Quantum Simulation

with analog and digital quantum computers

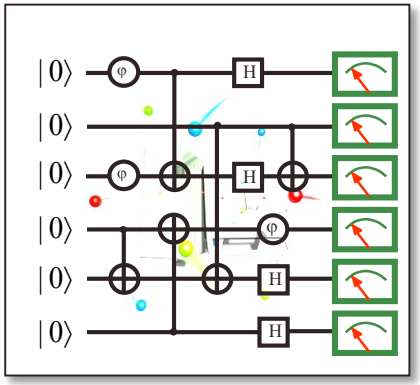
Inernational Iran Conferences on Quantum Information

University of Sharif, May 13th, 2021

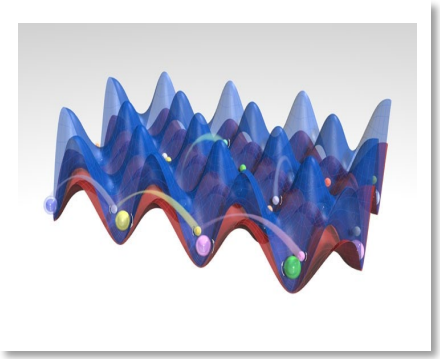
J. Ignacio Cirac

QUANTUM COMPUTING

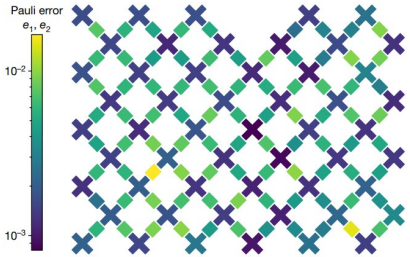
DIGITAL
(gate-based)



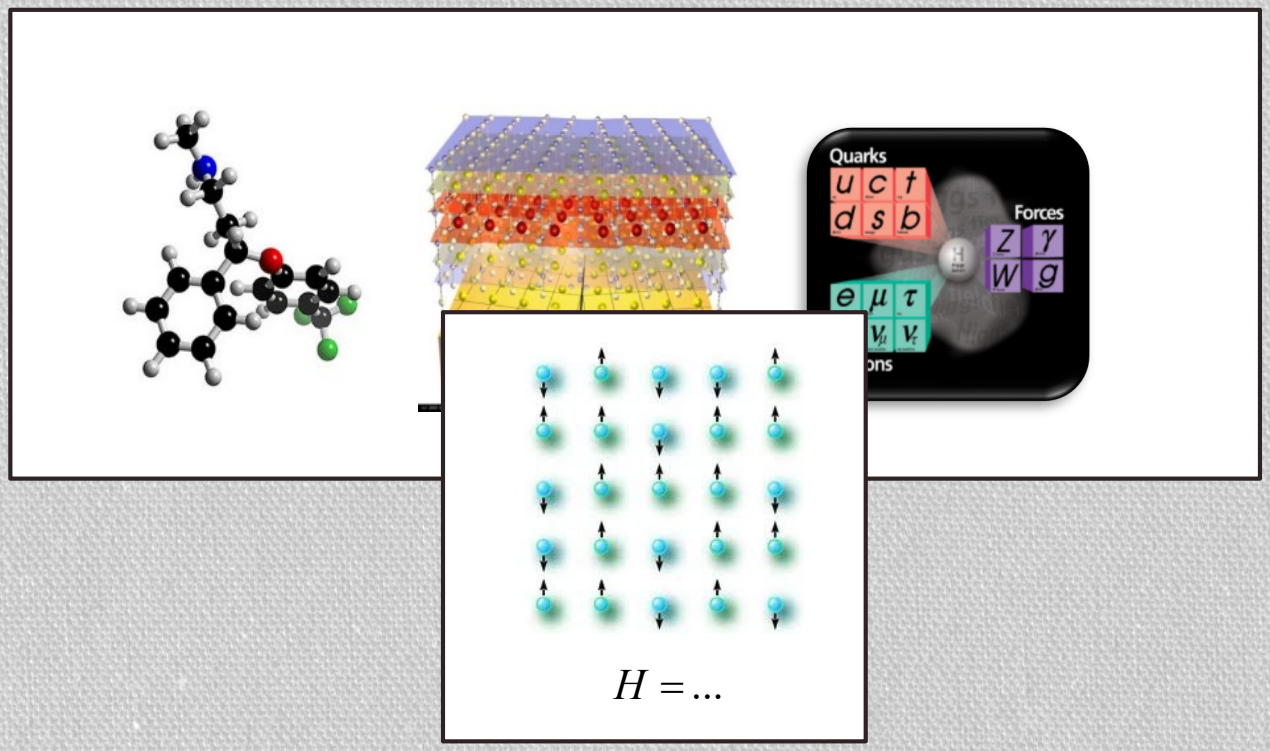
ANALOG
(continuous)



NISQ
(noise intermediate scale)



