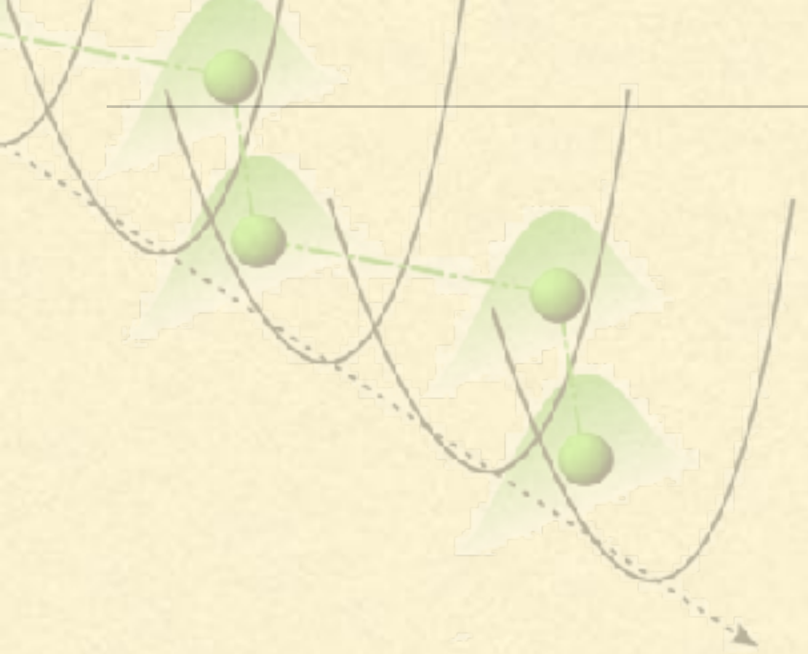
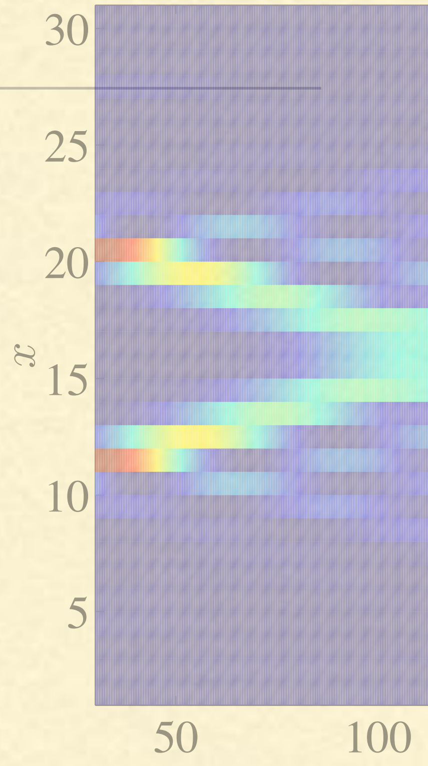
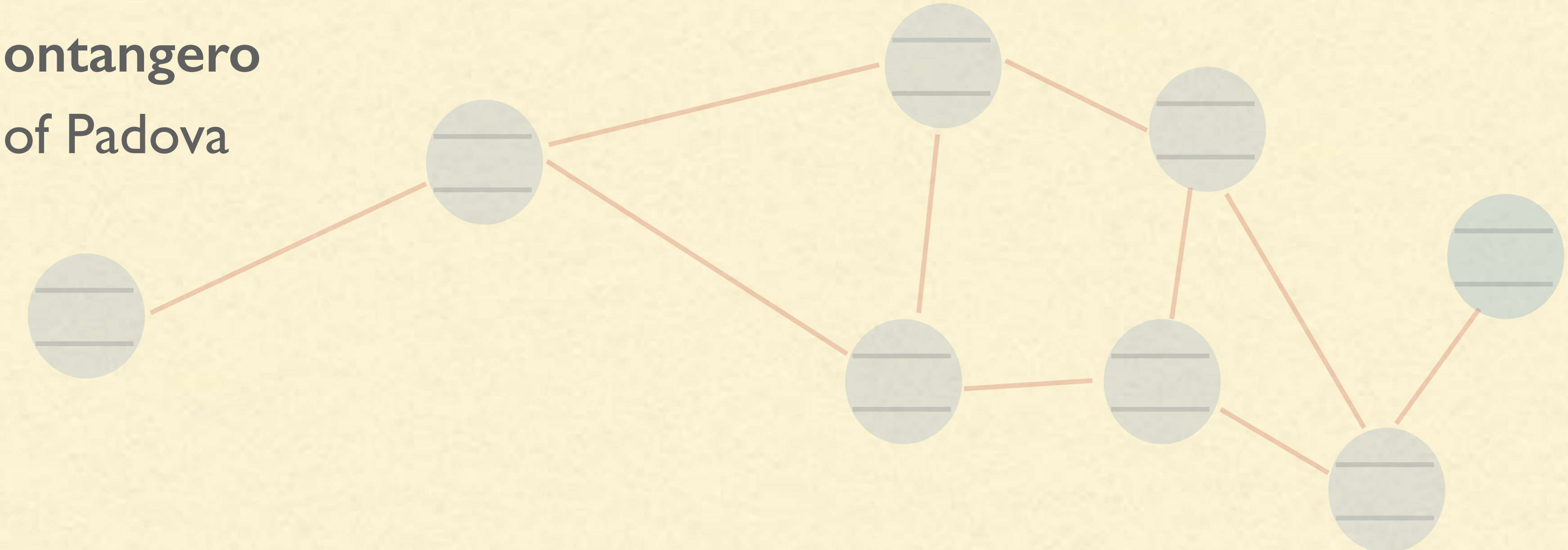
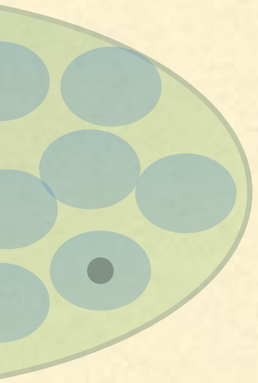




EXTREME SIMULATIONS FOR QUANTUM TECHNOLOGIES

Simone Montangero
University of Padova





Verona 25/10/18

(QUANTUM) TECHNOLOGIES

1800

1950

2000

Thermodynamics

Electromagnetism

Quantum mechanics

Quantum science

Engines

Circuits

Lasers, semiconductors..

2nd quantum revolution

Hz

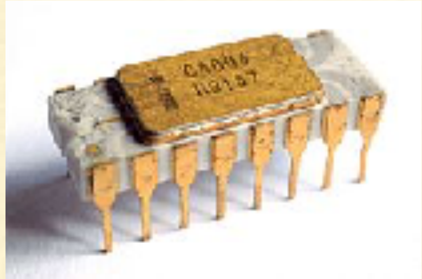
KHz

GHz

???

Babbage difference engine

Zuse's Z3



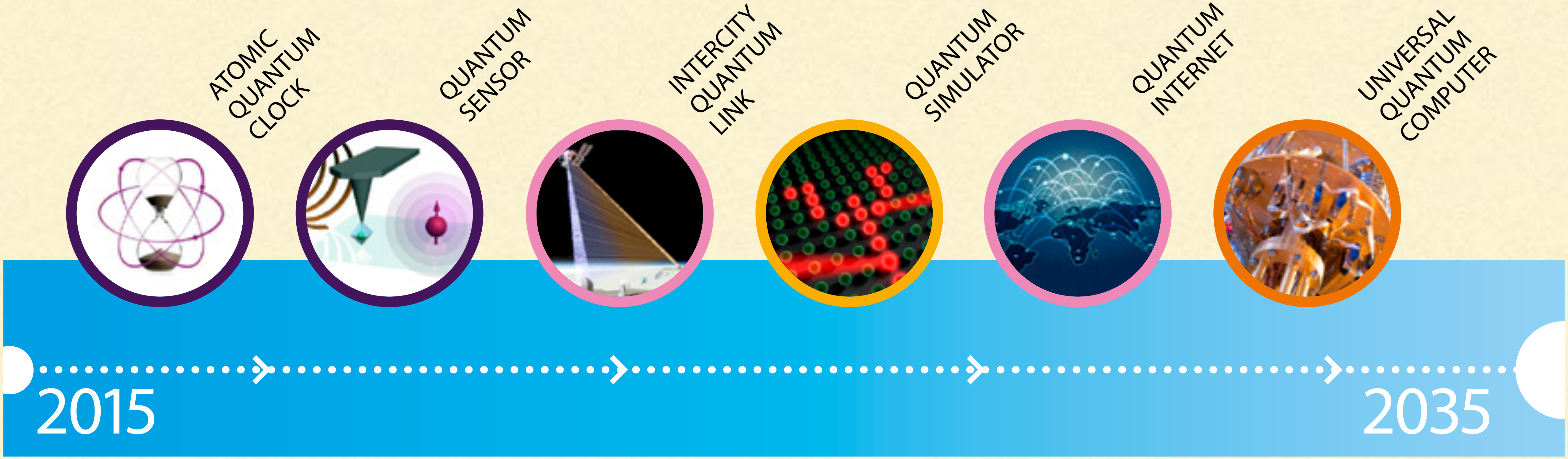
Intel 4004

Numerical solution of PDEs

Lattice calculations
Density Functional theory
Tensor networks…

2ND QUANTUM REVOLUTION

Quantum Technologies Timeline



ATOMIC QUANTUM CLOCK

QUANTUM SENSOR

INTERCITY QUANTUM LINK

QUANTUM SIMULATOR

QUANTUM INTERNET

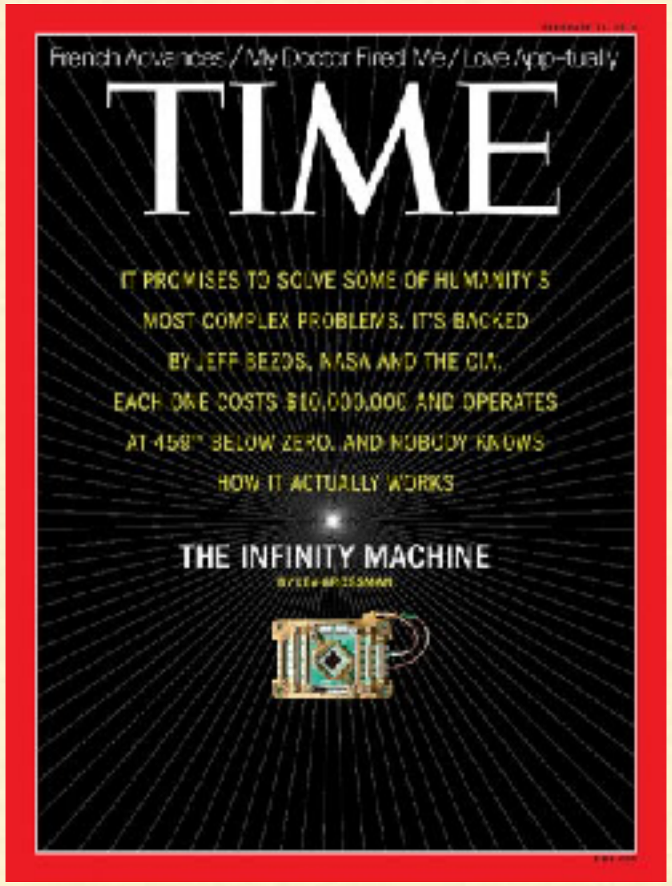
UNIVERSAL QUANTUM COMPUTER

2015

2035

Quantum Manifesto (2015)

CURRENT EFFORTS



French Advances / My Doctor Fired Me / Love App-tually

TIME

IT PROMISES TO SOLVE SOME OF HUMANITY'S MOST COMPLEX PROBLEMS. IT'S BACKED BY JEFF BEZOS, NASA AND THE CIA. EACH ONE COSTS $10,000,000 AND OPERATES AT 458° BELOW ZERO. AND NOBODY KNOWS HOW IT ACTUALLY WORKS

THE INFINITY MACHINE

SEPTEMBER 13, 2016

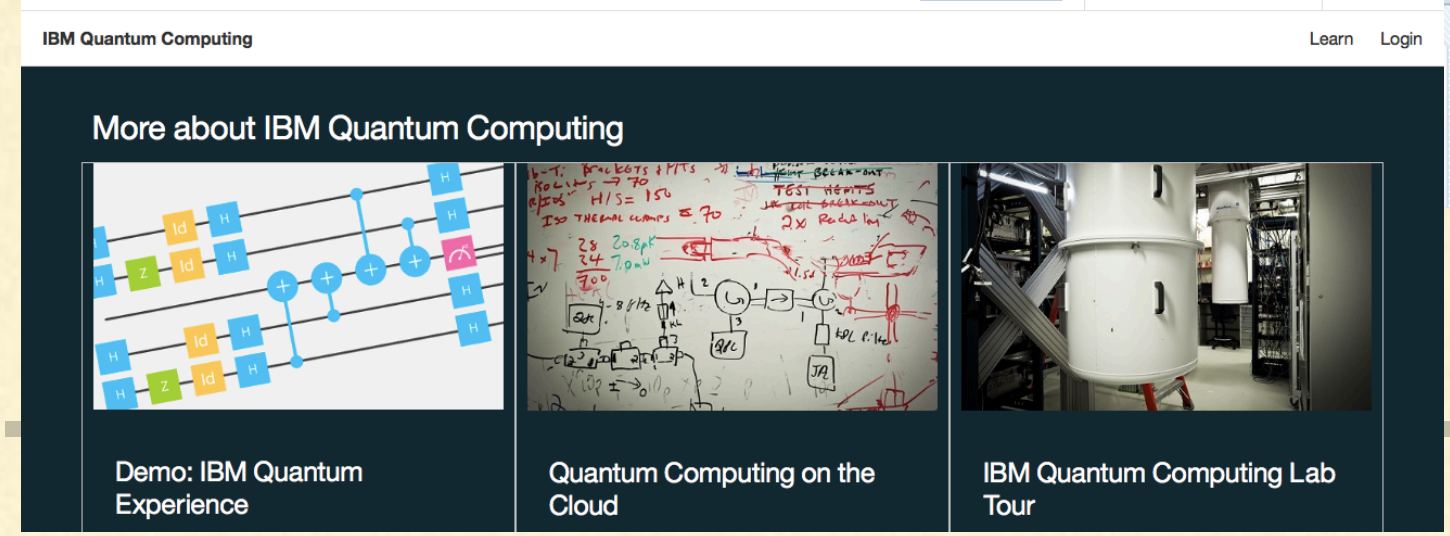
19 Corporations Working On Quantum Computing

