Variational Quantum Algorithms for NISQ Devices

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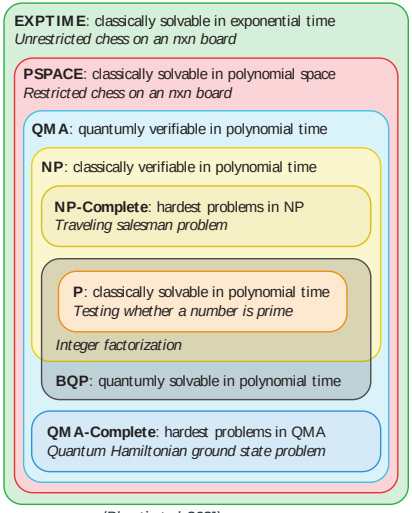
Overview of this Talk

1. **The Case for Variational Quantum Algorithms**
2. **Building Blocks of Variational Quantum Algorithms**
3. **Limitations of Variational Quantum Algorithms**
4. **The Barren Plateaux Phenomenon**
5. **Parameter Initialization and Ansatz Strategies**
6. **Variational Quantum Eigensolver**
7. **Quantum Approximate Optimization Algorithm**
8. **Applications of Variational Quantum Algorithms**

Why Variational Quantum Algorithms?

- **Noisy Intermediate-Scale Quantum** (NISQ) devices are currently realizable quantum devices whose qubits and quantum operations are not **quantum error correctable**, and therefore are imperfect (Preskill 2018).
- **VQAs** have emerged as the dominant technique to realize **quantum advantage** on NISQ devices.
- VQAs are **universal**, and they are in principle as powerful as any other **universal model of quantum computation** (Biamonte 2021; Lloyd 2018).
- VQAs have the capacity to realize **quantum supremacy** and a competitive edge over **classical supercomputers** (Dalzell et al. 2020).
  - **Instantaneous Quantum Polynomial-Time** (IQP) circuits require **208 Qubits and 500 gates**.
  - **Quantum Approximate Optimization Algorithm** (QAOA) circuits require **420 qubits and 500 constraints**.

Computational Complexity Primer



(Bharti et al. 2021)

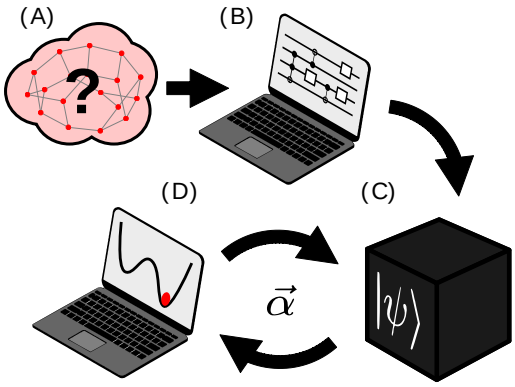
- **Complexity classes** classify problems by their **hardness**, or the **scaling of the cost** of solving the problem with respect to some resource.
- Despite their capabilities, quantum computers are not anticipated to solve **NP-Complete problems** in polynomial time.
- However, quantum algorithms **may outperform** classical algorithms for **NP-Complete problems**.

Variational Quantum Algorithms in a Nutshell

- **Variational Quantum Algorithms** (VQA) focus on **combining** the capabilities of quantum and classical computers.
- They delegate the **classically intractable** parts of computing to **quantum computers** while performing the tractable parts on **powerful classical devices**.
- The **Variational Quantum Eigensolver** (VQE) and the **Quantum Approximate Optimization Algorithm** (QAOA) were the first proposals for VQA.
- **QVE** and **QAOA** are often considered as the VQA family's parents.

Building Blocks of Variational Quantum Algorithms

1. **Objective Function**: The function which encodes the problem that is to be **variationally minimized**.
2. **Ansatz**: **Parameterized Quantum Circuits** which consist of **unitaries** whose parameters are manipulated in the minimization of the objective function.
3. **Measurement Scheme**: Required to extract the **expectation values** needed to evaluate the objective function.
4. **Classical Optimizer**: The method used to obtain the **optimal circuit parameters** that minimize the objective function.



