Variational Quantum Eigensolver

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Quantum Computing in the NISQ era and beyond

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Quantum **2**, 79 (2018)
arXiv: 1801.00862

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30 July 2018

Noisy Intermediate-Scale Quantum (NISQ) technology will be available in the near future. **Quantum computers with 50-100 qubits may be able to perform tasks which surpass the capabilities of today's classical digital computers**, **but noise in quantum gates will limit the size of quantum circuits that can be executed reliably**. NISQ devices will be useful tools for exploring many-body quantum physics, and may have other useful applications, but the 100-qubit quantum computer will not change the world right away — we should regard it as a significant step toward the more powerful quantum technologies of the future. Quantum technologists should continue to strive for more accurate quantum gates and, eventually, fully fault-tolerant quantum computing.

Hybrid Quantum-Classical Algorithm

- **NISQ (Noisy Intermediate Scale Quantum)** Devices:
  - **Imperfect gates, noise measurements and decoherence of the qubits (No error correction)**
- **NISQ algorithm solution**: **small number of qubits and low circuit depth**
- **Hybrid Quantum-Classical (HQC) Algorithm**: **leverage strengths of quantum and classical computation**
- **Variational quantum circuit algorithm is the most popular Hybrid Quantum-Classical algorithm**.

Hybrid Quantum-Classical Algorithm

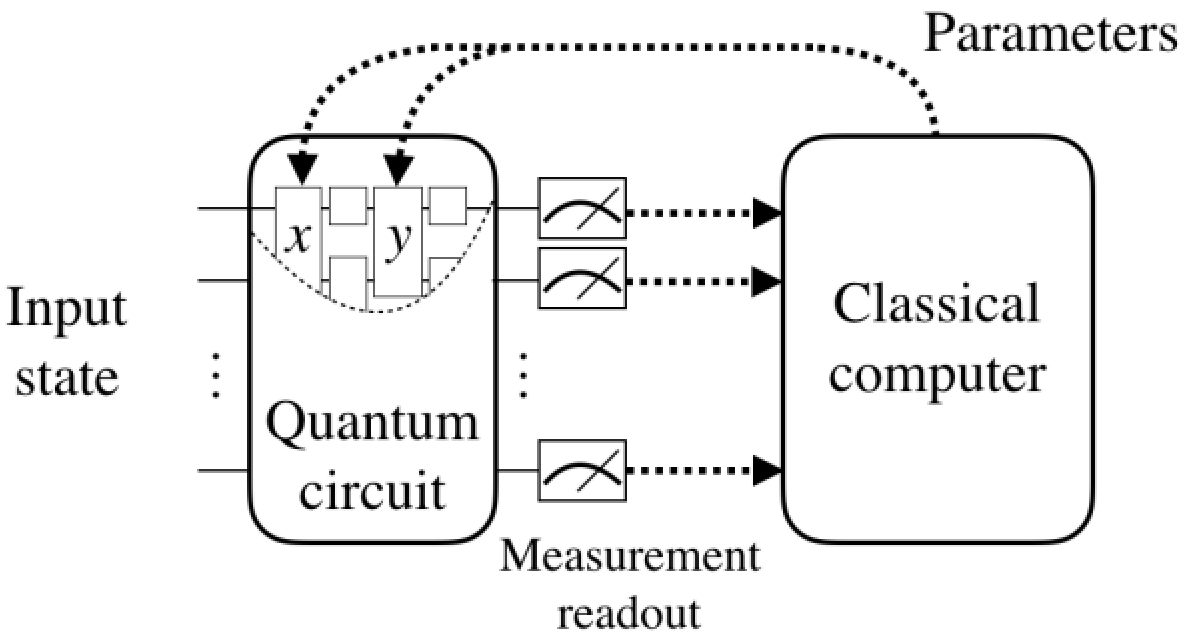
- **NISQ (Noisy Intermediate Scale Quantum)** Devices:
  - **Imperfect gates, noise measurements and decoherence of the qubits**
    (No error correction)

- **NISQ algorithm solution**: **small number of qubits and low circuit depth**

- **Hybrid Quantum-Classical (HQC) Algorithm**: **leverage strengths of quantum and classical computation**

