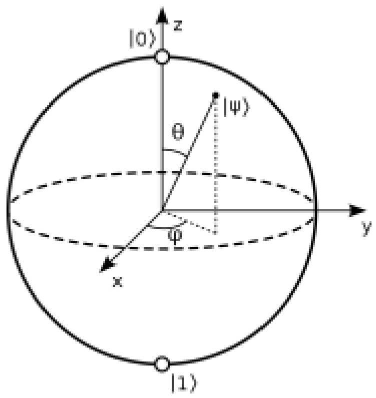
A BRIEF INTRO TO QUANTUM COMPUTING AND VQE

- INTRO TO QUANTUM COMPUTING:

The basic operational units of quantum computers are qubits. Qubits in turn are two-state quantum systems, be they atomic spins or photon polarizations. The quantum computer consists of the qubits, the connections between them, and the apparatus used to manipulate their states. In most cases, the qubits are very sensitive to mechanical and thermal perturbations, which can cause them to decohere and lose their quantum properties. To prevent this from happening the whole machine is encased in a multistage dilution refrigerator to keep it cold and housed in a shock-absorbent chamber to keep it very still. Even with all of these precautions, qubits still typically decohere in a matter of microseconds. Calculations are performed on a quantum computer by acting on single or multiple qubits via quantum logic gates and thereby changing their states. Since these are quantum systems, they can exhibit superposition and entanglement, which are key to their computational power. When a qubit is in superposition it has a probability of being measured in either of its two states. Entanglement refers to a state involving two qubits which can't be described independently. If we measure one of them, we automatically know the state of the other. We can conceptualize a qubit as a complex two-component vector:

$$|q\rangle = \alpha|0\rangle + \beta|1\rangle \quad , \qquad \|\alpha\|^2 + \|\beta\|^2 = 1$$

Here α and β represent the probability amplitudes for the qubit being in its two states, so the sum of their squares must be one. With this in hand, we can think of single-qubit quantum gates as 2×2 unitary matrices. They must be unitary to conserve probability. This formalism also allows us to think of the state of a qubit as existing on the surface of a unit sphere called the Bloch sphere:



Using the two angles θ and φ, we can express α and β as:

$$\alpha = \cos\frac{\theta}{2} \qquad \beta = e^{i\varphi}\sin\frac{\theta}{2}$$

So quantum logic gates simply move the point representing the state of the qubit along the Bloch sphere. Some single-qubit gates include rotations about the x, y and z-axes, the familiar Pauli matrices, and the Hadamard gate which can put a qubit into superposition. Arguably the most important 2-qubit gate is the controlled-not or "CNOT" gate, which is commonly used to entangle two neighboring qubits. Quantum gates are used to build up quantum circuits, which take our set of qubits to the desired state. Typically a circuit will end with all the qubits being measured to get the result. Since we are dealing with probabilistic objects, we can't get an "answer" from a single measurement; we need to run the circuit many times and histogram all the results to get a probability distribution. The peaks in the distribution tell us what the outcome of the quantum program.

- INTRO TO THE VARIATIONAL QAUNTUM EIGENSOLVER (VQE) ALGORITHM :

The VQE algorithm tries to approximate the ground state energy of a given matrix Hamiltonian through a hybrid classical/quantum optimization process. We start by initializing our qubits with a trial state populated with guessed parameters. The quantum computer then evaluates the expectation value of this state with the given Hamiltonian. Using the returned value, a classical optimization algorithm varies the parameters. These two steps cycle until a user-set goal is set, either for number of steps or stability of the calculated energy. In actuality, the algorithm is not run on the whole Hamiltonian at once, since in most cases it can't be represented as a single layer of quantum gates. To be fed into the VQE algorithm the Hamiltonian matrix must be decomposed into a sum of tensor products of Pauli matrices. This can be done because the Pauli matrices and the identity matrix form a complete basis for complex 2×2 matrices, and their complete set of tensor products does the same for larger matrices.

- This Brief Overview is token from this paper: https://arxiv.org/abs/1812.01044