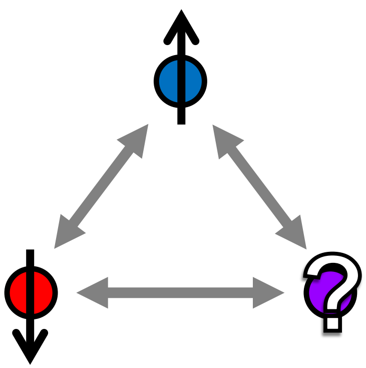
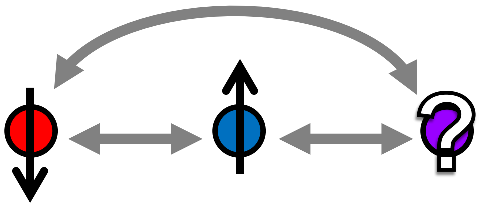
Quantum Simulation of Materials and Chemistry with Trapped Atomic Ions



Phil Richerme
Indiana University
Department of Physics

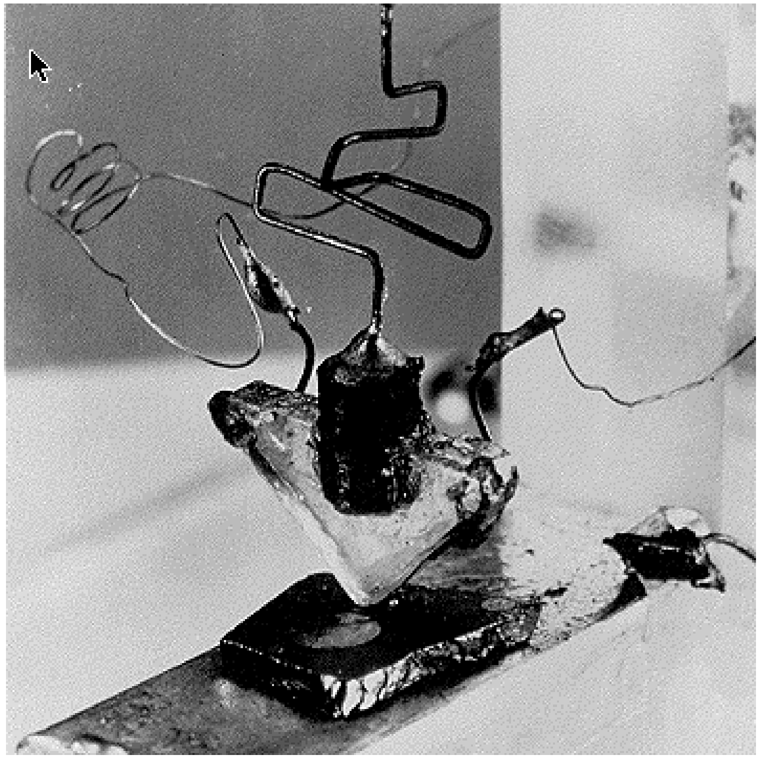


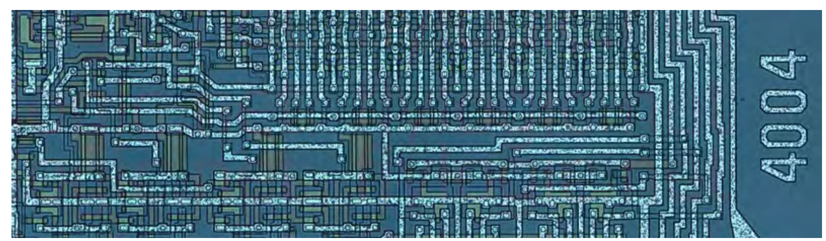
Fossil Energy Workshop on Quantum Information Science & Technology
NETL-Pittsburgh, PA
November 19, 2019