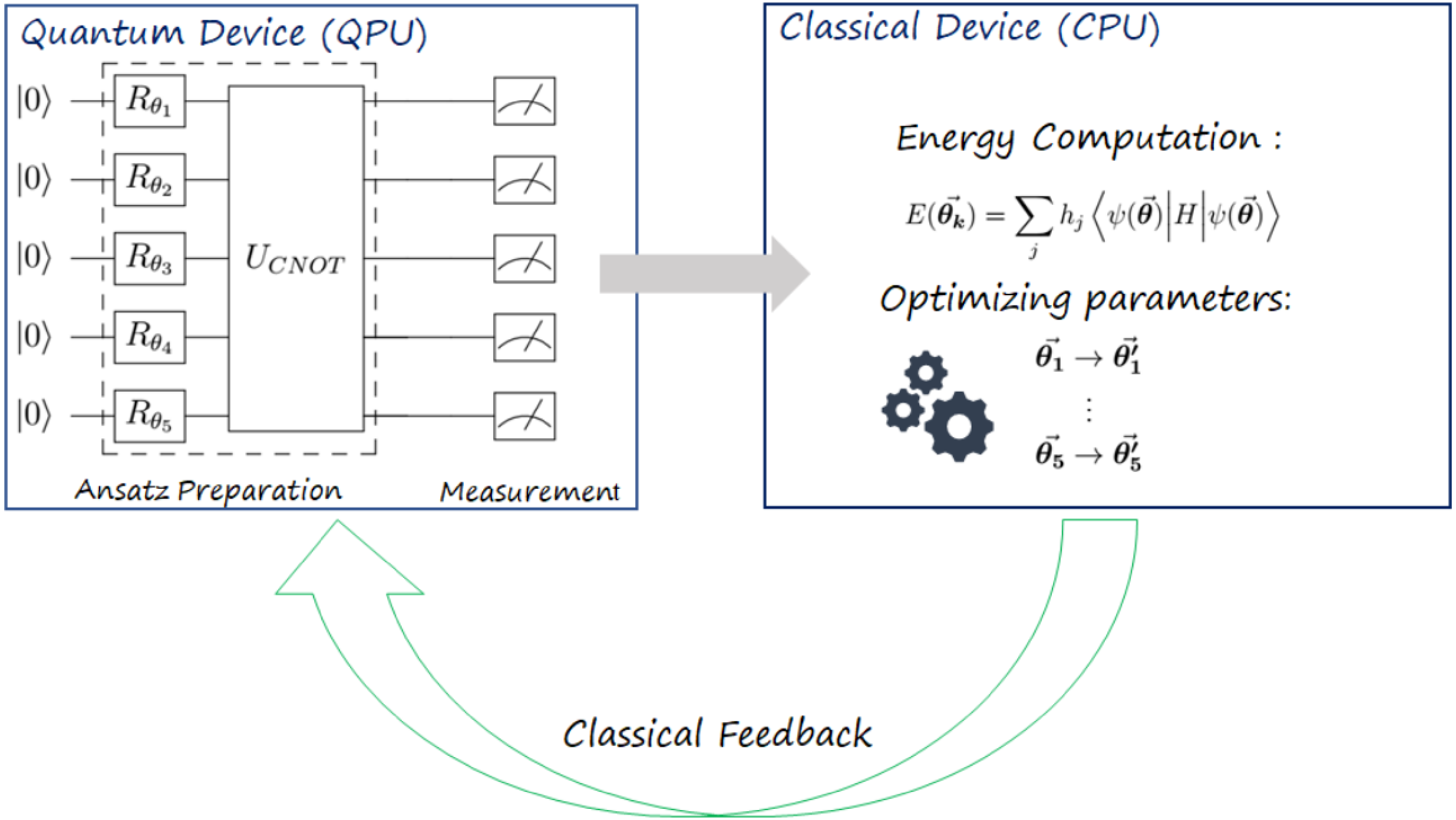
- **Variational quantum eigensolver (VQE) is the most famous Hybrid Quantum-Classical algorithm**.

Scheme of HQC Algorithm



- **QPU**: Input and output states
- **CPU**: Classical Optimization

Variational Quantum Eigensolver (VQE)



Variational principle

$$\mathcal{H}|\psi_\alpha\rangle = \varepsilon_\alpha|\psi_\alpha\rangle\,, \quad \alpha = 0, 1, \ldots$$

where

$$\mathcal{E}_0 \leq \mathcal{E}_1 \leq \mathcal{E}_2 \leq \cdots \leq \mathcal{E}_\alpha \leq \cdots\,, \quad \langle\psi_\alpha|\psi_\beta\rangle = \delta_{\alpha\beta}$$

Theorem - the variational principle

Given *any normalized function* $\widetilde{\psi}$ (that satisfies the appropriate boundary conditions), then the expectation value of the Hamiltonian represents an upper bound to the *exact* ground state energy

$$\langle\widetilde{\psi}|\mathcal{H}|\widetilde{\psi}\rangle \geq \mathcal{E}_0\,.$$

What if $\widetilde{\psi}$ is a ground state w.f.?

$$\langle\widetilde{\psi}|\mathcal{H}|\widetilde{\psi}\rangle = \mathcal{E}_0$$

Proof

$\widetilde{\psi}$ are normalized $\Rightarrow \langle\widetilde{\psi}|\widetilde{\psi}\rangle = 1$

On the other hand, (unknown) ψ_α form a complete set $\Rightarrow |\widetilde{\psi}\rangle = \sum_\alpha c_\alpha|\psi_\alpha\rangle$

