

# VQE Algorithm

Given a hamiltonian  $\mathcal{H}$  acting on  $n$ -qubits, we wish to find its ground state.

1. Write  $\mathcal{H}$  in its Pauli-basis (Pauli group on  $n$ -qubits).
2. Start with a random initial vector  $|\psi_0\rangle$  created by rotating every qubit in the  $x$  and  $z$  directions by two random qubit-dependent angles:  $\theta_i$  and  $\phi_i$ .
3. For  $j \in [trials]$ , calculate the expectations:

$$E_{\pm} := \langle \psi_j(\pm\varepsilon) | \mathcal{H} | \psi_j(\pm\varepsilon) \rangle$$

where  $\psi_j(\pm\varepsilon)$  is given by setting  $\theta_i^j := \theta_i^{j-1} \pm \varepsilon$  (similarly for  $\phi_i^j$ ).

1. We are essentially *rotating each qubit* a little bit at each step, and recomputing its energy.
4. Given the positive expectation and the negative expectation, compute the gradient via finite difference:

$$\nabla \approx \frac{E_+ - E_-}{2\varepsilon}$$

5. Update the angles as:

$$\theta_i^{j+1} := \theta_i^j - \nabla$$

Similarly for  $\phi_i^{j+1}$ .

6. Repeat and hope you can reach convergence.