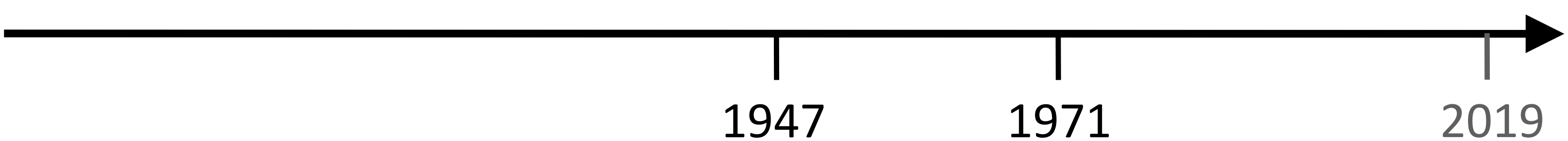
Universal Classical Computing

2019

Universal Classical Computing







Pre-Universal Classical Computing

Build a classical device to solve classical problem of interest

1880 — 1947 — 1971 — 2019

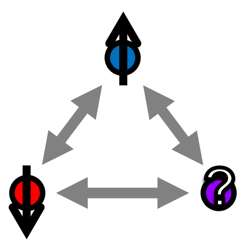
Pre-Universal Quantum Computing

Build a quantum device to solve quantum problem of interest

$$i\hbar\frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle$$

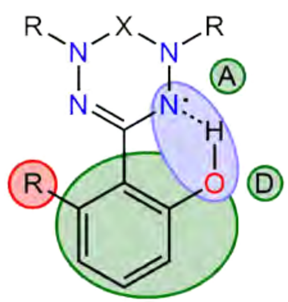
Quantum Materials

- Physical properties emerge from quantum behavior
- Examples:
  - Spin Liquids
  - Topological Insulators
  - High-Temp. Superconductors

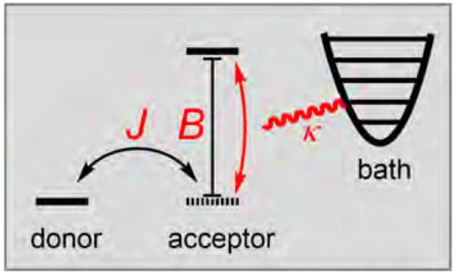


Quantum Chemistry

- Problems in chemistry where protons & electrons are both transferred



X = CH_2, CO, CS



changing the magnitude of B:

- *torsion modified by R group*
- *O-H distance modified by donor group*

Pre-Universal Quantum Computing

Build a quantum device to solve quantum problem of interest

$$i\hbar\frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle$$

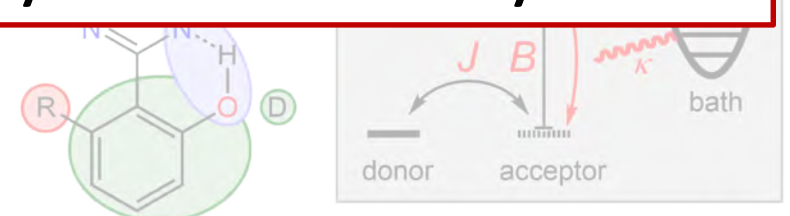
Quantum Materials

- Physical properties emerge from quantum behavior
    - Topological Insulators
    - High-Temp. Superconductors