So,

$$\langle\widetilde{\psi}|\widetilde{\psi}\rangle = \Big\langle \sum_\beta c_\beta\psi_\beta \Big| \sum_\alpha c_\alpha\psi_\alpha \Big\rangle = \sum_{\alpha\,\beta} c_\beta^* c_\alpha \underbrace{\langle\psi_\beta|\psi_\alpha\rangle}_{\delta_{\alpha\beta}} = \sum_\alpha |c_\alpha|^2 = 1$$

Now

$$\langle\widetilde{\psi}|\mathcal{H}|\widetilde{\psi}\rangle = \Big\langle \sum_\beta c_\beta\psi_\beta \Big| \underbrace{\mathcal{H} \Big| \sum_\alpha c_\alpha\psi_\alpha \Big\rangle}_{\sum_\alpha c_\alpha \underbrace{\mathcal{H}|\psi_\alpha\rangle}_{\mathcal{E}_\alpha|\psi_\alpha\rangle}} = \sum_{\alpha\,\beta} c_\beta^* c_\alpha \mathcal{E}_\alpha \underbrace{\langle\psi_\beta|\psi_\alpha\rangle}_{\delta_{\alpha\beta}} = \sum_\alpha \mathcal{E}_\alpha |c_\alpha|^2$$

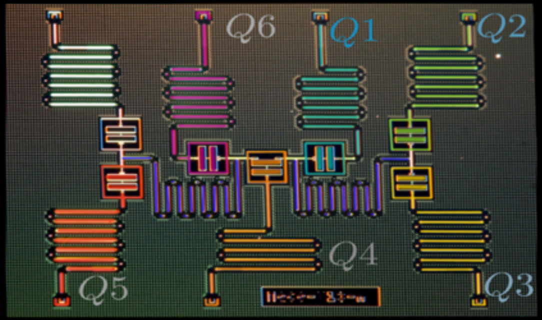
But $\mathcal{E}_\alpha \geq \mathcal{E}_0$, $\forall\alpha$, hence

$$\langle\widetilde{\psi}|\mathcal{H}|\widetilde{\psi}\rangle \geq \sum_\alpha \mathcal{E}_0 |c_\alpha|^2 = \mathcal{E}_0 \sum_\alpha |c_\alpha|^2 = \mathcal{E}_0$$

Hybrid Algorithms for NISQ Devices - VQE

IBM **Q**

A simple hybrid quantum-classical algorithm can be used to solve problems where the goal is to minimize the energy of a system



Prepare a trial state $|\psi(\theta)\rangle$ and compute its energy $E(\theta)$

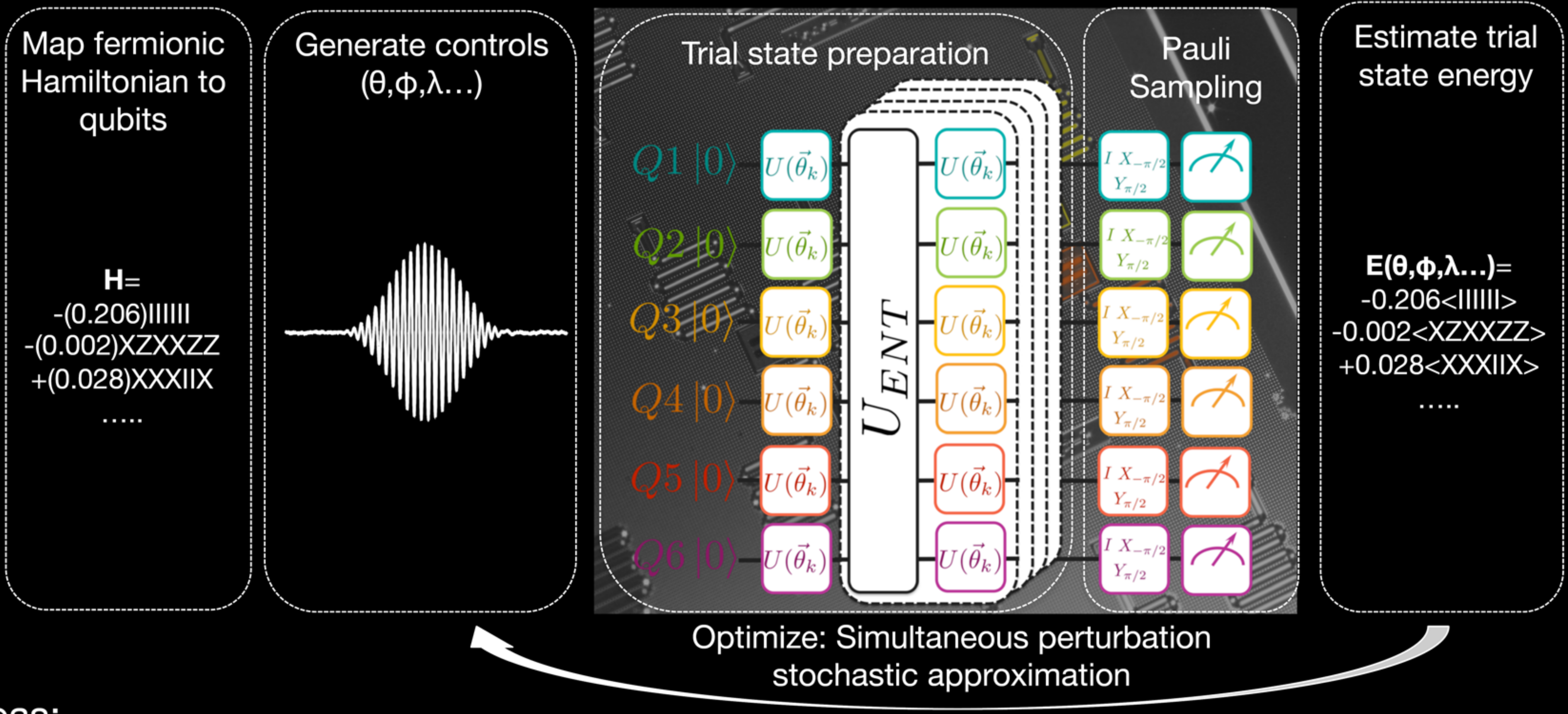
Use classical optimizer to choose a new value of θ to try

