ANALOG QUANTUM SIMULATION:
Quantum Chemistry

Solvay Workshop on Quantum Simulation

ULB, Brussels, February 18th, 2019

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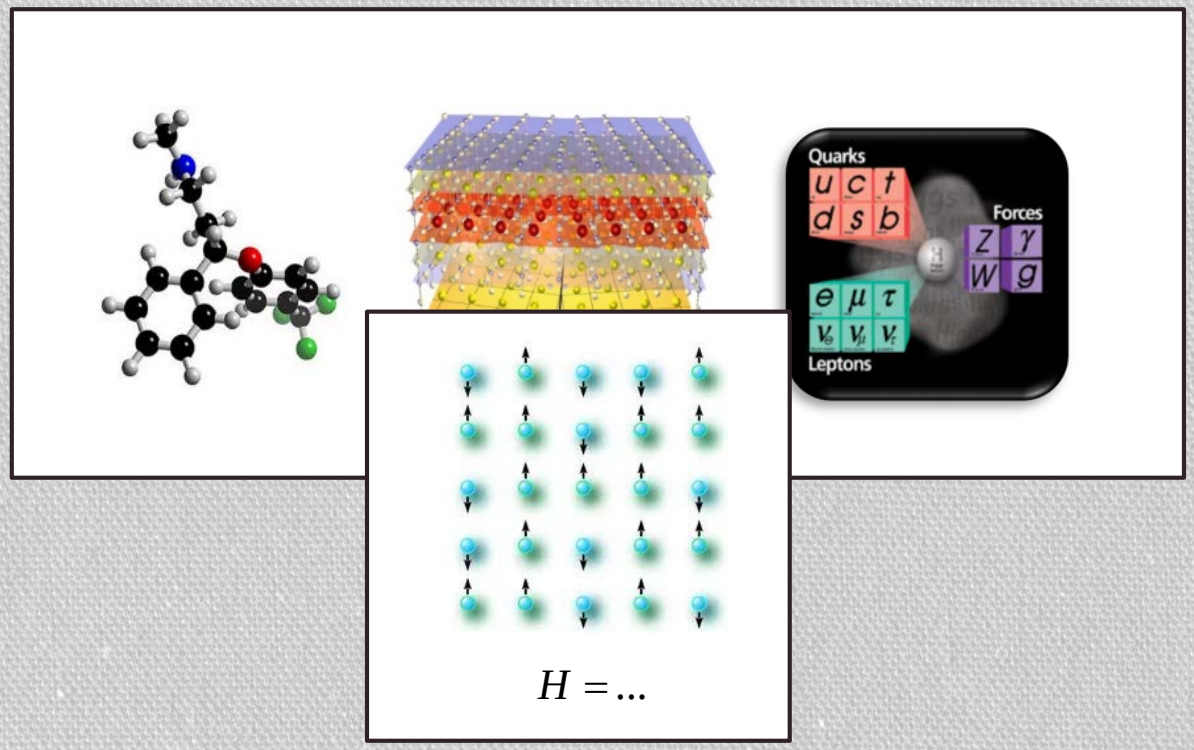
MPQ
Max-Planck-Institut
für Quantenoptik

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

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

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 COMPUTING

DYNAMICS:

- Efficient: Lloyd, Scince 273, 5278 (1996)

$$e^{-iHt} \approx \left(e^{-ih_1 t/M} \ldots e^{-ih_N t/M} \right)^M$$

$$T \approx \left(N \| h \| t \right)^2 / \varepsilon$$

- Very efficient: Haah, Hstings, Kothari, Low, arXiv: 1801.03922

$$T \approx N \| h \| t \log(1/\varepsilon)$$

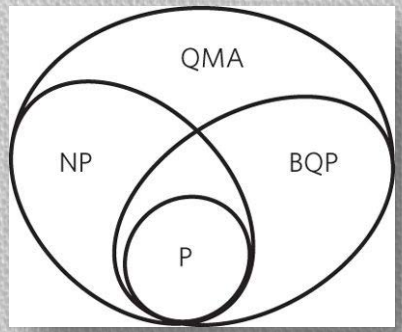
Compare $T \approx 2^{N^2}$

QUANTUM COMPUTING

GROUND STATE:

- Compute the energy
- Prepare the state

  - Difficult: Kempe, Kitaev, Regev, SIAM 5, 1070 (2006)



Compare $T \approx 2^{N^2}$

  - Heuristic: Farhi, Goldstone, Gutmann, Sipser, Science 292, 472 (2001)

QUANTUM COMPUTING

SCALING-UP:

- Fault-tolerant error correction

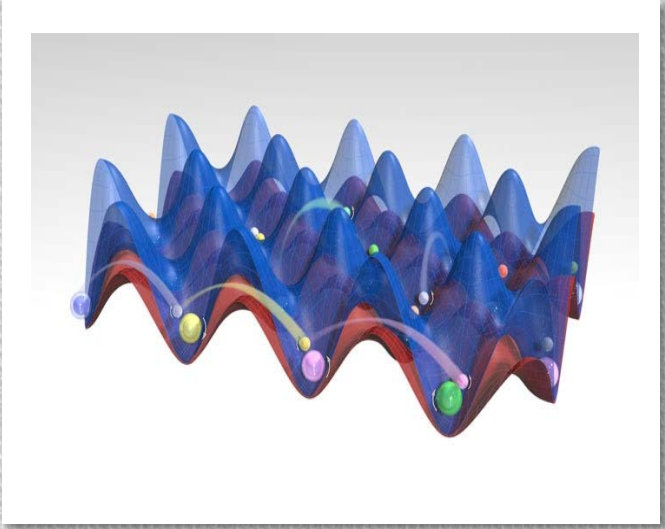
  Overhead $\sim 10^4$ (@ 10^{-3} error/gate with surface codes)