QUANTUM MANY-BODY PROBLEMS



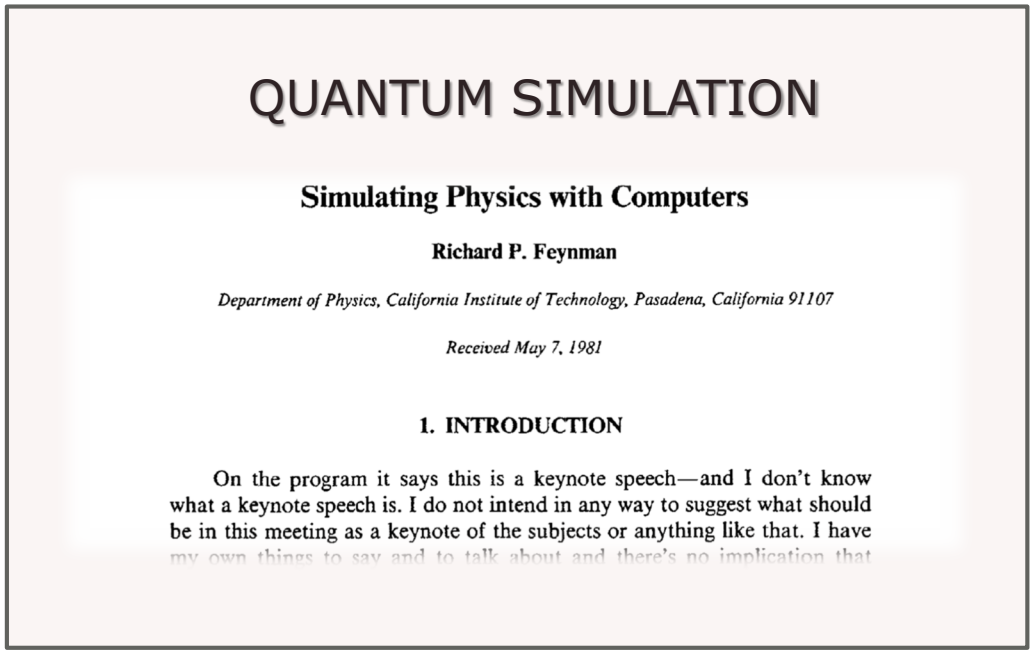
$$|\Psi\rangle = c_{0,0,\ldots,0}\,|0,0,\ldots,0\rangle + c_{0,0,\ldots,1}\,|0,0,\ldots,1\rangle + \ldots + c_{1,1,\ldots,1}\,|1,1,\ldots,1\rangle$$

- Memory: Exponential in N
- Time: Exponential in N

$$\Rightarrow \quad \tau \approx (2^N)^{\mathrm{O(depth)}} \rightarrow \left(2^N\right)^N$$

QUANTUM INFORMATION

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



QUANTUM SIMULATION

Simulating Physics with Computers

Richard P. Feynman

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

Received May 7, 1981

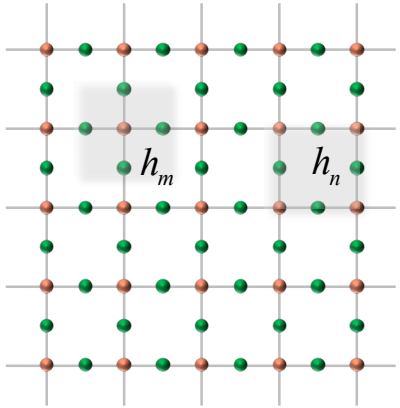
1. INTRODUCTION

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

Memory: linear in N

Time: $\tau \leq N, \ldots, 2^N, ???$

THIS TALK



Hamilonian

$$H = \sum_{n=1}^{N} h_n$$

QUANTUM ALGORITHMS:

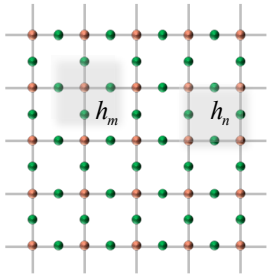
DYNAMICS
ZERO TEMPERATURE
FINITE TEMPERATURE

APPLICATIONS:

CONDENSED MATTER
HIGH-ENERGY
CHEMISTRY

QUANTUM ALGORITHMS:
Dynamics and zero temperture

DYNAMICS



- We want to compute $\langle \Psi | O | \Psi \rangle$

$$|\Psi\rangle = e^{-iHt} |\Psi_0\rangle$$

easy to prepare, eg, product state

- Prepare the state Ψ and measure:
  Lloyd, Scince 273, 5278 (1996)

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

- Very efficient:

  Haah, Hastings, Kothari, Low, arXiv: 1801.03922

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

Compare $\tau \approx 2^N$

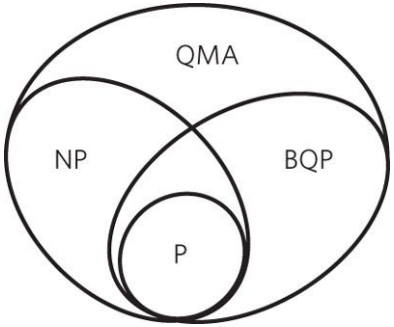
Not very natural for NISQ
With analog, straightforward algorithms