$$\langle\psi(\theta)|H|\psi(\theta)\rangle \geq \langle\psi_0|H|\psi_0\rangle$$

Variational Principle

Variational Quantum Eigensolver (VQE)

IBM Q



Focus areas:

- Reduce number of qubits (qubit tapering)
- Trial states (the ansatz)
- Fast, robust classical optimizers

Major steps in VQE

- **Variational Principle**: Minimize $\langle \Psi | H | \Psi \rangle$
- **Transformation of $\mathcal{H}$ into**: $\mathcal{H} = h^i_\alpha \sigma^i_\alpha + h^{ij}_{\alpha\beta}\sigma^i_\alpha \sigma^j_\beta + h^{ijk}_{\alpha\beta\gamma}\sigma^i_\alpha\sigma^j_\beta\sigma^k_\gamma + \ldots$
- **Linearity**: $\langle\psi|\mathcal{H}|\psi\rangle \equiv \langle\mathcal{H}\rangle = \mathcal{H} = h^i_\alpha\langle\sigma^i_\alpha\rangle + h^{ij}_{\alpha\beta}\langle\sigma^i_\alpha\sigma^j_\beta\rangle + h^{ijk}_{\alpha\beta\gamma}\langle\sigma^i_\alpha\sigma^j_\beta\sigma^k_\gamma\rangle + \ldots$

Easy for a Quantum Computer: $\boxed{\langle\sigma^i_\alpha\sigma^j_\beta\sigma^k_\gamma\ldots\rangle}$ $\longrightarrow$ Easy for a Classical Computer: $\boxed{+,\times \rightarrow \langle H\rangle}$

Outline of the VQE Algorithm

- Goal: Find the lowest eigenvalue of a given Hamiltonian

$$E(\theta) \equiv \langle H \rangle = \langle \psi(\theta) | H | \psi(\theta) \rangle \geq E_0 = \langle \psi_0 | H | \psi_0 \rangle.$$

- Method:
  - **Quantum**: Preparation of trial wavefunction ansatz with variational parameters θ, measurements of the expectation values
  - **Classical**: Sum the individual expectation value result and optimize the parameters
  - Iterate this procedure until it converges

- Applications: Quantum Chemistry, Optimization, Quantum Machine Learning…

Variation-Based Quantum Chemistry

Classical preparation

Choose basis set and SCF calculation

↓

Molecular Hamiltonian

↓

Qubit Hamiltonian

⬇

VQE Implementation

Ansatz selection and preparation (UCC/Heuristic)

↓

Measurement and classical feedback

⬇

Reconstruct PES

Hamiltonian of the quantum chemistry problem

- Molecule Hamiltonian consist *M* nuclei and *N* electron

$$H = -\sum_A \frac{\nabla_A^2}{2M_A} - \sum_i \frac{\nabla_i^2}{2} - \sum_{i,A} \frac{Z_A}{|r_i - R_A|} + \frac{1}{2}\sum_{i\neq j} \frac{1}{|r_i - r_j|} + \frac{1}{2}\sum_{A\neq B} \frac{Z_A Z_B}{|R_A - R_B|}.$$

