ANALOG QUANTUM SIMULATION
from Physics to Chemistry

Quantum Science Seminar

Garching, April 16th, 2020

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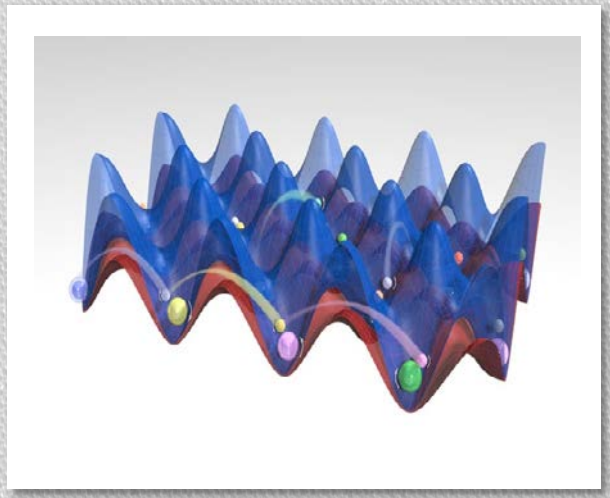
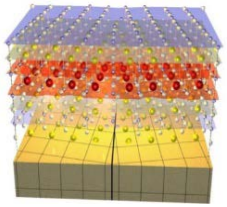
MPQ
Max-Planck-Institut
für Quantenoptik

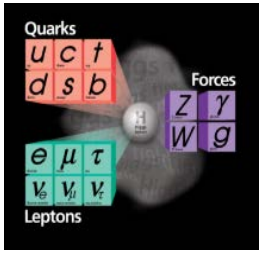
ANALOG QUANTUM SIMULATION: COLD ATOMS IN OPTICAL LATTICES



Condensed matter



High-Energy



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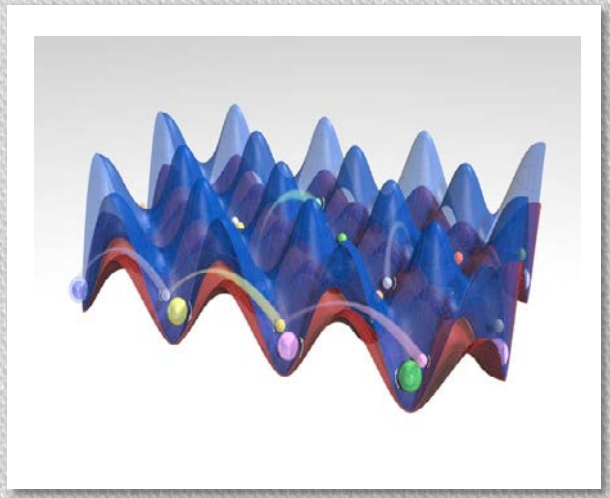

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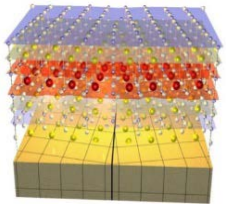

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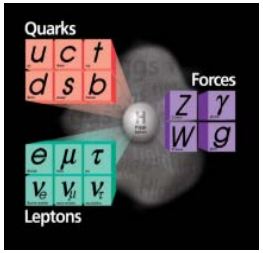
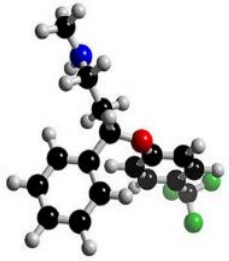


Chemistry



A different perspective …

QUANTUM CHEMISTRY

QUANTUM CHEMISTRY

ELECTRONIC PROBLEM

Fixing the positions of the nuclei,
find the ground state energy:

Born-Oppenheimer approximation:

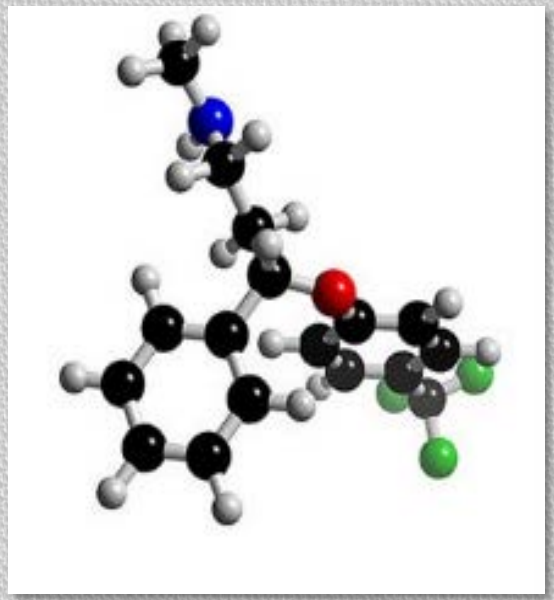
$$H \approx H_{\text{nuc}} - \sum_n \nabla_n^2 - \sum_{n,X} \frac{1}{|R_X - r_n|} + \sum_{n,m} \frac{1}{|r_n - r_m|}$$

Electron

Electron-Electron

Schrödinger Equation:

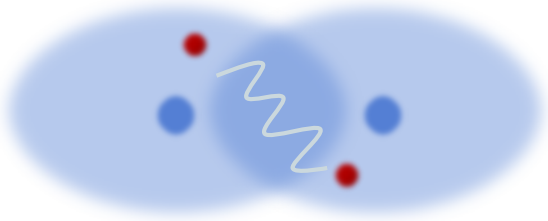
$$H(R_1,...,R_N)\,|\Psi_{\text{electrons}}\rangle = E_0(R_1,...,R_N)\,|\Psi_{\text{electrons}}\rangle$$

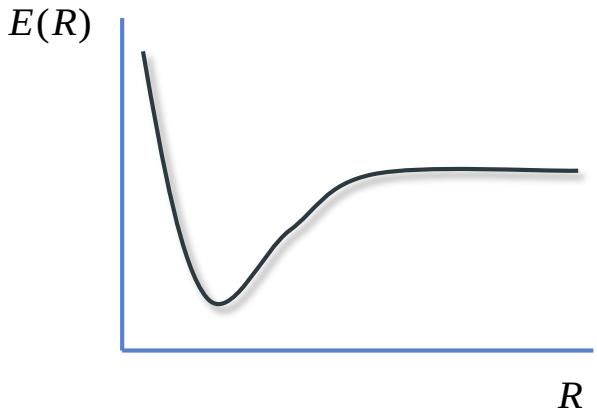


NUCLEAR PROBLEM

$$i\partial_t\,|\Phi_{\text{nuclei}}\rangle = \left[\sum_{n=1}^{N} \frac{P^2}{2M} + E_0(R_1,...,R_N)\right]|\Phi_{\text{nuclei}}\rangle$$

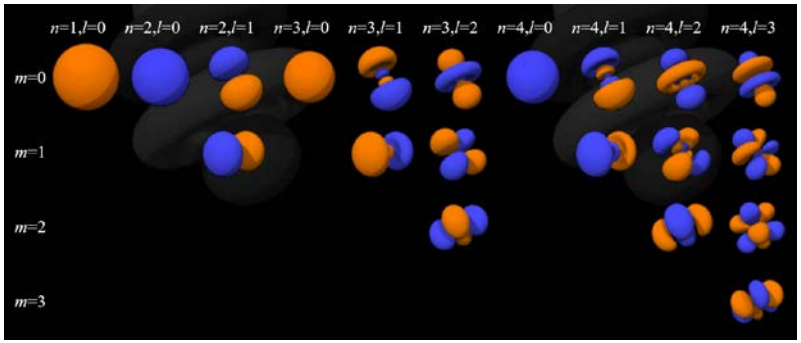
QUANTUM CHEMISTRY





- Dissociation
- Vibrations, Rotations
- Electronic properties
- Dynamics of electrons, etc

QUANTUM CHEMISTRY
MOLECULAR ORBITALS



www.orbitals.com

ORBITALS:

Single-electron wavefunctions

$$\varphi_1(r), \varphi_2(r), ..., \varphi_M(r)$$

Determined with approximate (eg Hartree-Fock or heuristic methods (modified Hidrogen orbitals)

$$\Psi_{electron}(r_1, r_2, .., r_L) = A\sum c_{i_1, i_2, .., i_L} \varphi_{i_1}(r_1)\varphi_{i_2}(r_2)...\varphi_{i_L}(r_L)$$

SECOND QUANTIZATION:

$$H_{\text{electrons}} = \sum_{i,j=1}^{M} t_{i,j} a_i^{\dagger} a_j + \sum_{i,j,k,l=1}^{M} V_{i,j,k,l} a_i^{\dagger} a_j^{\dagger} a_k a_l$$

- Hubbard model
- M^4 parameters

QUANTUM CHEMISTRY
NUMERICAL METHODS

$$H_{\text{electrons}} = \sum_{i,j=1}^{M} t_{i,j} a_i^\dagger a_j + \sum_{i,j,k,l=1}^{M} V_{i,j,k,l} a_i^\dagger a_j^\dagger a_k a_l$$

- Exact
- Perturbation theory
- Coupled-cluster method
- ...
- Density Functional Theory

QUANTUM CHEMISTRY
NUMERICAL METHODS

DENSITY FUNCTIONAL THEORY:

Total energy: $E(n)$

electron density

$$E_0 = \min_n E(n)$$

$$K_{kinetic}(n) + V_{nuclear}(n) + X_{exchange}(n) + F(n)$$

Density functional

- Extremely efficient
- Can give very accurate results
- Widely used
- Question: how to choose the density functional *F(n)*?

