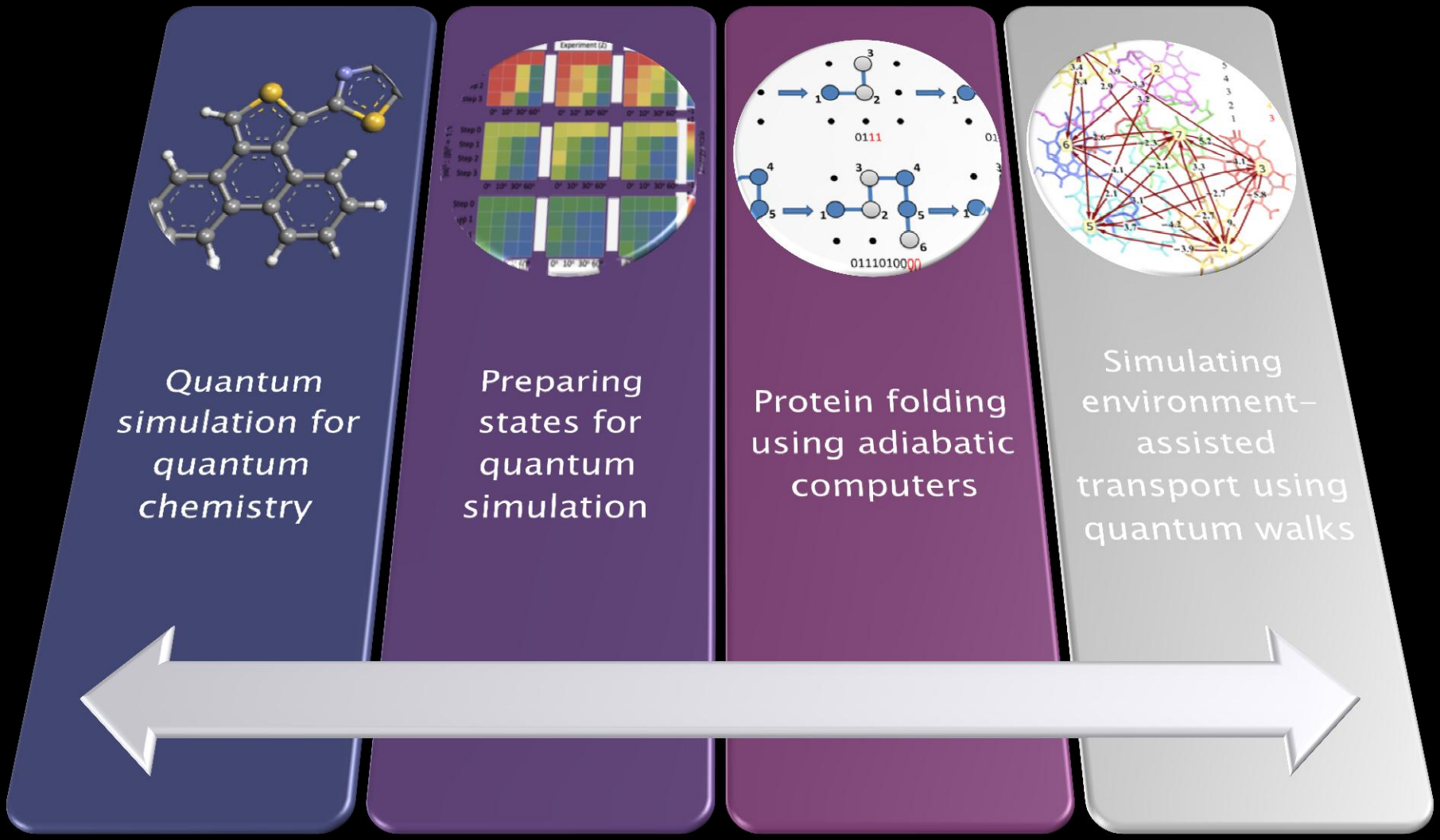
Quantum Information Processing for Chemistry

NASA Quantum Technologies Conference
Stanford, CA, 2011

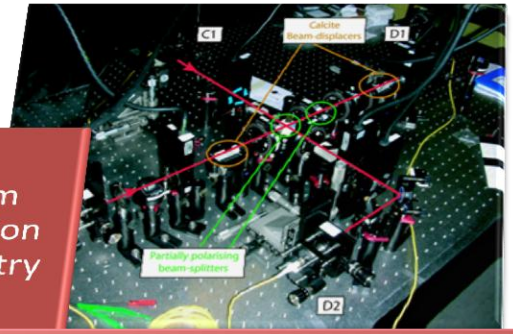
Alán Aspuru-Guzik
Associate Professor
Department of Chemistry and Chemical Biology
Harvard University

Cast of characters…


Quantum simulation for quantum chemistry
Preparing states for quantum simulation
Protein folding using adiabatic computers
Simulating environment-assisted transport using quantum walks

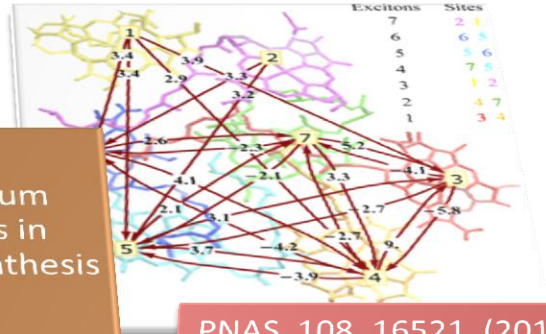
PV

Aspuru-Guzik group Research (2006-2012)



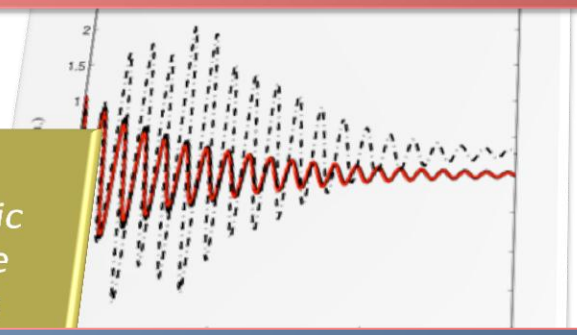
Quantum computation for chemistry

Nature Chemistry, 2, 106, (2010)
Ann. Rev. Phys. Chem. 62, 185 (2011)
PNAS, 109 (2012) Early Edition Online



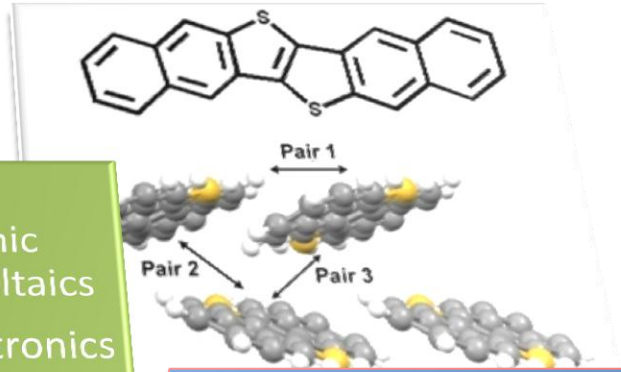
Quantum effects in photosynthesis

PNAS, 108, 16521 (2011)
PNAS, 108, 17615 (2011)



Electronic structure methods

Phys Rev. Lett 104, 043001 (2011)
Phys. Rev. Lett. 107, 183002 (2011)



Organic photovoltaics and electronics

Nature Comm. 2, 437 (2011)
Nature 480, 504 (2011)

TDDFT for open quantum systems, ultrafast quantum process tomography,
First algorithms and experiments for quantum computer simulations of chemistry
Distributed computing for search of organic photovotaics materials

QIQC

- Sabre Kais – Purdue
- Daniel Lidar – USC
- Ken Brown – Georgia Tech
- Peter Love – Haverford
- Alán Aspuru-Guzik – Harvard

QUANTUM INFORMATION FOR QUANTUM CHEMISTRY

An NSF Center for Chemical Innovation

Experimental collaborators

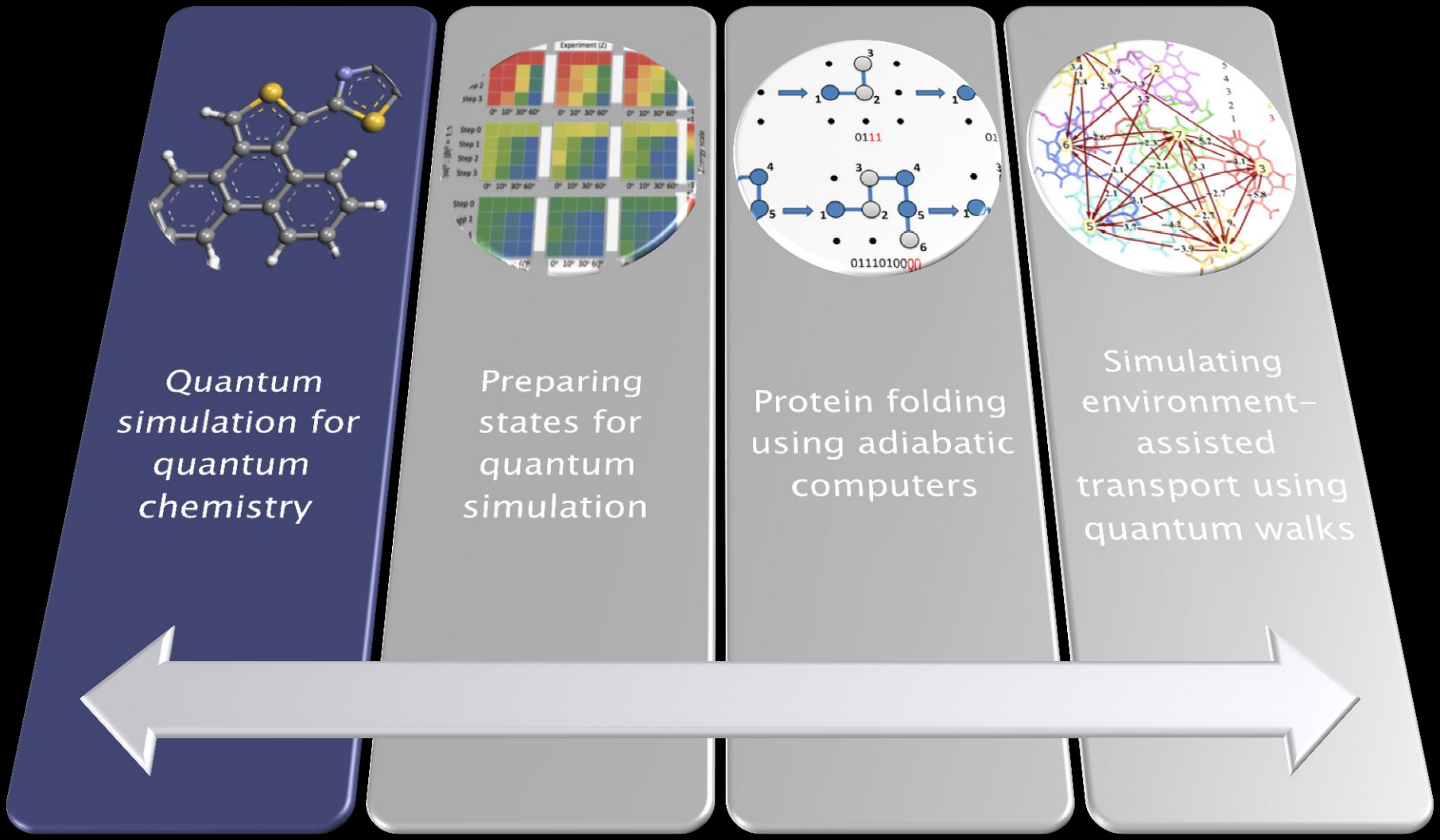
- Andrew White – Queensland
- Philip Walther – Vienna
- Jianfeng Du – USTC, China
- Guan-Can Guo – USTC, China
- Jonathan Baugh – Waterloo

Simulating Chemistry Using Quantum Computers

Ivan Kassal,* James D. Whitfield,*
Alejandro Perdomo-Ortiz, Man-Hong Yung,
and Alán Aspuru-Guzik

Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts 02138; email: aspuru@chemistry.harvard.edu

Annual Review of Physical Chemistry
62, 185–207 (2011) arxiv:1007.2648


Quantum simulation for quantum chemistry
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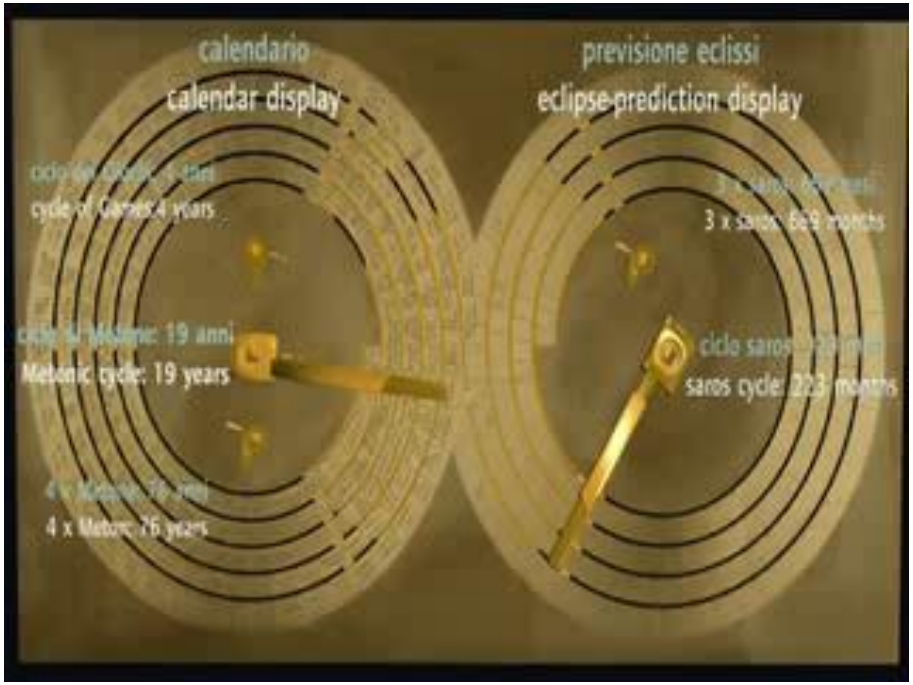
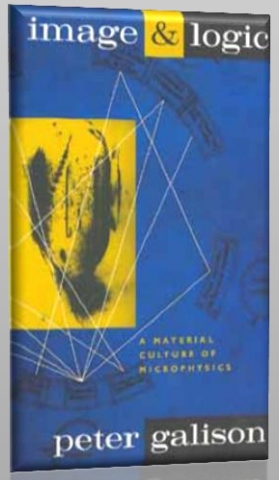
Analog Simulation



Antikythera Mechanism circa 200 BC

Digital Computer simulation

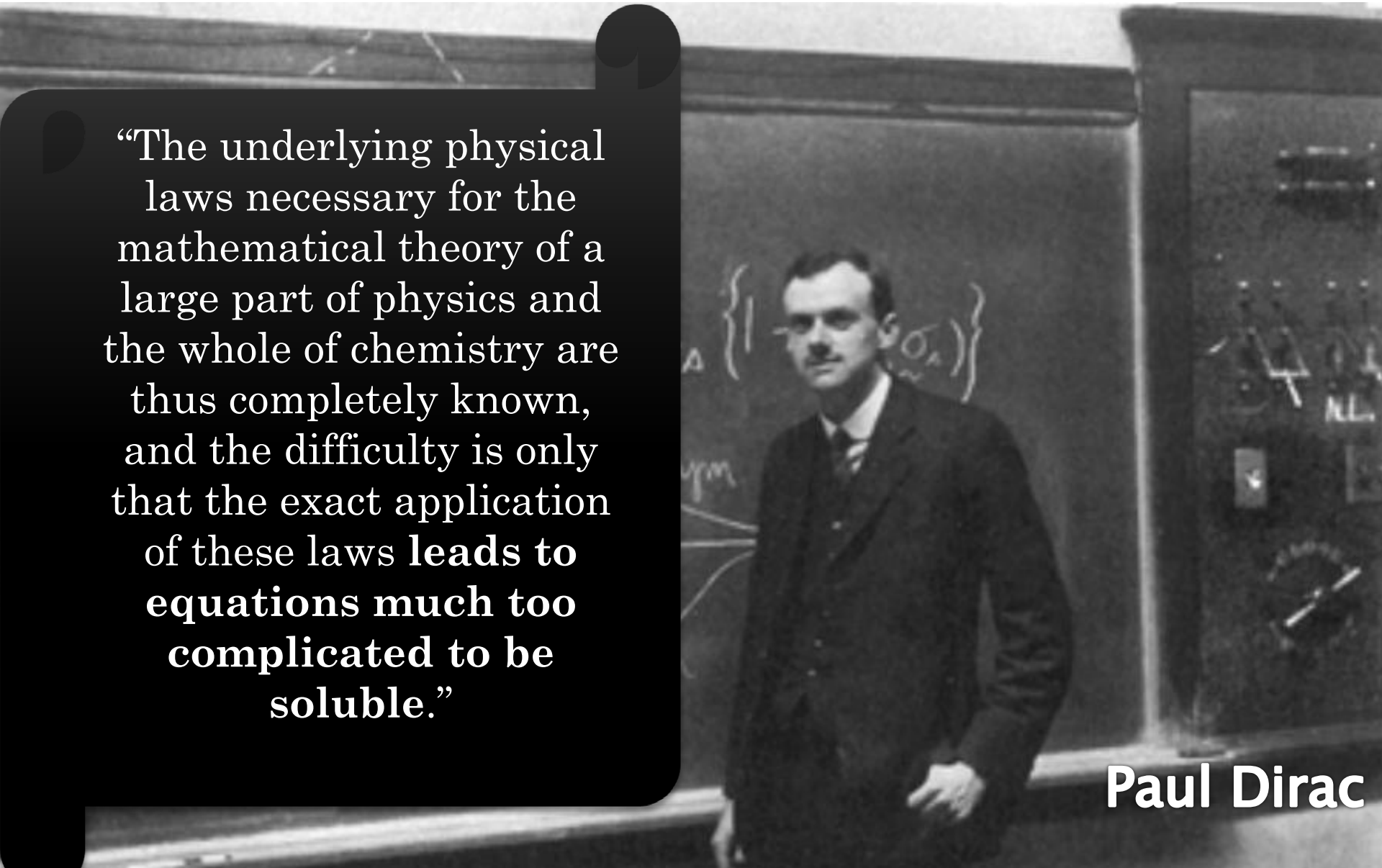
Without the computer-based simulation, the material culture of late-twentieth-century microphysics is not merely inconvenienced – It does not exist. [...] Machines [...] are inseparable from their virtual counterparts – all are bound to simulations.



–Peter Galison

From *Image and Logic: A material culture of microphysics* (1997)

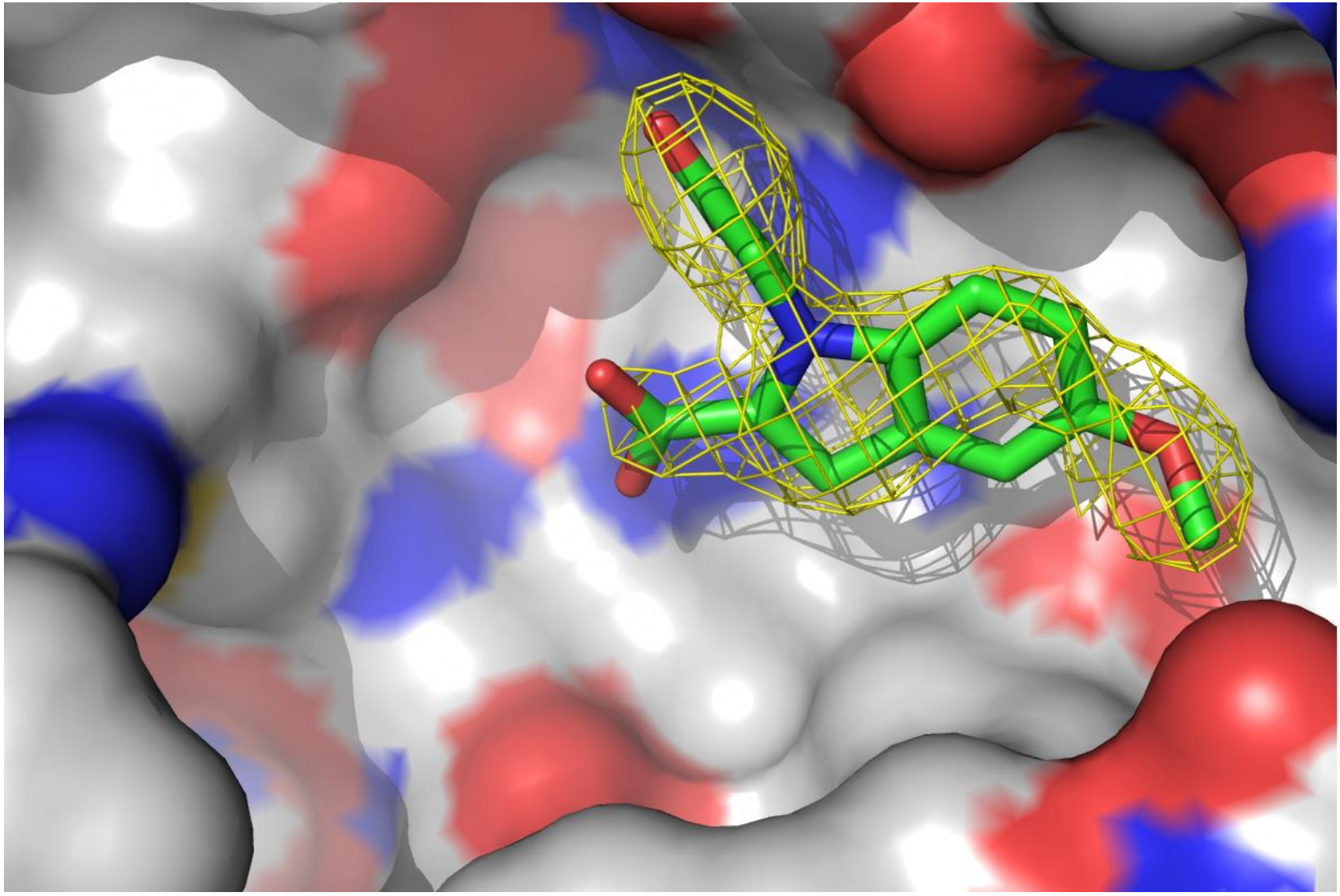
The current simulation paradigm (1929–)



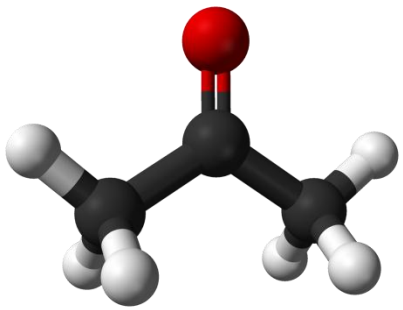
"The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws **leads to equations much too complicated to be soluble.**"

Paul Dirac

Computational chemistry and drug design



The current paradigm



quantum system

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

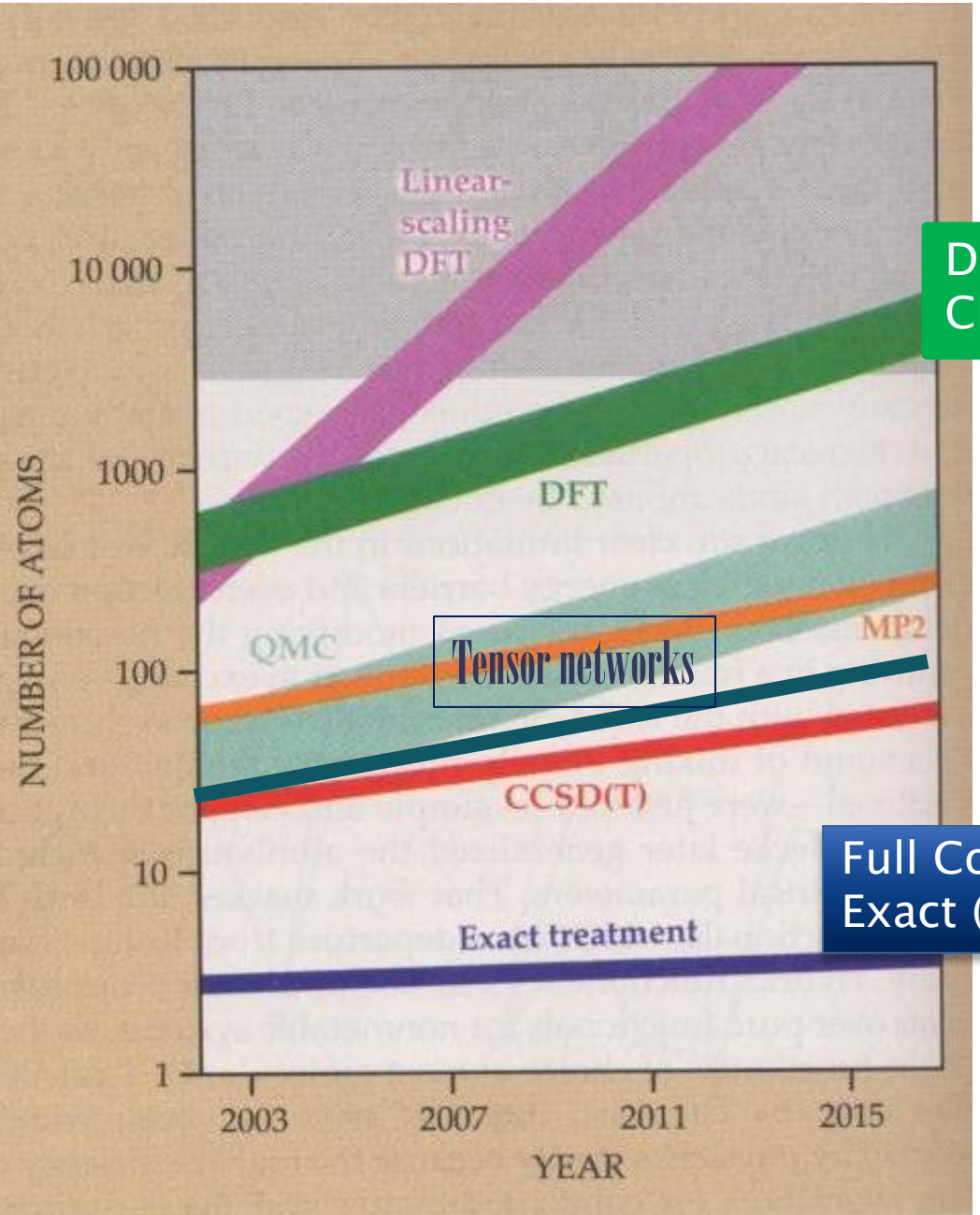
Quantum model
(quantum information)

Classical information
processor

E = −192.0492 Hartree

Classical information

Some alternatives



DFT: Errors in transition states,
Charge transfer excitations, anions,...

Full Configuration Interaction:
Exact (within a basis)

M. Head-Gordon, M. Artacho,
Physics Today 4 (2008)

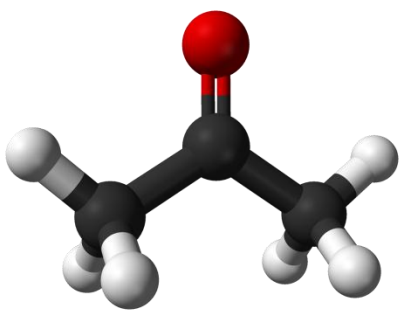
Quantum computer simulation of physical systems

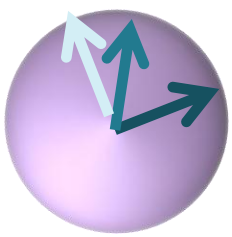
Richard P. Feynman
1982

Quantum computer simulation

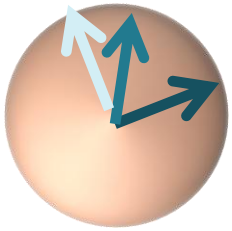
$$|\Psi^{mol}\rangle \quad \rightarrow \quad |\Psi^{QC}\rangle$$

$$\hat{U}^{mol}(t) = e^{-i\hat{H}^{mol}t} \quad \rightarrow \quad \hat{U}^{QC}(t) = e^{-i\hat{H}^{QC}t}$$





$\longrightarrow$

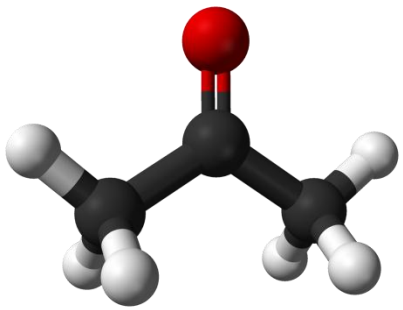


quantum system

quantum system
(quantum information)

R. P. Feynman, *Int. J. Theor. Phys.* (1982)

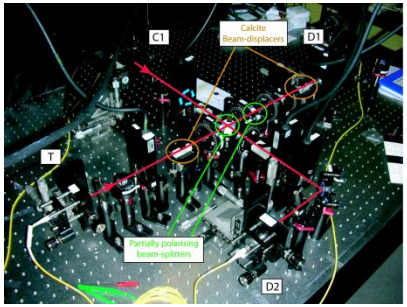
The quantum computing paradigm



quantum system

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

Quantum model
(quantum information)



Quantum information
processor

E = −192.0492 Hartree

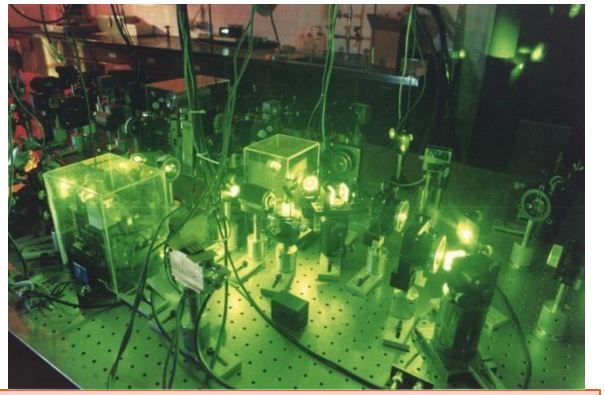
Classical information

The quantum advantage

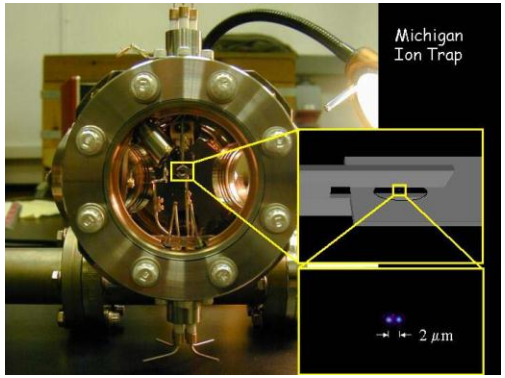
Computational task	Classical cost	Quantum cost
Factoring	$e^{O(n^{1/3}\log^{2/3} n)}$	$O(n^2 \log n \log\log n)$
Search	$O(n)$	$O(\sqrt{n})$
Full CI	$e^{O(n)}$	$O(n^5)$
Chemical dynamics	$e^{O(n)}$	$O(n^2)$
Protein folding	$e^{O(n)}$	?

- Full CI: Aspuru-Guzik et. al, **Science** (2005). Huang, Kais, Aspuru-Guzik, Hoffman, **Phys. Chem. Chem. Phys.** 10, 5388 (2008); Molecular Properties: Kassal, Aspuru-Guzik, **J. Chem. Phys.** 121, 224102 (2009), Experiments: Lanyon *et al.*, **Nature Chemistry** 2, 106 (2010). Du *et al.* **Phys. Rev. Lett.** 104, 103502 (2010)
- Chemical dynamics: Kassal, Jordan, Mohseni, Love, Aspuru-Guzik, **Proc. Nat. Acad. Sci.** 105, 1868 (2008), Ward, Kassal, Aspuru-Guzik, **J. Chem. Phys.** 130, 194105 (2009)
- Protein folding (random heteropolymer minima): Perdomo, Truncik, Tubert-Brohman, Rose, Aspuru-Guzik. **Phys. Rev. A.** 78, 1, 021320 (2008) Experiment: Perdomo *et al.* **In Preparation.**

Quantum computer hardware

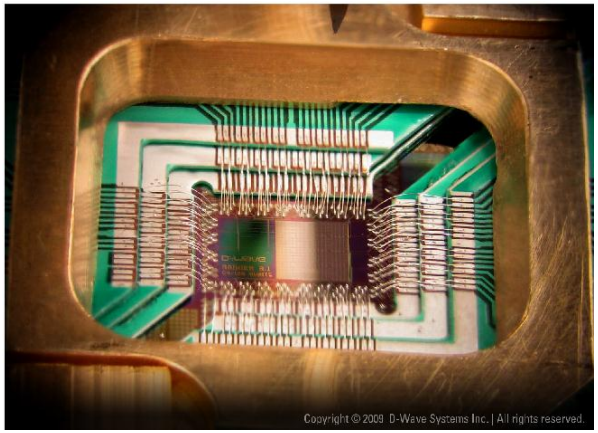


quantum optics

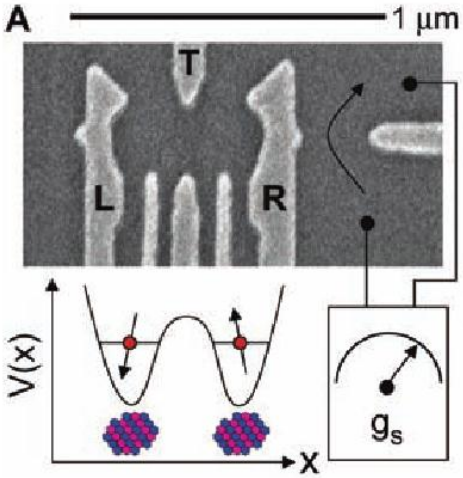


trapped ions

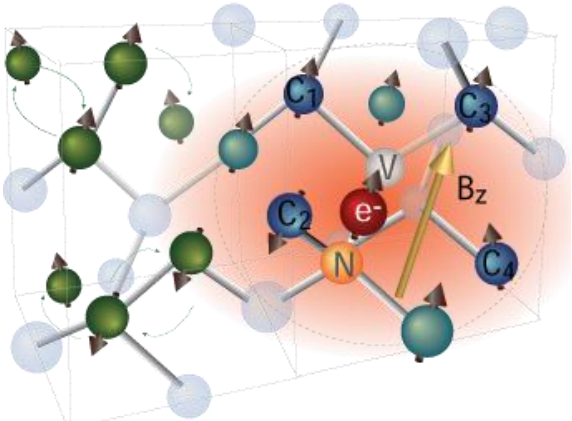
nuclear magnetic resonance



superconducting loops

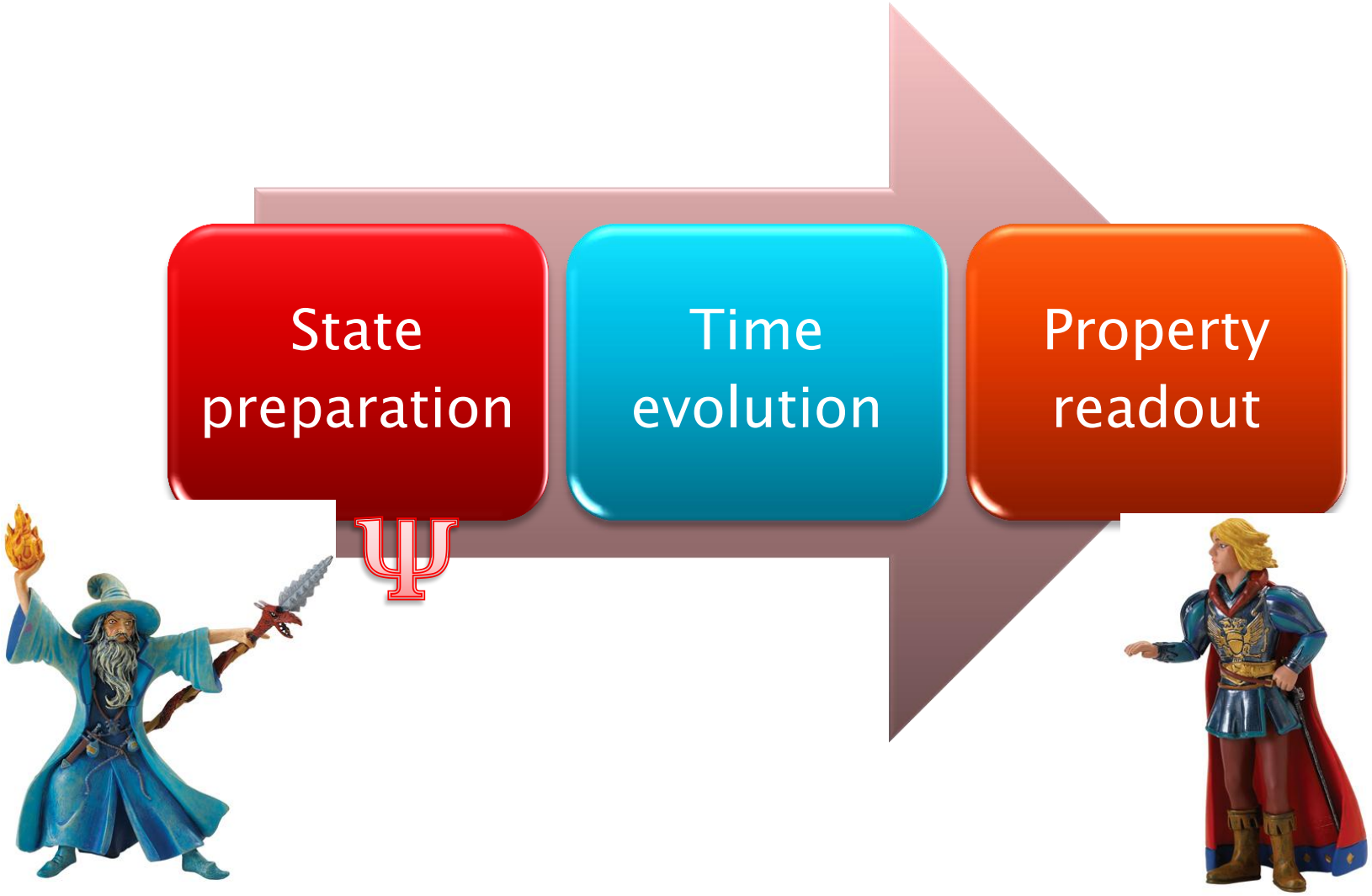


semiconductor quantum dots



nitrogen vacancies in diamond

Quantum computer simulation



Merlin

Arthur

Complexity classes

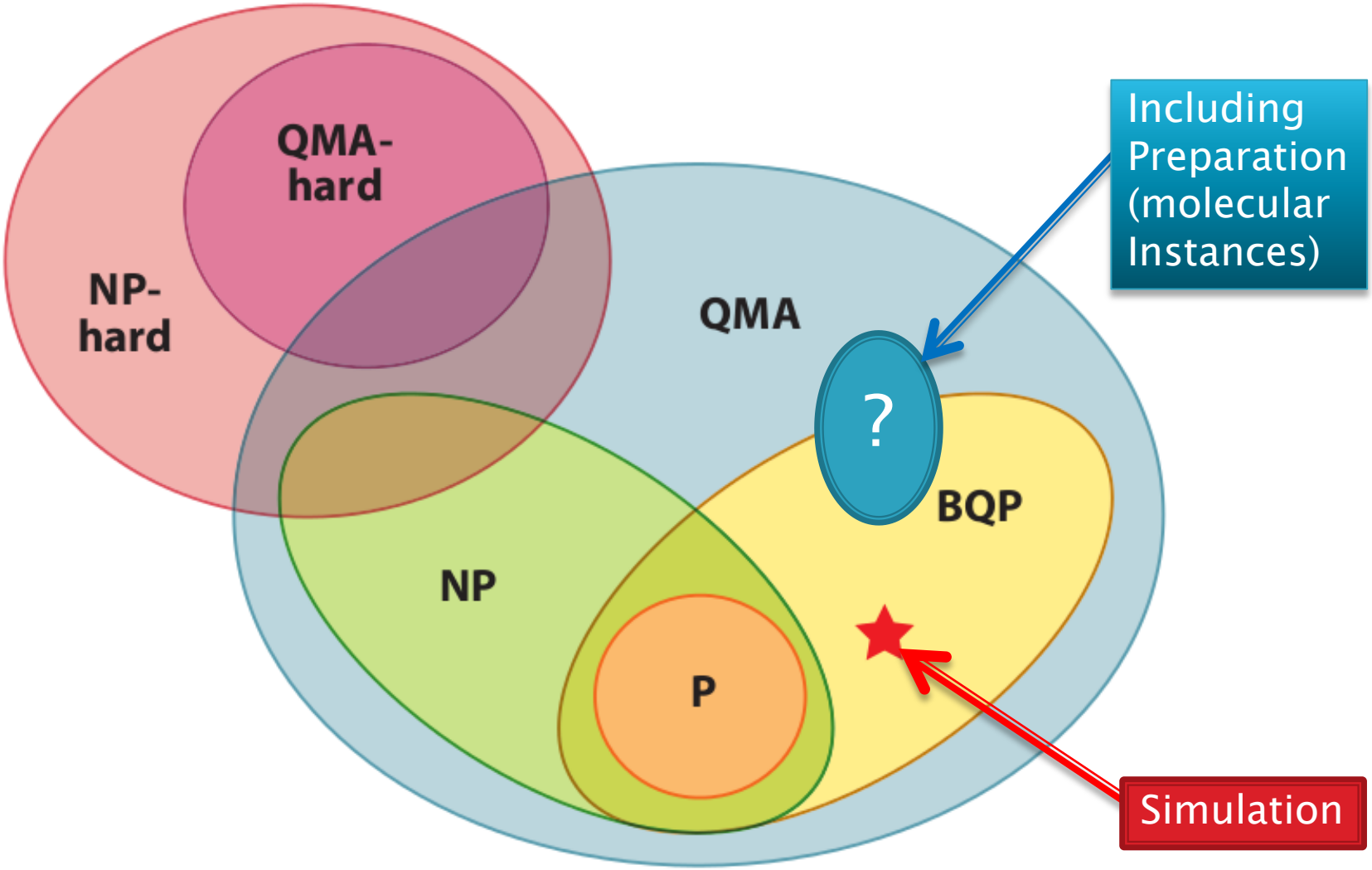
- Quantum Merlin Arthur
  (**Complete**: two-body Hamiltonian problem)