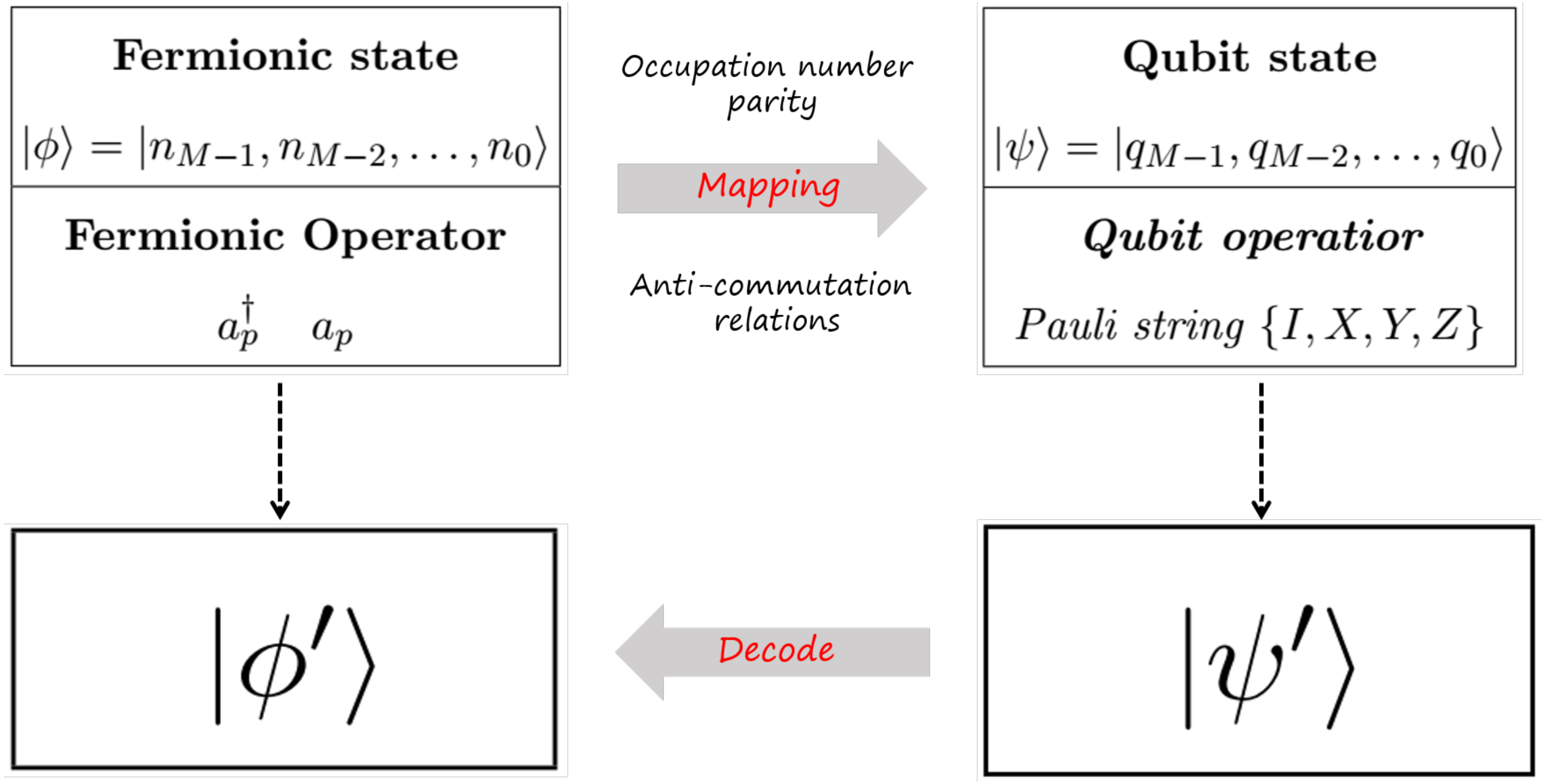
- Electronic Hamiltonian in second-quantization representation

$$H_{\mathrm{elec}} = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2}\sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s.$$

$$h_{pq} = \int d\sigma \phi_p^*(\sigma)\left(\frac{\nabla_r^2}{2} - \sum_i \frac{Z_i}{|R_i - r|}\right)\phi_q(\sigma),$$

$$h_{pqrs} = \int d\sigma_1 d\sigma_2 \frac{\phi_p^*(\sigma_1)\phi_q^*(\sigma_2)\phi_s(\sigma_1)\phi_r(\sigma_2)}{|r_1 - r_2|}.$$