Objective Function

- The problem to be solved is formulated as a **Hamiltonian** whose ***expectation value*** *is often used as the objective* that is to be minimised.
- To encode the Hamiltonian onto a quantum circuit, we express it as a **linear combination of tensor products** of Pauli matrices σ_x, σ_y, σ_z.
- These tensor products are often referred to as **Pauli strings** and expressed as

$$P = \bigotimes_{j=1}^{n} \sigma$$

- The **Hamiltonian** can be decomposed as

$$H = \sum_{k=1}^{M} c_k P_k$$

- The **expectation value** then naturally decomposes into a set of expectation values, each defined by a **single Pauli string**

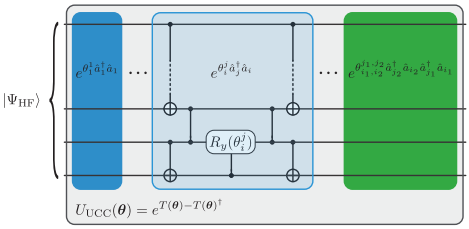
$$\langle H \rangle = \sum_{k=1}^{M} c_k \langle P_k \rangle$$

Ansatz and Parameterized Quantum Circuits

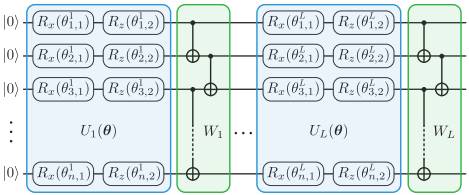
- **Ansatz** determines the form of the **parameterized quantum circuit** that prepares the **desired state**.
- The states are formed by **unitary operations** that depends on a series of parameters.
- A classical optimisation subroutine finds the optimal *unitary ansatz parameters*.
- The ansatz influences a VQA's performance substantially. Most developed ansatzes are of two sorts.

1. **Problem Inspired Ansatz**: Information of the problem to be solved is used to **tailor an effective ansatz**.
2. **Hardware Efficient Ansatz**: Ansatz that are aimed at **reducing the circuit depth** needed to implement when using a given quantum hardware.

a Problem Inspired Ansatz



b Hardware Efficent Ansatz



(Bharti et al. 2021)

Measurement of Pauli String

- To estimate the expectation value of the **objective function**, by measuring the probabilities of the **computational basis states** $|0\rangle$ or $|1\rangle$.
- The **expectation value** of the σ_z operator on a particular qubit can be measured as

$$\langle \psi | \hat{\sigma}_z | \psi \rangle \equiv \langle \sigma_z \rangle = |\alpha|^2 - |\beta|^2$$

  where $|\alpha|^2$ and $|\beta|^2$ are the probabilities of measuring the qubit in states $|0\rangle$ and $|1\rangle$.
- Measurements defined by σ_x and σ_y can be defined similarly by transforming them into the σ_z basis first.

$$\sigma_x = R_y^\dagger(\pi/2)\sigma_z R_y(\pi/2)$$
$$\sigma_y = R_x^\dagger(\pi/2)\sigma_z R_x(\pi/2)$$

- **Arbitrary Pauli strings** P with **Pauli operations** $\sigma_{f(k)} \in \{\sigma_x, \sigma_y, \sigma_z\}$ on qubits $k \in K$ can then be measured by the same procedure on each individual qubit as

$$\langle P \rangle = \left\langle \prod_{k \in K} \sigma_z(k) \right\rangle$$

Classical Optimization of Ansatz Parameters

- Standard classical methods applied for **multivariate optimization** procedures are applicable to the optimization of ansatz's parameters.
- Generally the **quantum circuit's parameter space** can be navigated by using gradient based methods.
- The **objective function** $f(\boldsymbol{\theta})$ with M parameters $\boldsymbol{\theta} = (\theta_1, \cdots, \theta_M)$ can be optimised by starting from some initial parameter value $\boldsymbol{\theta}^{(0)}$ and **iteratively updating** $\boldsymbol{\theta}^{(t)}$ for discrete steps t by following

$$\theta_i^{(t+1)} = \theta_i^{(t)} - \eta \partial_i f(\boldsymbol{\theta})$$

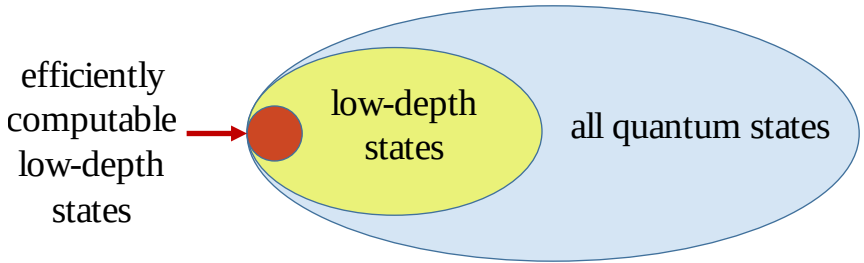
  where η is the **learning rate** and

$$\partial_i \equiv \frac{\partial}{\partial \theta_i}, \quad \nabla = (\partial_1, \cdots, \partial_M)$$