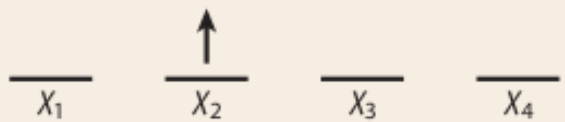
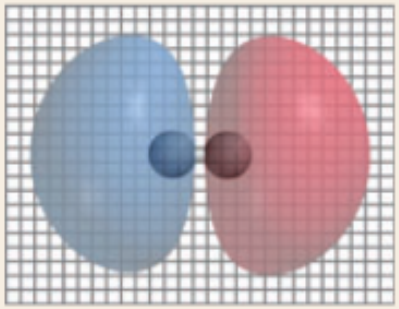
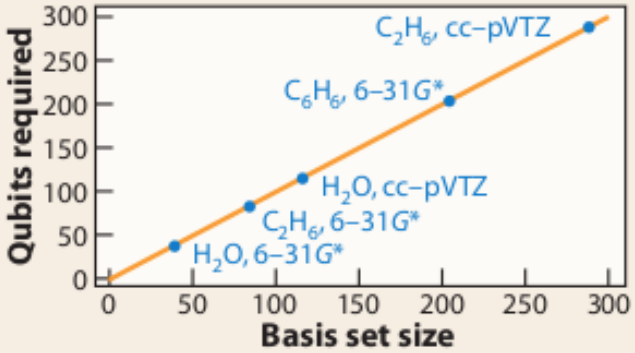
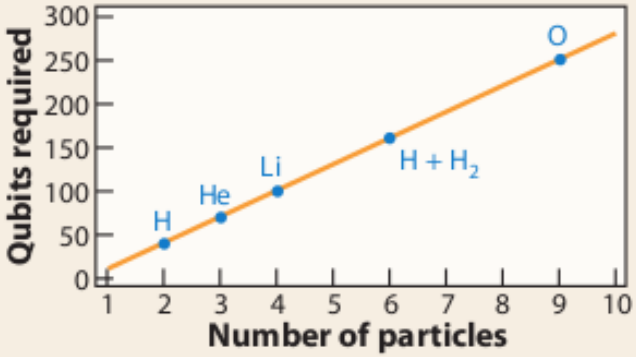
Decision problems that have a proof that can be verified by a quantum computer

- Bounded Quantum Polynomial (BQP)

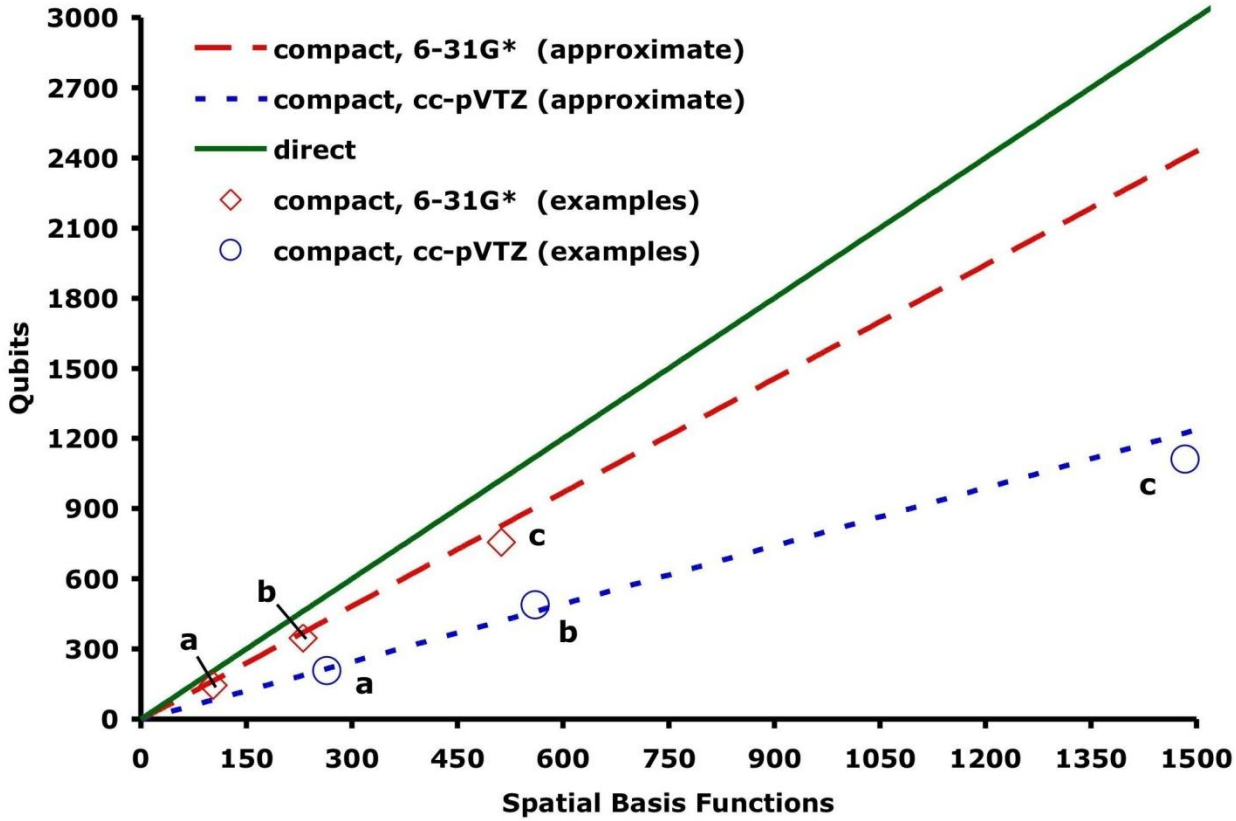
The class of decision problems **solvable in polynomial time** by a quantum computer

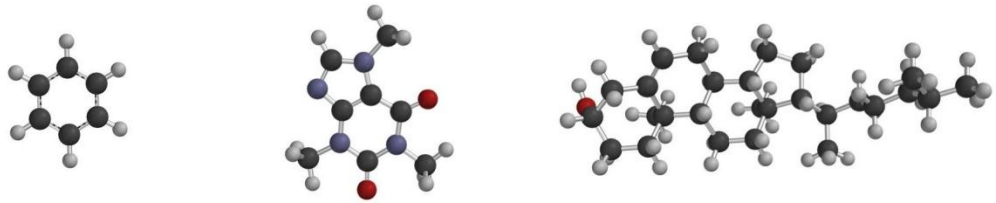
Quantum complexity of chemical simulation



	Second quantized	First quantized
Wave-function encoding	Fock state in a given basis:  $\lvert\psi\rangle = \lvert 0100\rangle$	On a grid of 2^n sites per dimension: $\lvert\psi\rangle = \sum_x a_x \lvert x\rangle$ 
Qubits required to represent the wave function	One per basis state (spin-orbital): 	$3n$ per particle (nuclei and electrons): 
Molecular Hamiltonian	Coefficients precomputed classically: $\sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$	Interaction calculated on the fly: $\sum_i \frac{p_i^2}{2m_i} + \sum_{i<j} \frac{q_i q_j}{r_{ij}}$
Quantum gates required for simulation	$O(M^5)$ with number of basis states	$O(B^2)$ with number of particles
	• Compact wave-function representation (requires fewer qubits)	• Better asymptotic scaling (requires fewer gates)

First- Quantized qubit requirements





a benzene b caffeine c cholesterol

A. Aspuru-Guzik, A. D. Dutoi, P. J. Love, M. Head-Gordon, *Science* (2005)

Time Evolution

Molecular Hamiltonian

$$\hat{H} = \sum_X \hat{h}_X = \sum_{p,q} \langle p| \hat{T} + \hat{V}_N |q\rangle \hat{a}_p^\dagger \hat{a}_q - \frac{1}{2} \sum_{p,q,r,s} \langle p|\langle q| \hat{V}_e |r\rangle |s\rangle \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

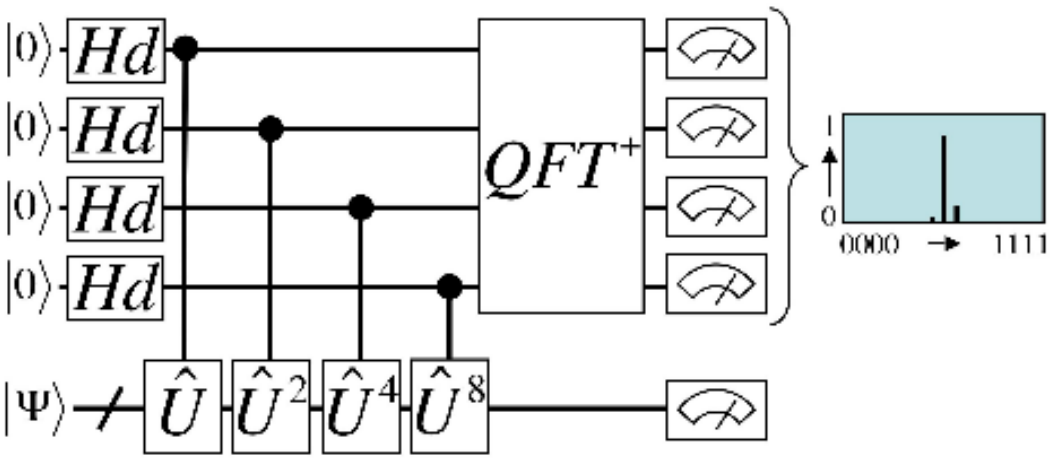
Trotter Expansion and Jordan-Wigner Transformation

$$e^{-i\hat{H}t} \approx \left[\prod_X e^{-i\hat{h}_X t/M} \right]^M \qquad \hat{a}_p^\dagger \hat{a}_q \rightarrow \hat{X}^p \hat{X}^q \left[\prod_{i=p+1}^{q-1} \hat{\sigma}_z^i \right] \hat{P}_0^p \hat{P}_1^q$$

- Number of Terms in $\hat{H}$ grows as N_{basis}^4
- Each term involves a controlled action on at most 4 qubits
- Few gates required by term

Read-out

Phase estimation algorithm



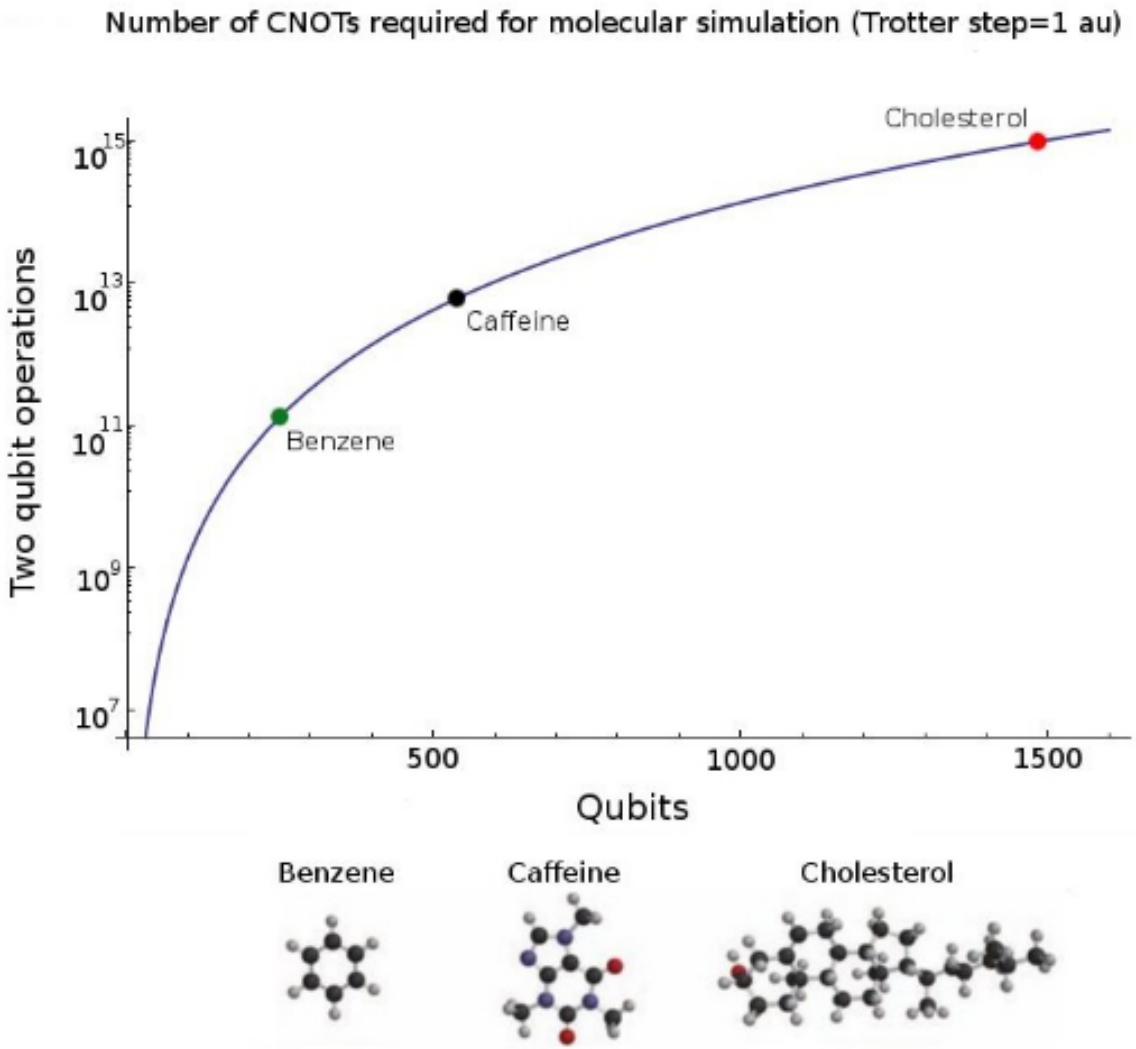
Choose t; $Et = -2\pi\phi$

$$\hat{U}(t)|\Psi\rangle = e^{-i\hat{H}t}|\Psi\rangle = e^{-iEt}|\Psi\rangle$$

Abrams, Lloyd, Phys. Rev. Lett (1997)

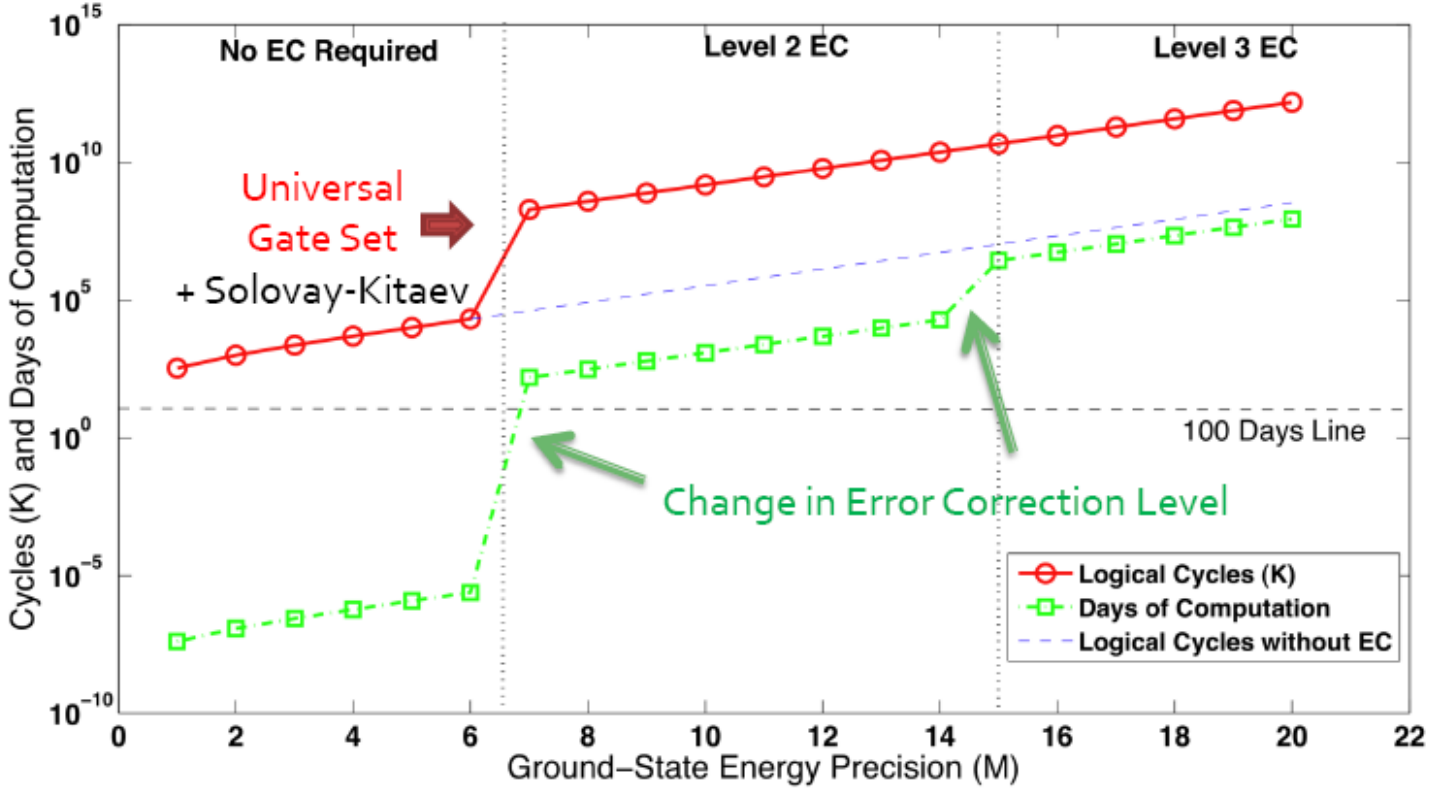
Two-qubit gates required for simulating molecules

Whitfield, Biamonte, Aspuru-Guzik, Molecular Physics, 109, 735–750 (2011)



Error correction scaling

Ising model in Transverse magnetic field : Ken Brown (GATech)



N=100 TIM

Gates and time required for simulating 100 spins on ion trap QC

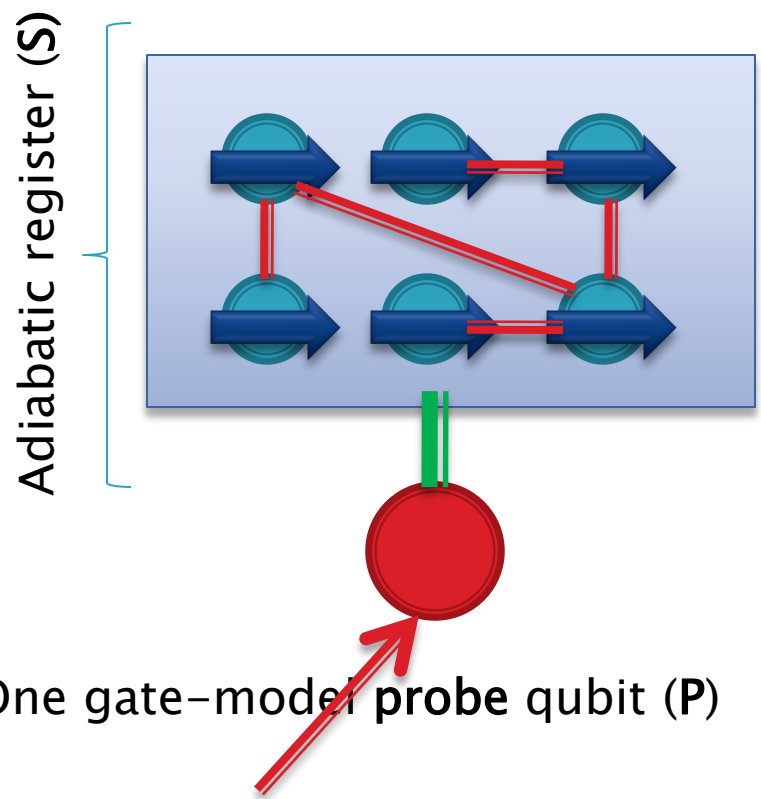
Clark et al, PRA (2009)

The Simulation decision tree

Kassal, Whitfield, Perdomo, Yung, Aspuru-Guzik,
A Annual Review of Physical Chemistry 62, 185-207 (2011) arxiv:1007.2648

Hybrid adiabatic gate-model

J. D. Biamonte, V. Bergholm, J. Fitzimmons, J. D. Whitfield, A. Aspuru-Guzik, Adiabatic quantum simulators. AIP Advances 1, 022126 (2011)



Hamiltonian to simulate

$$H_T = \sum_{v \in V} L_v + \sum_{e \in E} K_e.$$

Start with: (eg. Transverse field)

$$H_0 = H_{S,I} \otimes \mathbb{1}_P + \mathbb{1}_S \otimes H_P.$$

Adiabatically turn on Hs

$$H_1 = H_{S,T} \otimes \mathbb{1}_P + \mathbb{1}_S \otimes H_P.$$

Slowly interact using operator **A**

$$H_2 = H_1 + \underbrace{A \otimes |p_1\rangle\langle p_1|}_{H_{SP}},$$

Progress in full CI algorithm

Molecular Properties

- **O(D) evaluation of forces and derivatives**
- Kassal, AAG, ***J. Chem. Phys.*** (2009)

State preparation

- Kassal, Ward, AAG, ***J. Chem. Phys.*** (2009)
- Huang, Kais, AAG, ***Phys Chem .Chem. Phys.*** (2008)

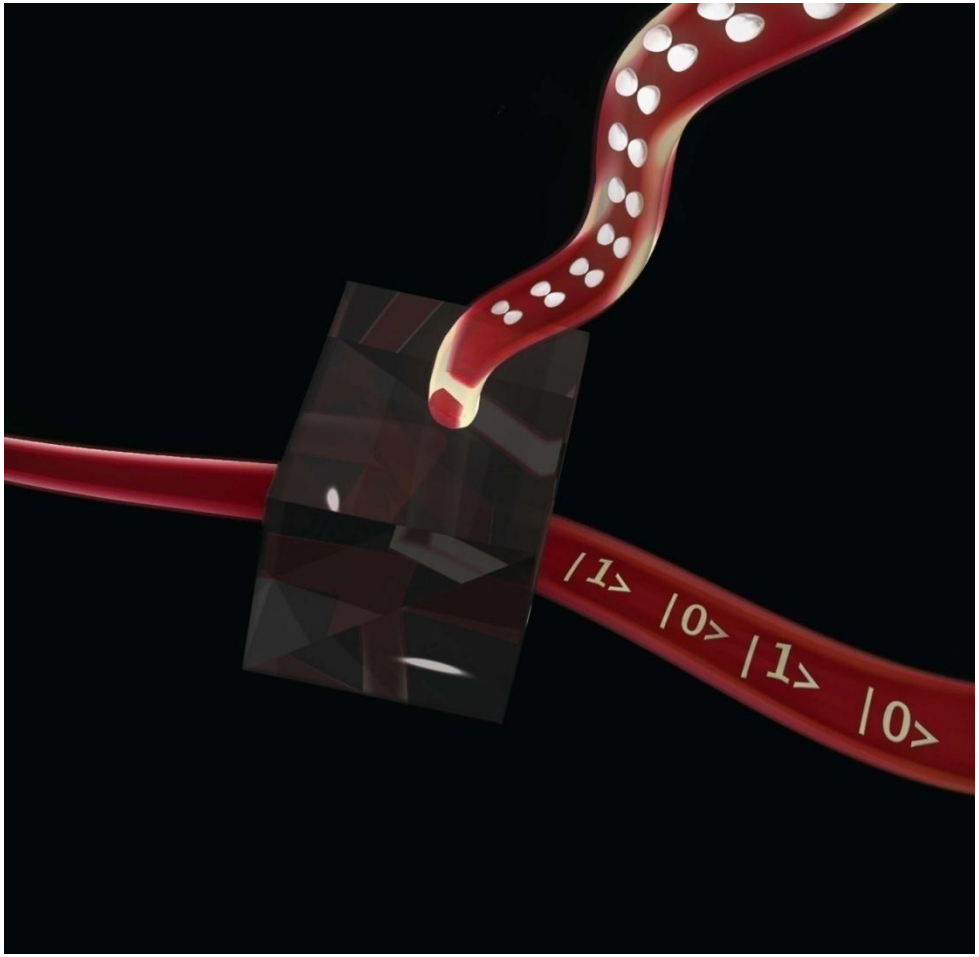
Resource estimation

- Whitfield, Biamonte, AAG, ***(Molecular Physics.*** (2011))

Error Correction

- C. R. Clark, …, K. Brown, **Phys. Rev. A. (2009)**

Quantum optics experiment



The first quantum computing for chemistry experiment

Quantum Technology Lab - Brisbane, Australia

Ben Lanyon

Andrew White

M. DeAlmeida

Geoff Gillet

Aspuru-Guzik research group - Harvard, USA

James Whitfield

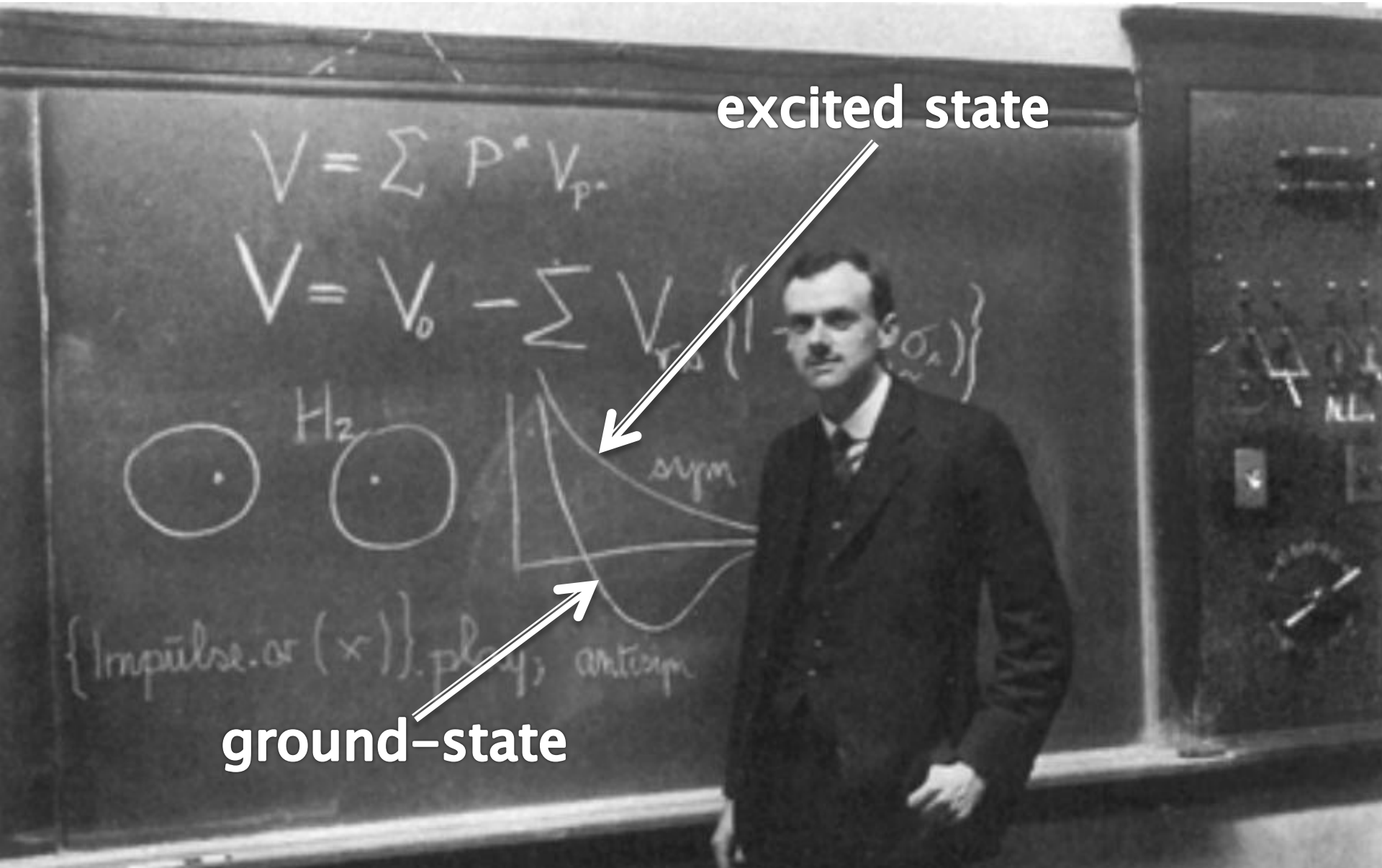
Ivan Kassal

Alejandro Perdomo

Masoud Mohseni

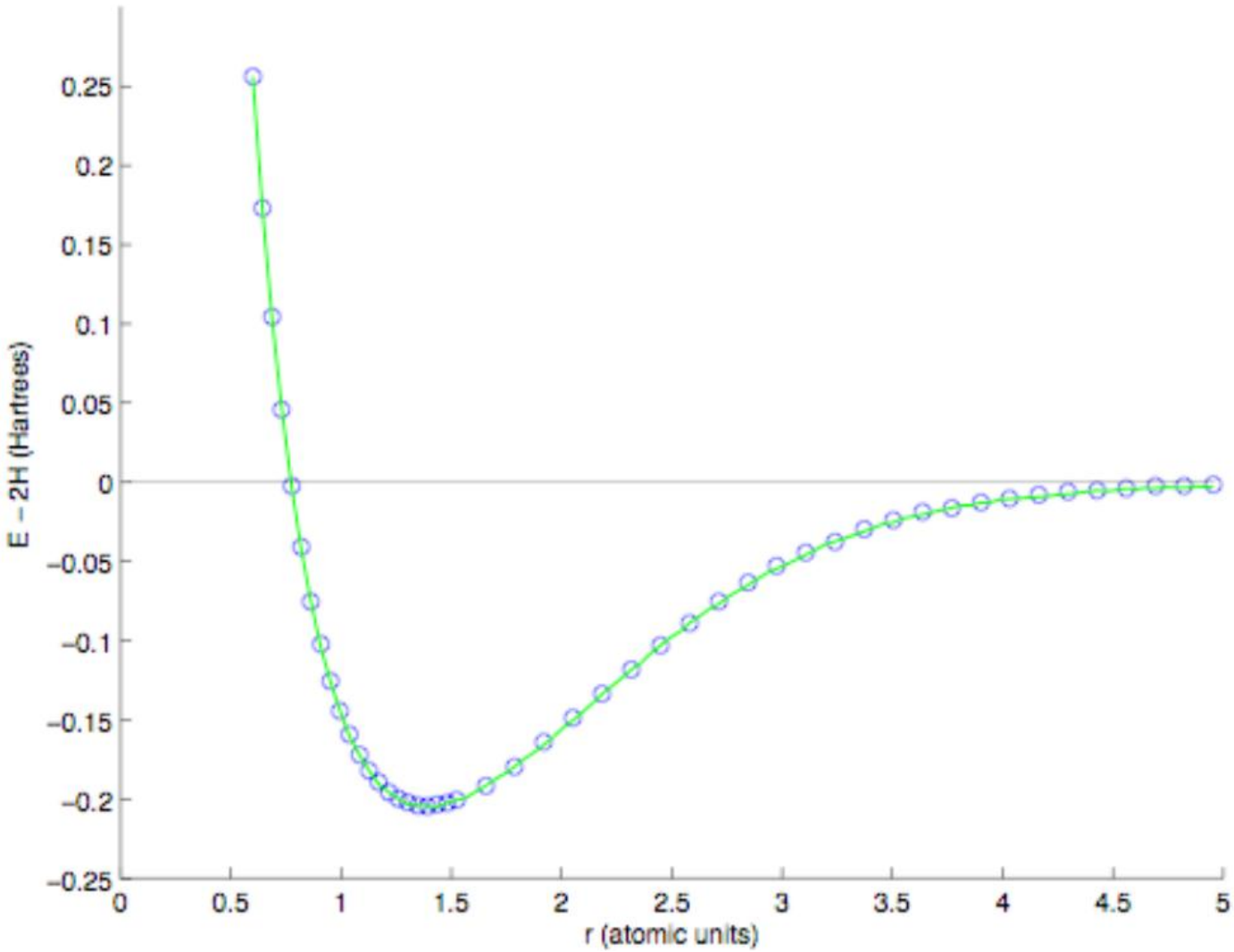
Lanyon, Whitfield, …, Kassal, Aspuru-Guzik, White, **Nature Chemistry** (2010)

