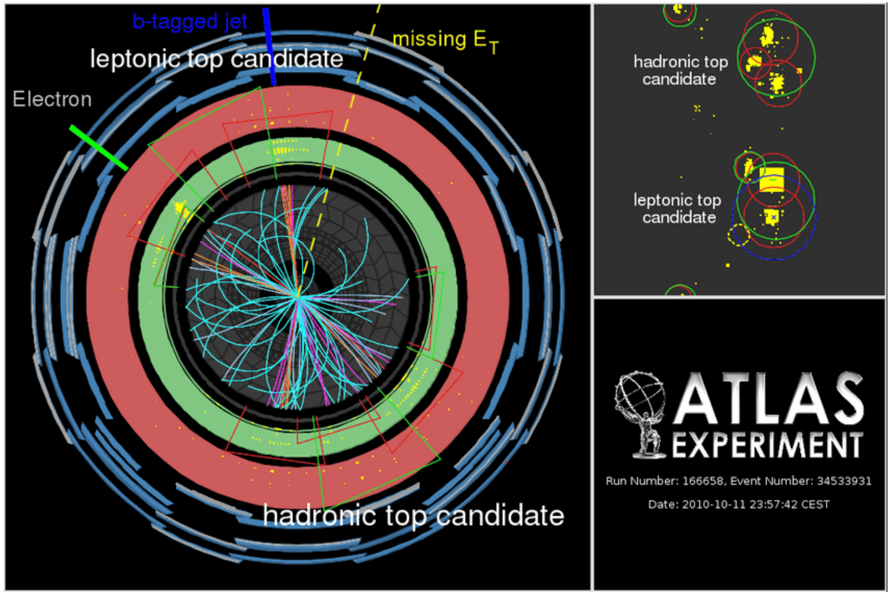


- One needs to identify (reconstruct) a particle with information from various sub-detectors.

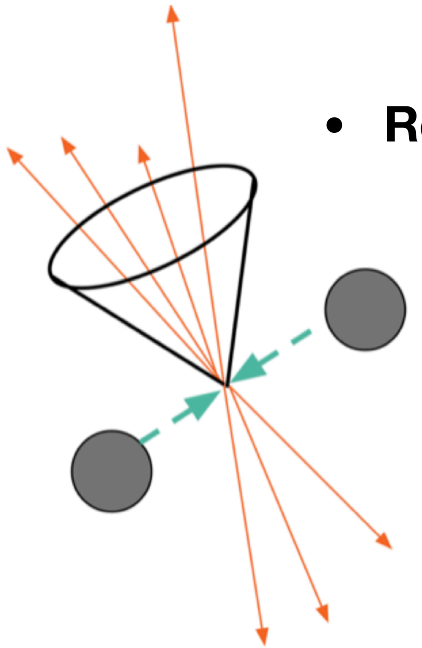


- **Reconstructing a particle**

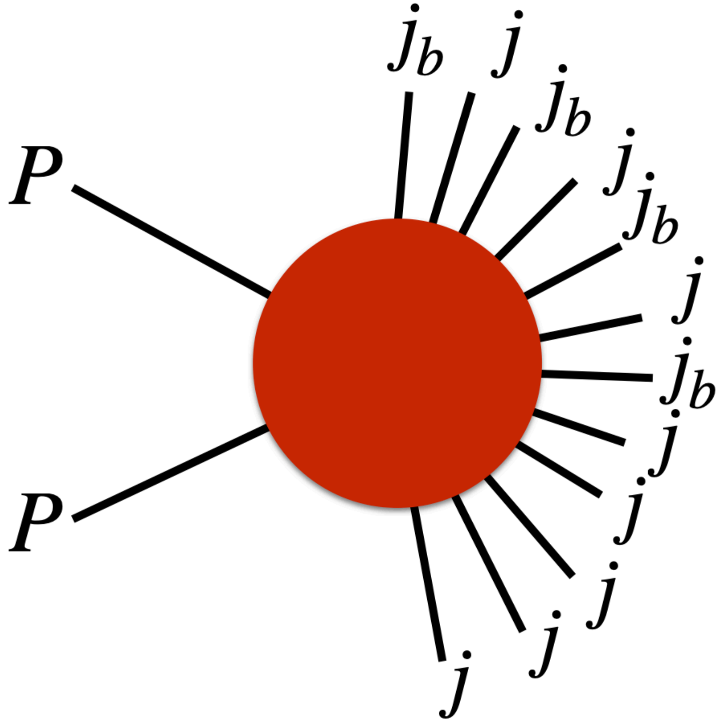




- **Reconstructing an object**

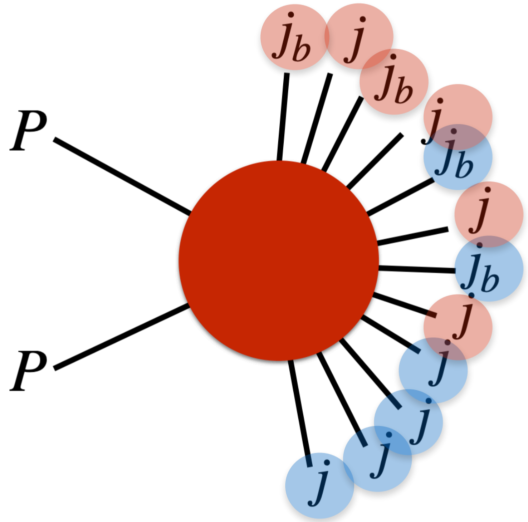


Examples (multi-jets)