Mapping the problem into Pauli's matrices



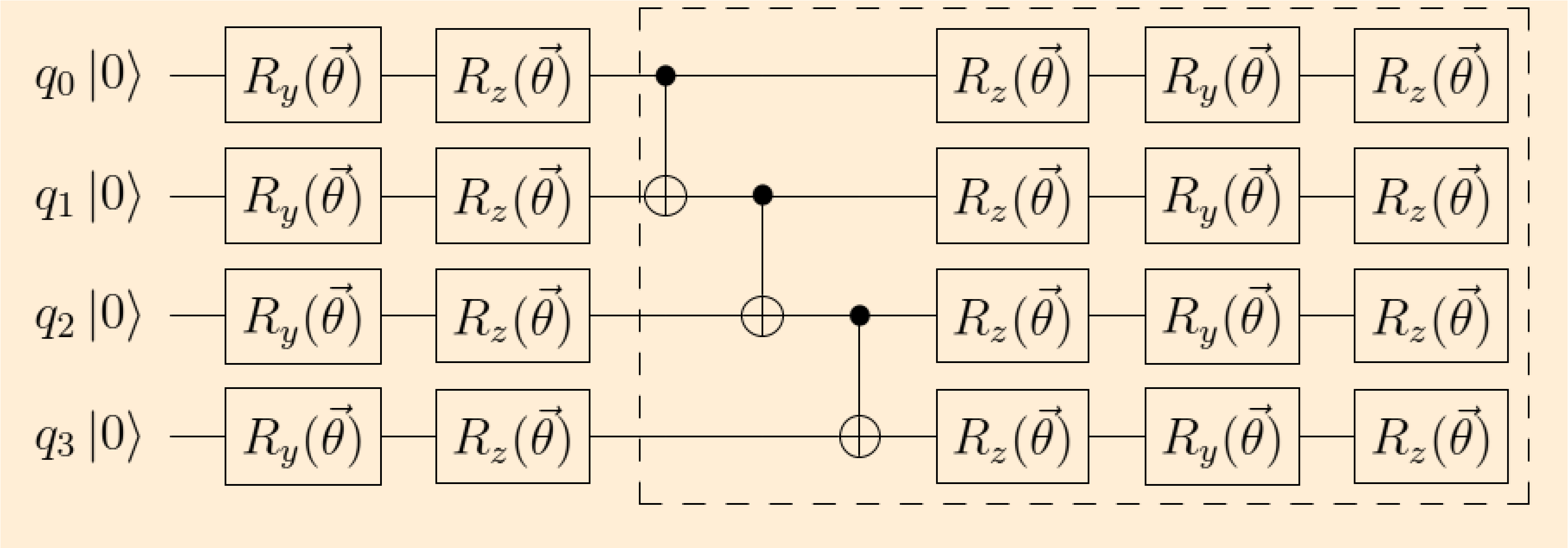
Hamiltonian in Pauli's matrix representation

- **Qubit Hamiltonian**: String of Pauli matrices

```
Representation: paulis, qubits: 4, size: 15
IIII    (-0.8121706073608677+0j)
IIIZ    (0.1714128263940238+0j)
IIZI    (-0.22343153674664057+0j)
IZII    (0.1714128263940239+0j)
ZIII    (-0.22343153674664057+0j)
IIZZ    (0.12062523481381844+0j)
IZIZ    (0.1686889816869329+0j)
XXYY    (0.04530261550868937+0j)
YYYY    (0.04530261550868937+0j)
XXXX    (0.04530261550868937+0j)
YYXX    (0.04530261550868937+0j)
ZIIZ    (0.16592785032250779+0j)
IZZI    (0.16592785032250779+0j)
ZIZI    (0.17441287610651643+0j)
ZZII    (0.12062523481381844+0j)
```

Ansatz Preparation and trial waavefunction

- **General rotation ansatz**

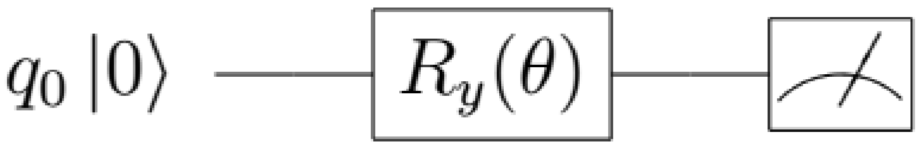


Measurements

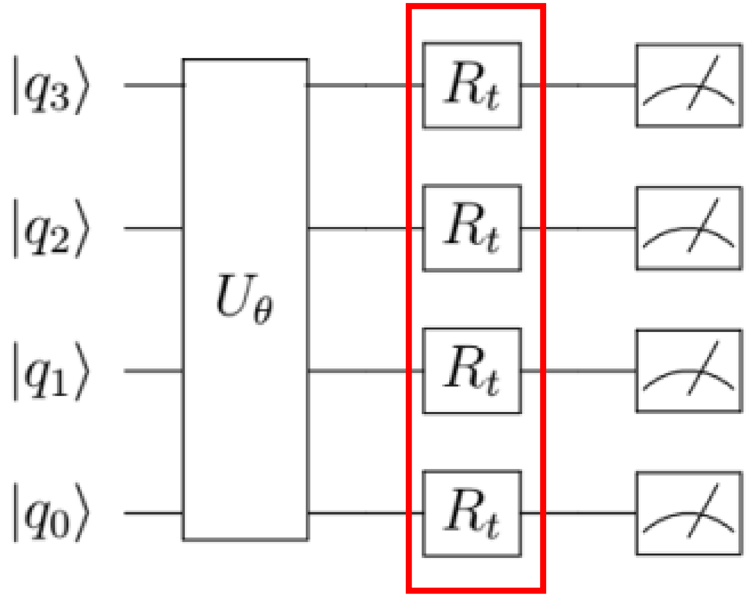
- Expectation value is easy to evaluate on a quantum computer

- How to measure the expectation value on a quantum computer ?