The hydrogen molecule



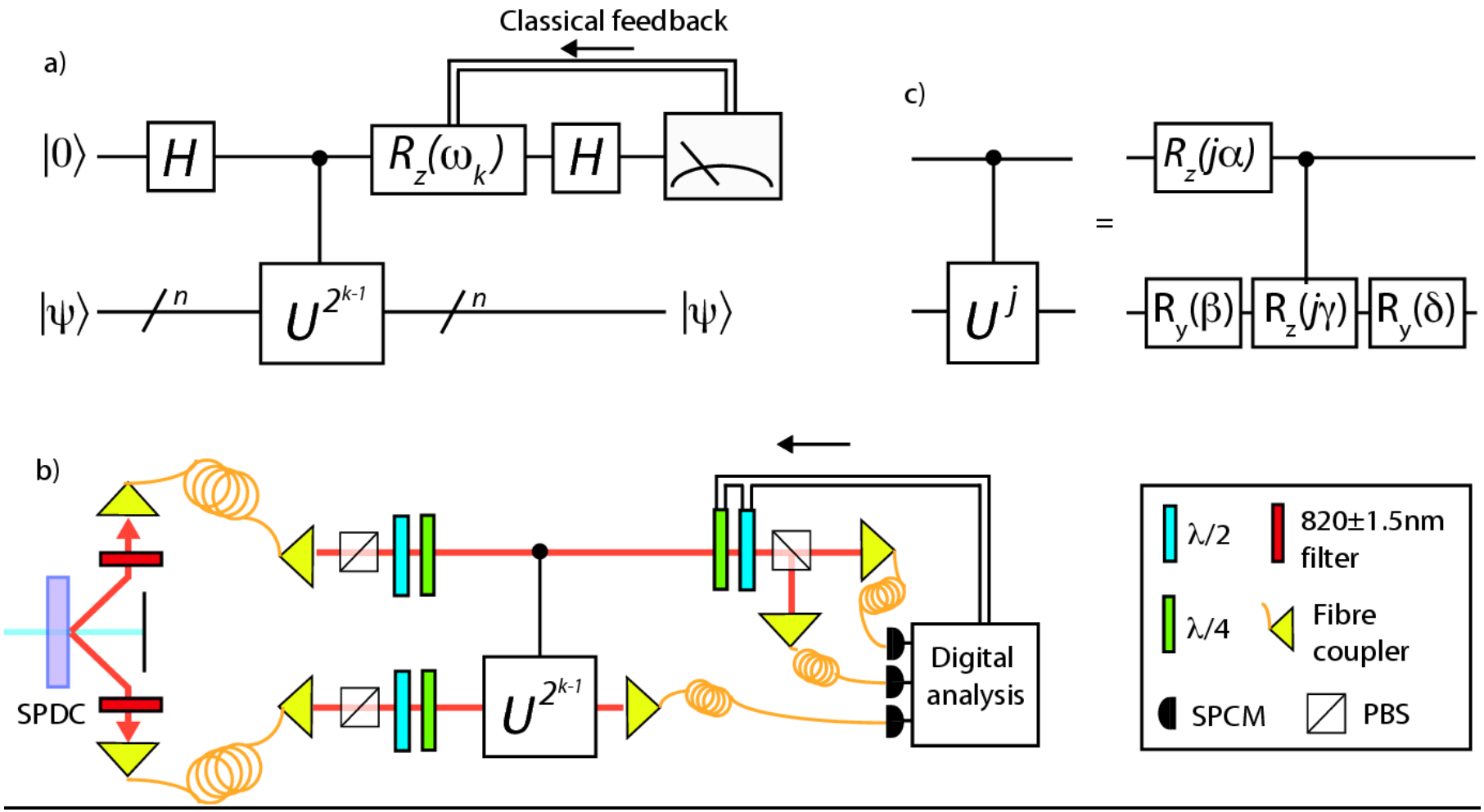
The hydrogen molecule

STO-3G Basis set, Full CI

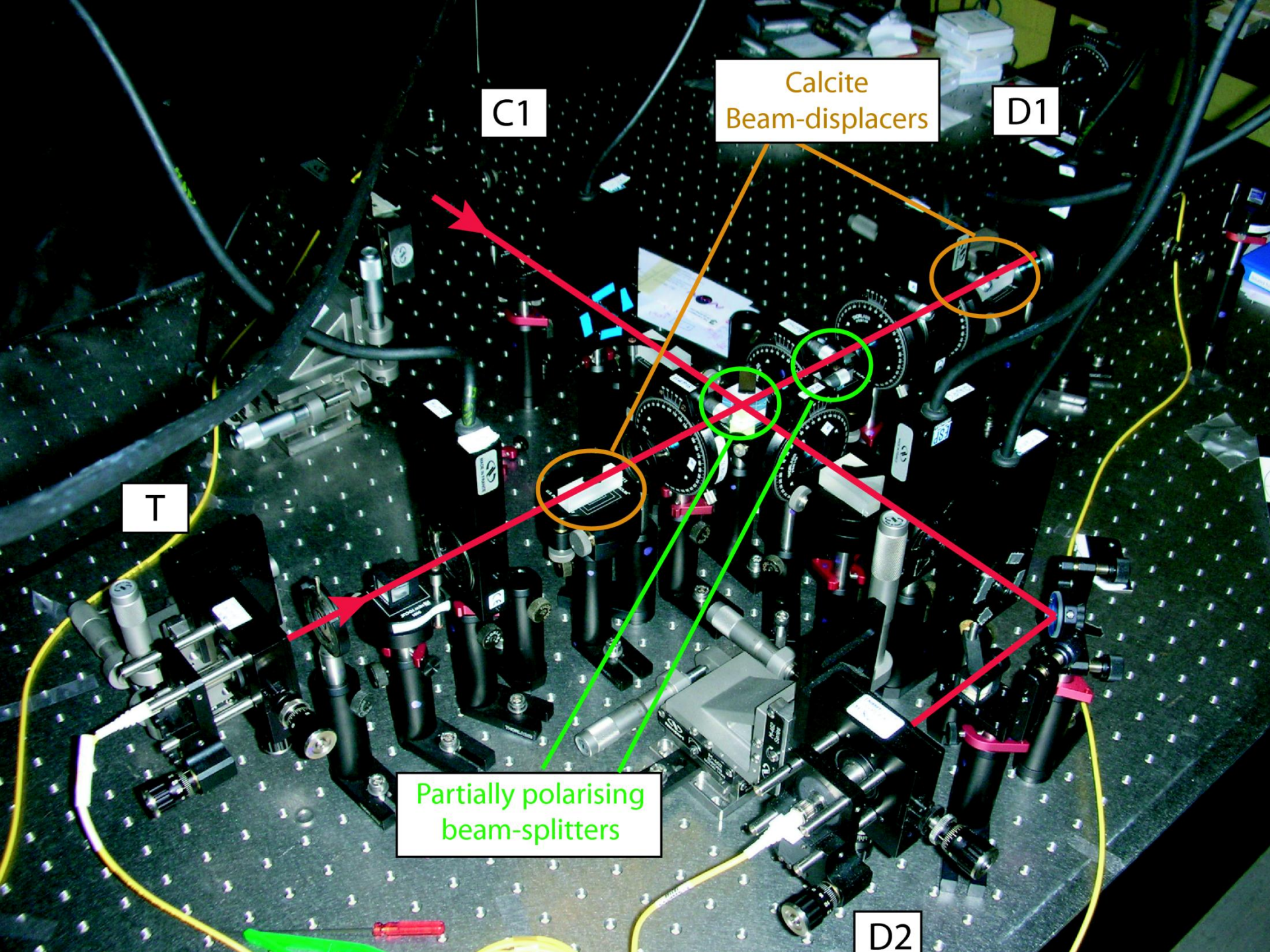


Lanyon, Whitfield, …, Kassal, Aspuru-Guzik, White, *Nature Chemistry* (2010)

Experimental setup

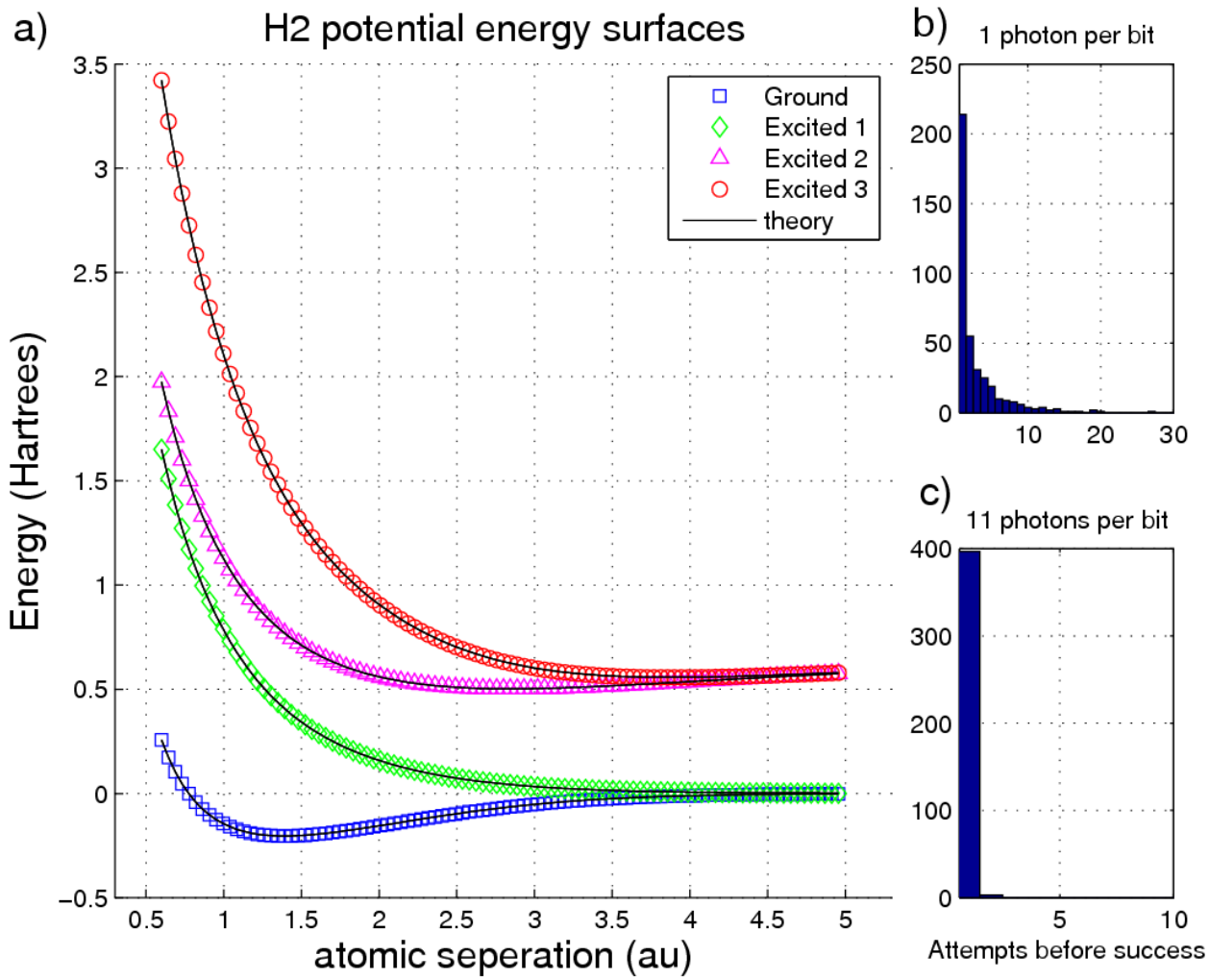


Lanyon, Whitfield, …, Kassal, Aspuru-Guzik, White, *Nature Chemistry* (2010)


C1
Calcite
Beam-displacers
D1
T
Partially polarising
beam-splitters
D2

Experimental energy curves

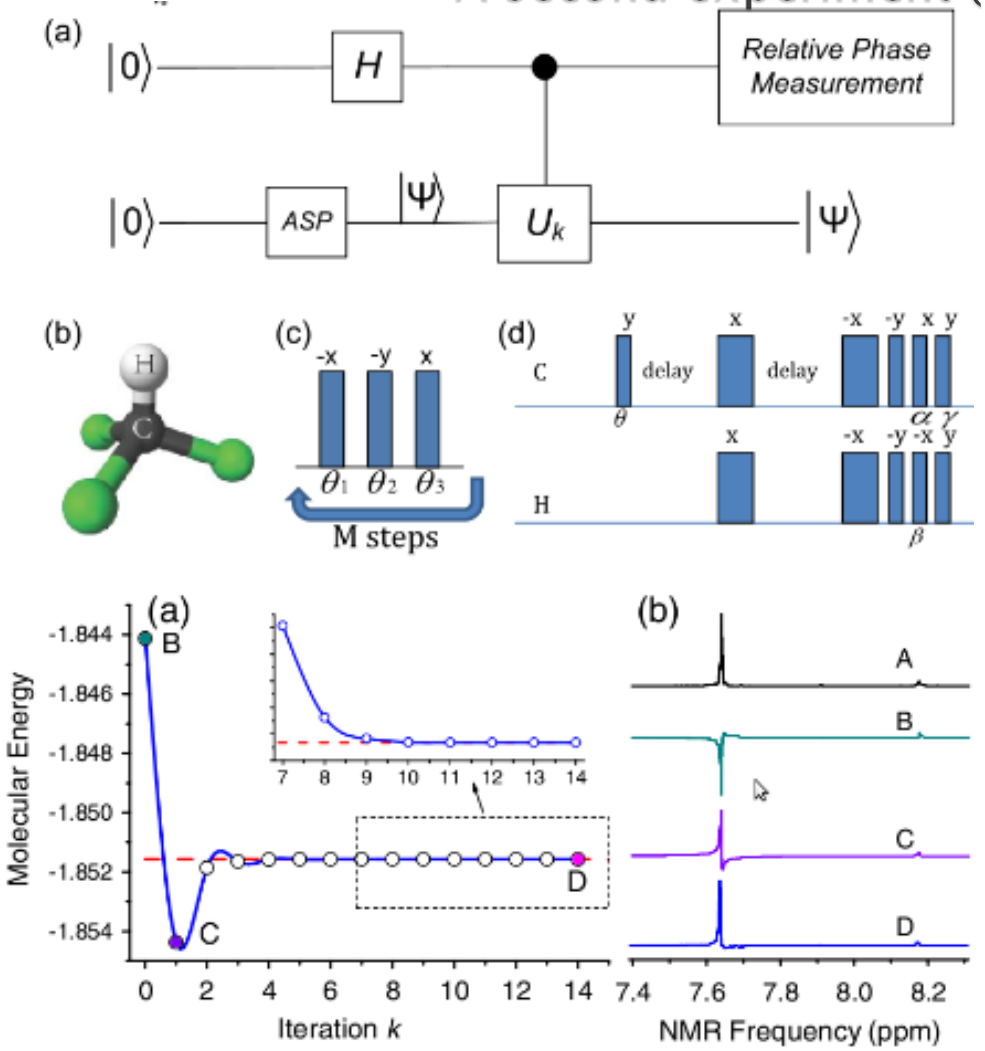
And photons per energy evaluation



Lanyon, Whitfield, …, Kassal, Aspuru-Guzik, White, *Nature Chemistry* (2010)

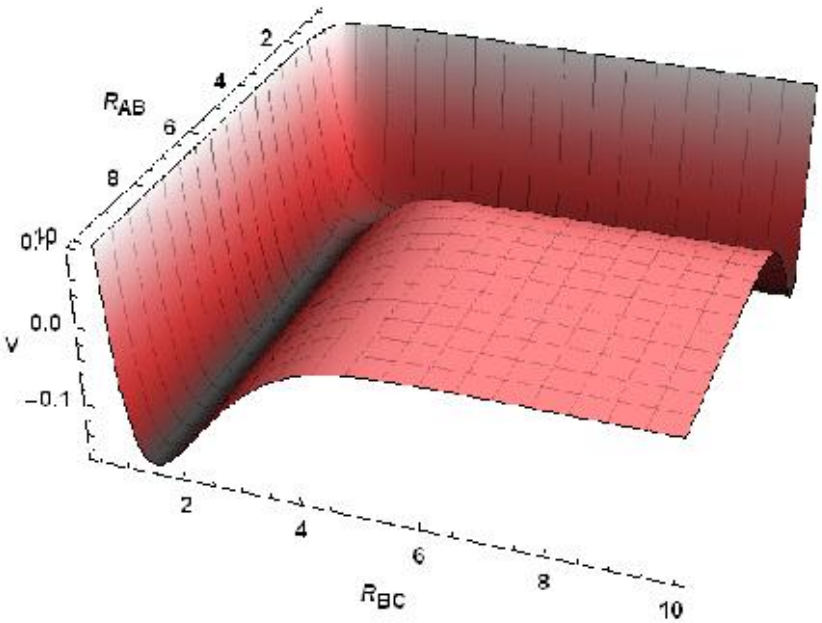
NMR calculation of H2 using chloroform!

A second experiment (3 months later)

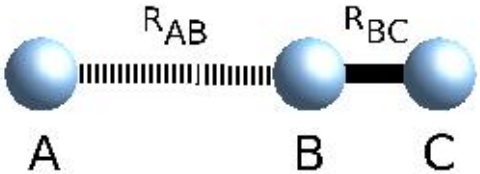


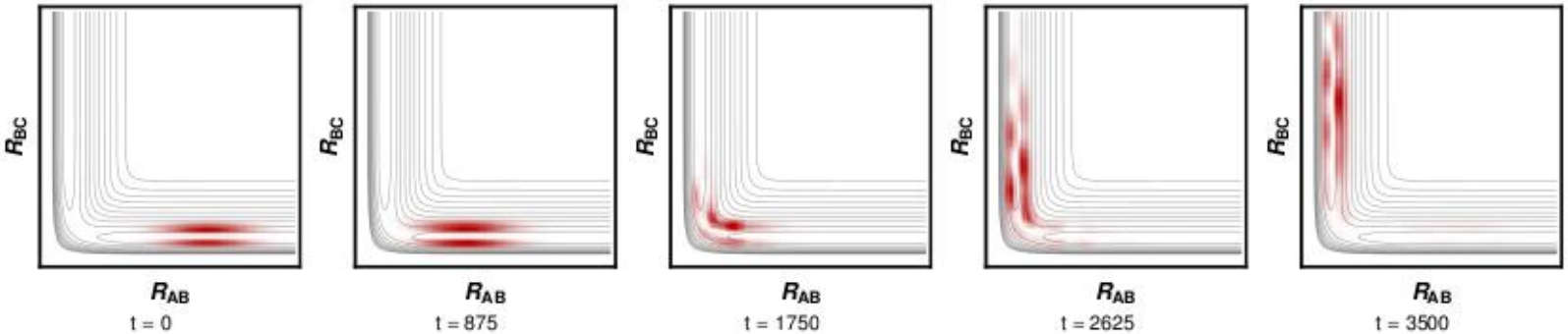
Du et al., *Phys. Rev. Lett.* (2010)

Chemical reaction dynamics



$$H + H_2 \longrightarrow H_2 + H$$

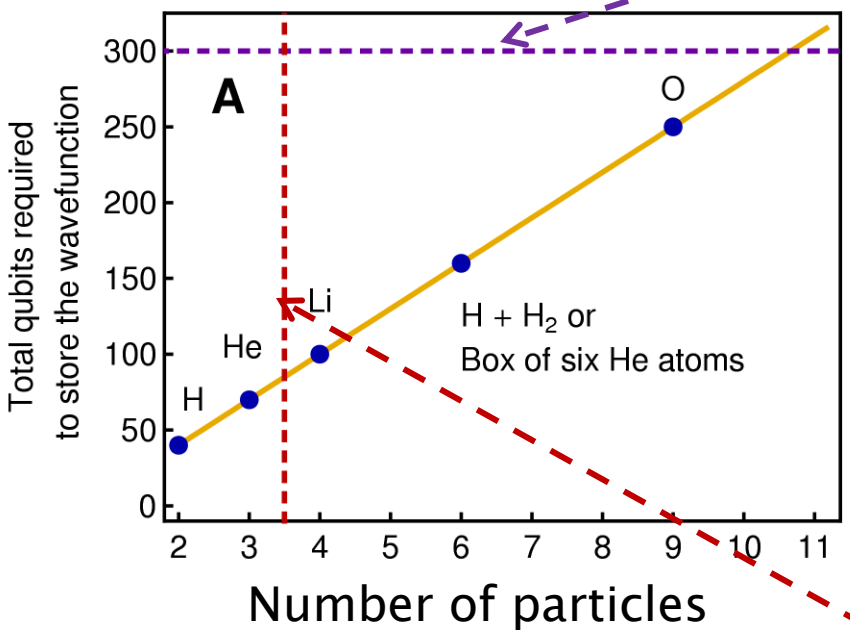


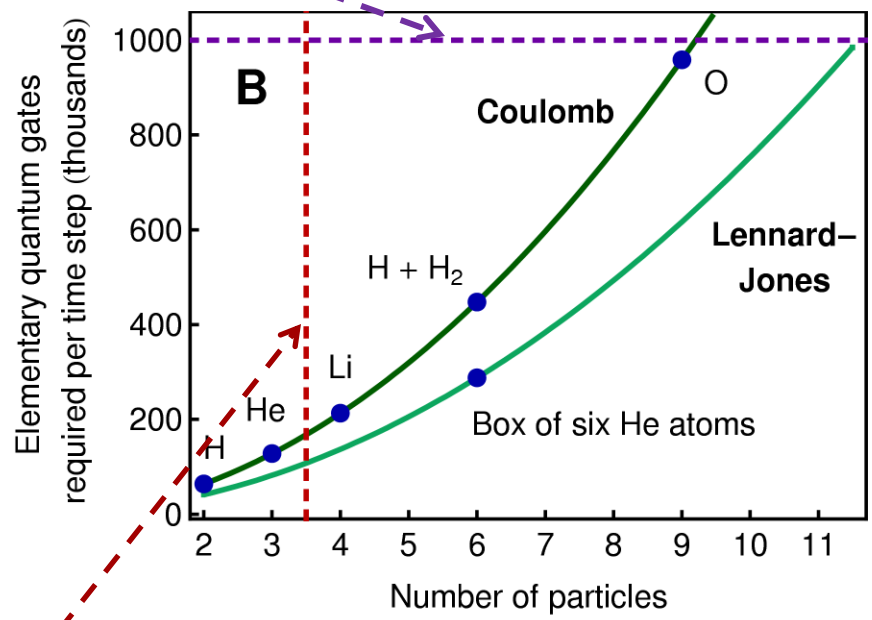


Kassal, …, Aspuru-Guzik *Proc. Nat. Acad. Sci.* (2008)

Chemical dynamics

300 bit, 1 giga-op quantum computer



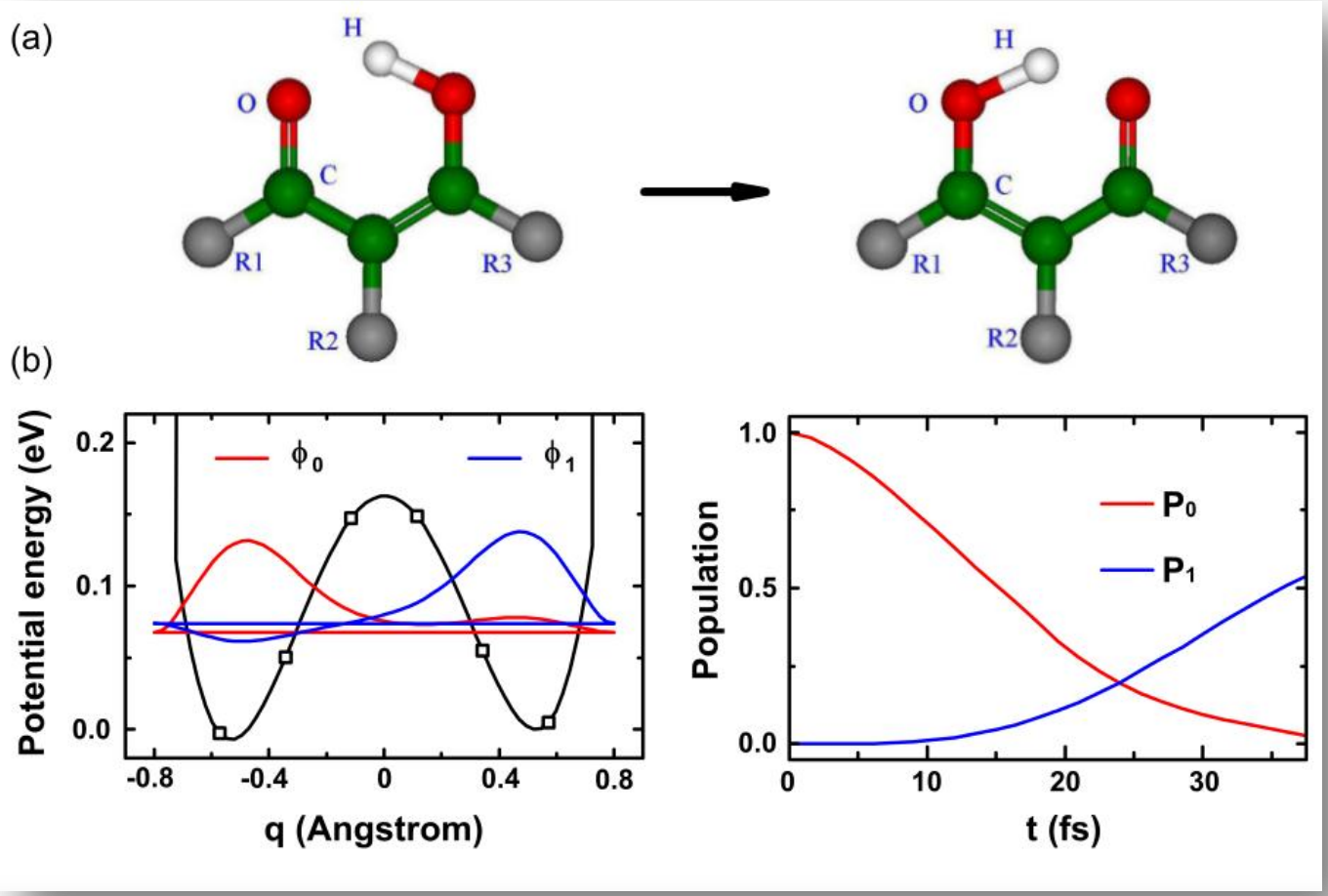


Supercomputer

Kassal, ..., Aspuru-Guzik *Proc. Nat. Acad. Sci.* (2008)

A. P. Steane, *Quant. Inf. And Comp.* (2007)

Chemical dynamics experiment

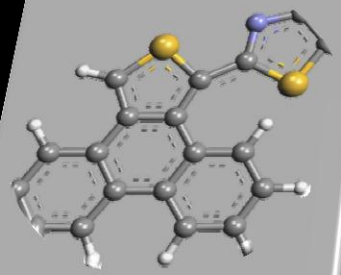


PRL **107,** 020501 (2011) PHYSICAL REVIEW LETTERS week ending 8 JULY 2011

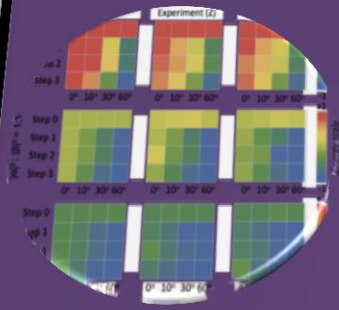
Simulation of Chemical Isomerization Reaction Dynamics on a NMR Quantum Simulator

Dawei Lu,[1] Nanyang Xu,[1] Ruixue Xu,[1] Hongwei Chen,[1] Jiangbin Gong,[2,3] Xinhua Peng,[1] and Jiangfeng Du[1,*]

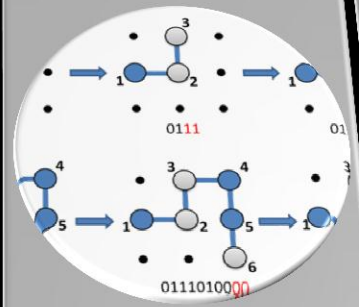
[1]*Hefei National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei, Anhui, 230026, China*



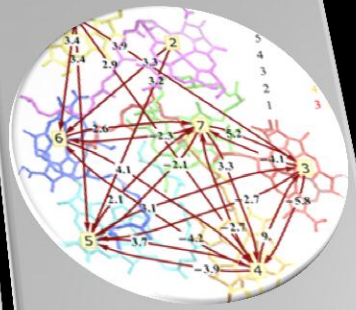
Quantum simulation for quantum chemistry



Preparing states for quantum simulation



Protein folding using adiabatic computers



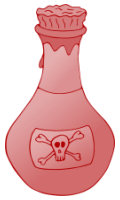
Simulating environment-assisted transport using quantum walks

What about state preparation?

Or how Arthur has to pick a poison

Adiabatic preparation

Projection using phase estimation



Cooling it, like a Demon! ™

Prepare a polynomially-scaling approximation from quantum chemistry

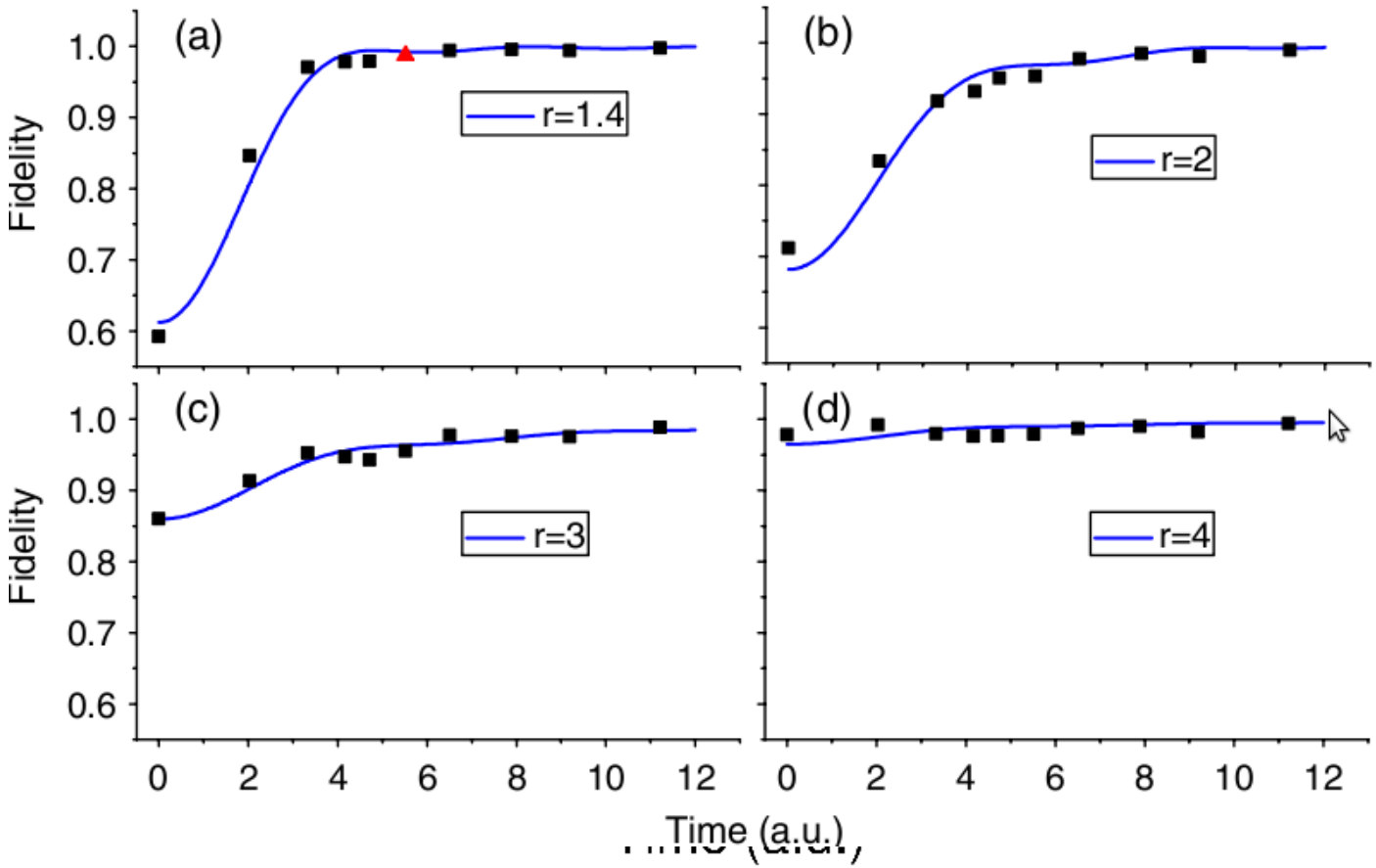
Adiabatic preparation

$$H_0 = H_{HartreeFock} \qquad H(\lambda) = (1-\lambda)H_{H_0} + \lambda H_{Full} \qquad H_f = H_{Full}$$

Start with a Hamiltonian that is easy to prepare and then deform adiabatically to the Full Hamiltonian.

If slow enough, you will have a high probability of remaining in the ground state

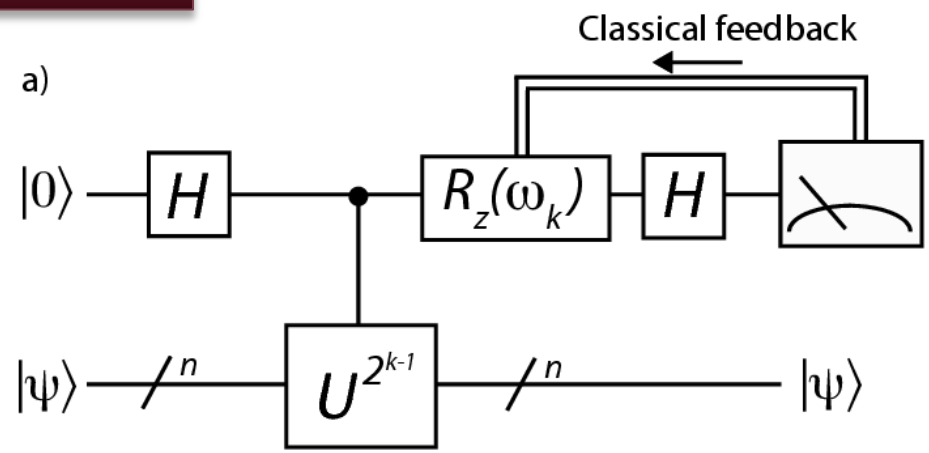
Adiabatic preparation

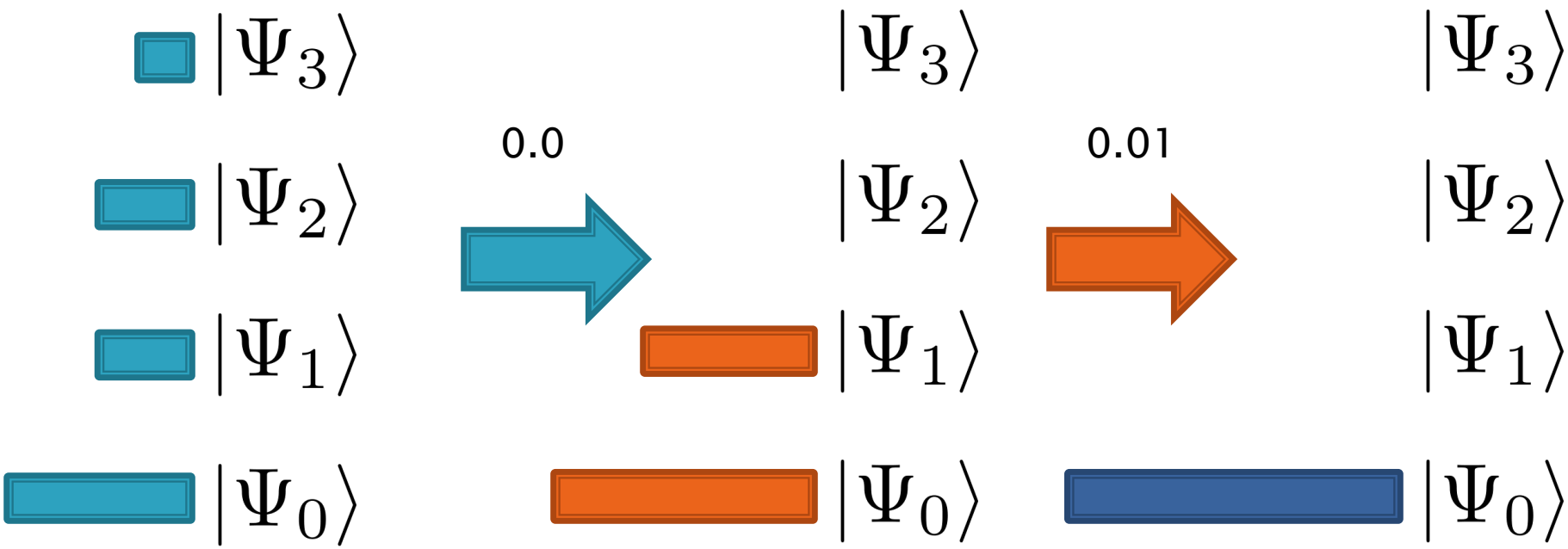


A. Aspuru-Guzik, A. D. Dutoi, P. J. Love, M. Head-Gordon, *Science* (2005)

Du et al., *Phys. Rev. Lett.* (2010)

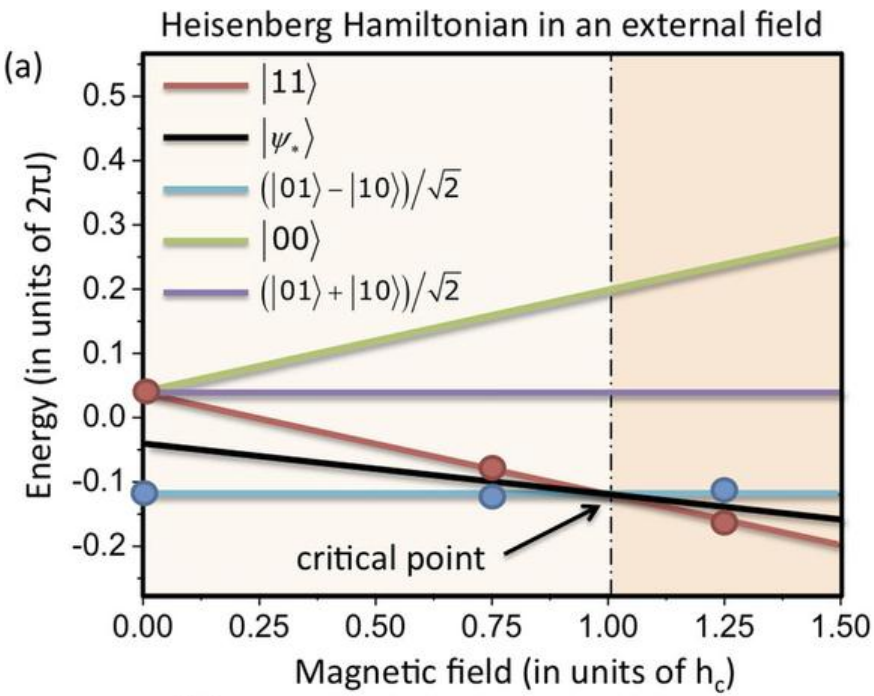
Adiabatic preparation



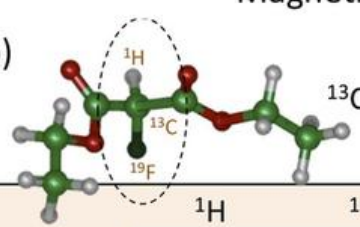


Solving Quantum Ground-State Problems with Nuclear Magnetic Resonance

Zhaokai Li[1]*, Man-Hong Yung[2]*, Hongwei Chen[1], Dawei Lu[1], James D. Whitfield[2], Xinhua Peng[1], Alán Aspuru-Guzik[2] & Jiangfeng Du[1]



(b)



^{13}C-labeled diethyl-fluoromalonate

	^{1}H	^{13}C	^{19}F	T1	T2
^{1}H	400 MHz			2.8 s	1.2 s
^{13}C	160.7 Hz	100 MHz		2.9 s	1.1 s
^{19}F	47.6 Hz	-194.4 Hz	376 MHz	3.1 s	1.3 s

Two-qubit experiment to demonstrate state preparation to 10-5 precision in the phase and simulate 2-qubit Heisienberg model "phase transition"

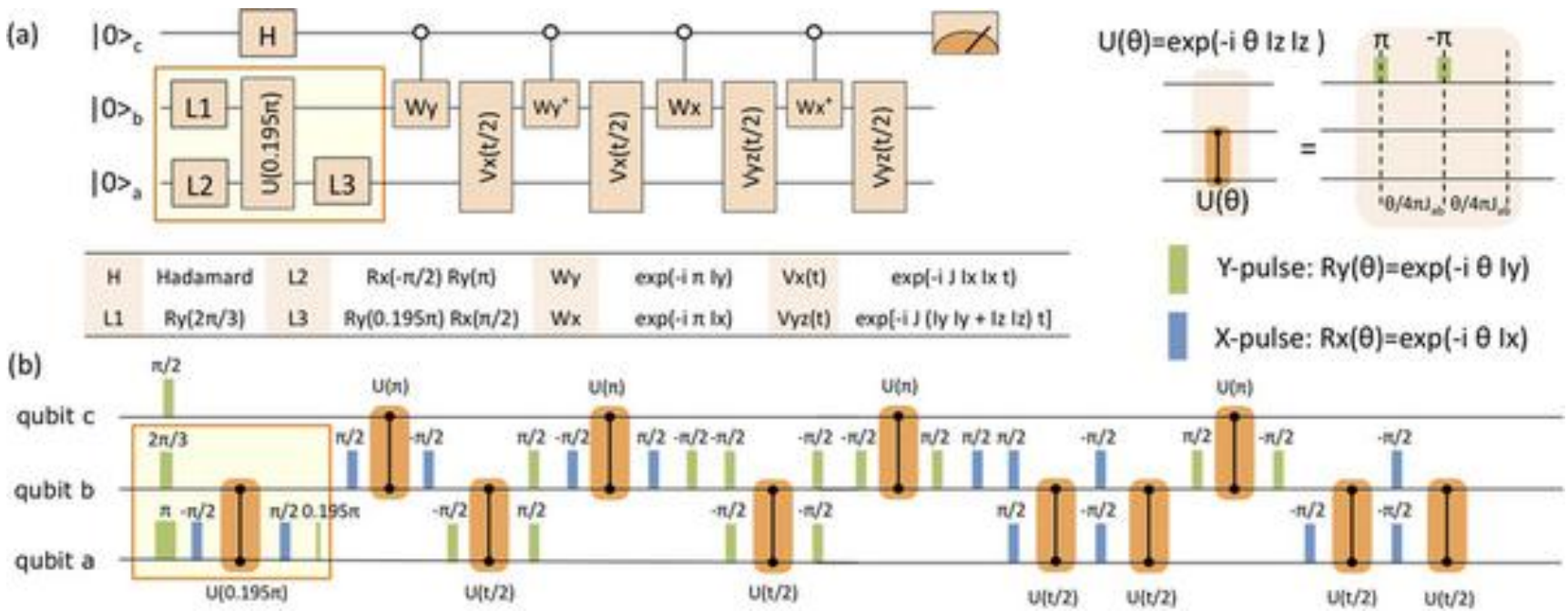
Li et al., Aspuru-Guzik, Du Scientific Reports 1:88 (2011)

Projection using phase estimation

SCIENTIFIC REPORTS

Solving Quantum Ground-State Problems with Nuclear Magnetic Resonance

Zhaokai Li[1]*, Man-Hong Yung[2]*, Hongwei Chen[1], Dawei Lu[1], James D. Whitfield[2], Xinhua Peng[1], Alán Aspuru-Guzik[2] & Jiangfeng Du[1]

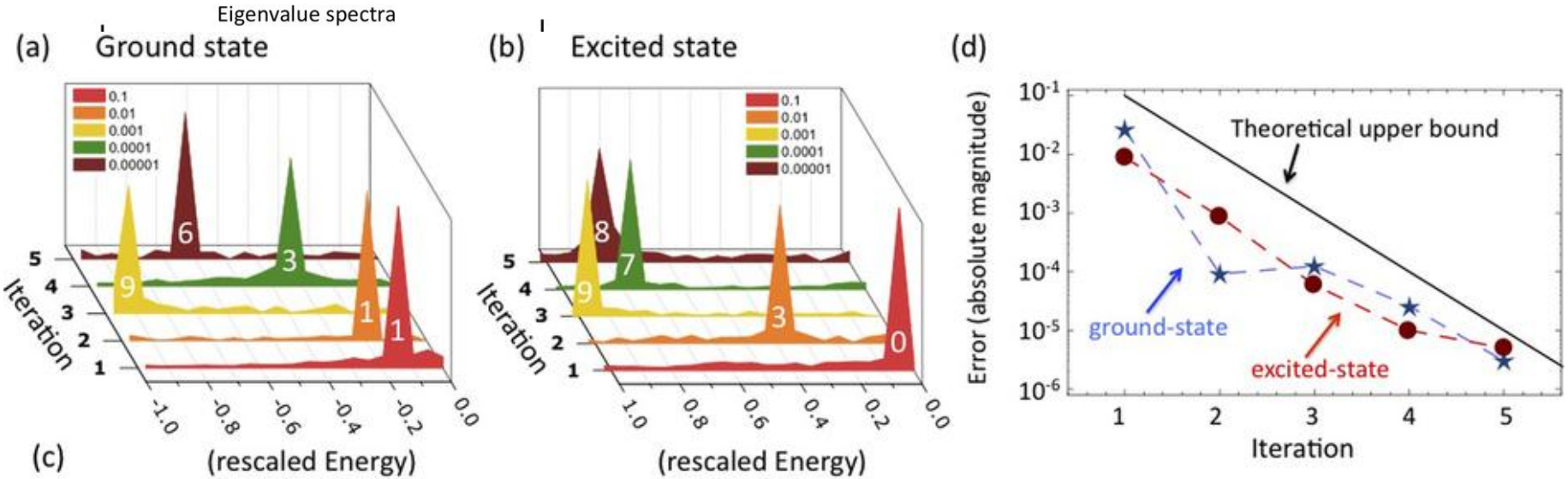


Projection using phase estimation

Li et al., Aspuru-Guzik, Du Scientific Reports 1:88 (2011)

Solving Quantum Ground-State Problems with Nuclear Magnetic Resonance

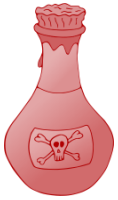
Zhaokai Li[1]*, Man-Hong Yung[2]*, Hongwei Chen[1], Dawei Lu[1], James D. Whitfield[2], Xinhua Peng[1], Alán Aspuru-Guzik[2] & Jiangfeng Du[1]



Iteration	1	2	3	4	5	Theory
Ground state	-0.145937	-0.119458	-0.119242	-0.119340	-0.119363	-0.119366
Excited state	0.048645	0. 038916	0.039729	0.039778	0.039783	0.039788

Projection using phase estimation

Li et al., Aspuru-Guzik, Du Scientific Reports 1:88 (2011)



Cooling it, like a Demon! ™

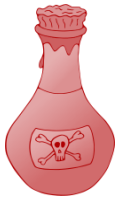
Quantum Cooling via Random Walk

State preparation (and cooling) remains one of the hardest quantum computation tasks

We present a simple, experimentally implementable cooling algorithm

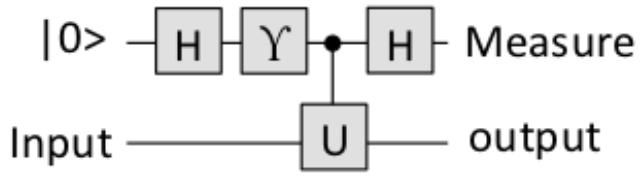
The method is related to: imaginary time evolution, evaporative cooling, weak measurements...