1. Under the a simple assumption: $pp \to X, Y \to \{j_x\} \cup \{j_y\}$

2. Find a right **combination** to reconstruct X and Y particles.



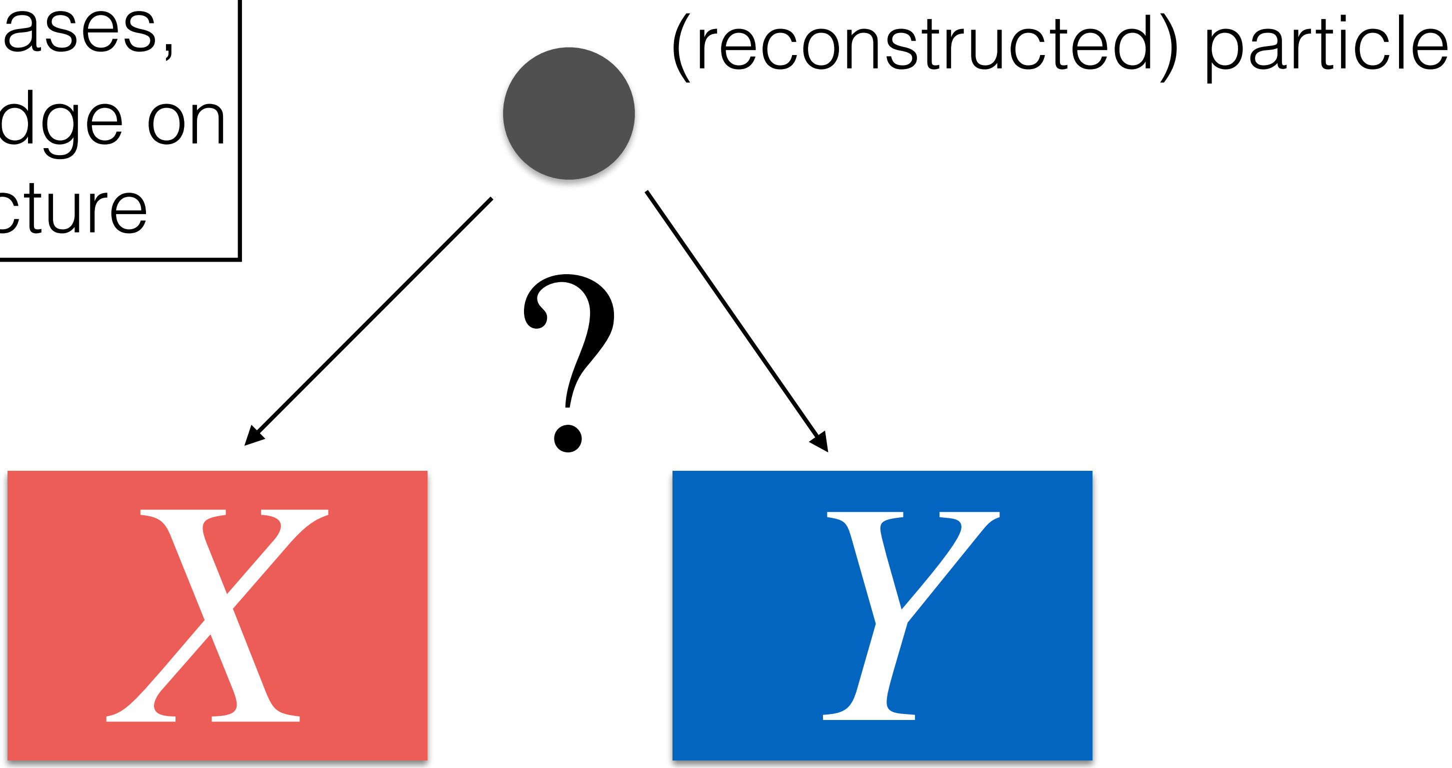
- Complicate situation (12 jets)

$$pp \to o\tilde{o} \to \{t, \bar{t}\} \cup \{t, \bar{t}\}$$

$$o \to t\bar{t} \to \{j_b, (W \to jj)\} \cup \{j_b, (W \to jj)\}$$

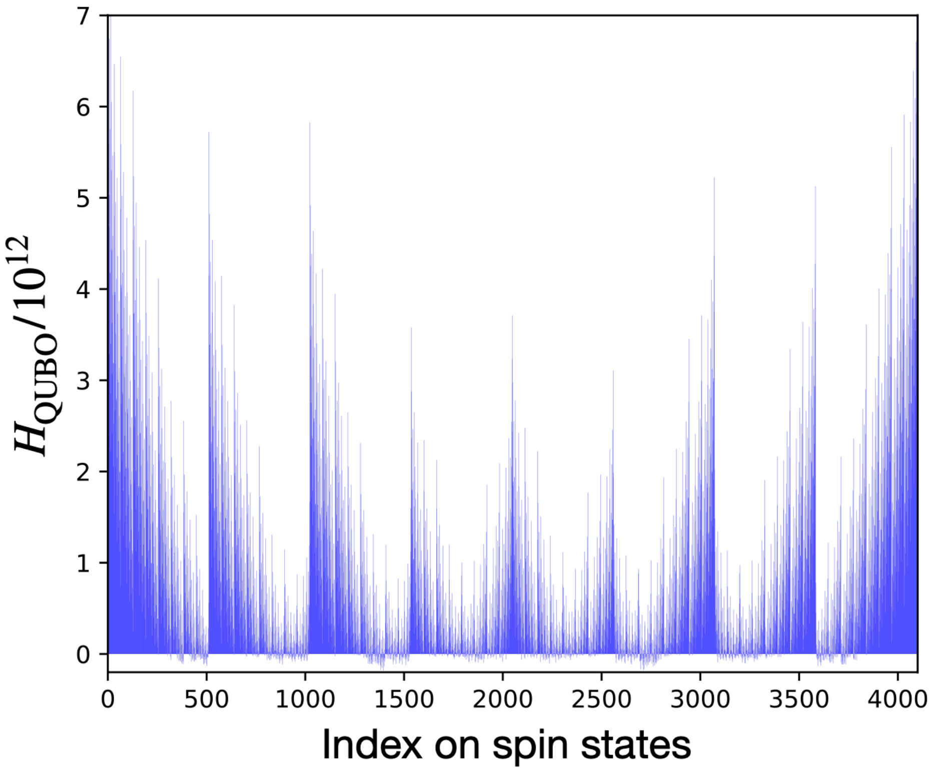
$$\tilde{o} \to t\bar{t} \to \{j_b, (W \to jj)\} \cup \{j_b, (W \to jj)\}$$