GROUND STATE

- We want to compute $\langle \Psi_0 | O | \Psi_0 \rangle$

  ground state

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



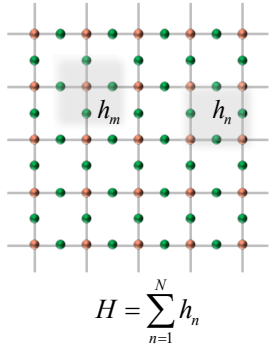
$\tau \approx 2^{\alpha N}$

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

Ge, Tura, JIC, PRL (2018)

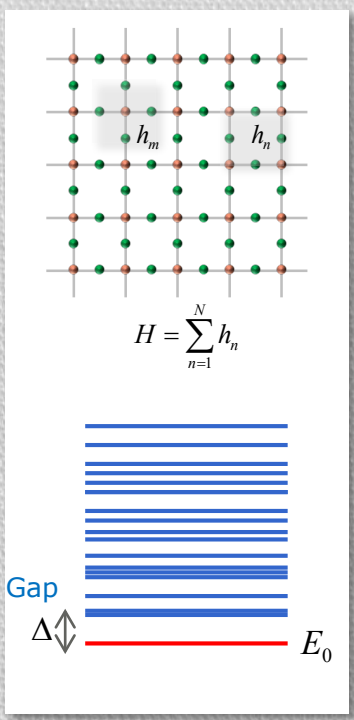
$$\tau \approx \frac{2^{N/2}}{\Delta} \log(1/\varepsilon)$$

Not applicable to NISQ or analog



GROUND STATE

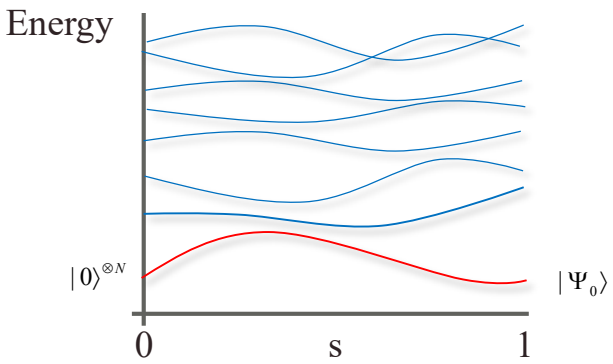
Heuristic algorithms



- **Adiabatic algorithm**

  See, eg, Farhi, Goldstone, Gutmann, Sipser, Science 292, 472 (2001)

$$H(0) = \sum_{n=1}^{N} \sigma_z^n \qquad H(s) \qquad H(1) = \sum_{n=1}^{N} h_n$$



„slow" change of s

- **Variational algorithms**

  Farhi, Goldstone, Gutmann, arXiv:1411.4028
  A. Peruzzo et al Nat. Comm.5, 4213 (2014)

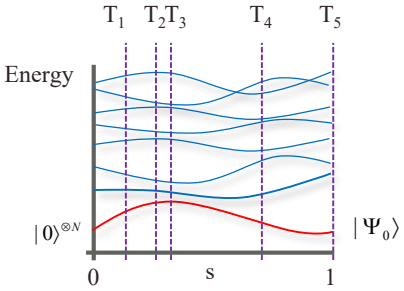
$$|\Psi(p)\rangle = U_m(p_m)...U_1(p_1)\,|0\rangle^{\otimes N}$$