THIS AND MOST METHODS NEED BENCHMARKING

QUANTUM CHEMISTRY
QUANTUM COMPUTING

$$H_{\text{electrons}} = \sum_{i,j=1}^{M} t_{i,j} a_i^\dagger a_j + \sum_{i,j,k,l=1}^{M} V_{i,j,k,l} a_i^\dagger a_j^\dagger a_k a_l$$

GROUND STATE ALGORITHMS

- Computational time grows exponentially with *M (*or *N)*

PRACTICAL ALGORITHMS

- Adiabatic preparation
- Variational methods

Theory: Aspuru-Guzik, Hasting, Childs, Troyer, Simon, Ge et al, …
Experiments: photons (Vienna), superconducting (IBM), ions (Ibk)
cold atoms (Hamburg), …

QUANTUM CHEMISTRY

$$H_{\text{electrons}} = \sum_{i,j=1}^{M} t_{i,j} a_i^\dagger a_j + \sum_{i,j,k,l=1}^{M} V_{i,j,k,l} a_i^\dagger a_j^\dagger a_k a_l$$

- Rely on the selection of orbitals

CLASSICAL COMPUTERS

- Exact methods: hard
- Approximate methods

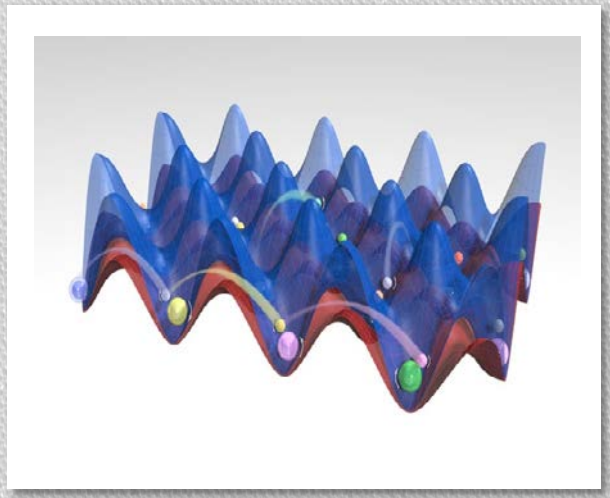
BENCHMARKING?

QUANTUM COMPUTERS

- Full quantum computers: hard to build
- NISQ: approximate methods

BENCHMARKING?

ANALOG QUANTUM SIMULATION: COLD ATOMS IN OPTICAL LATTICES



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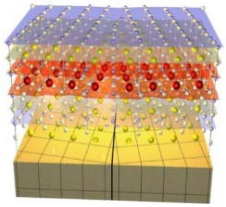

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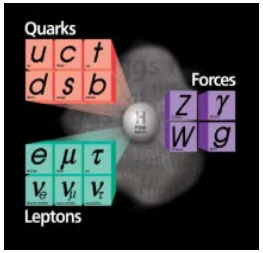

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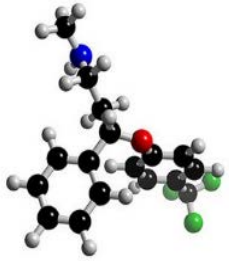

ANALOG QUANTUM CHEMISTRY

Argüello, Shi, González-Tudela, Zoller, JIC, 574, 215, Nature (2019)

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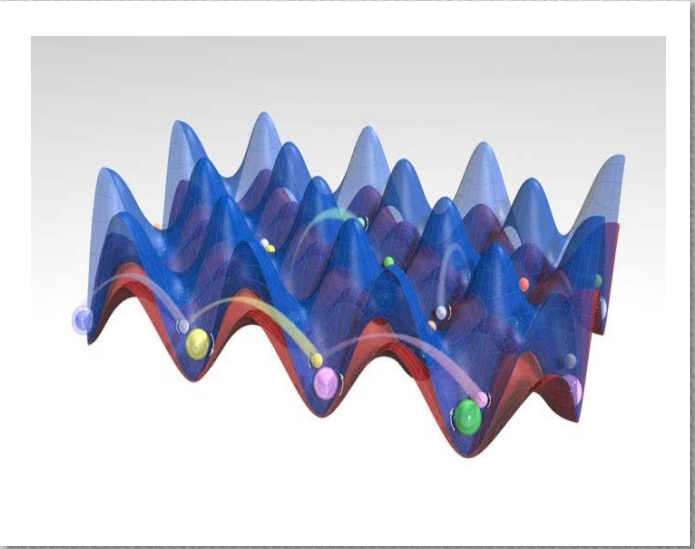
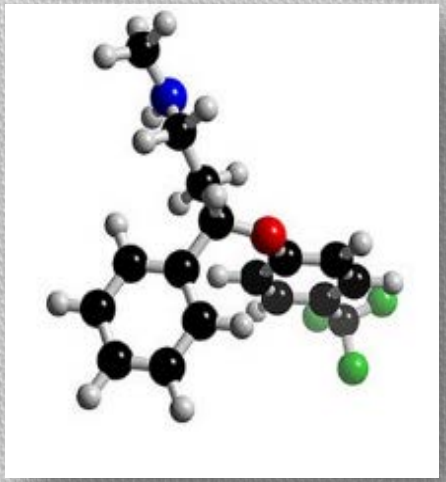


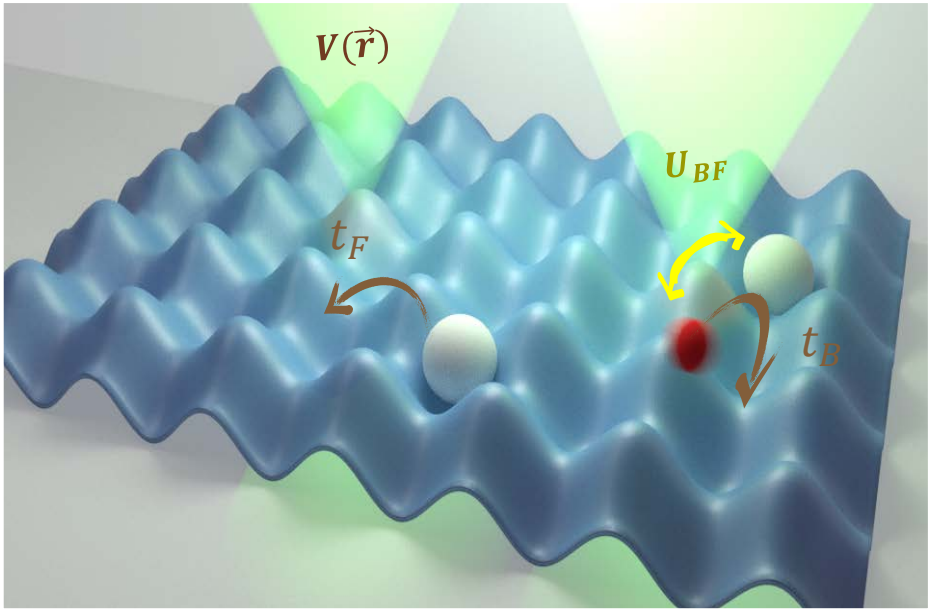


$$H = -\sum_{\substack{<n,m> \\ \sigma,\sigma'}} \left(t_{\sigma,\sigma'} a^{\dagger}_{n,\sigma} a_{m,\sigma'} + h.c \right) + \sum_{\substack{n \\ \sigma,\sigma'}} U_{\sigma,\sigma'} a^{\dagger}_{n,\sigma} a^{\dagger}_{n,\sigma'} a_{n,\sigma'} a_{n,\sigma}$$

$$H_{electrons} = \sum_{i,j=1}^{M} t_{i,j} a_i^{\dagger} a_j + \sum_{i,j,k,l=1}^{M} V_{i,j,k,l} a_i^{\dagger} a_j^{\dagger} a_k a_l$$

Local Interactions

QUANTUM CHEMISTRY SIMULATION GENERAL IDEA



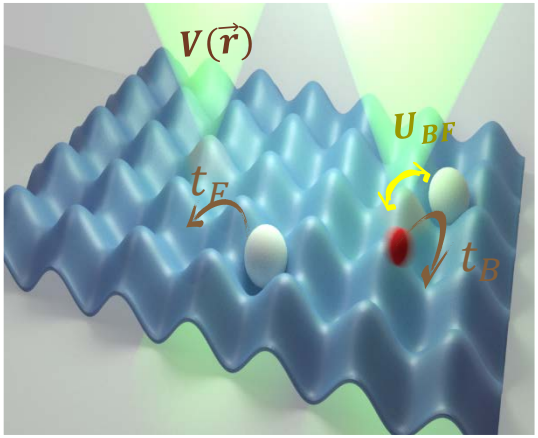
$$H \approx H_{\text{nuc}} - \sum_n \nabla_n^2 - \sum_{n,X} \frac{1}{|R_X - r_n|} + \sum_{n,m} \frac{1}{|r_n - r_m|}$$

