⟨Womanium|Quantum⟩ Hackathon 2022

UCLA Bruinium

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Beginner

Trying different backends

Backends	Ground State Energy of LiH (Hartree)*
AerBackend	-0.835072
ProjectQBackend	-0.8350720000000006

*at equilibrium bond length, not accounting for energy shifts due to the filling of inner orbitals and the Coulomb repulsion between nuclei

Knowledgeable

Optimizing the Depth of Jordan-Wigner Mapper Ansatz

LiH	Before Optimization	After Optimization
Circuit Depth	9834	8573
Depth CNOT	7964	7330

H_2	Before Optimization	After Optimization
Circuit Depth	83	65
Depth CNOT	52	44

Advanced

Calculating the ground state energy of LiH

Molecular

$$H = -\sum_i \frac{\nabla_{R_i}^2}{2M_i} - \sum_i \frac{\nabla_{r_i}^2}{2} - \sum_{i,j} \frac{Z_i}{|R_i - r_i|} + \sum_{i,j>i} \frac{Z_i Z_j}{|R_i - R_j|} + \sum_{i,j>i} \frac{1}{|r_i - r_j|}$$

KE(n) *KE(e)* *PE(n–e)* *PE(n–n)* *PE(e–e)*

Assumes…
- Borne-Oppenheimer
- Independent single particle wavefunctions

Second Quantization

$$H = \sum_{\alpha,\beta=1}^{M} t_{\alpha\beta} a_\alpha^\dagger a_\beta + \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta=1}^{M} u_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\gamma^\dagger a_\delta a_\beta$$

One-body *Two-body*

Hamiltonian Mapping

Molecular Hamiltonian ⇨ Qubit Hamiltonian

Second Quantization

$$H = \sum_{\alpha,\beta=1}^{M} t_{\alpha\beta} a_\alpha^\dagger a_\beta + \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta=1}^{M} u_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\gamma^\dagger a_\delta a_\beta$$

One-body *Two-body*

Qubit

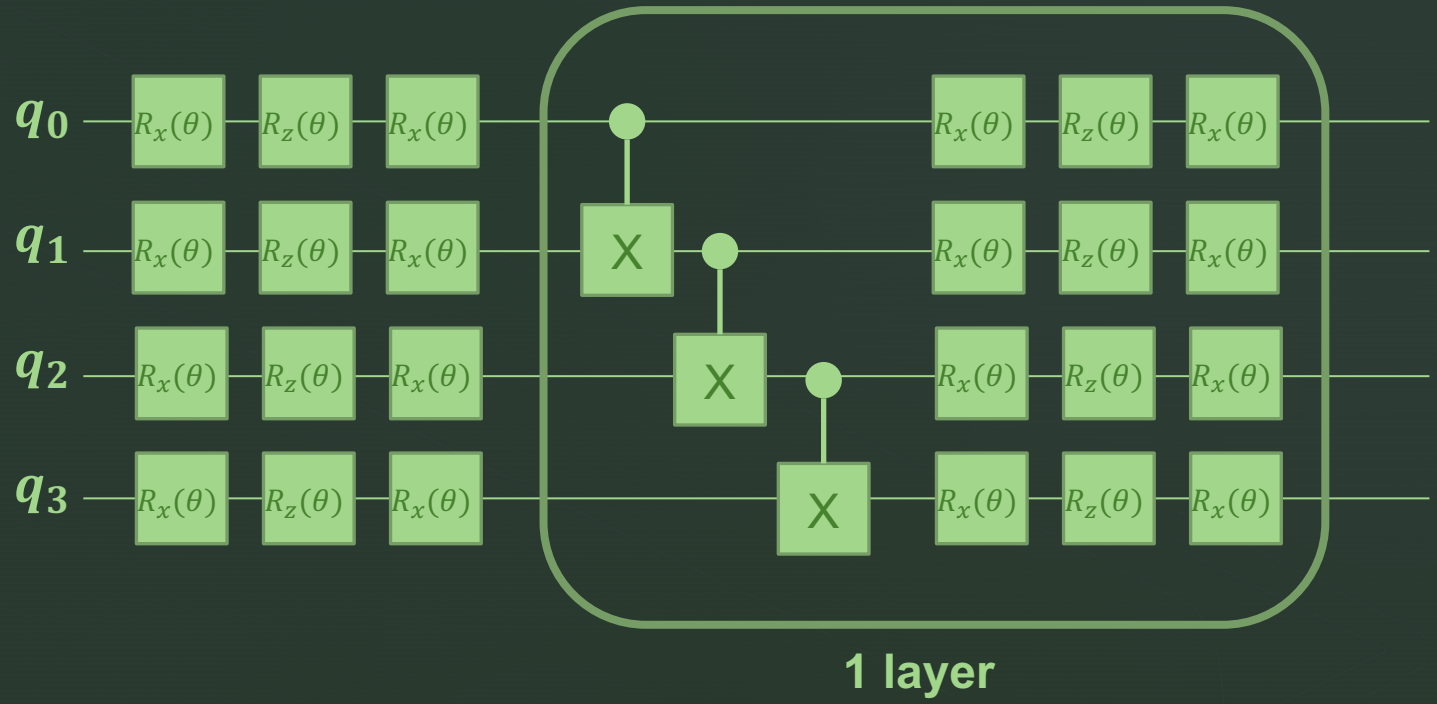
$$H = J \sum_{\langle i,j \rangle} \left(X_i X_j + Y_i Y_j + Z_i Z_j \right) + B \sum_i Z_i$$