  is the partial derivative with respect to the parameter θ_i and the **gradient vector**.
- Parameters can also be optimised via **gradient-free methods** by means of
  - Evolutionary Algorithms
  - Reinforcement Learning
  - Sequential Minimal Optimisation
  - Surrogate Model-based Optimisation

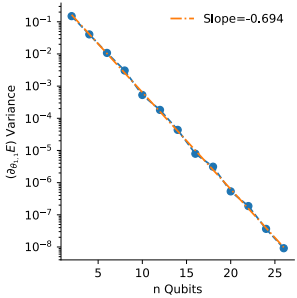
Limitations of VQA

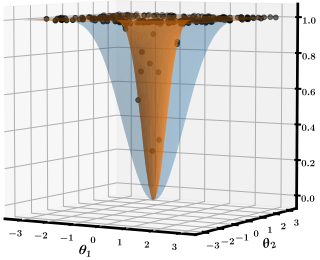
- **Hardware Limitations**: Depth of the state preparation circuit must be small enough to enable reliable implementation on NISQ devices. **Qubit connectivity** may be limited, e.g. only 2D or 3D. **Highly entangled ground states** are out of scope.
- **Algorithmic Limitations**: The number of variational parameters must be small enough to enable **efficient energy minimization**. **Large-scale VQA** with an extensive number of variational parameters may give rise to intractable optimization problems.



The Barren Plateaux Phenomenon

- The **Barren Plateaux** phenomenon was originally discovered when executing ***deep unstructured parameterized*** *quantum circuits* with **randomly** initialised parameters (McClean et al. 2018).
- This occurs because the ansatz must search an **exponentially large Hilbert space** for the answer.
- The analysis of Barren Plateaux has been extended to variety of variational quantum circuits and can be induced by reasons such as
  - Cost Function and its Locality (Marco Cerezo, Sone, et al. 2021)
  - Intrinsic Randomness of Problems (Holmes et al. 2021)
  - Amount of Entanglement between Qubits (Marrero et al. 2021)
  - Increased Circuit Depth and Problem Size
  - Noise and Accumulation of Error (Wang et al. 2021)





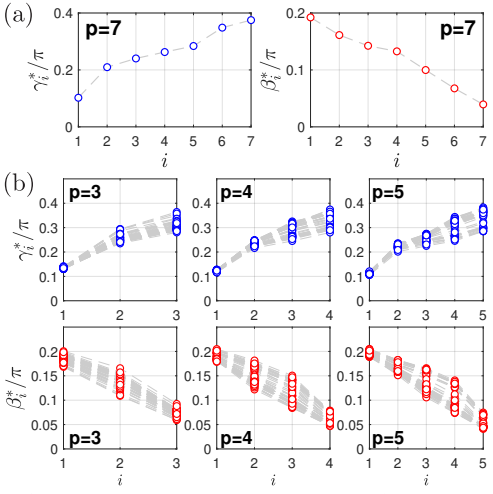
Parameter Initialization and Ansatz Strategies

1. **Parameter Initialization**

   - Instead of random initialization, *optimally choosing* the seed parameters can help avoid **Barren Plateaux**.
   - The importance of parameter initialization was made clear when the optimal parameters in QAOA exhibited **persistent patterns**.
   - The pattern observed in the optimal parameters can be then **extrapolated** for circuits with larger depth.

2. **Ansatz Strategies**

   - Barren plateaux can also be avoided by designing **structured ansatz** that restricts the space explored during the optimization.
   - Another approach is to learn a **mixed state** using the target Hamiltonian's information to generate a **Hamiltonian variational ansatz**.