Fermions:
Single particle:
lattice + laser

Fermions:
Mediated by boson

"Few atoms" scenario

QUANTUM CHEMISTRY SIMLUATION
ATOMS IN OPTICAL LATTICES

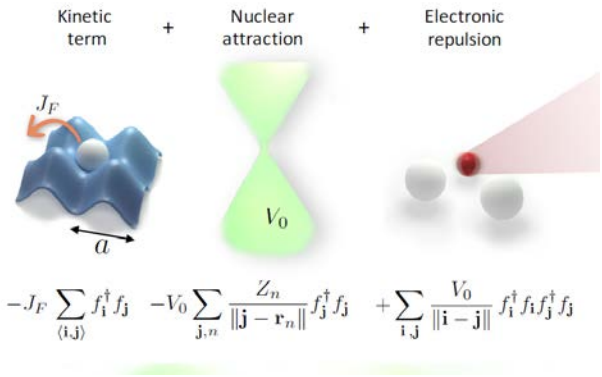


- Different from QS in CMP or HEP:
  - Long-range interactions
  - Small densities (few fermions / site)
- Different from standar Qchemistry:
  - No orbitals (space orbitals)
- Discrete: continuum limit
- One could include the dynamics of the nuclei

ANALOG QUANTUM SIMULATION
COLD ATOMS IN OPTICAL LATTICES

MAIN QUESTIONS:

- External Coulomb potential
- Electron-electron Coulomb interaction
- Discretization

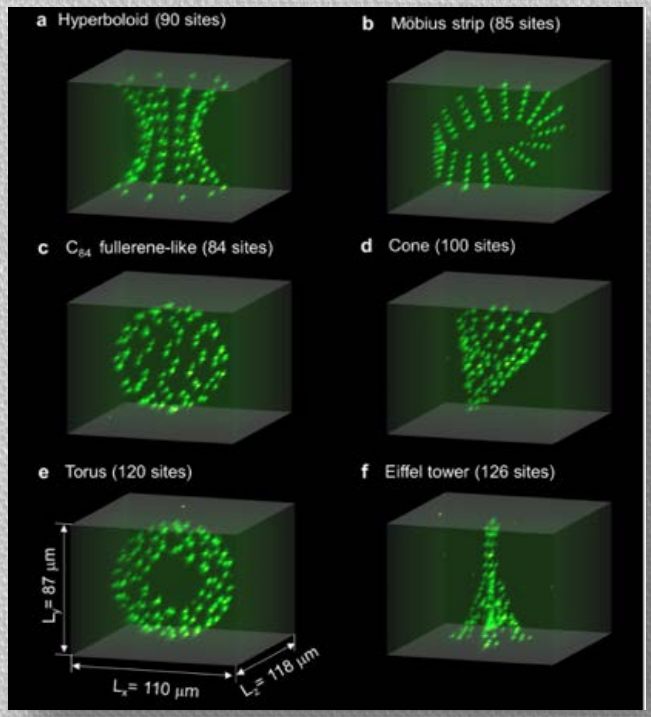


TECHNICAL QUESTIONS:

- Which atoms
- How to prepare
- How to measure
- Disadjustments, decoherence, finite temperatures, etc

EXTERNAL COULOMB POTENTIAL

$$H \approx H_{\text{nuc}} - \sum_n \nabla_n^2 - \sum_{n,X} \frac{1}{|R_X - r_n|} + \sum_{n,m} \frac{1}{|r_n - r_m|}$$

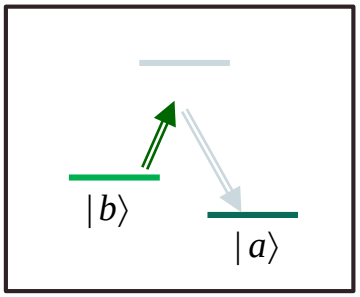


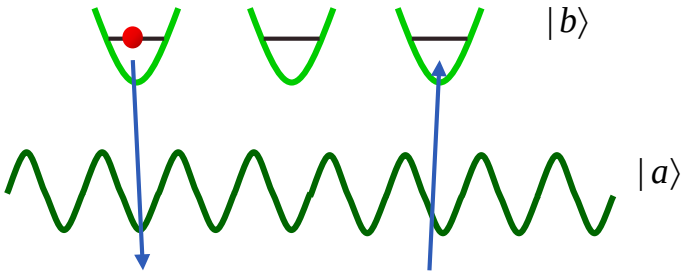
Broaways et al, Nature **561**, 79 (2018)

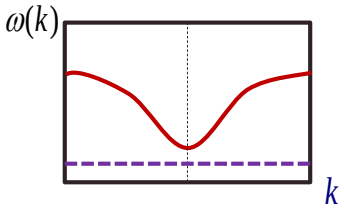
ELECTRON-ELECTRON INTERACTION

$$H \approx H_{\text{nuc}} - \sum_{n} \nabla_n^2 - \sum_{n,X} \frac{1}{|R_X - r_n|} + \sum_{n,m} \frac{1}{|r_n - r_m|}$$

ELECTRON-ELECTRON INTERACTION
Quantum Optics simulation

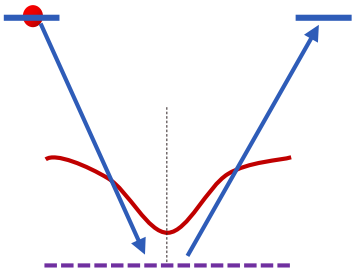






Vega, Porras, JIC, Phys. Rev. Lett. **101**, 260404 (2008),
Navarrete, Vega, Porras, JIC, New J. Phys.**13**, 023024 (2011)

Experiments: Stoneybrook (Schneble), MPQ (Blatt)

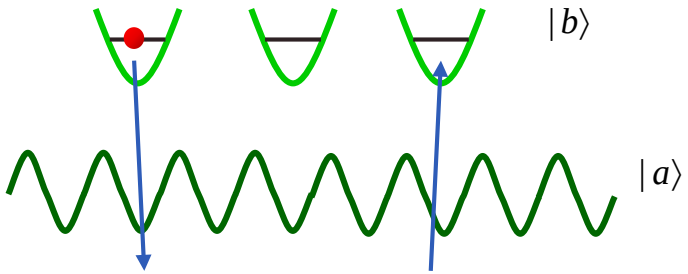


$$\Omega_{eff} \approx \int dk \frac{\Omega^2 e^{ikd}}{\Delta + ak^2}$$

ELECTRON-ELECTRON INTERACTION
Quantum Optics simulation

Cubic lattice:

$$\Omega_{eff} \approx \int dk^3 \frac{e^{ikd}}{\Delta + ak^2}$$



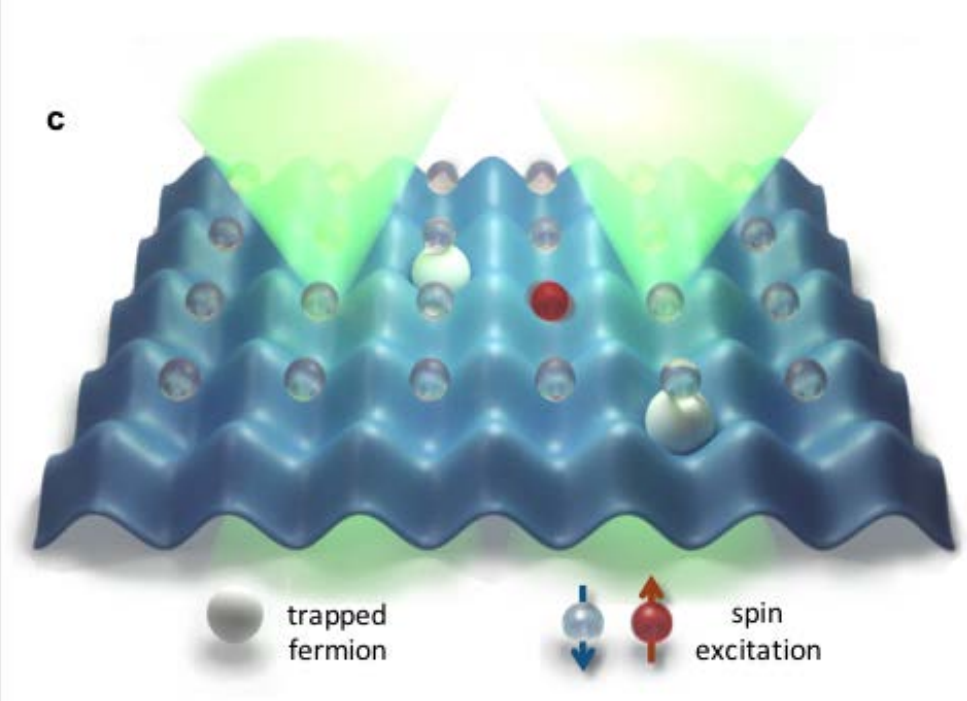
$$H \approx \sum_{n,m} V(n-m)\left[\sigma_n^+\sigma_m^- + \sigma_m^+\sigma_n^-\right]$$

$$V(r) \approx \frac{\Omega^2}{J}\frac{e^{-r/\xi}}{r} \xrightarrow{r \ll \xi} \sim \frac{1}{r}$$