DIGITAL SINGLE MARKET

Digital Economy & Society

European Commission > European Commission will launch €1 billion quantum technologies flagship

European Commission will launch €1 billion quantum technologies flagship



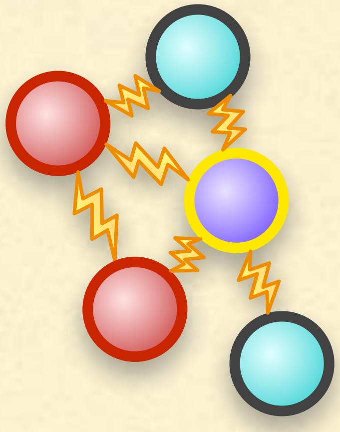
IBM Quantum Computing

More about IBM Quantum Computing

- Demo: IBM Quantum Experience
- Quantum Computing on the Cloud
- IBM Quantum Computing Lab Tour

QUANTUM SIMULATORS

System



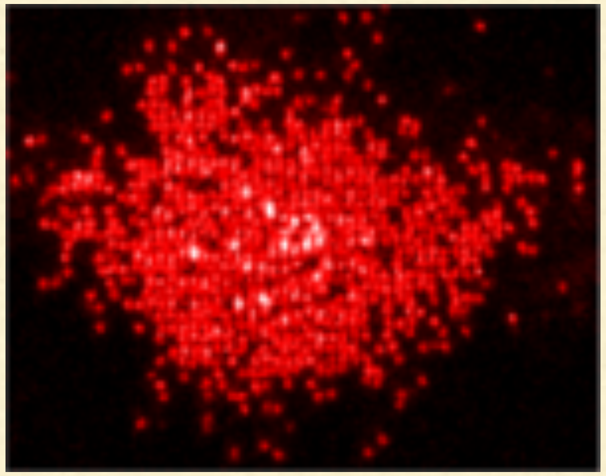
Model

$$H = \sum \sigma_i^z \sigma_{i+1}^z + \sum_i \sigma_x$$

Energy function

Simulator

classical



quantum

- Original Feynman’s motivation for QC
- Cold atoms, trapped ions, superconductors…
- Adiabatic quantum computation

J. I. Cirac and P. Zoller, Nat. Phys. (2012).

CLASSICAL PROBLEMS AND AQC

Partitioning problem

$$S = \{n_1, \ldots, n_N\}$$

Is it possible to divide it in two sets of equal value?

NP-complete

Define the energy function:

$$H = A\left(\sum_{i=1}^{N} n_i s_i\right)^2$$

$$s_i = \{\uparrow, \downarrow\}$$

For every configuration H>0

If the ground state is s.t.

$$E_{gs} = 0$$

the solution exists!

If $E_{gs} > 0$

the mismatch is minimized (NP-hard)

Graph partitioning

Complete subgraph finding (clique)

Binary integer programming

Covering and packaging problems

k-sat problems

Minimal maximal matching…

A. Lucas, Front. Phys. 2, 5 (2014)

ALL-TO-ALL TO LGT MAPPING

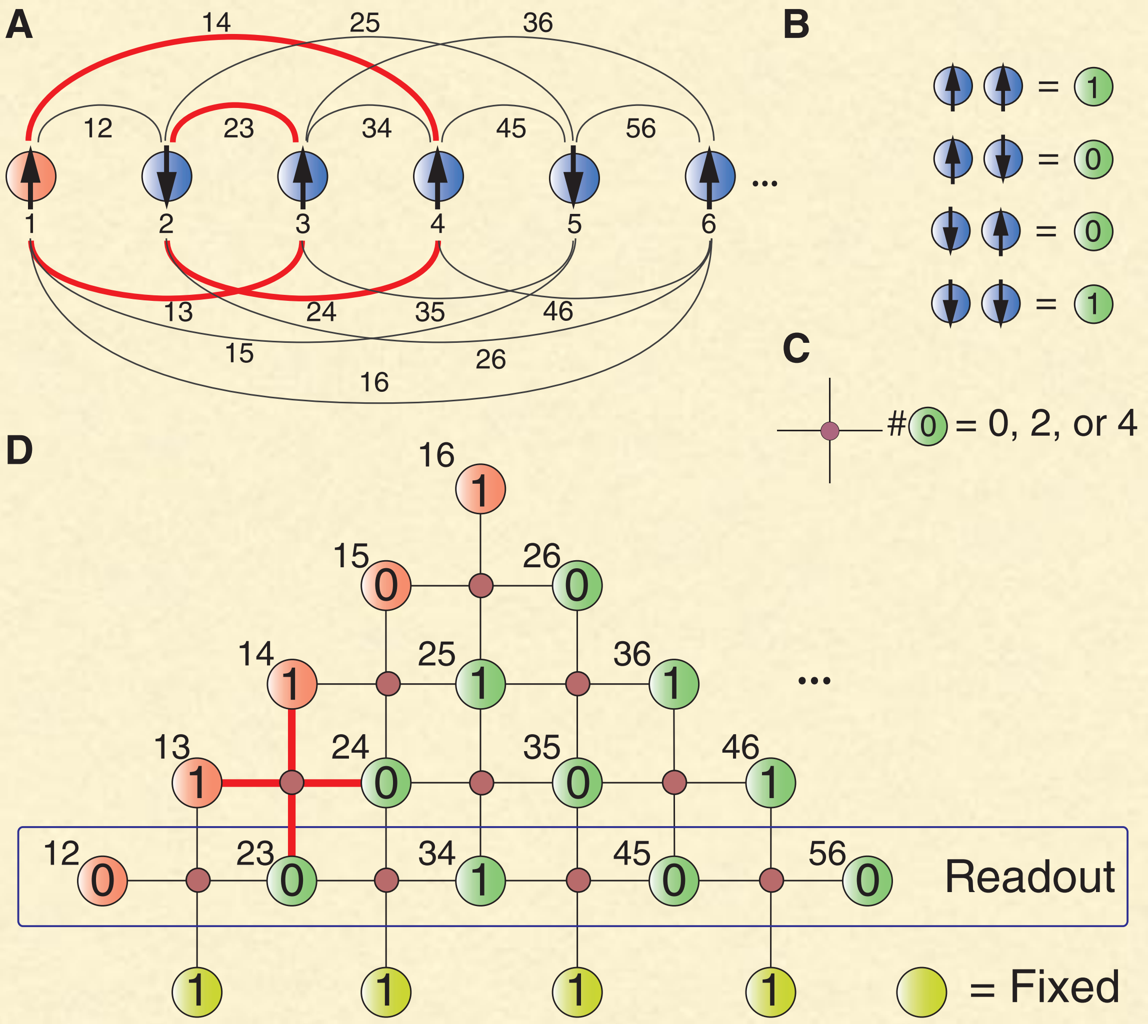
$$H_I = \sum \sigma_x^{[k]}$$

$$H_F = \sum_{i<j} V^{[i,j]} \sigma_z^{[i]} \sigma_z^{[j]}$$

$$\Big\downarrow$$

$$H_F = \sum_{k=1}^{K} f^{[k]} \sigma_z^{[k]} +$$

$$H_C = -\sum_{p=1}^{P} c^{[p]} \sigma_z^{[k_1]} \sigma_z^{[k_2]} \sigma_z^{[k_3]} \sigma_z^{[k_4]}$$



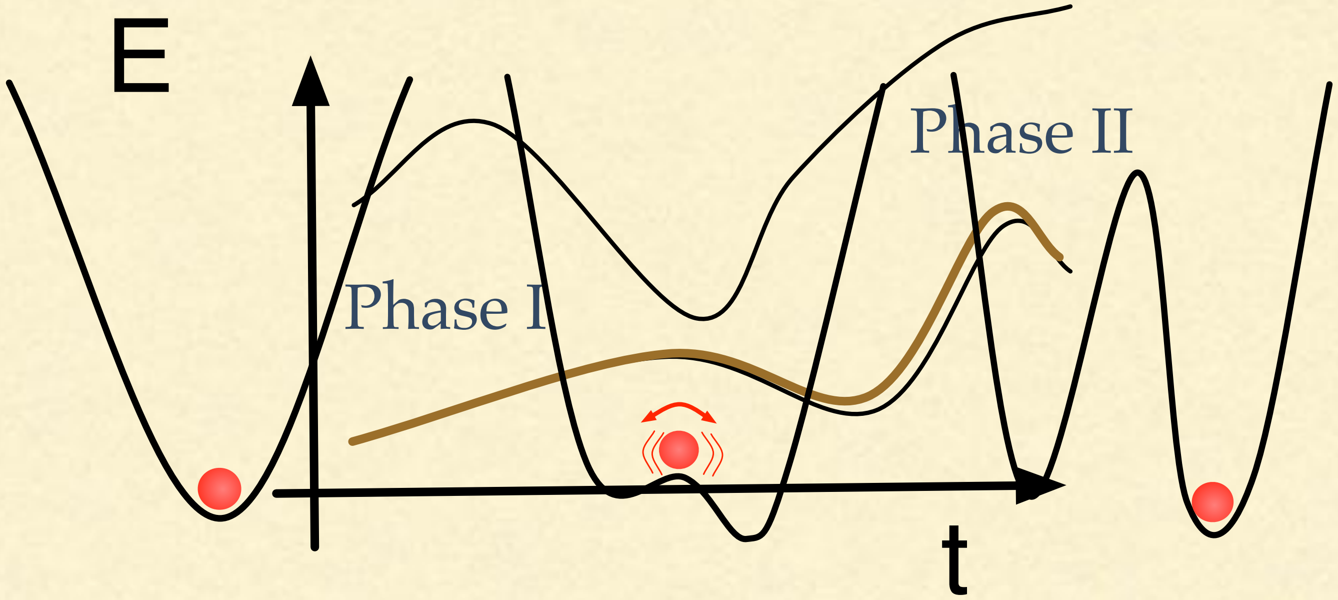
W. Lechner, P. Hauke, and P. Zoller, Sci. Adv.. (2015).

ADIABATIC QUANTUM COMPUTATION

- Preparation of the system in an "easy" state $\downarrow\downarrow\downarrow\ldots\downarrow\downarrow\downarrow$
- Change of a system parameter to reach another ground state which encodes the problem solution $\downarrow\uparrow\downarrow\ldots\downarrow\downarrow\uparrow$

$$H_0 = -h_0 \sum_{i=1}^{N} s_i \qquad s_i = \{\uparrow, \downarrow\} \qquad H(t) = \left(1 - \frac{t}{T}\right) H_0 + \frac{t}{T} H_P$$

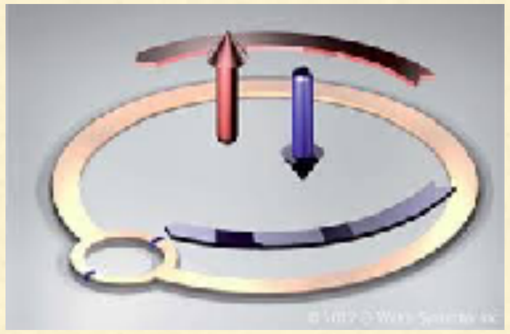
Slow



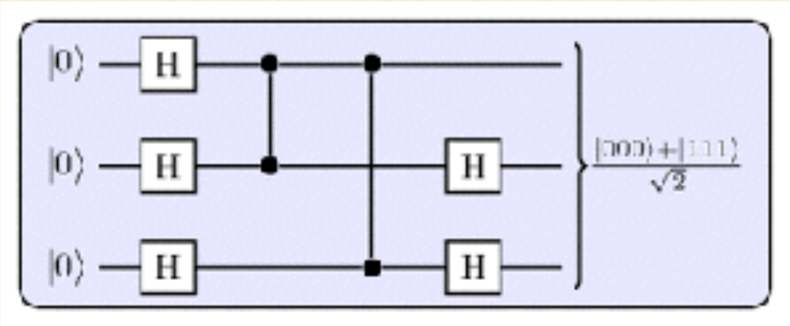
Adiabatic strategy

WHAT IS NEEDED?

Quantum hardware



Algorithms/Protocols



Validation and certification

Calls for:

- Classical numerical simulations
- Optimisation
- Software engineering

CHALLENGES?

