Quantum Simulation

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Outline

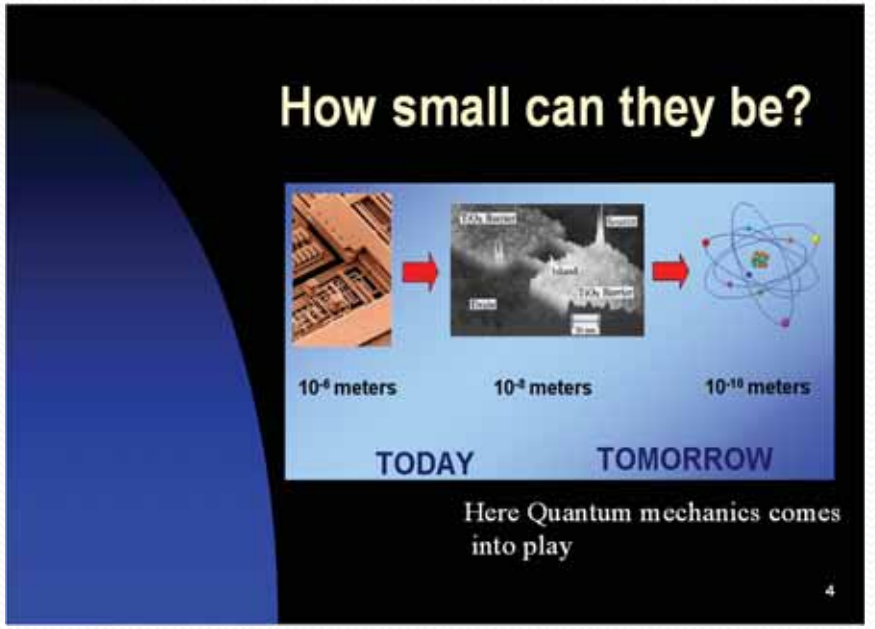
- What is Quantum Computer and Quantum Simulation?
- Categories, Resources and Errors
- Possible Physical Realization
- Applications of Quantum Simulation

- **What is Quantum Computer and Quantum Simulation?**
- Categories, Resources and Errors
- Possible Physical Realization
- Applications of Quantum Simulation

Bottleneck of Classical Computers

Limitation of Classical Computers:

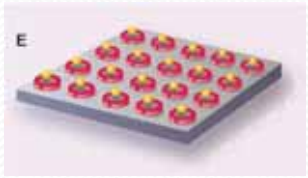
Heat dissipation and Quantum effect



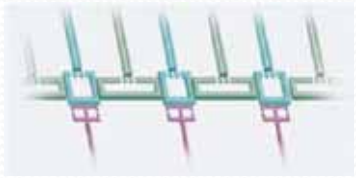
We need a new type of computation!

What is a Quantum Computer?

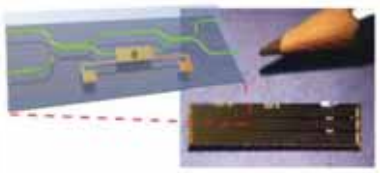
Classical Computers



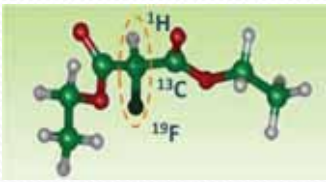
Ion Trap



Superconducting



Photons



NMR

A quantum computer is not a bigger, smaller of faster version.
It is a new computer version by controlling coherent quantum mechanical waves.

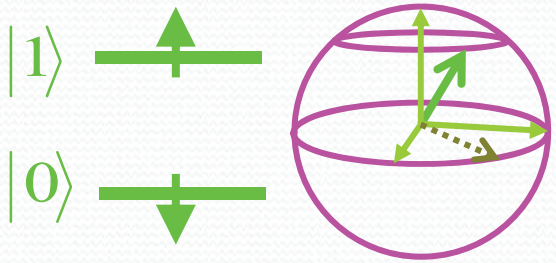
How it Works?

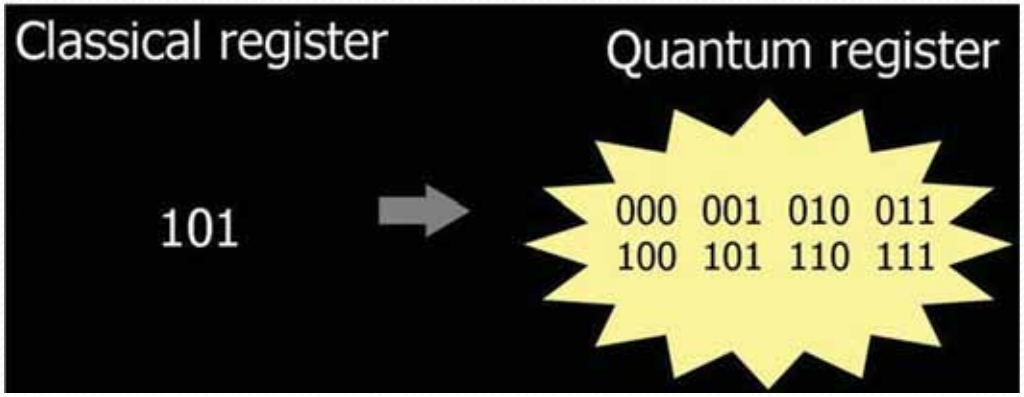
Quantum computing exploits properties of quantum bits (qubits).