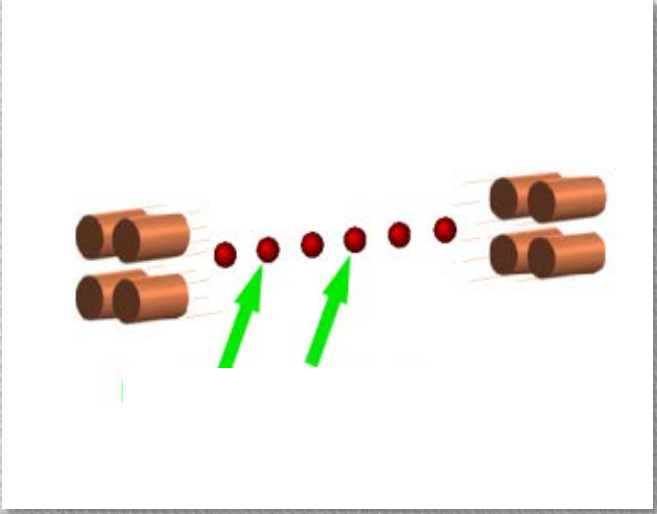
- Error scaling

  Error/gate independent of the size

Scientific and Technological challenge

ANALOG QUANTUM SIMULATION





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

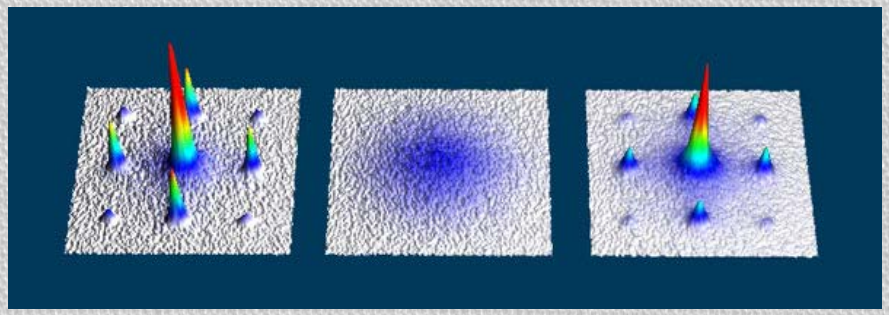
ADVANTAGES/DISADVANTAGES

Errors are extensive

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

Observables are intensive

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



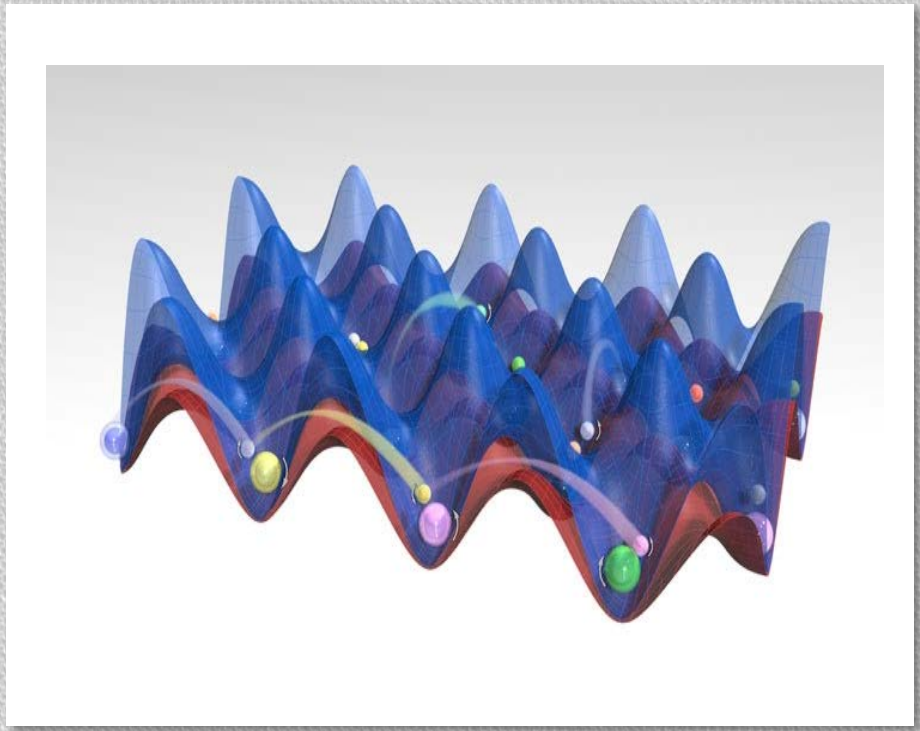
Bloch, Esslinger, Greiner

ANALOG QUANTUM SIMULATION

GOALS:

- Solve specific models
- Provide understanding
- Benchmark theory

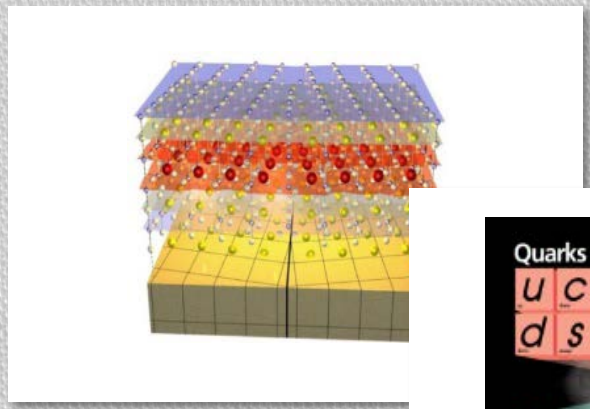
ANALOG QUANTUM SIMULATION: COLD ATOMS IN OPTICAL LATTICES



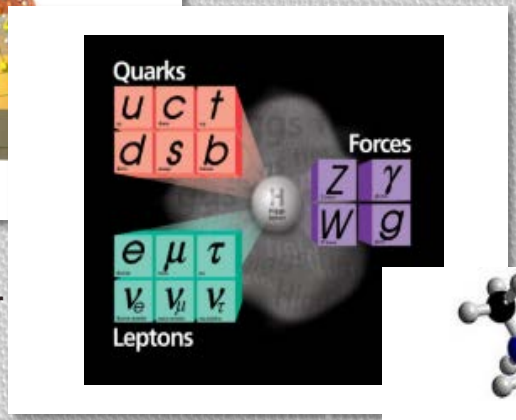
$$H = -\sum_{\substack{<n,m> \\ \sigma,\sigma'}} \left(t_{\sigma,\sigma'} a^{\dagger}_{n,\sigma} a_{m,\sigma'} + h.c \right) + \sum_{\substack{n \\ \sigma,\sigma'}} U_{\sigma,\sigma'} a^{\dagger}_{n,\sigma} a^{\dagger}_{n,\sigma'} a_{n,\sigma'} a_{n,\sigma}$$

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

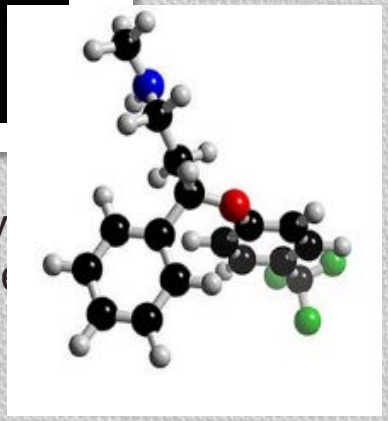
ANALOG QUANTUM SIMULATION
COLD ATOMS IN OPTICAL LATTICES



Condensed matter
Hubbard and spin



High-energy Phy
Lattice gauge th

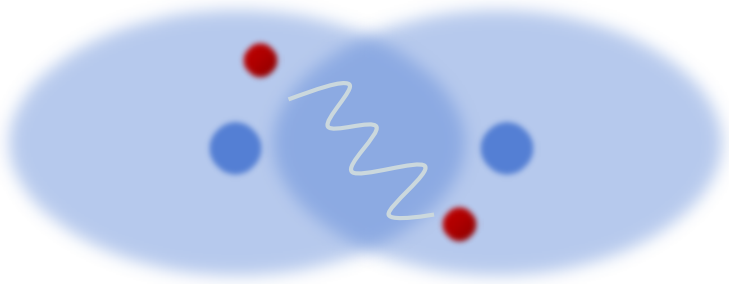


Quantum chemistry:

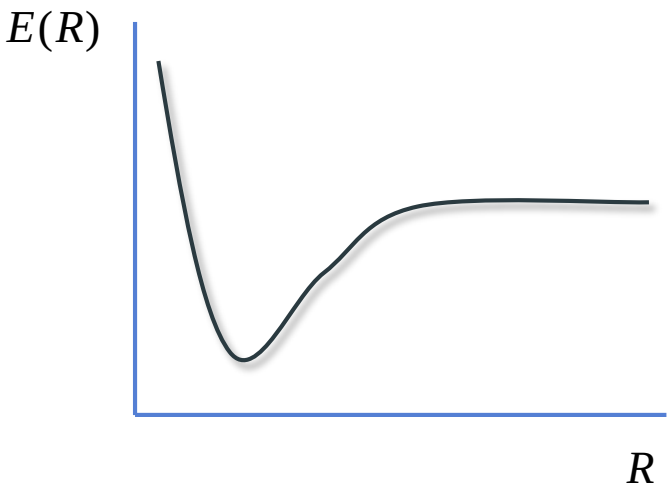
QUANTUM CHEMISTRY SIMULATIONS

Argüello, Shi, González-Tudela, Zoller, JIC, arXiv: 1807.09228

QUANTUM CHEMISTRY



Molecular potential



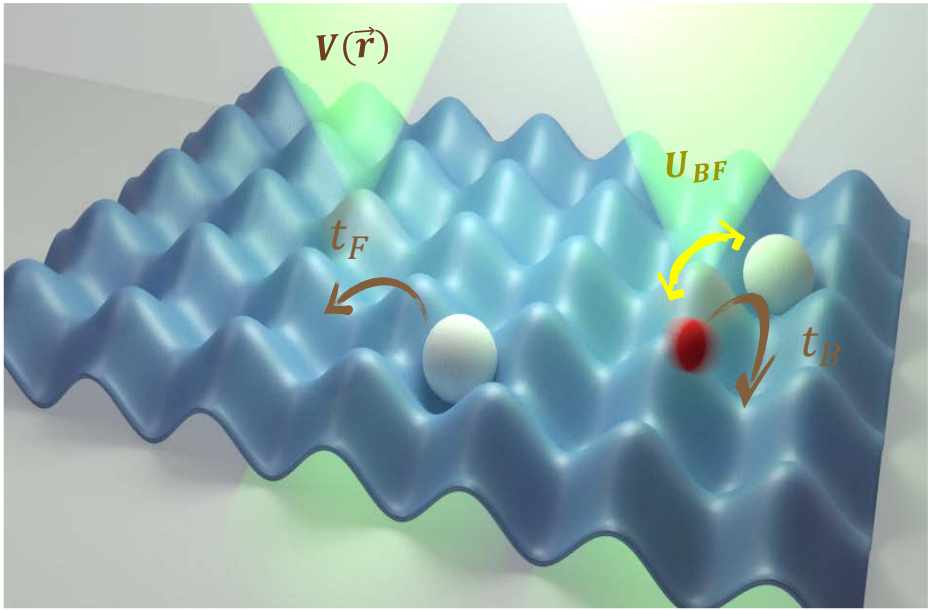
Born-Oppenheimer approximation:

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

Electron

Electron-Electron

QUANTUM CHEMISTRY SIMLUATION
ATOMS IN OPTICAL LATTICES

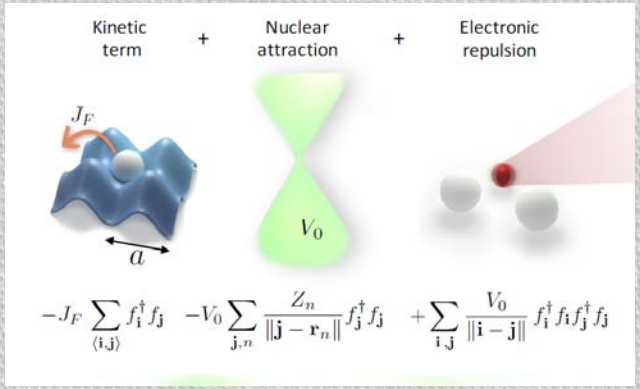


$$H \approx H_{\text{nuc}} - \sum_n \nabla_n^2 - \sum_{n,X} \frac{1}{|R_X - r_n|} + \sum_{n,m} \frac{1}{|r_n - r_m|}$$

Fermions:
Single particle:
lattice + laser

Fermions:
Mediated by boson

ANALOG QUANTUM SIMULATION
COLD ATOMS IN OPTICAL LATTICES



MAIN QUESTIONS:

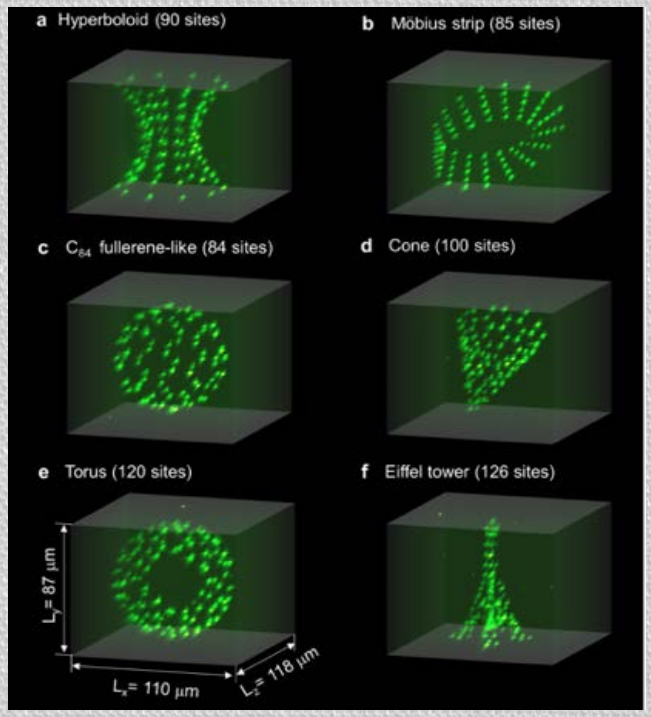
- External Coulomb potential
- Electron-electron Coulomb interaction
- Discretization

TECHNICAL QUESTIONS:

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

1. EXTERNAL COULOMB POTENTIAL

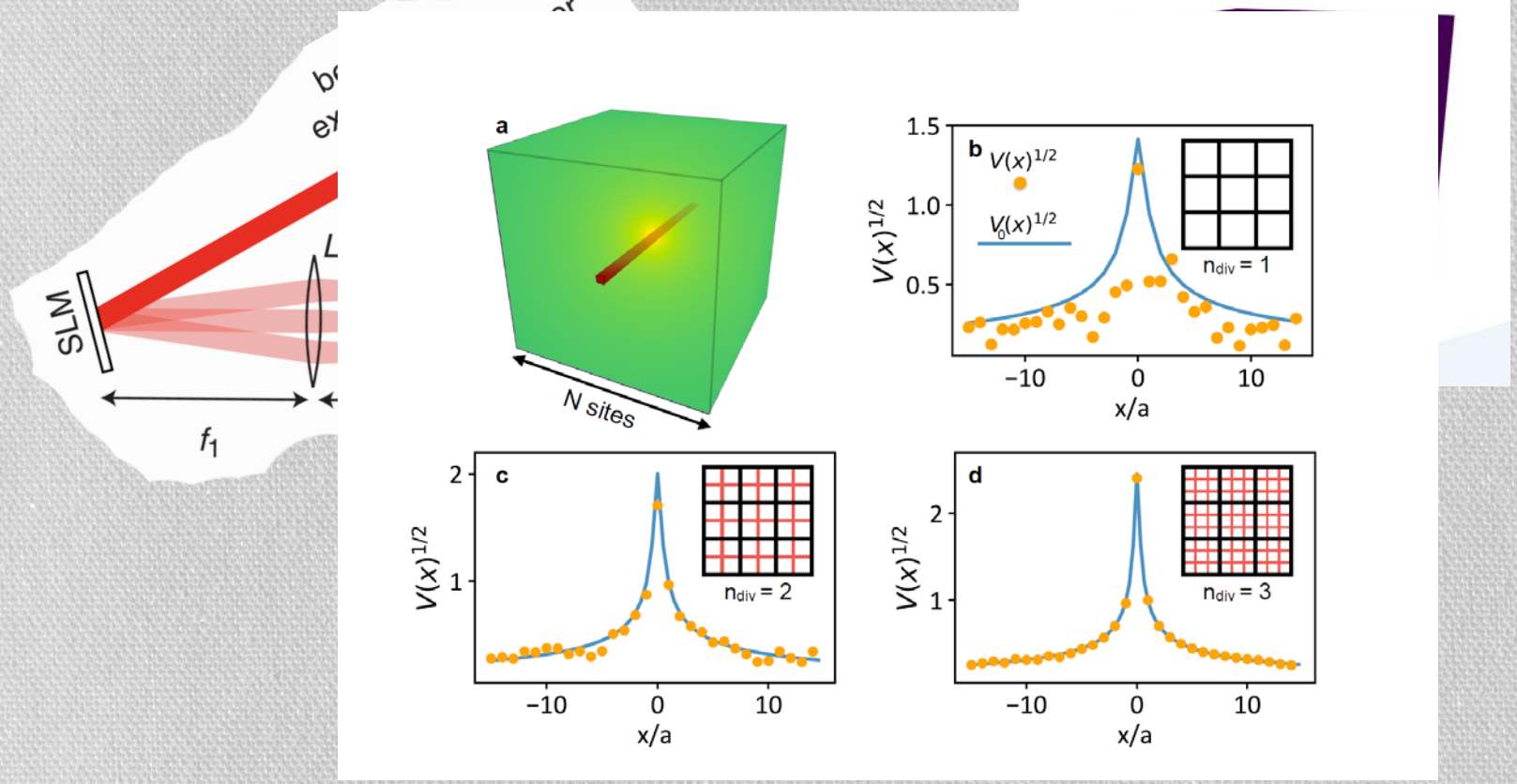
$$H \approx H_{\text{nuc}} - \sum_n \nabla_n^2 - \sum_{n,X} \frac{1}{|R_X - r_n|} + \sum_{n,m} \frac{1}{|r_n - r_m|}$$



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

1. EXTERNAL COULOMB POTENTIAL

Holographic technique: phase pattern

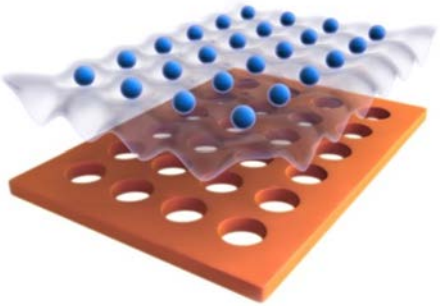


2. ELECTRON-ELECTRON INTERACTION

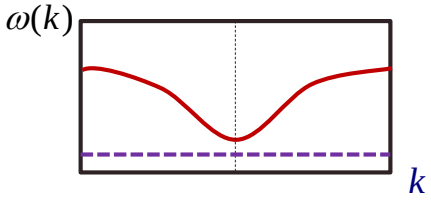
$$H \approx H_{\text{nuc}} - \sum_{n} \nabla_n^2 - \sum_{n,X} \frac{1}{|R_X - r_n|} + \sum_{n,m} \frac{1}{|r_n - r_m|}$$

2. ELECTRON-ELECTRON INTERACTION

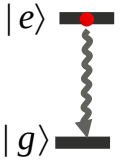
EMITTERS IN STRUCTURED BATHS



$$H = \Delta \sum_i |e\rangle_i\langle e| + \sum_k \omega_k \hat{a}_k^\dagger \hat{a}_k + \sum_i g\left(\sigma_i^+ a_i + a_i^\dagger \sigma_i^-\right)$$



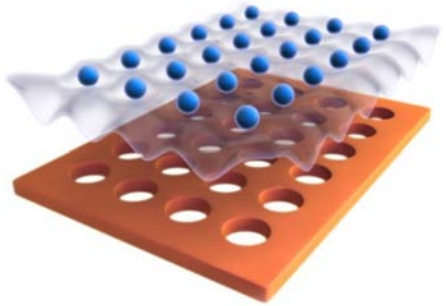
PHOTONIC CRYSTAL



EMITTERS

2. ELECTRON-ELECTRON INTERACTION

EMITTERS IN STRUCTURED BATHS



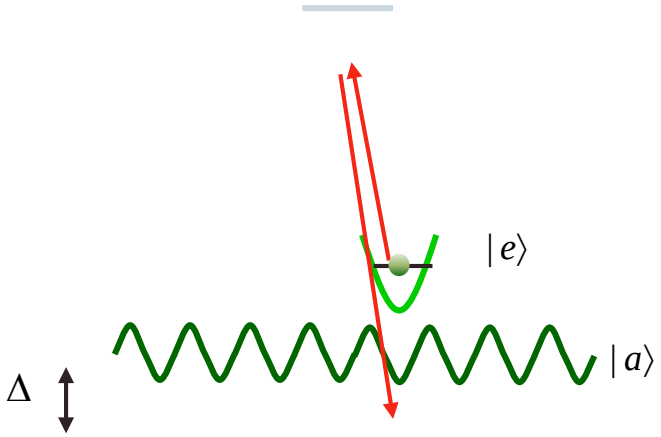
$$H \approx \sum_{n,m} V(n-m)\left[\sigma_n^+\sigma_m^- + \sigma_m^+\sigma_n^-\right]$$

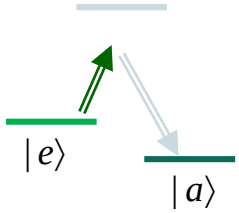
$$V(\mathbf{d}) \prec \int d^D\mathbf{k}\,\frac{e^{i\mathbf{kd}}}{\omega_0-\omega_k} \quad = \frac{e^{-d/\xi}}{d} \xrightarrow{d\ll\xi} \frac{1}{d}$$

In 3D

2. ELECTRON-ELECTRON INTERACTION

ATOMS IN OPTICAL LATTICES





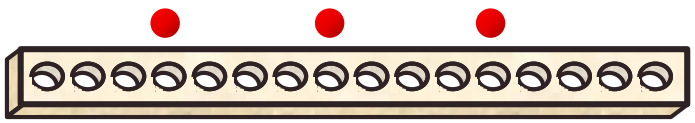
$$H = \Delta |e\rangle\langle e| + \sum_k \omega_k \hat{a}_k^\dagger \hat{a}_k + g\left(\sigma^+ a_0 + a_0^\dagger \sigma^-\right)$$