$$\xi \approx \sqrt{J/\Delta}$$

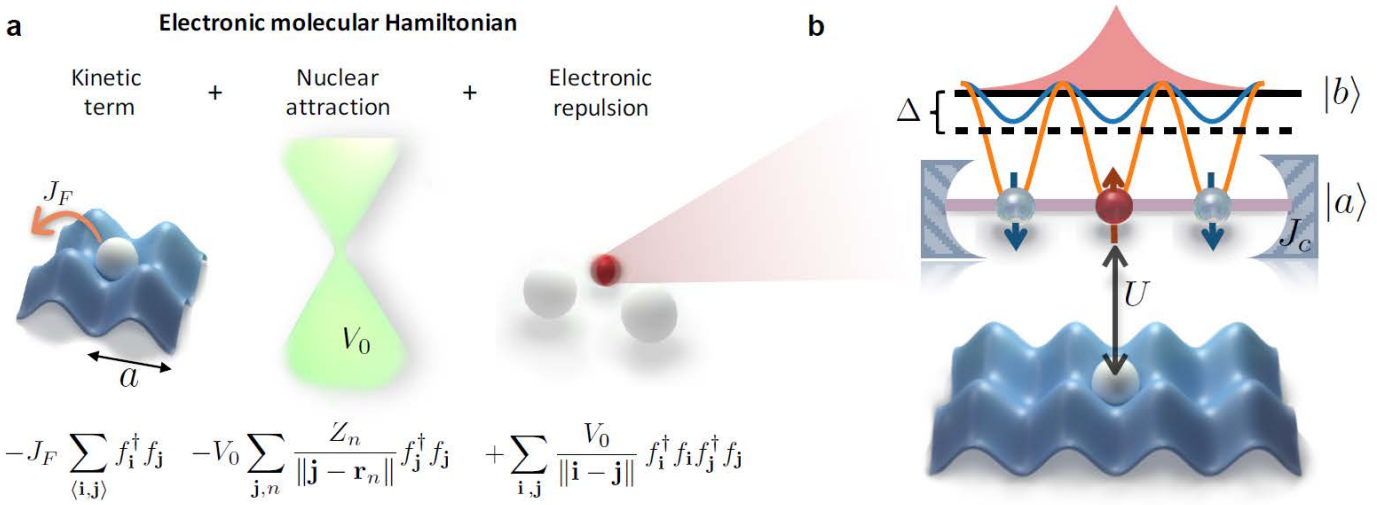
González-Tudela, JIC, Quantum **2**, 97 (2018)

ELECTRON-ELECTRON INTERACTION



- But the interaction between electrons is obtained in second order perturbation theory…
- It only works for two particles…

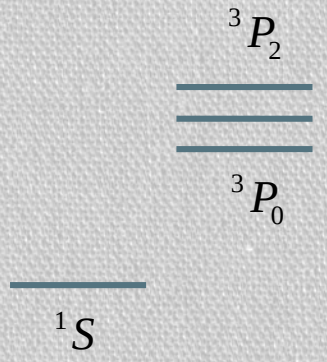
ANALOG QUANTUM CHEMISTRY



- Possible “in principle”
- Requires combination of technologies

TECHNICAL QUESTIONS

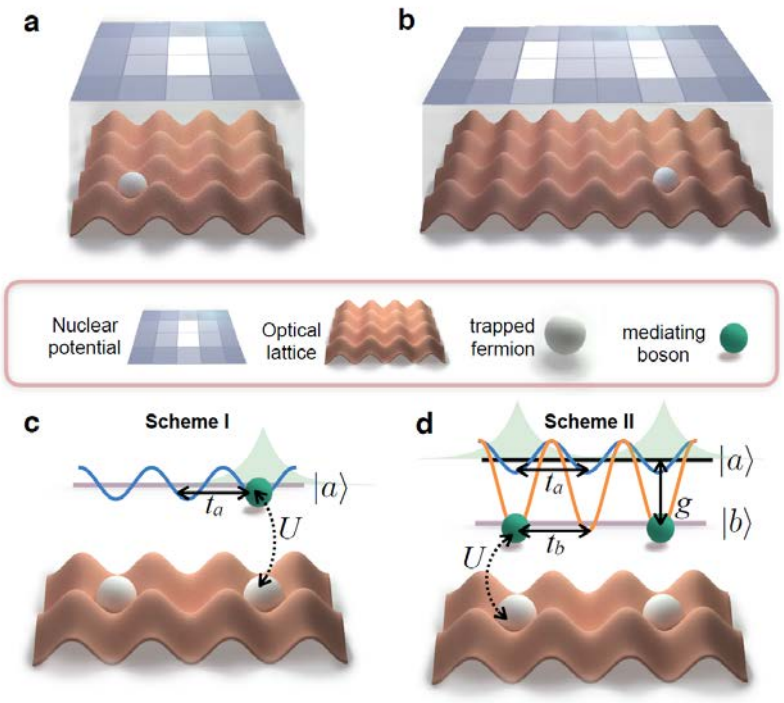
- Atoms: two earth-alkali isotopes
  - Fermion/Boson isotopes
  - Similar transition frequencies (isotopes shifts)
  - Magic wavelenghts
  - Interactions in the right states
  - Cavity mode: only bosons in state a
- Preparation: Adiabatic procedure
  - Prepare atoms locally
  - Adiabatically switch on interactions
- Measurement: Energy
  - Measure density
  - Measure energy by time-of-flight
  - Observables via Helmann-Feynman theorem



ANALOG QUANTUM CHEMISTRY
Simplified setups

Argüello, Shi, González-Tudela, Zoller, JIC, arXiv 2002.09373

QUANTUM CHEMISTRY IN 2D LATTICES

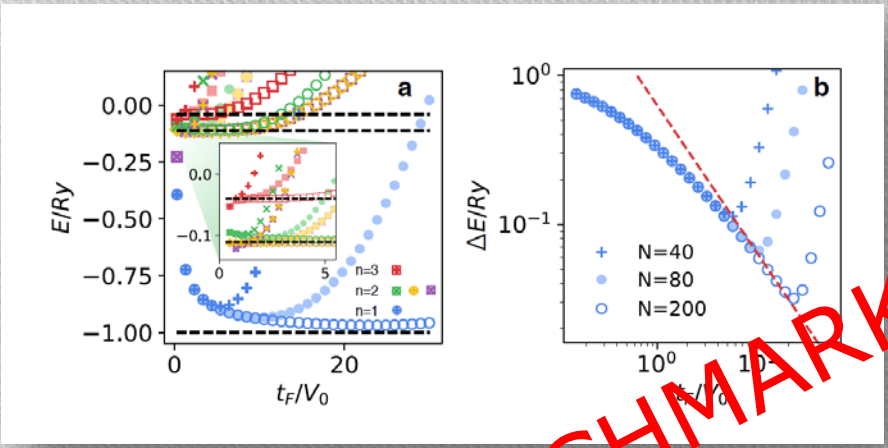


For two electrons, Coulomb law ($1/r$)

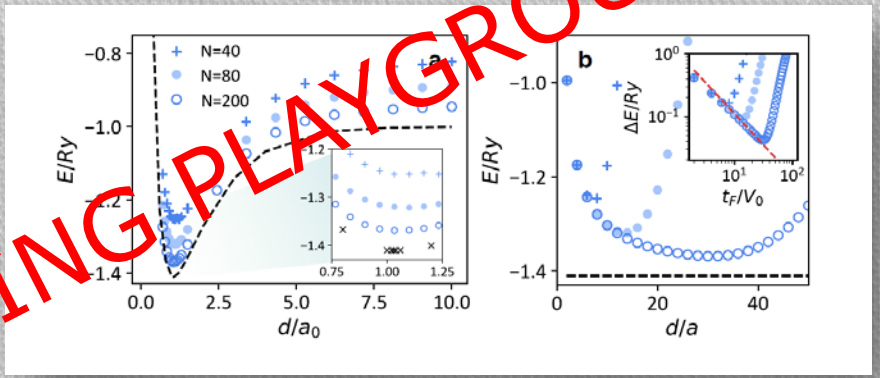
For more electrons, different law ($e^{-r/d}$)