Quantum Chemistry

- Problems in chemistry where protons & electrons are both transferred

Classical computing can only solve *small* systems



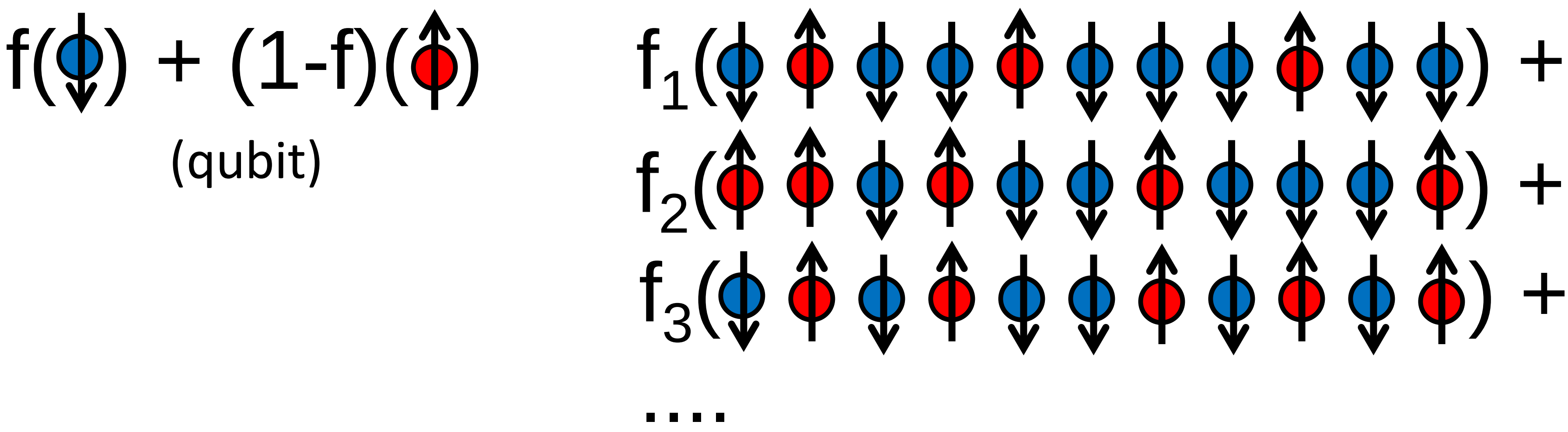
X = CH_2, CO, CS

changing the magnitude of B:

- *torsion modified by R group*
- *O-H distance modified by donor group*

Why Quantum Problems are Hard to Solve

Quantum objects can exist in multiple different configurations *at the same time*