System description

Control

NUMERICAL SIMULATIONS

The art of high-performance computing

MANY-BODY WAVE FUNCTION

$$|\psi\rangle = \psi_0|0\rangle + \psi_1|1\rangle$$

N=1

$$|\psi\rangle = \psi_{00}|00\rangle + \psi_{10}|10\rangle + \psi_{01}|01\rangle + \psi_{11}|11\rangle$$

N=2

$$|\psi\rangle = \psi_{000}|000\rangle + \psi_{010}|010\rangle + \psi_{001}|001\rangle + \psi_{011}|011\rangle + \psi_{100}|100\rangle + \psi_{110}|110\rangle + \psi_{101}|101\rangle + \psi_{111}|111\rangle$$

N=3

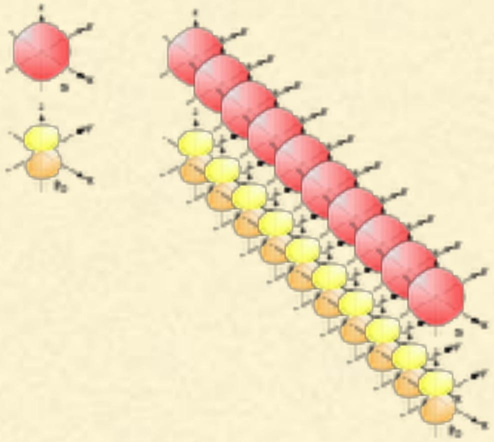
$$\begin{aligned}|\psi\rangle =\, &\psi_{0000}|0000\rangle + \psi_{0010}|0010\rangle + \psi_{0001}|0001\rangle + \psi_{0011}|0011\rangle + \psi_{0100}|0100\rangle + \psi_{0110}|0110\rangle + \psi_{0101}|0101\rangle + \\ &\psi_{0111}|0111\rangle + \psi_{1000}|1000\rangle + \psi_{1010}|1010\rangle + \psi_{1001}|1001\rangle + \psi_{1011}|1011\rangle + \psi_{1100}|1100\rangle + \psi_{1110}|1110\rangle + \\ &\psi_{1101}|1101\rangle + \psi_{1111}|1111\rangle\end{aligned}$$

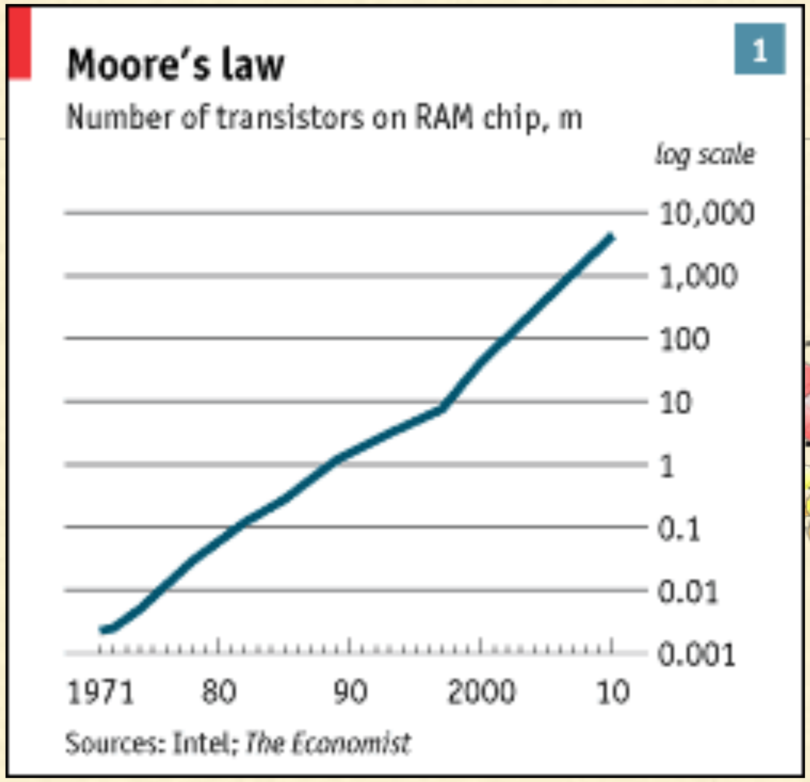
N=4

$$|\psi\rangle = \sum \psi_{\alpha_1,\alpha_2,\ldots\alpha_N}|\alpha_1, \alpha_2, \ldots \alpha_N\rangle$$

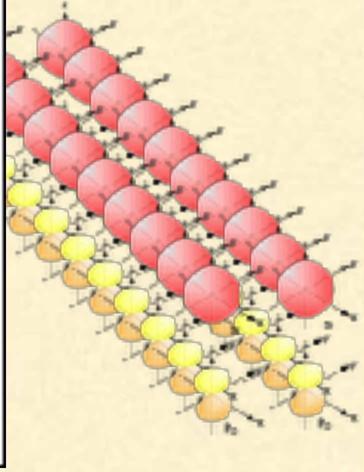
MANY-BODY WAVE FUNCTION

N=11



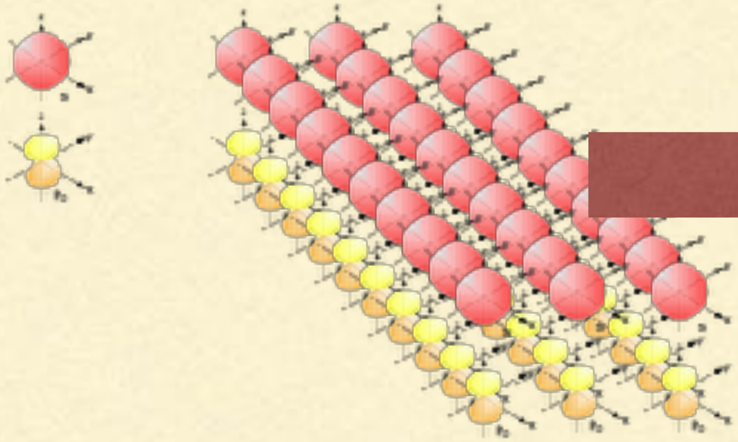


Sources: Intel; *The Economist*



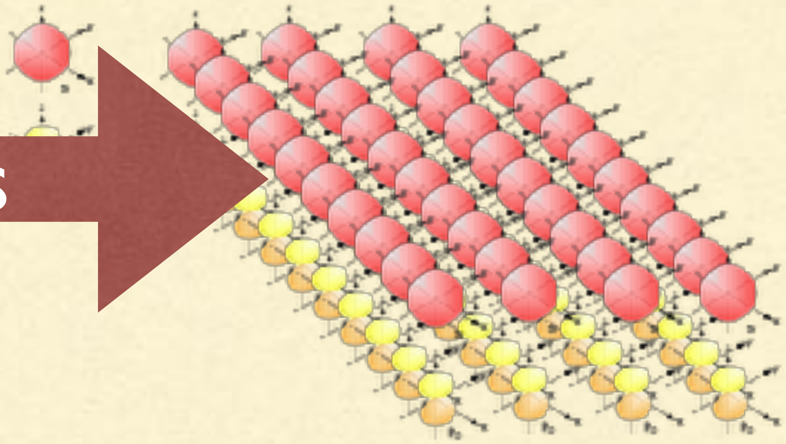
1GB

N=31



~20 years

N=41

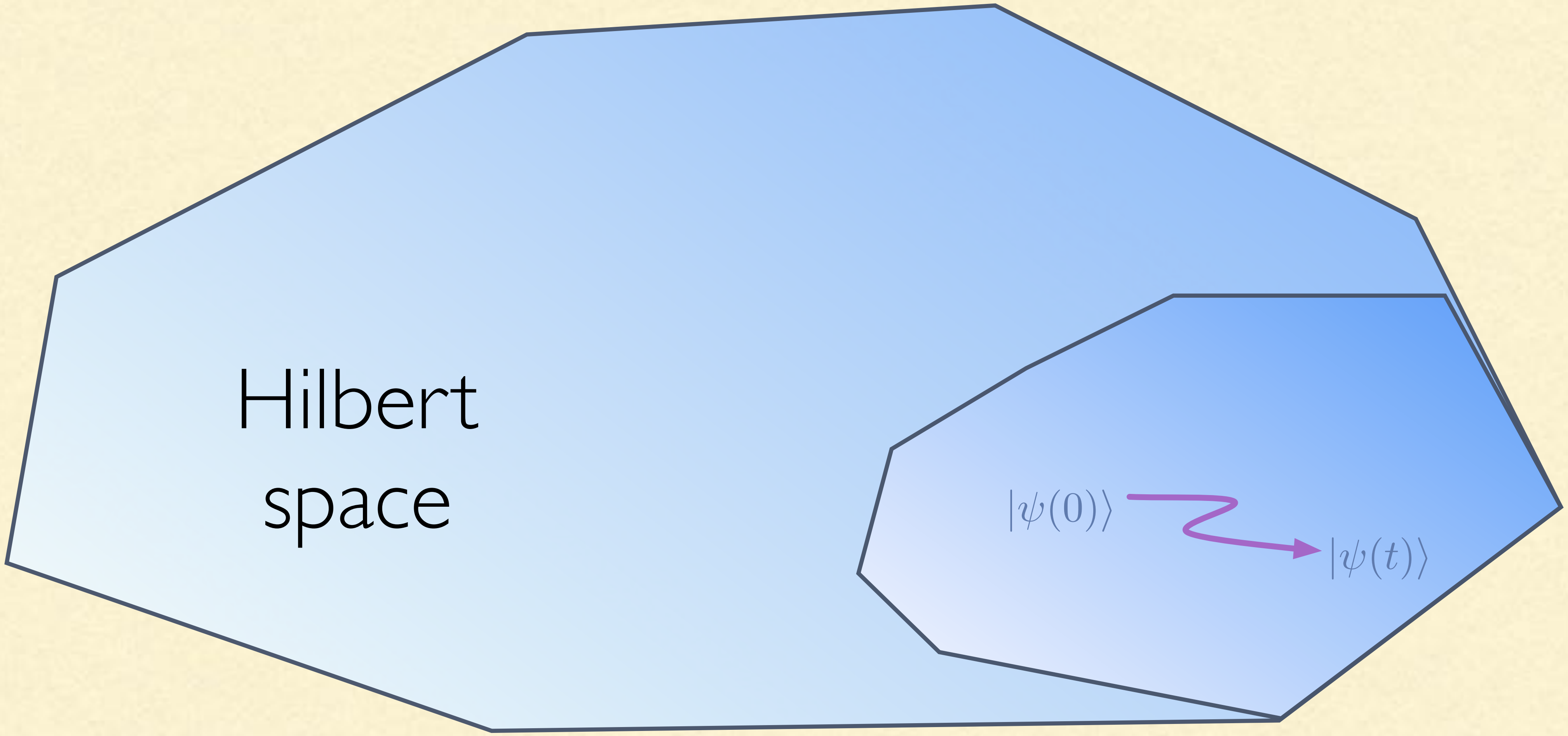


1PB

$$|\psi\rangle = \sum \psi_{\alpha_1,\alpha_2,\ldots\alpha_N}|\alpha_1,\alpha_2,\ldots\alpha_N\rangle$$

TENSOR NETWORK STATES

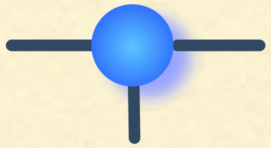
"Simple" variational Ansatz to describe faithfully interesting quantum dynamics!



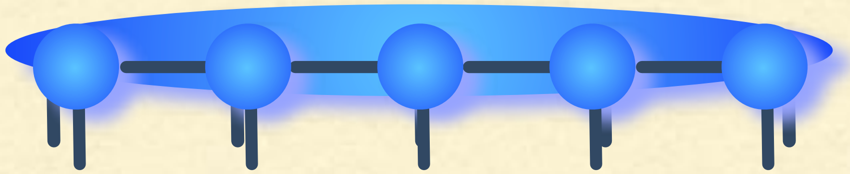
Adaptive system description tunable between mean field and exact

TENSOR NETWORKS

$A_{\alpha_i}^{\beta_i,\beta_{i+1}} \equiv$

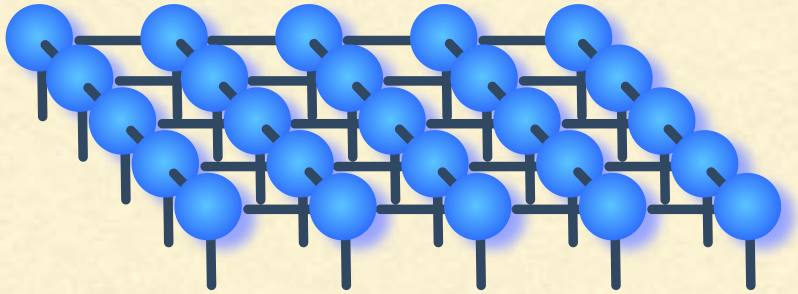


$$\psi_{\alpha_1,\alpha_2,\ldots\alpha_N} \qquad \mathcal{O}(d^N)$$

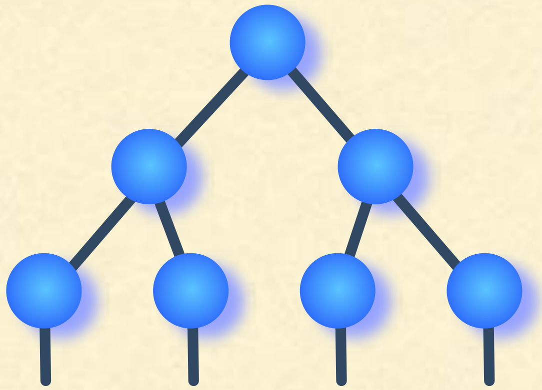


$$A_{\alpha_1}^{\beta_1} A_{\alpha_2}^{\beta_1\beta_2} \ldots A_{\alpha_N}^{\beta_{N-1}}$$

$$\mathcal{O}(Ndm^2)$$

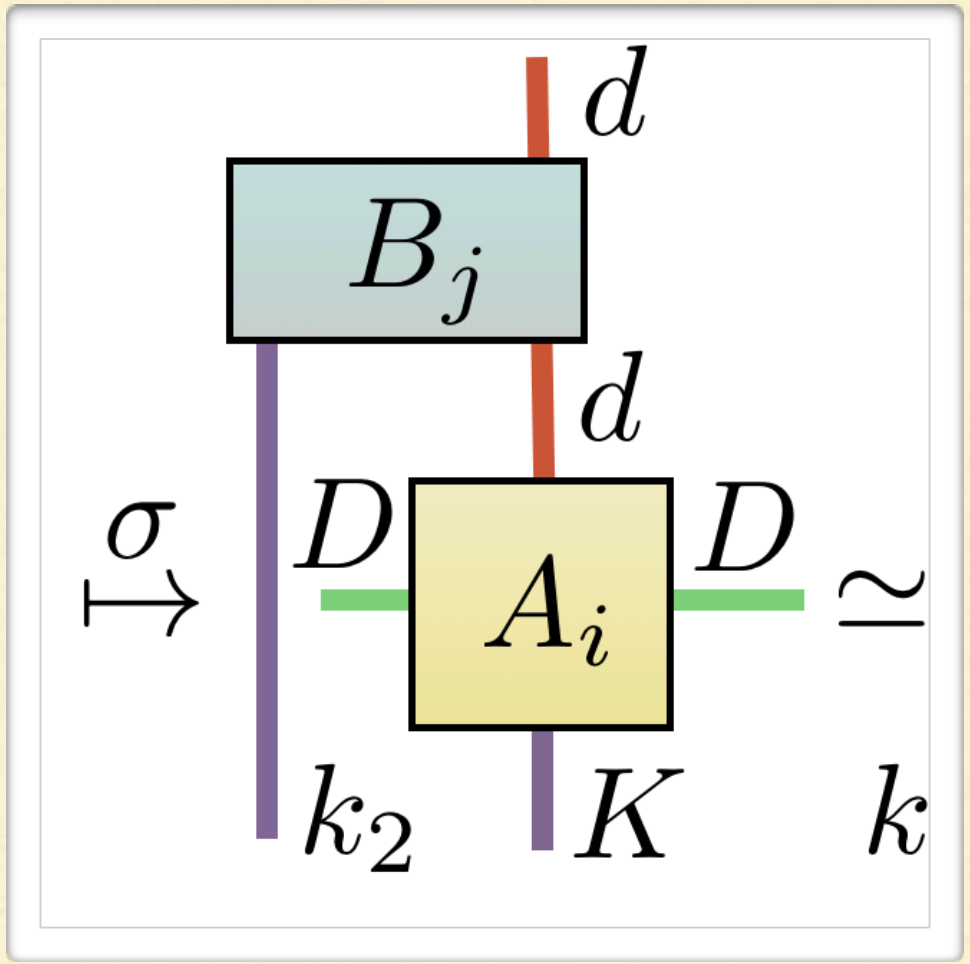


PEPS



Tree Tensor Network
(Hierarchical Tucker decomposition)