QUANTUM CHEMISTRY IN 2D LATTICES

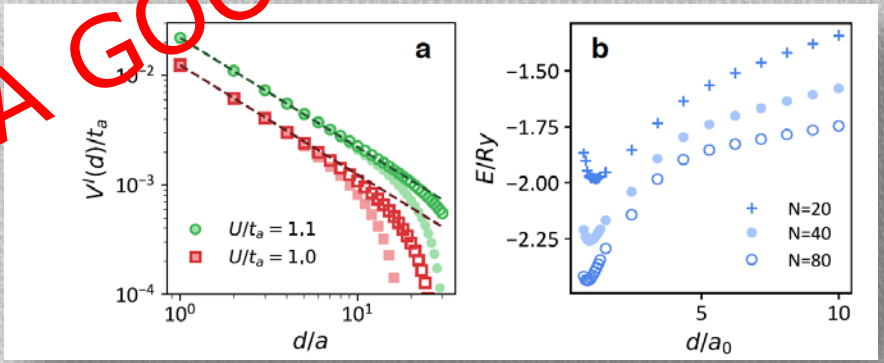
HIDROGEN-LIKE ATOM



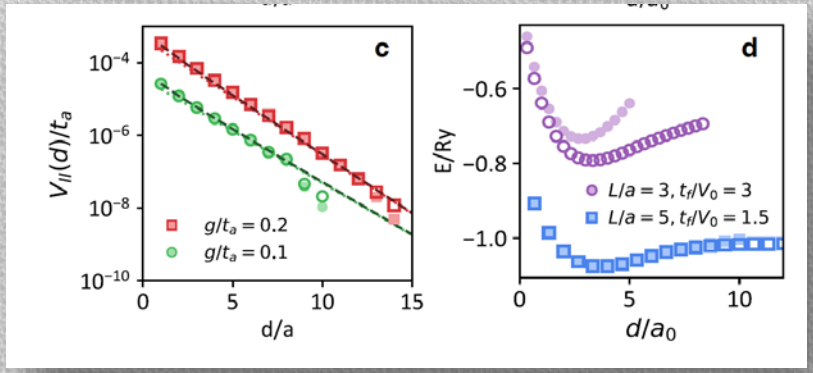
HIDROGEN-LIKE ION-MOLECULE



HIDROGEN-LIKE MOLECULE
Single boson mediating

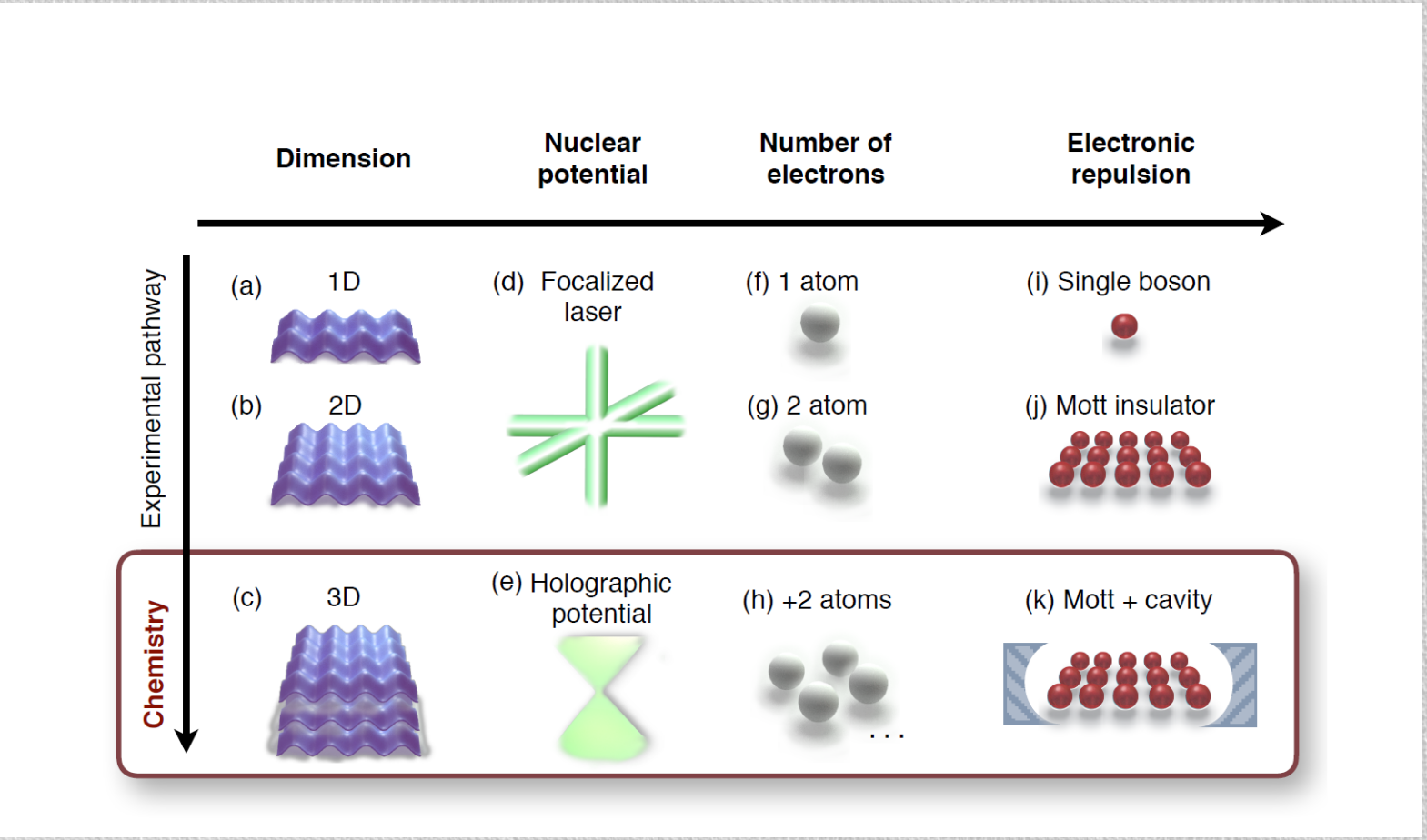


HIDROGEN-LIKE MOLECULE
Scalable scheme



A GOOD BENCHMARKING PLAYGROUND

QUANTUM SIMULATION QUANTUM CHEMISTRY ROADMAP



+ other setups

SUMMARY

- Simulating molecules is hard
- Classical methods and NISQ prototypes would benefit from Benchmarking
  - Orbital selection
  - Density functional / variatonal methods
- Analog quantum chemistry with cold atoms in optical lattices
  - Full solution: In principle, possible.

    Requires beyond the art techniques
  - Toy models: 1-2D lattices, in the discrete, different potentials

    A key tool for benchmarking
- Outlook:
  - Other systems (Rydberg atoms / ions / atomic arrays on PC)
  - Continuum (semiconductors)
  - Nuclear motion

Fruitful connection between cold atoms / condensed matter / high-energy / Chemistry

ANALOG QUANTUM SIMULATION

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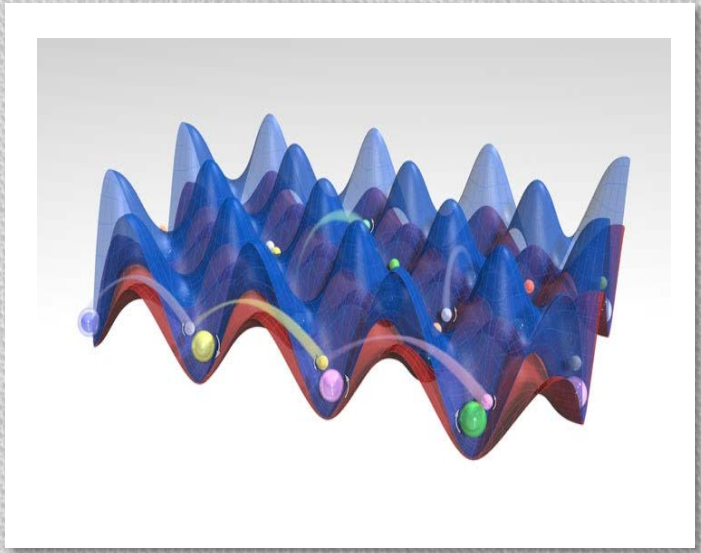

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Bosons, Fermions, Spins, Geometry, Dimensions, ...

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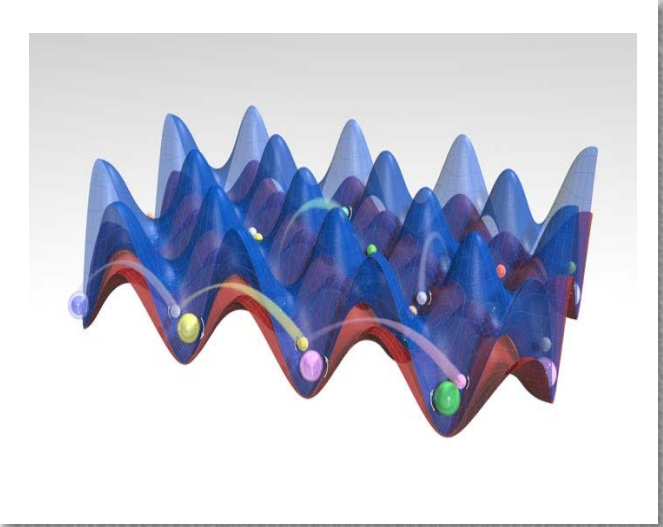
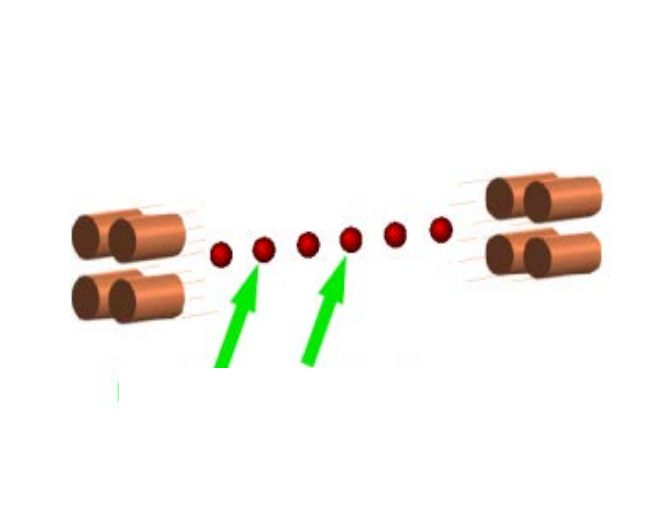
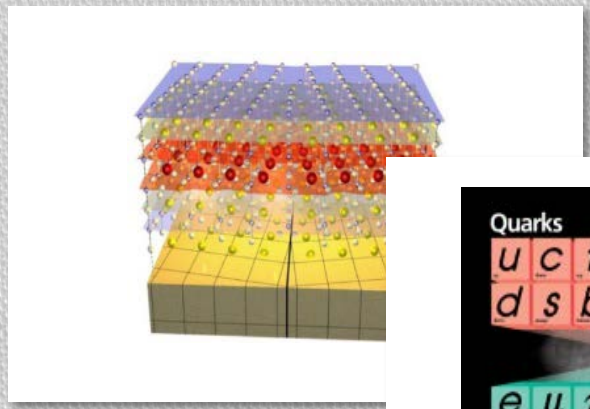