Classical bits are 0 and 1

Qubits have a probability of being either 0 or 1, denoted

$$\cos\theta|0\rangle + e^{i\phi}\sin\theta|1\rangle$$

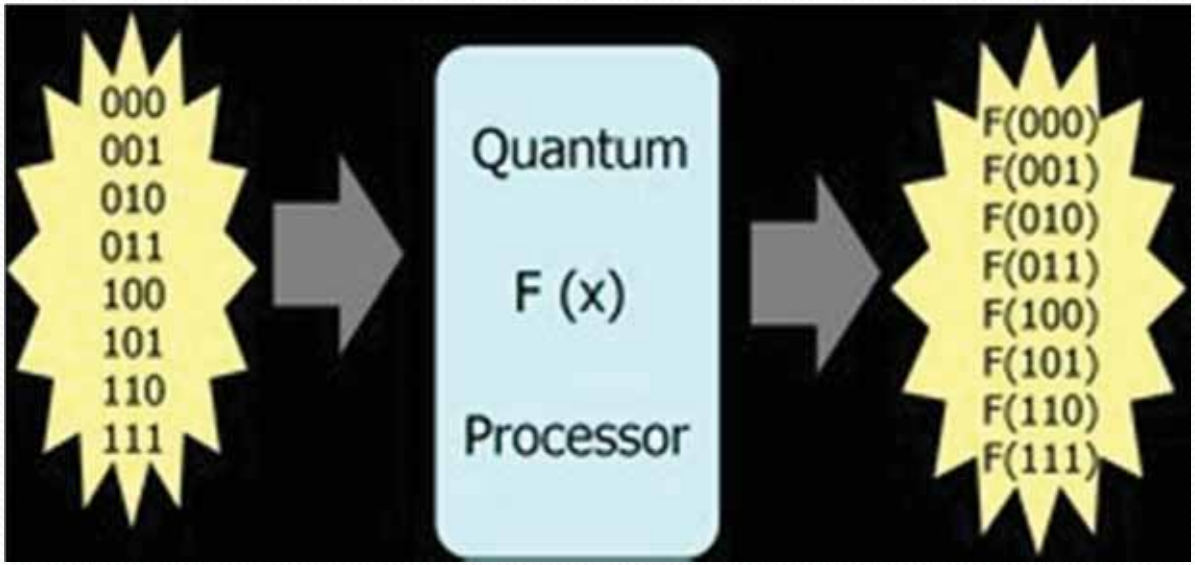




General Concepts

Each qubit represents two possible states with different probabilities.
For *n* qubits, 2^n states are represented.

- Multiple states of qubits leads to 2^n computations performed on *n* qubits



- Simultaneous calculations can be made on **all** qubits

Applications

Quantum Computation

Algorithms

Shor's Algorithm

Factoring a 512-bit integer:

8400 years with MIPS

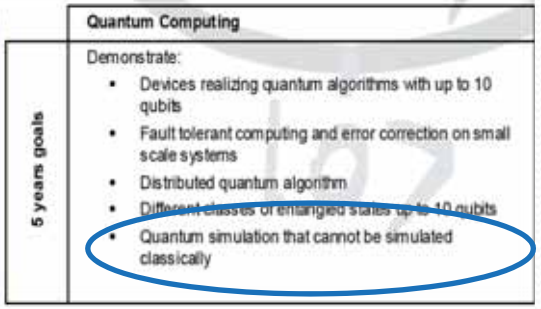
3.5 hours with QC

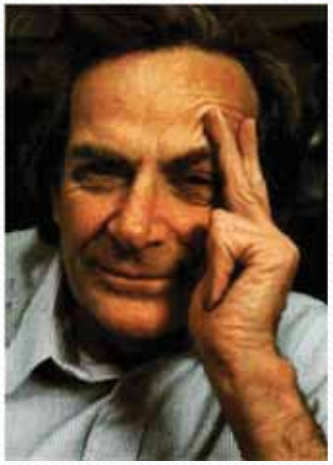
Require thousands of qubits

P. W. Shor, *Proc. 35nd Annual Symposium on Foundations of Computer Science* (1994)

Simulation

Quantum Simulators





Require 30-100 qubits

Feynman, *Int. J. Theor. Phys.* 21, 467 (1982)
Lloyd, *Science* 273, 1073-1078 (1996)

Definition of Quantum Simulation

Feynman's Question:

What kind of computer are we going to use to simulate physics?

--- "Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws."

--- "The rule of simulation that I would like to have is that the number of computer elements required to simulate a large physical system is only to be proportional to the space-time volume of the physical system. I don't want to have an explosion. "

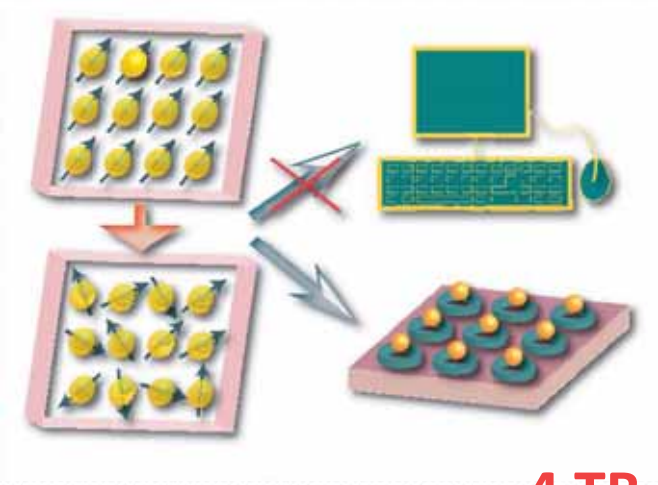
--- "... there is to be an exact simulation, that the computer will do exactly the same as nature."

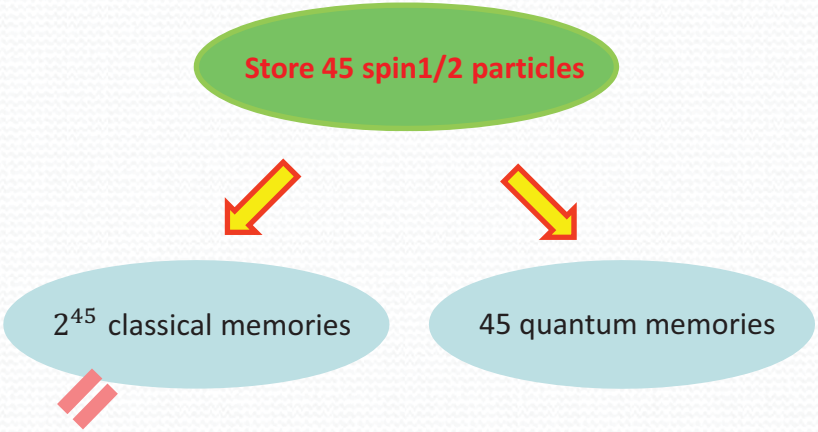
A loosely definition

Simulating Quantum Systems by Quantum Mechanical Means

Why Quantum Simulator?