Jin-Shi Xu, Man-Hong Yung, Xiao-Ye Xu, Sergio Boixo, Zheng-Wei Zhou,Chuan-Feng Li, Alan Aspuru-Guzik, and Guang-Can Guo, Submitted (2011)



Cooling it, like a Demon! ™

Meet the cooling module



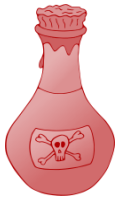
H_S = System Hamiltonian; $U = \exp(-iH_S t)$,

H = Hadamard gate; $\Upsilon = |0\rangle\langle 0| - i\, e^{i\Upsilon} |1\rangle\langle 1|$

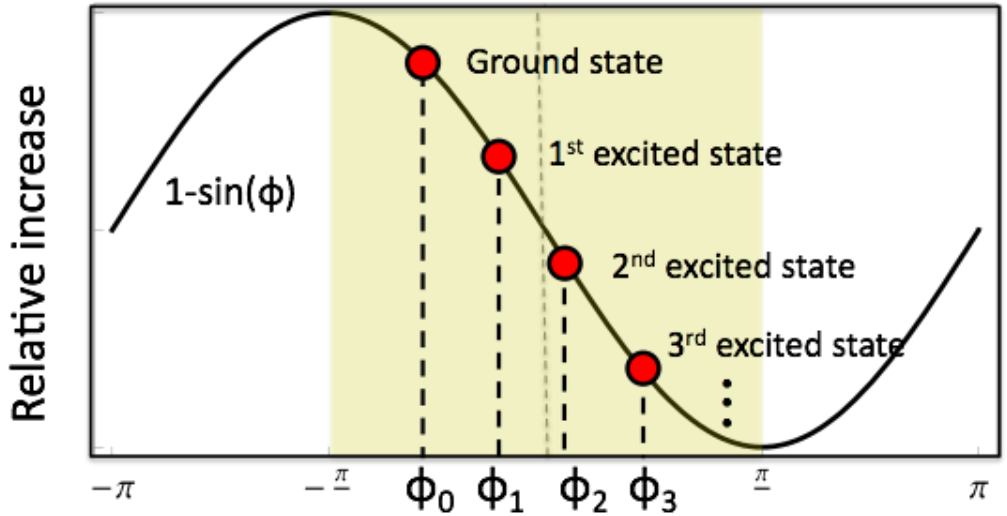
Before measurement…

the state becomes

Cooling modules are cool.

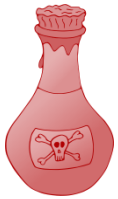


Cooling it, like a Demon! ™

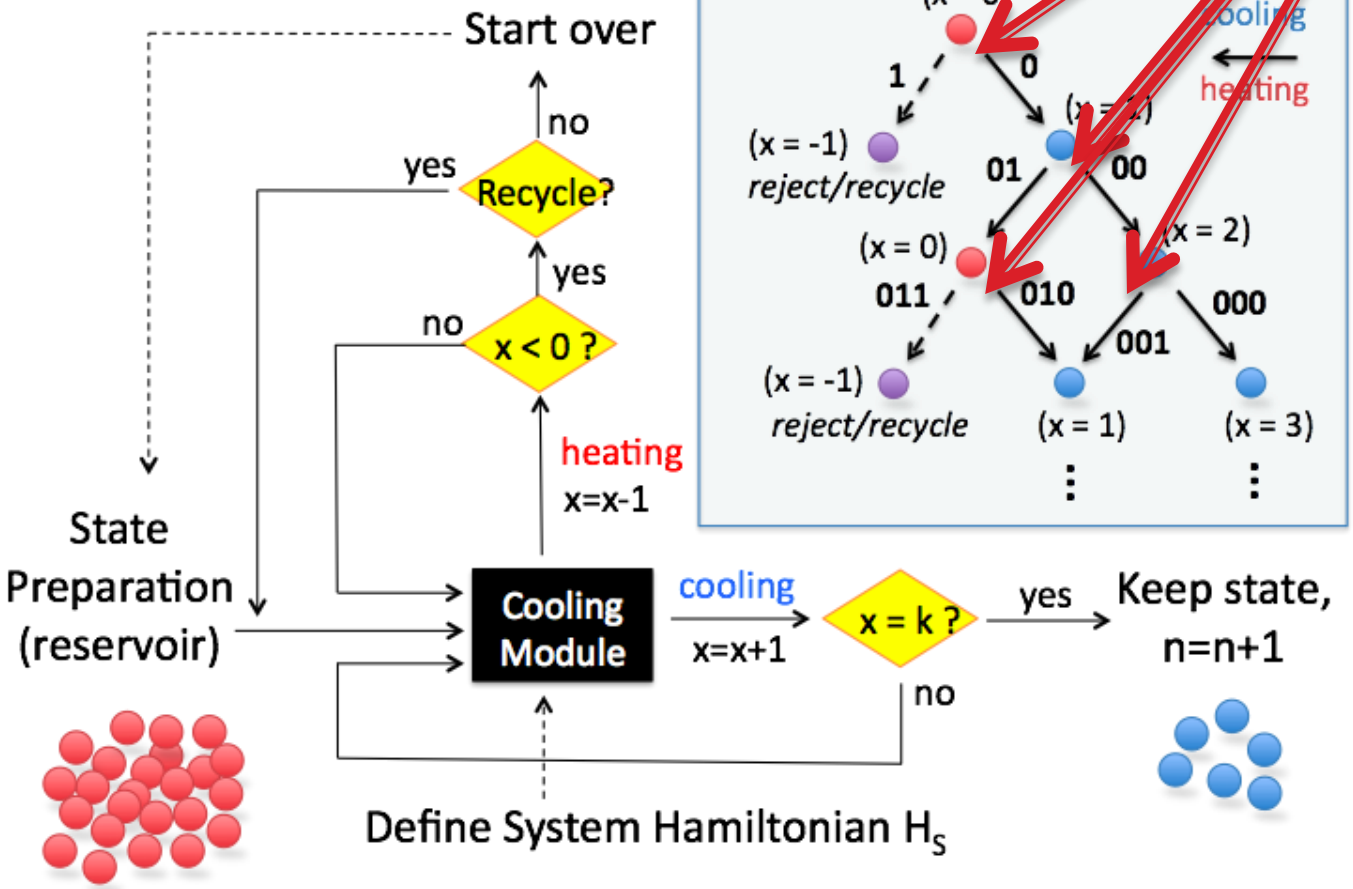


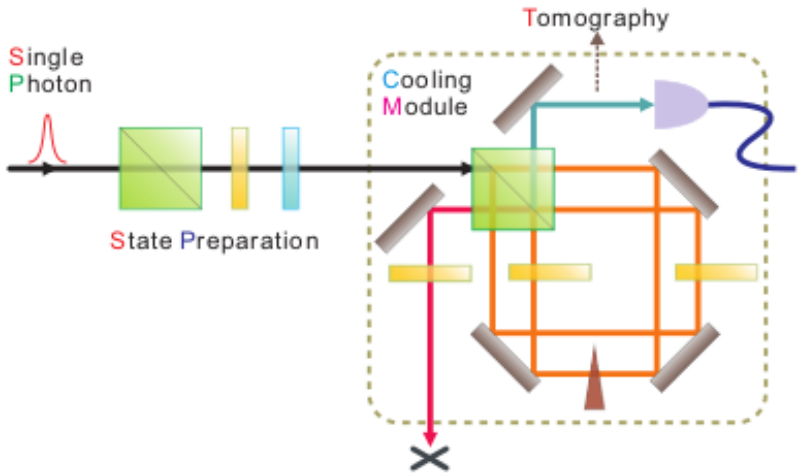
Input state	any state $\|\psi\rangle$, $\|\psi\rangle = \Sigma_k\ c_k\ \|e_k\rangle$, where $H\ \|e_k\rangle = E_k\ \|e_k\rangle$
Output state	$(1+i\ e^{i\Upsilon}\ U)\|\psi\rangle$ or $(1-i\ e^{i\Upsilon}\ U)\|\psi\rangle$ (up to a normalization constant)
Cooling	$\|\psi\rangle \rightarrow (1-i\ e^{i\Upsilon}\ U)\|\psi\rangle$, $\|c_k\|^2 \rightarrow \|c_k\|^2 \times (1-\sin(\phi_k))$, where $\phi_k = E_k t - \Upsilon$

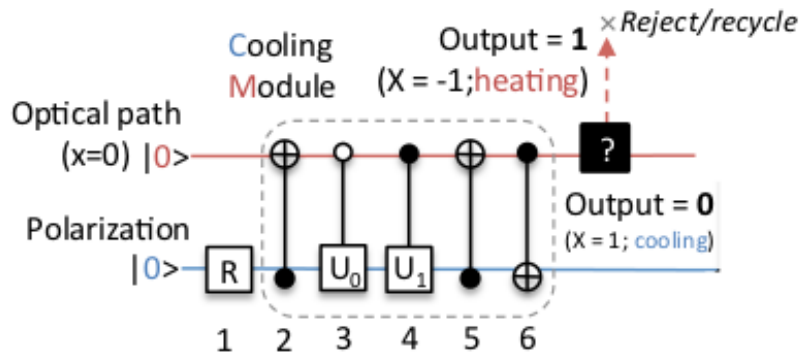
Cooling via Random Walk



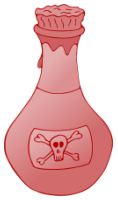
Cooling it, like a Demon! ™





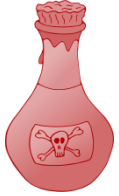


Step 1:	$(\alpha\,\|0\rangle + \beta\,\|1\rangle)\|0\rangle$	Step 4:	$\alpha\,(a\|0\rangle + b\|1\rangle)\|0\rangle + \beta\,(a\|0\rangle + b\|1\rangle)\|1\rangle$		$R\|0\rangle = \alpha\,\|0\rangle + \beta\,\|1\rangle$
Step 2:	$\alpha\,\|0\rangle\|0\rangle + \beta\|1\rangle\|1\rangle$	Step 5:	$(\alpha\,a\|0\rangle + \beta\,b\|1\rangle)\|0\rangle + (\alpha\,b\|1\rangle + \beta\,a\,\|0\rangle)\,\|1\rangle$	Where:	$U_0\,\|0\rangle = U_1\,\|1\rangle = a\,\|0\rangle + b\,\|1\rangle$
Step 3:	$\alpha\,(a\|0\rangle + b\|1\rangle)\|0\rangle + \beta\,\|1\rangle\|1\rangle$	Step 6:	$(\alpha\,a\|0\rangle + \beta\,b\|1\rangle)\|0\rangle + (\alpha\,b\|0\rangle + \beta\,a\,\|1\rangle)\,\|1\rangle$		$a = (1+i\,e^{i\theta})/2,\ b = (1-i\,e^{i\theta})/2$

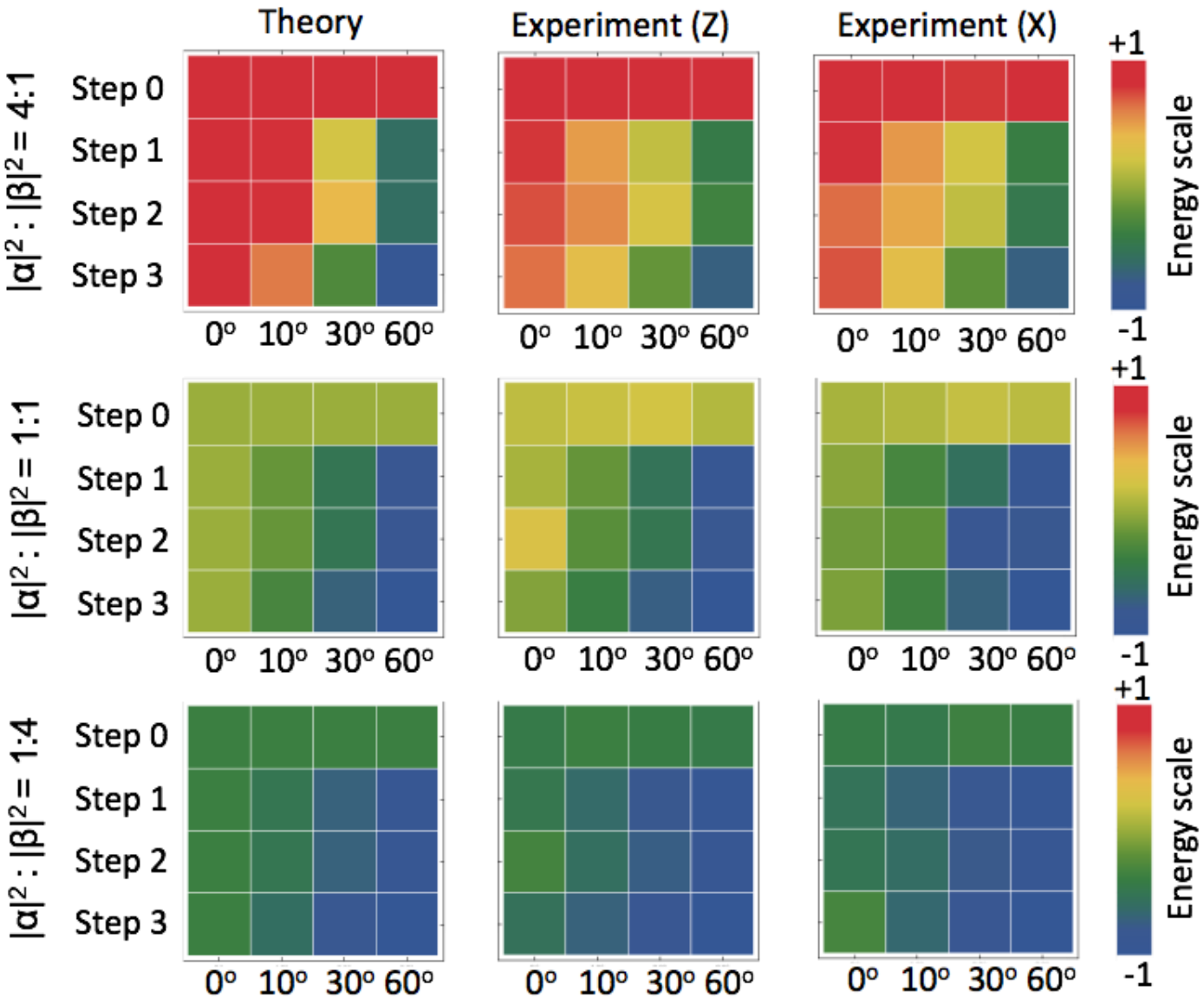


Cooling it, like a Demon! ™

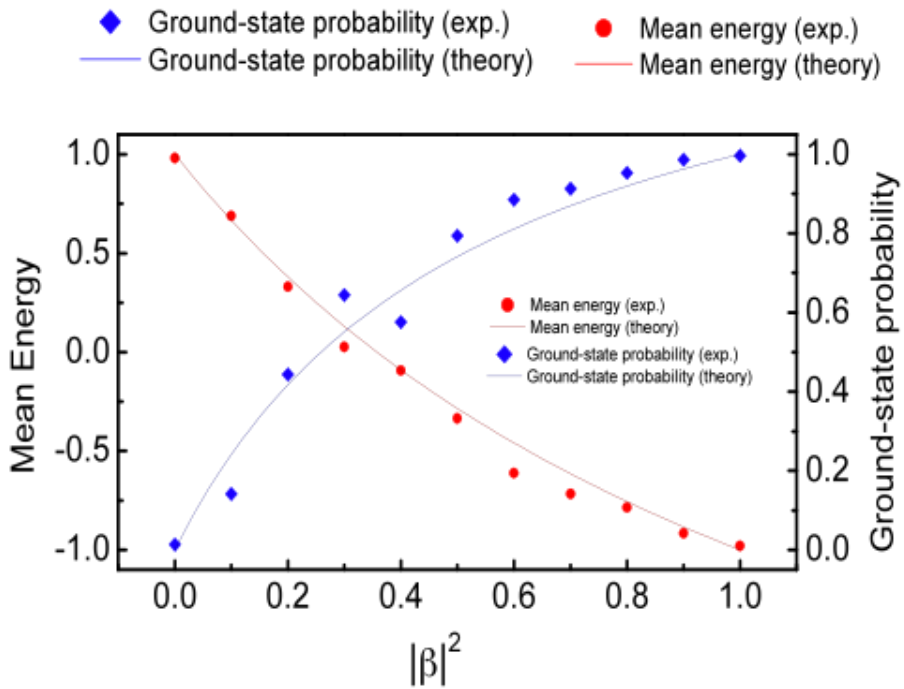
Experimental data

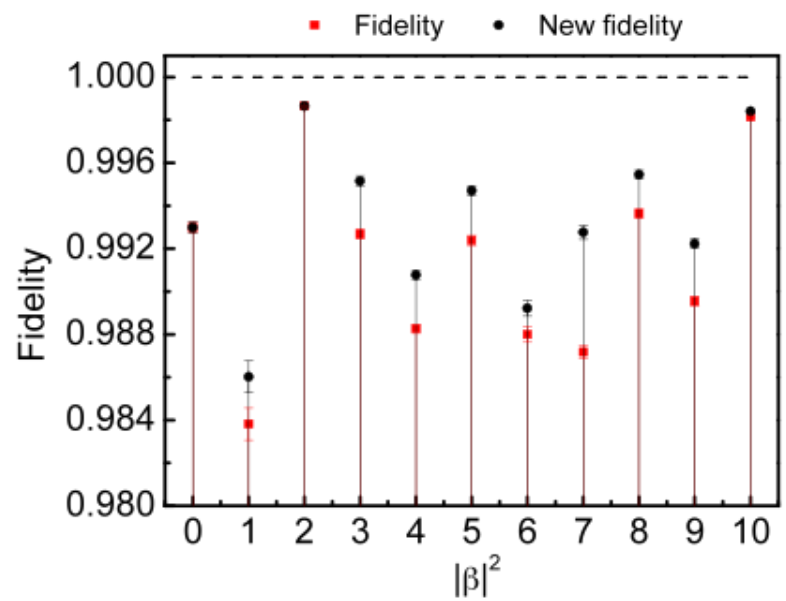


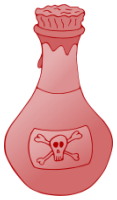
Cooling it, like a Demon! ™



Three cooling steps fidelity



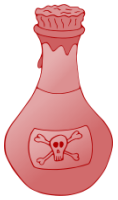




Cooling it, like a Demon! ™

General basic scaling

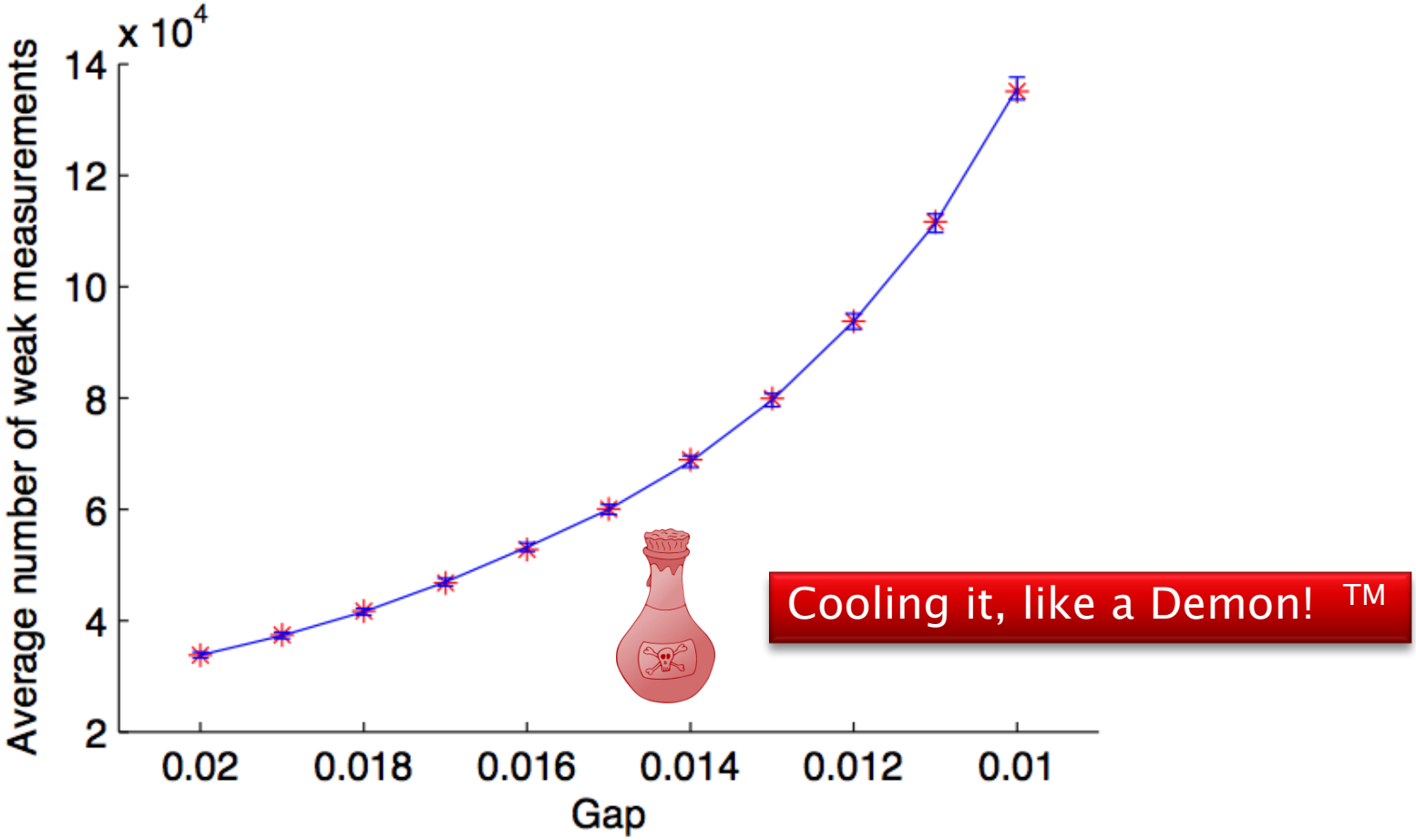
	Projection	Amplitude amplification
Weak measurement	$\Delta^{-2}p^{-1}$	$\Delta^{-2}p^{-1/2}$
Phase estimation	$\Delta^{-1}p^{-1}$	$\Delta^{-1}p^{-1/2}$



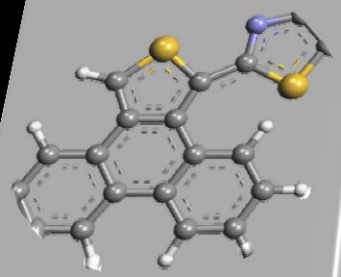
Cooling it, like a Demon! ™

Quadratic gap scaling

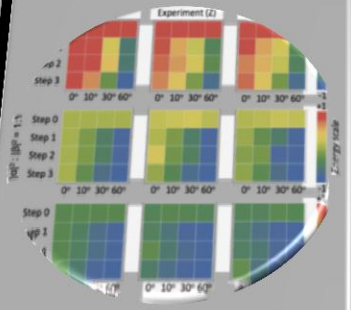
Optimal refreshing



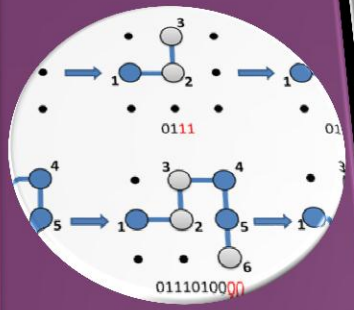
Initial ground state pop.: 0.2. Final: 0.95



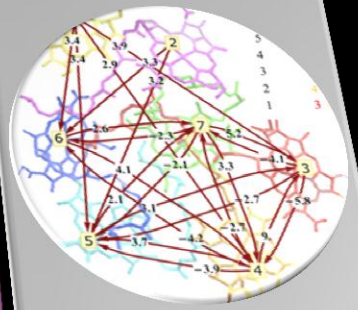
Quantum simulation for quantum chemistry



Preparing states for quantum simulation

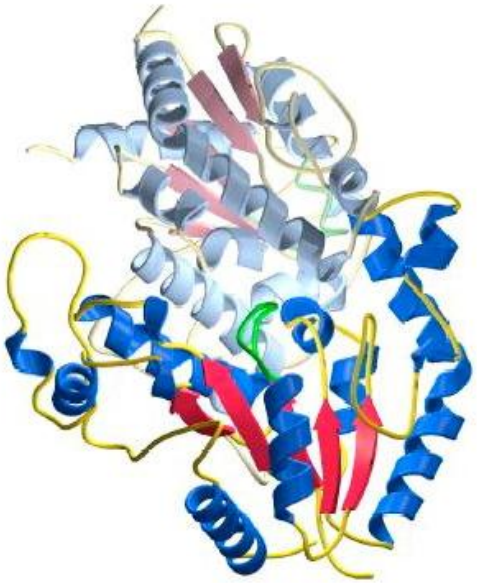


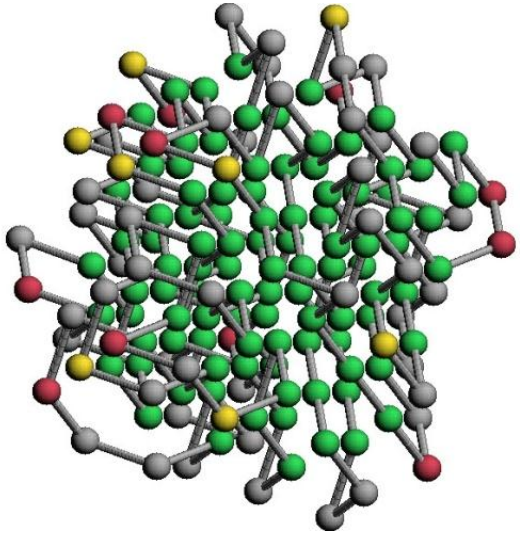
Protein folding using adiabatic computers



Simulating environment-assisted transport using quantum walks

Towards lattice folding on a quantum device



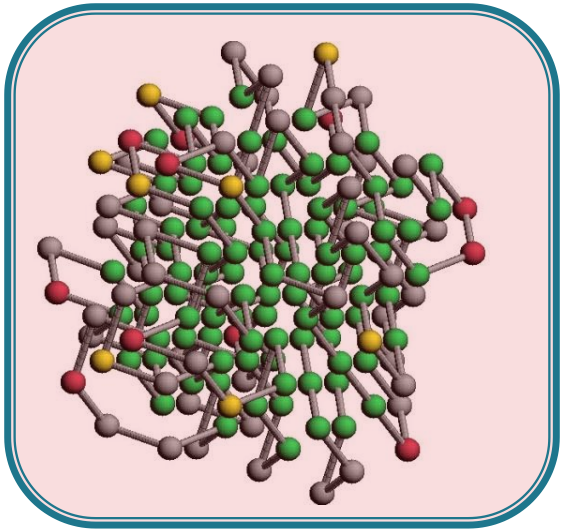


Continuum protein → Lattice model → Quantum annealing machine

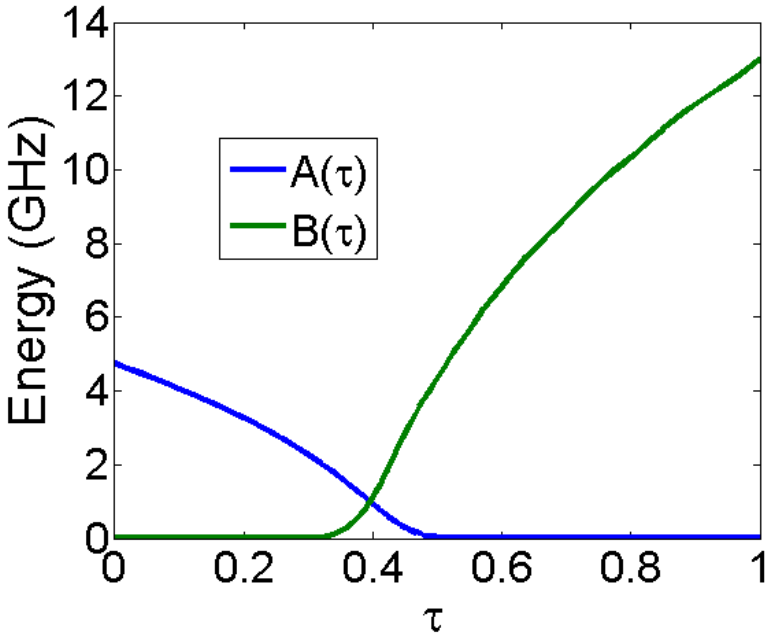
1) A. Perdomo, C. Truncik, I. Tubert-Brohman, G. Rose, and A. Aspuru-Guzik. *Phys. Rev. A,* 78(1):012320, 2008.