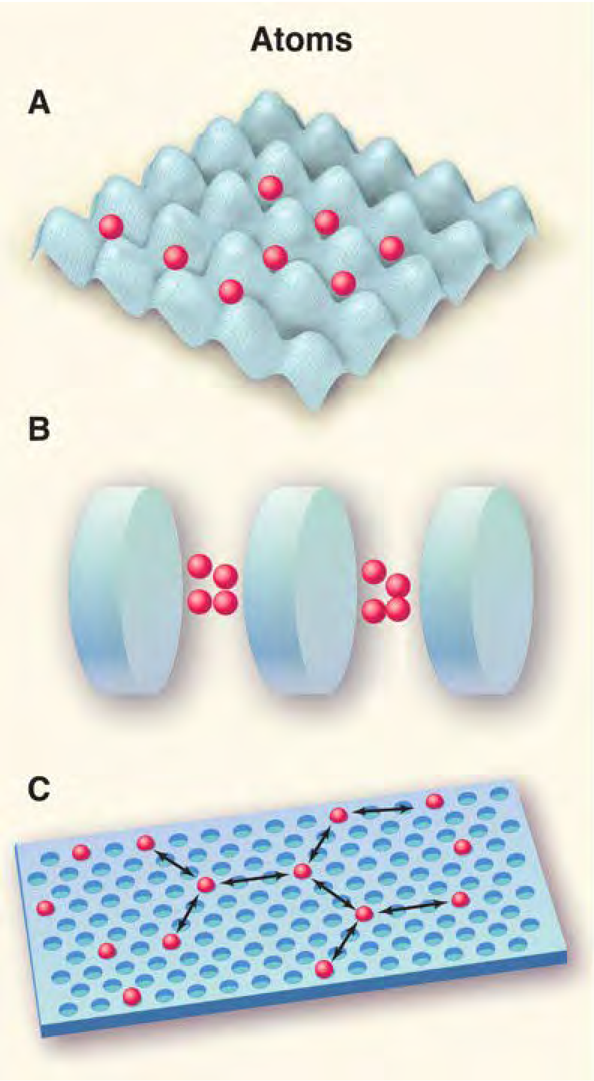


Exponentially large number of possible configurations

Requires quantum hardware to store and process

