Simulating the Hydrogen Molecule Using a Quantum Computer

Amir H. Karamlou

Quantum Summer Camp

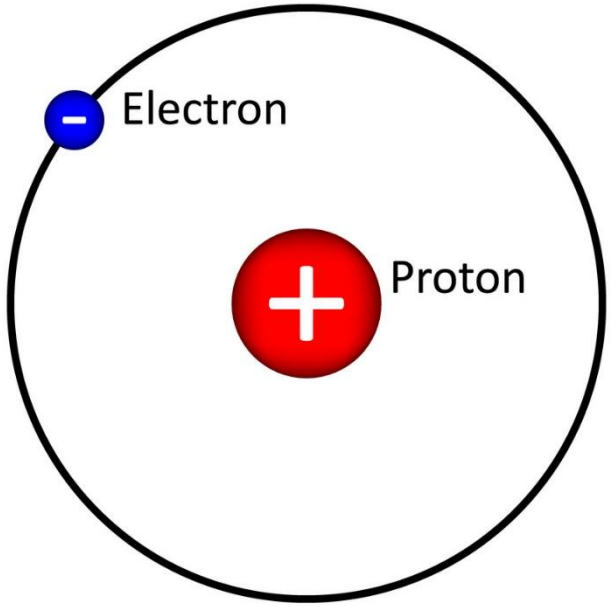
14 July 2020

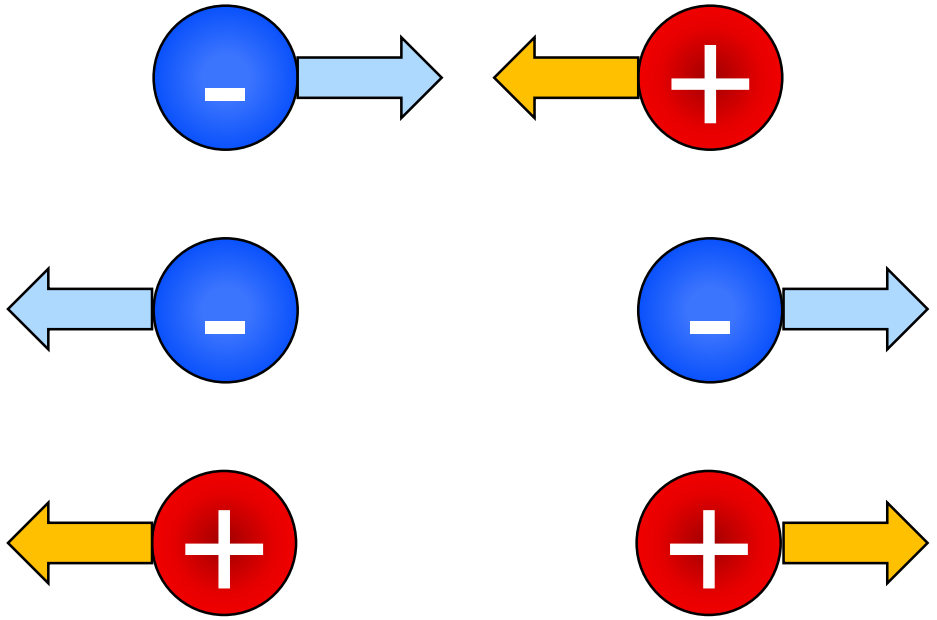
EQuS
ENGINEERING QUANTUM SYSTEMS

LINCOLN LABORATORY
MASSACHUSETTS INSTITUTE OF TECHNOLOGY

NSF

Hydrogen Atom





Coulomb's law:

q_1, q_2: electric charge
$|r|$: distance between charges
k: Coulomb's constant

$$|F| = -\frac{kq_1q_2}{|r|^2}$$

Force

$$U = \frac{kq_1q_2}{|r|}$$

Energy

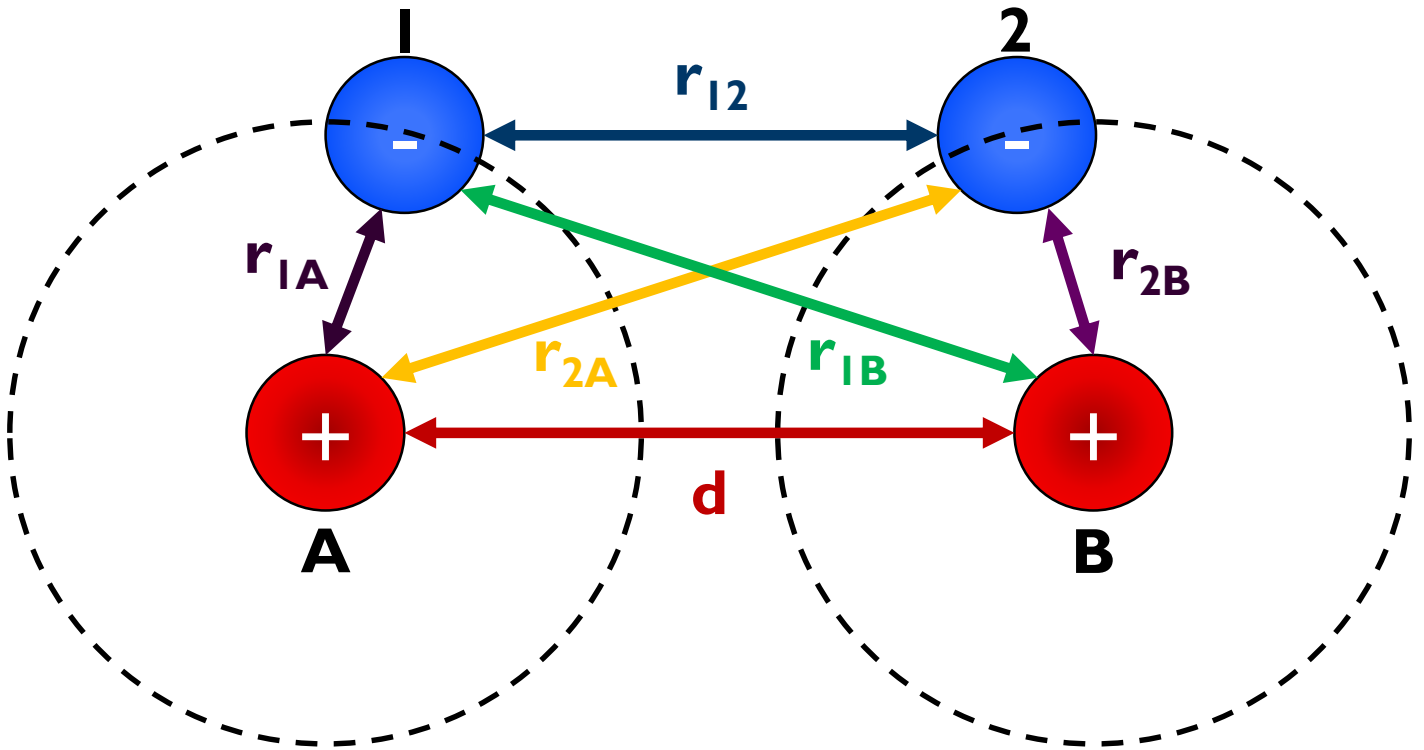
Hydrogen Molecule

$$E = KE$$

$$-\frac{ke^2}{r_{1A}} - \frac{ke^2}{r_{2B}}$$

$$-\frac{ke^2}{r_{1B}} - \frac{ke^2}{r_{2A}}$$

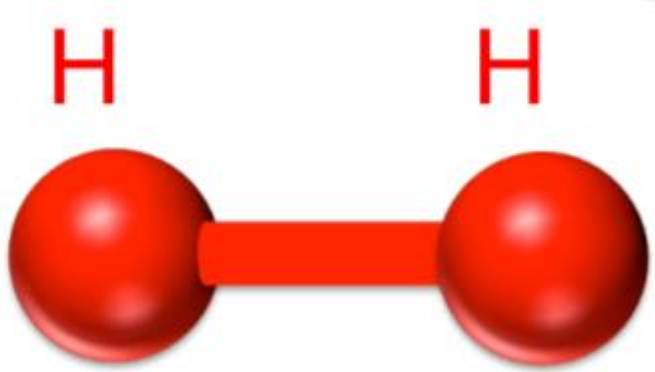
$$+\frac{ke^2}{r_{12}} + \frac{ke^2}{d}$$