2) A. Perdomo-Ortiz, S. Venegas-Andraca, and A. Aspuru-Guzik. A study of heuristic guesses for adiabatic quantum computation. *Quantum Inf. Process.*, 10, 33-52 (2011)

Lattice folding into spin-glass Hamiltonian



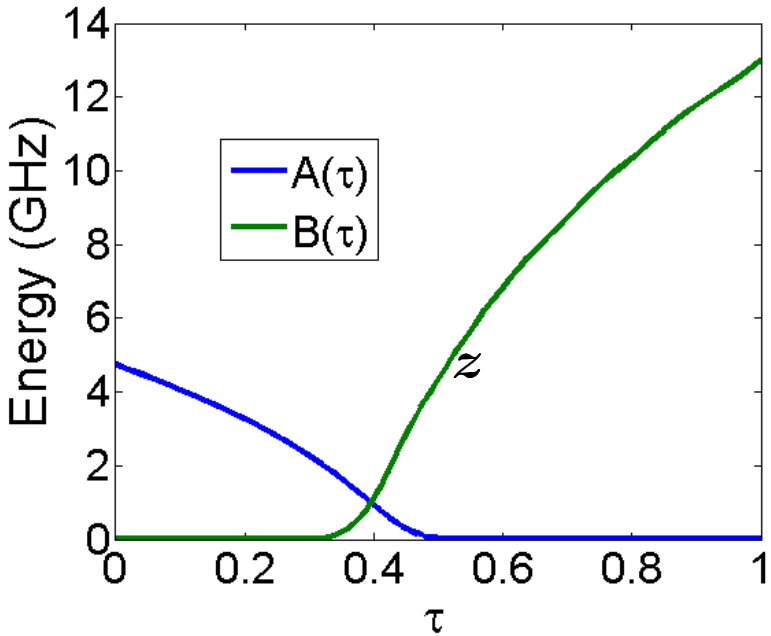
$$H_p = \sum_i^N h_i \sigma_i^z + \sum_{j>i}^N J_{ij} \sigma_i^z \sigma_j^z$$



Quantum annealing

$$H(\tau) = A(\tau) \sum_i \sigma_i^x + B(\tau) H_p$$

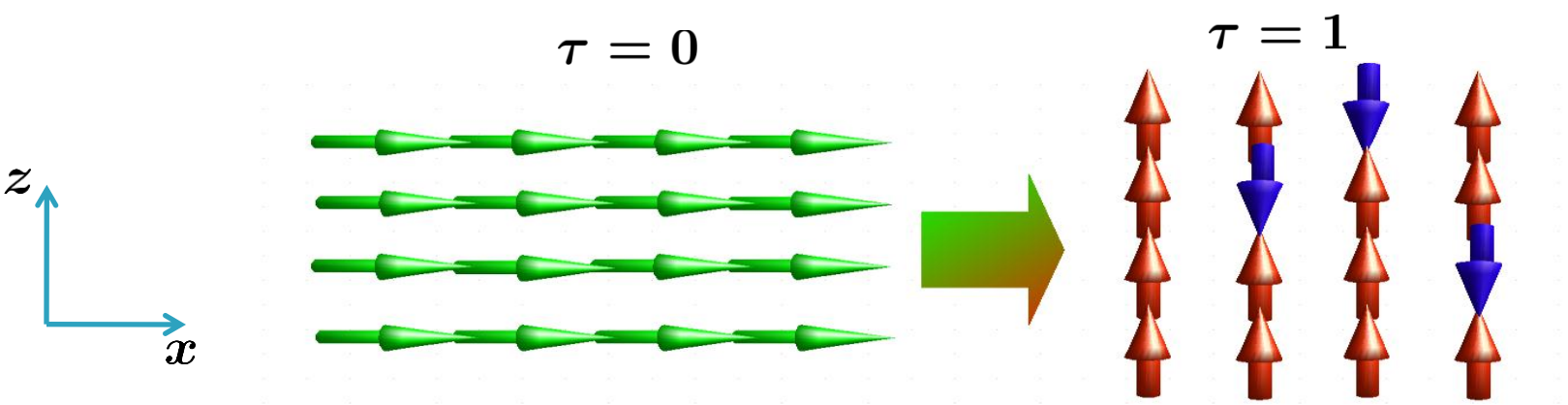
$$\tau = t/t_{run} \qquad t_{run} = 148 \mu s$$



Quantum annealing

$$H(\tau) = A(\tau)\sum_i \sigma_i^x + B(\tau)H_p$$

$$\tau = t/t_{run} \qquad t_{run} = 148\mu s$$



Transverse field ON
Longitudinal field OFF

Transverse field OFF
Longitudinal field ON

Rules of the game: Hydrophobic-Polar (HP) model

Assumptions:

1) Protein as a chain of beads (amino acids) joined by strings (peptide bonds)

2) Only two types of amino acids:

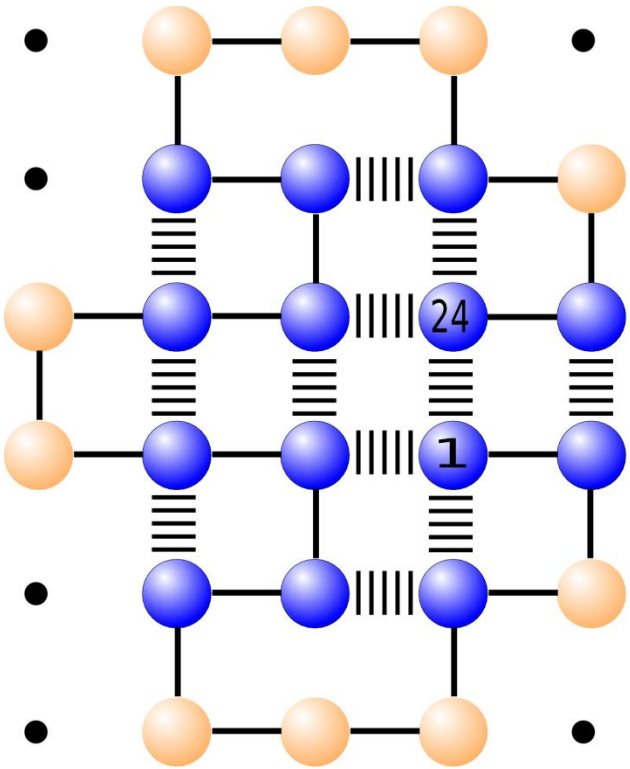
Hydrophobic =

Polar =

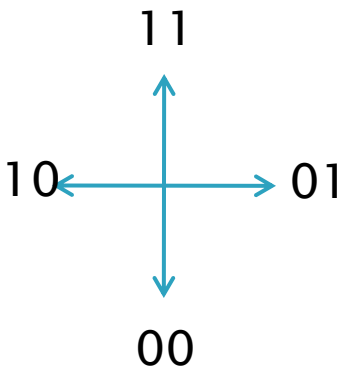
3) Amino acids allowed to move in a 2D or 3D square lattice

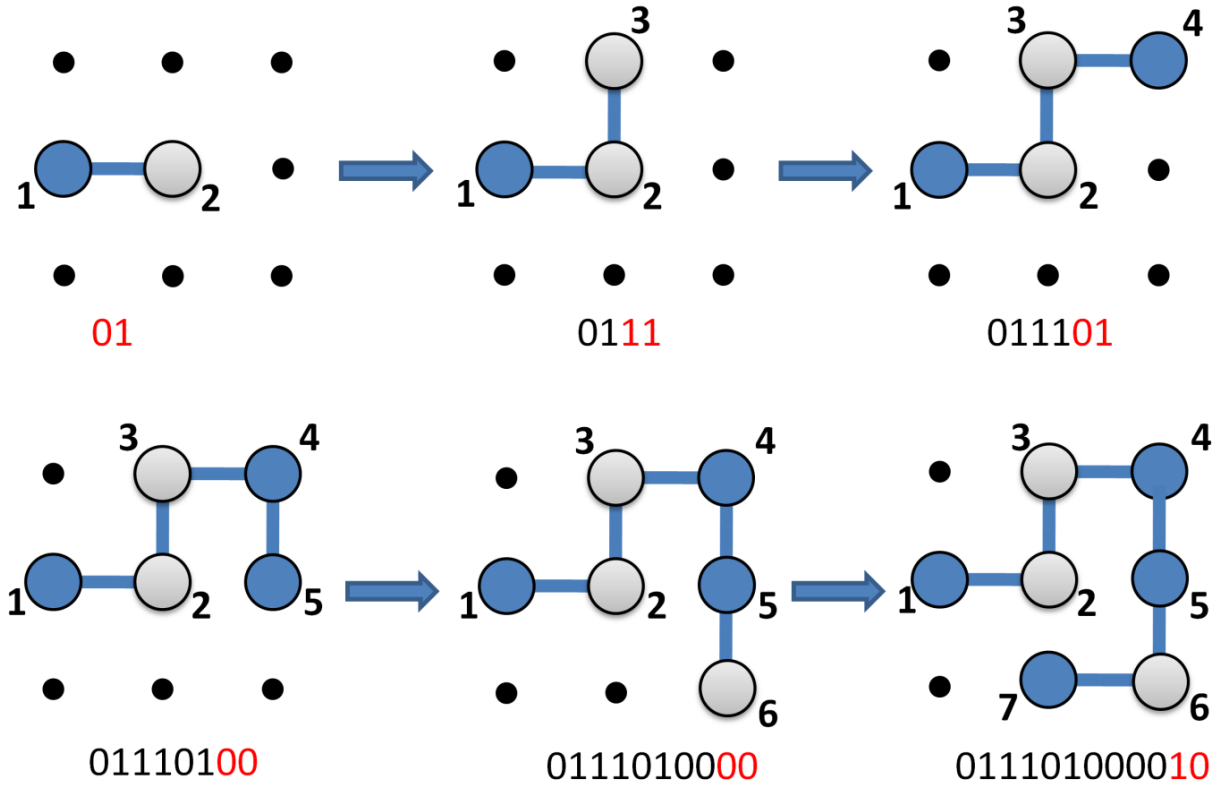
4) Only nearest neighbor interactions

$$\boldsymbol{E}_{HH} = -1, \quad \boldsymbol{E}_{PP} = \boldsymbol{E}_{HP} = 0$$



How to encode the folding pattern?





$$\boldsymbol{q} = \underbrace{01}_{turn1}\ \underbrace{q_1 q_2}_{turn2}\ \underbrace{q_3 q_4}_{turn3} \cdots \underbrace{q_{2(N-2)-1} q_{2(N-2)}}_{turn(N-1)}$$

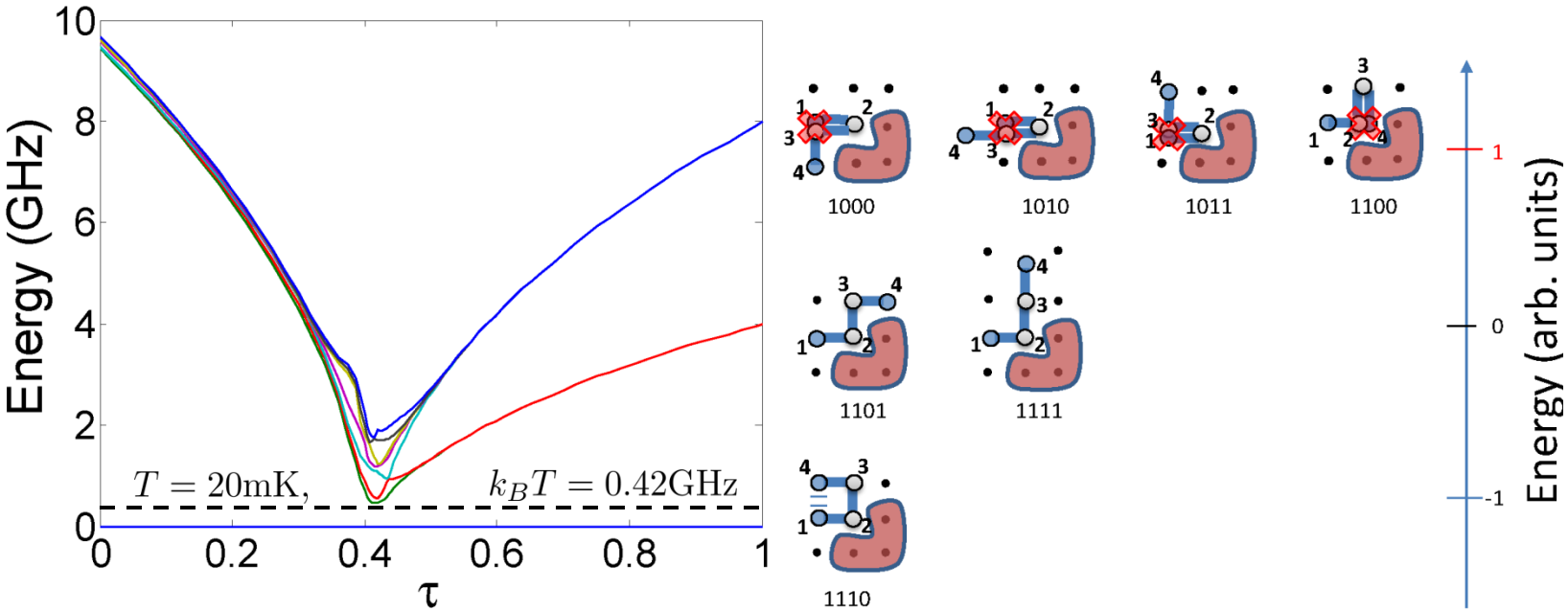
Number of resources for A *D*–dimensional lattice:

$$\ell = D(N-2)$$

Previous mapping (Perdomo *et al.* PRA2008):

$$\ell = D(N-2)\log_2 N$$

Time-dependent spectrum and energy landscape

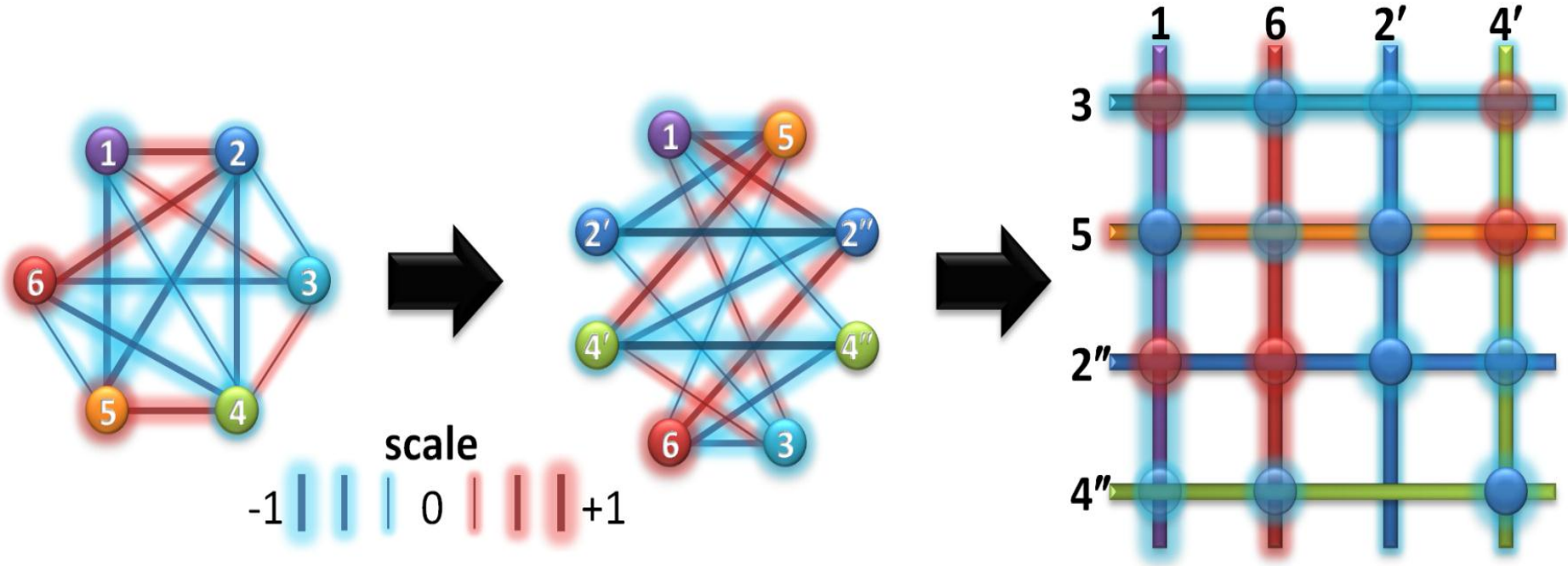


$$H(\tau) = A(\tau)\sum_i \sigma_i^x + B(\tau) H_p$$

$$H_p = \sum_i^N h_i \sigma_i^z + \sum_{j>i}^N J_{ij}\sigma_i^z \sigma_j^z$$

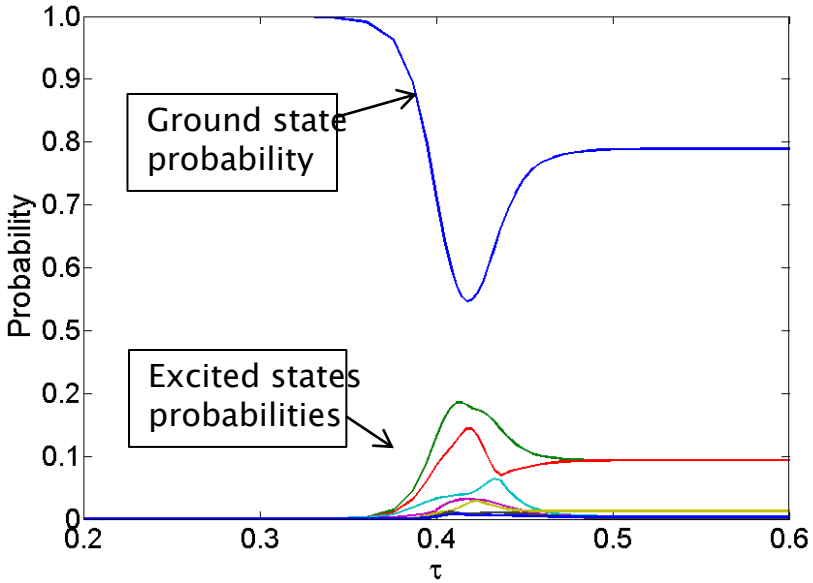
Embedding of the problem into the quantum device

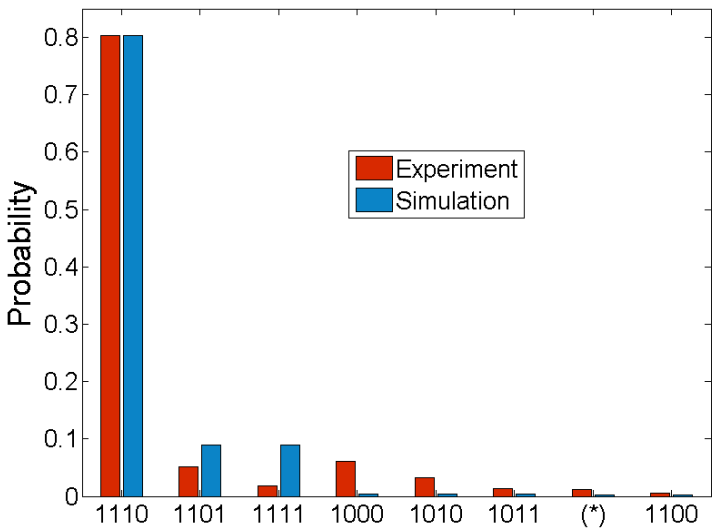
$$H_p = \sum_{i}^{N} h_i \sigma_i^z + \sum_{j>i}^{N} J_{ij} \sigma_i^z \sigma_j^z$$



Results: Theory vs. Experiment

Results at Temperature = 20mK





Ground state probability
- *Experiment: 80.3%*
- *Theory: 80.4%*

As expected, most non-adiabatic dynamics happen around $\tau \approx 0.4$ (min. gap region)

Bloch-Redfield simulations considering thermal and noise effects, using a Markovian model. All bath parameters (spectral densities, etc) are extracted from measurements on the device. *No adjustable parameters.*

Example with Miyazawa-Jernigan interaction energies

Example:

P =Proline S =Serine V =Valine

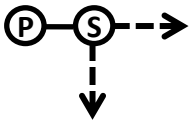
K =Lysine M =Methionine A =Alanine

Six amino-acid problem: P–S–V–K–M–A

Interaction	ΔE
P III K	-1
P III A	-2
S III M	-3
V III A	-4

Scheme 1

1 experiment
7 qubits, 7-local

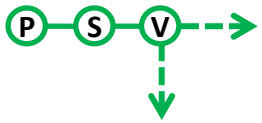


01 0q_1 q_2q_3 q_4q_5 q_6q_7

Scheme 2

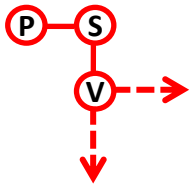
3 experiments
5 qubits, 5-local (each)

Experiment #1



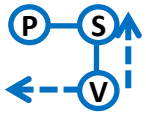
01 01 0q_1 q_2q_3 q_4q_5

Experiment #2



01 00 0q_1 q_2q_3 q_4q_5

Experiment #3

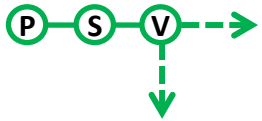


01 00 1q_1 q_2q_3 q_4q_5

Scheme 3

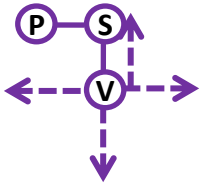
1 experiment
6 qubits, 6-local
+
1 experiment
5 qubits, 5-local

Experiment #1



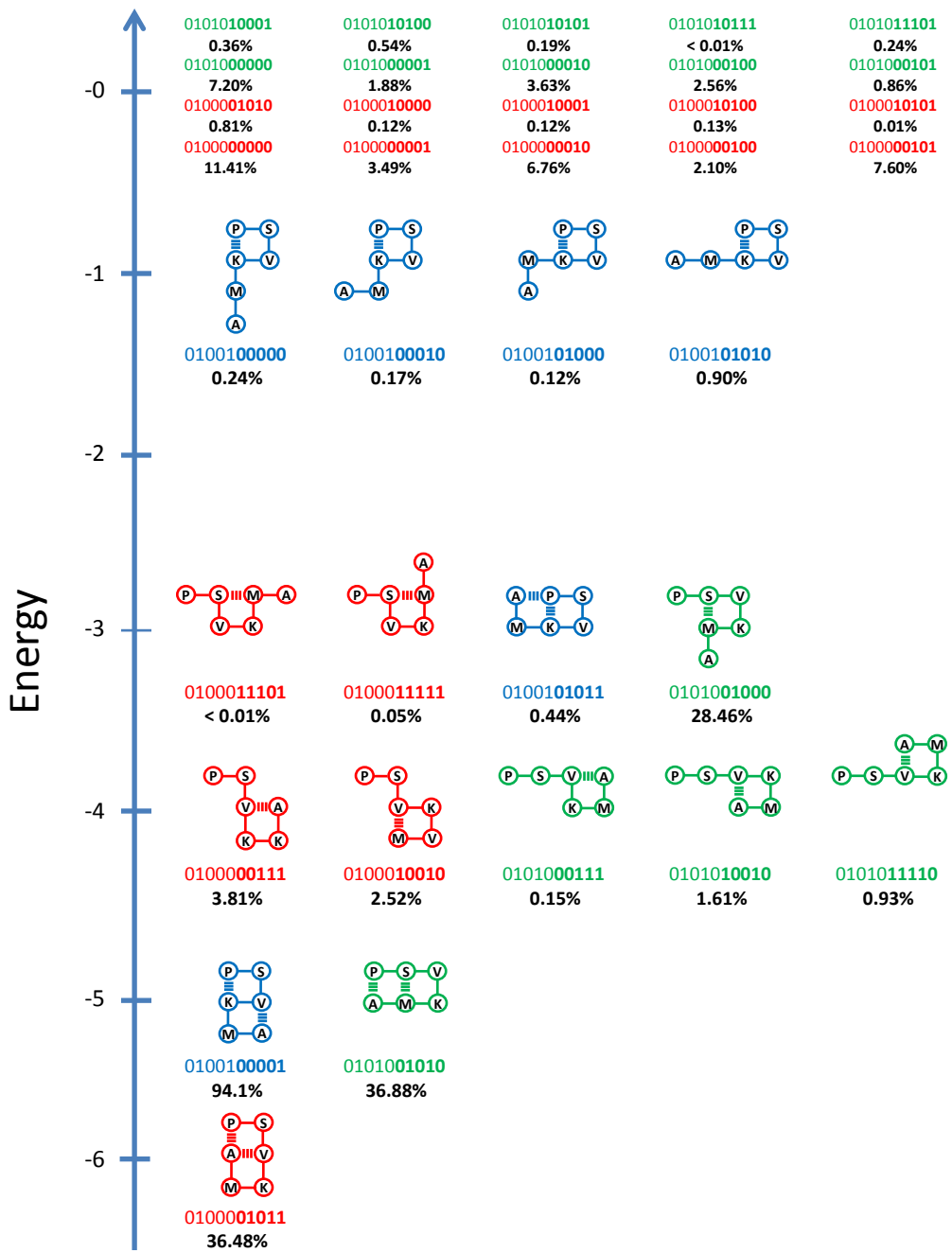
01 01 0q_1 q_2q_3 q_4q_5

Experiment #2



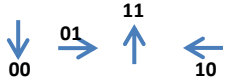
01 00 q_1q_2 q_3q_4 q_5q_6

Energy landscape for six amino-acid sequence P–S–V–K–M–A

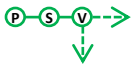


24 states in the E=0 manifold

Turn encoding:



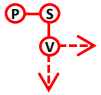
Experiment #1



01 01 0q_1 q_2q_3 q_4q_5

Originally: 5 qubit, 5 local
Transformed to: 10 qubit, 2-local
Experiment: 28 qubits

Experiment #2



01 00 0q_1 q_2q_3 q_4q_5

Originally: 5 qubit, 5 local
Transformed to: 10 qubit, 2-local
Experiment: 27 qubits

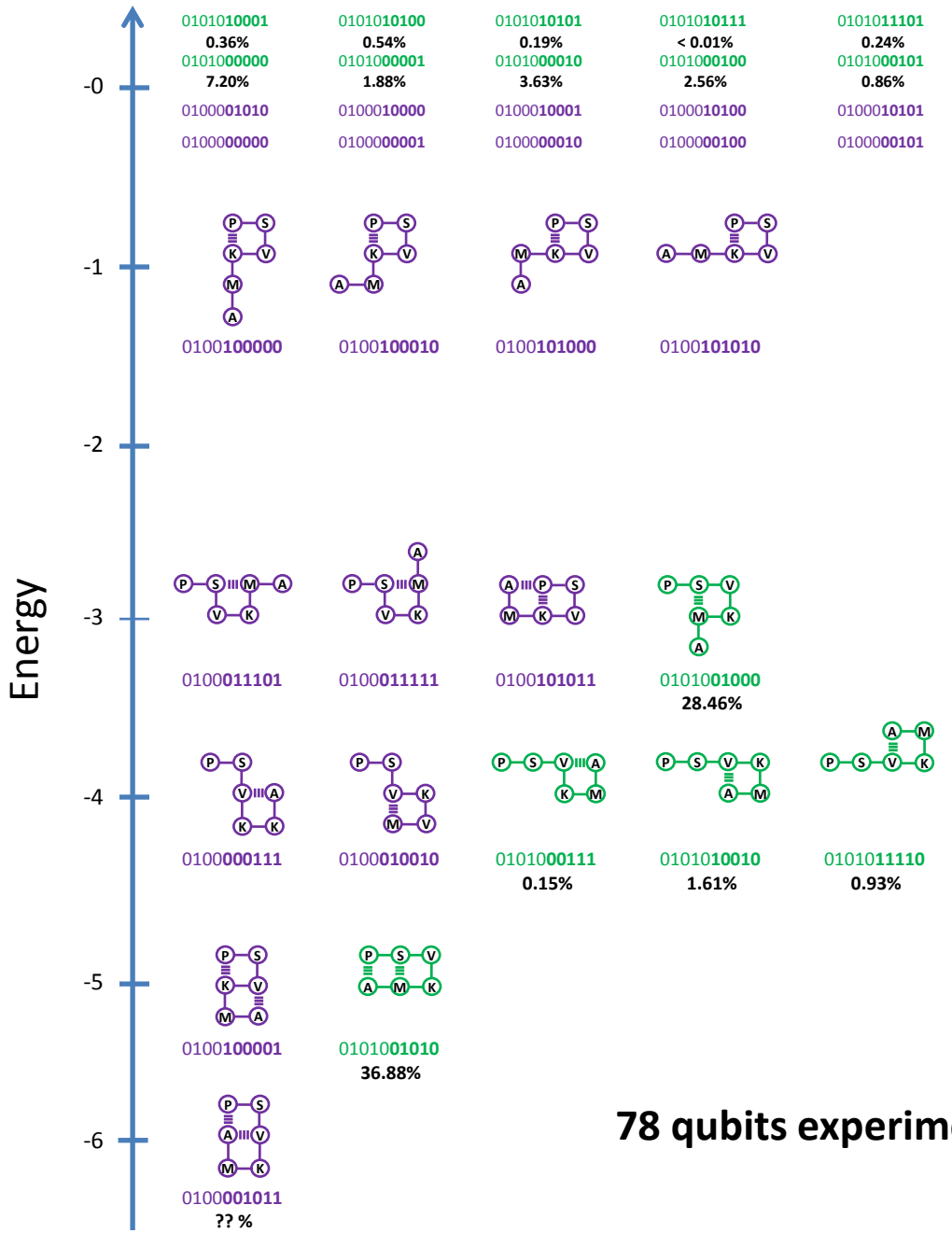
Experiment #3

01 00 1q_1 q_2q_3 q_4q_5

Originally: 5 qubit, 5 local
Transformed to: 10 qubit, 2-local
Experiment: 28 qubits

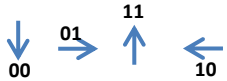
Interaction	ΔE
P III K	-1
P III A	-2
S III M	-3
V III A	-4

Energy landscape for six amino-acid sequence P–S–V–K–M–A

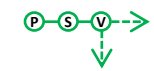


24 states in the E=0 manifold

Turn encoding:



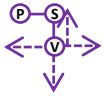
Experiment #1



01 01 0q_1 q_2q_3 q_4q_5

Originally: 5 qubit, 5 local
Transformed to: 10 qubit, 2-local
Experiment: 28 qubits

Experiment #2



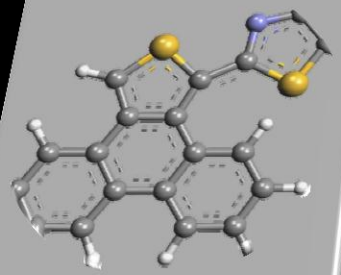
01 00 q_1q_2 q_3q_4 q_5q_6

Originally: 6 qubit, 6-local
Transformed to: 19 qubit, 2-local
Experiment: 78 qubits

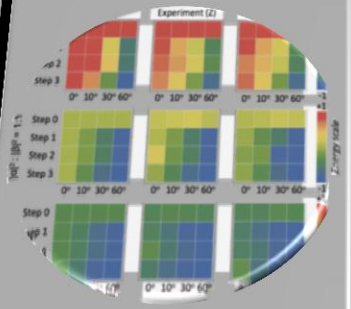
Interaction	ΔE
P III K	-1
P III A	-2
S III M	-3
V III A	-4

78 qubits experiment in progress!

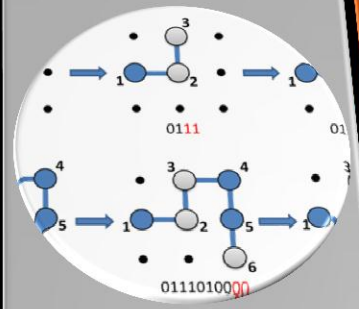
EXIT



Quantum simulation for quantum chemistry

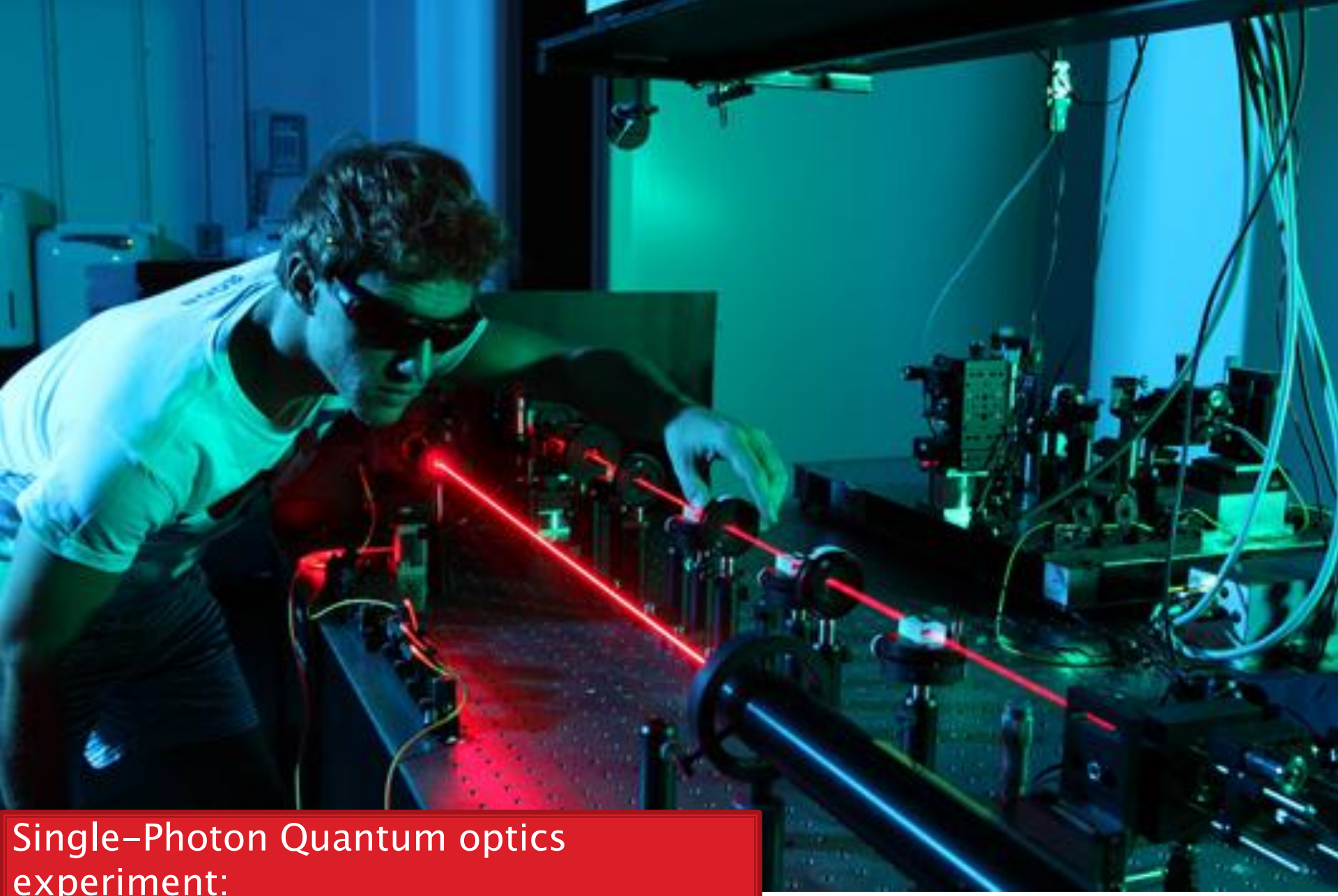


Preparing states for quantum simulation



Protein folding using adiabatic computers

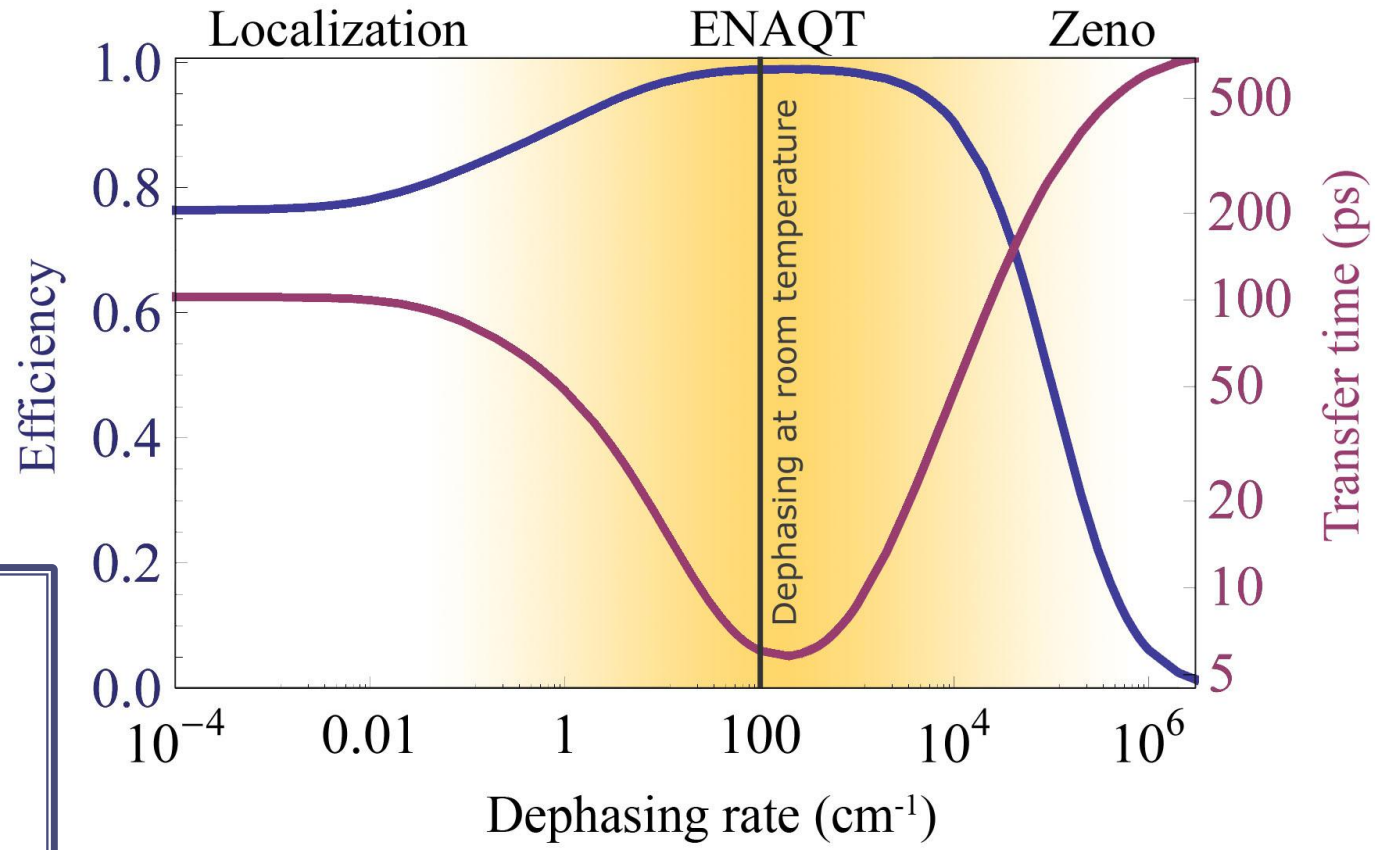
Simulating environment-assisted transport using quantum walks



Single-Photon Quantum optics experiment:
Physical Review Letters 104, 153602 (2010)

Collaboration with Andrew White (Queensland)

Environment-Assisted Quantum Transport

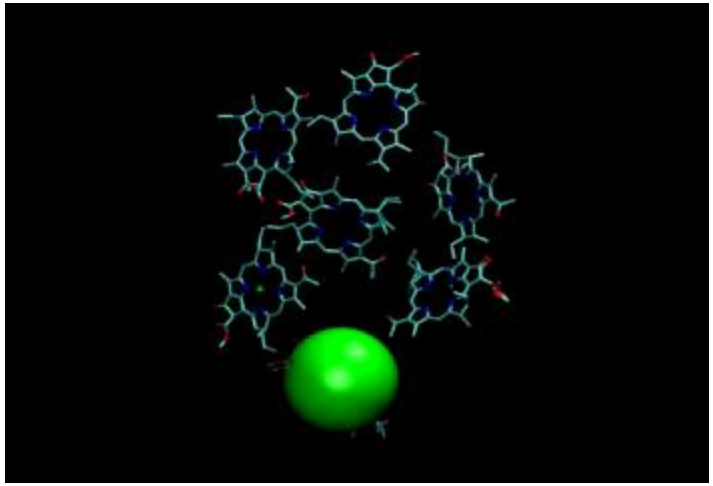


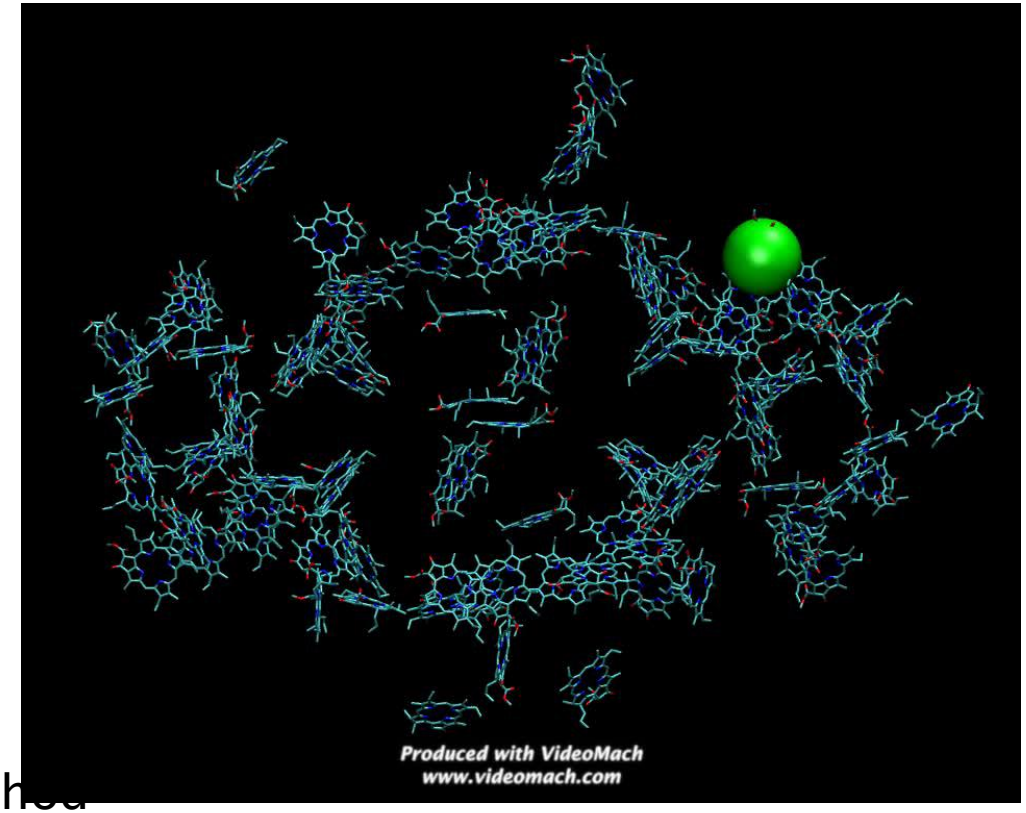
Haken-Strobl model

- Gaussian fluctuations
- Classical noise
- Pure dephasing
- Arbitrary coupling strength

Rebentrost et. al, *New J. Phys*.**11** 003303 2009 Environment-assisted quantum transport
Selected by Journal as Best of 2009