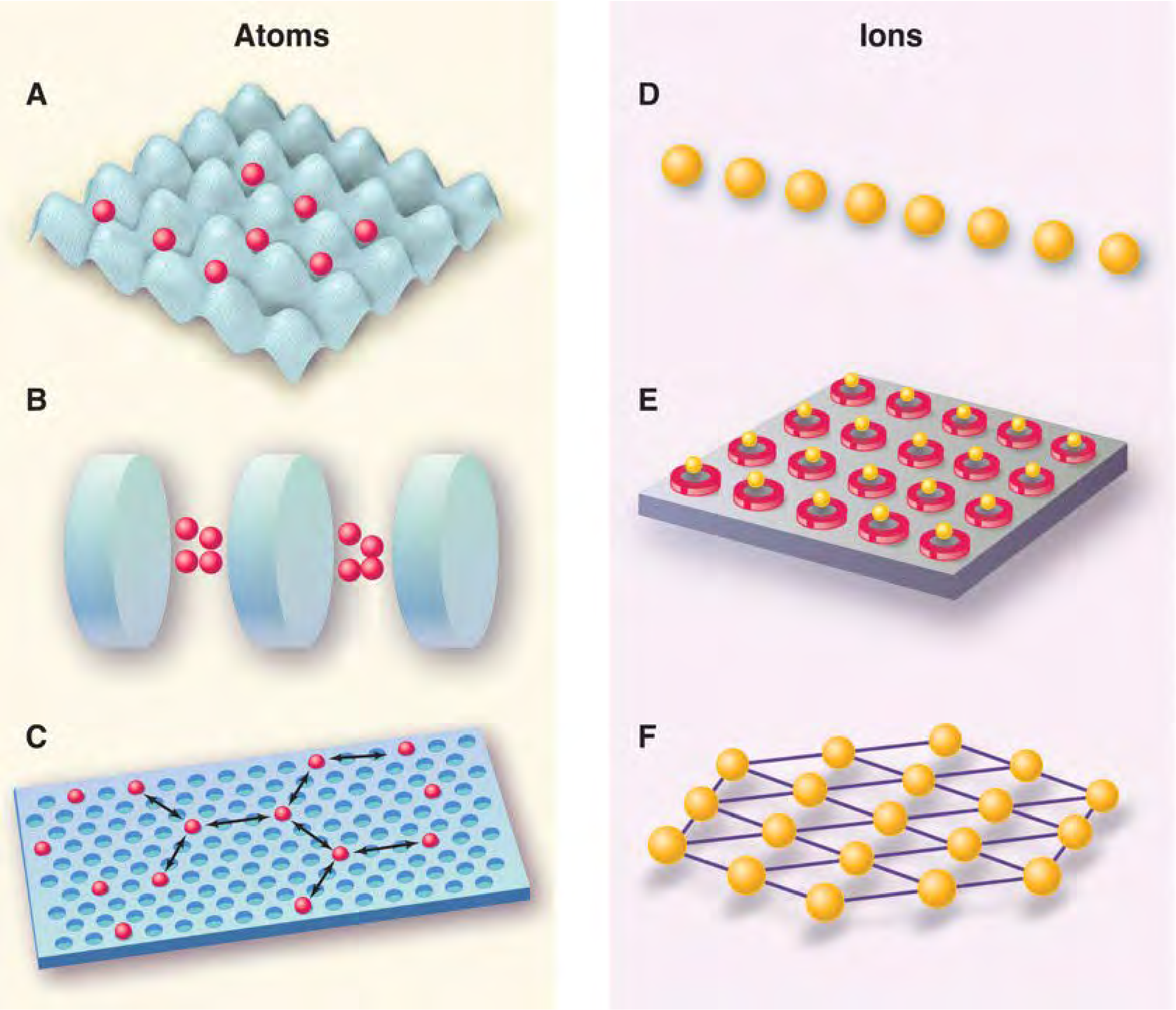
Quantum Hardware

Quantum Hardware



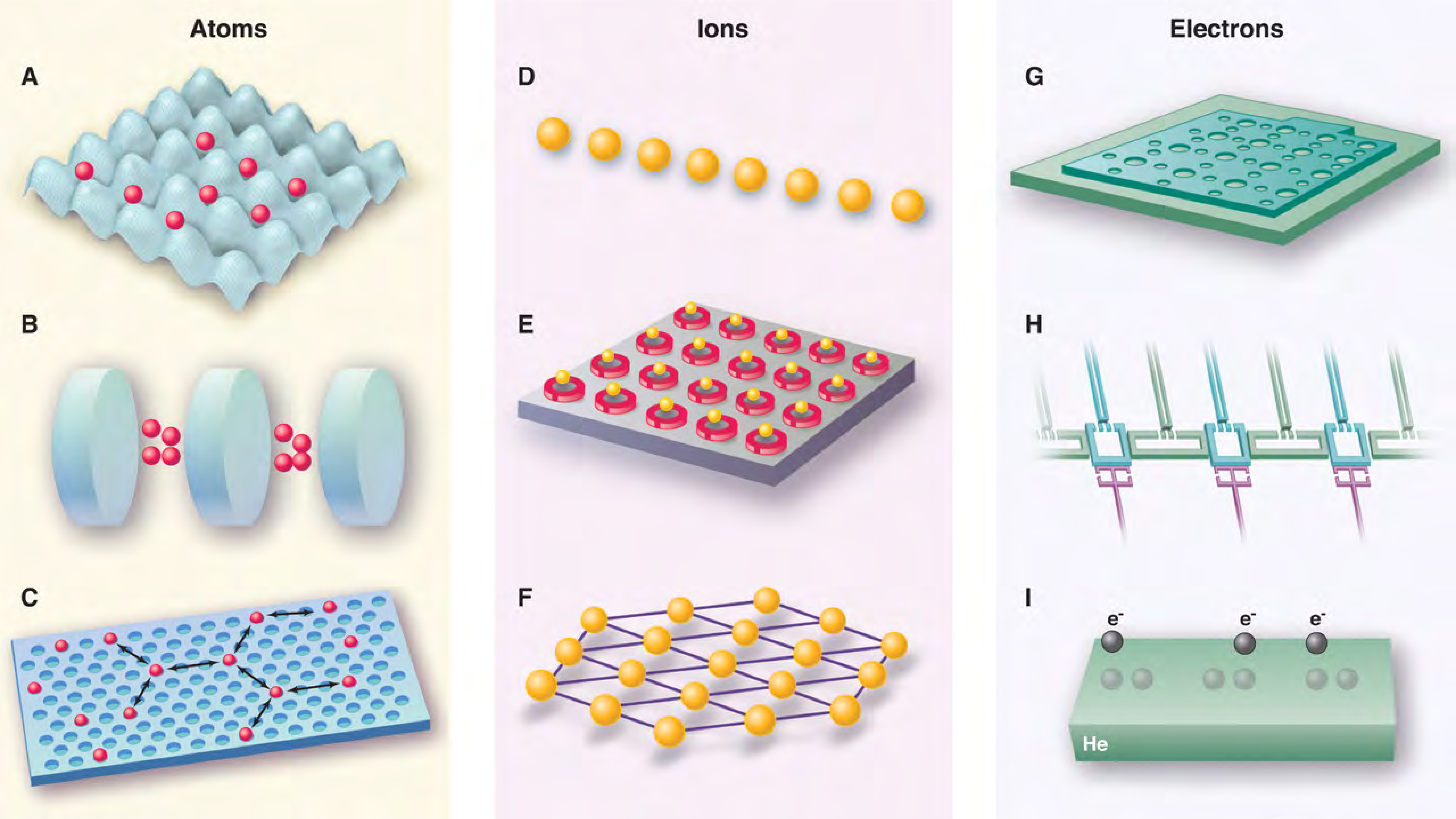
I. Buluta and F. Nori, Science **326**, 108 (2009)

