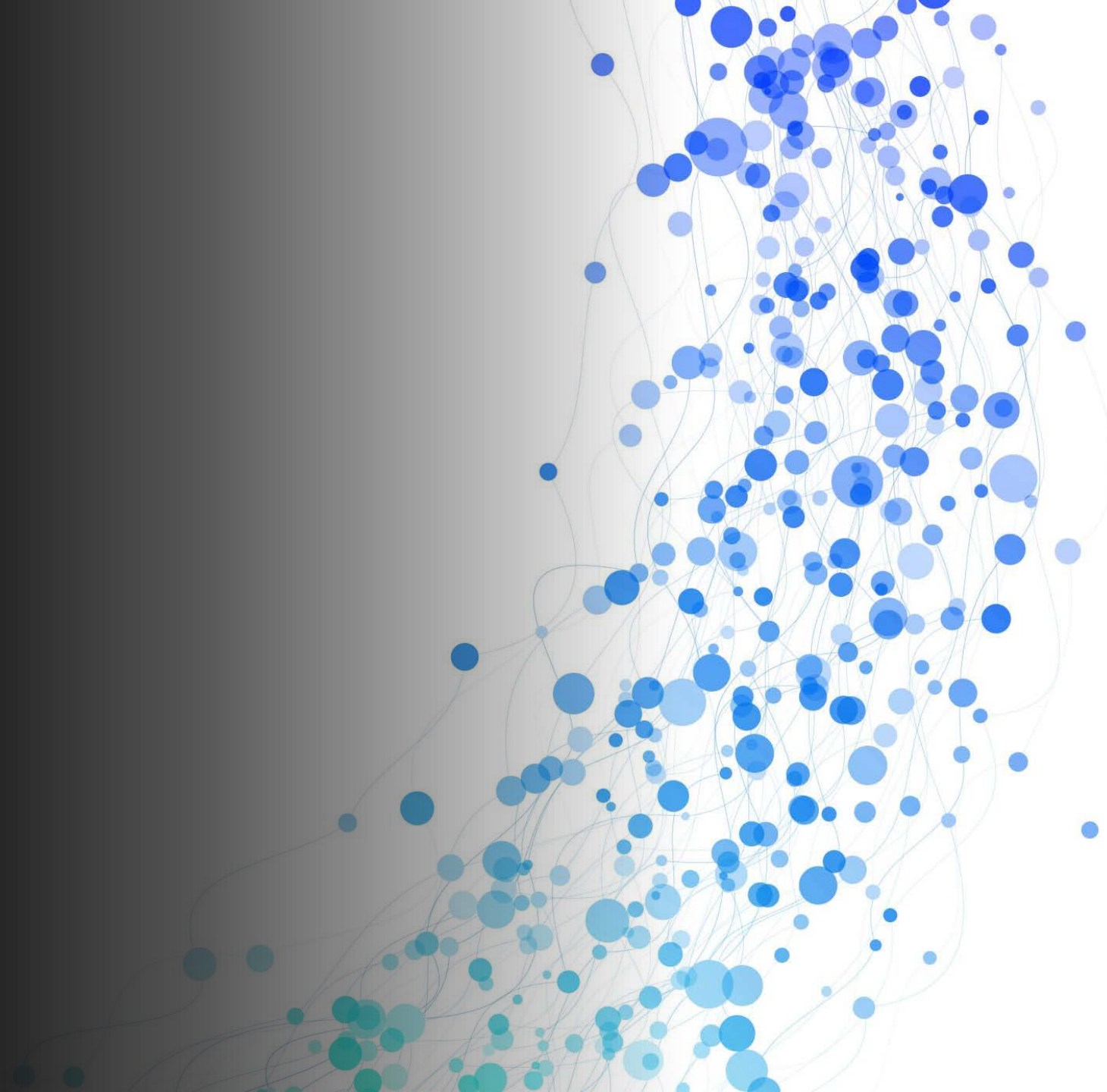




Probing quantum metaverse with Qiskit

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Outline

Understanding Preliminaries of a Quantum Circuit- Training parameterized unitaries

Applications

Writing code in qiskit

M. Sajjan, J. Li, R. Selvarajan, S. H. Sureshababu, S. S. Kale, R. Gupta, V. Singh, and S. Kais, Quantum machine learning for chemistry and physics, Chemical Society Reviews (2022).



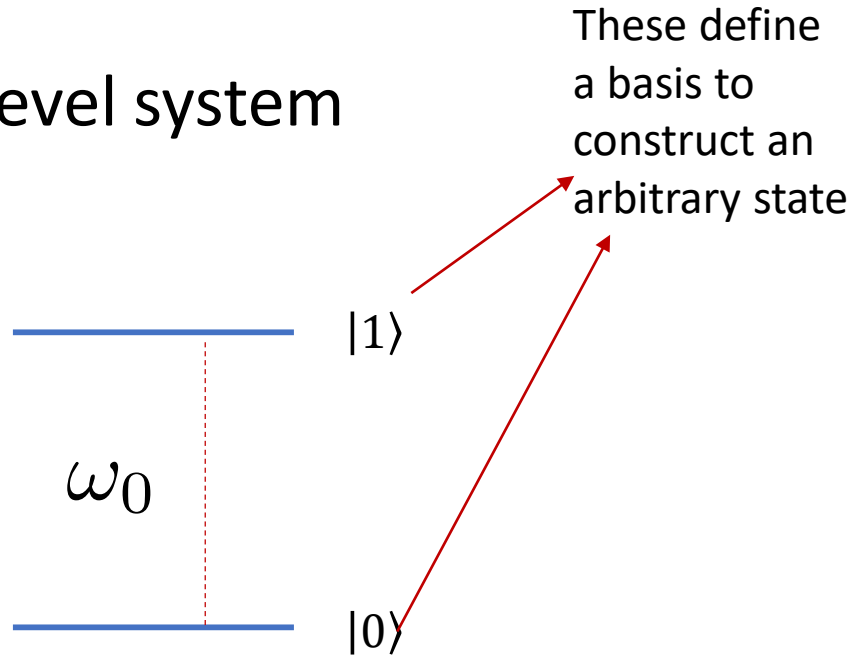
Understanding preliminary architectural features of a quantum circuit