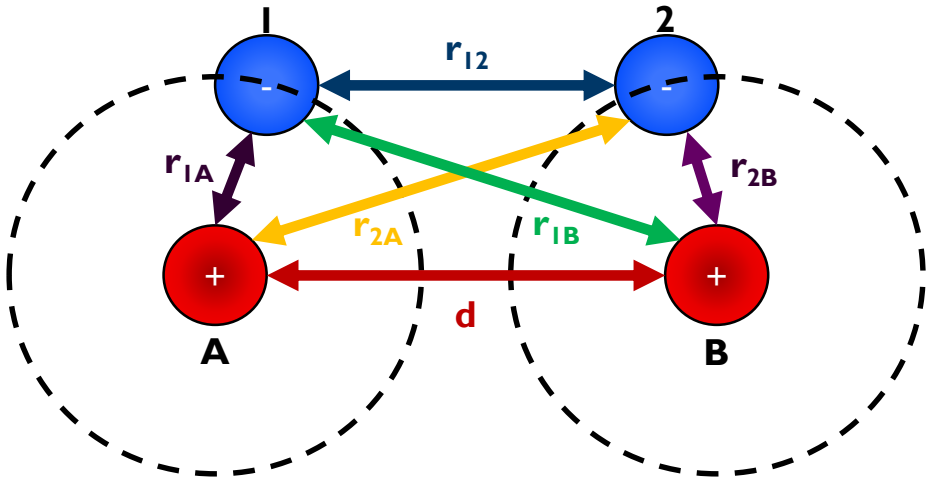


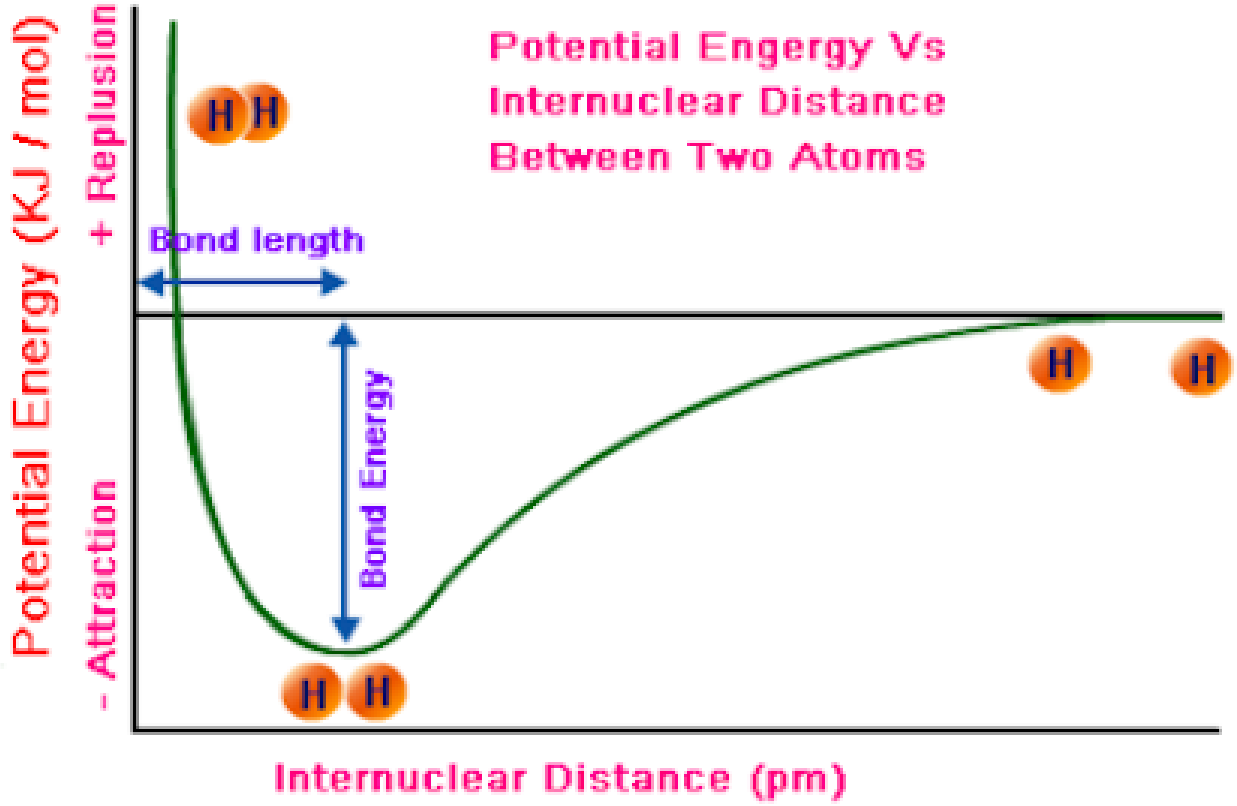
$$H = H_A + H_B + H_{AB}$$

Energy $U = \frac{kq_1q_2}{|r|}$

Hydrogen Molecule Energy Spectrum







Quantum Computers for Chemistry Simulations

- Quantum computers can solve quantum chemistry problems efficiently
- Chemistry simulations are likely the first application of quantum computers
- State of the art: classical-quantum hybrid approach
- Today: Use a quantum computer to solve the hydrogen molecule energy spectrum