$2^{12} = 4096$ cases, no prior knowledge on a decay-structure



Combinatorial complexity arises (in a random Ising model)

Landscape of energy distribution

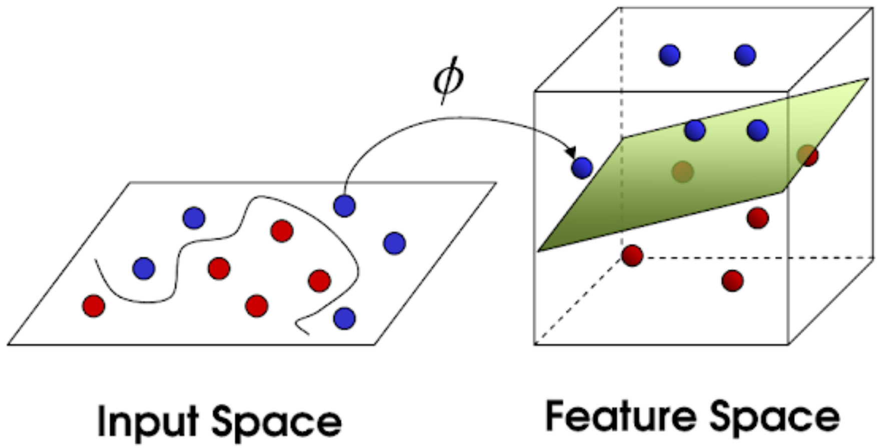


$\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \rightarrow \uparrow\uparrow\uparrow\uparrow\uparrow\downarrow \rightarrow \cdots \rightarrow \downarrow\downarrow\downarrow\downarrow\downarrow\downarrow \quad (n_{\mathrm{spin}} = 2^{12} = 4096)$

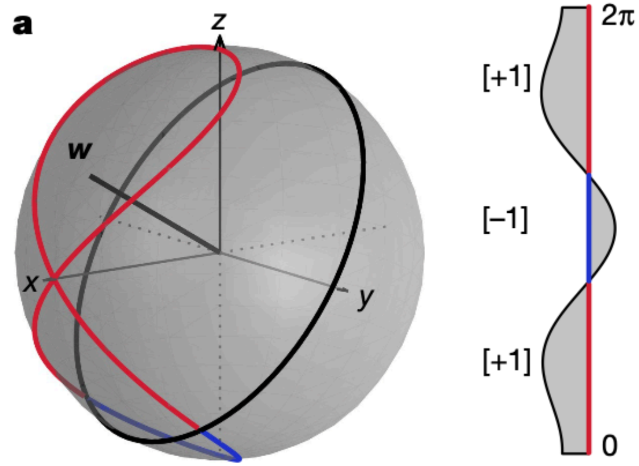
Any classical algorithm (except a brute force scanning) cannot find a global minimum for this random potential!

4) Quantum Machine Learning

classical ML Kernel Method



Quantum kernel function



$$|\Psi\rangle = \sum a_{i_1 i_2 \cdots i_n} |s_{i_1} s_{i_2} \cdots s_{i_n}\rangle$$

- Data embedding on the Hilbert space provides a good "kernel"

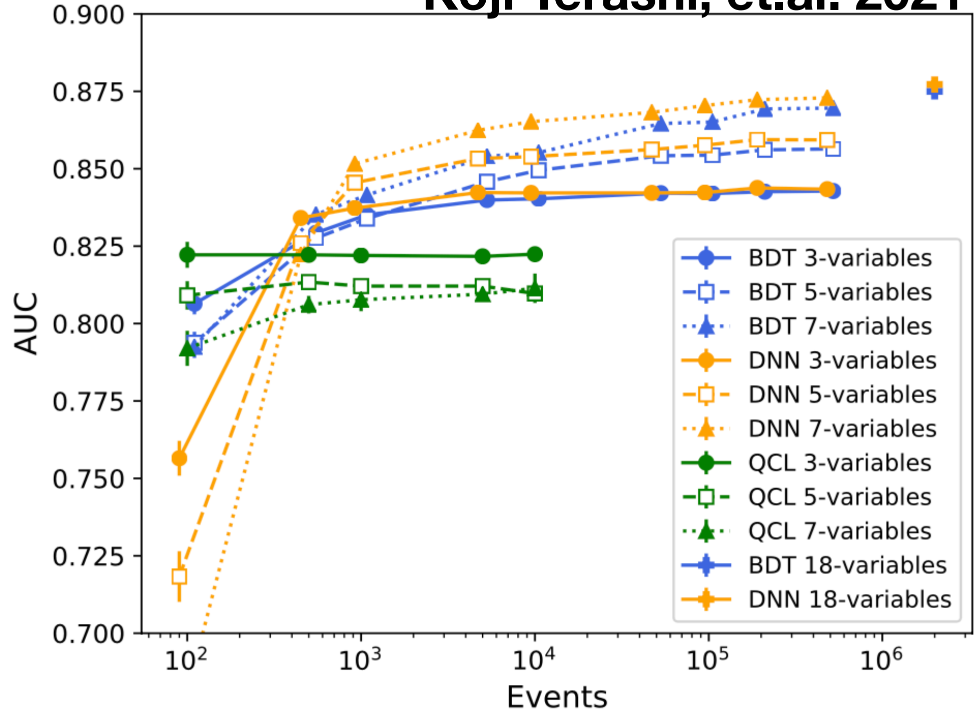
QML as Effective numerical method with a few training data

- A dream of totally bottom-up approach, a data-driven method
  with controlled data samples, instead of utilizing artificial data from Monte Carlo