- Qubit
- Single-qubit gates
- Two-qubit gates
- Understanding quantum circuits
- Parameterized quantum circuits-Training and Optimization
- Data-encoding

A quick review of essential building blocks of a digital quantum algorithm

• Qubit

Simple two-level system



$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Examples

- Electronic spin
- Energy levels of an atom/ion
- Polarization states of a photon
- Energy levels of a molecule
- Energy levels of artificial atoms like quantum dots

General states of a qubit

$$\rho = \left(\frac{1}{2} + n_z\right)|0\rangle\langle 0| + (n_x + in_y)|0\rangle\langle 1| \\ + (n_x - in_y)|1\rangle\langle 0| + \left(\frac{1}{2} - n_z\right)|1\rangle\langle 1|$$

$$n_x^2 + n_y^2 + n_z^2 \leq 1 \quad (n_x, n_y, n_z)^T \in \mathbb{R}^3$$

(pure states)

$$\rho^2 = \rho$$

$$(n_x, n_y, n_z)^T = (\cos\theta \sin\phi, \sin\theta \cos\phi, \cos\theta)^T$$

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi} \sin\left(\frac{\theta}{2}\right)|1\rangle$$

$$\rho^2 \neq \rho \quad (\text{mixed states})$$

We can't do much here. We will have to represent the state as above

Visual Representation of a qubit state

Any point on the surface of the sphere will satisfy

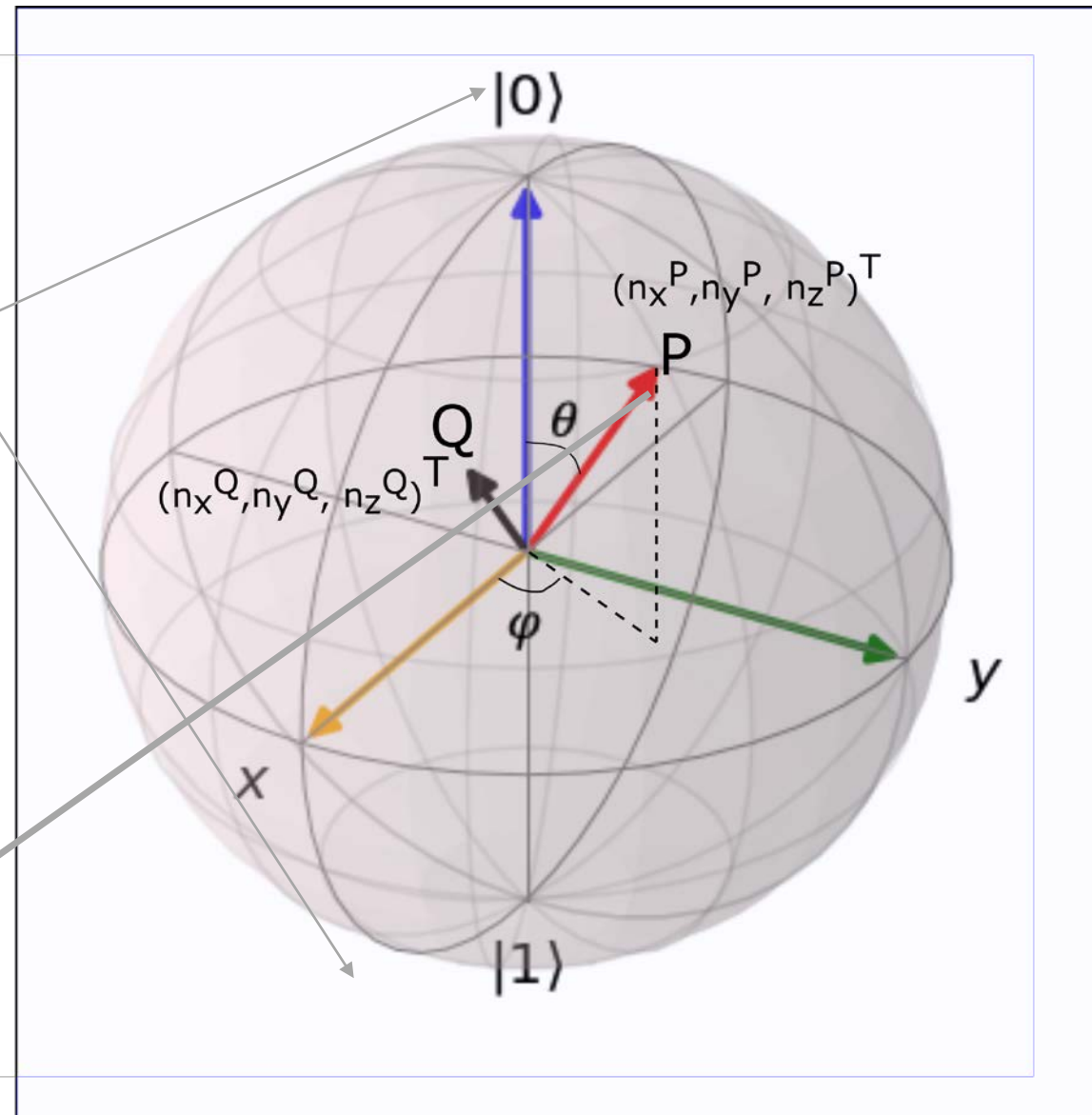
$$n_x^2 + n_y^2 + n_z^2 = 1$$

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle$$

$$= \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) \\ e^{i\phi}\sin\left(\frac{\theta}{2}\right) \end{pmatrix}$$

$$\rho^2 = \rho$$

————— $|1\rangle$
————— $|0\rangle$



A quick review of essential building blocks of a digital quantum algorithm

<https://lewisla.gitbook.io/learning-quantum/quantum-circuits/single-qubit-gates>