GROUND STATE

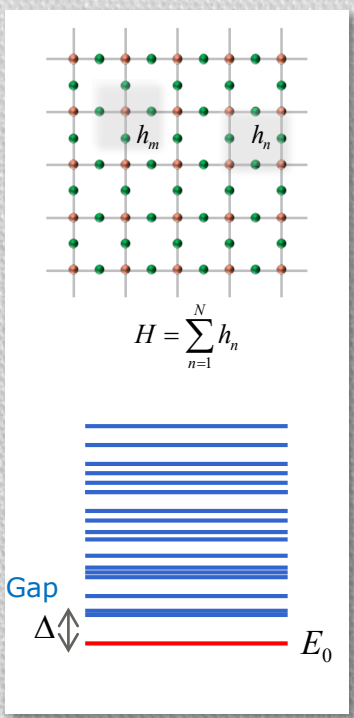
Heuristic algorithms

- **Variational adiabatic algorithm**

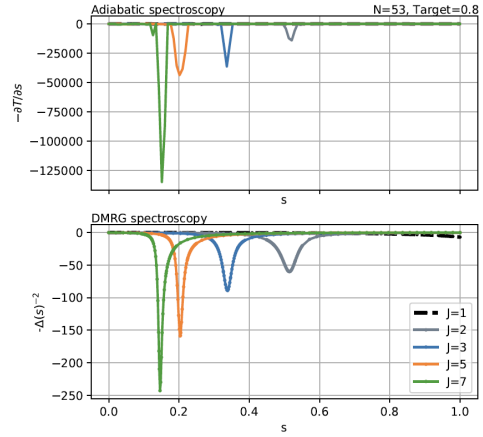
  Schiffer, Tura, JIC, arXiv:2103.01226



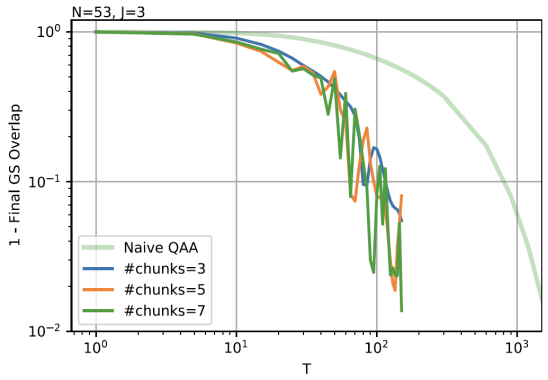
$$H = \sum_{j=1}^{N} J\sigma_i^z\sigma_{i+1}^z + h\sigma_i^x + g\sigma_i^z$$



Adiabatic spectroscopy

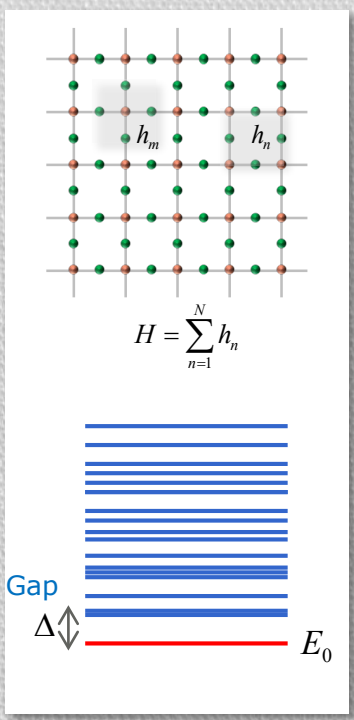


VQAA



GROUND STATE

Heuristic algorithms



- Adiabatic algorithm for local Hamiltonians

Promise: Lower bound to the gap

$$\delta \leq \Delta(t)$$

- Standard: $\tau = O(N\delta^{-3}\varepsilon^{-1})$

  Jansen, Ruskai, Seiler (2007)

- Sequential: $\tau = O(\delta^{-3}\mathrm{polylog}(N/\varepsilon\delta))$

  Ge, Molnar, JIC (2017)
  Molnar, Schuch, JIC (in preparation)

For a NISQ, it gives the circuit depth

QUANTUM ALGORITHMS:
Finite energies / temperatures

Lu, Banuls, JIC, PRXQuantum (2020)

FINITE TEMPERATURE

- We want to compute $\langle O \rangle = \mathrm{tr}(\rho O)$

Microcanonical

Energy spectrum

Canonical

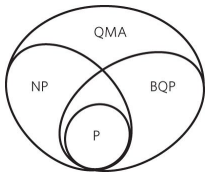
Energy spectrum

- Exponential, in general:

Kempe, Kitaev, Regev, SIAM 5, 1070 (2006)

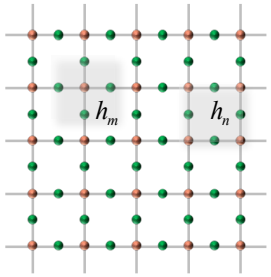
Temme et al, Nature 471, 87 (2011)
Mota et al, Nat. Phys. 16, 205 (2020)
Cohn et al, arXiv:1812.03607

They include the $T=0$ case

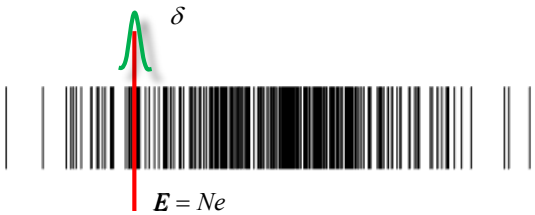


However, starting from some temperature/ energy, this may change

FINITE ENERGIES



PROBLEM:



Formulation (not precise):

- Fix the energy density: e
- Take an observable: O
- Compute $\langle \Psi | O | \Psi \rangle$

  For some Ψ with $\langle \Psi | H | \Psi \rangle = E$

  $\langle \Psi | (H - E)^2 | \Psi \rangle = \delta$

  with some prescribed precision, ε and variance δ

- **How does the computational time scale with N?**

  and ε and δ?

*For physically relevant problems, $\delta = O(1/N)$

Dymarsky, Liu, PRE **99**, 010102 (2019).