Optimal QAOA Parameters of Maxcut on 16 Vertex Unweighted 3-Regular Graph (Zhou et al. 2020)

Variational Quantum Eigensolver (VQE)

- **Electronic structure problems** involve solving for the **ground-state energy** of many-body interacting fermionic Hamiltonians.
- The electronic Hamiltonian in second **quantization** is given by mapping between fermionic and qubit operators as

$$H_F = \sum_{ij} t_{ij} a_i^\dagger a_j + \sum_{ijkl} u_{ijkl} a_i^\dagger a_k^\dagger a_l a_j$$

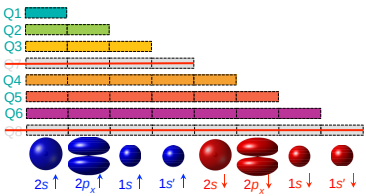
- The solution for a *k*-**local Hamiltonian** H amounts to finding its **ground-state eigenvalue** E_G and **ground state** $|\Phi_G\rangle$ which satisfy

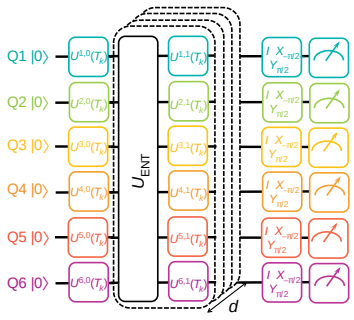
$$H|\Phi_G\rangle = E_G|\Phi_G\rangle$$

- **N-qubit trials** are obtained from the state $|00\ldots0\rangle$, applying d entanglers U_{ENT} that alternate with N Euler rotations, giving

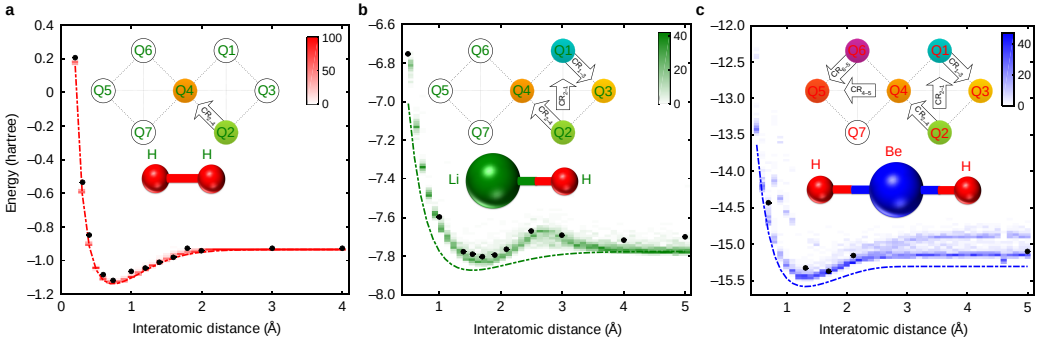
$$|\Phi(\theta)\rangle = \prod_{q=1}^{N}\left[U^{q,d}(\theta)\right] \times U_{\text{ENT}} \times \prod_{q=1}^{N}\left[U^{q,d-1}(\theta)\right] \times \cdots \times U_{\text{ENT}} \times \prod_{q=1}^{N}\left[U^{q,0}(\theta)\right] |00\ldots0\rangle$$

where $U_{\text{ENT}} = \exp(-iH_0\tau)$ and $U^{q,i}(\boldsymbol{\theta}) = Z^q_{\theta_1^{q,i}} X^q_{\theta_2^{q,i}} Z^q_{\theta_3^{q,i}}$.





Variational Quantum Eigensolver (VQE)



Application to Quantum Chemistry (Kandala et al. 2017)

- **Experimental Results** - Black Filled Circles
- **Dotted Lines** - Exact Energy Surfaces
- **Density Plots** - 100 Outcomes from numerical simulations at each interatomic distance

Quantum Approximate Optimization Algorithm

- QAOA (Farhi et al. 2014) takes the approach of **classical approximate algorithms** and looks for a quantum analogue to produce an **approximate solution** in polynomial-time.
- It consists of a **Problem Hamiltonian**

$$U(C,\gamma) = e^{-i\gamma C} = \prod_{\alpha=1}^{m} e^{-i\gamma C_\alpha}$$

and a **Mixing Hamiltonian**

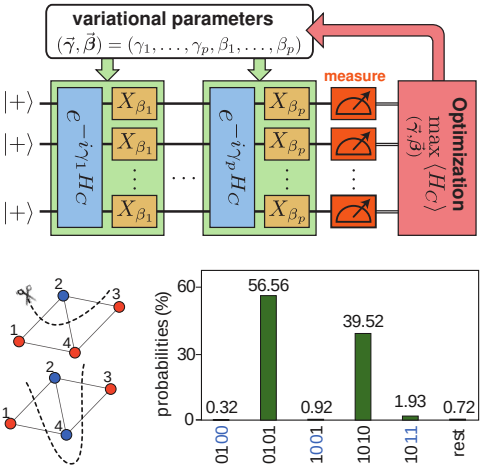
$$U(B,\beta) = e^{-i\beta B} = \prod_{j=1}^{n} e^{-i\beta\sigma_j^X}$$