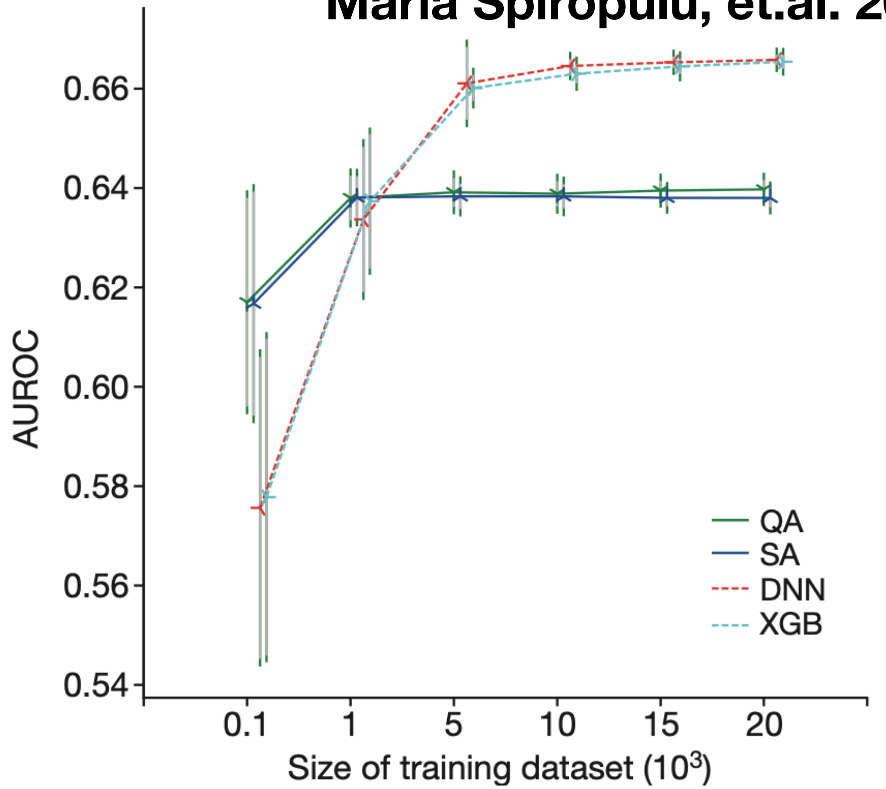
Data driven Machine Learning

- Compared to traditional GPU based ML, Quantum Machine learning provides a better performance with a small number of training samples

Koji Terashi, et.al. 2021



Maria Spiropulu, et.al. 2017



- VQA (Variational Quantum Algorithm) $(pp \to \tilde{\chi}^+\tilde{\chi}^- \to W^+W^- \to \ell^+\ell^-\nu\bar{\nu})$

- Quantum annealer to construct "energy (loss) function" $(pp \to H \to \gamma\gamma)$

Data-expensive GPU ML

- Due to the curse of dimensionality, current ML requires a BIG data

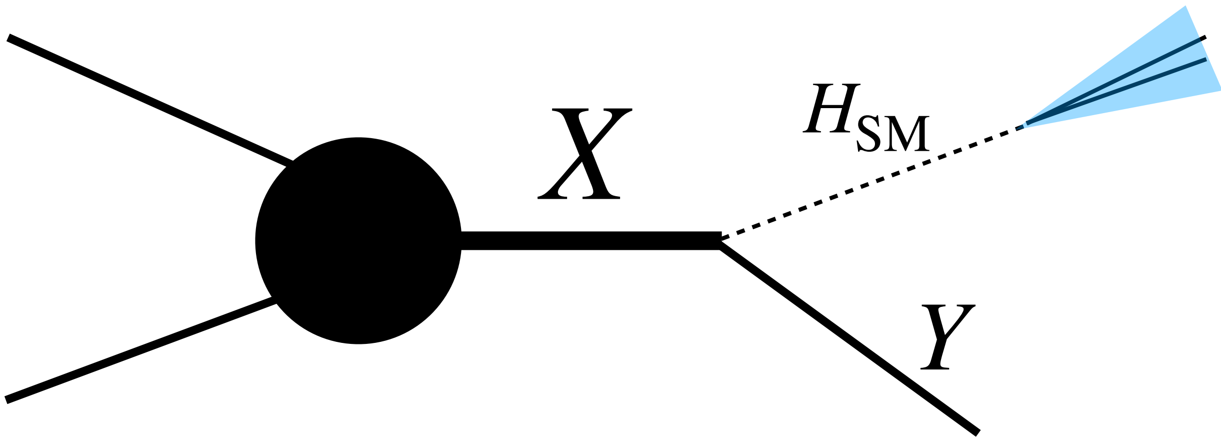
Chat gpt 4 vs gpt 3

Features	GPT-3 **570 gigabytes**	GPT-4
Parameters	**175 billion** $\mathcal{O}(10^{11})$	100 Trillion $\mathcal{O}(10^{14})$
Supported	Only Text	Both Te x t and Image
Word limit	approx 1500-2000 Words	25,000 words
Model complexity	High	Expected to be even higher