We cannot use classical computers to simulate quantum phenomena





4 TB hard disk

160

800

400,000

2,000,000

Classical Data We Have

US Library of Congress

Data: 160 TB = 50 Spins

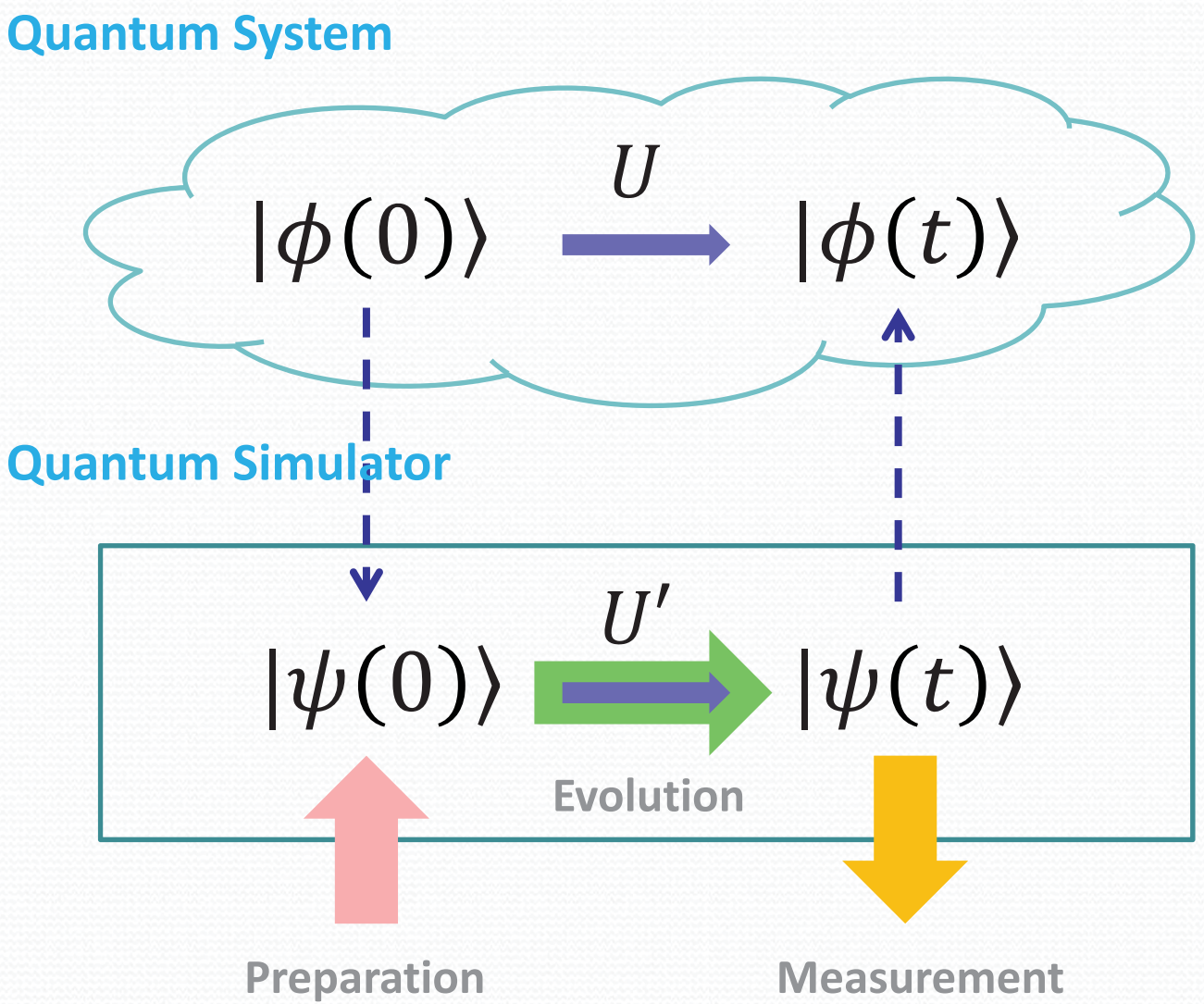
Information of Humankind

2.2×10^9 TB = 71 spins

M. Hilbert and P. Lopez, "The world's technological capacity to store, communicate and computer information", Science.

- What is Quantum Computer and Quantum Simulation?
- **Categories, Resources and Errors**
- Possible Physical Realization
- Applications of Quantum Simulation

Schematic Representation



DQS and AQS

Digital Quantum Simulation

Similar to circuit-based quantum computation

a. Initial state preparation
b. Unitary evolution which can be decomposed efficiently
c. Measurement of the final state

S. Lloyd, Science 273, 1073-1078 (1996)
D. Abrams and S. Lloyd, Phys. Rev. Lett. 79, 2586 (1997)

Analog Quantum Simulation

One quantum system would mimic the evolution of another

Core: Finding the mapping of the system onto the AQS.
Initial state preparation and measurement have not been discussed thoroughly.