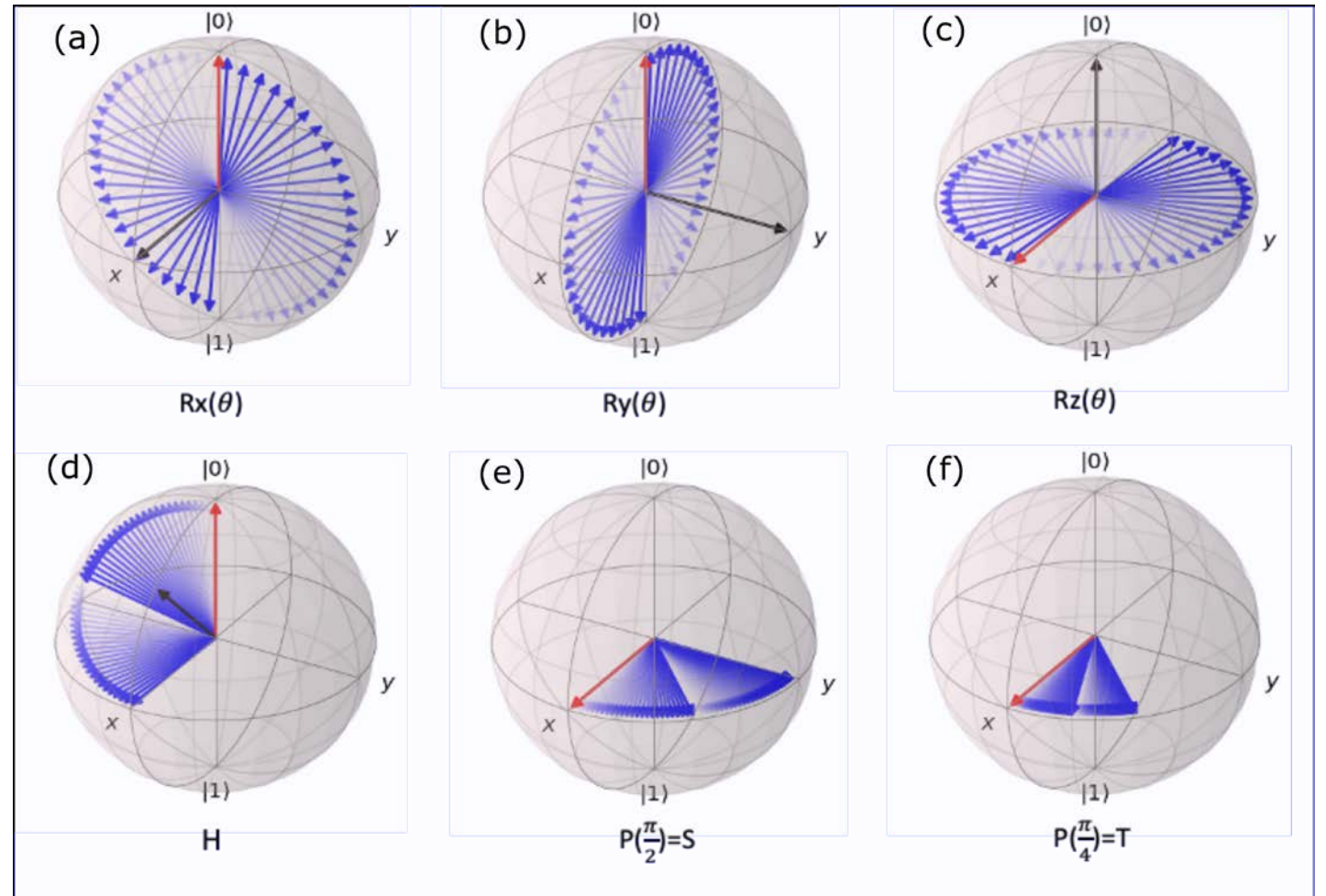
• Single-qubit gates

➤ Rotation of state on the Bloch sphere

➤ Denoted as



➤ Example : $H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

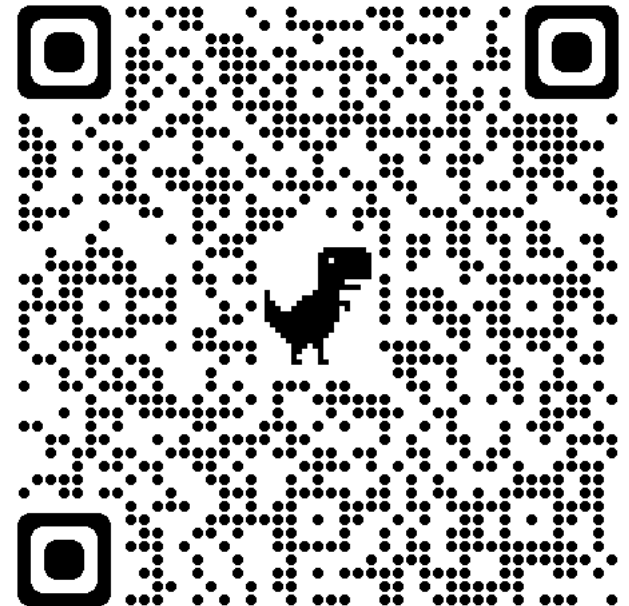


How to introduce single qubit gates in qiskit

For a comprehensive tutorial on implementing a single qubit gate and constructing a 1 qubit circuit lets look at

https://qiskit.org/documentation/tutorials/circuits/3_summary_of_quantum_operations.html

https://qiskit.org/documentation/tutorials/circuits/1_getting_started_with_qiskit.html