- For any integer $p \geq 1$, $\gamma_1 \dots \gamma_p \equiv \vec{\gamma}$, and $\beta_1 \dots \beta_p \equiv \vec{\beta}$ define the angle dependent quantum state:

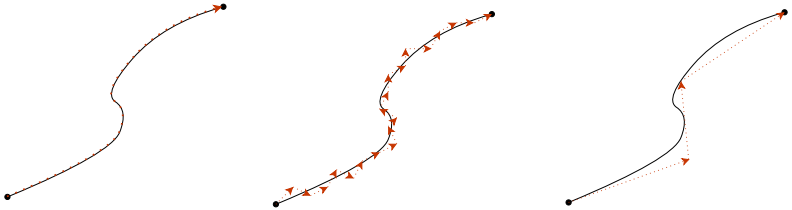
$$|\vec{\gamma},\vec{\beta}\rangle = U(B,\beta_p)\, U(C,\gamma_p) \cdots U(B,\beta_1)\, U(C,\gamma_1)\, H^{\otimes n}|0\rangle^{\otimes n}$$

- The **expectation value** of C, F_p, can be calculated as

$$F_p(\vec{\gamma},\vec{\beta}) = \langle\vec{\gamma},\vec{\beta}|C|\vec{\gamma},\vec{\beta}\rangle$$



Relation to Quantum Adiabatic Algorithm



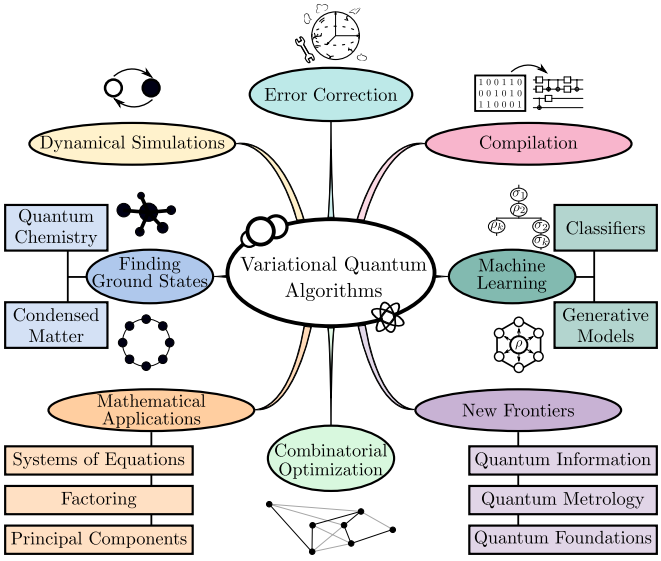
- Consider the following time dependent **Hamiltonian**.

$$H(t) = (1 - t/T)B + (t/T)C$$

Starting in $H^{\otimes n}|0\rangle^{\otimes n}$, the **adiabatic algorithm** would find the highest energy **eigenstate** of C in time T.

- A **Trotterized approximation** of the operators to the evolution consists of alternating the operators $U(C, \gamma)$ and $U(B, \beta)$ where the sum of angles is the total run time.

Applications of Variational Quantum Algorithms

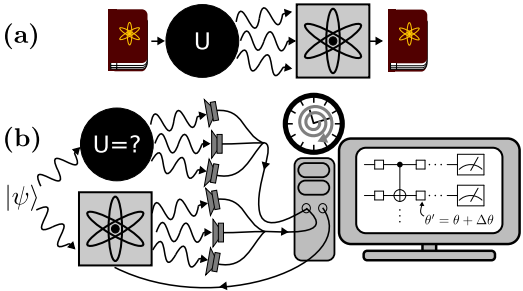


VQAs for Quantum Information Theory

- Using NISQ computers to compute quantum information quantities like **von Neumann entropy** or distinguishability metrics like **trace distance** is one possible area of investigation.
- While these problems are hard for general quantum states (Rosgen et al. 2005), there exists VQAs such as **Variational Quantum Fidelity Estimation** to estimate the **quantum fidelity** between an arbitrary state σ and a low-rank state ρ (Marco Cerezo, Poremba, et al. 2020).
- There is also potential for using the **Quantum Autoencoder** algorithm to learn encodings and achievable rates for quantum channel transmission (Romero et al. 2017).