D. Porras and J. Cirac, Phys. Rev. Lett. 92, 207901 (2004)
A. Smirnov et al., Euro. Phys. Lett. 80, 67008 (2007)

Digital Quantum Simulation

Initial State Preparation

How to realize $|000\ldots\rangle$ to $|\phi(0)\rangle$

Only particular cases efficient preparation is possible

- ✓ **Generating an antisymmetrized superposition of n! states**

  D. Abrams and S. Lloyd, Phys. Rev. Lett. 79, 2586 (1997)

- ✓ **Preparation of N-particle fermionic states**

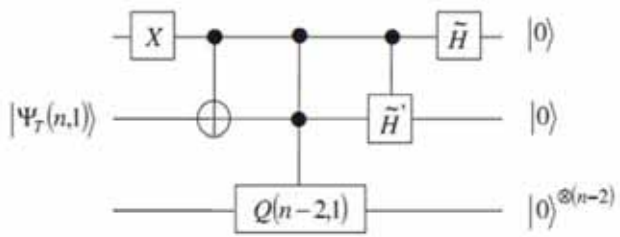
  G. Ortiz et al., Phys. Rev. A 64, 022319 (2001)

- ✓ **Chemical wave functions**

  I. Kassal et al., PNAS 105, 18681 (2008)

- ✓ **Molecular system with m electrons occupying n spin orbitals**

  H. Wang et al., Phys. Rev. A 79, 042335 (2009)



This method starts from the target state and transforms it back to the initial state.

Digital Quantum Simulation

Unitary Evolution (a)

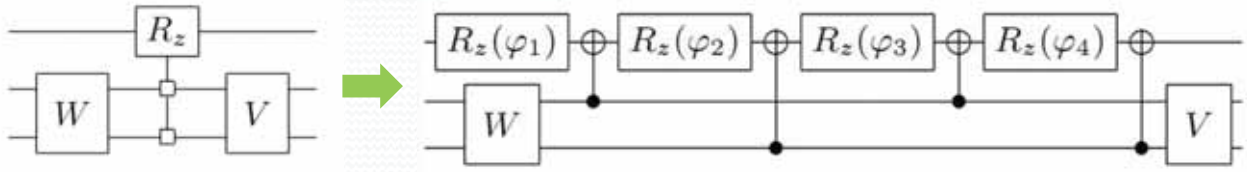
✓ **First Order Trotter-Suzuki Formula:**

$$U(\Delta t) = \prod_l e^{-i\hbar H_l \Delta t} + O(\Delta t^2)$$

Very small Δt induces very large number of gates

K. Brown, I. Clark and I. Chuang, Phys. Rev. Lett. 97, 050504 (2006)
C. Clark et al., Phys. Rev. A 79, 062314 (2009)

✓ **Generation of Many-body Interactions**



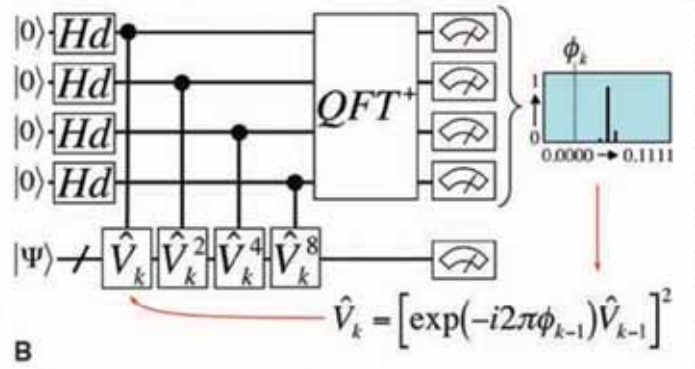
It is not easy and usually requires ancilla qubits

M. Nielson et al., Phys. Rev. A 66, 022317 (2002)
L. Veis et al., arxiv 1111.3490v1 (2011)
K. Brown, S. De, V. Kendon and W. Murno, arxiv 1011.2984v2 (2011)

Digital Quantum Simulation

Unitary Evolution (b)

✓ **Calculation of Molecular energies**



Recursive phase estimation algorithm. *K* iterations are needed to obtain *k* bits of the phase ϕ.

A. Aspuru-Guzik et al., Science, 309, 1704 (2005)

✓ **Continuous Evolution of a Quantum System**

M. McKague, M. Mosca and N. Gisin, Phys. Rev. Lett. 102, 020505 (2009)

✓ **Under Translational Symmetry**

C. Kraus, M. Wolf and J. Cirac, Phys. Rev. A 75, 022303 (2007)

Digital Quantum Simulation

Measurement

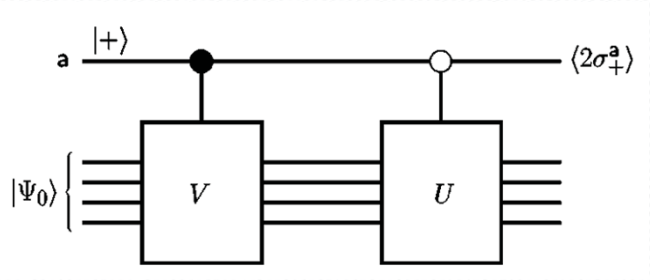
- ✓ **Quantum State Tomography**

  The most common approach but scales exponentially.

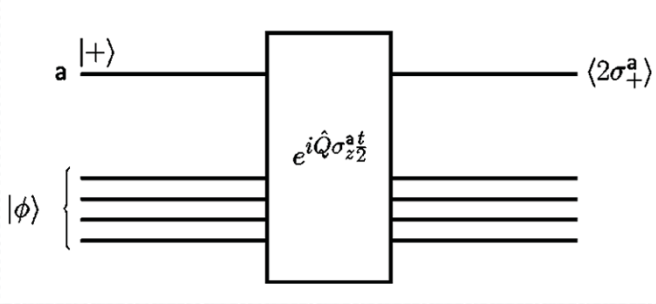
  G. D'Ariano, M. Paris and M. Sacchi, Advances in Imaging and Electron Physics 128, 205 (2003)

- ✓ **Correlation Functions or Spectrum of Operators**

  G. Ortiz et al., Phys. Rev. A 64, 022319 (2001)
  R. Somma et al., Phys. Rev. A 65, 042323 (2002)



Measure $\langle U^\dagger V \rangle$



Measure Hermitian operator Q

Comparison

	Digital	Analogue
Quantum simulation via	Manipulation of symbols	Evolution equations
Output	Logical quantum state	Physical quantum state
Determined by	Number of active qubits	Accuracy of realization
Errors controlled	Yes	No
Errors fatal to calculation	Yes	No
Required fidelity	Higher	Lower
Ancilla qubits	Yes	No
Hardware/software	General purpose	Problem-specific
Target problems	Any problem	Restricted set