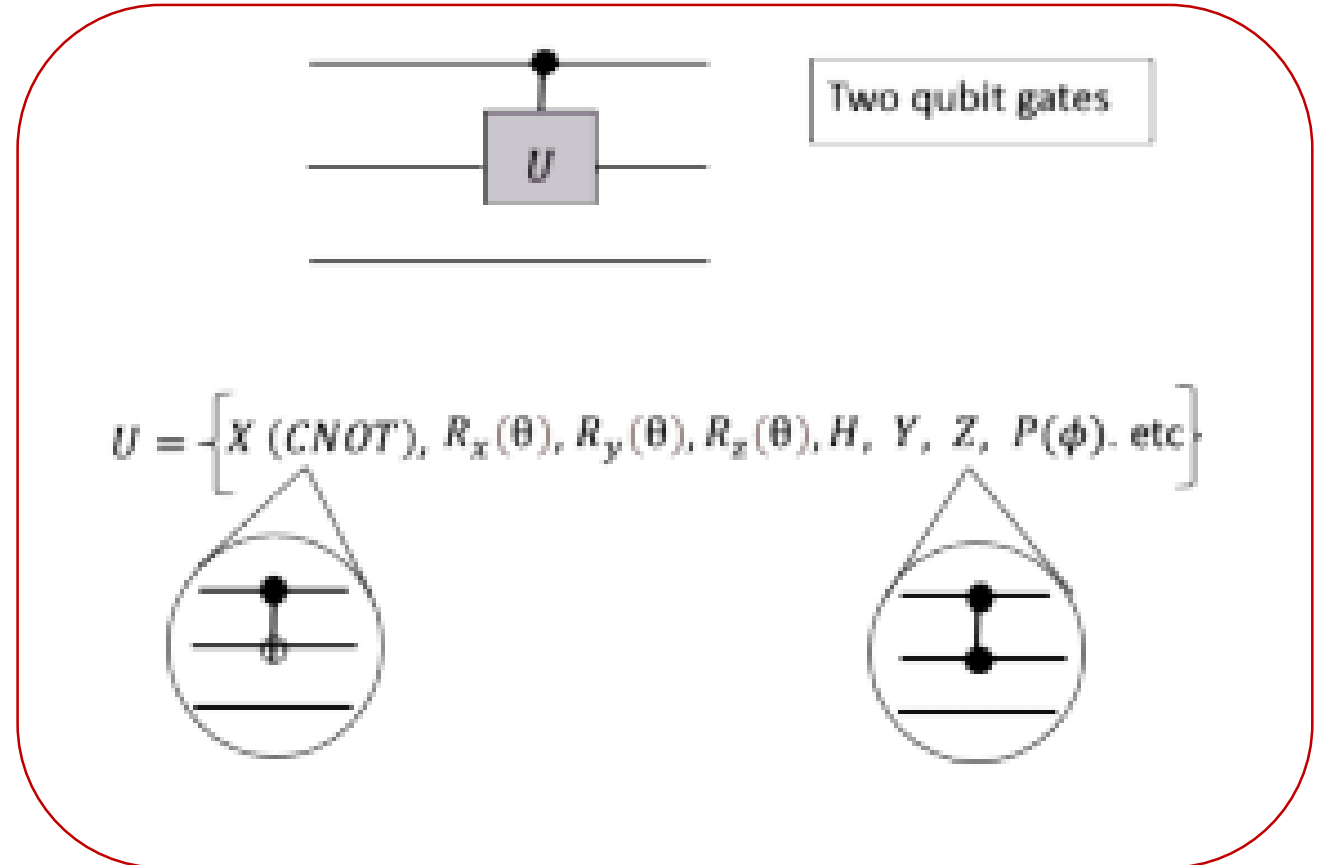
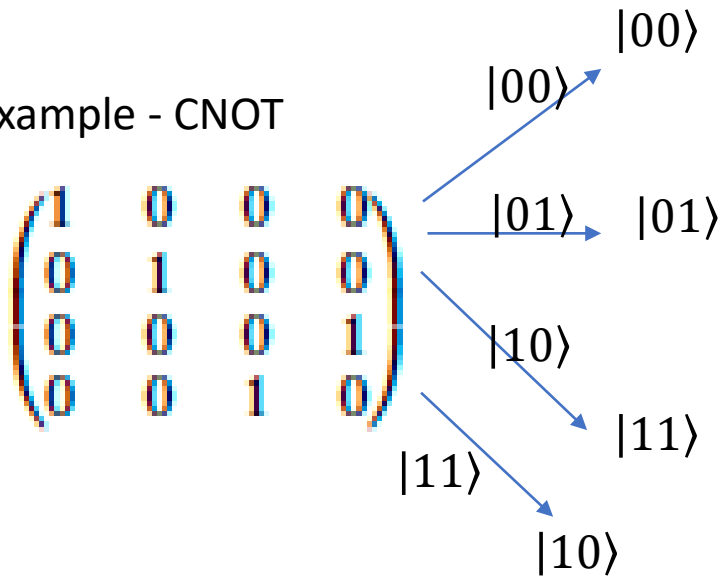