TENSOR NETWORK ALGORITHMS



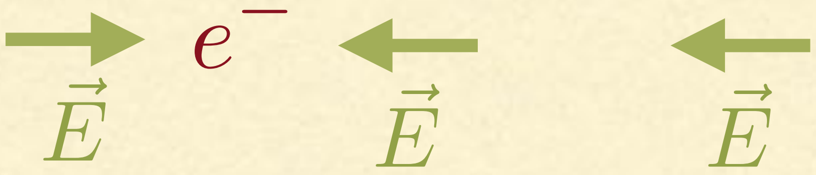
- Polynomial effort
  (state of the art in 1D)
- No sign problem
- Works also with open system
  (Lindblad master equation)
- Increasingly applied in quantum chemistry
- Recently extended to Lattice Gauge Theories

U. Schollwock, Rev. Mod. Phys. (2005)

GAUGE THEORIES

Theories with local symmetries (to be satisfied at every point)

CLASSICAL (electrodynamics)



$$\rho = \vec{\nabla} \cdot \vec{E}$$

Gauss' law

QUANTUM (QED)

$$\psi_x^\dagger \psi_x |\Psi\rangle = \Delta E_{x,x+a} |\Psi\rangle$$

Cirac, Lewenstein, Zoller, Verstraete, Reznik, QTFLAG…

LGT HAVE APPLICATIONS IN

High-energy physics

QED,
QCD, …

Condensed matter

Quantum spin ice,
Kitaev model, …

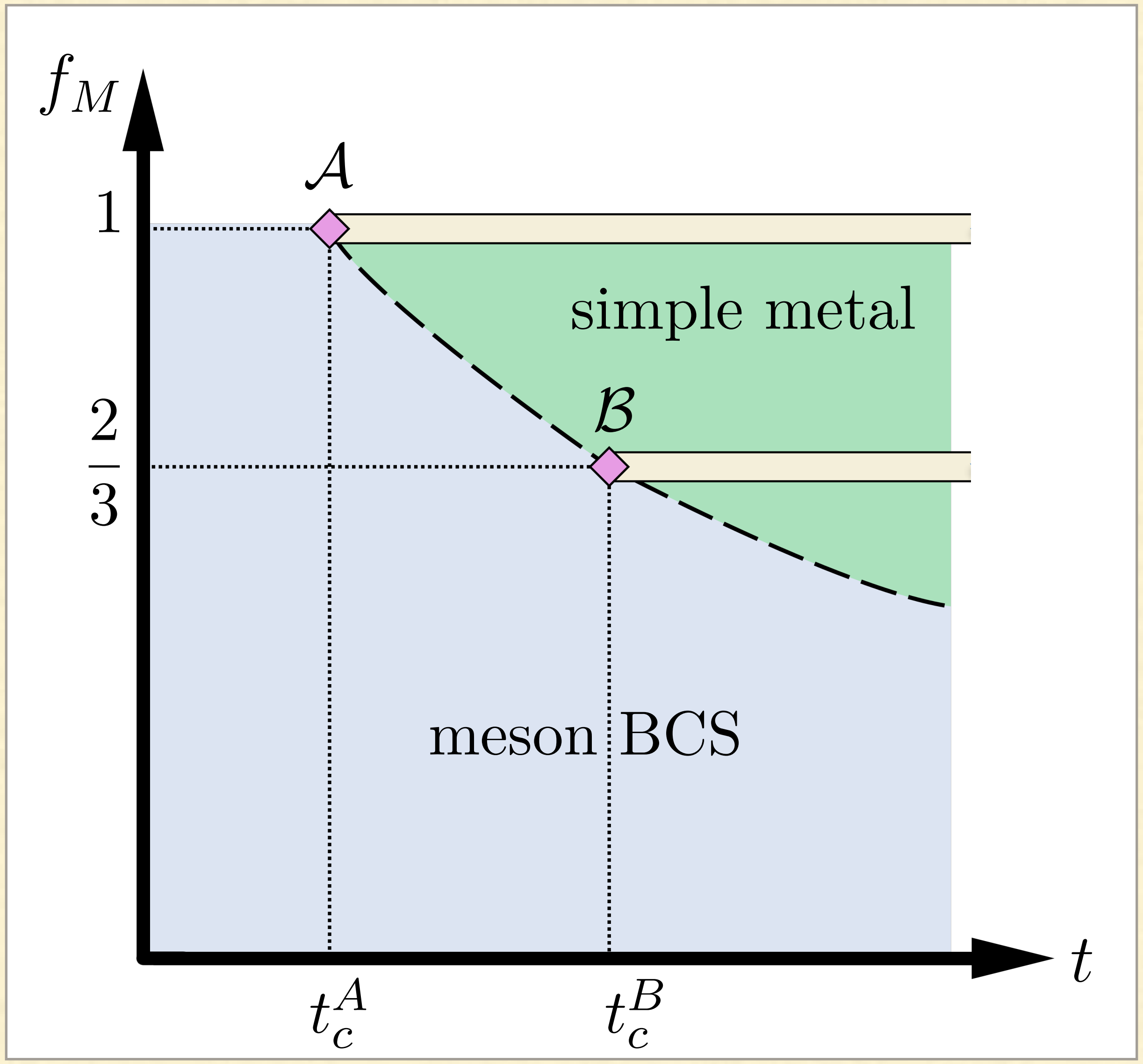
Quantum science

Quantum
simulations, …

Computer science

Adiabatic
computation

SU(2) LATTICE GAUGE THEORY



$$H = H_{\text{coupl}} + H_{\text{free}} + H_{\text{break}}$$

$$H_{\text{coupl}} = t \sum_{j=1}^{\mathrm{L}-1} \sum_{s,s'=\uparrow,\downarrow} c_{j,s}^{[M]\dagger} U_{j,j+1;s,s'} c_{j+1,s'}^{[M]} + \text{h.c.}$$

$$H_{\text{free}} = \frac{g_0^2}{2} \sum_{j=1}^{\mathrm{L}} \left[\vec{J}_{j-1,j}^{[R]}\right]^2 + \left[\vec{J}_{j,j+1}^{[L]}\right]^2$$

Phase diagram at
finite chemical potential

P. Silvi, E. Rico2 F. Tschirsich1, M. Dalmonte, and SM, Quantum 1 (2017)

ADDITIONAL APPLICATIONS

Tensor decomposition for Big Data and Optimization

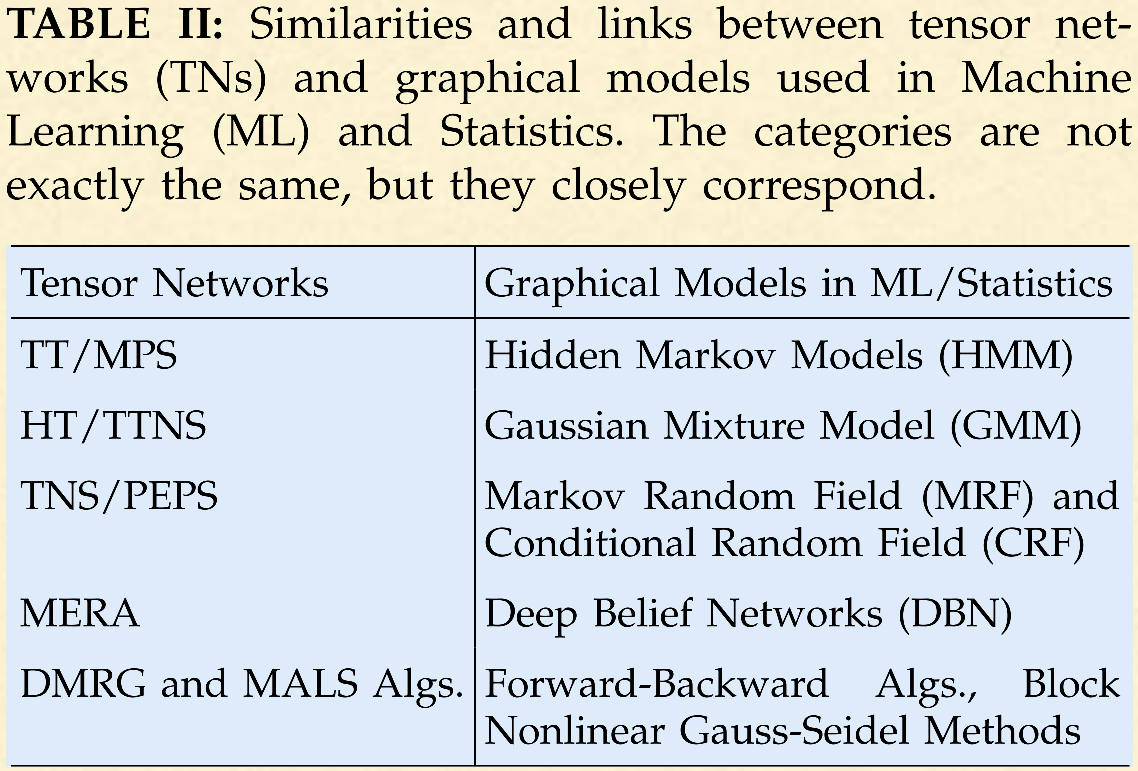


TABLE II: Similarities and links between tensor networks (TNs) and graphical models used in Machine Learning (ML) and Statistics. The categories are not exactly the same, but they closely correspond.

Tensor Networks	Graphical Models in ML/Statistics
TT/MPS	Hidden Markov Models (HMM)
HT/TTNS	Gaussian Mixture Model (GMM)
TNS/PEPS	Markov Random Field (MRF) and Conditional Random Field (CRF)
MERA	Deep Belief Networks (DBN)
DMRG and MALS Algs.	Forward-Backward Algs., Block Nonlinear Gauss-Seidel Methods

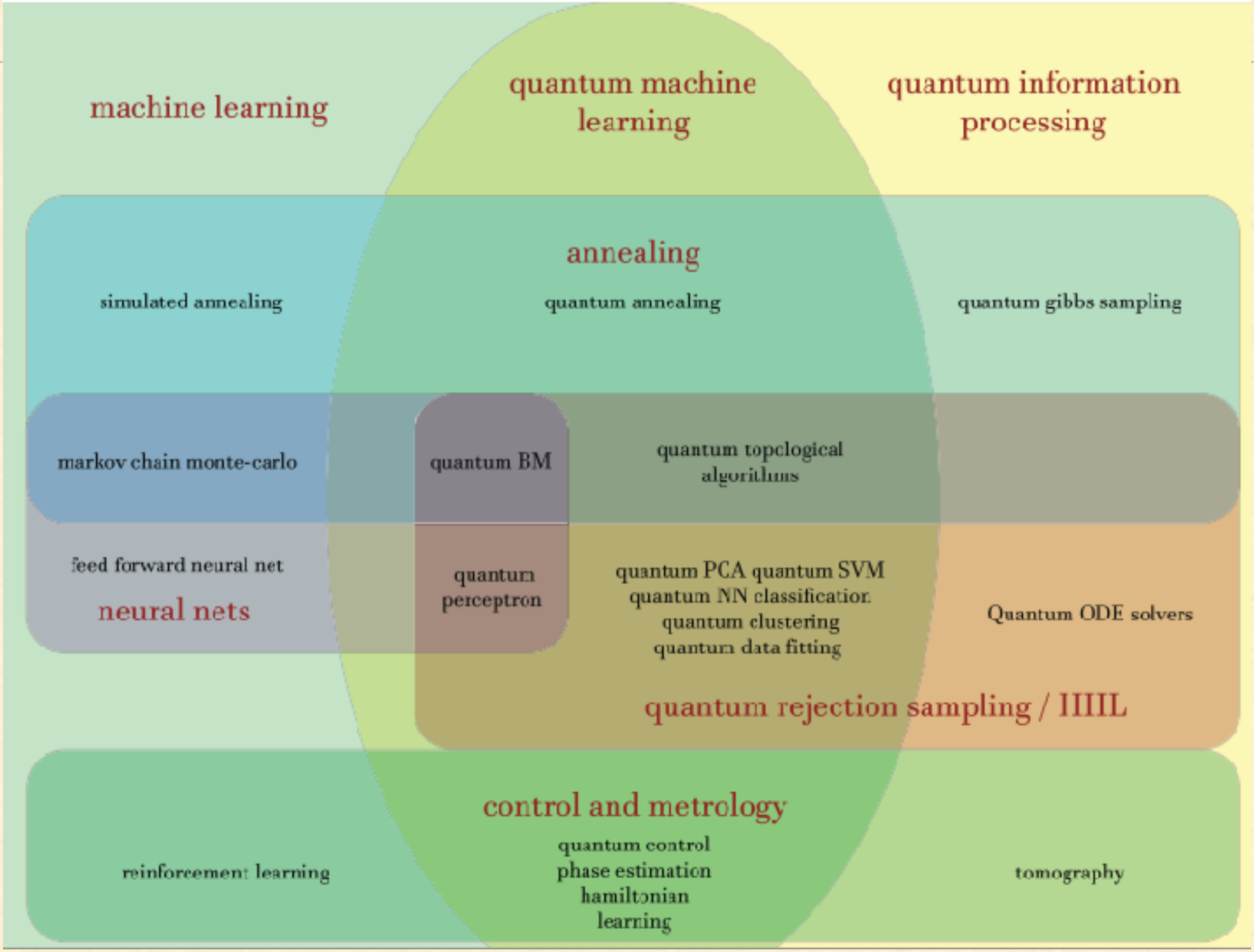
A. Cichocki, ECM (2013).