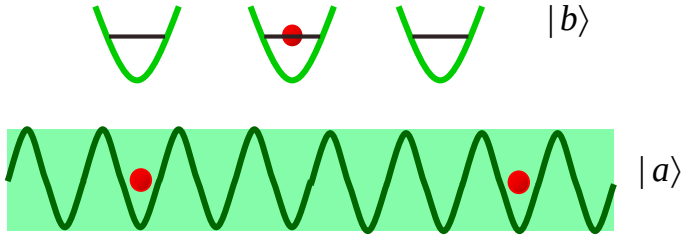
Vega, Porras, JIC, Phys. Rev. Lett. **101**, 260404 (2008),
Navarrete, Vega, Porras, JIC, New J. Phys.**13**, 023024 (2011)

Experiments: Stoneybrook (Schneble), MPQ (Blatt)

2. ELECTRON-ELECTRON INTERACTION

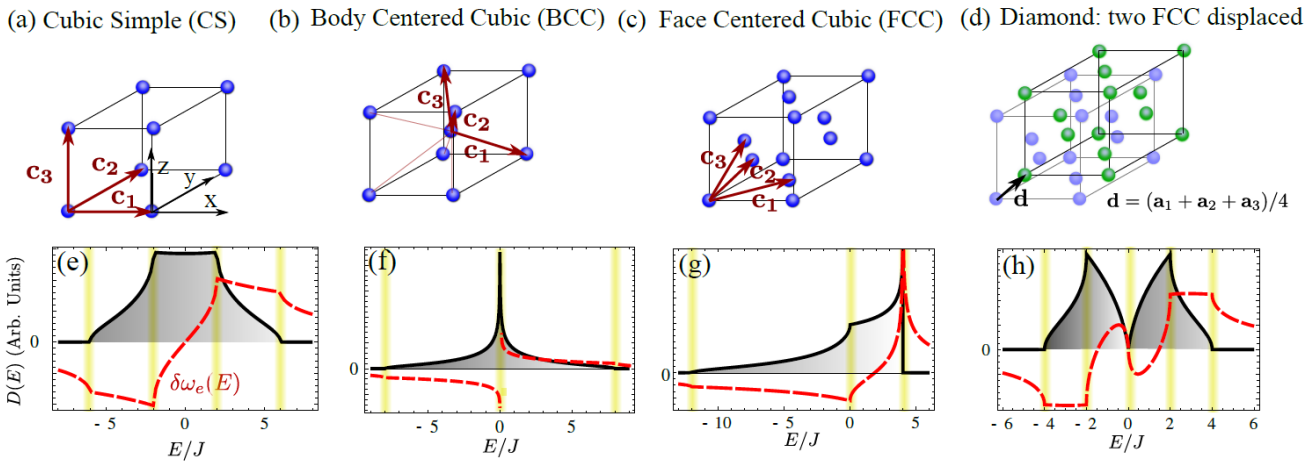
$$H = \Delta \sum_n |e\rangle_n \langle e| + \sum_k \omega_k \hat{a}_k^\dagger \hat{a}_k + \sum_n g_n \left(\sigma_n^+ a_n + a_n^\dagger \sigma_n^- \right)$$





- Different regimes
- Dimension & geometries
- Exotic baths

2. ELECTRON-ELECTRON INTERACTION



- Cubic lattice:

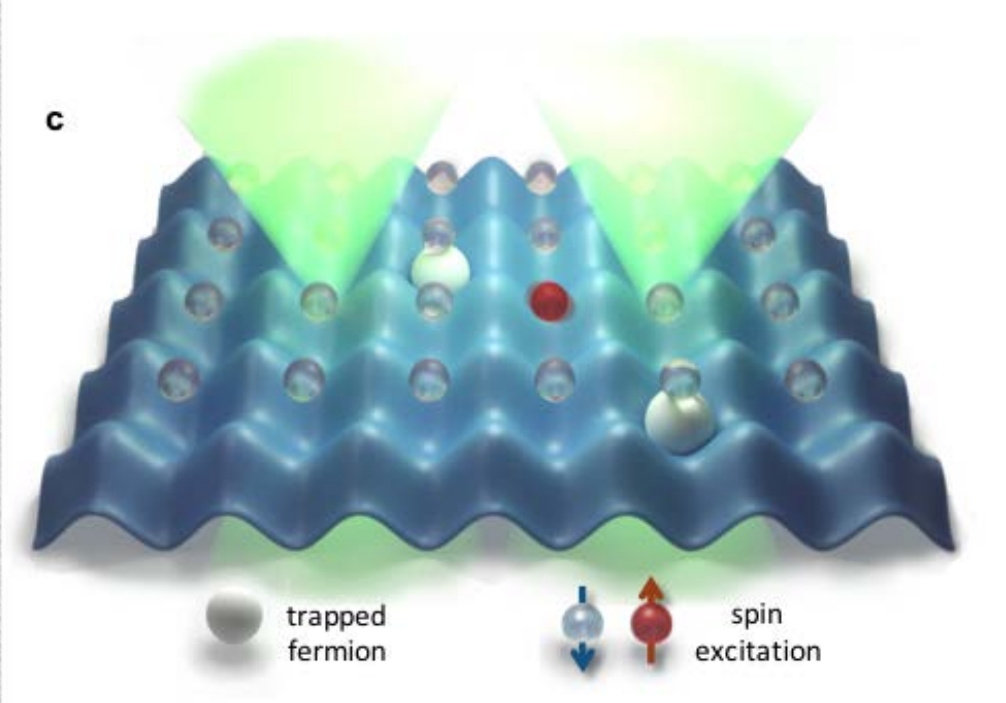
$$H \approx \sum_{n,m} V(n-m)\left[\sigma_n^+\sigma_m^- + \sigma_m^+\sigma_n^-\right]$$

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

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

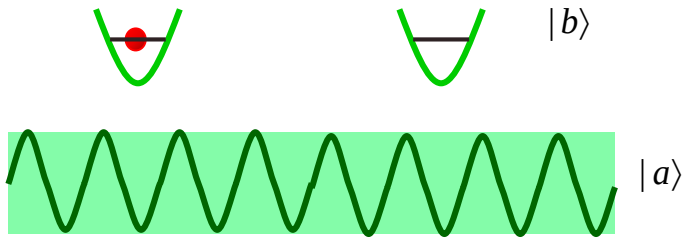
González-Tudela, JIC, Quantum **2**, 97 (2018)

2. ELECTRON-ELECTRON INTERACTION



But the interaction between electrons is obtained in second order perturbation theory…