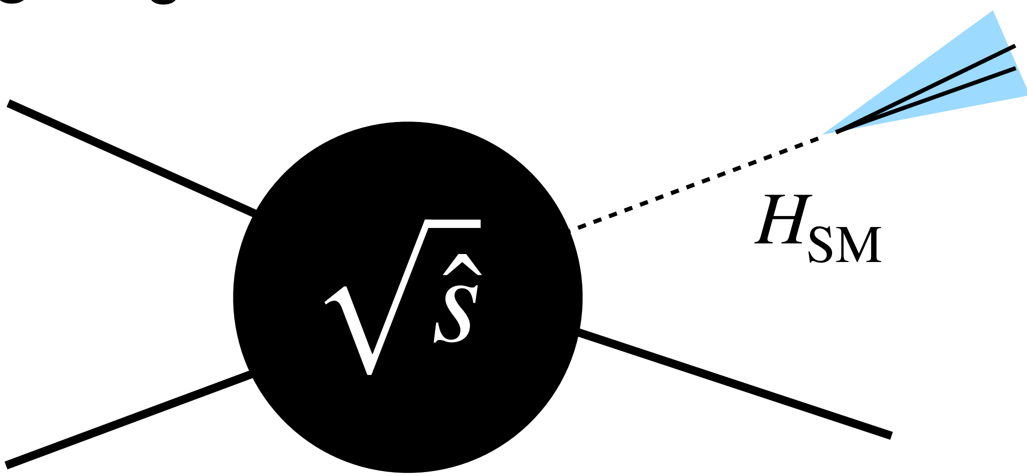
ML only with four qubits

Higgs in the Boosted region

- A new **heavier** state X, which $X \to H_{\text{SM}} + Y$ process



- The **edge** region where we can observe the effects of the **EFT**

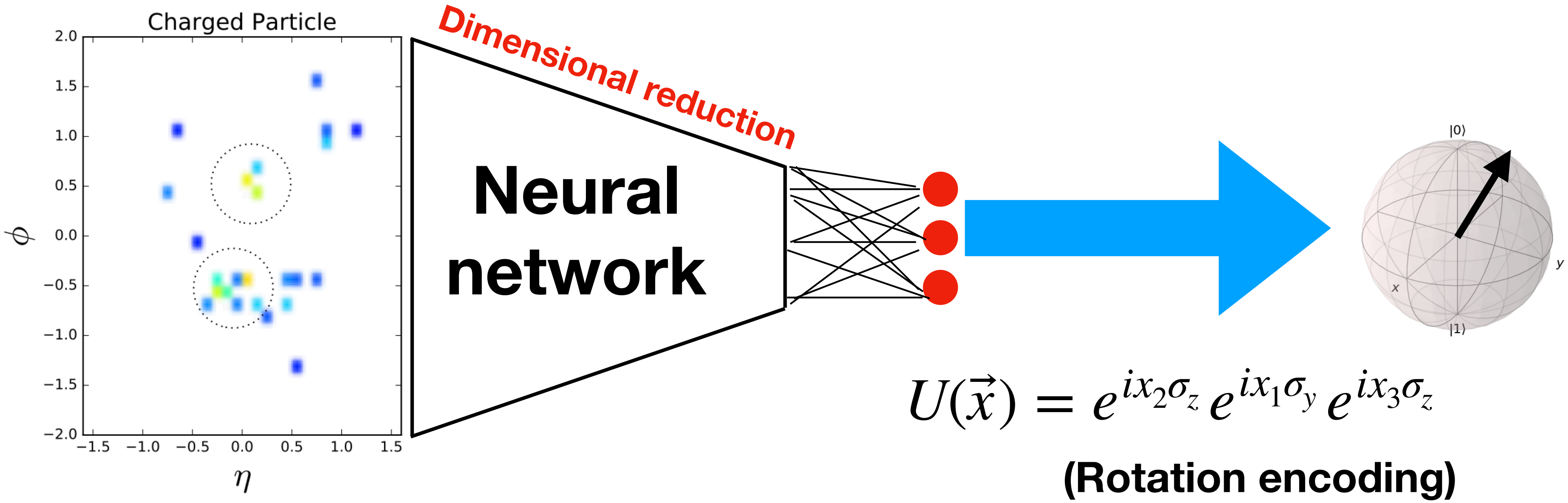


$$\frac{\sqrt{\hat{s}}}{\Lambda} \leq \mathcal{O}(1)$$

Hybrid QC with Neural Net

- We use a Classical CNN to reduce a dimension of input data.

(based on a work by Seth Lloyd et.al. 2020)



$$U(\vec{x}) = e^{ix_2\sigma_z} e^{ix_1\sigma_y} e^{ix_3\sigma_z}$$

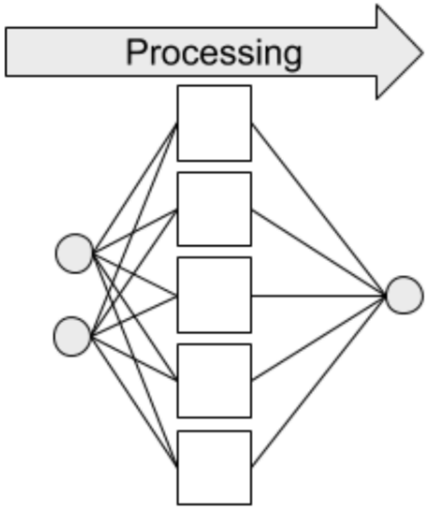
(Rotation encoding)

- The dimension of a latent space is a hyper-parameter.
- We can put a number of data as much as the d.o.f of $SU(2)$
- Any single qubit unitary gate can be decomposed as $U(\vec{x}) = e^{ix_2\sigma_z} e^{ix_1\sigma_y} e^{ix_3\sigma_z}$

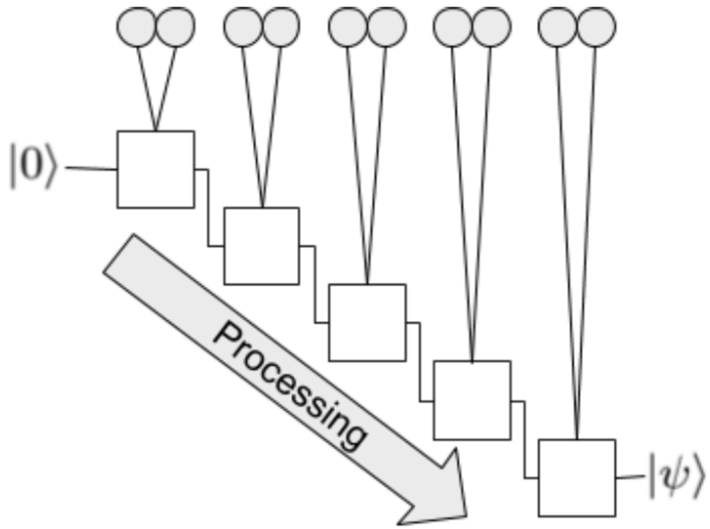
Quantum hidden layer

- Quantum circuit can mimic a multi-node structure to achieve "**universal approximation**" using a date re-uploading technique.