A quick review of essential building blocks of a digital quantum algorithm

- **Two-qubit gates**

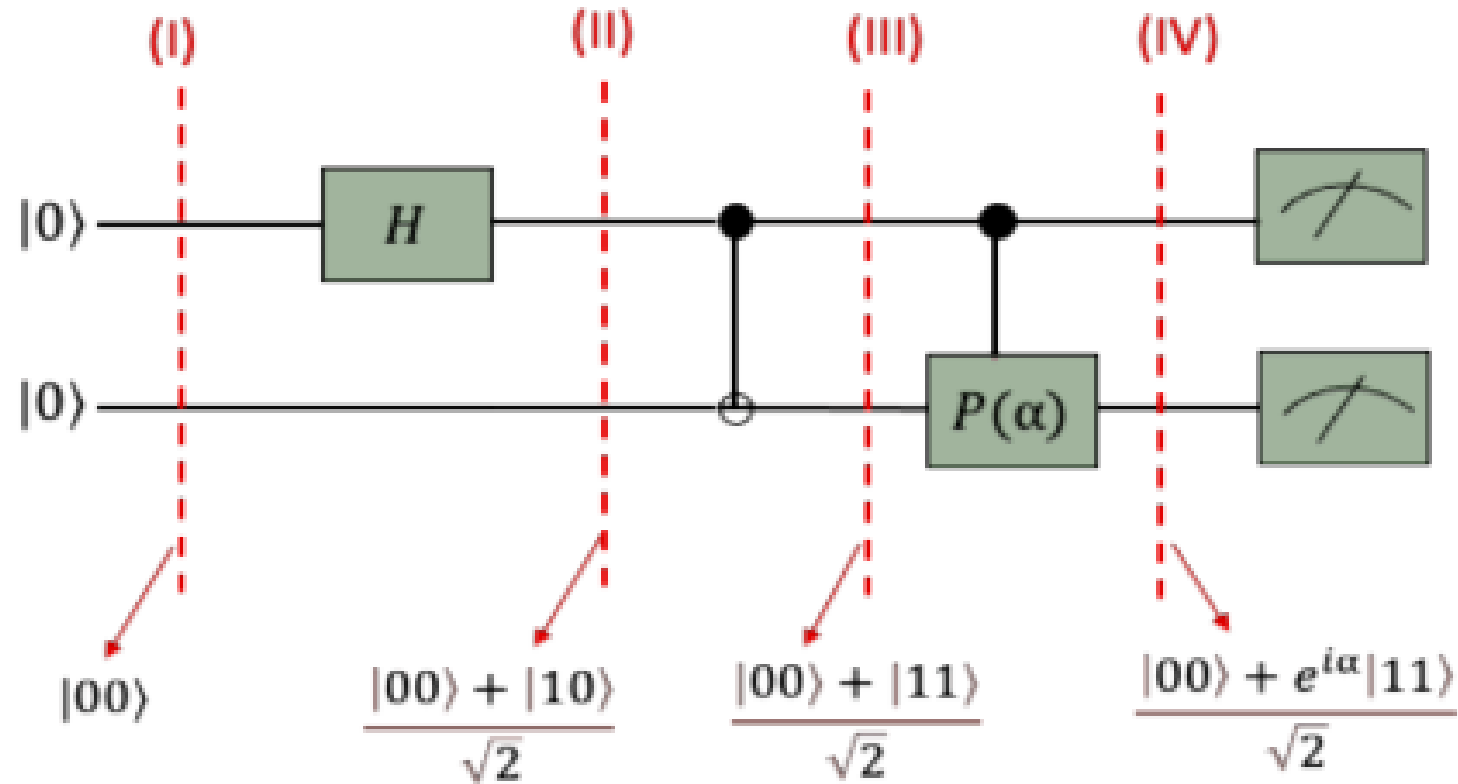
Can be used to generate correlation between two qubits

Example - CNOT



Understanding a quantum circuit

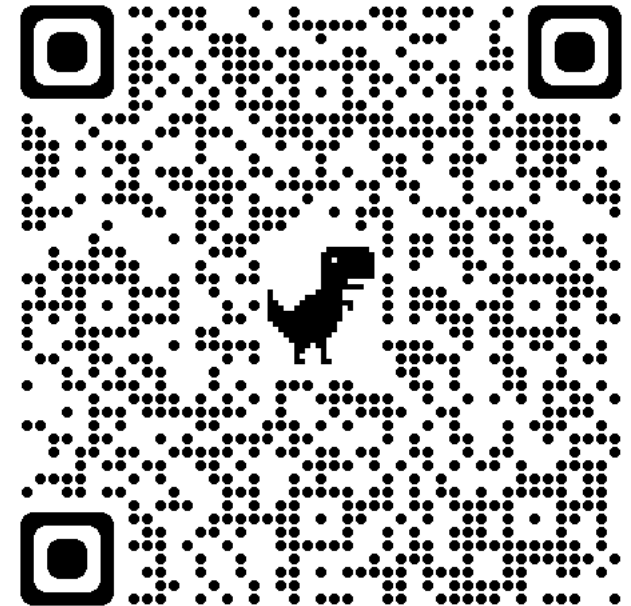
The usual technique to analyze a quantum circuit is to read from left to right and construct the joint state of the qubit array at each junction between every non-trivial operations



How to introduce multi-qubit gates in qiskit

For a comprehensive tutorial on implementing a single qubit gate and constructing a 1 qubit circuit lets look at

https://qiskit.org/documentation/tutorials/circuits/3_summary_of_quantum_operations.html