Visualizing ENAQT in single quantum trajectories





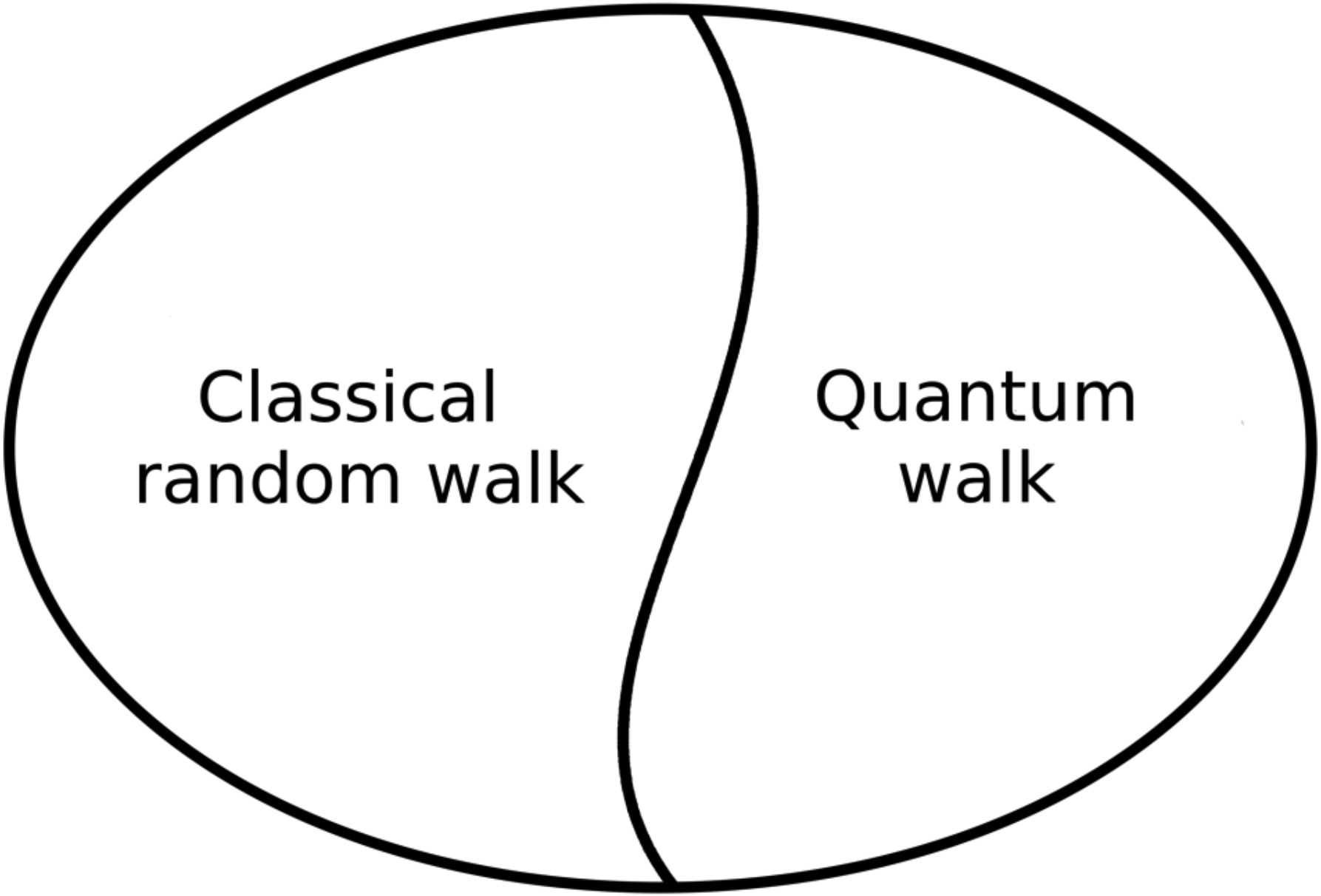
Simulation of Haken-Strobl Equaiton using Stochastic Schrodinger Equation (SSE) method

Stochastic Schrödinger Equation (SSE) simulation of FMO and PSI (higher plants)
Rupak Chakraborty , Patrick Rebentrost, Aspuru-Guzik, *In Preparation* 2010

Classical Random Walk vs. Quantum Walk

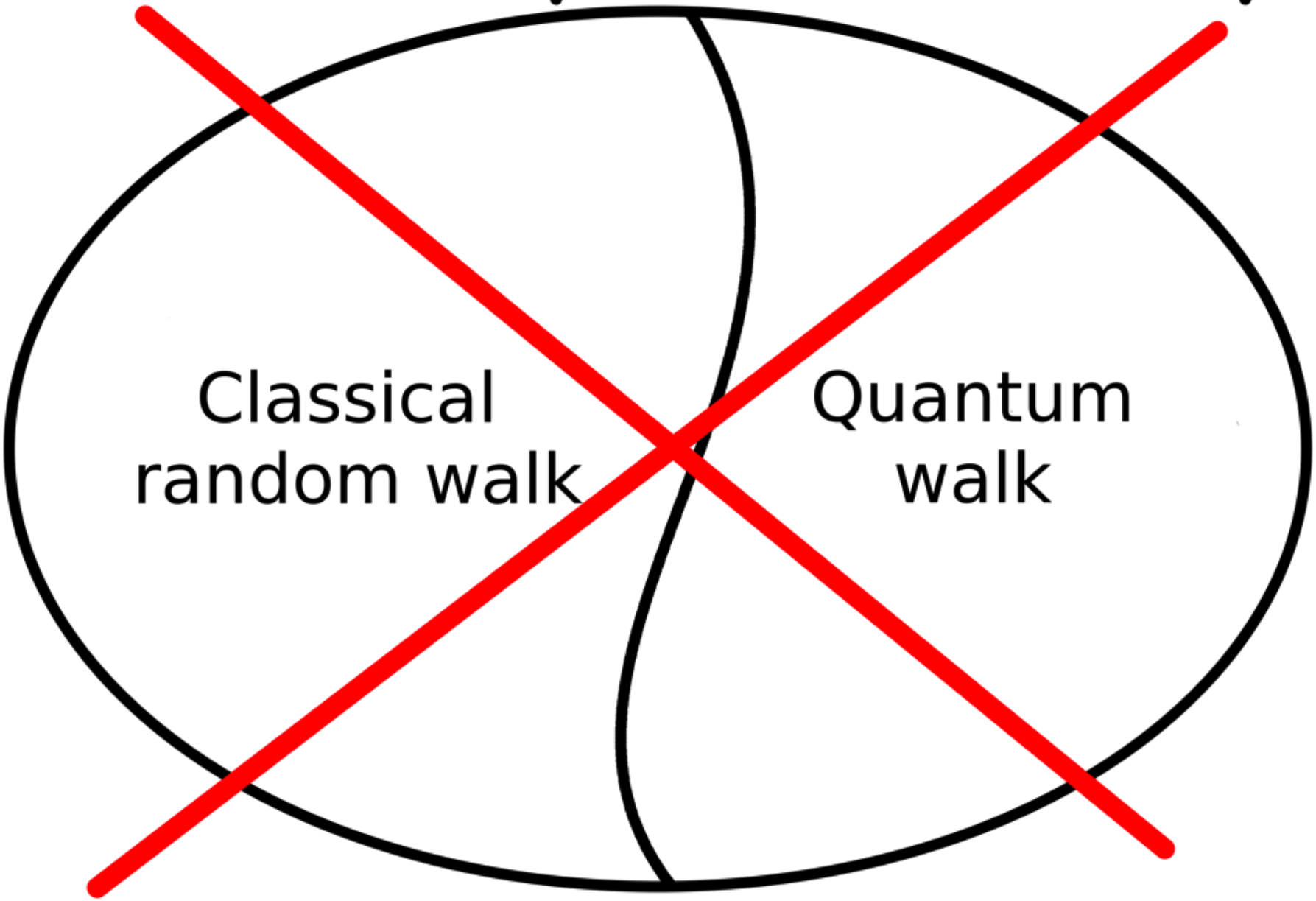
Walk	Classical random walk	Quantum walk
State function	Probability Vector p	State Vector (Wave Function) $\lvert\psi\rangle$
Equation of Motion	Stochastic Process $\frac{dp_b}{dt} = \sum L_{b,a} p_a$	Schrödinger Equation $\frac{\partial \psi_b}{\partial t} = -i \sum H_{b,a} \psi_a$
Graph Correspondence	Irreversible Operator = Laplacian $L = M$	Reversible Operator = Laplacian $H = M$

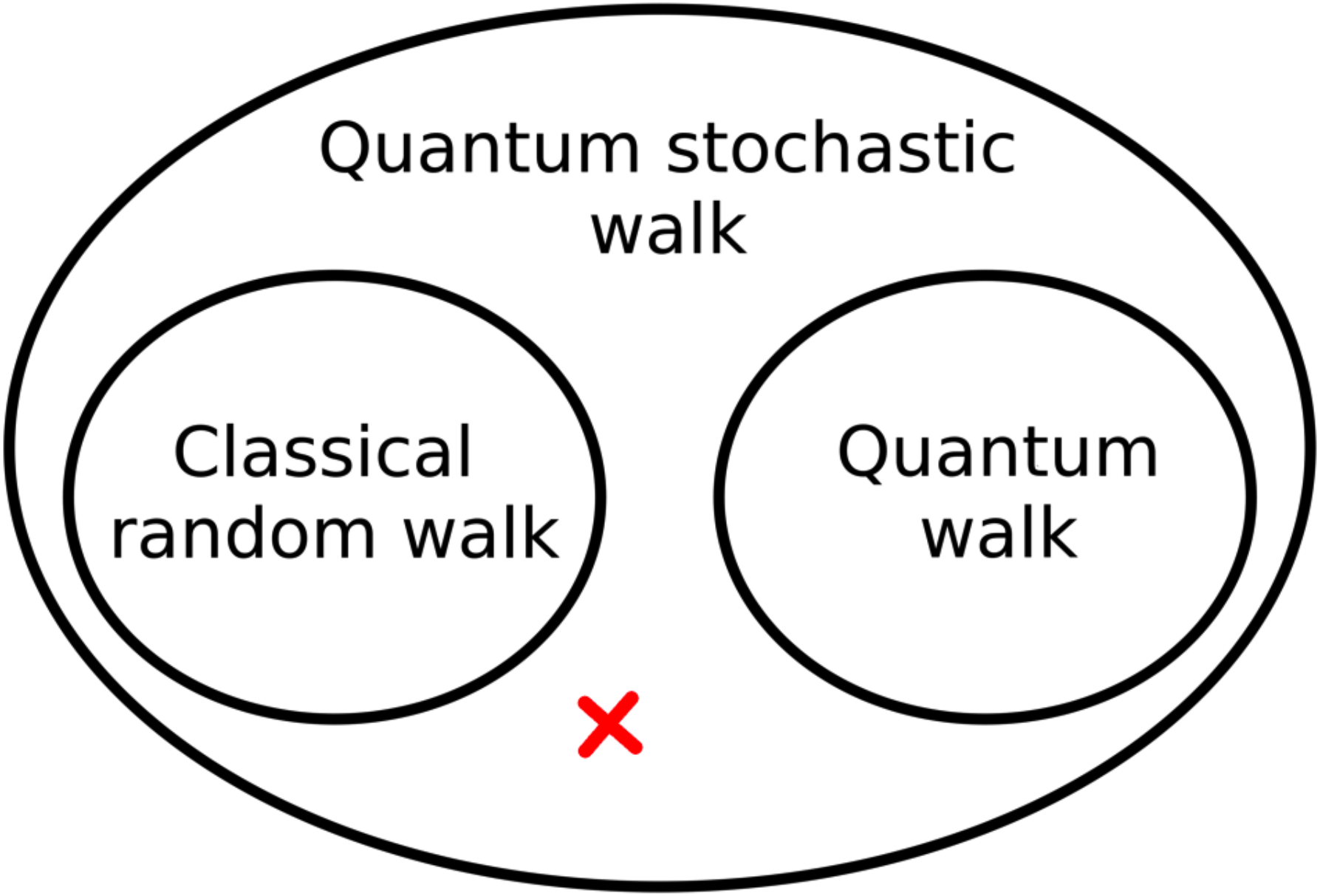
J. D. Whitfield, C. A. Rodriguez-Rosario, A. Aspuru-Guzik
Phys. Rev. A 81, 022323 (2010)



For example: Work of Viv Kendon and co-worke

Non-unitary effects are key

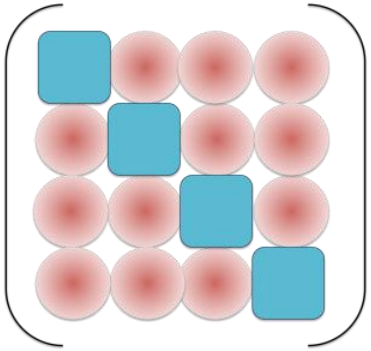


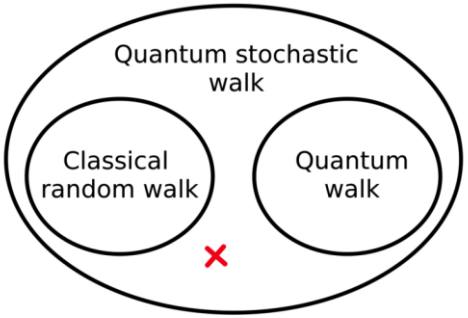

Quantum stochastic walk
Classical random walk
Quantum walk

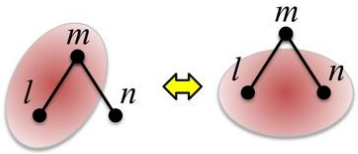
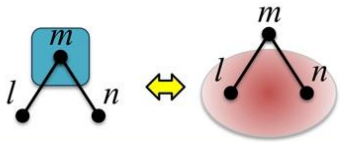
Walk	State function	Equation of Motion	Graph Correspondence
Classical	p	$Lp = \dot{p}$	L=M
Quantum	$\|\psi\rangle$	$H\|\psi\rangle = -i\partial_t\|\psi\rangle$	H=M
Q Stochastic	ρ	$\mathcal{L}\rho = \dot{\rho}$	???

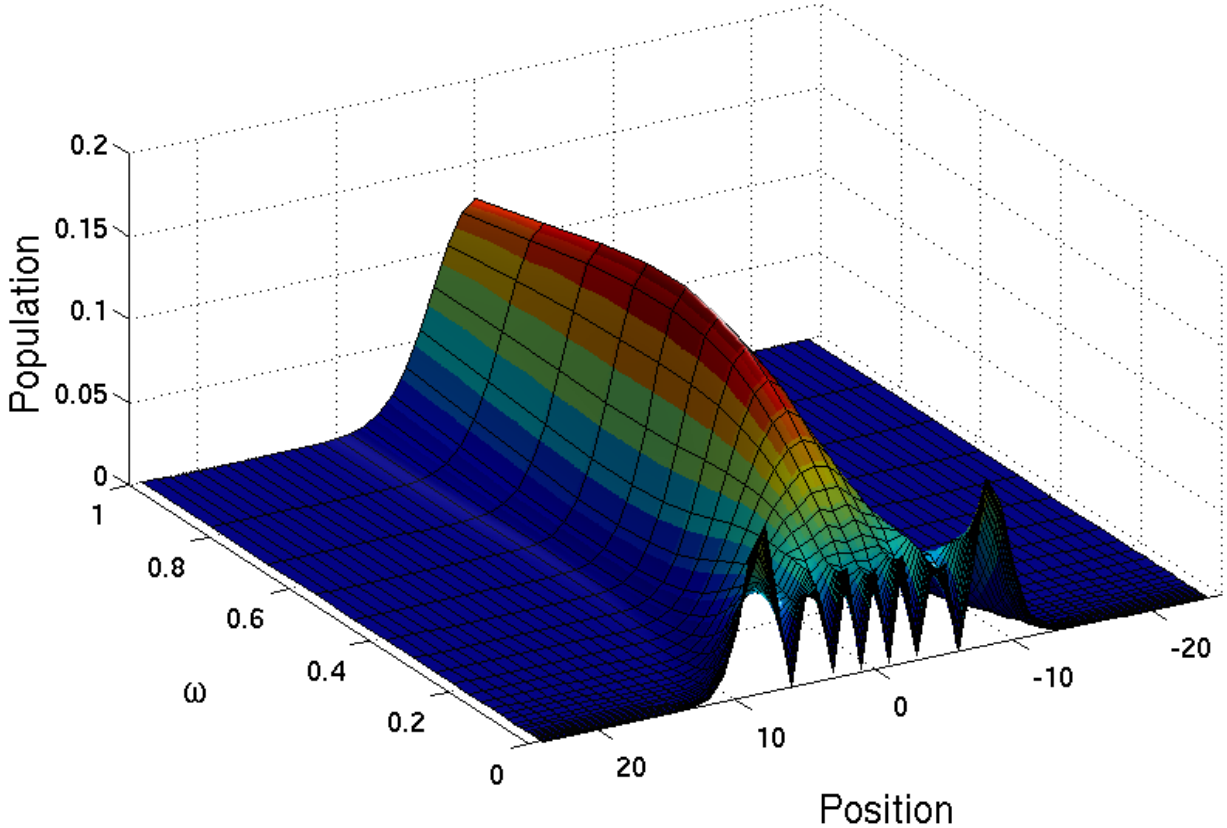
J. D. Whitfield, C. A. Rodriguez-Rosario, A. A.-G. Phys. Rev. A 81, 022322 (2010)

Walk	State function	Equation of Motion	Graph Correspondence
Classical	p	$Lp = \dot{p}$	L=M
Quantum	$\|\psi\rangle$	$H\|\psi\rangle = -i\partial_t\|\psi\rangle$	H=M
Q Stochastic	ρ	$\mathcal{L}\rho = \dot{\rho}$	???





Density Matrix Elements	Transition Operators	Characteristics
	$\{L_k\}$	Classical Random Walk
	$H, \{L_k\}$	Quantum Walk + <u>MORE</u>
	$H, \{L_k\}$	Quantum Walk + <u>MORE</u>
	$\{L_k\}$	<u>MORE</u>!!!

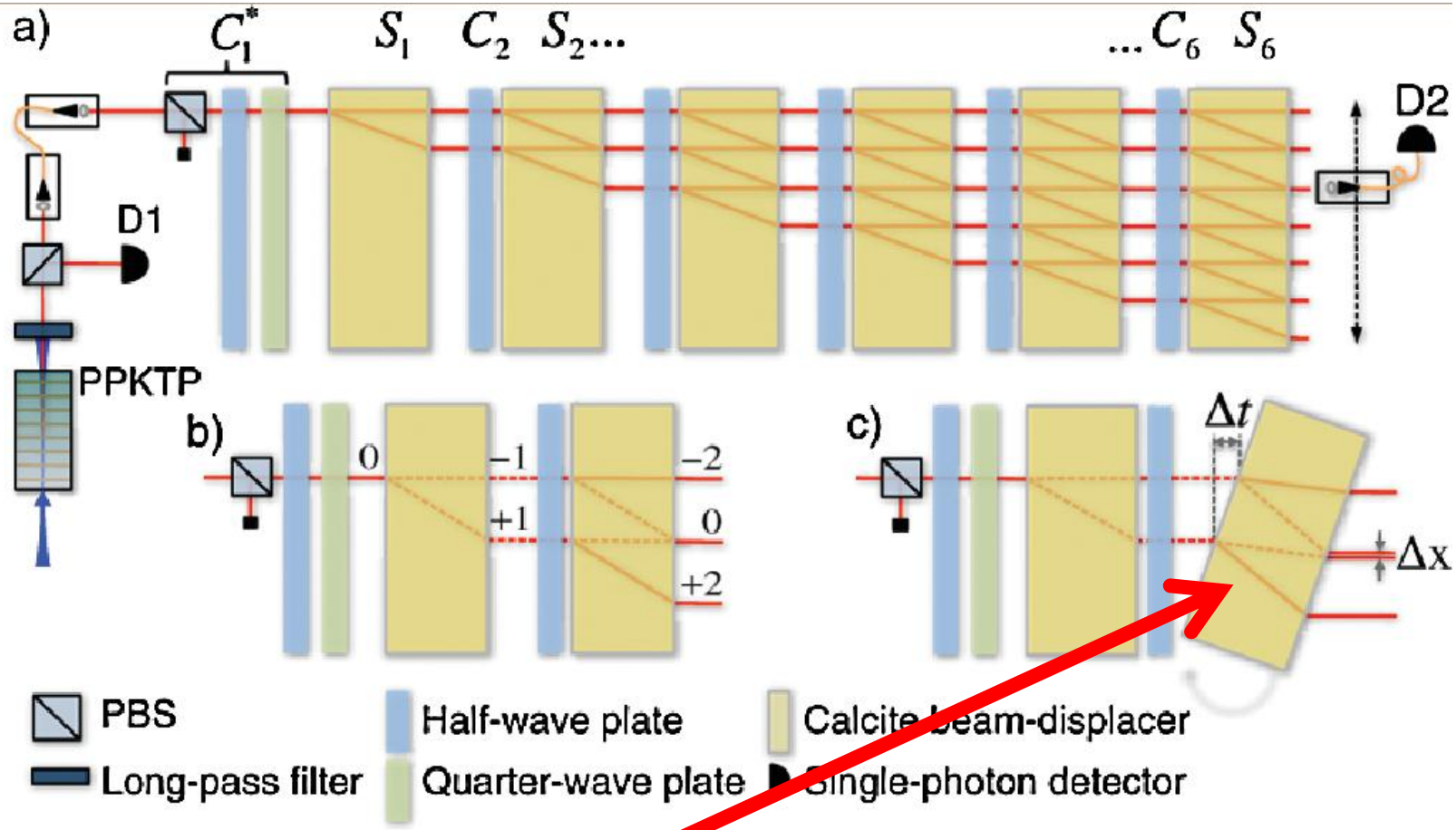


Single parameter interpolation

- Quantum walk: use von Neumann equation
- Classical random walk: use $L_{(k,k')} = M_{k,k'} |k\rangle\langle k'|$

$$\mathcal{L}_\omega[\rho] = -(1-\omega)\, i\,[H,\rho] + \omega \sum_k \left(-\tfrac{1}{2} L_k^\dagger L_k \rho - \tfrac{1}{2} \rho L_k^\dagger L_k + L_k \rho L_k^\dagger \right)$$

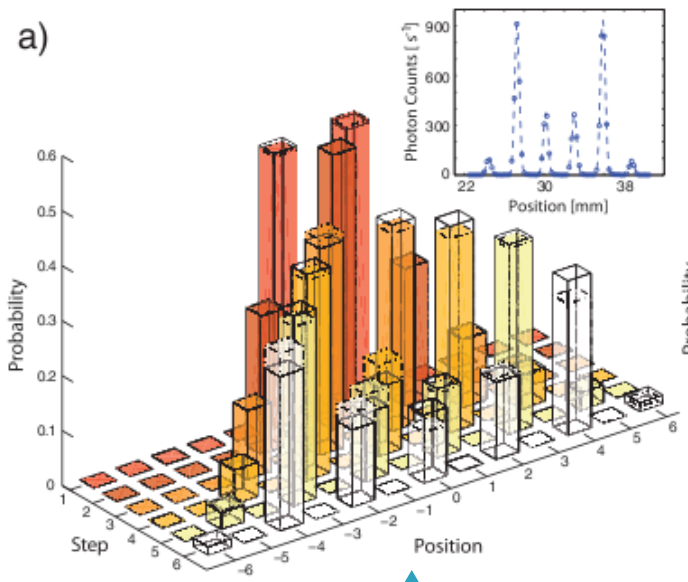
Discrete-time quantum walk: Optical setup

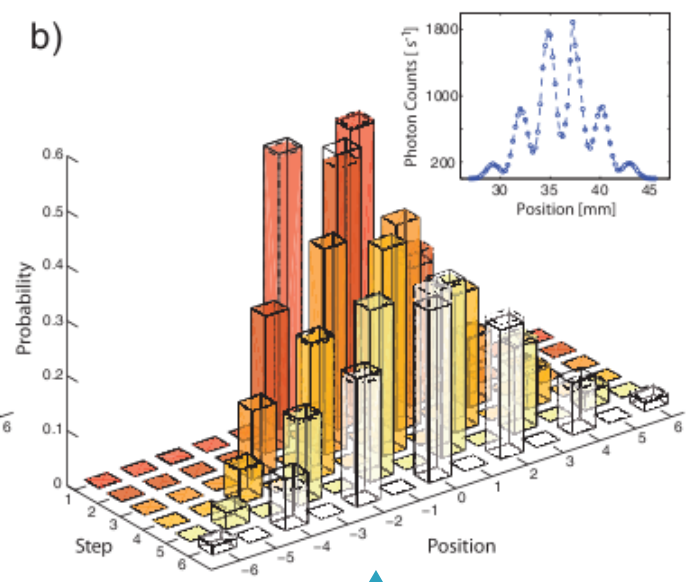


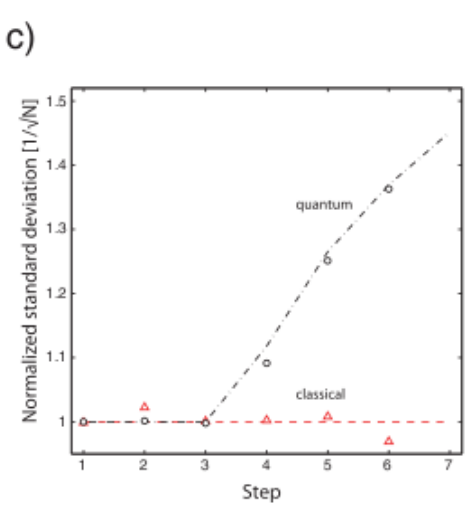
Turn to induce decoherence

W = SC (shift + coin)

Experimental results





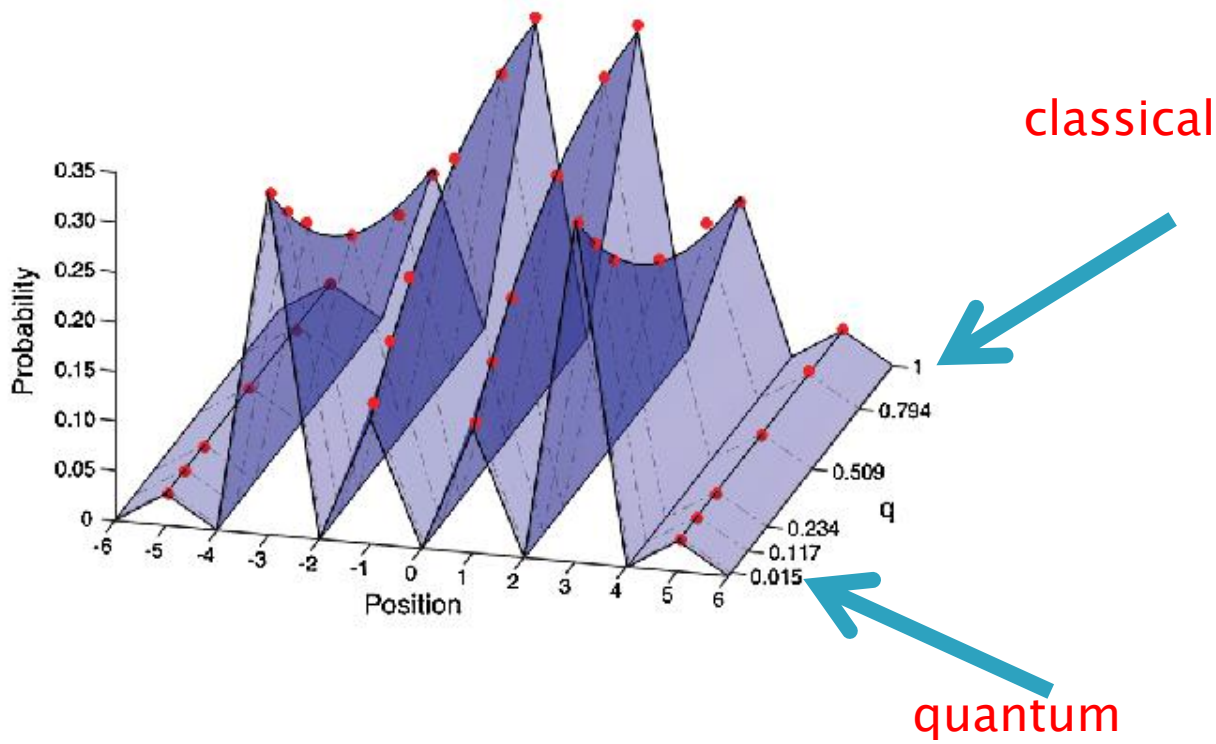


quantum walk

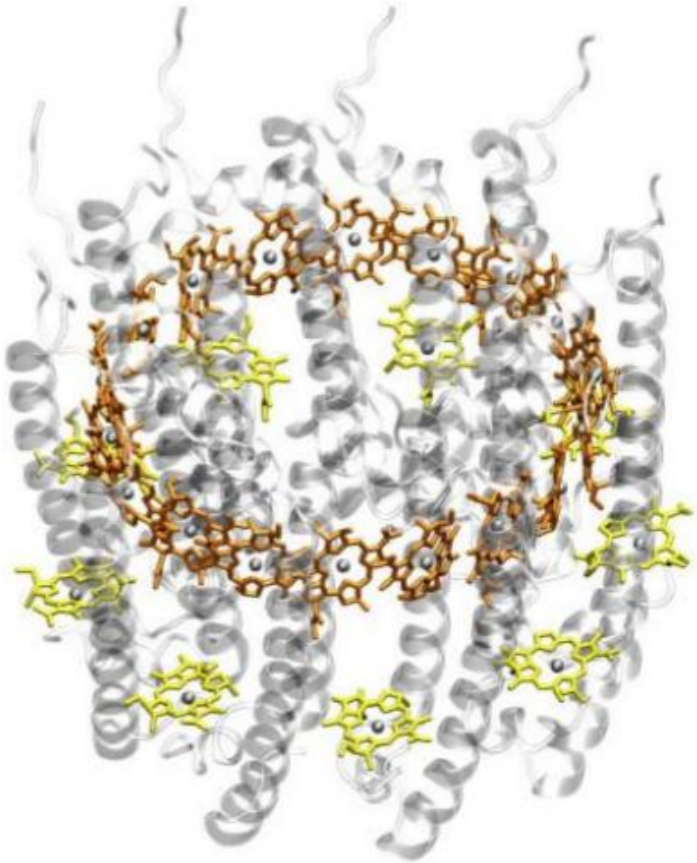
discrete-time classical walk

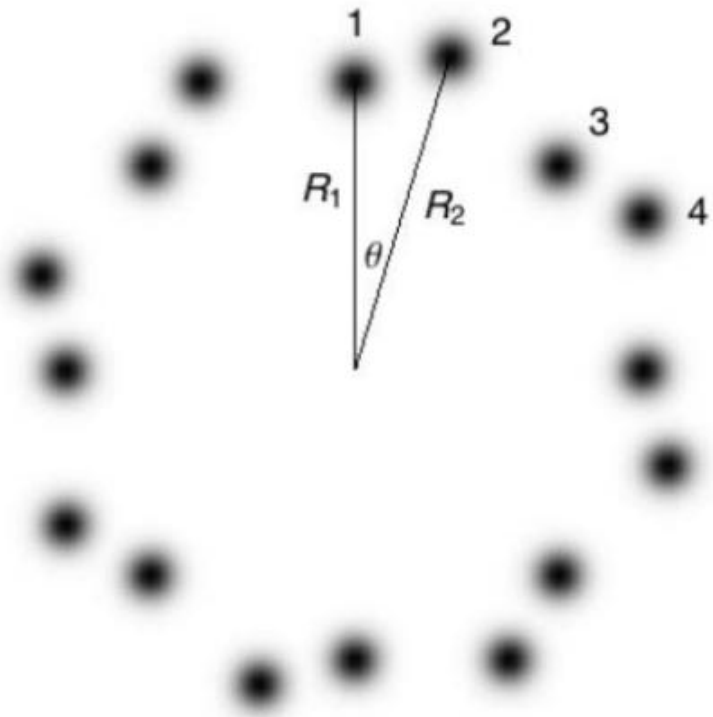
Standard deviation

Quantum to classical transition (dephasing-induced)



ENAQT in Photosynthesis using wave guides (In progress)





Just 54 years ago…

AUTOMATIC FUNDAMENTAL CALCULATIONS OF MOLECULAR STRUCTURE

By Dr. S. F. BOYS, Dr. G. B. COOK, C. M. REEVES and I. SHAVITT
Theoretical Chemistry Department, University of Cambridge

S. F. Boys, et. al, *Nature* (1956)

Thank you!

Quantum simulation for chemistry
Is a promising direction:

- Electronic Structure
- Chemical Dynamics
- Statistitical models (proteins)

http://aspuru.chem.harvard.edu
aspuru@chemistry.harvard.edu

James Whitfield, Ivan Kassal, Alejandro Perdomo, Man-Hong Yung, Sarah Mostame, Sergio Boixo, Patrick Rebentrost, Masoud Mohseni

Patrick Rebentrost, Leslie Vogt, Joel Yuen-Zhou, Sangwoo Shim Cesar Rodriguez-Rosario,, Lauren Kaye, Sule Atahan, Johannes Hachmann, Jacob Krich, Roberto Olivares, Dmtrij Rappoport, Semion Saikin, David Tempel, Mark Watson

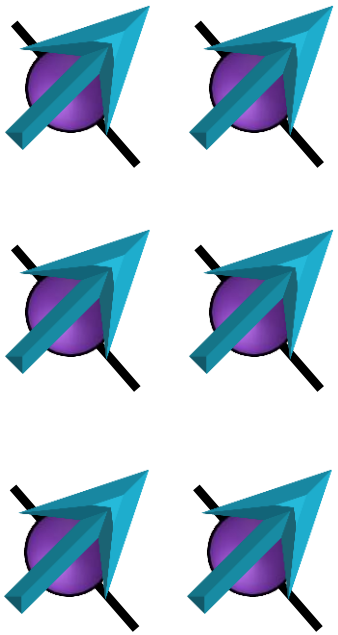
Peter Love, Ben Lanyon, Andrew White

In the bottom of the ocean,

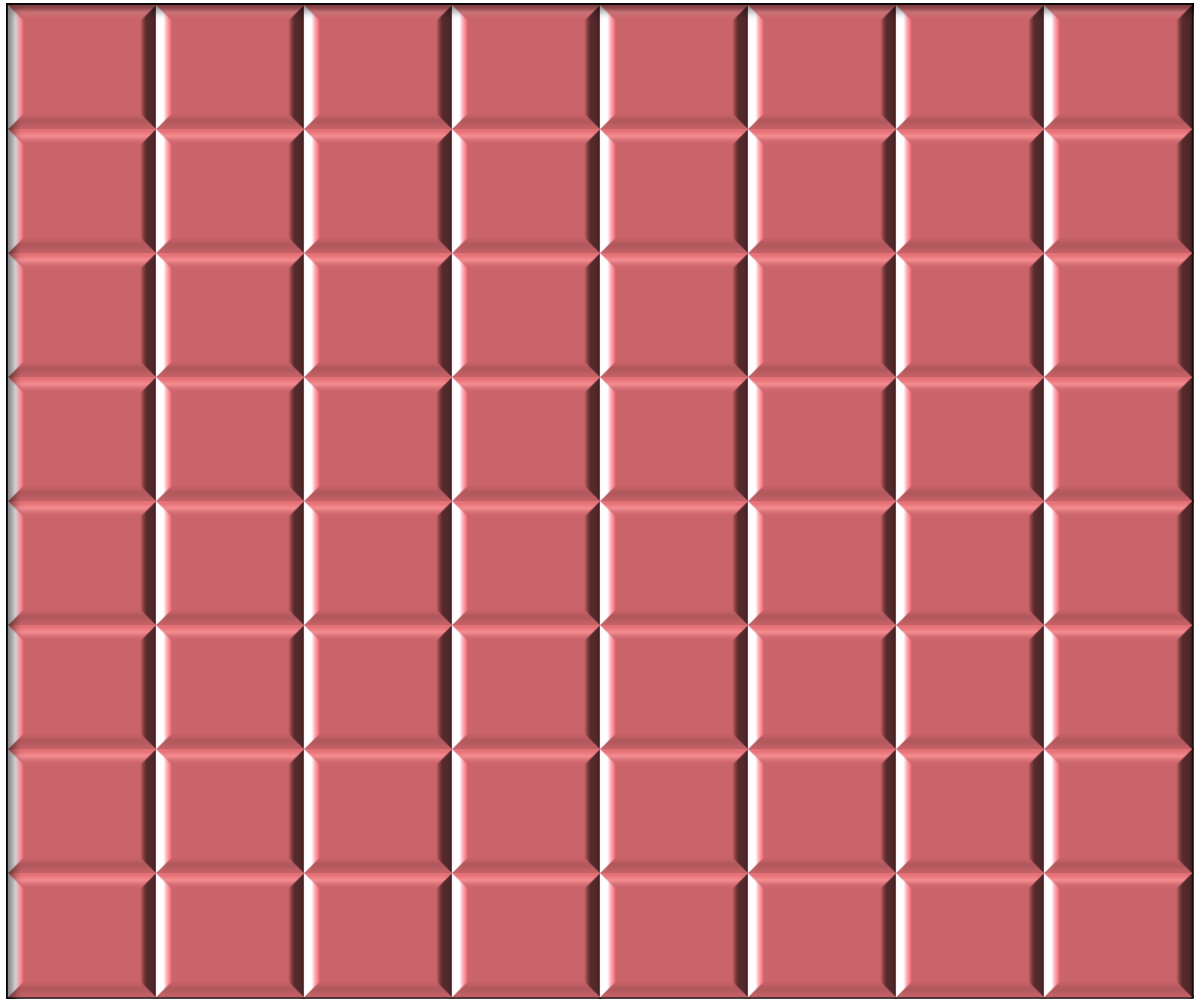
At a depth very far below…

Chemical dynamics

Spatial grid scaling



x

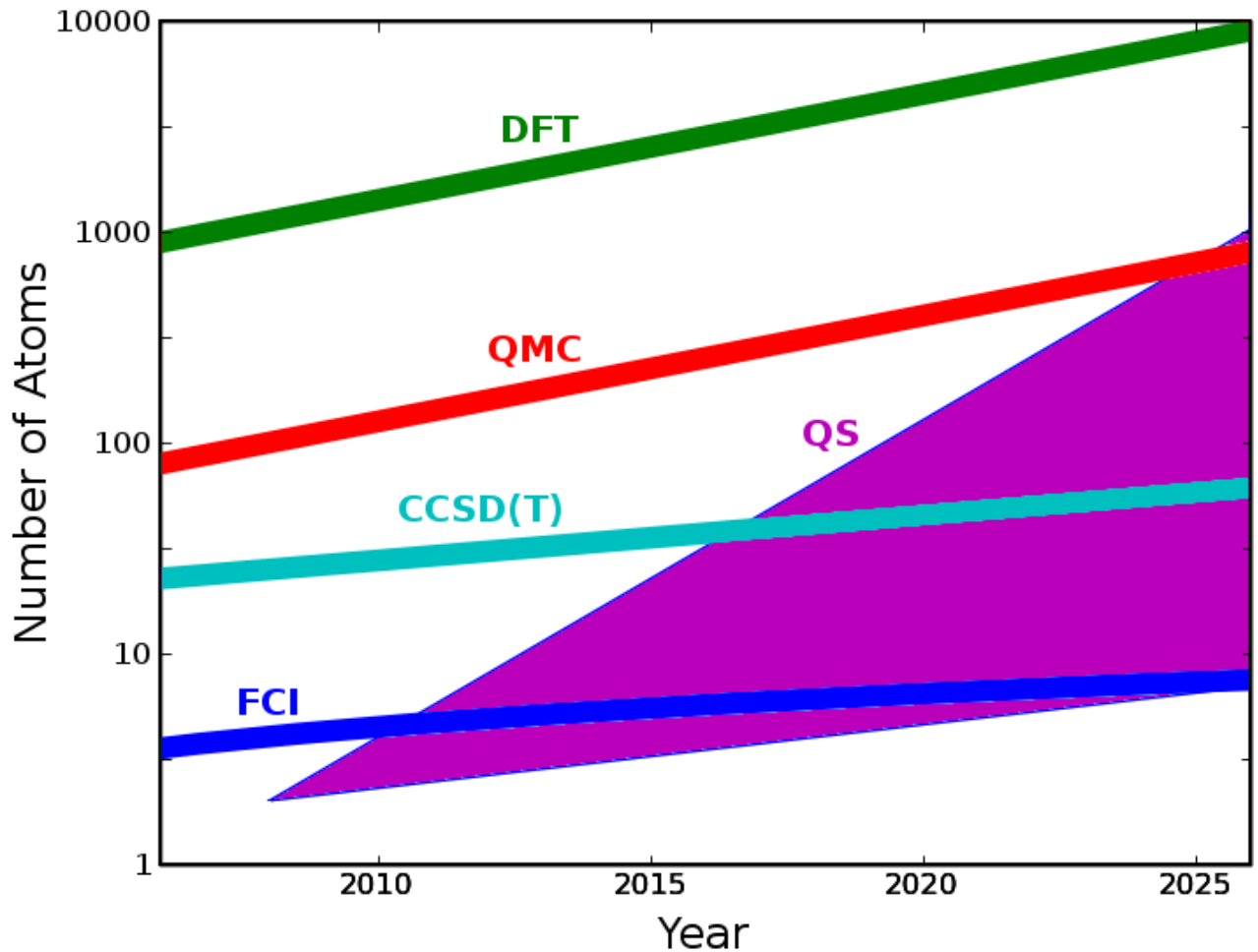


y

Kassal, …, Aspuru-Guzik *Proc. Nat. Acad. Sci.* (2008)

Optimistic prospects?