(Adrian Perez-Salinas et.al. 2020)



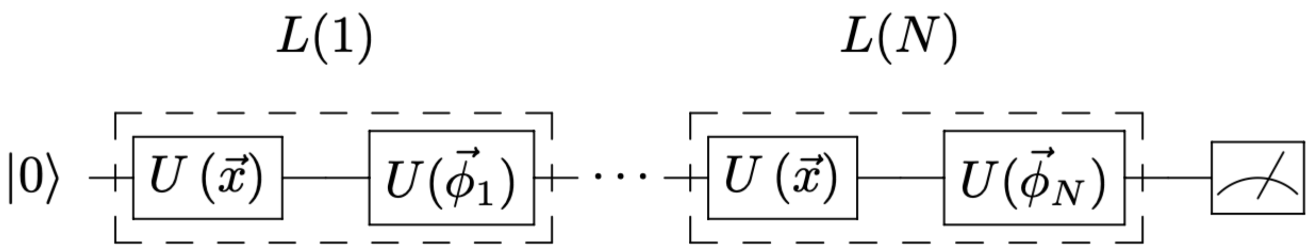
"Classical" Neural net



Quantum circuit

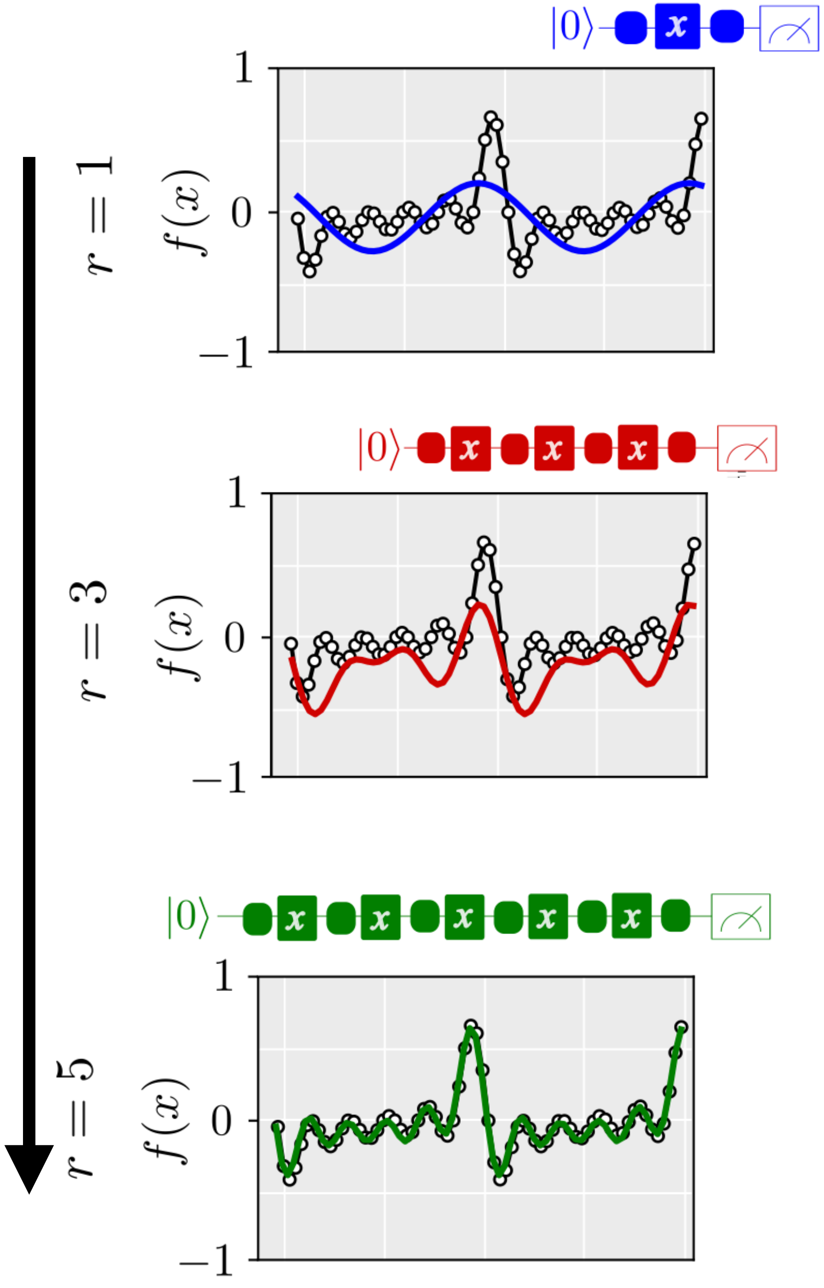
N-times of (N-nodes)

1) data re-uploading
2) weights to be learned



Quantum expressibility

Maria Schuld et.al. **2021**

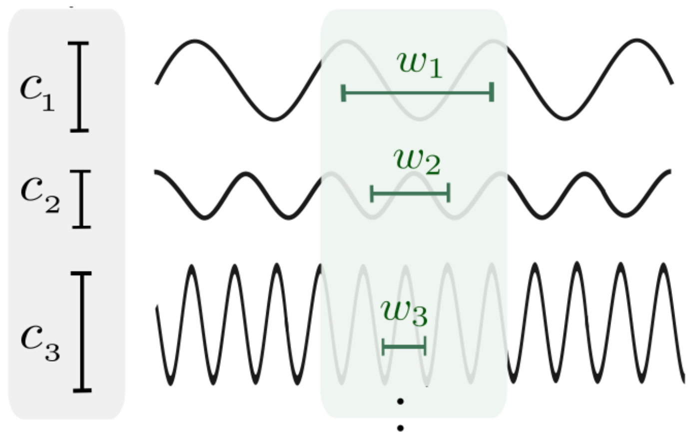


- Data re-uploading can be understood as Fourier analysis.