Nearest neighbor spin-spin interaction *Magnetic field*

Circuit Design

Hardware Structure

Hardware-Efficient Ansatz

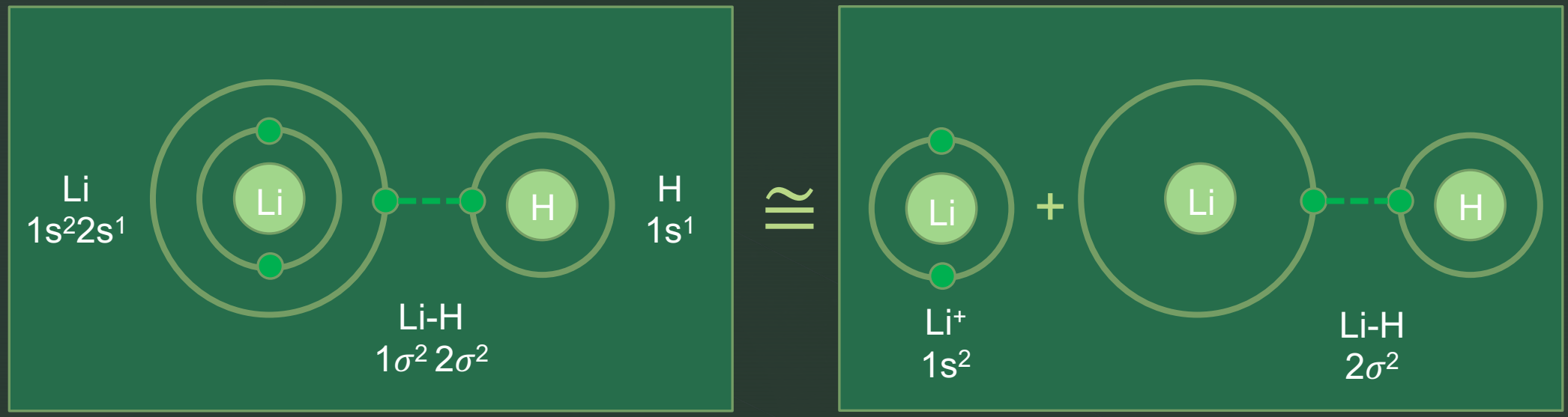


Approach

A

Chemistry-inspired simulation of LiH

Li-H($1\sigma^2\,2\sigma^2$) ≅ $Li^+(1s^2)$ + Li-H($2\sigma^2$)



Our Hamiltonian $H_{LiH} = H_{LiH(1\sigma^2)} + H_{LiH(2\sigma^2)} \approx H_{Li^+(1s)} + H_{LiH(2\sigma^2)}$

Approach

B

Potential energy surface of LiH

Varying the Hamiltonian for different bond lengths