Quantum Hardware



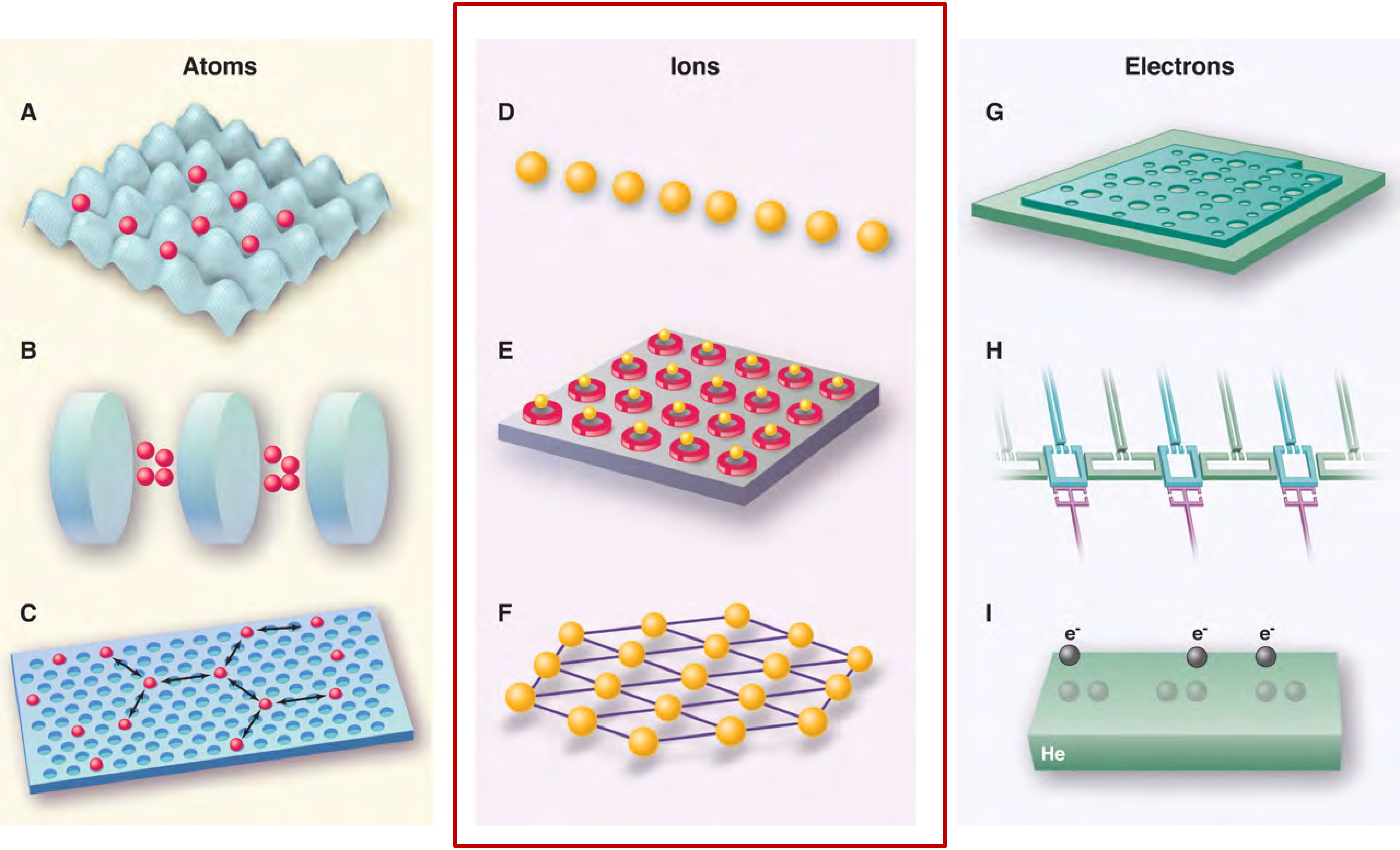
I. Buluta and F. Nori, Science **326**, 108 (2009)

Quantum Hardware



I. Buluta and F. Nori, Science **326**, 108 (2009)

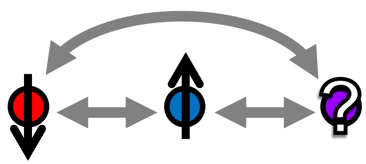
Quantum Hardware



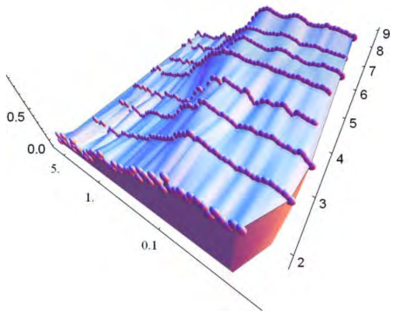
I. Buluta and F. Nori, Science **326**, 108 (2009)