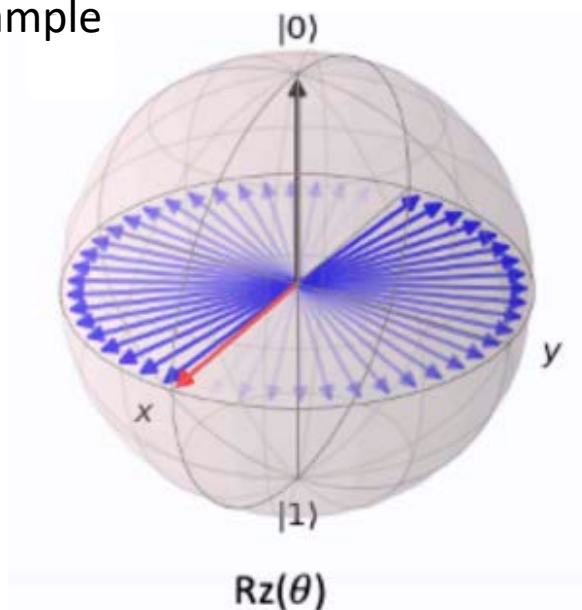


Quantum circuit with tunable parameters – Essential building block for most QML applications

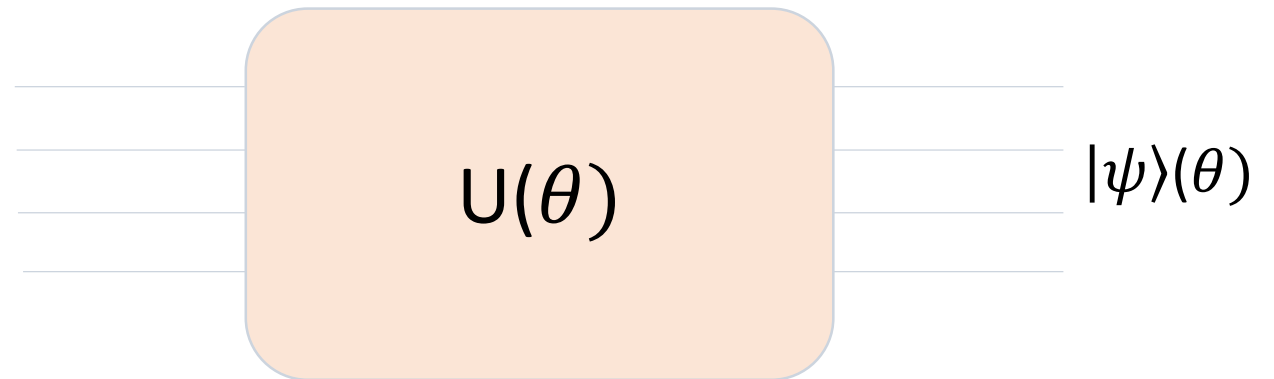
- Parameterized quantum circuits- PQC

Unlike in previous cases ,the circuit here consists of free trainable parameters which are not fixed apriori once and for all . These parameters are ‘learnt’(optimized) to perform a certain task

Example



$|\psi\rangle(0)$

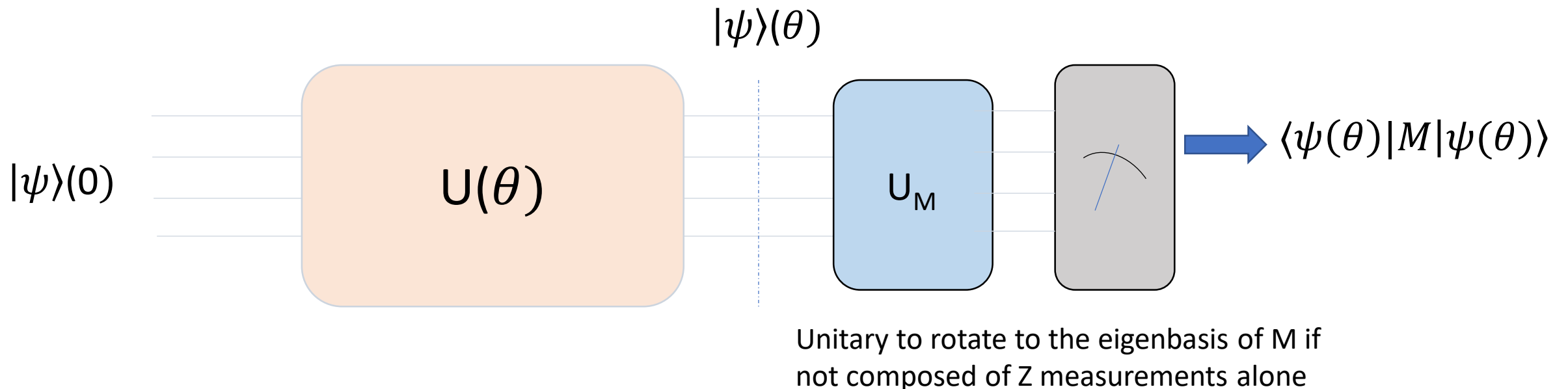


$$|\psi\rangle(\theta) = U(\theta)|\psi\rangle(0)$$

How are the parameters optimized

Parameters can be trained using the following steps

Step 1 : Using measurement results from the circuit on appropriate operator (say M) construct a suitable loss function / cost function whose minimization guarantees the solution desired