Resources

With ten or less qubits:

✓ Quantum Chaos

J. Howell and J. Yeaze, Phys. Rev. A 61, 012304 (2000)
Y. Weinstein et al., Phys. Rev. Lett. 89, 157902 (2002)

✓ Simple Chemical Reactions

A. Smirnov et al., Euro. Phys. Lett. 80, 67008 (2007)

✓ Dirac Particles

A. Bermudez et al., Phys. Rev. A 76, 041801 (2007)
R. Gerritsma et al., Nature, 463, 68 (2010)
L. Lamata et al., Phys. Rev. Lett. 98, 253005 (2007)

✓ Unruh Effect

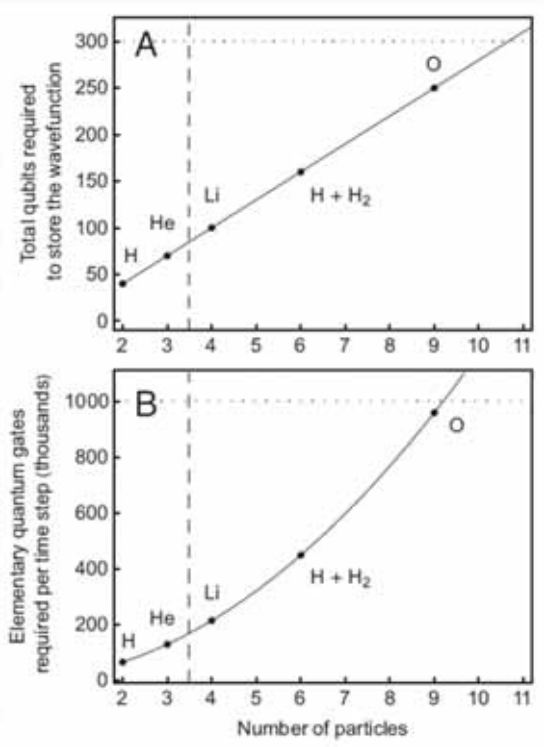
P. Alsing, J. Dowling and G. Milburn, Phys. Rev. Lett. 94, 220401 (2005)

✓ Anyons

C. Lu et al., Phys. Rev. Lett. 102, 030502 (2009)
J. You et al., Phys. Rev. B 81, 014505 (2010)

Resources: An Example

Simulating reaction dynamics



The number of qubits scales linear with molecular size

Total number of qubits:

$$n(3N-6)+4m$$

The number of operations scales polynomial with molecular size

Total number of gates:

$$O(N^2m^2)$$

To outperform classical computers:
100 qubits and 200,000 gates!

I. Kassal et. al., PNAS 105, 18681 (2008)

Errors

Compared to quantum algorithms, only limited precision is required in quantum simulation.