Tensor networks for image processing

FIG. 3: Comparison of the original 512x512 8-bit grayscale image (upper-left) with images compressed with the MPS algorithm (upper-right, DCR=17.97, SSIM=0.8311, and lower-left, DCR=7.64, SSIM=0.9014) and JPEG (lower-right, DCR=33.14, SSIM=0.8311). Note how the compression artifacts are characteristic of each algorithm, even though the quality measure is the same.

A. Bloque and J.I Latorre

QT, TN & MACHINE LEARNING



J. Biamonte et al. Nature (2017).

I. Glasser, et al. Phys. Rev. X (2018).

GAME OF LIFE (CONWAY'S)

Cellular automata

Two states: "dead" or "alive"

Set of simple rules that generate complexity, self-organization

Universal Turing machine

Non unitary

from wikipedia

M. Gardner, Sci. Am.,(1970)

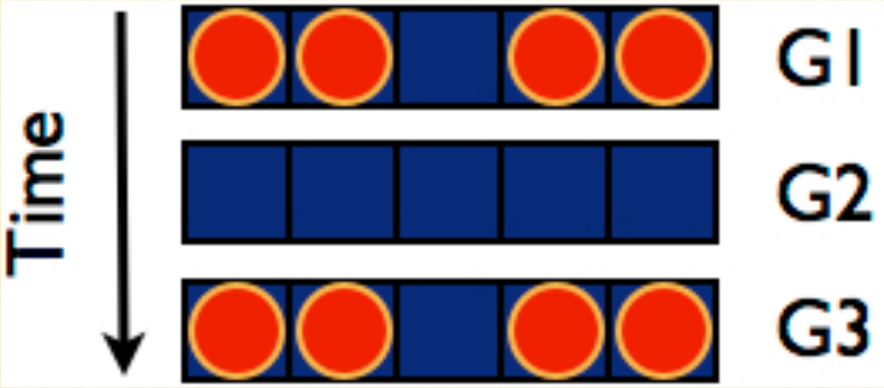
QUANTUM GAME OF LIFE

Unitary
One dimensional

$$H = \sum_{i=3}^{L-2} (b_i + b_i^\dagger) \cdot \left(\mathcal{N}_i^3 + \mathcal{N}_i^2\right)$$

$$\mathcal{N}_i^2 = \sum\nolimits_P n_\alpha n_\beta \bar{n}_\gamma \bar{n}_\delta$$

$$\mathcal{N}_i^3 = \sum\nolimits_{P'} n_\alpha n_\beta n_\gamma \bar{n}_\delta$$

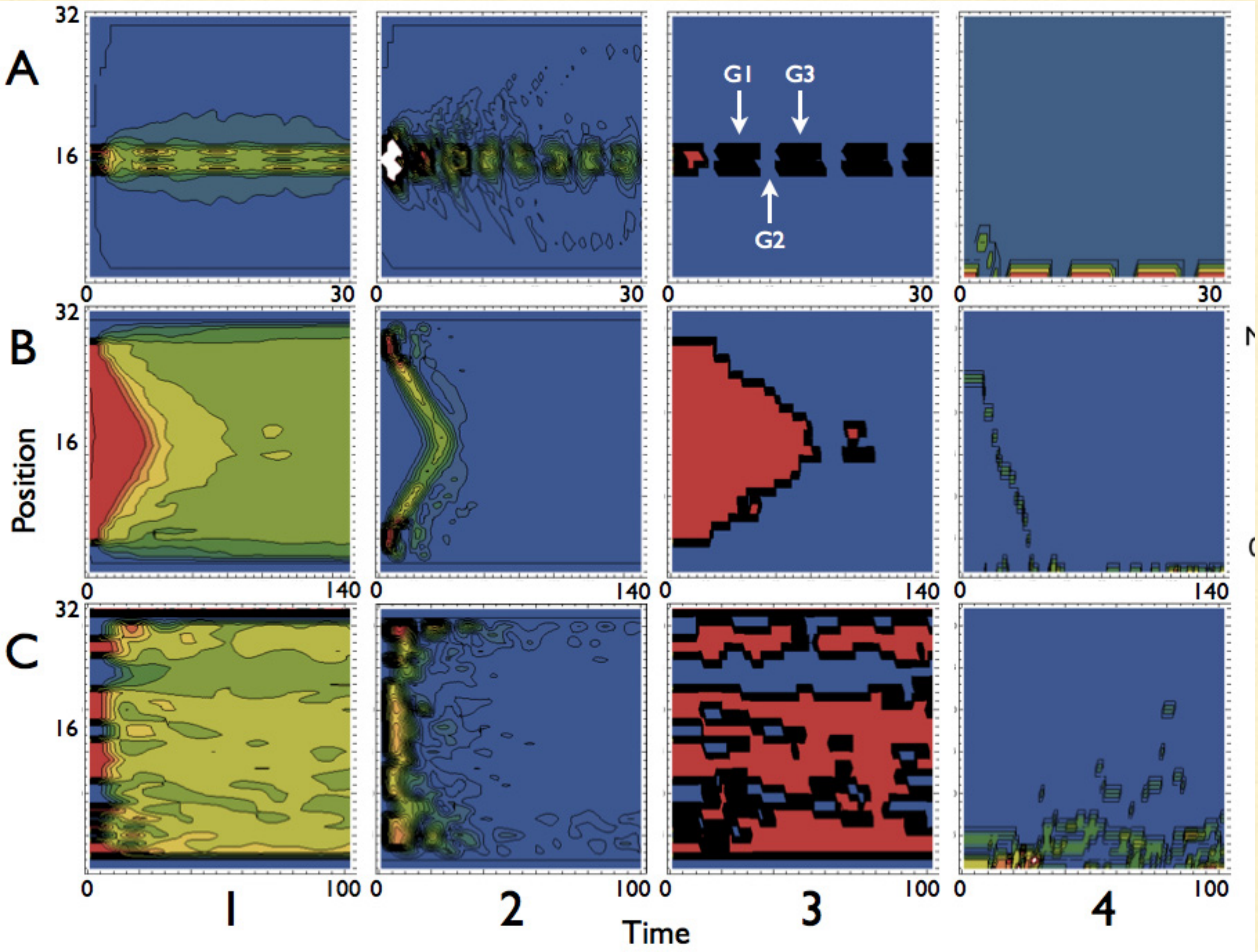


Blinker

Two possible states:
"active only if surrounded by 2 or 3 alive sites"

D. Bleh, T. Calarco, SM EPL, 97 (2012) 20012

Population Activity Discrete Pop. Clustering



D. Bleh, T. Calarco, SM EPL, 97 (2012) 20012

OPTIMAL CONTROL

Steering quantum systems at your will

Classical OCT problem

+

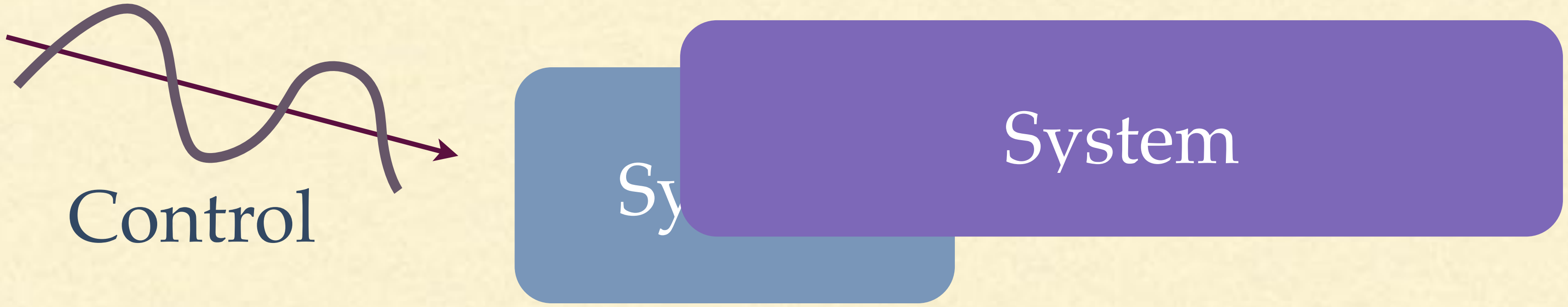
=

+

$\overset{?}{=}$

Quantum OCT problem

QUANTUM OPTIMAL CONTROL

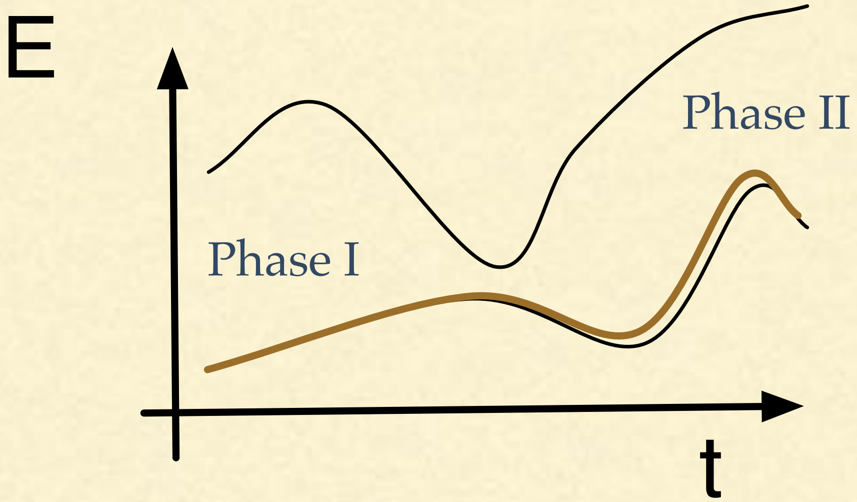


$$i\frac{\partial}{\partial t}|\psi(t)\rangle = (H_0 + f(t)H_1)\,|\psi(t)\rangle \qquad \min_{f(t)} J(|\psi(T)\rangle)$$

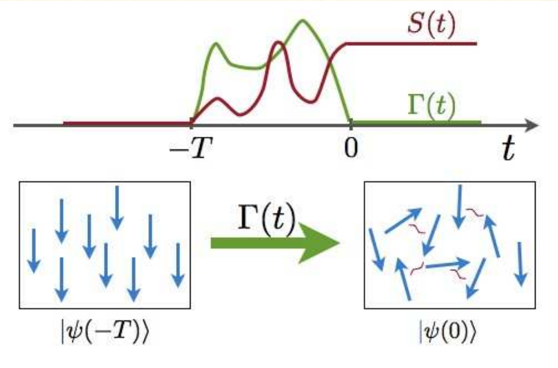
- Few-body: standard optimal control
  (high-accuracy, many iterations, complete knowledge…)
- Many-body: dCRAB
  (high-efficiency, few iterations, minimal knowledge…)

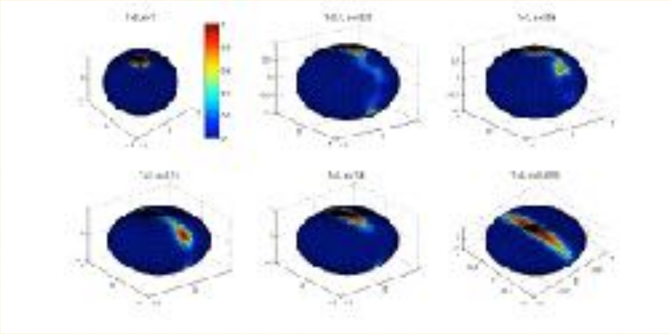
H. Rabitz et.al., NJP (2009) P. Doria, T. Calarco, SM PRL (2011)