Constructing a loss function with the measurement result (say)

$$J(\theta) = f(\langle\psi(\theta)|M|\psi(\theta)\rangle)$$

How are the parameters optimized

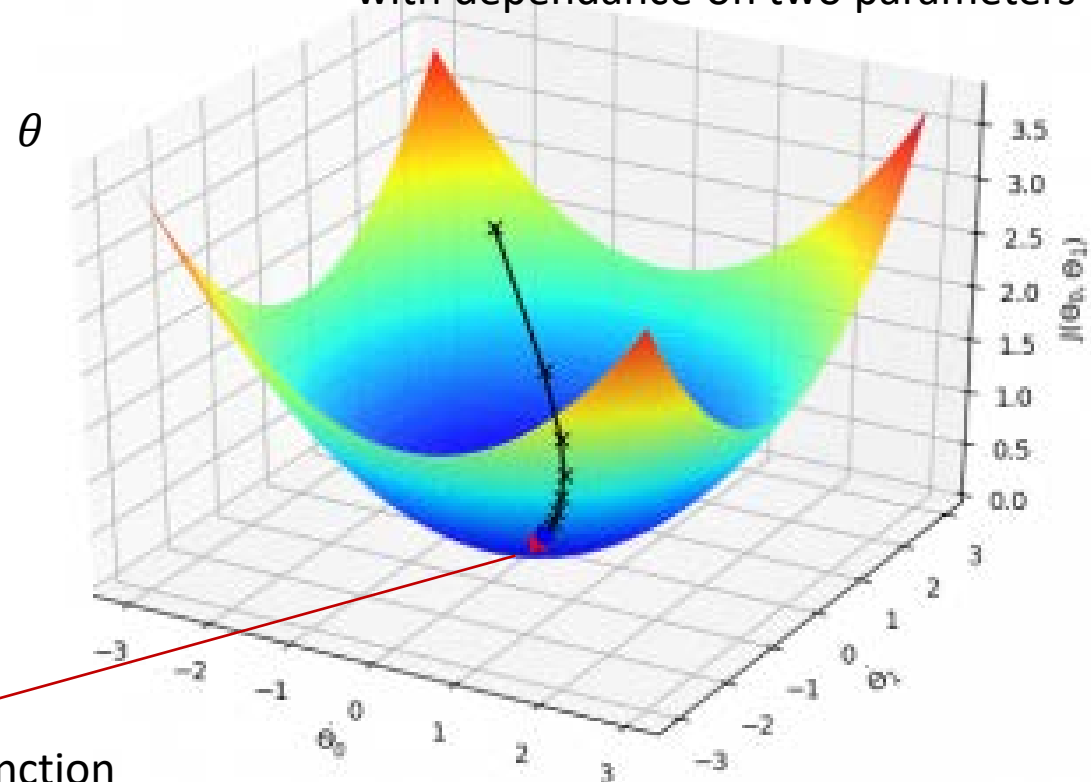
Parameters can be trained using the following steps

Step 2 : Loss function is optimized using a gradient-descent based algorithm

$$\theta^* = \operatorname{argmin}_{\theta} J(\theta) = f(\langle \psi(\theta) | M | \psi(\theta) \rangle)$$

Starting from arbitrary parameter set we want to minimize the cost function $J(\theta)$

A typical surface of $J(\theta)$ with dependence on two parameters



Minimum of cost function



Example study- Ground state simulation of molecules

- Encoding Hamiltonians into Pauli words
- Seeing simulation on jupyter notebook.

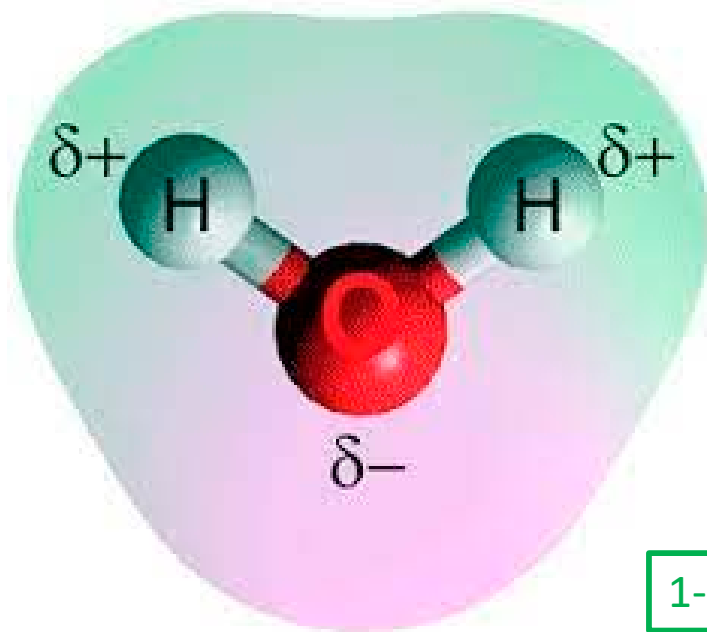
Electronic Structure Hamiltonian

6



Nonrelativistic Schrödinger equation

$$\hat{H}(\{\mathbf{r}\}, \{\mathbf{R}\})\Psi_j(\{\mathbf{r}\}, \{\mathbf{R}\}) = E_j\Psi_j(\{\mathbf{r}\}, \{\mathbf{R}\})$$