- ✓ **Pairing Hamiltonian Model**

  Systematic errors and Trotter approximations

  K. Brown, R. Clark and I. Chuang, Phys. Rev. Lett. 97, 050504 (2006)

- ✓ **Schrodinger's Equation**

  Amplitude errors

  G. Strini, Fortsch. Phys. 50, 171 (2002)

- ✓ **Dynamically Localized System**

  Small changes of Hamiltonian and chosen qubits

  S. Montangero, Phys. Rev. A 70, 032311 (2004)

- ✓ **Many-body Interaction Hamiltonian**

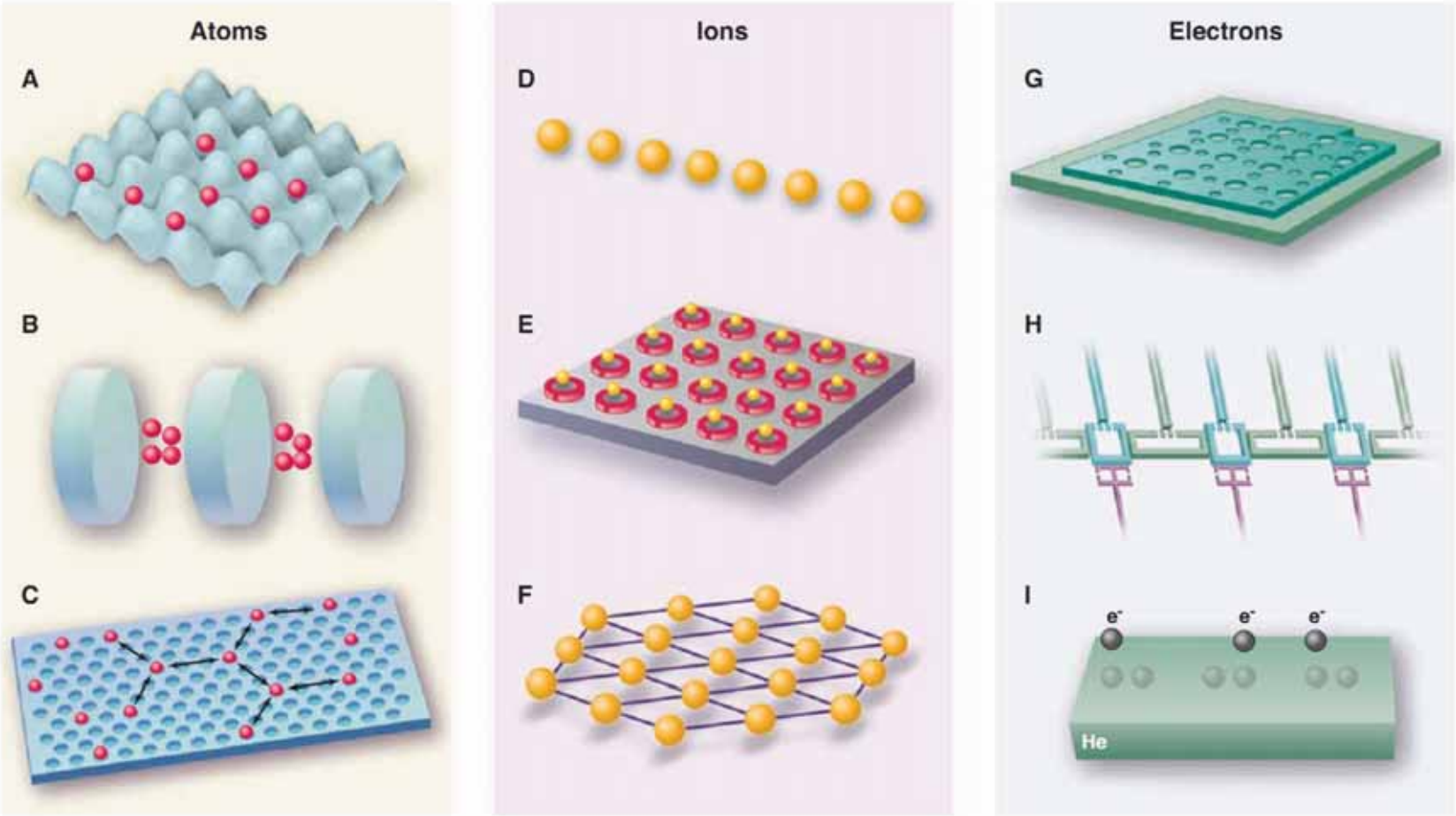
  Study of the effect of noise

  W. Dur, M. Bremne and H. Briegel, Phys. Rev. A 78, 052325 (2008)

- What is Quantum Computer and Quantum Simulation?
- Categories, Resources and Errors
- **Possible Physical Realization**
- Applications of Quantum Simulation

Potential Systems

Potential Systems



Photons

- ✓ **Qubits: Polarization states**
- ✓ **Single-qubit gate: Birefringent waveplates**
- ✓ **Two-qubit gate: Combining linear optical elements**
- ✓ **Initialize: Single-photon source**
- ✓ **Measure: Single-photon detector**

E. Knill, R. Laflamme and G. Milburn, Nature 409, 46 (2001)

Quantum Baker's Map

J. Howell and J. Yeaze, Phys. Rev. A 61, 012304 (2000)

Fractional Statistics of Anyons

C. Lu et al., Phys. Rev. Lett. 102, 030502 (2009)

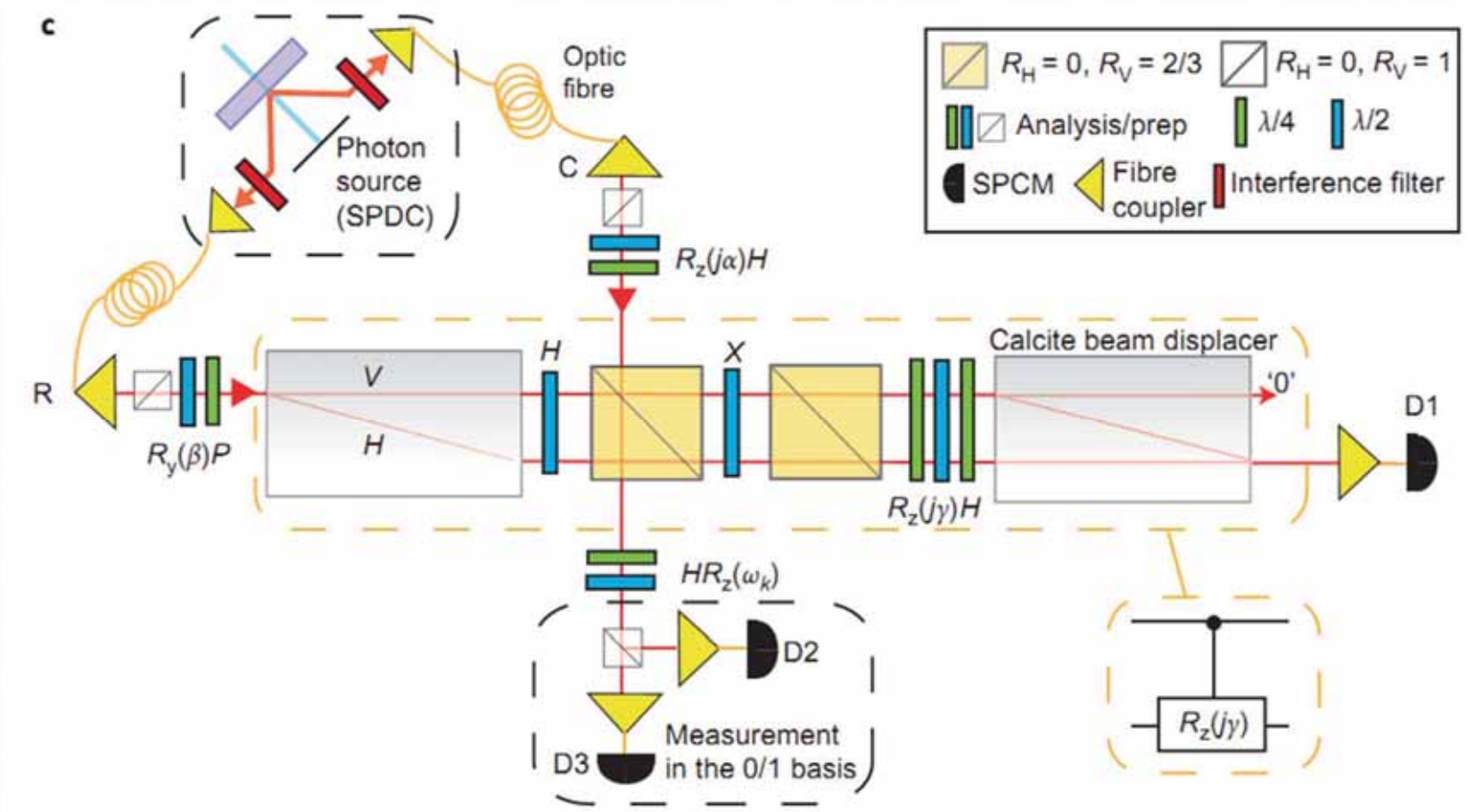
Energy of Hydrogen Molecule

B. Lanyon et al., Nat. Chem. 2, 483 (2010)

Little flexibility and limited scalability

Photons

Simulating Energy of Hydrogen Molecule in Photons



B. Lanyon et al., Nat. Chem. 2, 483 (2010)

Neutral Atoms

- ✓ **Qubits: Energy levels in trapped atoms**
- ✓ **Single-qubit gate: External laser beams**
- ✓ **Two-qubit gate: Appropriate laser and contact interactions**
- ✓ **Initialize: Optical pumping**
- ✓ **Measure: State-dependent optical fluorescence detection**