2. ELECTRON-ELECTRON INTERACTION



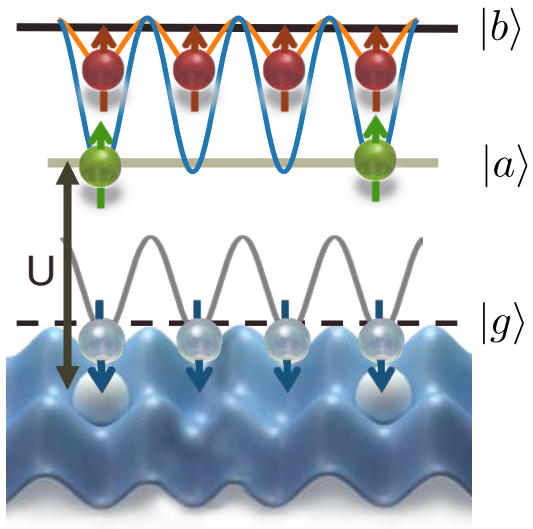
$$H \approx \sum_{n,m} \frac{1}{|r_1 - r_2|}\left[\sigma^+_{r_1}\sigma^-_{r_2} + \sigma^+_{r_2}\sigma^-_{r_1}\right]$$

The eigenstate state $(b^\dagger_{r_1} \pm b^\dagger_{r_2})|vac\rangle$ has energy $\pm\frac{1}{|r_1 - r_2|}$

Take an atom in that state (that adiabatically follows)

2. ELECTRON-ELECTRON INTERACTION

Use spin excitation:

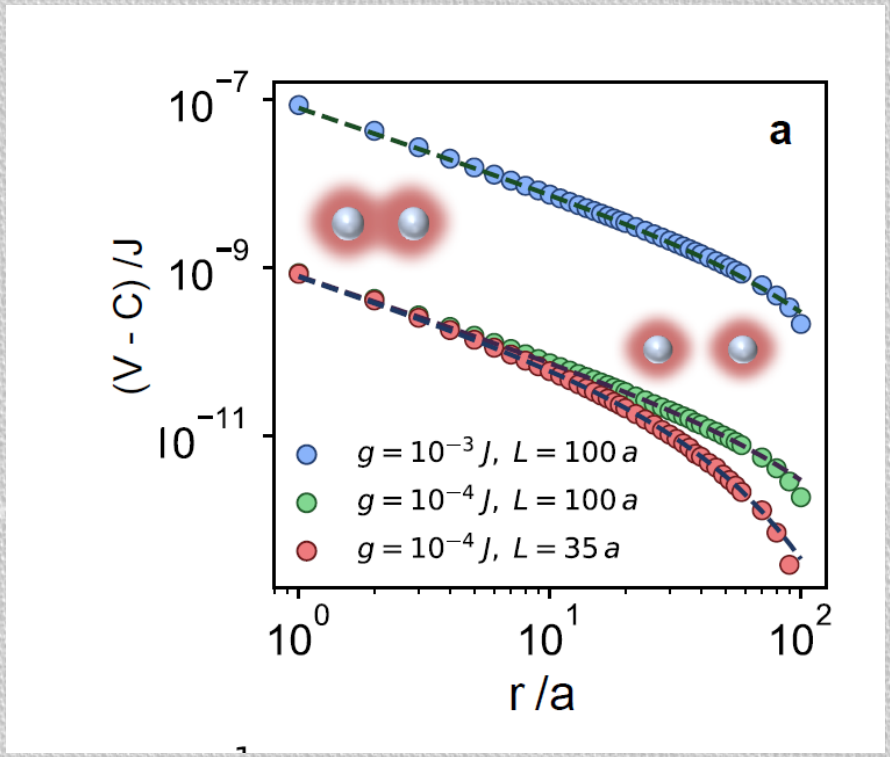


- Moving with the fermions
- In a symmetric state

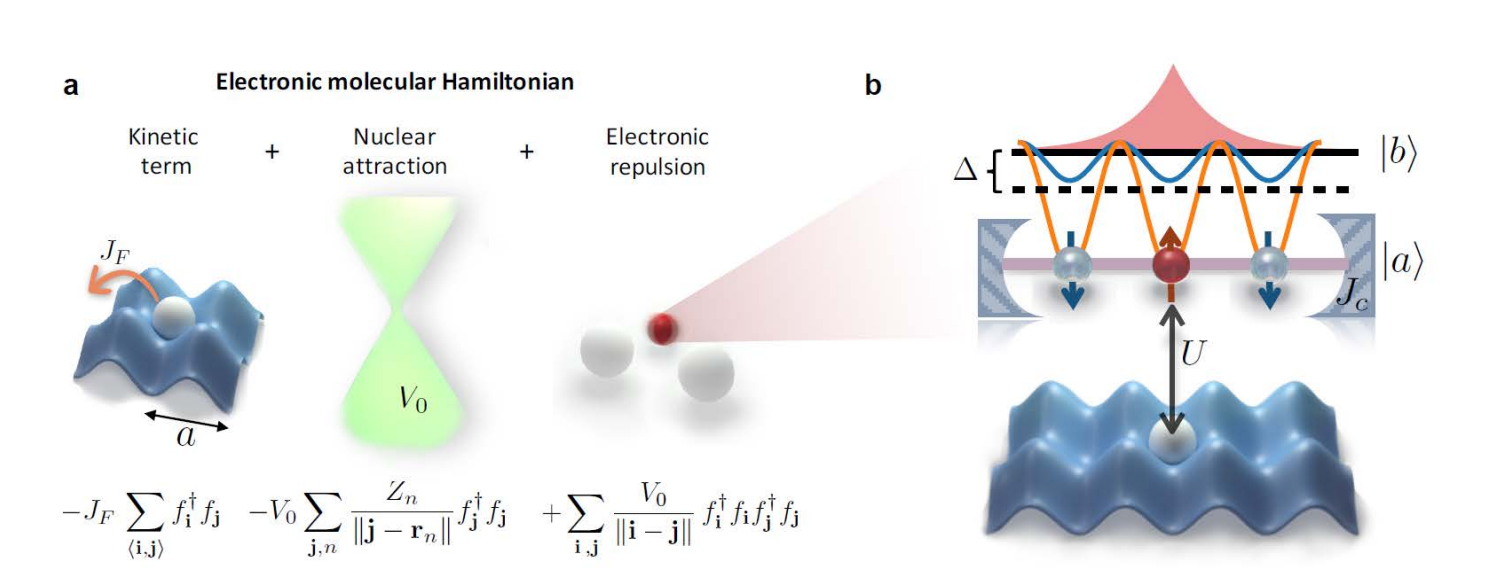
→ Cavity mode off resonance

2. ELECTRON-ELECTRON INTERACTION

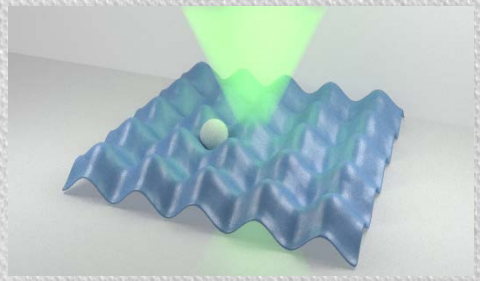
Effective fermion-fermion interaction



ANALOG QUANTUM CHEMISTRY



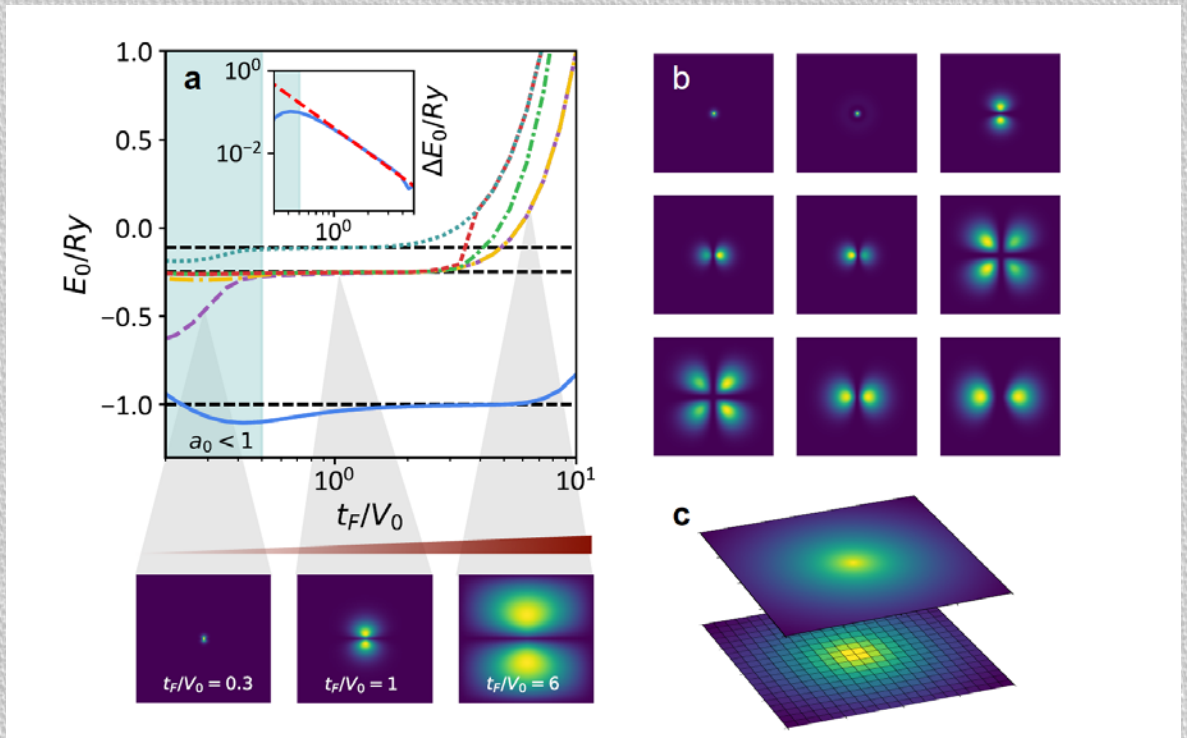
DISCRETIZATION: Hydrogen atom



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

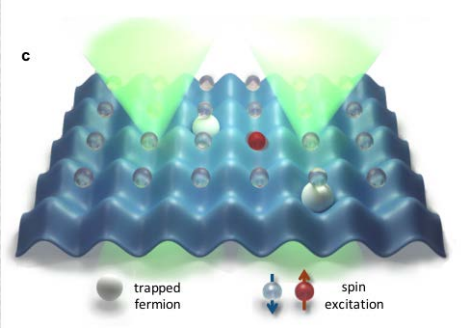
$$H_{hop} = -t_F \sum_{\langle i,j \rangle} \left(f_i^\dagger f_j + h.c. \right)$$

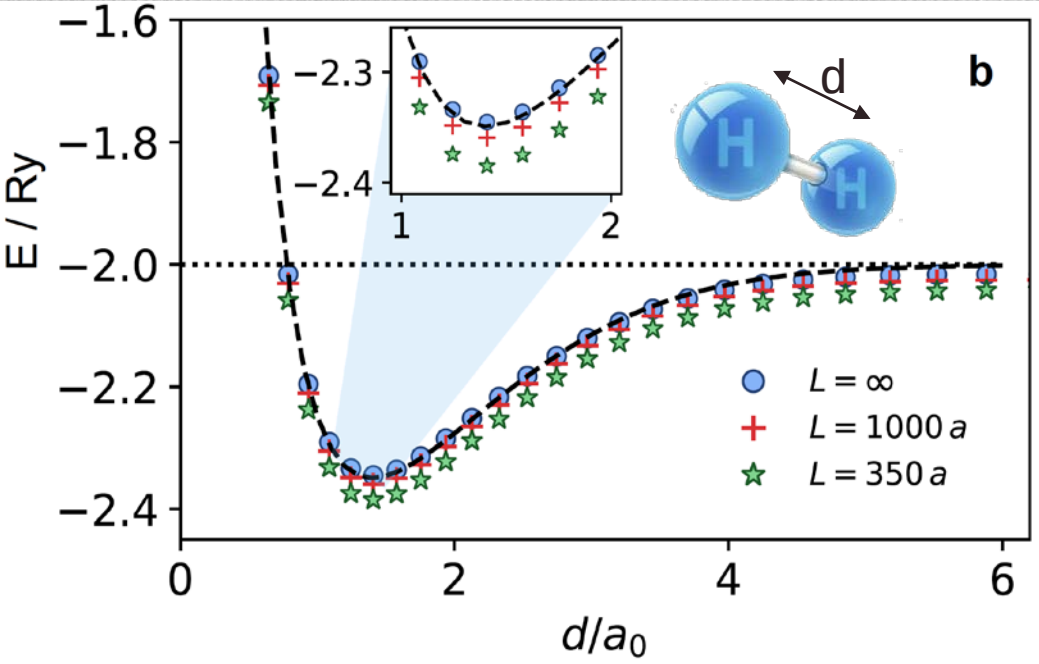
$$H_n = -V_0 \sum_j \left(\sum_{m=1}^{N_n} \frac{Z_m}{|j - R_m|} \right) f_j^\dagger f_j$$



System size determines the accuracy

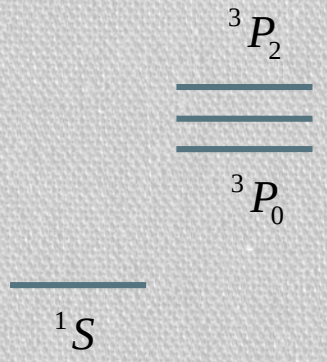
DISCRETIZATION:
Hydrogen Molecule (H_2)