APPLICATIONS



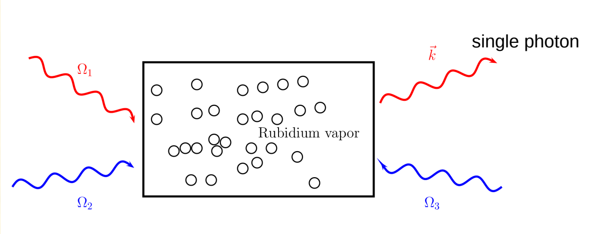
Quantum annealing

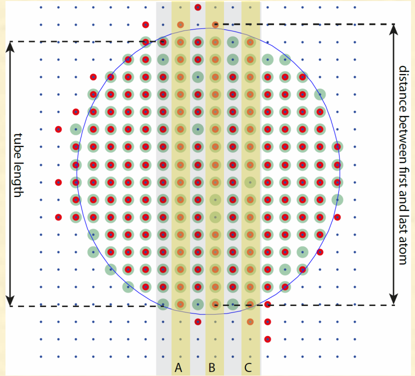


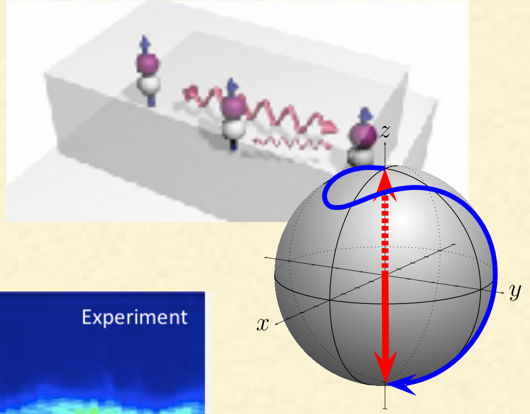


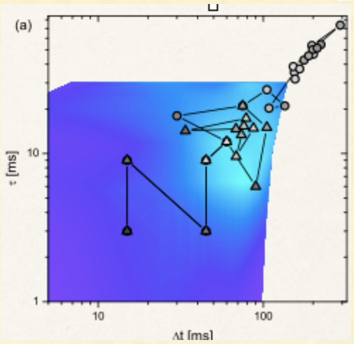
Entanglement/Squeezing manipulation

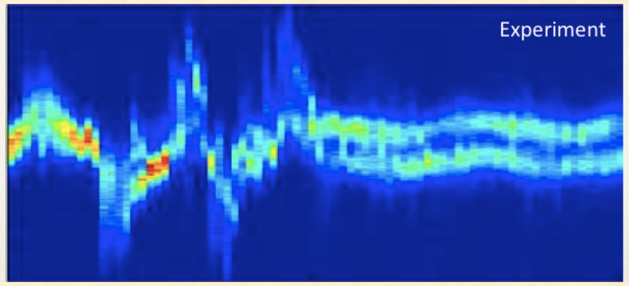
Light-harvesting dynamics







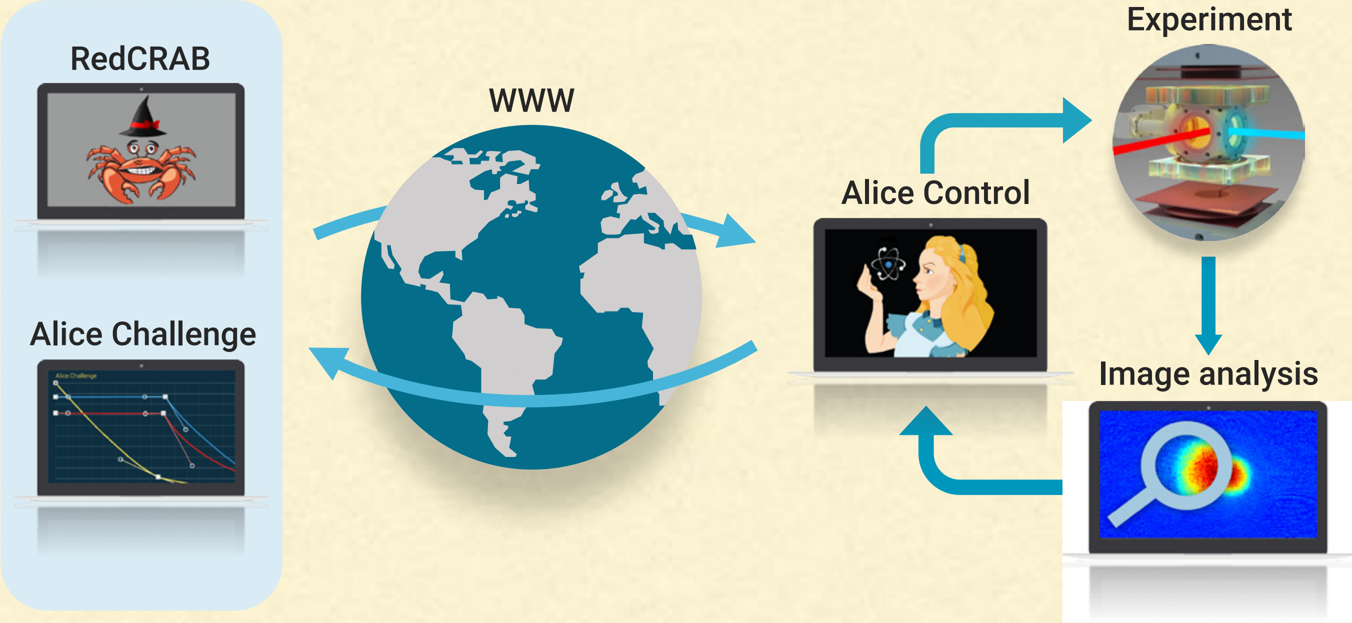




Optimal experimental protocols

RED CRAB

Server is online!



RedCRAB

Alice Challenge

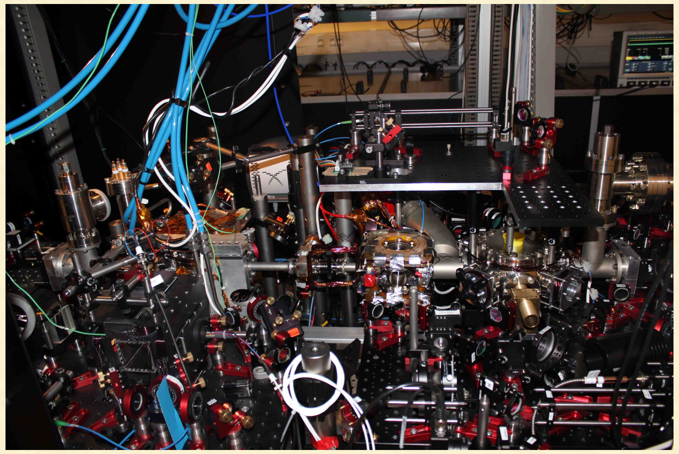
WWW

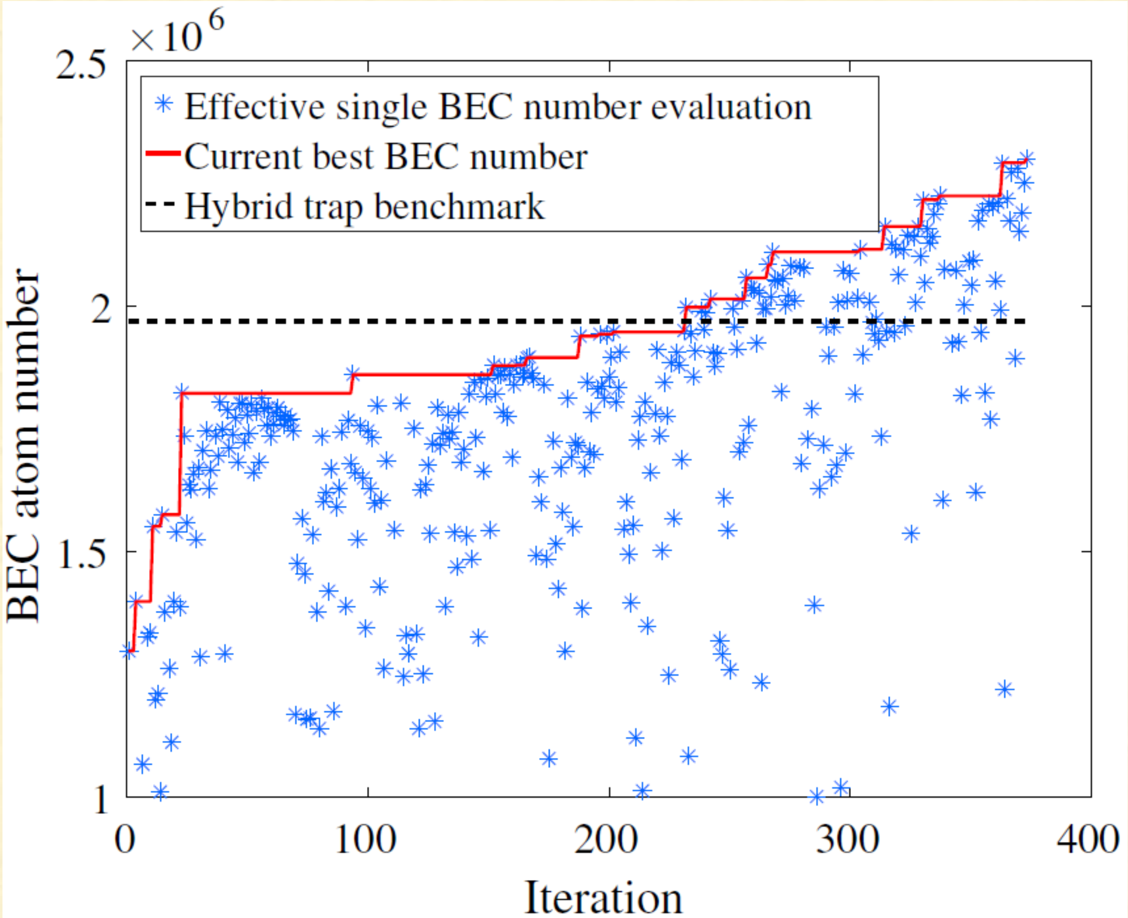
Alice Control

Experiment

Image analysis

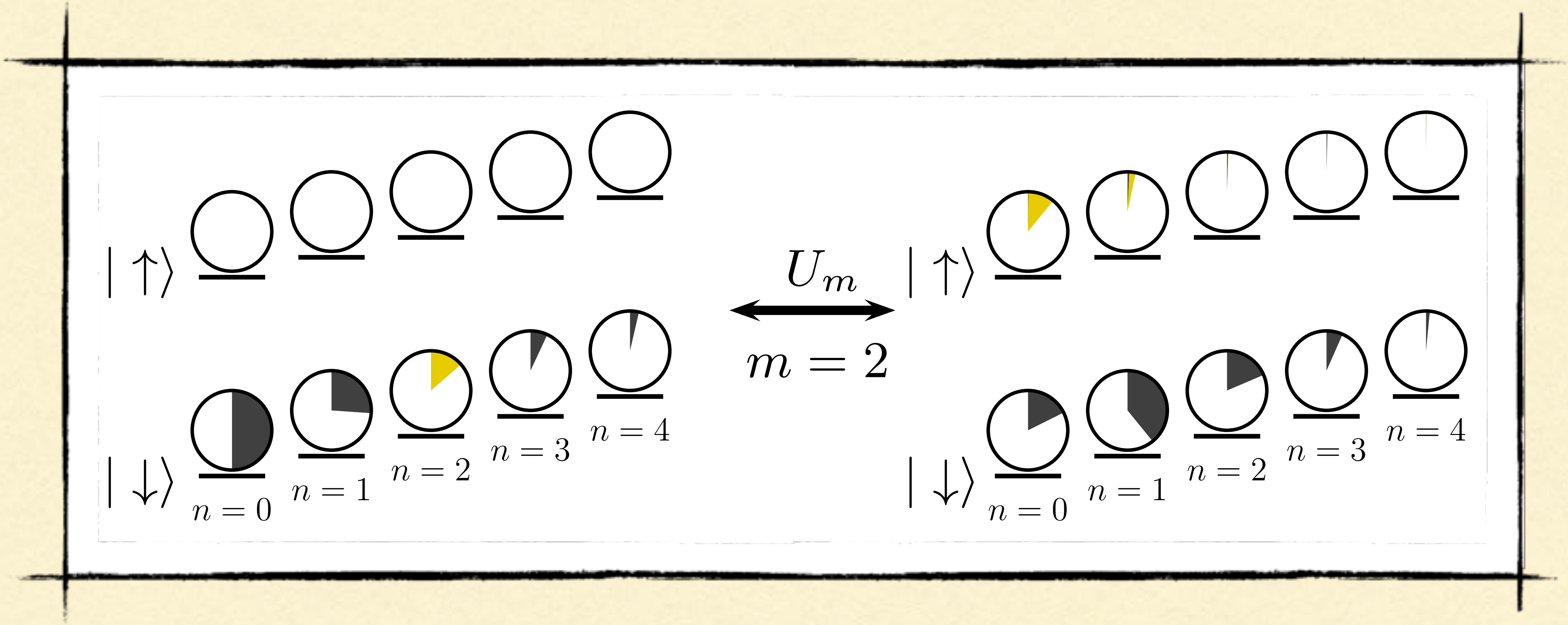
Maximize BEC atom number





www.scienceathome.org

PNAS (2018)



OPTIMAL EXPERIMENTAL PROTOCOLS

Cold atoms in optical lattices, Bose-Einstein condensates on atom chip, NV-centers in diamonds, Rydberg atoms, circuit QED, Trapped ions, Light-harvesting complexes…