Ion Trap Quantum Simulations

Early Experiments: just a few particles, easily predicted results

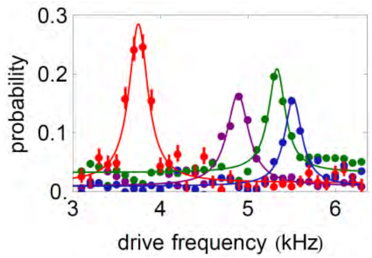


Long-Range Frustration

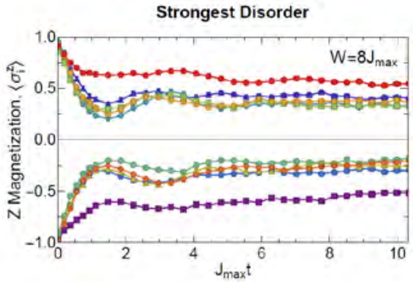


Onset of a Quantum Phase Transition

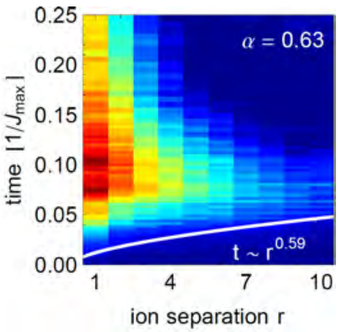
Recent Experiments: many more particles, edge of known physics