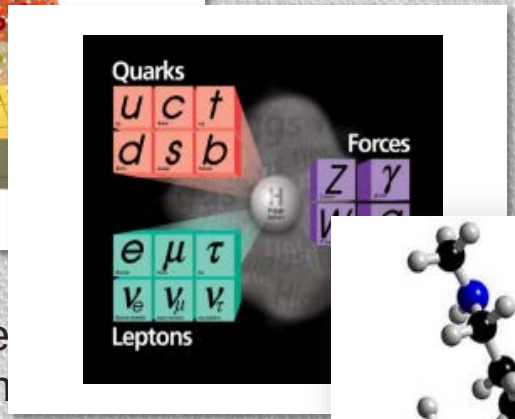
Quantum dots, SC-qubits, photons, etc

$$|\Psi\rangle = c_{0,0,\ldots,0}\,|0,0,\ldots,0\rangle + c_{0,0,\ldots,1}\,|0,0,\ldots,1\rangle + \ldots c_{1,1,\ldots,1}\,|1,1,\ldots,1\rangle$$

ANALOG QUANTUM SIMULATION
COLD ATOMS IN OPTICAL LATTICES



Condensed matte
Hubbard and spin



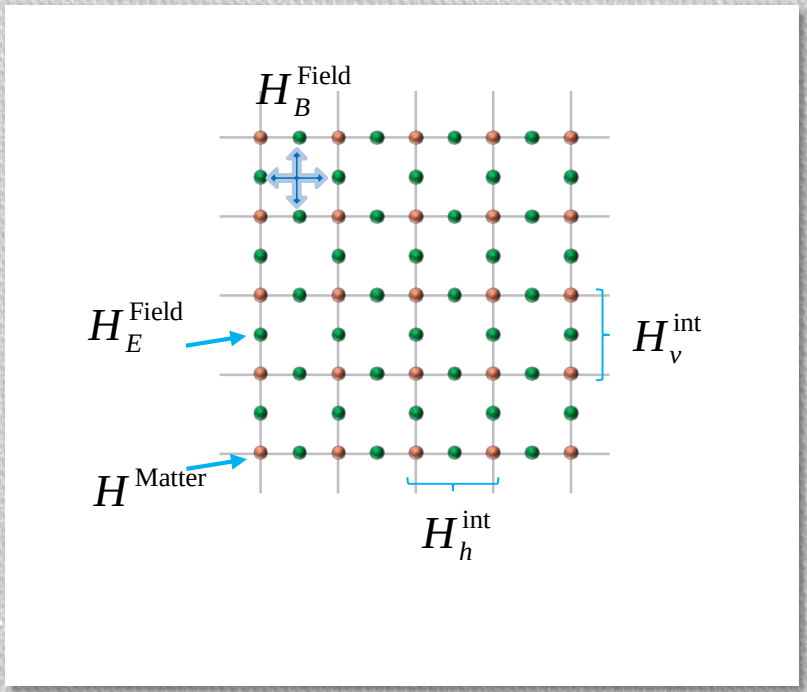
High-energy P
Lattice gauge

Quantum chemistry:

LATTICE GAUGE THEORIES REMOVING FERMIONS

- Unitary transformation:

$$\mathcal{U} = \prod_{\lambda} \mathcal{U}_{\lambda} \quad \Rightarrow \quad \mathcal{U} H \mathcal{U}^{\dagger} = H'$$



We end up with a new Hamiltonian

$$H = H^{\text{Matter}} + H^{\text{Field}} + H^{\text{int}}$$

That is local, and fermins are replaced by hard-core bosons

Zohar, JIC, PRD **97**, 034510 (2018)
Verstraete, JIC, J. Stat. Mech., P09012 (2005)
Ball, PRL 95 (2005) 176407.

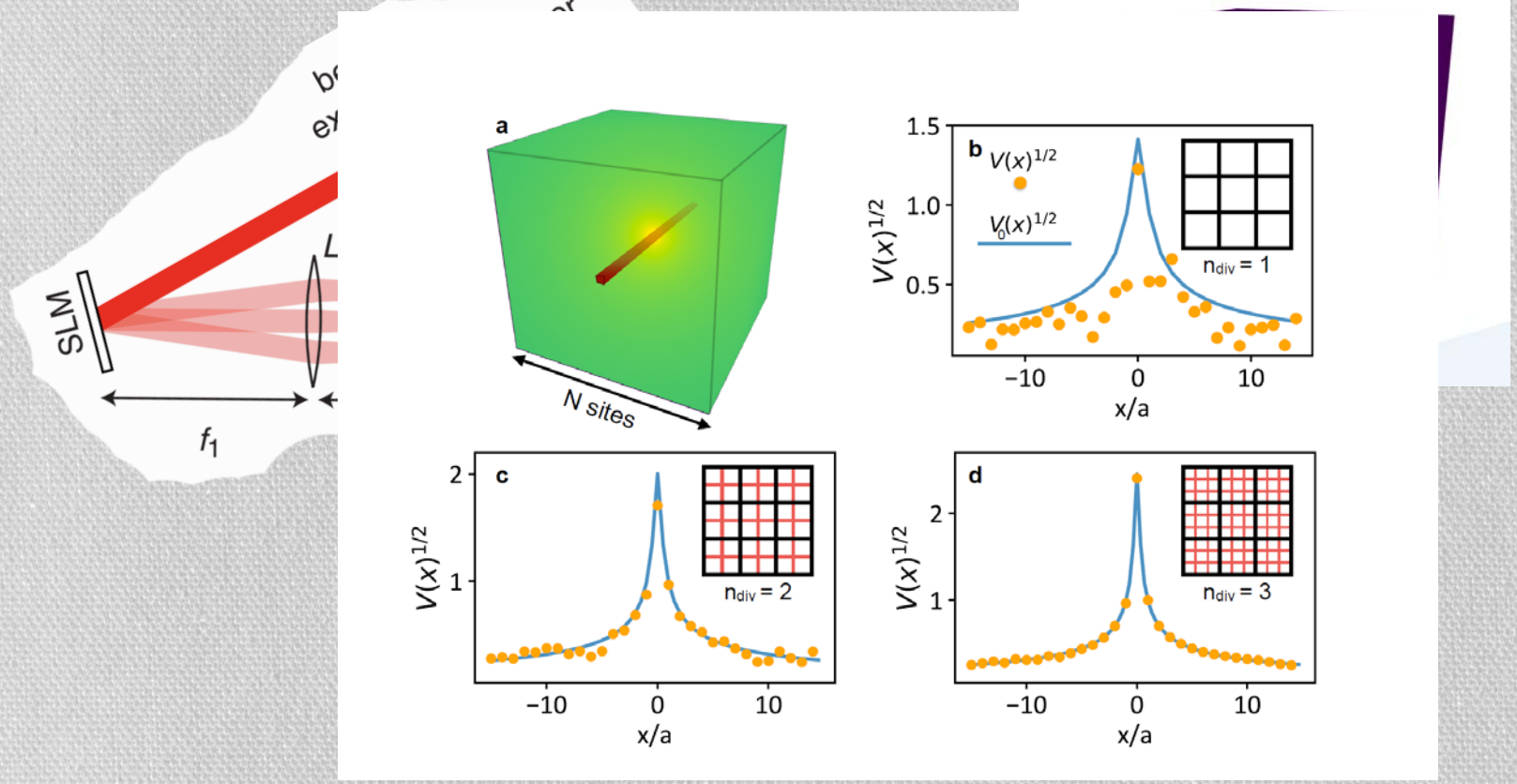
LATTICE GAUGE THEORIES
REMOVING FERMIONS

It is possible to do the same for any LGT

- Consequences:
  - Fermions are not required
  - Quantum computing
  - Analog quantum simulation
  - Quantm gravity?