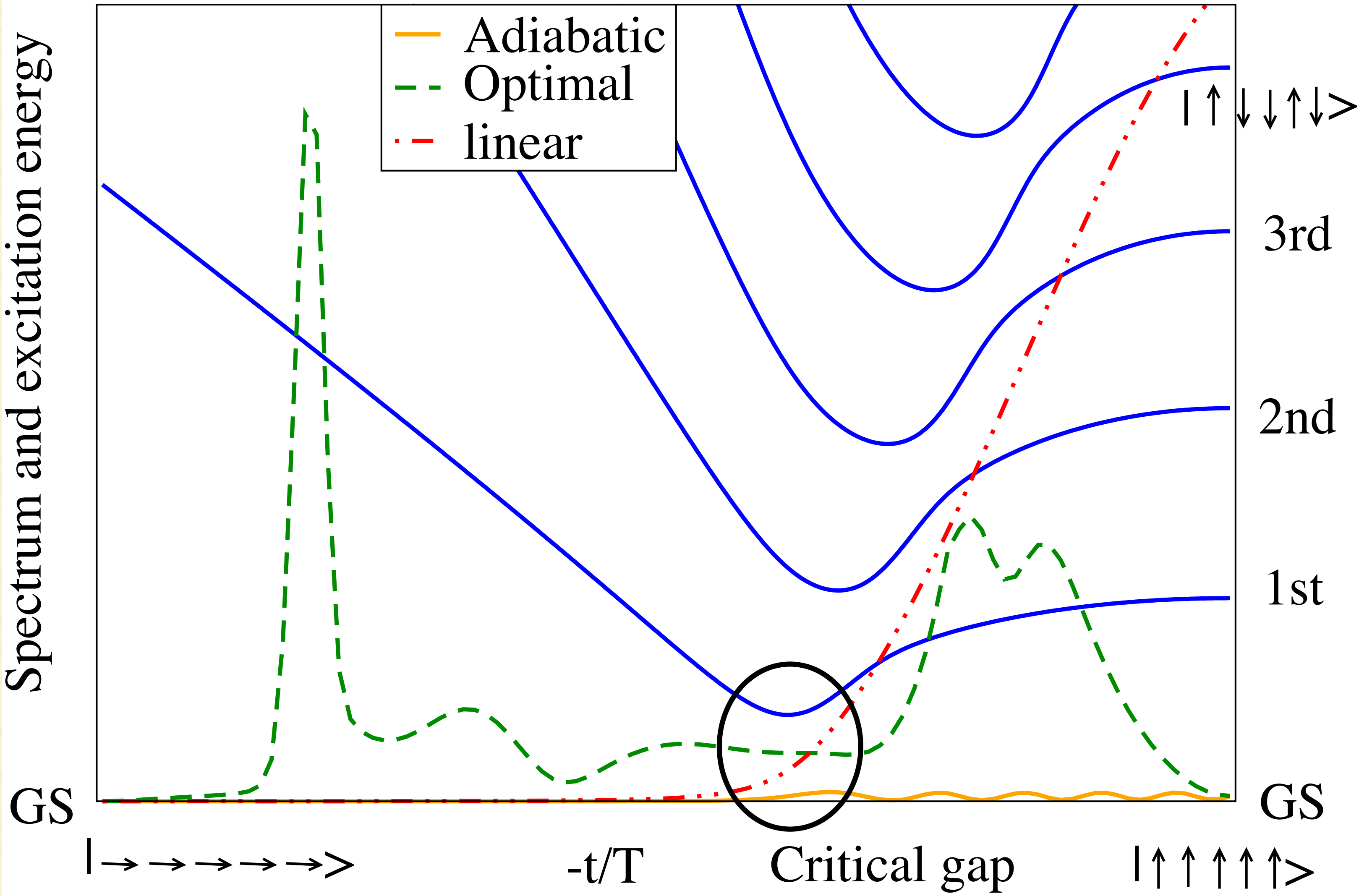
OPTIMAL QPT CROSSING

Slow

iabatic
ategy

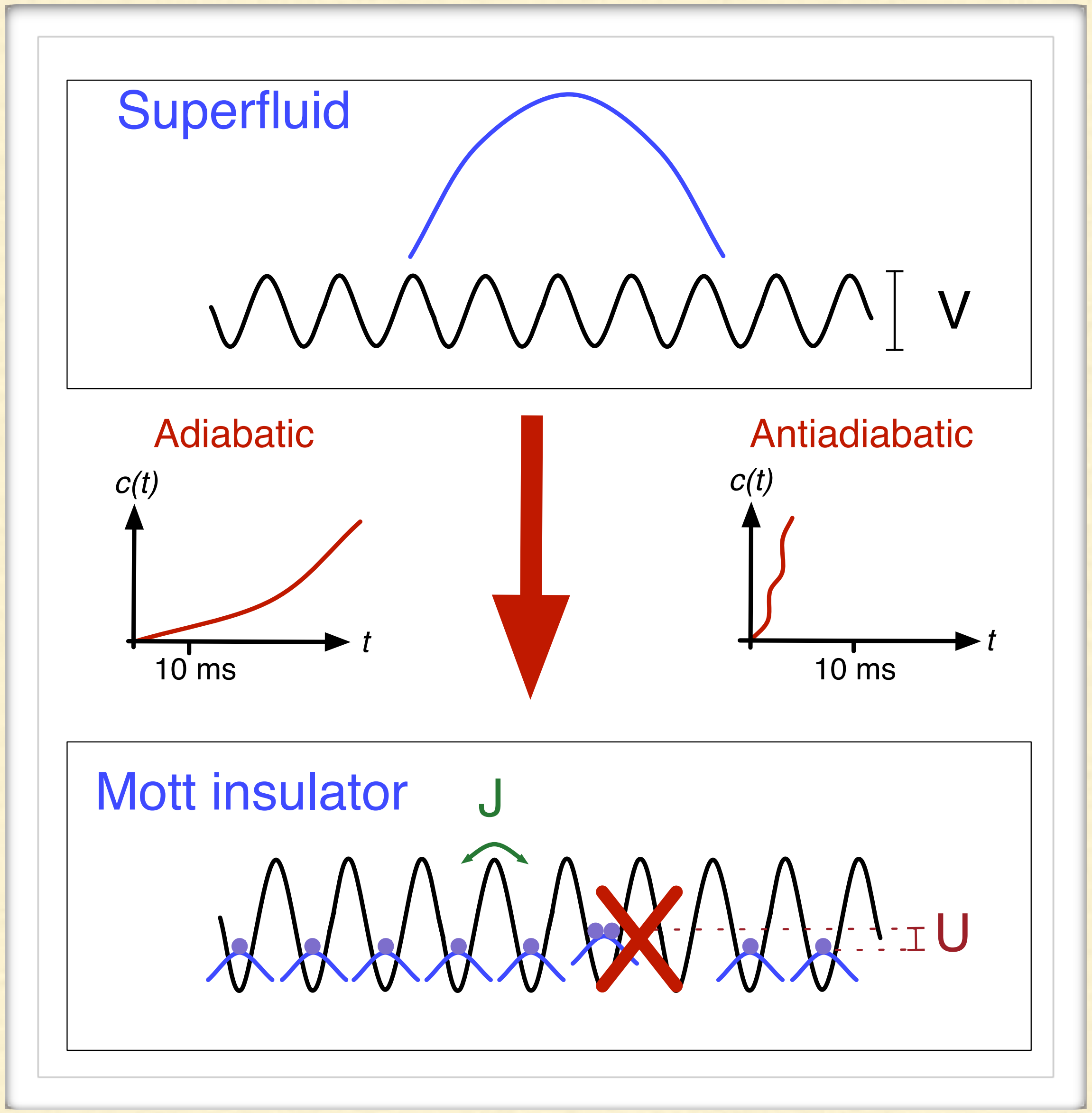
Fast

ptimal
ontrol

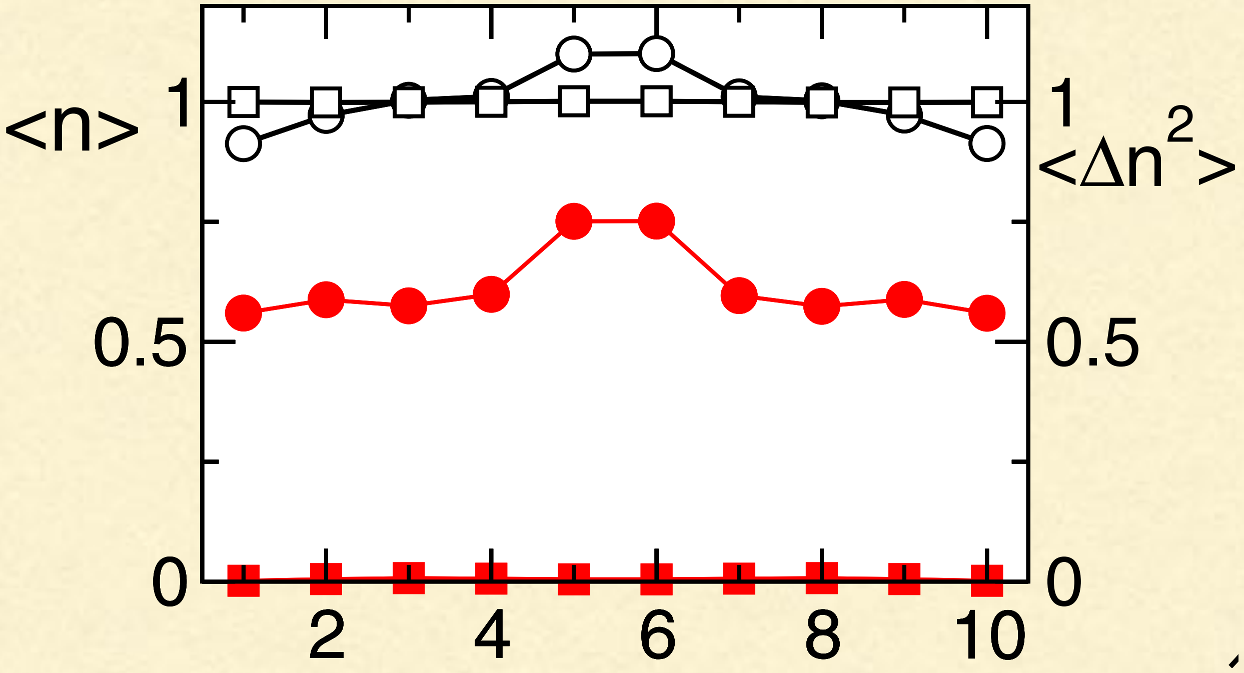


$$H = -\frac{1}{N}\sum_{i<j}(\sigma_i^x\sigma_j^x + \gamma\sigma_i^y\sigma_j^y) - \Gamma(t)\sum_i^N \sigma_i^z$$

SUPERFLUID-MOTT INS. QPT



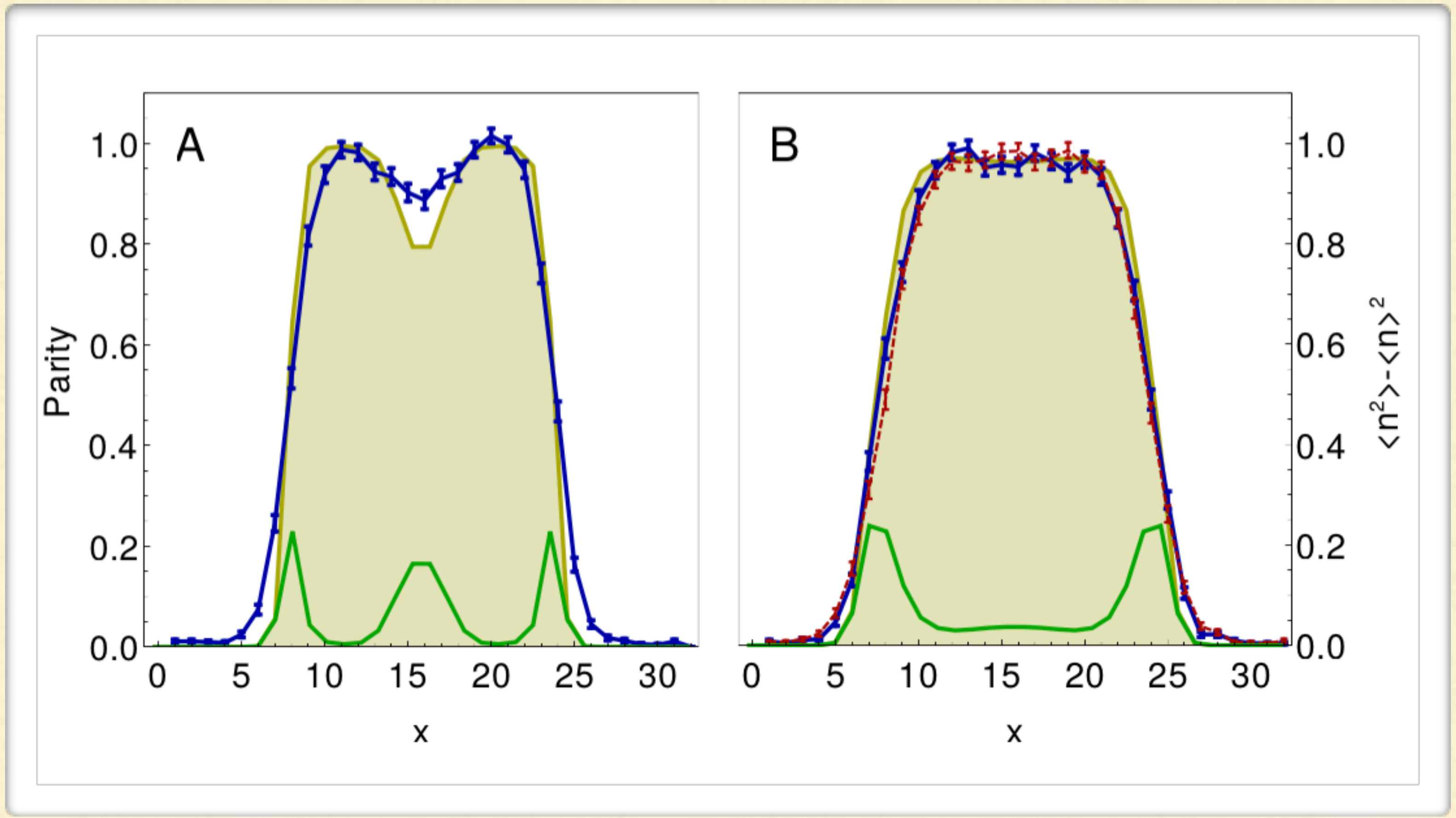
Optimal loading of cold atoms
in optical lattices