  (a practice problem)



probability difference $P(+1) - P(-1)$.



Post-rotations to Z-basis

Variational Quantum Eigensolver (VQE)

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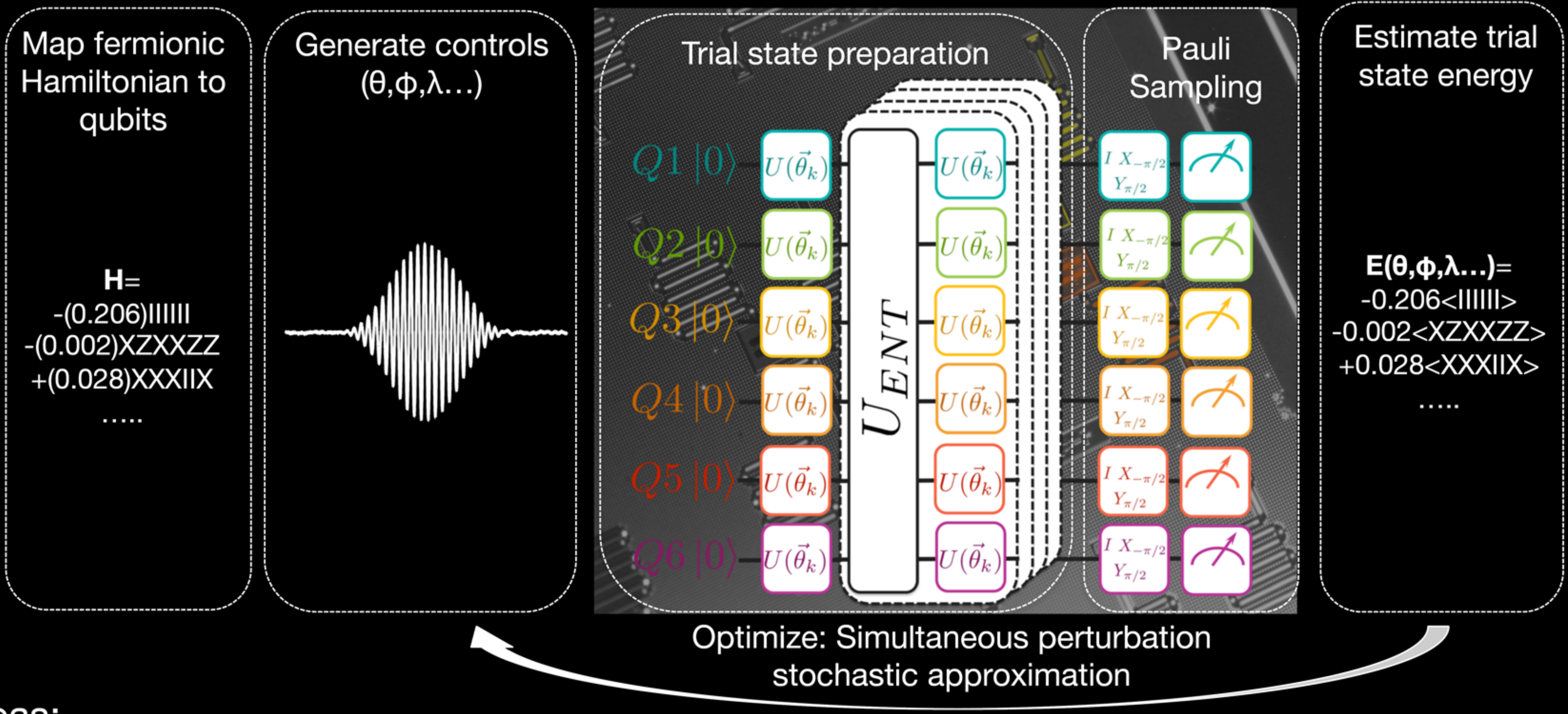