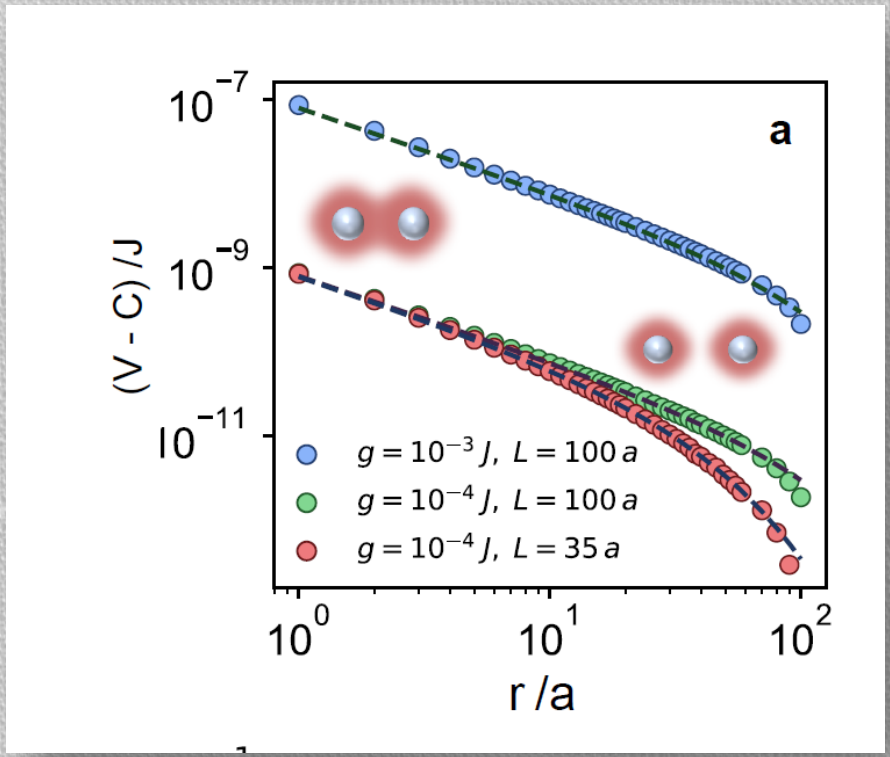
1. EXTERNAL COULOMB POTENTIAL

Holographic technique: phase pattern

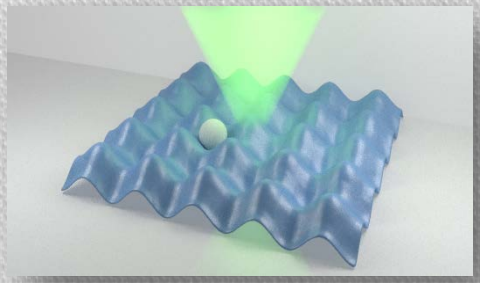


2. ELECTRON-ELECTRON INTERACTION

Effective fermion-fermion interaction



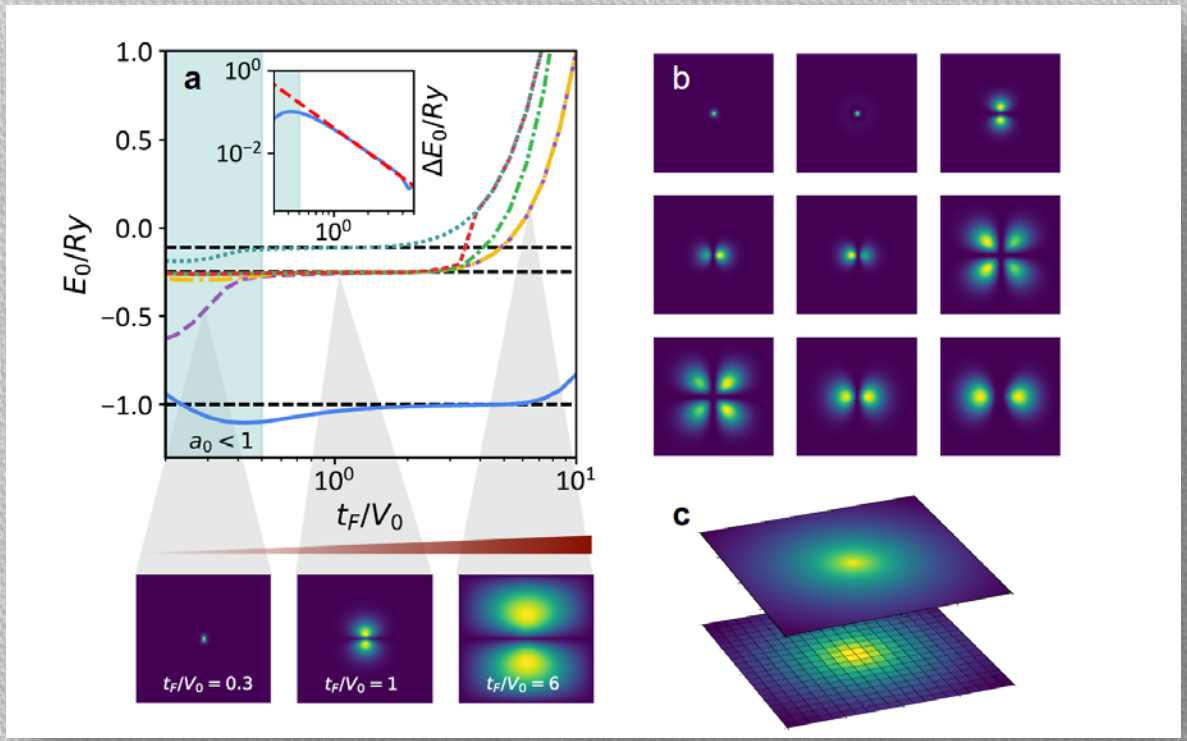
DISCRETIZATION: Hydrogen atom



$$a_{\mathrm{Bohr}} = 2\frac{t_F}{V_0}a_0 \qquad R_H = \frac{V_0^2}{4t_F}$$

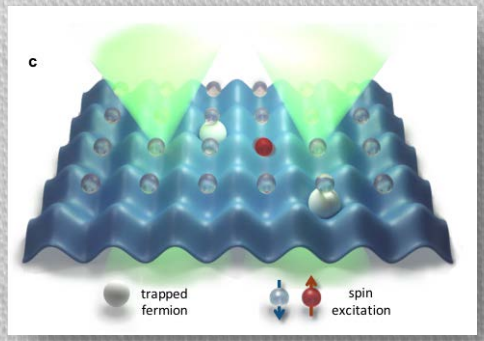
$$H_{hop} = -t_F \sum_{\langle i,j \rangle} \left(f_i^\dagger f_j + h.c. \right)$$

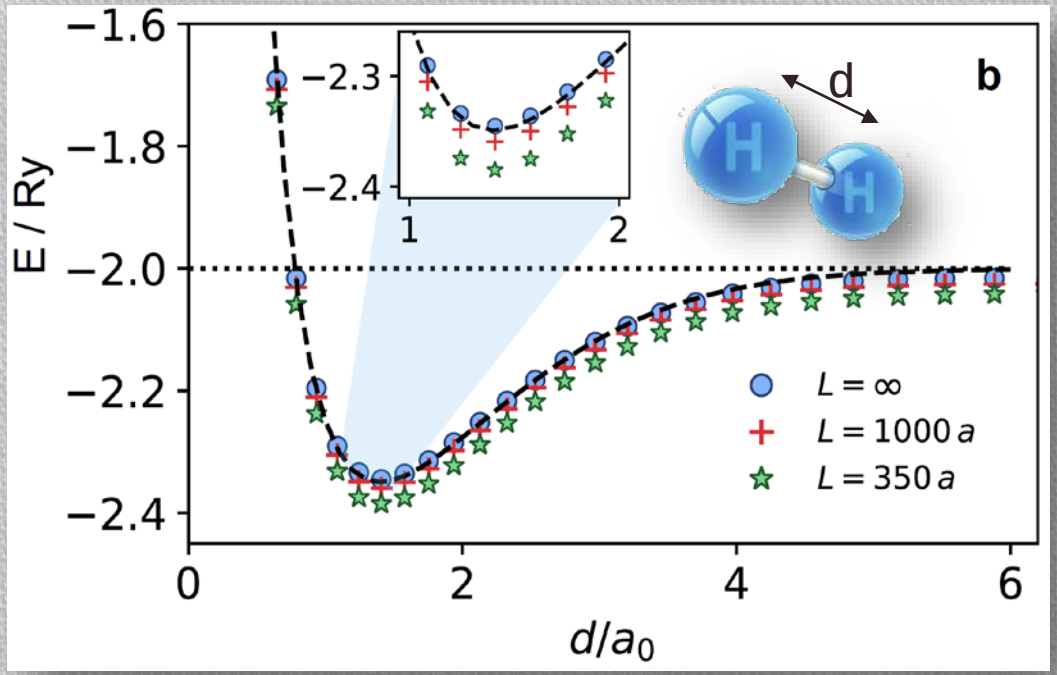
$$H_n = -V_0 \sum_j \left(\sum_{m=1}^{N_n} \frac{Z_m}{|j - R_m|} \right) f_j^\dagger f_j$$



System size determines the accuracy

DISCRETIZATION:
Hydrogen Molecule (H_2)





ANALOG QUANTUM SIMULATION

ADVANTAGES/DISADVANTAGES

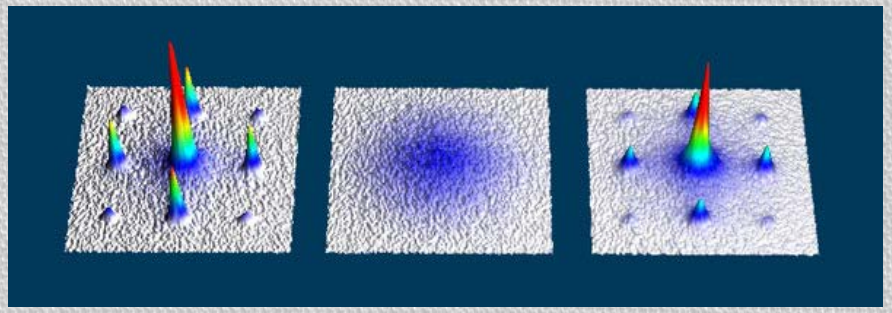
- CONTROL
- ERRORS:

Errors are extensive

$$H = \sum_n h_n + \varepsilon \sum_n v_n$$

Observables are intensive

$$m = \frac{1}{N} \sum_n \langle s_n^z \rangle$$

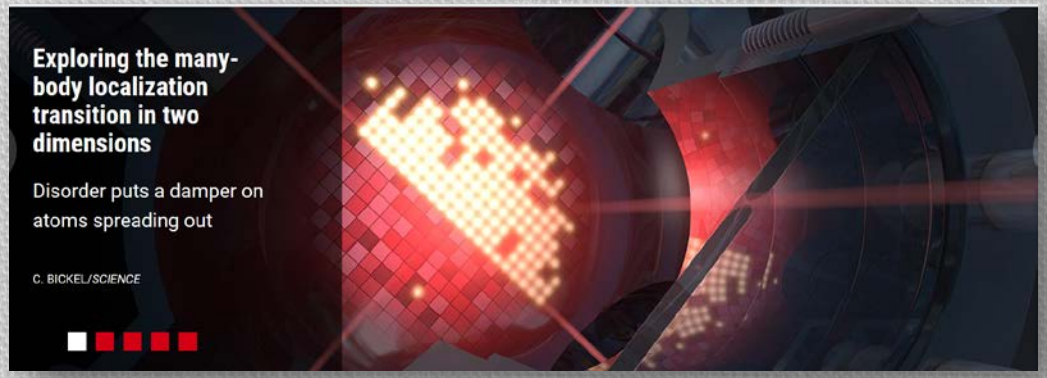


Bloch, Esslinger, Greiner

ANALOG QUANTUM SIMULATION

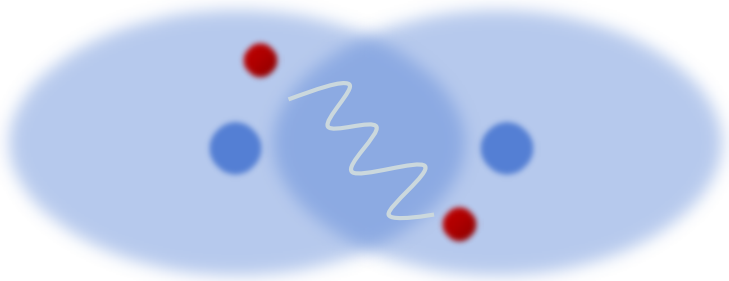
GOALS:

- Solve specific models
- Provide understanding
- Benchmark theory

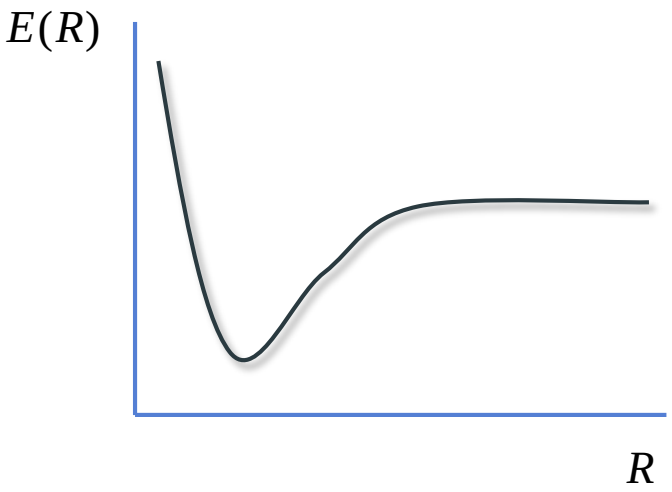


Bloch, Gross, et al

QUANTUM CHEMISTRY



Molecular potential



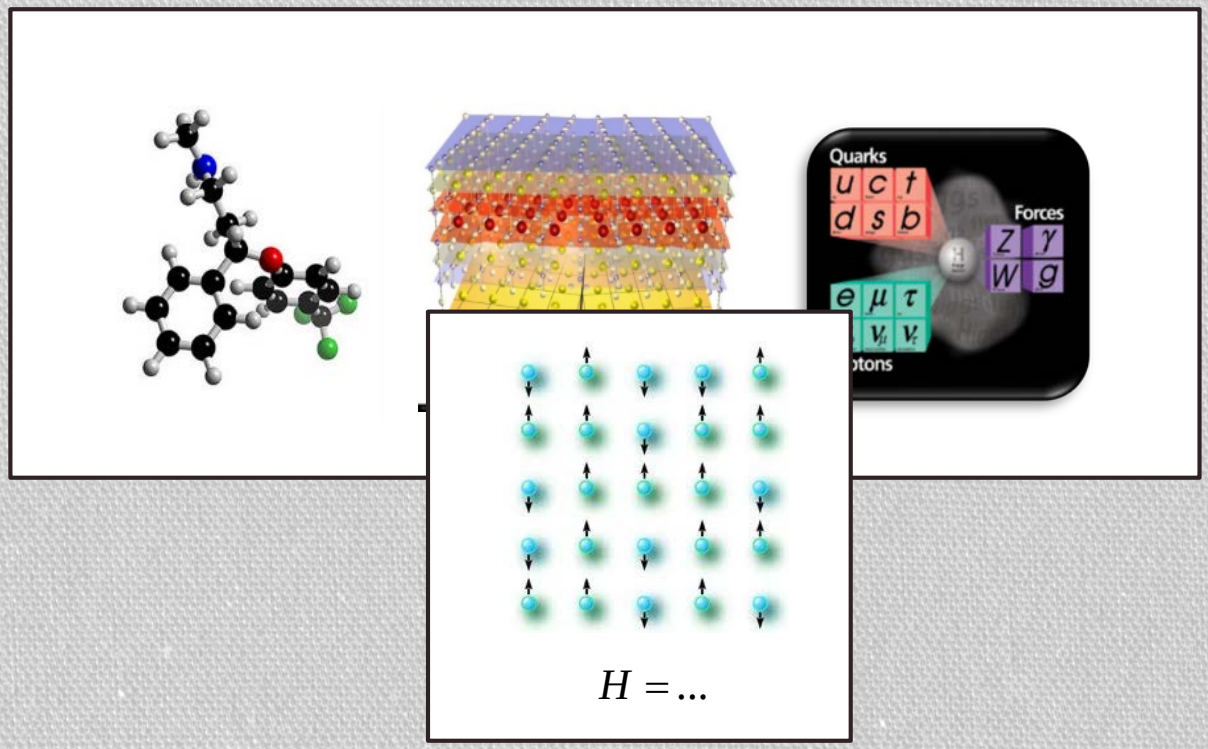
Born-Oppenheimer approximation:

$$H \approx H_{\text{nuc}} - \sum_{n} \nabla_n^2 - \sum_{n,X} \frac{1}{|R_X - r_n|} + \sum_{n,m} \frac{1}{|r_n - r_m|}$$

Electron

Electron-Electron

QUANTUM MANY-BODY PROBLEMS



$$|\Psi\rangle = c_{0,0,\ldots,0}\,|0,0,\ldots,0\rangle + c_{0,0,\ldots,1}\,|0,0,\ldots,1\rangle + \ldots c_{1,1,\ldots,1}\,|1,1,\ldots,1\rangle$$

- Exponential in space
- Exponential in time

$$T \approx (2^N)^{\mathrm{O(depth)}}$$

QUANTUM SIMULATION

Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

1. INTRODUCTION

On the program it says this is a keynote speech—and I don't know what a keynote speech is. I do not intend in any way to suggest what should be in this meeting as a keynote of the subjects or anything like that. I have my own things to say and to talk about and there's no implication that

$$|\Psi\rangle = c_{0,0,\ldots,0}\,|0,0,\ldots,0\rangle + c_{0,0,\ldots,1}\,|0,0,\ldots,1\rangle + \ldots c_{1,1,\ldots,1}\,|1,1,\ldots,1\rangle$$

QUANTUM SIMULATION

DYNAMICS:

- Efficient: $T \approx N \,||\, h \,||\, t \log(1/\varepsilon)$

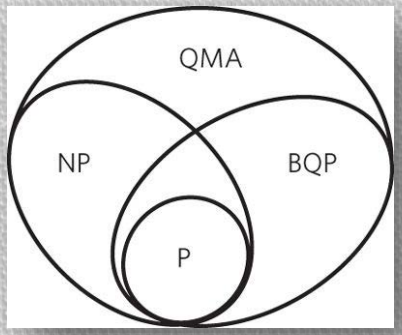
  Lloyd, Scince 273, 5278 (1996)

  Haah, Hstings, Kothari, Low, arXiv: 1801.03922

Compare $T \approx 2^{NO(t)}$

GROUND STATE (zero temperature):

- Difficult: $T \approx 2^{\alpha N}$



Compare $T \approx (2^N)^N$

QUANTUM SIMULATION

SCALING-UP:

- Fault-tolerant error correction
- Error scaling

Scientific and Technological challenge

NISQ (noise intermediate scale quantum computers):

- Exact dynamics: hundreds of qubits and thousands of gates
- Ground state: Heuristic methods: adiabatic, variational, etc