I. Bloch, J. Dalibard and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008)
M. Lewenstein et al., Advances in Physics 56, 243 (2007)

Superfluid to Mott Insulator

M. Greiner et al., Nature 415, 39 (2002)

Creation of Tonks-Girardeau Gas

B. Paredes et al., Nature 429, 277 (2004)

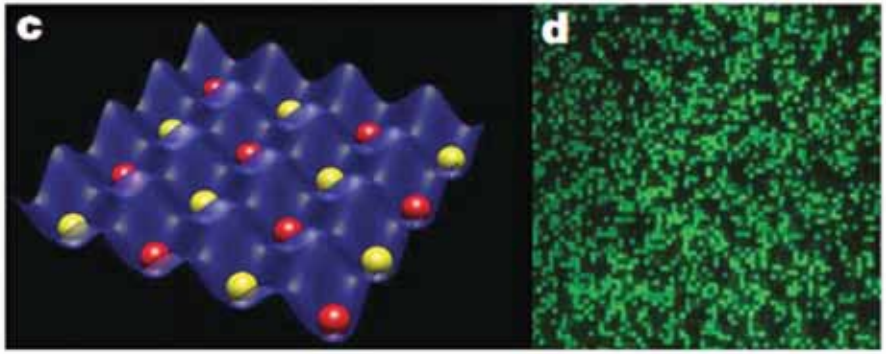
Observe BCS-BEC Crossover

M. Zwierlein et al., Nature 435, 1047 (2005)

Disordered Systems

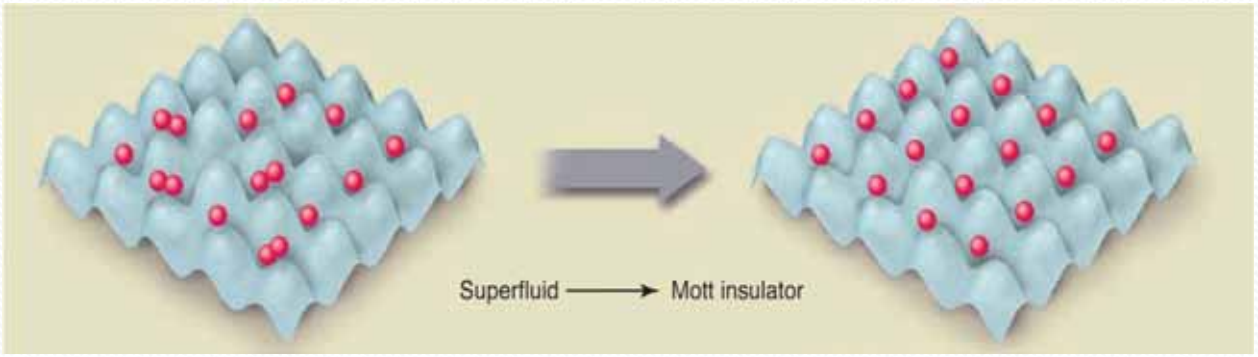
T. Schulte et al., Phys. Rev. Lett. 95, 170411 (2005)
L. Fallani et al., Phys. Rev. Lett. 98, 130404 (2007)

Neutral Atoms



T. Ladd et al., Nature 464, 45 (2010)

Simulating Quantum Phase Transition in Neutral Atoms



M. Greiner et al., Nature 415, 39 (2002)

Trapped Ions

- ✓ Qubits: Phonons
- ✓ Single-qubit gate: External laser beams
- ✓ Two-qubit gate: Appropriate interactions
- ✓ Initialize: Cooling to the hyperfine ground state
- ✓ Measure: Distribution of the hyperfine status