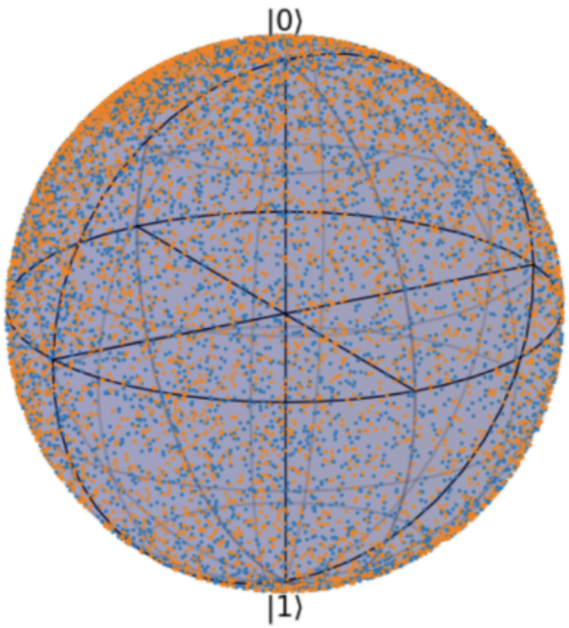
$$S(x) = e^{-i\frac{x}{2}\sigma_r}$$

$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{\boldsymbol{\omega}\in\Omega} c_{\boldsymbol{\omega}}(\boldsymbol{\theta})e^{i\boldsymbol{\omega}\boldsymbol{x}},$$

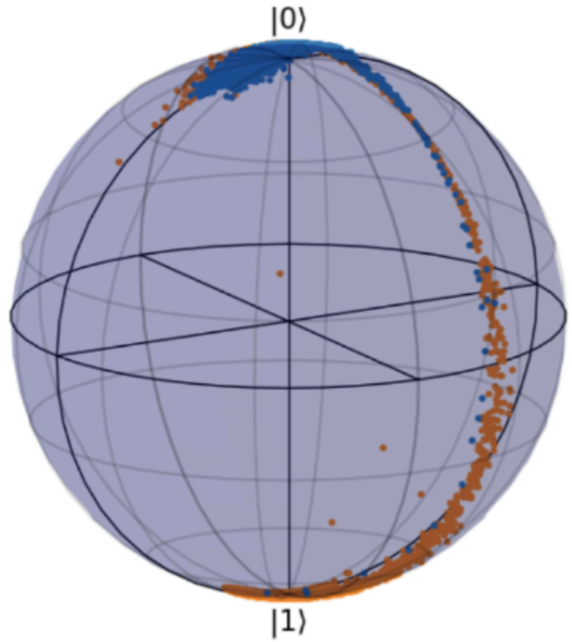
- Coefficient $c_\omega(\theta)$ can be adjusted with variational method.



Result of training



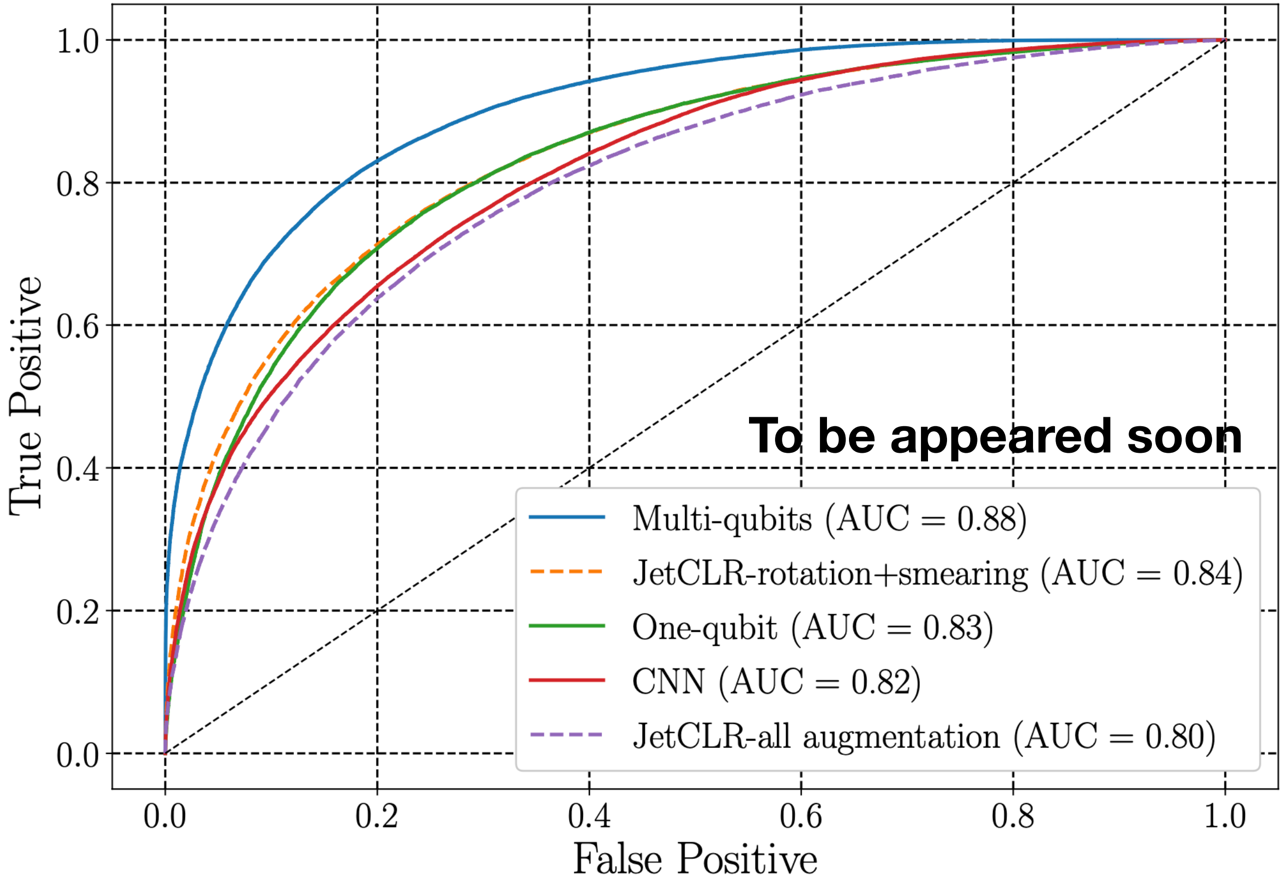
Before training



After training

- Through training, distances between signal points and background points on the Bloch sphere get maximized.