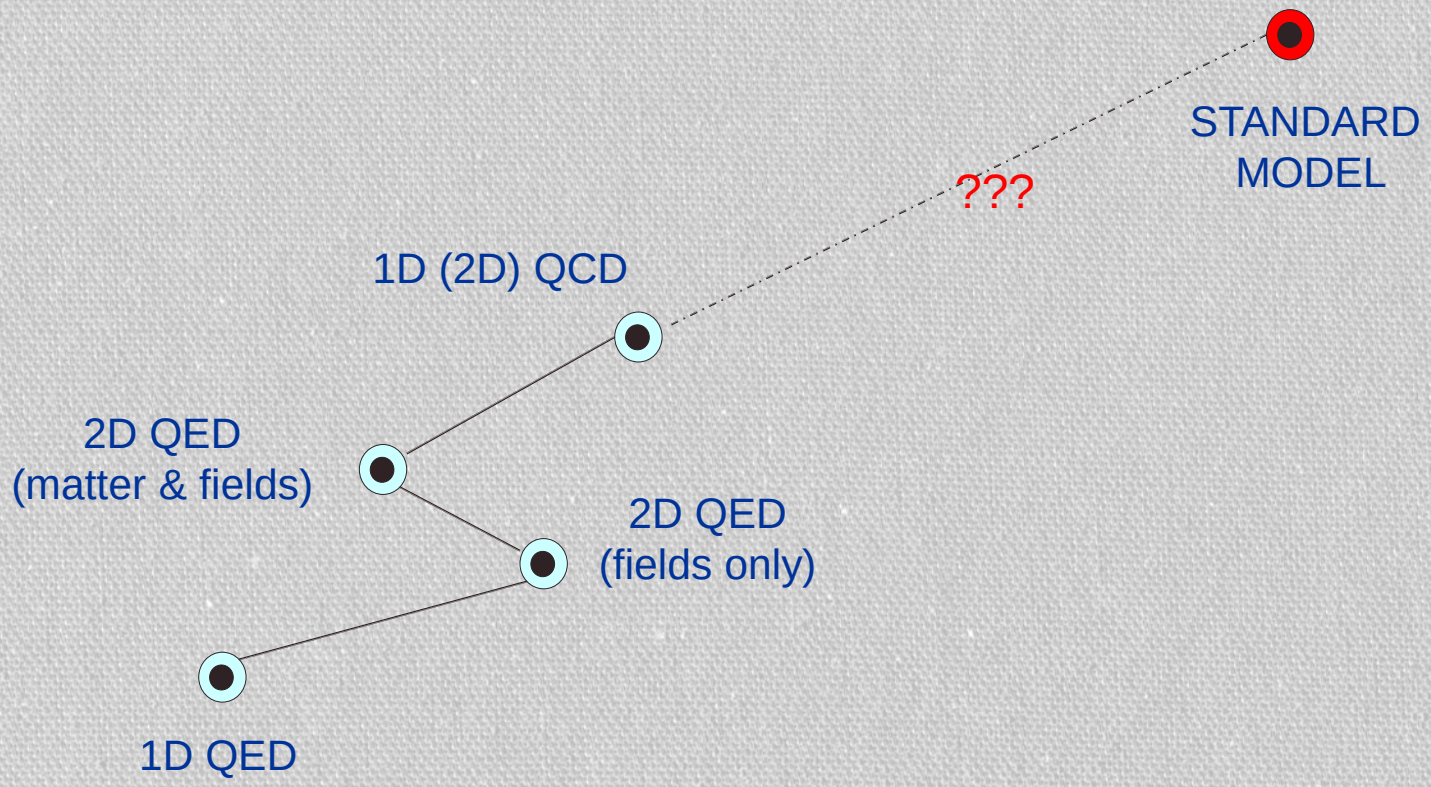


TECHNICAL QUESTIONS

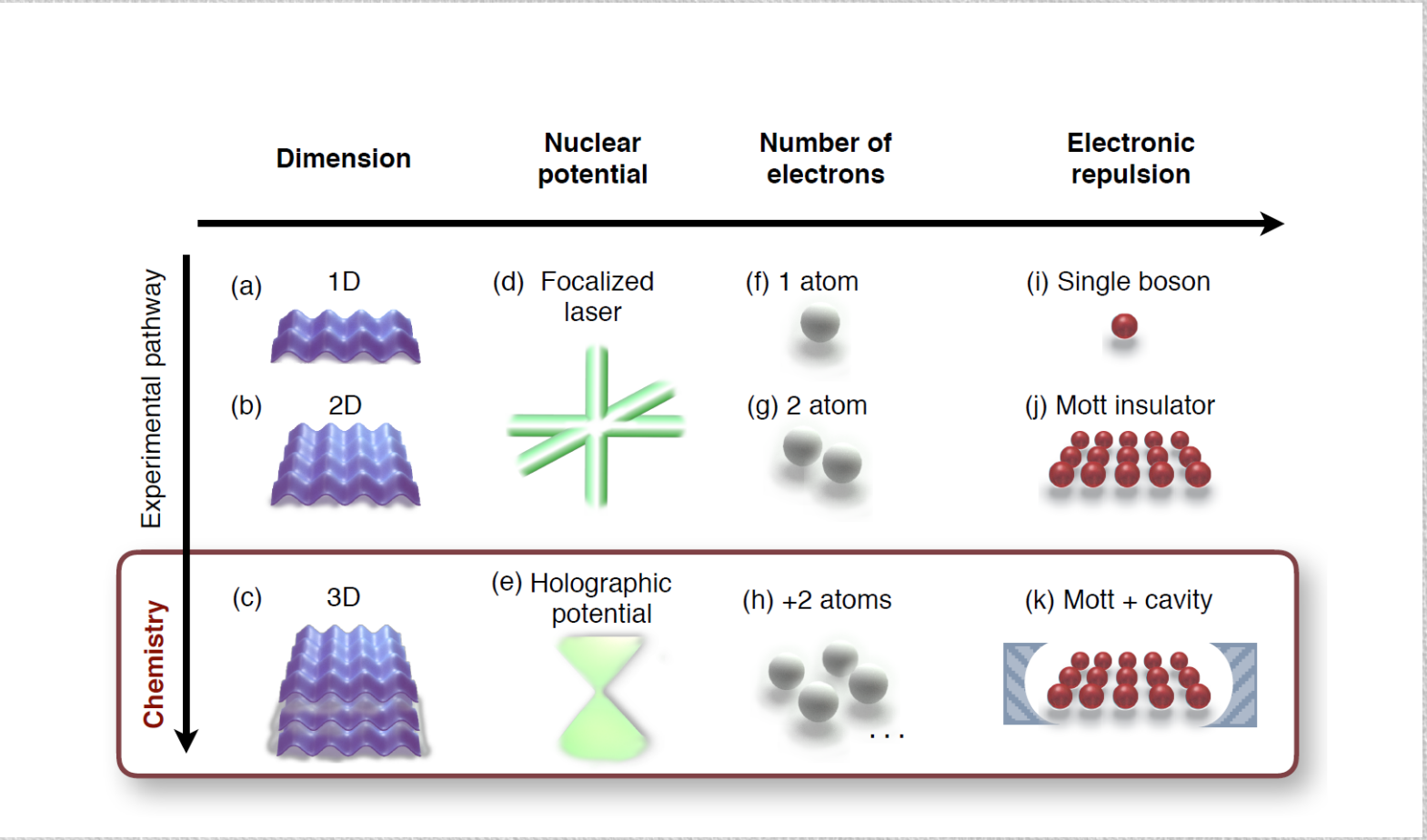
- Atoms: two earth-alkali isotopes
  - Fermion/Boson isotopes
  - Similar transition frequencies (isotopes shifts)
  - Magic wavelenghts
  - Interactions in the right states
  - Cavity mode: only bosons in state a
- Preparation: Adiabatic procedure
  - Prepare atoms locally
  - Adiabatically switch on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



QUANTUM SIMULATION HEP MODELS ROADMAP



QUANTUM SIMULATION HEP MODELS ROADMAP



+ other setups

Acknowledgments



Argüello, Shi, González-Tudela, Zoller, JIC, arXiv: 1807.09228