FINITE ENERGIES

Classical algorithms

Finite energies: Tensor networks (in 1D)

Banuls, Huse, JIC (2020)

- To compute expectation values of a state with a variance δ

$$\tau \sim \min\left[\exp(1/\delta), \exp(N)\right]$$

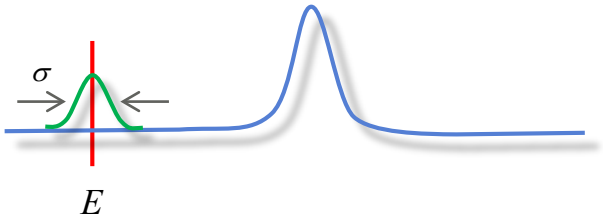
- To obtain relevant information, we need $\delta \sim 1/N$

➡ Classical algorithms require exponential time

Quantum algorithm:

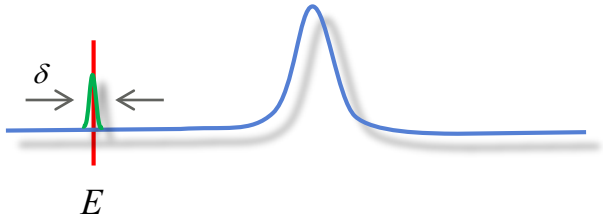
Lu, Banuls, JIC (2020)

1. Take a state that is easy to prepare



restriction

2. Apply a spectral filter to decrease the variance



$$|\Psi\rangle = G_\delta(H)\,|p\rangle$$

$$G_\delta(H) = e^{-(H-E)^2/\delta^2} = \sum c_m e^{iEt_m} e^{-iHt_m}$$

3. Do not create the state:

Time series: Somma et al, PRA 65, 042323 (2002)

$$\langle O\rangle = \frac{\langle\Psi\,|\,O\,|\,\Psi\rangle}{\langle\Psi\,|\,\Psi\rangle}$$

Use the quantum simulator to obtain quantities needed to compute the observables

$$a(t) = \langle p\,|\,e^{-iHt}\,|\,p\rangle$$

$$b(t_n, t_m) = \langle p\,|\,e^{iHt_n} O e^{-iHt_m}\,|\,p\rangle$$

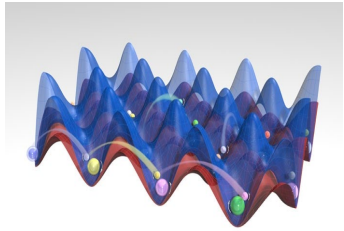
RETRIEVING $a(t) = \langle p | e^{-iHt} | p \rangle$

With an analog quantum simulator:

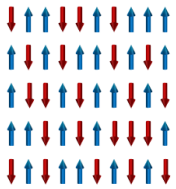
- Measure: $|a(t)|^2$

it can be computed classically

For many problems, $a(t) = |a(t)| e^{i\phi(t)}$

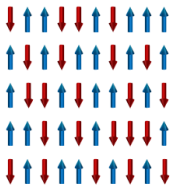


Prepare state with E_0:



Evolve for different times t_n

Measure the spins



FINITE ENERGIES

Summary

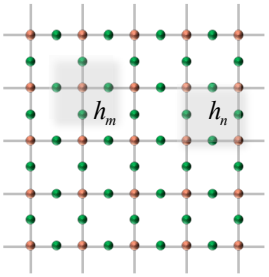
PROBLEM:

$\langle e|O|e\rangle$

EFFICIENCY:

- Time: $\tau = \mathrm{poly}(N, 1/\delta, 1/\varepsilon)$
- Efficient to compute thermodynamic properties: $\delta \geq 1/N$

FINITE TEMPERATURE



PROBLEM

Finite temperature

$$\rho = \frac{e^{-H/kT}}{Z}$$

More precise formulation:

- Fix the temperature: T
- Take an observable: O
- Compute $\langle O \rangle = \mathrm{tr}(\rho O)$
  with some prescribed precision, ε
  where $\rho = \frac{e^{-H/kT}}{Z}$
- How does the computational time scale with N?
  and ε and T?
- Heuristic algorithm that overcomes the sign problem

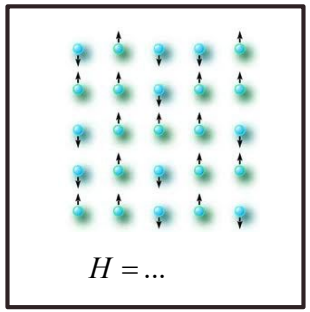
QUANTUM MONTE CARLO

Classical algorithm

THERMAL EQUILIBRIUM:

- Sample configuration n with probability P_n

$$\mathrm{tr}(O\rho) = \frac{\sum_n \langle n | e^{-H/T} | n \rangle \, O_n}{\sum_n \langle n | e^{-H/T} | n \rangle} = \frac{\sum_n P_n \, O_n}{\sum_n P_n}$$



$$\rho = \frac{e^{-H/kT}}{\mathrm{tr}\left[e^{-H/kT} \right]}$$

- We need to compute $P_n = \langle n | e^{-H/T} | n \rangle$

  This is a many-body calculation

- Approximate

$$P_n = \sum_{n_1, n_2, \ldots, n_M} Q_{n,n_1} Q_{n_1,n_2} \ldots$$

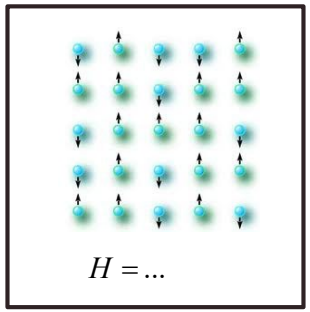
- If $Q_{n,m} \geq 0$, then we can sample $n_1, n_2, \ldots$