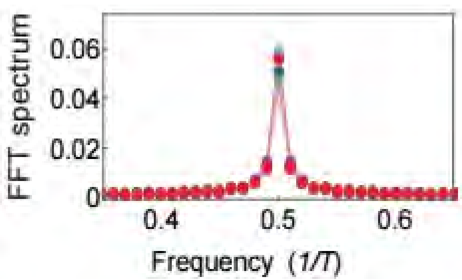
Many-body spectroscopy



Non-Thermalizing Systems

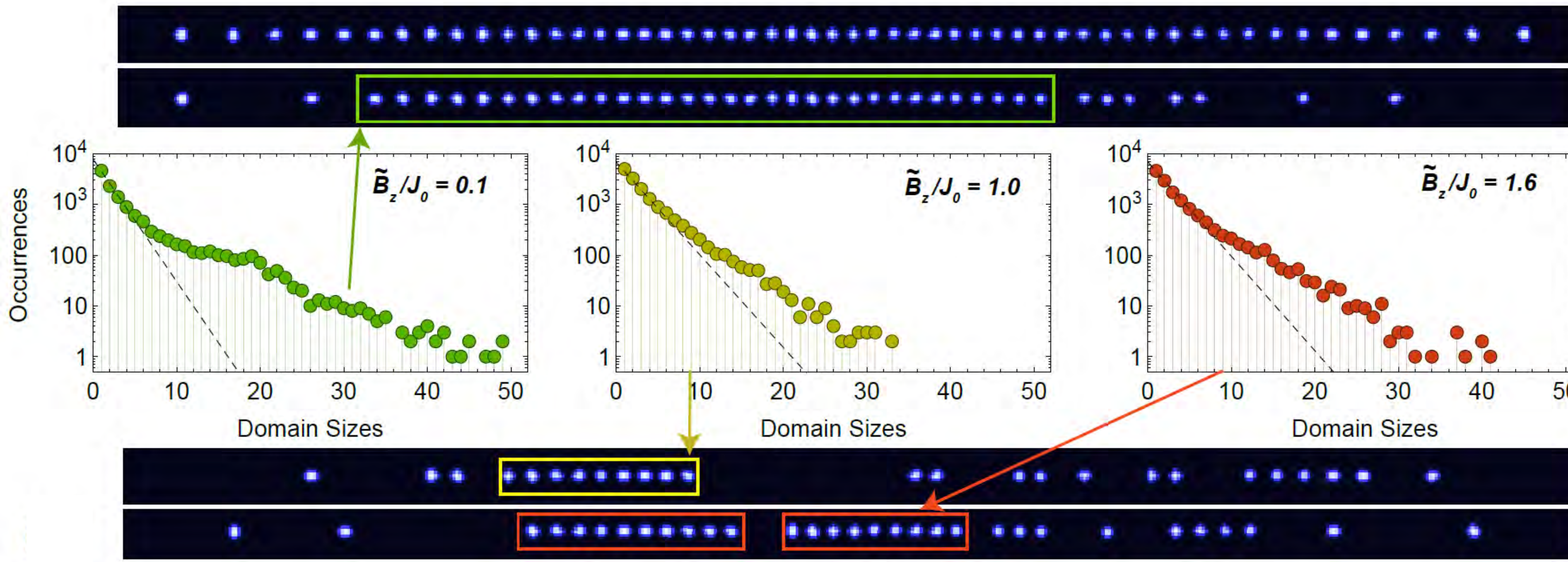


Lieb-Robinson bounds for entanglement and correlation growth



Time Crystals

Dynamics of Phase Transitions (N=53 qubits)

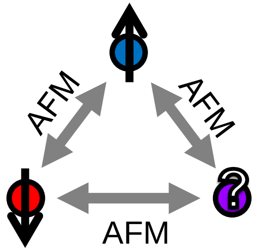


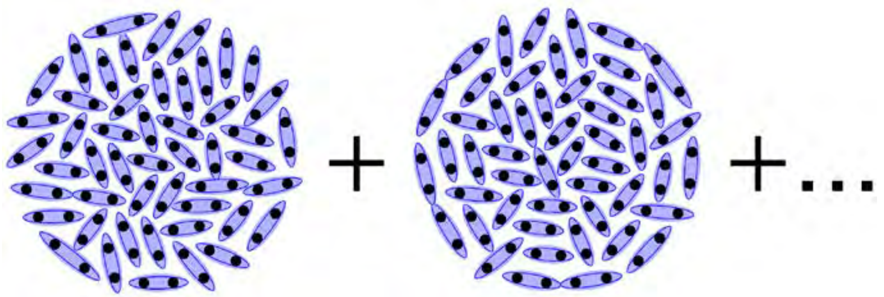
This system is too large to compute classically

J. Zhang et al., Nature **551,** 601 (2017)

2D ion traps for Quantum Simulation

- Goal: build a 2D quantum simulator to create and probe new states of quantum matter
- Applications:
  - Geometric Frustration and the relationship with quantum entanglement
  - Determine low-energy states and dynamic behavior for “unsolved” spin models
  - Search for evidence of spin-liquid behavior





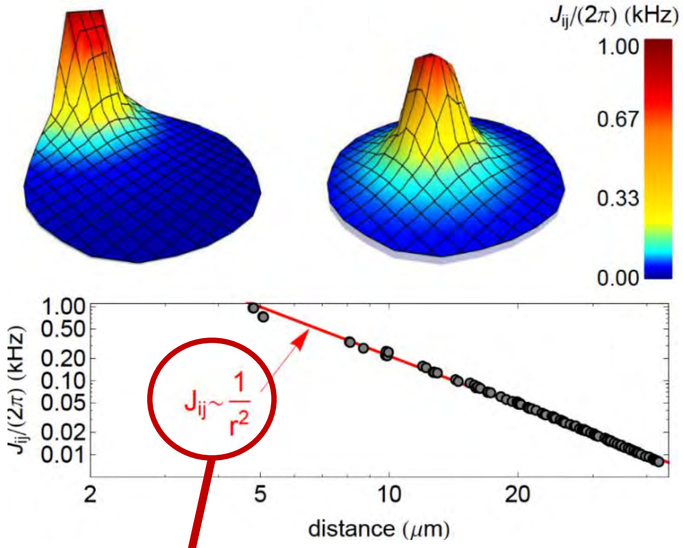
Modeling Quantum Materials

$$H_{Ising} = \sum_{i<j} J_{ij} \sigma_i^x \sigma_j^x$$

$$J_{ij} \approx \frac{J_0}{|i-j|^\alpha}$$

$$0 < \alpha < 3$$

$$H_{XY} = \sum_{i<j} J_{ij} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y)$$



$$H_{XYZ} = \sum_{i<j} J_{ij} (\vec{\sigma}_i \cdot \vec{\sigma}_j)$$

Ideal for studying quantum spin liquids

Summary

- Quantum Simulators solve specific problems without need for universal quantum computer
- Variety of physical realizations
- Ion traps: ideal for studies of new quantum materials or problems in quantum chemistry