A quantum "Moore's law?"



Whitfield, Kassal and Aspuru-Guzik, *In Preparation*

Quantum Simulation for Quantum Chemistry
Quantum Stochastic Walks

Beyond classical and quantum walks

Alán Aspuru-Guzik
Department of Chemistry and Chemical Biology
Harvard University

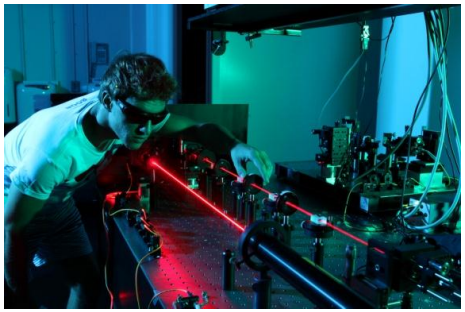
Quantum Computing Program Review
Cincinatti, OH, 2010

Quantum Computation for Quantum Chemistry

Alán Aspuru-Guzik, Harvard University
aspuru@chemistry.harvard.edu, http://aspuru.chem.harvard.edu

Objectives

- Fully characterize the efficiency of phase estimation algorithm for chemical problems (20-200 quantum bits)
- Develop methods for initial state preparation
- Develop embedding techniques



In 2010, we focused on the study of quantum walks as Possible simulators of tight-binding models such as Photosynthetic compleces.

Objective Approach

- Combine the theoretical approaches of the quantum information community with those of the quantum chemistry community
- Develop novel algorithms with specific gate sequences, resource and complexity estimation.

Status

- Developed the concept of quantum stochastic walks
- Collaborated on their implementation with Andrew White
- Developed an adiabatic quantum simulator approach.
- Developed a method for the preparation of thermal states on a quantum computer.

Quantum Computation for Quantum Chemistry

Alán Aspuru-Guzik, Harvard University

- Progress on last year's objectives

Seek first 2+ qubit experiments on quantum chemisty on quantum computer – Carried out quantum walk experiment

Algorithm for non-differential properties – Did not work on it

Explore the scaling limits of quantum simulation – Wrote a review paper on the work on quantum simulation to date.

- Research plan for the next 12 months

- Collaborate with experimental groups for the simulation of thermal states and matrix product states on gate-model quantum computers

-- Develop a fermionic adiabatic quantum simulation scheme.

- Long term objectives (demonstrations)

– **Develop a comprehensive picture of quantum simulation of chemical electronic structure problems using gate-model quantum computers**

–**Develop schemes for practical quantum simulation using different models (e.g. adiabatic model) and help with experimental realization.**

What I am not talking about today

Adiabatic quantum simulators

- Adiabatic system + gate-model qubit probe as a quantum simulator of many-body-systems. arxiv:1002.0368

Simulation of classical thermal sates on a QC

- Developed a method for preparing *coherently-encoded thermal states* (CETS) **directly** on a QC for many graphs (e.g. spin-ice) arxiv:1005.0020

Quantum simulation for chemistry

- Reported last year, but first experiment appeared this year in Nature Chemistry 2 106 (2010)

Photosynthesis 101

$$6CO_2 + 6H_2O \rightarrow C_6H_{12}O_6 + 6O_2$$

Efficient

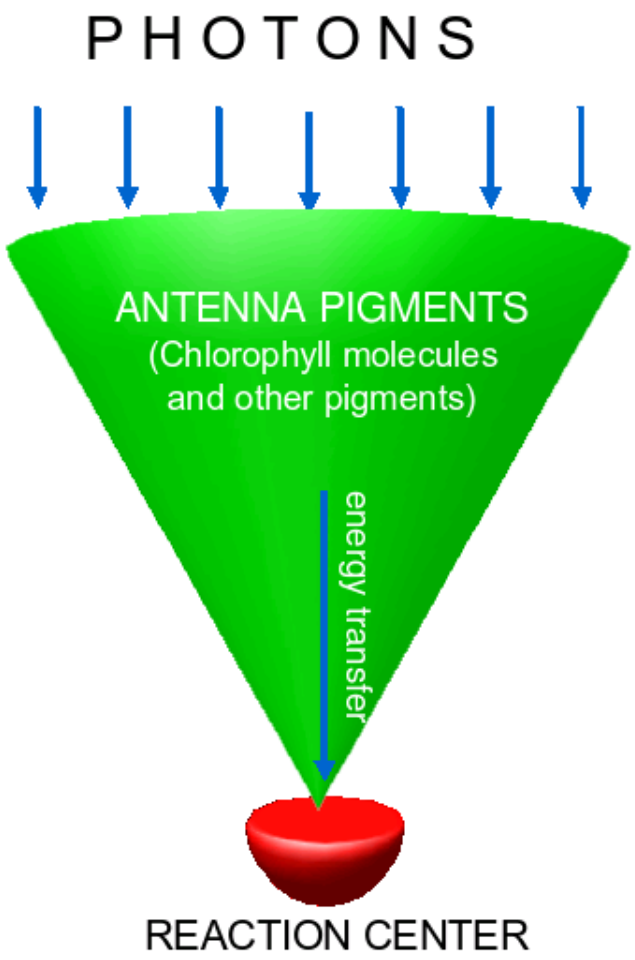
- >90% of energy absorbed initiates photosynthesis

Fast

- 300 turnover events / sec

Regulated

- ~75% energy dissipated within 1 sec



Continuous Time Quantum Walks in Graphs

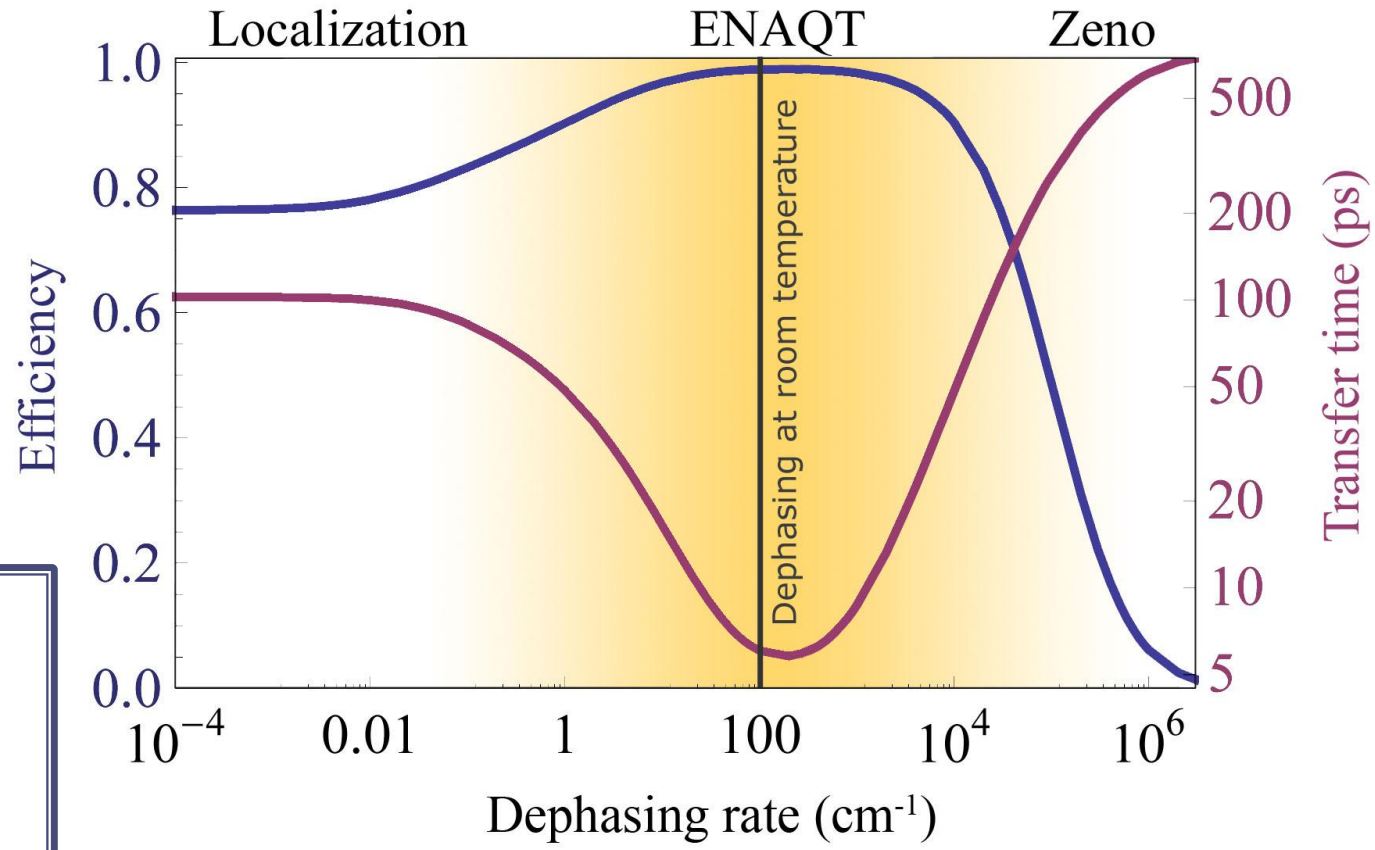
$$M_{ab} = \begin{cases} -\gamma & a \neq b,\ a \text{ and } b \text{ connected by edge} \\ 0 & a \neq b,\ a \text{ and } b \text{ not connected} \\ k\gamma & a = b,\ k \text{ is the valence of vertex } a \end{cases}$$

$$\frac{dp_a(t)}{dt} = -\sum_b M_{ab} p_b(t)$$

$$i\frac{d}{dt}\langle a|\psi(t)\rangle = \sum_b \langle a|H|b\rangle\langle b|\psi(t)\rangle$$

E. Farhi, S. Gutmann PRA 58, 915 (1998)
Introduced to Energy transfer by O. Muelken, Blumer

Environment-Assisted Quantum Transport

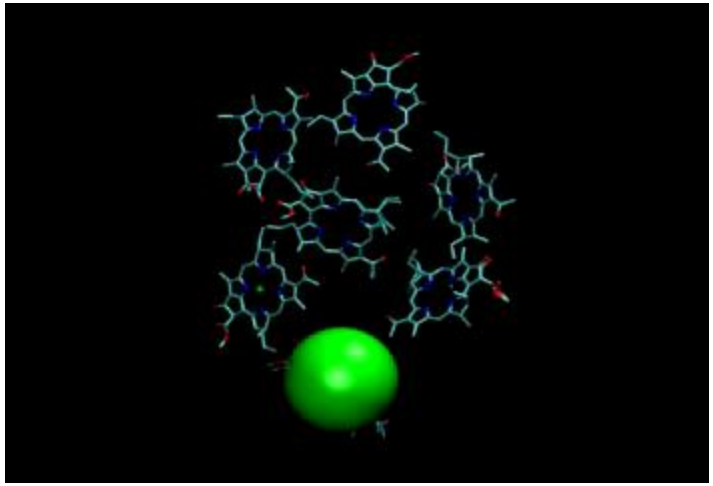


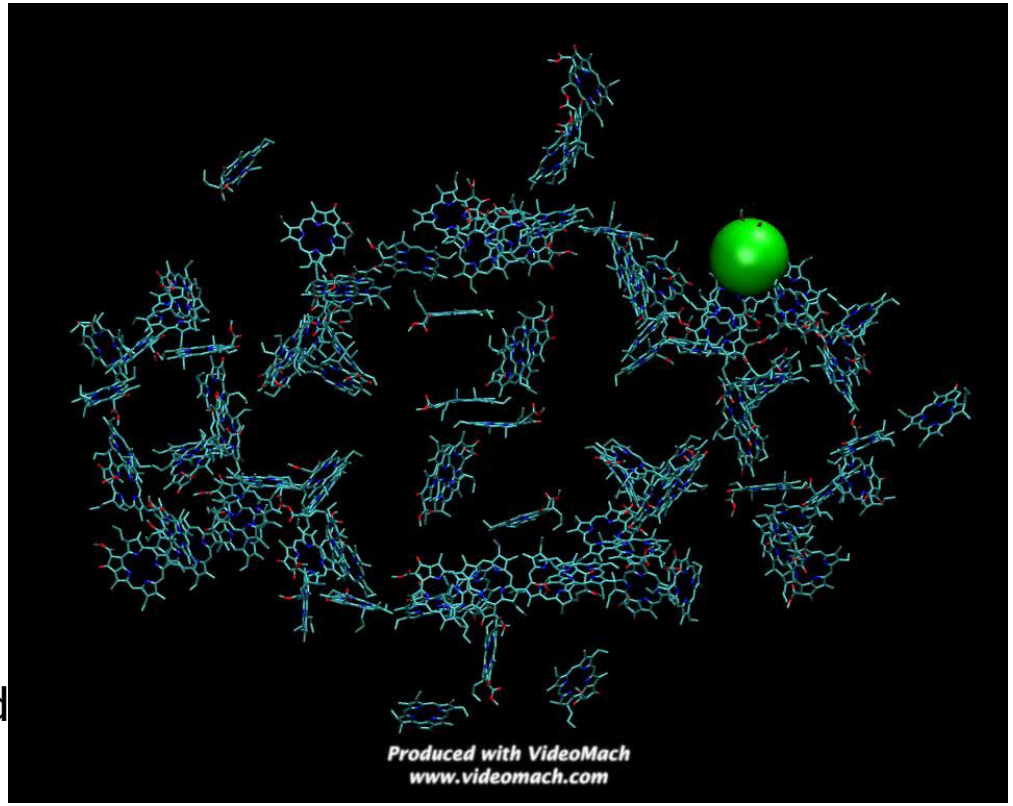
Haken-Strobl model

- Gaussian fluctuations
- Classical noise
- Pure dephasing
- Arbitrary coupling strength

Rebentrost et. al, ***New J. Phys*.11 003303 2009**
Selected by Journal as Best of 2009

Visualizing ENAQT in single quantum trajectories





Simulation of Haken-Strobl model using Stochastic Schrodinger Equation (SSE) method

Stochastic Schrödinger Equation (SSE) simulation of FMO and PSI (higher plants)
Rupak Chakraborty , Patrick Rebentrost, Aspuru-Guzik, *In Preparation* 2010

What is a Walk?

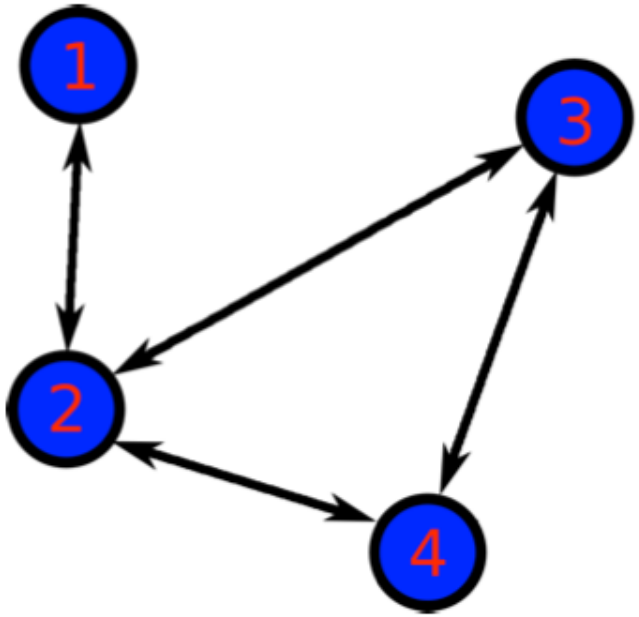
Walks	Space/Time Correspondence
State function	**Where is our walker?**
Equation of motion	**How does the walker move?**
Graph Correspondence	**How is space connected?**

Graph terminology

A graph $\mathcal{G}$ with vertex set $\mathcal{V}$ with $|\mathcal{V}|$ vertices and edge set $\mathcal{E}$ has

- Adjacency matrix
  - $A_{ij} = \begin{cases} 1 & \text{if vertex } i \text{ is connected to } j \\ 0 & \text{if not connected} \end{cases}$
- Degree matrix
  - $D_{ij} = \delta_{ij} deg(j)$
  - The degree of vertex i, $deg(i)$, is the number of vertices connected to it
- Laplacian Matrix
  - $M = D - A$

Example of a Graph



$$D = \begin{array}{c} \\ s1 \\ s2 \\ s3 \\ s4 \end{array} \begin{array}{c} \begin{array}{cccc} s1 & s2 & s3 & s4 \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix} \end{array}$$

$$A = \begin{array}{c} \\ s1 \\ s2 \\ s3 \\ s4 \end{array} \begin{array}{c} \begin{array}{cccc} s1 & s2 & s3 & s4 \end{array} \\ \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix} \end{array} \qquad M = \begin{array}{c} \\ s1 \\ s2 \\ s3 \\ s4 \end{array} \begin{array}{c} \begin{array}{cccc} s1 & s2 & s3 & s4 \end{array} \\ \begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 2 & -1 \\ 0 & -1 & -1 & 3 \end{pmatrix} \end{array}$$

Classical Random Walk vs. Quantum Walk

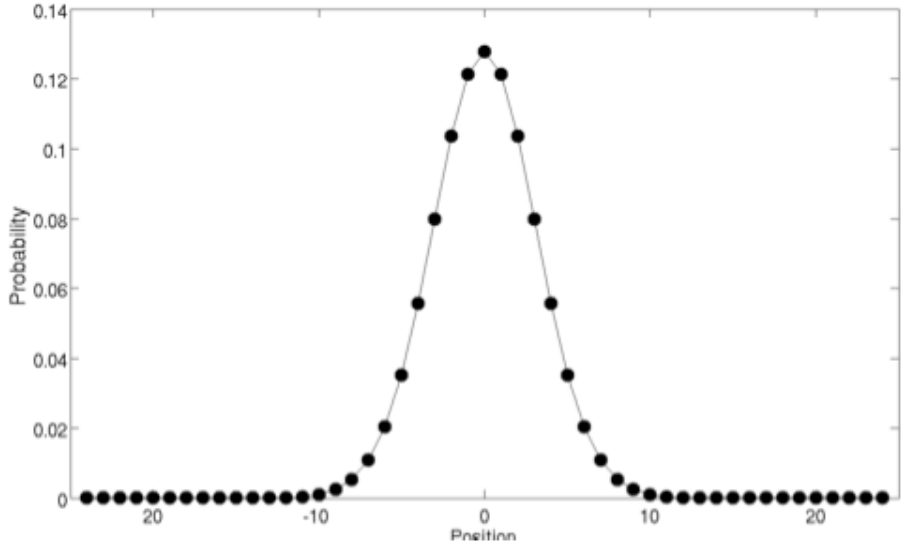
Walk	Classical random walk	Quantum walk
State function	Probability Vector p	State Vector (Wave Function) $\lvert\psi\rangle$
Equation of Motion	Stochastic Process $\frac{dp_b}{dt} = \sum L_{b,a} p_a$	Schrödinger Equation $\frac{\partial \psi_b}{\partial t} = -i \sum H_{b,a} \psi_a$
Graph Correspondence	Irreversible Operator = Laplacian $L = M$	Reversible Operator = Laplacian $H = M$

J. D. Whitfield, C. A. Rodriguez-Rosario, A. A.-G. Phys. Rev. A 81, 022323 (2010)

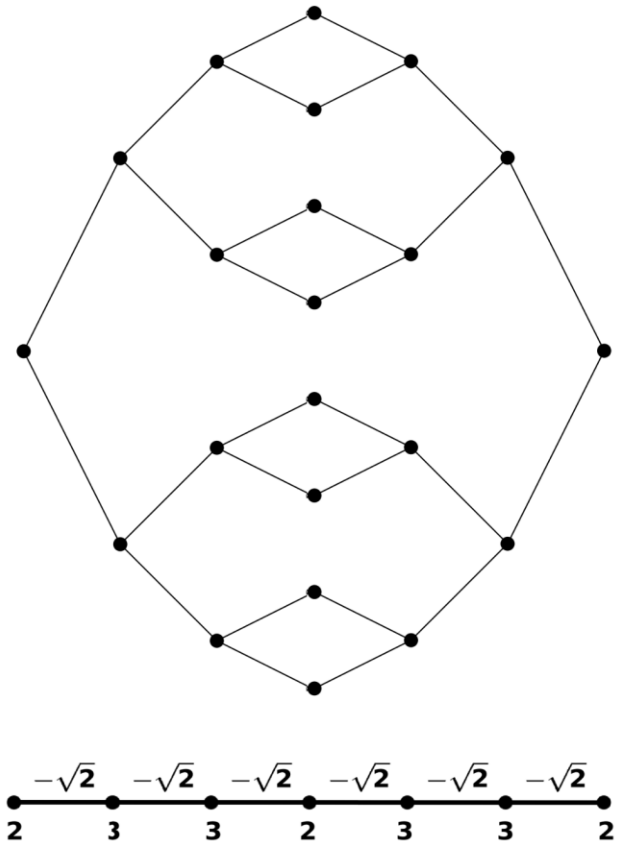
Walk on a Line

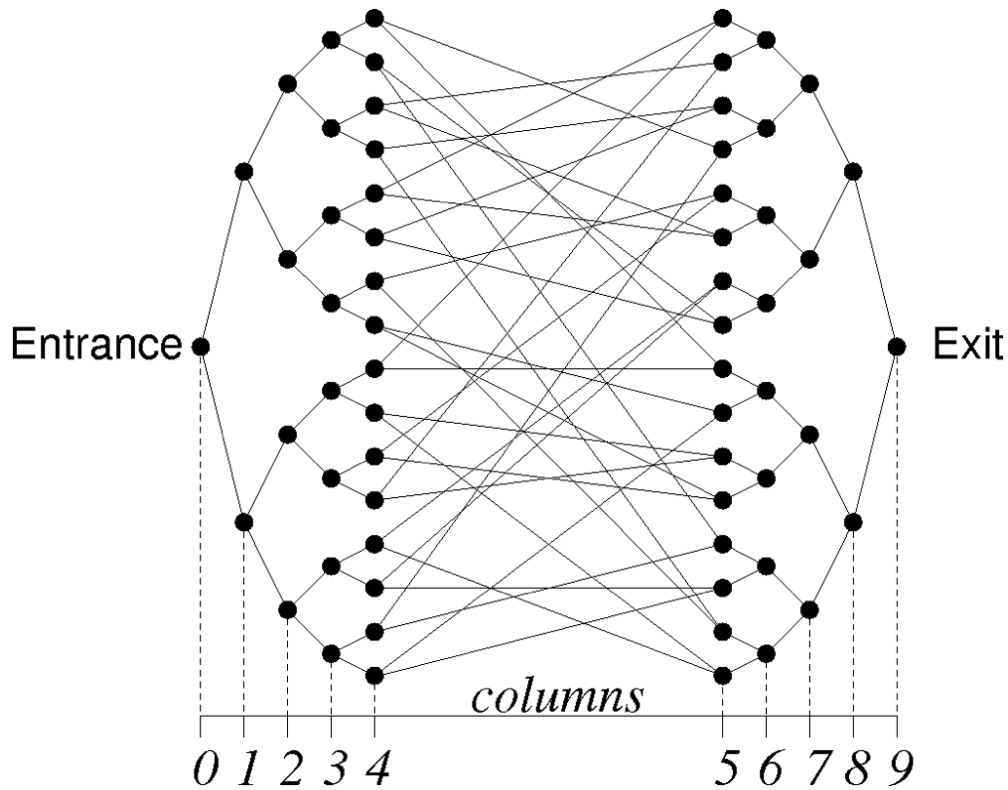
$$M = \begin{bmatrix} \ddots & \ddots & & & & \\ \ddots & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & -1 & 2 & -1 & \\ & & & \ddots & \ddots & \ddots \end{bmatrix}$$

Classical Random Walk

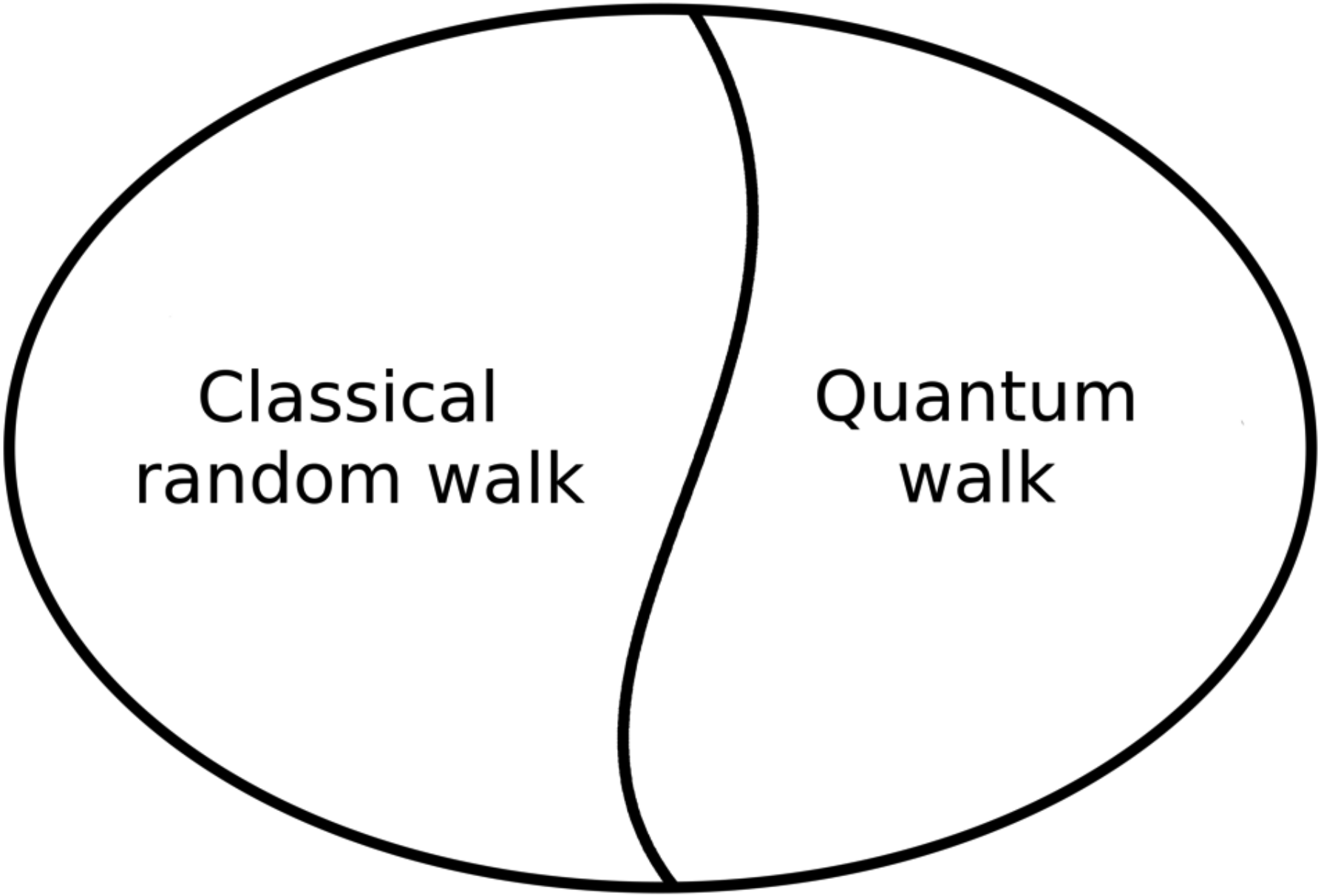


Quantum Walks and Speedups



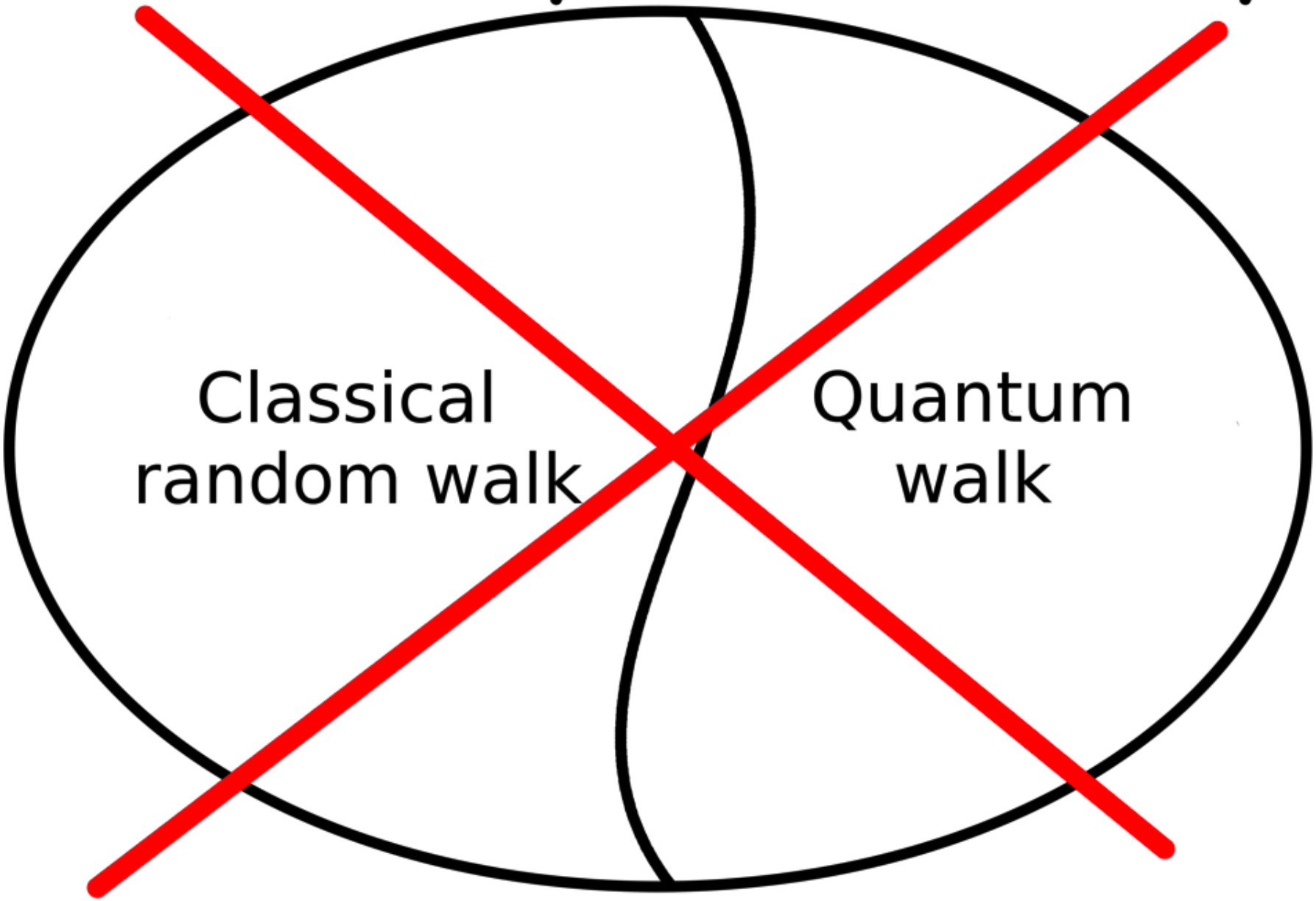


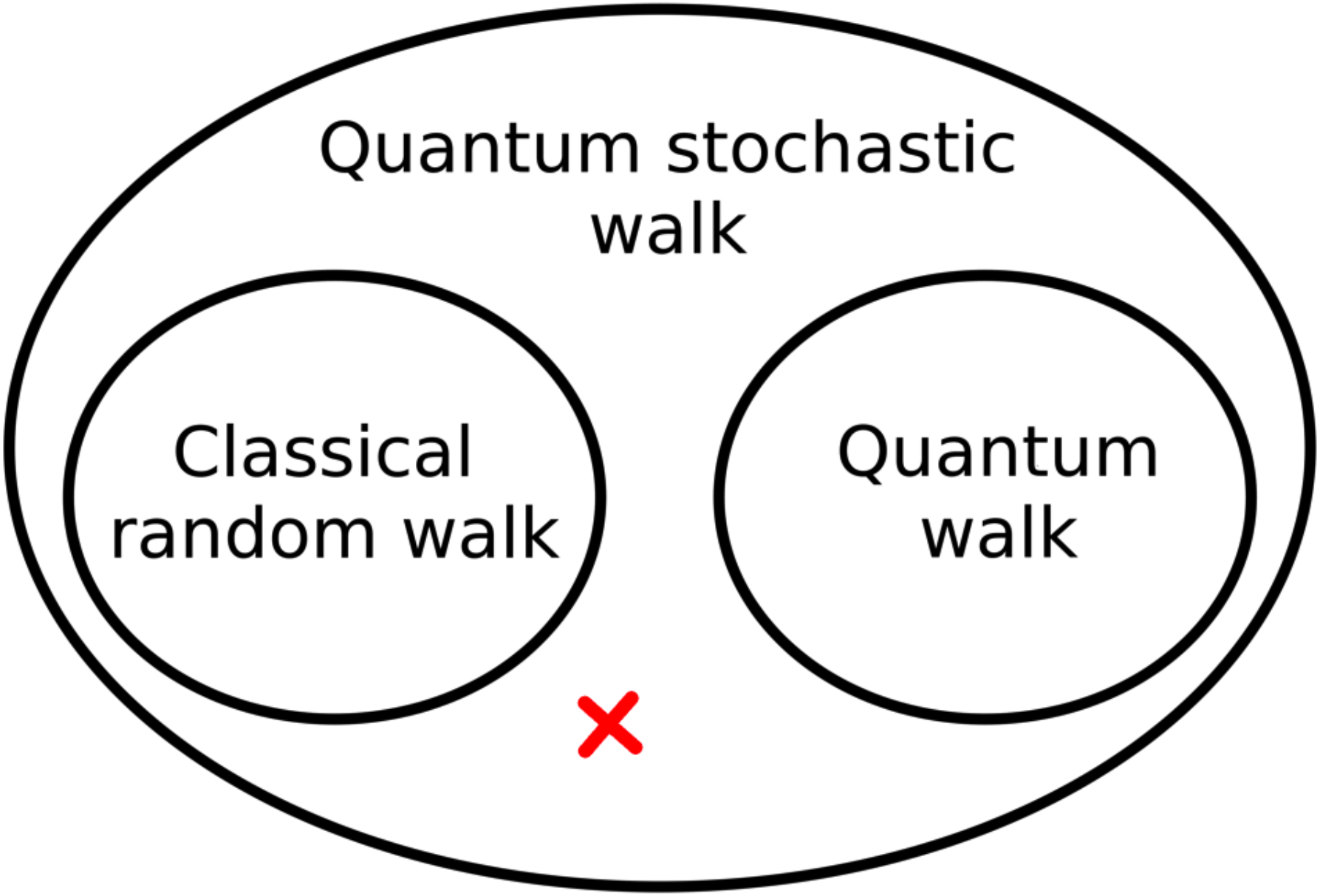
A. M. Childs, R. Cleve, E. Deotto, E. Farhi, S. Gutmann, and D.A. Spielman, Exponential Algorithmic Speedup by a Quantum walk quant-ph/0209131



For example: Work of Viv Kendon and co-worke

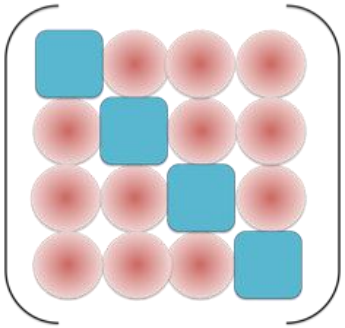
Non-unitary effects are key




Quantum stochastic walk
Classical random walk
Quantum walk

Density Matrices

- Quantum Generalization of Probability Distributions



Probability distributions of wave functions

Possible states: $\{\psi_k\}$
Prob of state ψ_k: p_k

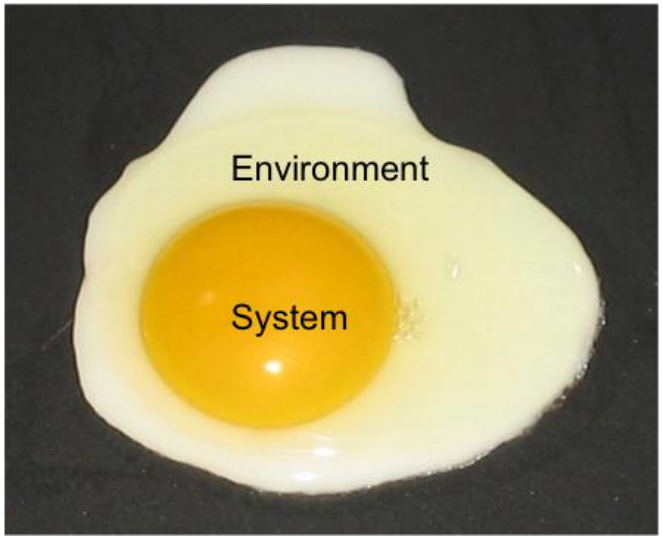
Density operator

$$\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|$$

Open Quantum Systems

The system interacts with the outside environment:

- Stochastic Processes give Thermodynamics
- Quantum Stochastic Processes give Quantum Thermodynamics



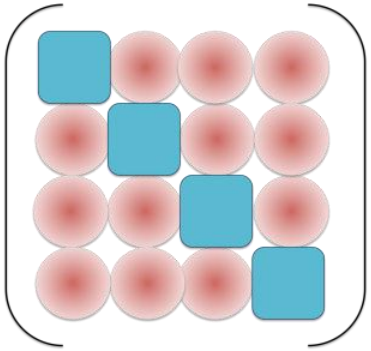
$$\dot{\rho} = \mathcal{L}\rho = -i[H,\rho] + \frac{1}{2}\sum_k 2L_k\rho L_k^\dagger - L_k^\dagger L_k\rho - \rho L_k^\dagger L_k$$

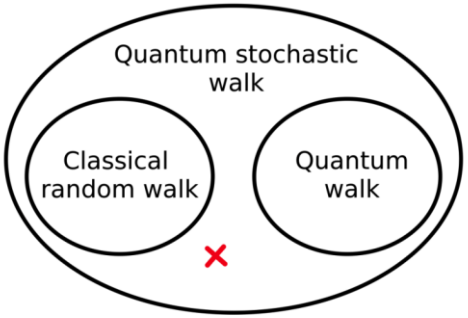
Coherent dynamics Stochastic evolution

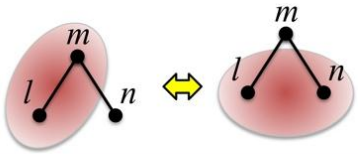
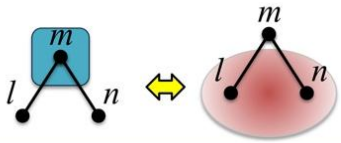
Walk	State function	Equation of Motion	Graph Correspondence
Classical	p	$Lp = \dot{p}$	L=M
Quantum	$\|\psi\rangle$	$H\|\psi\rangle = -i\partial_t\|\psi\rangle$	H=M
Q Stochastic	ρ	$\mathcal{L}\rho = \dot{\rho}$	???

