⟨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	-0.835072000000006

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

Assumes…
- Borne-Oppenheimer
- Independent single particle wavefunctions

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

$KE(n)$ $\quad\quad$ $KE(e)$ $\quad\quad$ $PE(n{-}e)$ $\quad\quad$ $PE(n{-}n)$ $\quad\quad$ $PE(e{-}e)$

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 $\quad\quad\quad\quad\quad\quad\quad$ *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

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

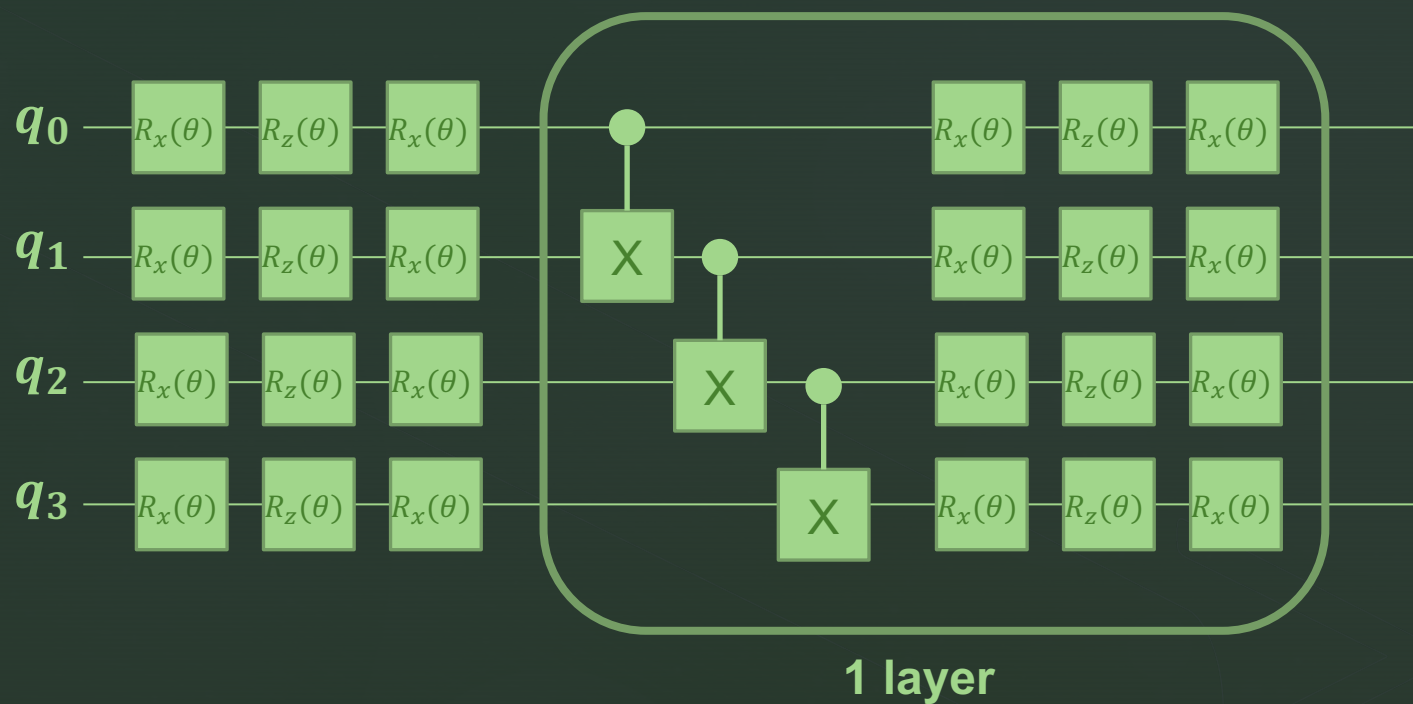*Nearest neighbor spin-spin interaction*   *Magnetic field*

Circuit Design

Hardware Structure

Hardware-Efficient Ansatz
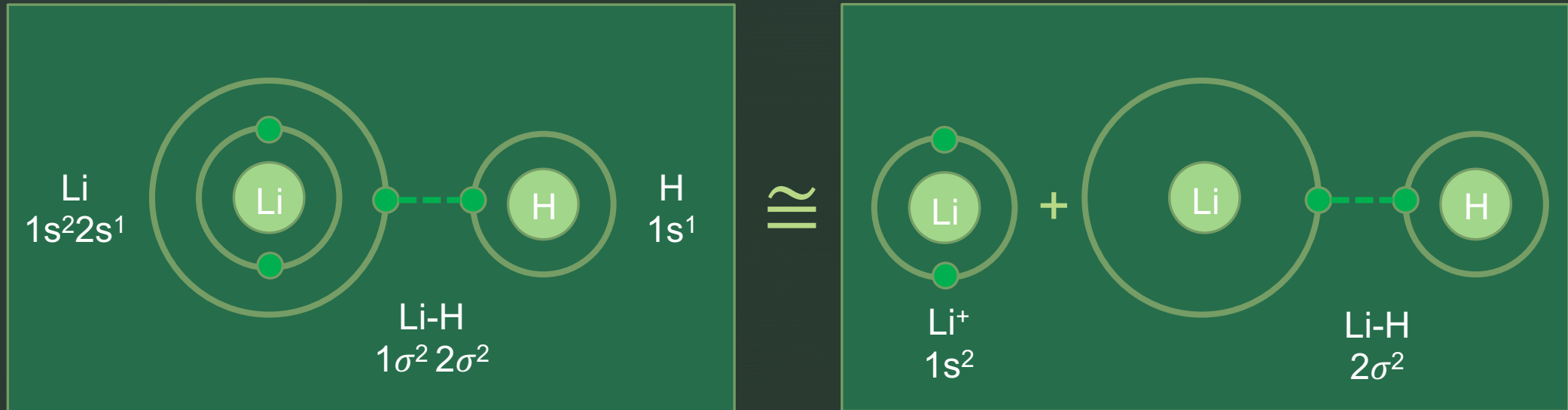

1 layer

Approach A

Chemistry-inspired simulation of LiH

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

Li
$1s^2 2s^1$

Li

H

H
$1s^1$

Li-H
$1\sigma^2 \, 2\sigma^2$

$\cong$

Li

+

Li

H

Li$^+$
$1s^2$

Li-H
$2\sigma^2$

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

Potential energy surface of LiH
Varying the Hamiltonian for different bond lengths