Ne= 10 electrons system
with three nuclei Nn =3 as

(O(Z=8), H(Z=1), H(Z=1))

$$\hat{H}(\{\mathbf{r}\}, \{\mathbf{R}\}) = \underbrace{\sum_{j=1}^{N_e} \left(-\frac{\nabla_j^2}{2} + V_e(\mathbf{r}_j) \right)}_{\text{1-body terms}} + \underbrace{\frac{1}{2} \sum_{j \neq k}^{N_e} \frac{1}{|\mathbf{r}_j - \mathbf{r}_k|}}_{\text{2-body term}} \left. \vphantom{\sum_{j=1}^{N_e}} \right\} \text{electronic Hamiltonian}$$

$$+ \sum_{j=1}^{N_n} \left(-\frac{\nabla_j^2}{2M_j} + V_{n,j}(\mathbf{R}_j) \right) + \frac{1}{2} \sum_{j \neq k}^{N_e} \frac{Z_j Z_k}{|\mathbf{R}_j - \mathbf{R}_k|} \left. \vphantom{\sum_{j=1}^{N_n}} \right\} \text{nuclear Hamiltonian}$$

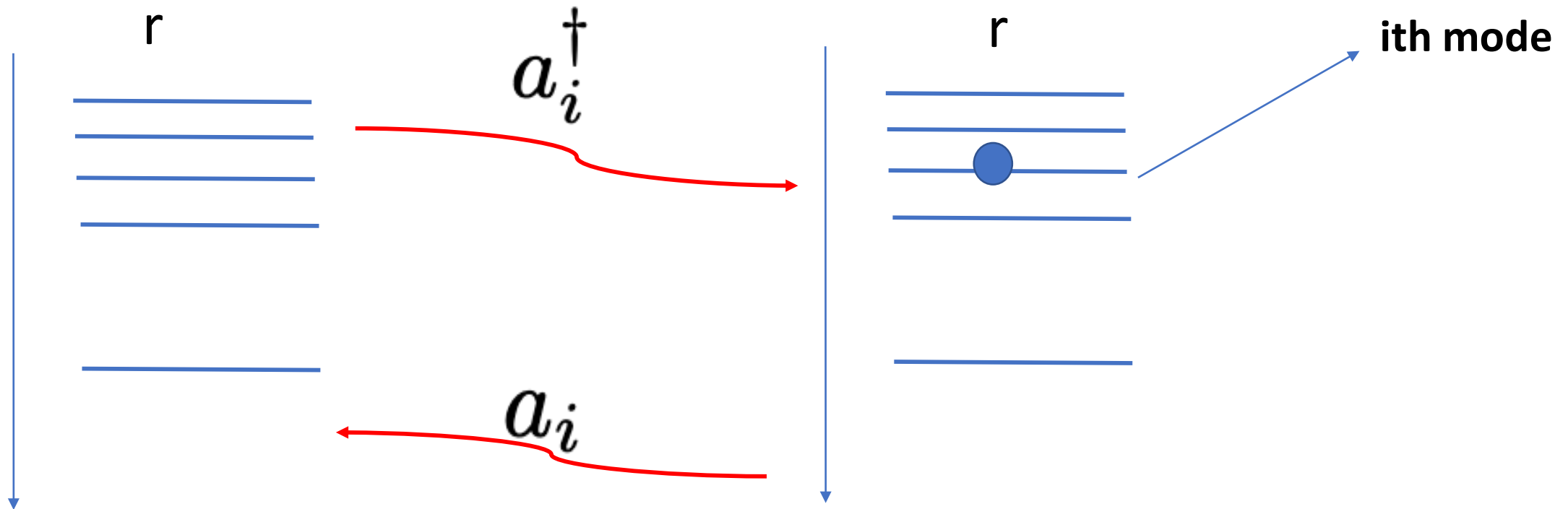
$$- \sum_{j=1}^{N_e} \sum_{k=1}^{N_n} \frac{Z_k}{|\mathbf{r}_j - \mathbf{R}_k|} \left. \vphantom{\sum_{j=1}^{N_e}} \right\} \text{electron-nuclear attraction}$$

$V_e(\mathbf{r}), V_n(\mathbf{R})$: external scalar potentials acting on the electrons/nuclei.

Fermionic modes and Second Quantization

FIRST ATTACK (MEAN FIELD BY CHOOSING AN ATOMIC ORBITAL BASIS)

Mean field (HF) solutions of the problem where each electron faces interaction with every other electron in an average way defines a bunch of single-particle functions (Molecular orbitals). Let their number be r



Fermionic modes and Second Quantization

$$\{a_i^\dagger, a_j\} = \delta_{ij}$$

$$\{a_i, a_j\} = 0 \quad \forall \{i, j\} \in \{1, 2..r\}$$

Using these properties it is easy to show that

1. $E_{ii} = a^\dagger a_i = E_{ii}^2$

2. $[E_{ii}, E_{pp}] = 0 \quad \forall i, p$

Eigenmodes of E_{pp}

$|1, 0, \dots, 0, 1, \dots, 0_r\rangle$

Occupation number representation, a convenient many-body basis

Fermion to Qubit Encoding – Jordan Wigner Transformation

Fermions

$\{a_i, a_i\} = 0, \{a_i^\dagger, a_i^\dagger\} = 0, \{a_i, a_i^\dagger\} = \delta_{i,j}$

mapping

Spins

$[\sigma_i, \sigma_i] = 0, [\sigma_i^\dagger, \sigma_i^\dagger] = 0, [\sigma_i, \sigma_j^\dagger] = \delta_{i,j}$

Jordan-Wigner

$$\hat{a}_j = \bigotimes_{i=1}^{j-1} \hat{\sigma}_i^z \otimes (\hat{\sigma}_j^x + i\hat{\sigma}_j^y)$$

$$\hat{a}_j^\dagger = \bigotimes_{i=1}^{j-1} \hat{\sigma}_i^z \otimes (\hat{\sigma}_j^x - i\hat{\sigma}_j^y)$$

$$\hat{H}_{elec} = \sum_{pq} h_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

$$\hat{H}_{elec} = \sum_i c_i \hat{P}_i$$

Case study for hydrogen molecule