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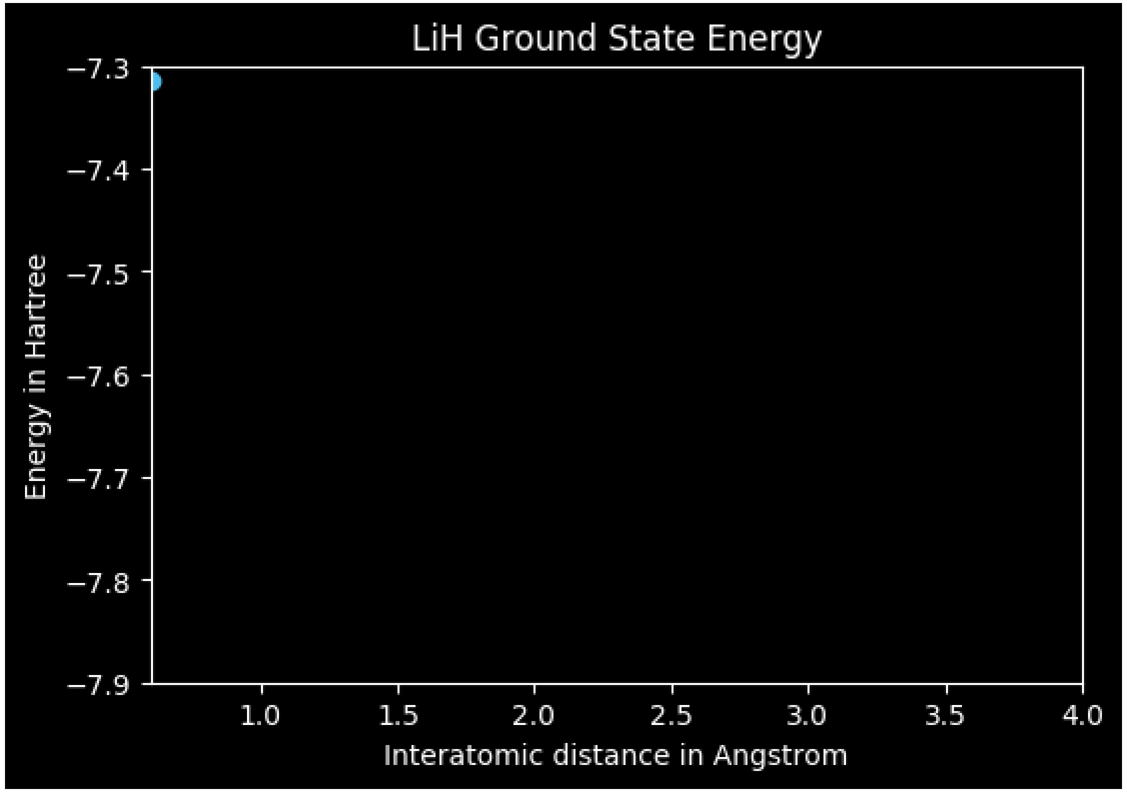
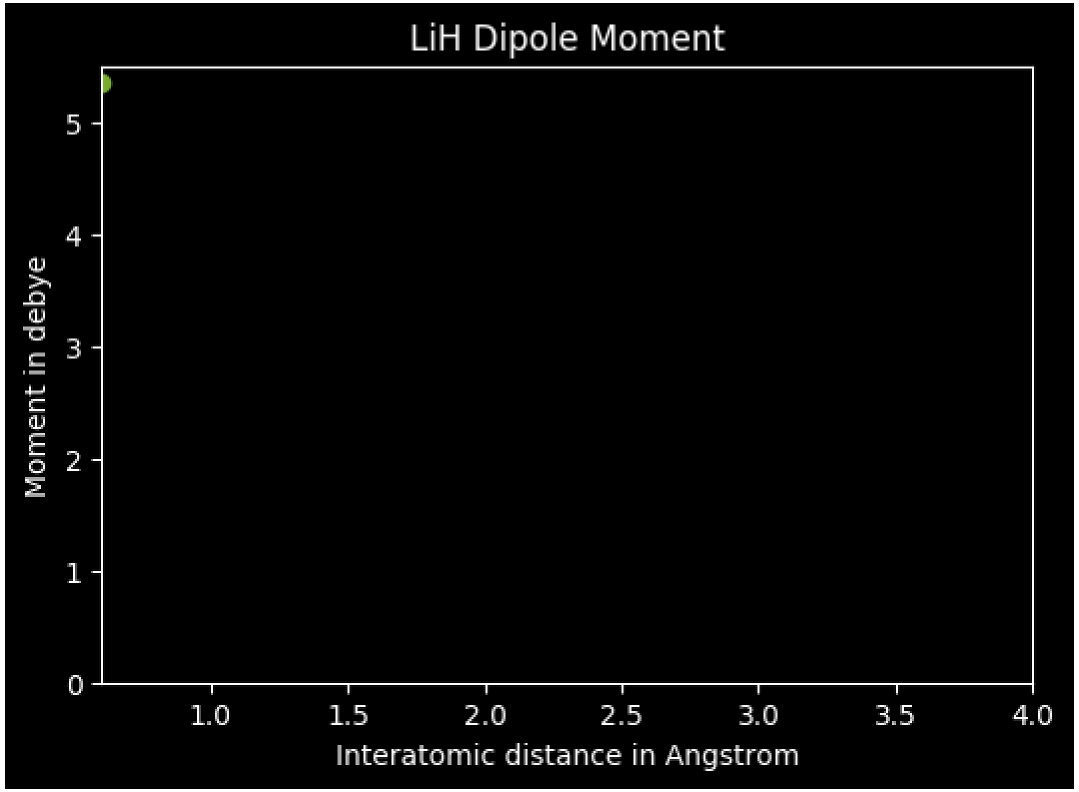
Simulation results for LiH





Simulation results for LiH