J. D. Whitfield, C. A. Rodriguez-Rosario, A. A.-G. Phys. Rev. A 81, 022322 (2010)

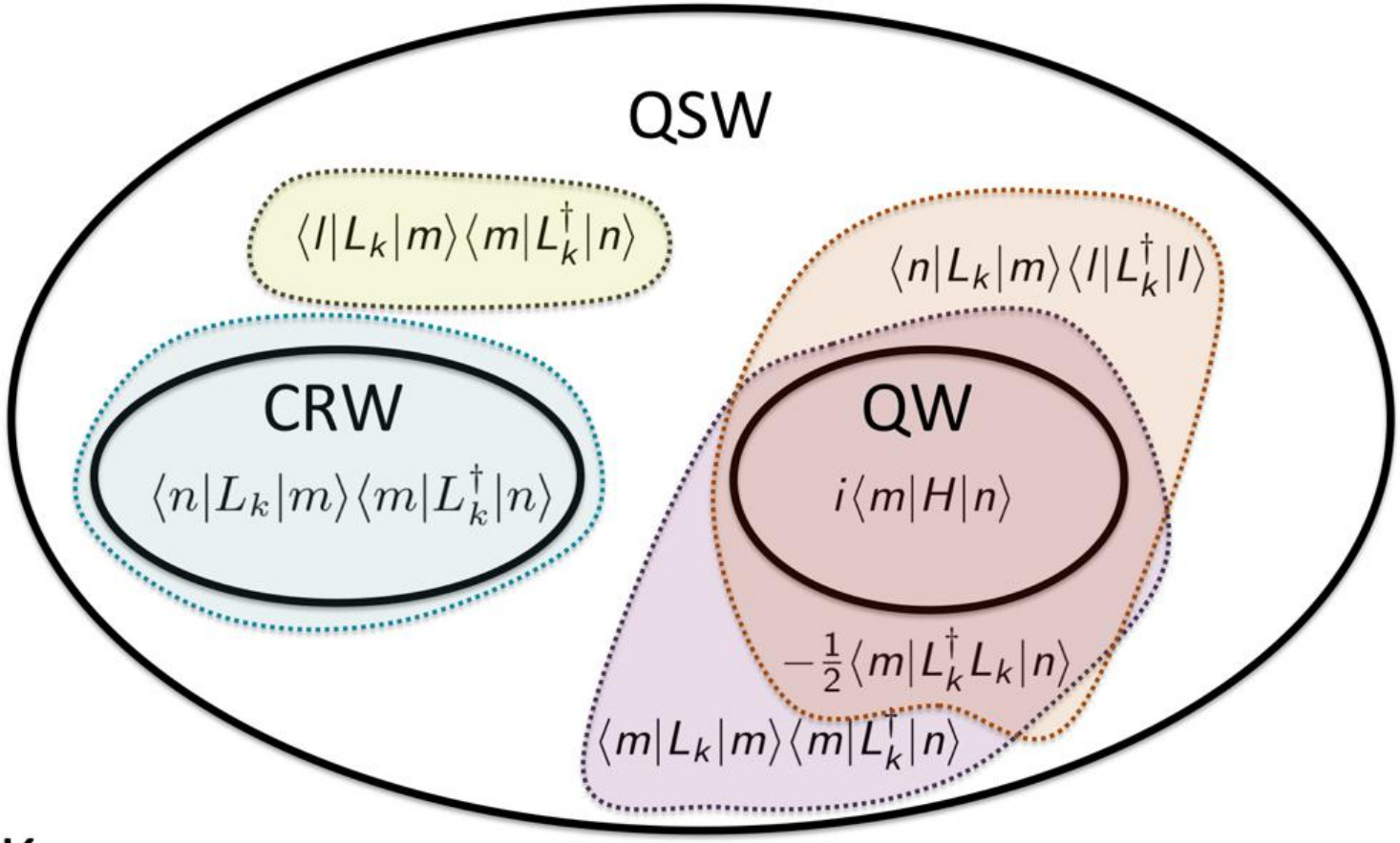
Walk	State function	Equation of Motion	Graph Correspondence
Classical	p	$Lp = \dot{p}$	L=M
Quantum	$\|\psi\rangle$	$H\|\psi\rangle = -i\partial_t\|\psi\rangle$	H=M
Q Stochastic	ρ	$\mathcal{L}\rho = \dot{\rho}$	???



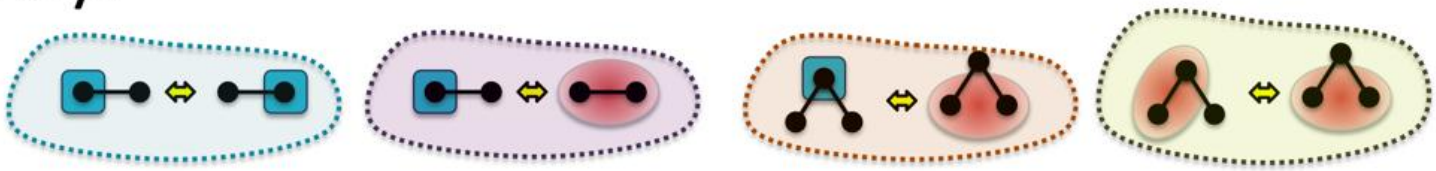


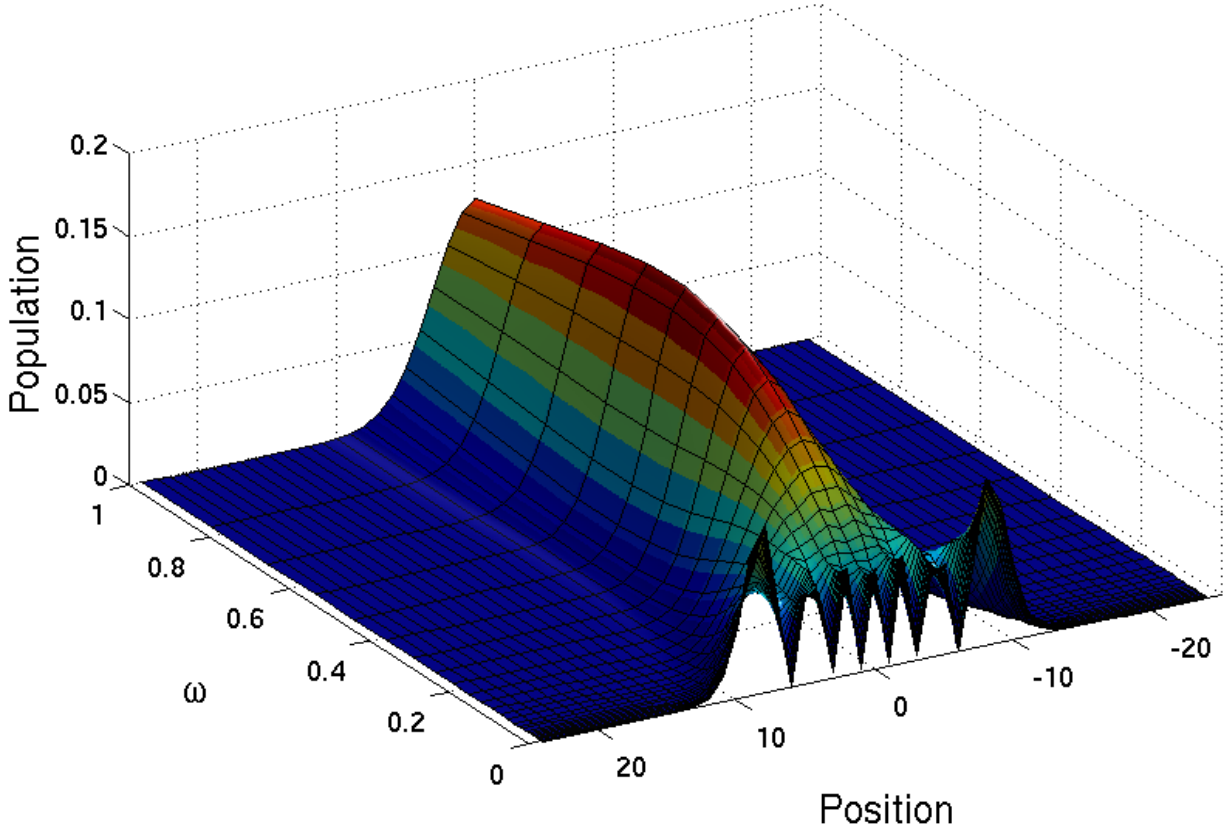
Density Matrix Elements	Transition Operators	Characteristics
	$\{L_k\}$	Classical Random Walk
	$H, \{L_k\}$	Quantum Walk + <u>MORE</u>
	$H, \{L_k\}$	Quantum Walk + <u>MORE</u>
	$\{L_k\}$	<u>MORE</u>!!!

Quantum Stochastic Walk: Rules



Key:



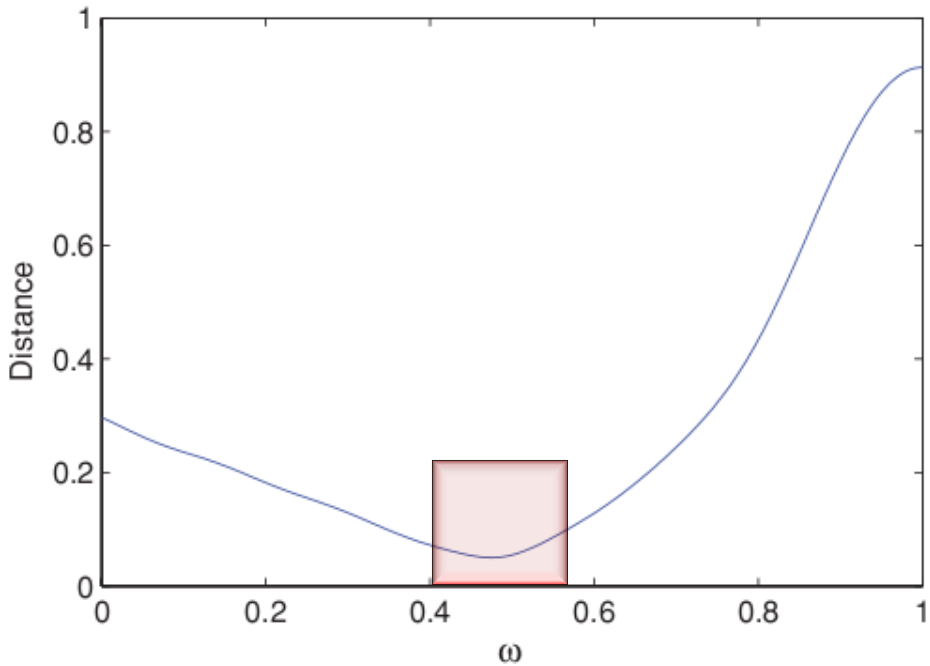


Single parameter interpolation

- Quantum walk: use von Neumann equation
- Classical random walk: use $L_{(k,k')} = M_{k,k'} |k\rangle\langle k'|$

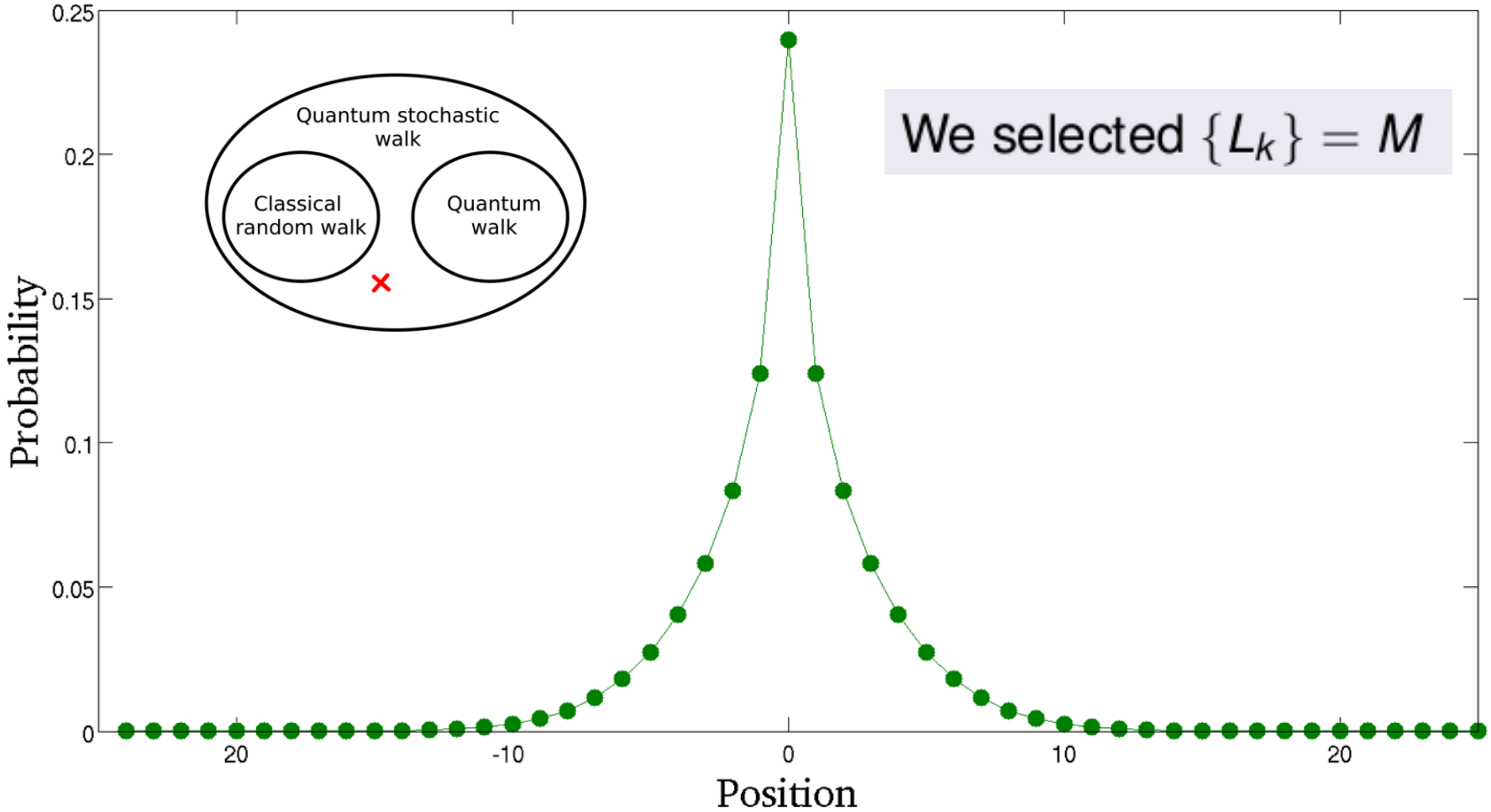
$$\mathcal{L}_\omega[\rho] = -(1-\omega)\, i\,[H,\rho] + \omega \sum_k \left(-\tfrac{1}{2} L_k^\dagger L_k \rho - \tfrac{1}{2} \rho L_k^\dagger L_k + L_k \rho L_k^\dagger \right)$$

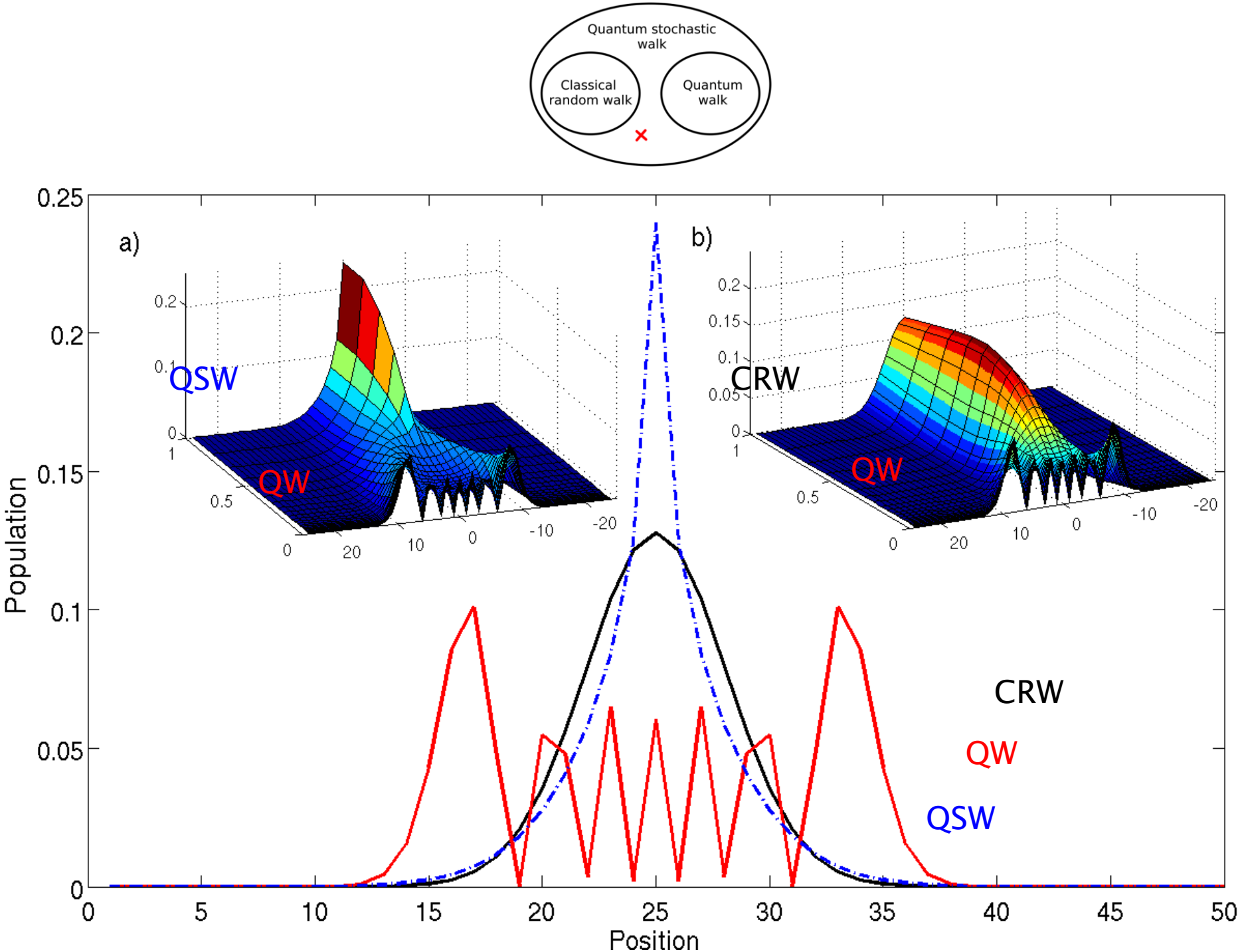
It never becomes a classical walk!



Euclidean distance metric between QSW and CRW as interpolation between the two using a pure-dephasing environment

Example of a QSW that is neither a CRW nor QW

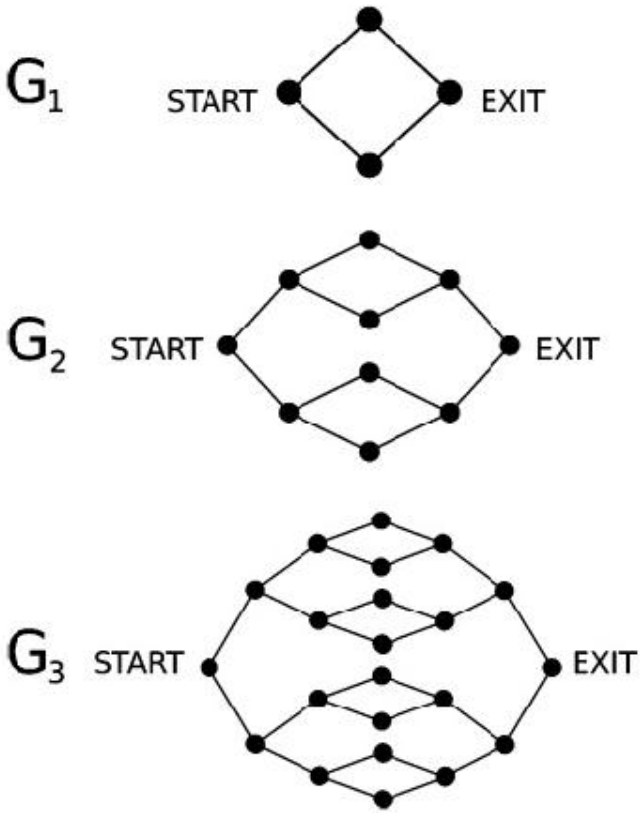



Quantum stochastic walk
Classical random walk
Quantum walk
a)
b)
QSW
QW
CRW
Population
Position
0.25
0.2
0.15
0.1
0.05
0
5
10
15
20
25
30
35
40
45
50

Ongoing Work

- Explorations of the QSW: Dephasing in Momentum space
- Connection between discrete (coined) walks and non-Markovian master equations
- More Graphs: beyond the line
- Classical to Quantum Transition of Algorithms
- Complexity Classes of QSW

Glued Trees: No smooth interpolation



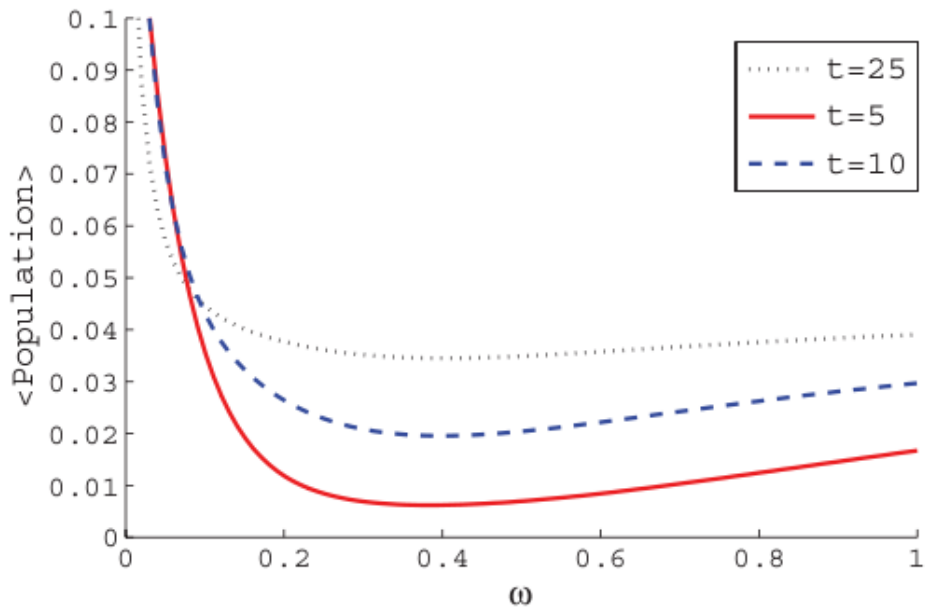
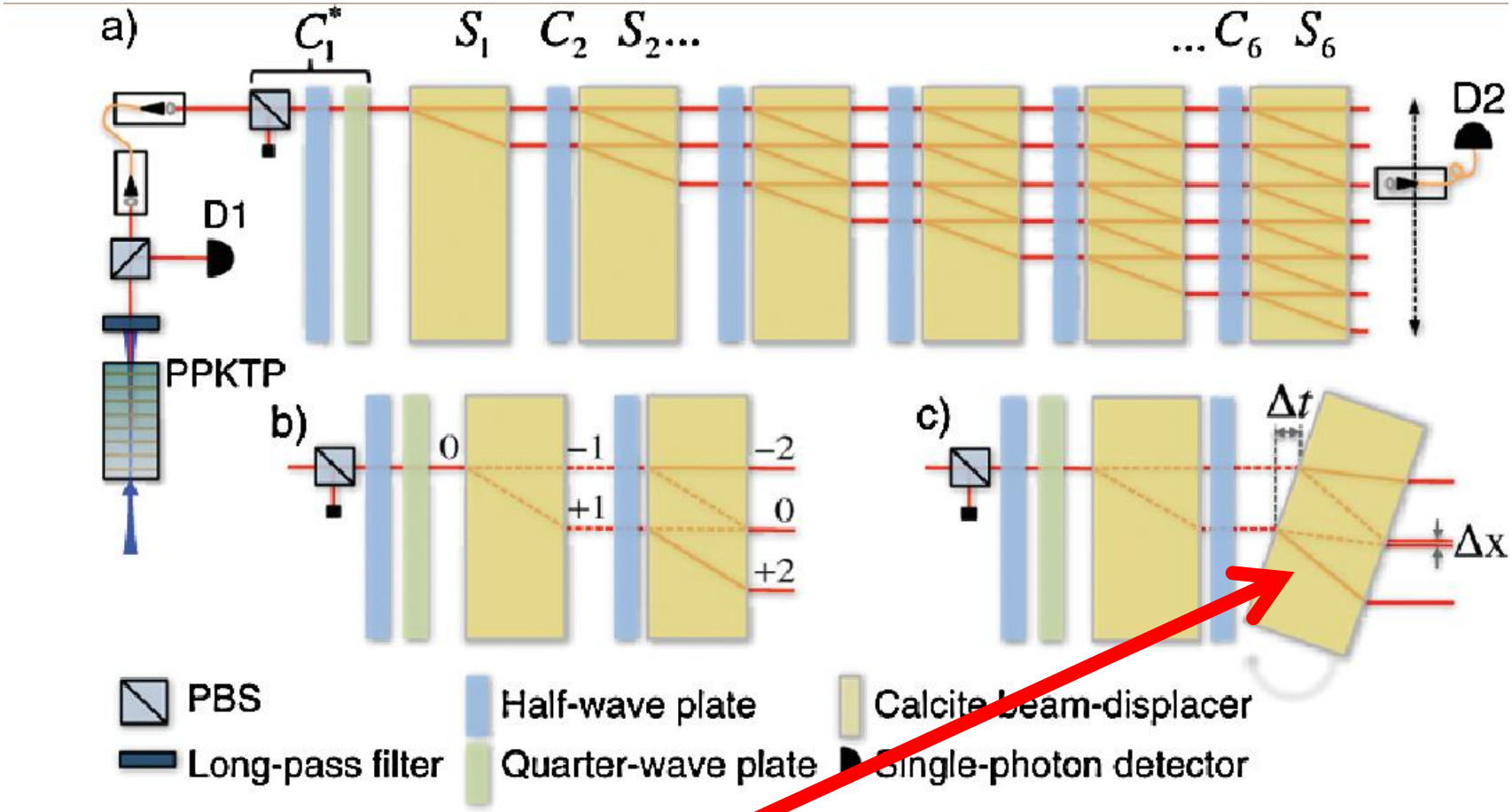


FIG. 5. (Color online) Plot of the time-averaged population for transport through the G_3 tree at three fixed times, $t = \{5, 10, 25\}$, as a function of the decoherence strength $\omega \in [0, 1]$ (atomic units). When $\omega = 1$, the classical walk is obtained, and when $\omega = 0$, the unitary walk is recovered. Notice that the probability is not a strictly decreasing function of the decoherence.

Single-Photon Quantum optics experiment:
Physical Review Letters 104, 153603

Collaboration with Andrew Whi
(Queensland)

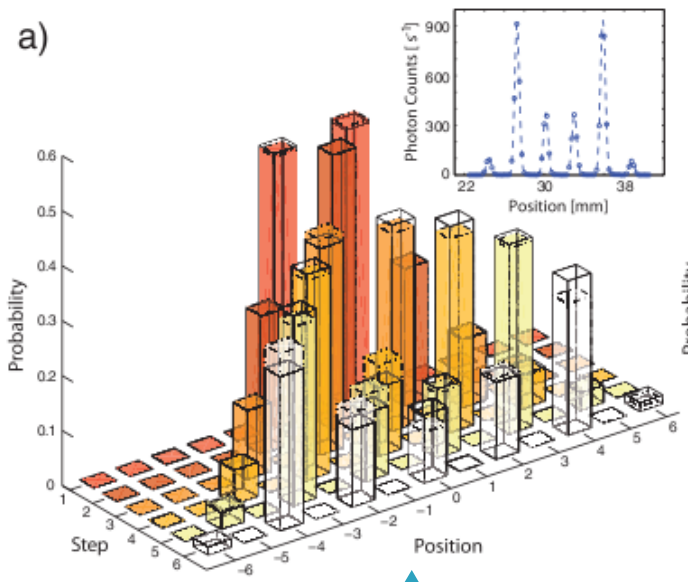
Discrete-time quantum walk: Optical setup

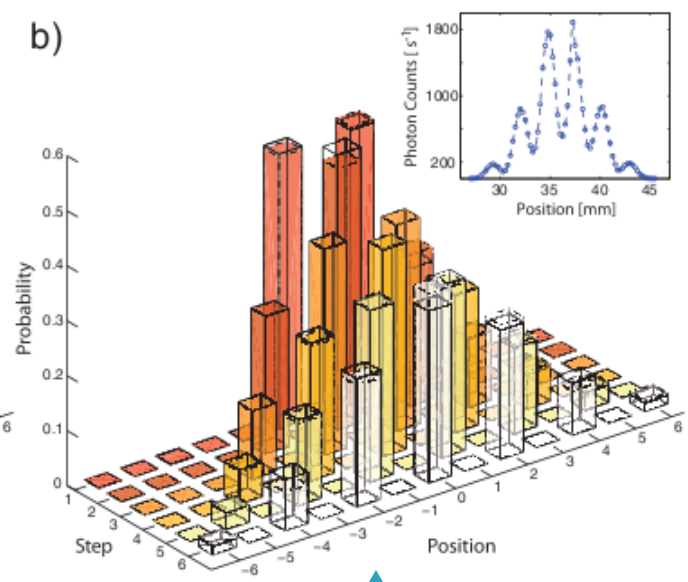


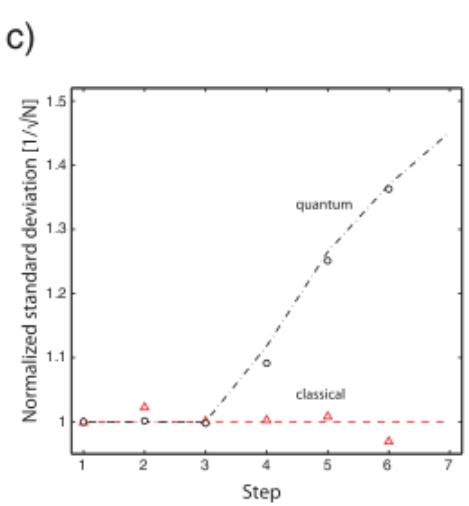
Jiggle to induce decoherence

W = SC (shift + coin)

Experimental results





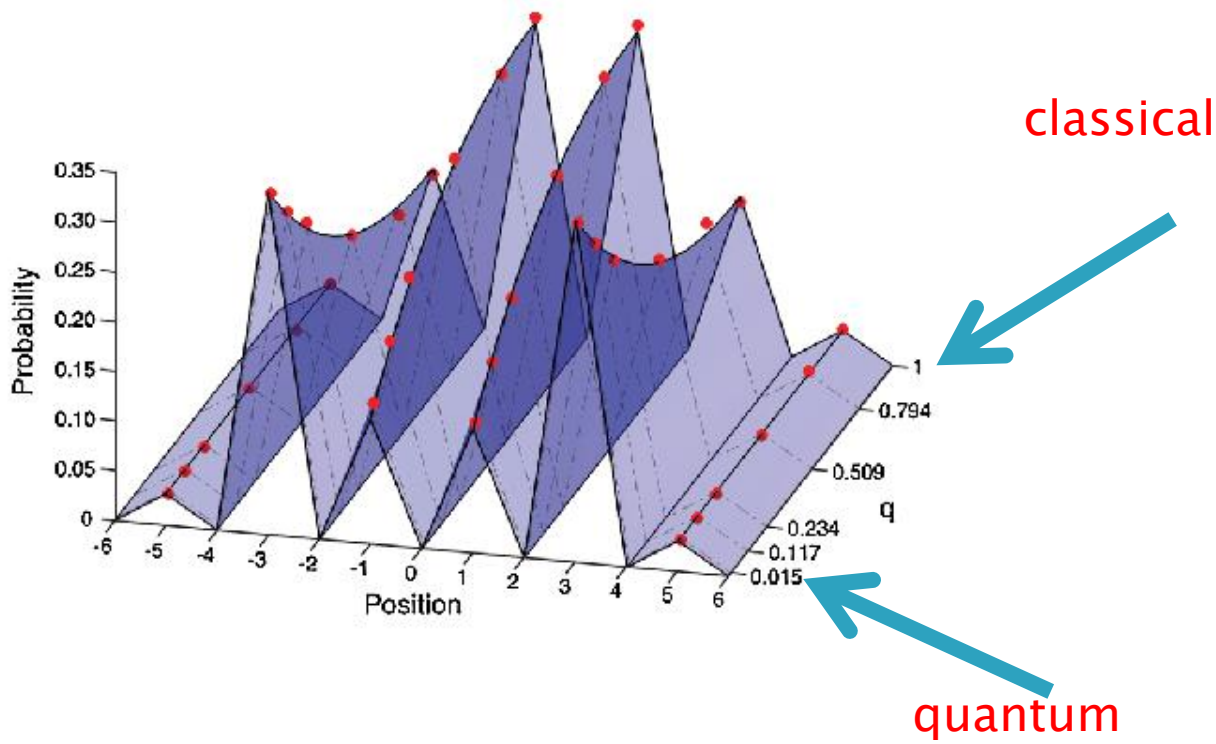


quantum walk

discrete-time classical walk

Standard deviation

Quantum to classical transition (dephasing-induced)

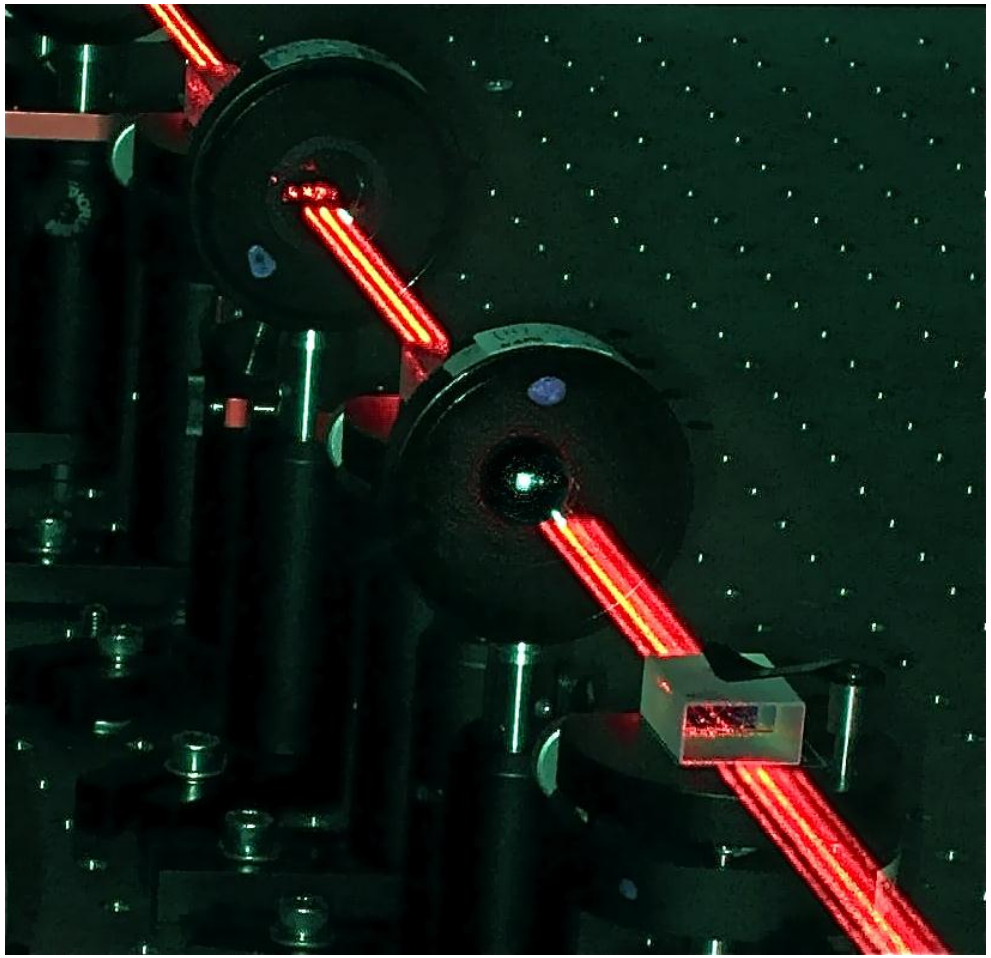


Outlook

Interpret ultra-fast experiments using quantum stochastic walks

Create a phase boundary in the DTQW experiment to seek for soliton states (topological insulators)

Seek quantum speedups for quantum stochastic walks



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Thank you!

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