Result



- With simple structure, Quantum machine learning can provide the better result compared to the classical counter part.

- One needs to be **careful in applying data augmentation** to collider data (0.84 vs 0.80)

Too early to be serious
with a toy QC ?

Look back on the History of ML

- **A game-changer (GPU) came suddenly** into the Machine Learning area

  - 2012 AlexNet utilized a GPU to enhance the performance from 74% to 84%, later on 96%

It would be too late
if we just wait for a realistic QC

Some activities in Korea

- Workshop

  - AI and Quantum Information Applications in Fundamental Physics (Feb. 2023) supported by **KIAS**

  - AI and Quantum Information for Particle Physics (Nov. 2023) supported by KAIST, **IBS-CTPU**

- Schools (to educate graduate students)

  - QUC (KIAS) school (2021, 2022, 2023)

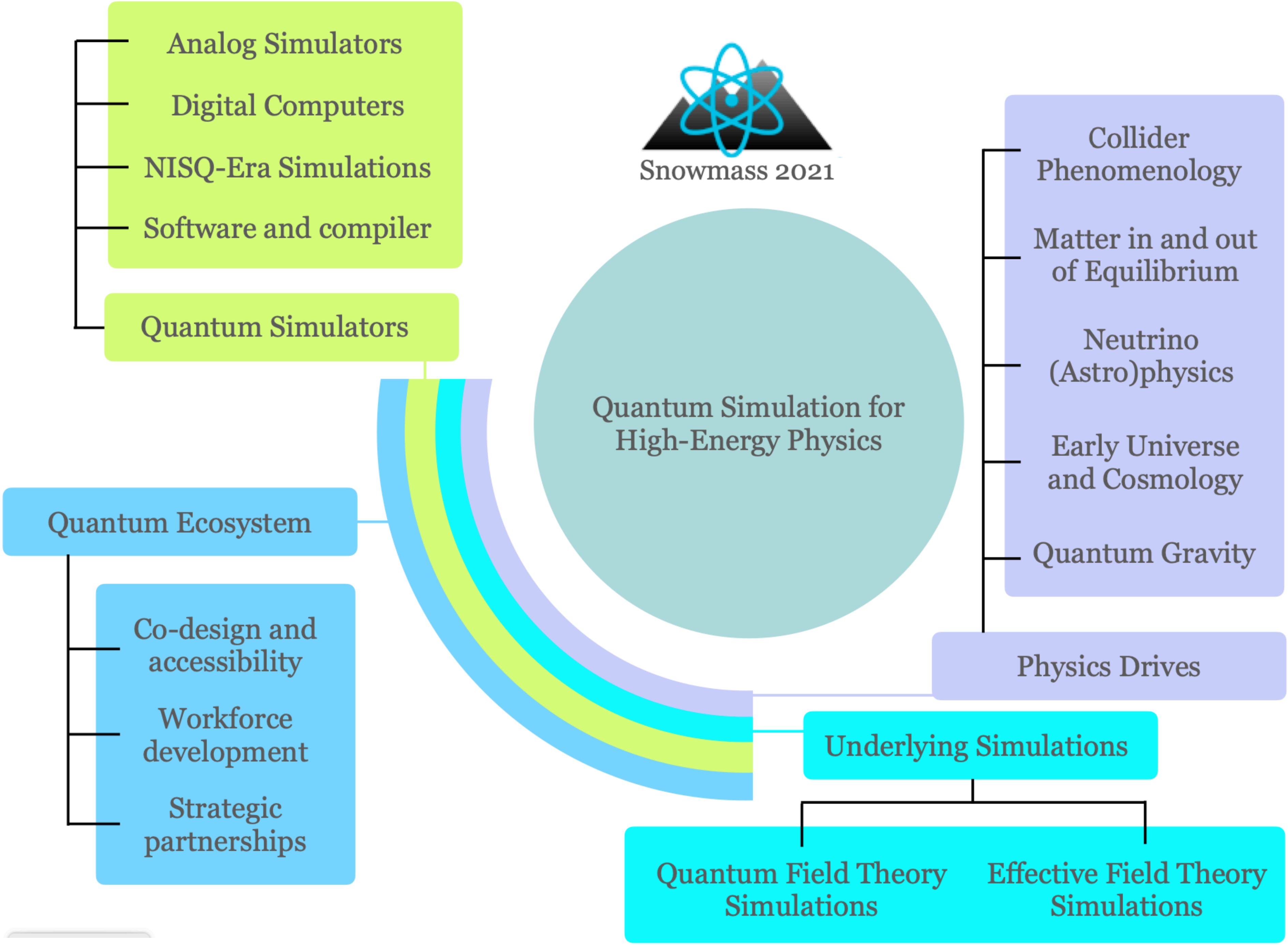
- **As a physicist, Quantum Computer has a lower hurdle, really low... compared to Machine Learning !**

  To be prepared by educating young students.

  - Currently many computer scientists are trying to "quantize" almost all classical neural networks.

- **Hope to have a network for "Quantum research activities" in high energy physics**

  - Broad applications, including Lattice QCD, neutrino physics, dark matter studies, data analyses in astrophysics, cosmology



- US snowmass report 2021