- Heuristics: $\tau \propto \frac{f(N)}{\varepsilon^2}$

QUANTUM MONTE CARLO

Classical algorithm

THERMAL EQUILIBRIUM:



- Sample configuration n with probability P_n

$$\mathrm{tr}(O\rho) = \frac{\sum_n \langle n | e^{-H/T} | n \rangle \, O_n}{\sum_n \langle n | e^{-H/T} | n \rangle} = \frac{\sum_n P_n \, O_n}{\sum_n P_n}$$

- We need to compute $P_n = \langle n | e^{-H/T} | n \rangle$

  This is a many-body calculation

- Approximate

$$P_n = \sum_{n_1, n_2, \ldots, n_M} Q_{n,n_1} Q_{n_1,n_2} \ldots$$

SIGN PROBLEM: This is not possible, in general

With sign problem, the computational time is exponential

FINITE TEMPERATURE

Heuristic Algorithms

CANONICAL:

Lu, Banuls, JIC (2020)

$$\langle O \rangle = \frac{\mathrm{tr}(Oe^{-H/T})}{\mathrm{tr}(e^{-H/T})}$$

$$\rho = \frac{e^{-H/kT}}{Z}$$

- It is based on (classical) Monte-Carlo methods
- Uses the QC as a subroutine
- Circumvents the sign problem

$$\langle O \rangle = \frac{\mathrm{tr}(Oe^{-H/T})}{\mathrm{tr}(e^{-H/T})} = \frac{\sum_E \sum_p P_p(E) \langle \Psi_p | O | \Psi_p \rangle}{\sum_E \sum_p P_p(E)}$$

$$a(t) = \langle p | e^{-iHt} | p \rangle$$

$$b(t_n, t_m) = \langle p | e^{iHt_n} O e^{-iHt_m} | p \rangle$$

As long as there are easily preparable states around the mean energy

FINITE TEMPERATURE
Heuristic Algorithms

CANONICAL:

Lu, Banuls, JIC (2020)

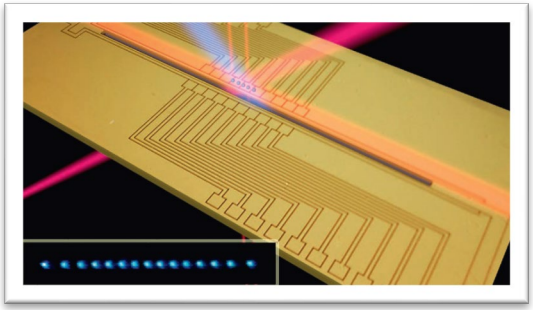
$$\langle O \rangle = \frac{\mathrm{tr}(Oe^{-H/T})}{\mathrm{tr}(e^{-H/T})}$$

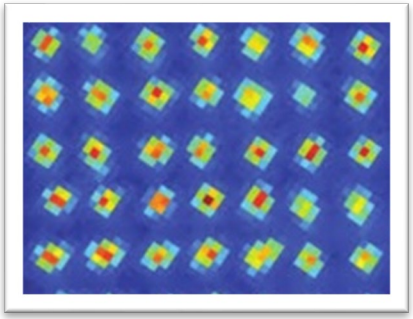
- It is based on (classical) Monte-Carlo methods
- Uses the QC as a subroutine
- Circumvents the sign problem

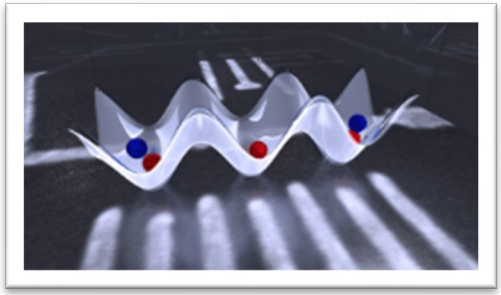
It can be used in analog quantum computers and NISQ devices