Bose-Hubbard model with external trapping potential

P. Doria, T. Calarco, SM Phys. Rev. Lett. (2011)

Parity density profiles



EXPERIMENTAL RESULTS

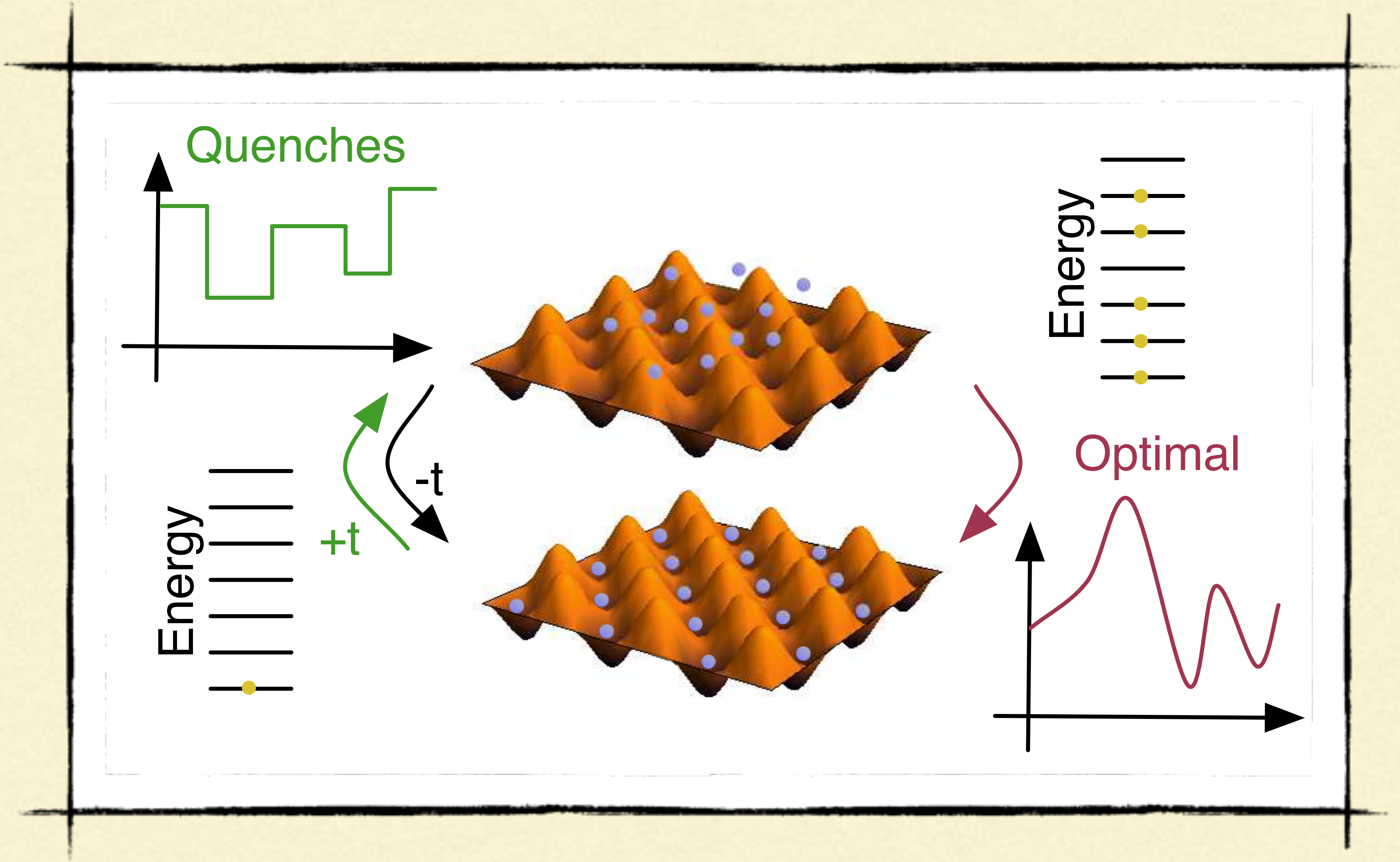
Speed up of one order of magnitude

Compatible with the quantum speed limit

I. Bloch's group (MPQ-Munich)

One dimensional tubes

Ulm-Munich collaboration, Scientific Reports (2016)



FUNDAMENTAL LIMITS AND COMPLEXITY

Where no man has gone before

PHYSICAL LIMITS

- Reachability

  Directions available

- Energy

  Power available

- Information

  Channel capacity

- Dynamical Lie algebra

$$V^{(0)} \equiv [[\mathrm{i}H_0', \mathrm{i}H_1], \mathrm{i}H_0']$$

$$V^{(\ell-1)} \equiv \left[\left[\mathrm{i}H_0', V^{(\ell-2)}\right], \mathrm{i}H_0'\right] - \omega_1^2 V^{(\ell-2)}$$

- Energy-time uncertainty

$$\Delta E \Delta t \geq \hbar/2$$

- Shannon-Hartley theorem

$$k_s = \log(1 + \mathcal{S})$$

OPTIMAL CONTROL COMPLEXITY

- The (smoothed) complexity of an optimal control problem scales polynomially with the size of (time-polynomial) reachable states $D_{\mathcal{W}^+}$
- Efficiently simulatable dynamics (Integrable, TN, DMFT, HF-like, etc…) can be efficiently optimally controlled
- Final error scales exponentially with the optimal control bandwidth

$$\varepsilon \geq 2^{-\frac{T\,\Delta\Omega\,\kappa_S}{D_{\mathcal{W}^+}}}$$

- The optimal control bandwidth, total time and the size of the set of reachable states are such that:

S. Lloyd and SM PRL (2014)

TAKE HOME MESSAGES

- Tensor network algorithms field of application is rapidly expanding
- What can be simulated can be controlled
- A large class of "complex quantum systems" can be efficiently characterized, simulated and controlled.
- We aim to support the development of quantum technologies and to study novel interesting phenomena

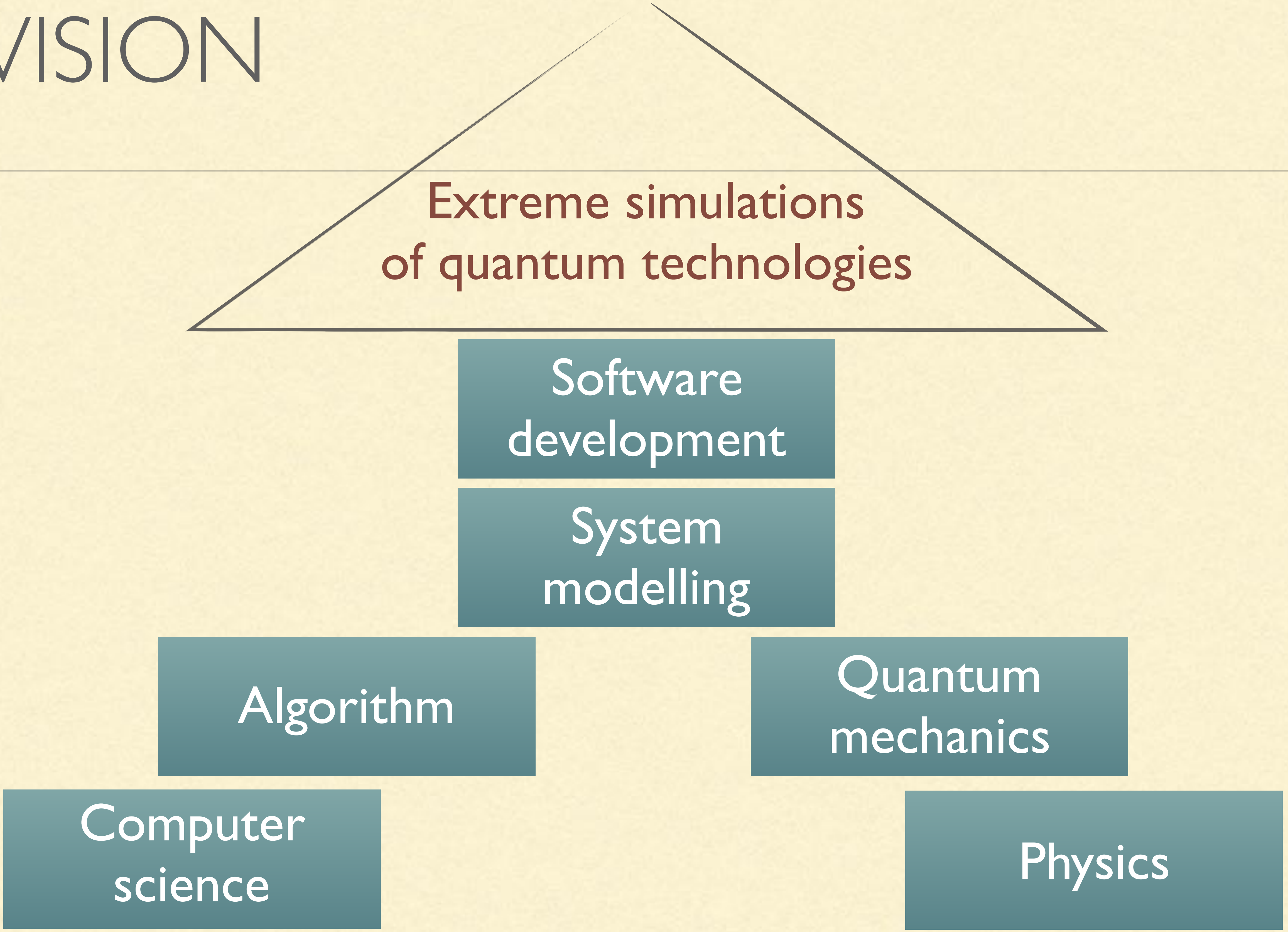
OUTLOOK

Every journey begins with a single step

OPEN QUESTIONS

- New tools and algorithms to simulate quantum systems
- Software engineering and optimization
- New protocols for quantum technologies
- Fundamental limits
- Classical versus quantum annealing
- Quantum advantage definition
- Universal quantum computers?
- …

VISION



Extreme simulations
of quantum technologies

Software development

System modelling

Algorithm

Quantum mechanics

Computer science

Physics

NECESSARY KNOW-HOW

- Algorithms
- Software engineering
- Complexity theory
- Graph theory
- Optimization
- High performance computing
- …

- Quantum information theory
- Many-body quantum systems
- Quantum hardware
- Tensor networks
- Optimal control
- Parallel computations
- …

OPTIMAL ENGINEERING OF COMPLEX QUANTUM PHENOMENA

- Dynamics of quantum phase transition
- Optimal driving of correlated matter
- Quantum chemistry
- Quantum transport
- Quantum thermodynamics
- Quantum technologies: sensing (NV-centers, graphene nano-ribbons), Quantum simulations (of LGT)…

Thank you for your attention!

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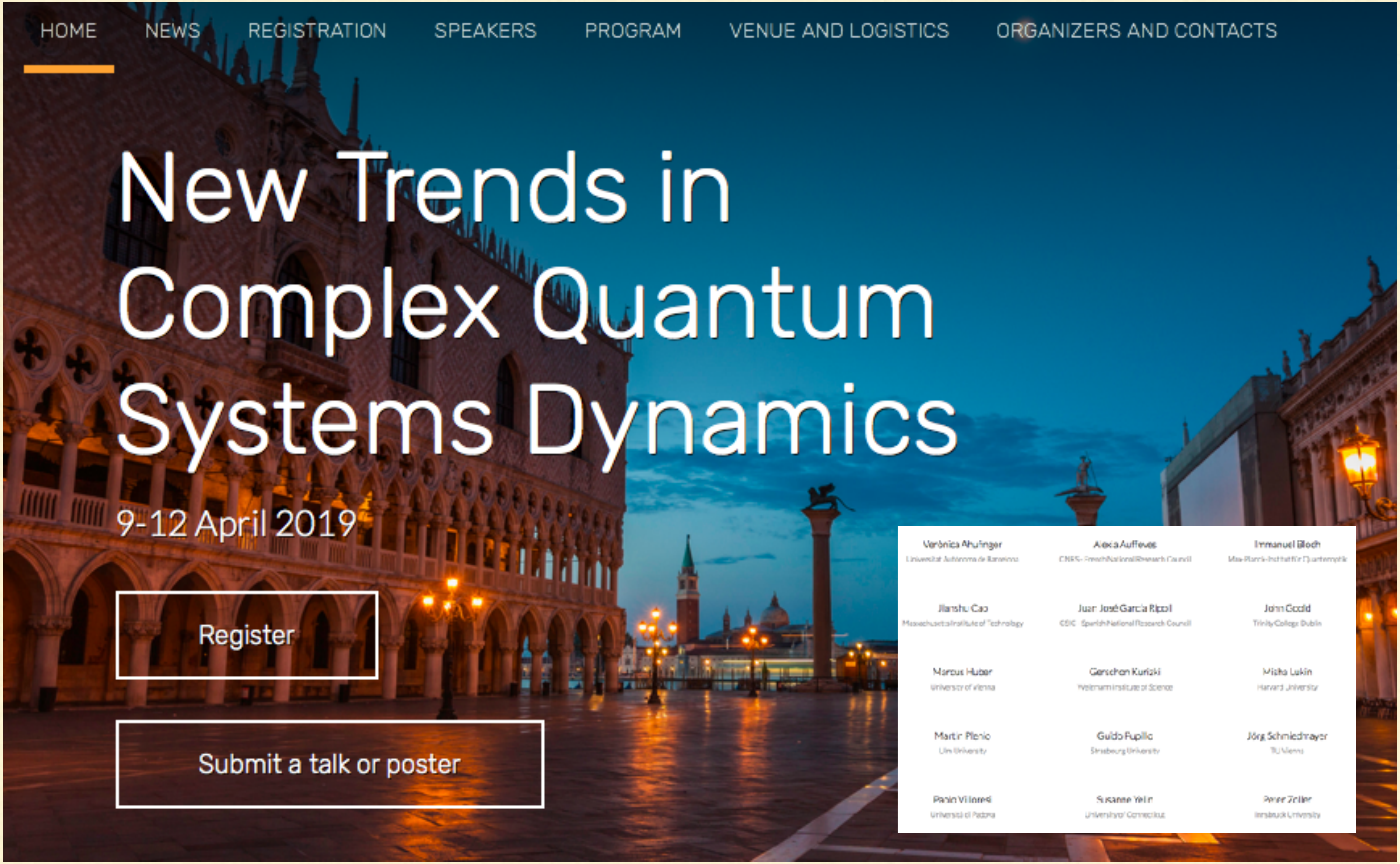
QUANTERA
QTFLAG
QUSCO

QuSCo

Numerics:

bwGRiD



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9-12 April 2019

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