VQAs for Foundations of Quantum Theory

- NISQ devices offer experimental platforms to test foundational ideas ranging from **quantum gravity** to **quantum Darwinism** (Zurek 2009).
- For example, the **emergence of classicality** in quantum systems will be soon be a computationally tractable field of study due to the increasing size of NISQ computers.
- The **Consistent Histories formulation** allows the study of the *quantum-to-classical transition* and *quantum cosmology*. The **Variational Consistent Histories** (VCH) algorithm allows one to efficiently examine the consistency of a set of histories (Arrasmith et al. 2019).
- (Holmes et al. 2021) showed that a **Full Unitary Matrix Compiling** (FUMC) strategy cannot efficiently learn a scrambling unitary which provides insight into the **black hole information paradox**.



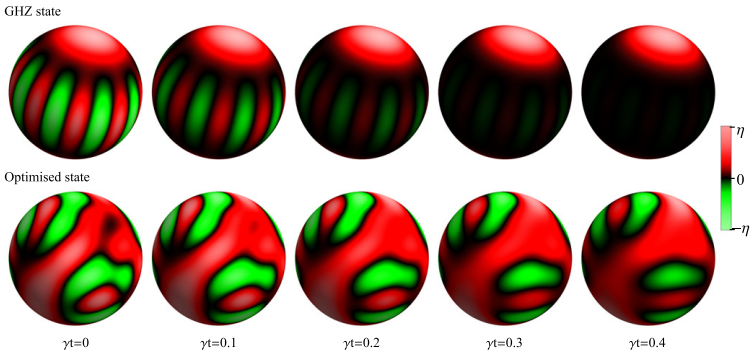
Learning a Scrambling Unitary: Panel (a) shows the famous Hayden-Preskill thought experiment where someone tries to extract data from a black hole (a scrambler). Panel (b) depicts the process of learning U.

VQAs for Quantum Metrology

- Quantum Metrology is a field where one seeks the **optimal setup** for probing a parameter of interest with **minimal shot noise** (M. Cerezo et al. 2021).
- In the **absence of noise** during the probing process, the ideal probe state may be derived analytically. However, general physical noises make **analytical solutions** difficult to obtain.
- In **Variational-State Quantum Metrology**
  1. one prepares a *probe state with variational parameters*
  2. probes the magnetic field with physical noises
  3. measures **Quantum Fisher Information (QFI)** as a cost function
  4. and updates the parameters to maximize it.

NOTE: Since QFI cannot be efficiently computed, an approximation of QFI can be heuristically found by optimizing the measurement basis, or by computing upper and lower bounds on the QFI (Beckey et al. 2020).

Variational-State Quantum Metrology



Finding (near) optimal states for metrology in the presence of noise (Koczor et al. 2020)

Wigner functions of permutation-symmetric **nine-qubit quantum states** that evolve under **dephasing noise**. Time increases left-to-right and γt is the dimensionless time expressed in units of the decay time γ^{-1}. **GHZ (upper) states** are the most sensitive to an external magnetic field, but their coherences rapidly deteriorate due to fluctuations of the external field. **The aim of this work is to find states (lower) that are optimally sensitive to the external field while being robust against noise using variational techniques.** Red and green colours show positive and negative values of the function while brightness represents the absolute value of the function relative to its global maximum η.

"The art of designing useful quantum algorithms hinges on somehow taking advantage of the hidden extravagance of the quantum world, overcoming our inability to glimpse any more than a meager shadow of the quantum reality whenever we read out our quantum device."

John Phillip Preskill

Further Reading on Variational Quantum Algorithms

1. **Noisy intermediate-scale quantum (NISQ) algorithms** - [K. Bharti et al. arXiv:2101.08448v2]

2. **Variational Quantum Algorithms** - [M. Cerezo et al. arXiv:2012.09265v2]

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