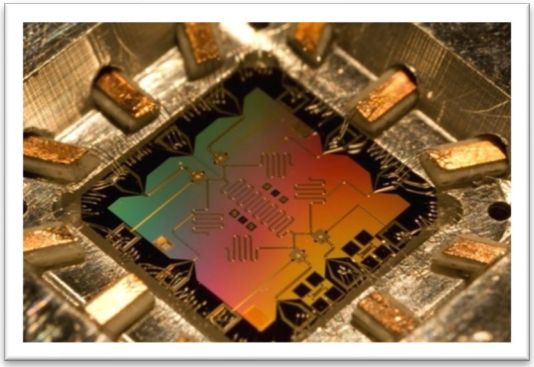
ANALOG vs DIGITAL QUANTUM COMPUTERS

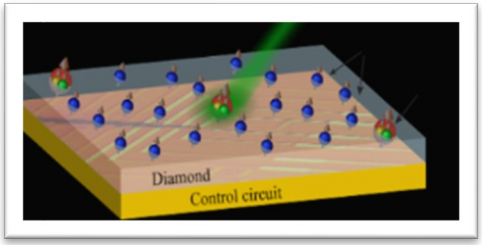
ANALOG vs DIGITAL

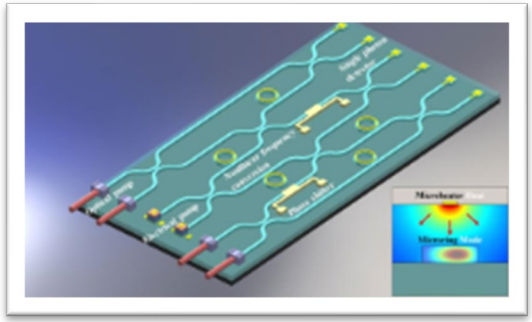












$$|\Psi\rangle = c_{0,0,\ldots,0}\,|0,0,\ldots,0\rangle + c_{0,0,\ldots,1}\,|0,0,\ldots,1\rangle + \ldots c_{1,1,\ldots,1}\,|1,1,\ldots,1\rangle$$

ANALOG vs DIGITAL

ADVANTAGES/DISADVANTAGES

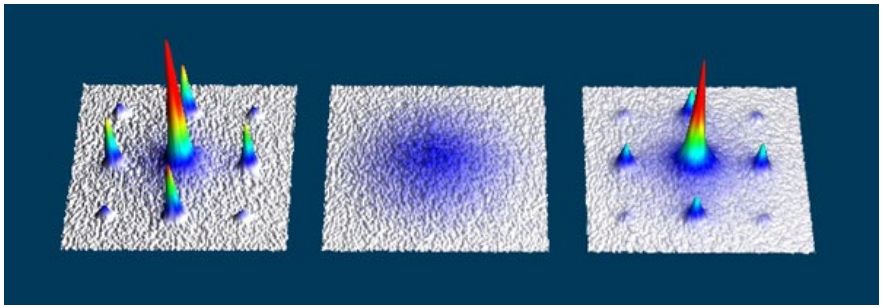
- Not universal
- No error correction
- Easier to build
- Errors

Errors are extensive

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

Observables are intensive

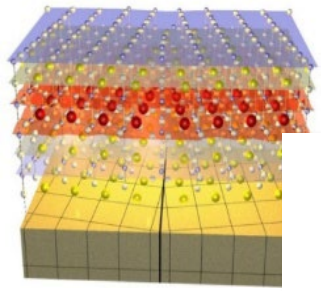
$$m = \frac{1}{N} \sum_n \langle s_n^z \rangle$$



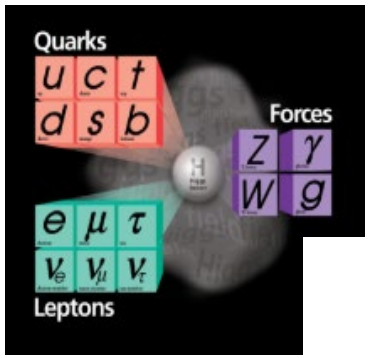
Bloch, Esslinger, Greiner, Hänsch (2002)

ATOMS IN OPTICAL LATTICES

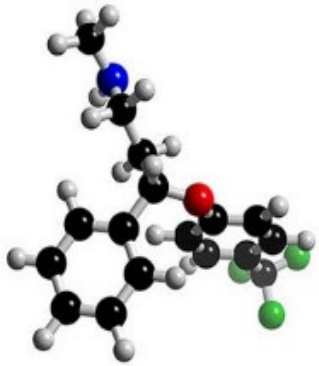
COLD ATOMS IN OPTICAL LATTICES



Condensed matter
Hubbard and spin

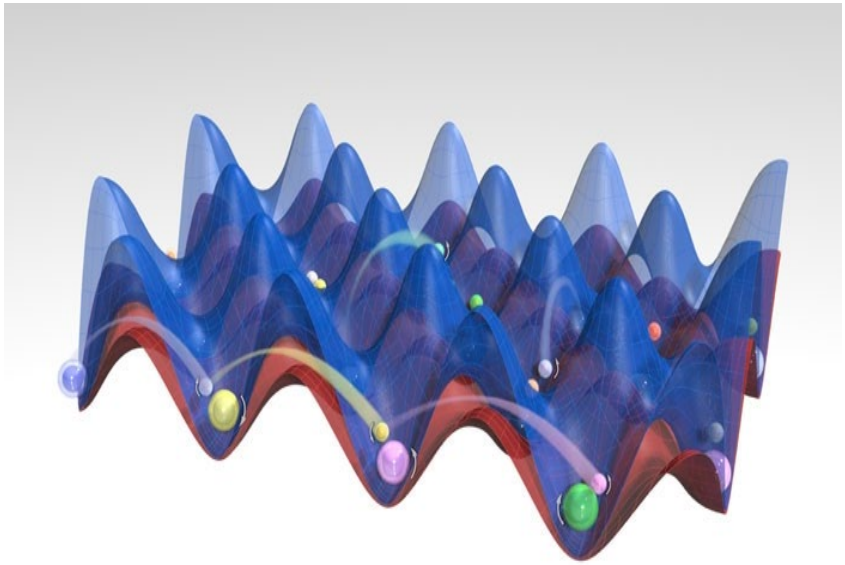


High-energy Phy
Lattice gauge th



Quantum chemistry:

CONDENSED MATTER PHYSICS



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

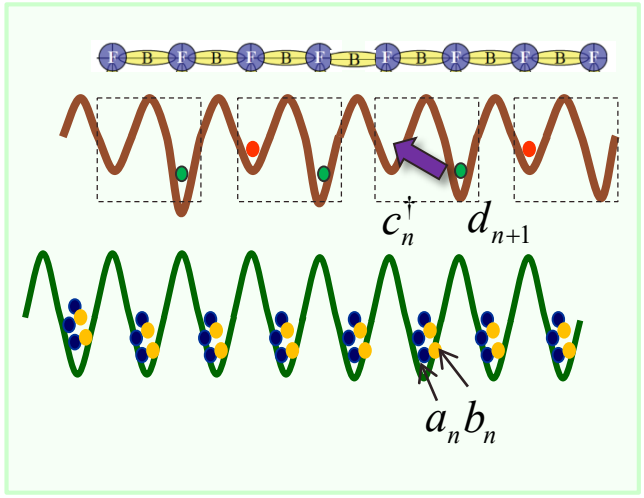
Bosons, Fermions, Spins, Geometry, Dimensions, …

Jaksch et al (1998)

HIGH-ENERGY PHYSICS

- 1+1 dimensioins

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

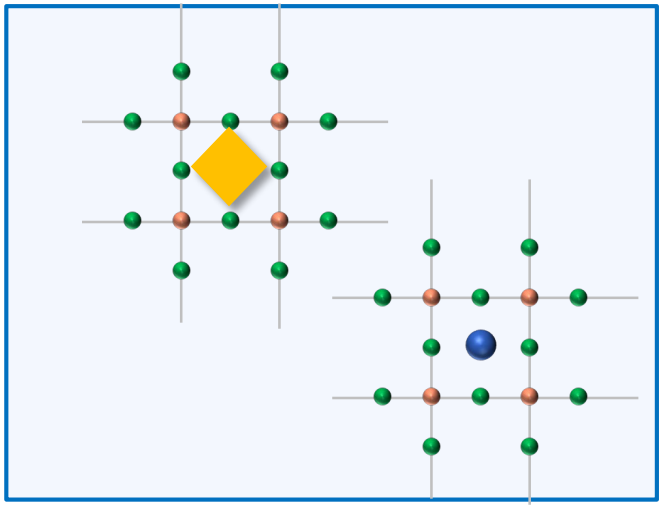


JIC, Maure, Pachos (2010)

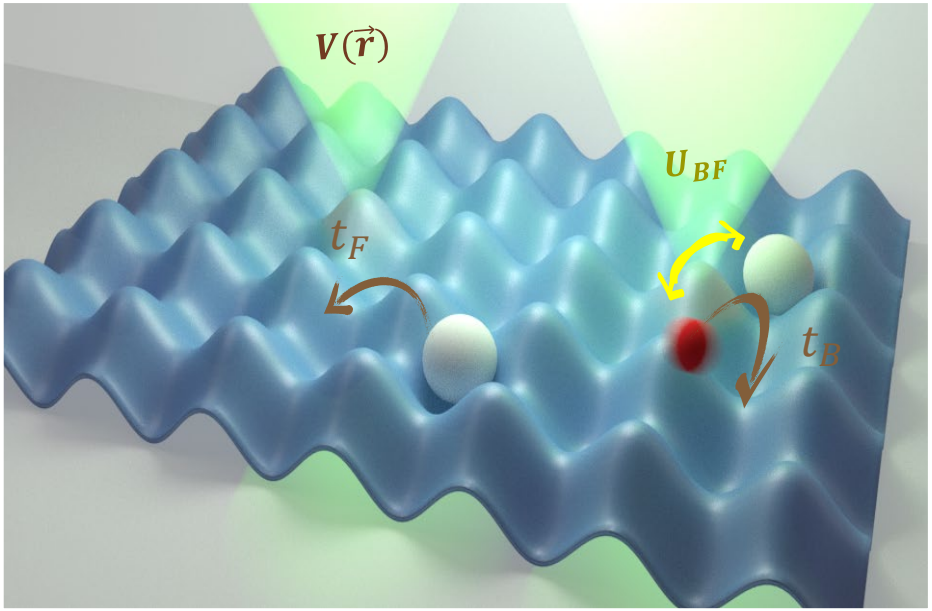
- Higher dimensions:

Main challenge: plaquette terms

- Perturbation theory
- Stroboscopic interactions



QUANTUM CHEMISTRY



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

Fermions:
Single particle:
lattice + laser

Fermions:
Mediated by boson

Argüello, Gonzalez, Shi, Zoller, JIC (2019)

QUANTUM SIMULATION

GOALS:

- Solve specific models
- Provide understanding
- Curiosity-driven research
- Benchmark theory

CHALLENGES:

- Experimental / technological
- New algorithms

  Adaptation to NISQ and analog
- Connect with industrial interests

MPQ Theory
Group Workshop
Jan 2021

Qoronolympics