R. Blatt and D. Wineland, Nature 453, 1008 (2008)

Nonlinear Interferometers

D. Leibfried et al., Phys. Rev. Lett. 89, 247901 (2002)

Paramagnetic to ferromagnetic

A. Friedenauer et al., Nat. Phys. 4, 757 (2008)

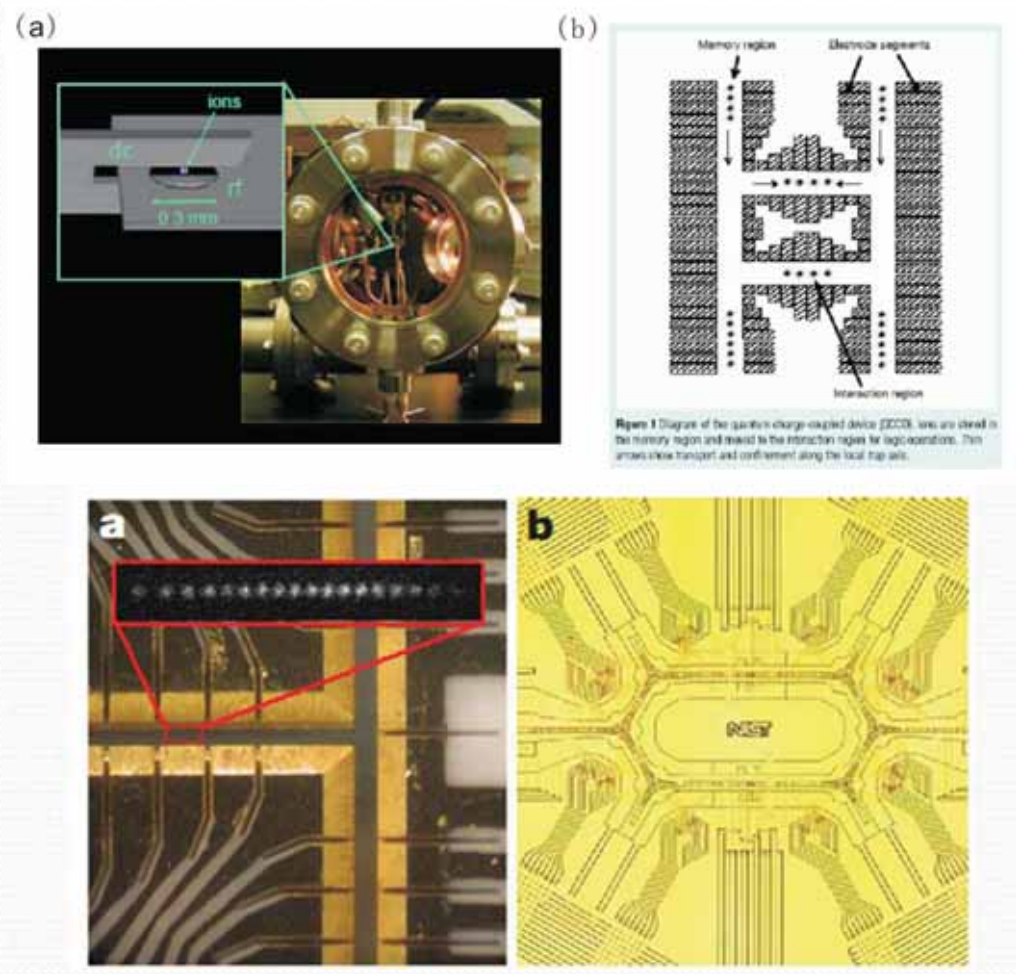
Dirac Particles

R. Gerritsma et al., Nature, 463, 68 (2010)

Unruh Effect

P. Alsing, J. Dowling and G. Milburn, Phys. Rev. Lett. 94, 220401 (2005)

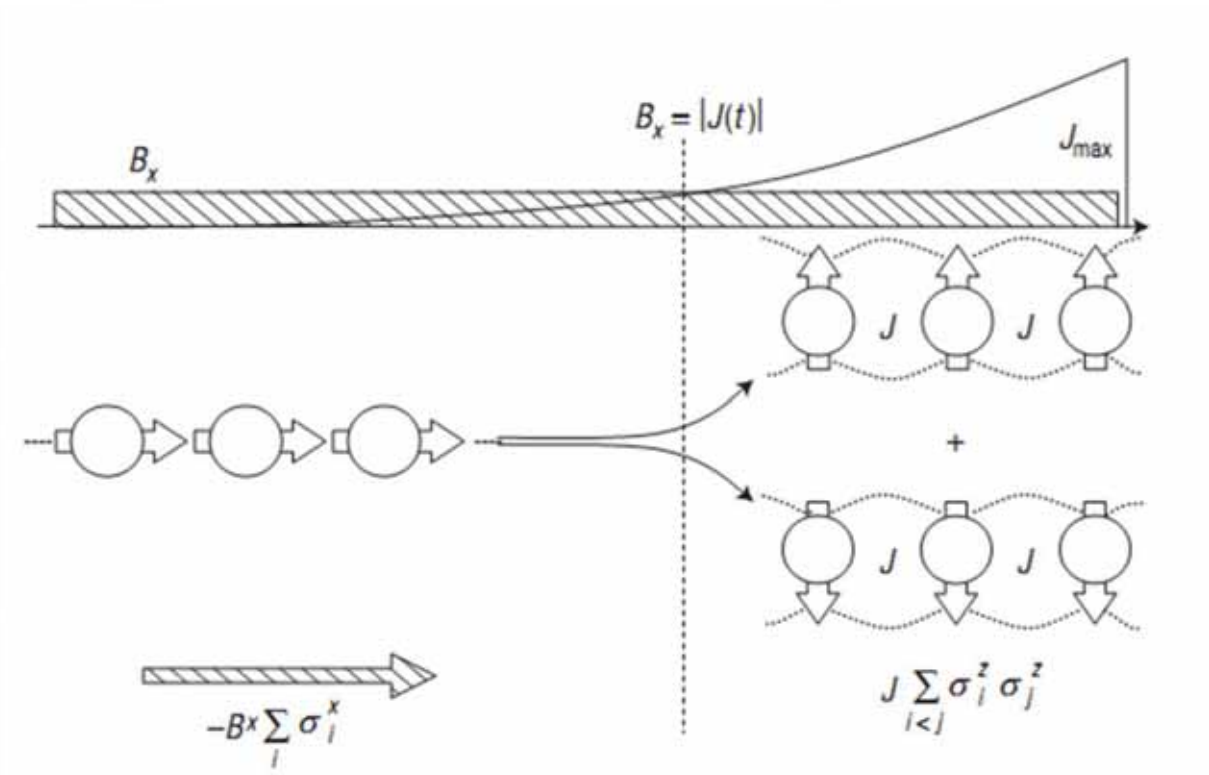
Trapped Ions



T. Ladd et al., Nature 464, 45 (2010)

Trapped Ions

Simulating a Quantum Magnet in Trapped Ions



A. Friedenauer et al., Nat. Phys. 4, 757 (2008)

Superconducting Circuits

- ✓ **Qubits: Quantized levels in the anharmonic potential**
- ✓ **Single-qubit gate: Resonant pulses**
- ✓ **Two-qubit gate: Capacitive or inductive couplings**
- ✓ **Initialize: Circuits designing and external signal**
- ✓ **Measure: Switching behavior of a current-biased Josephosn**

J. Clarke and F. Wilhelm, Nature 453, 1031 (2008)

Kitaev Model on a Honeycomb Lattice

J. You et al., Phys. Rev. B 81, 014505 (2010)

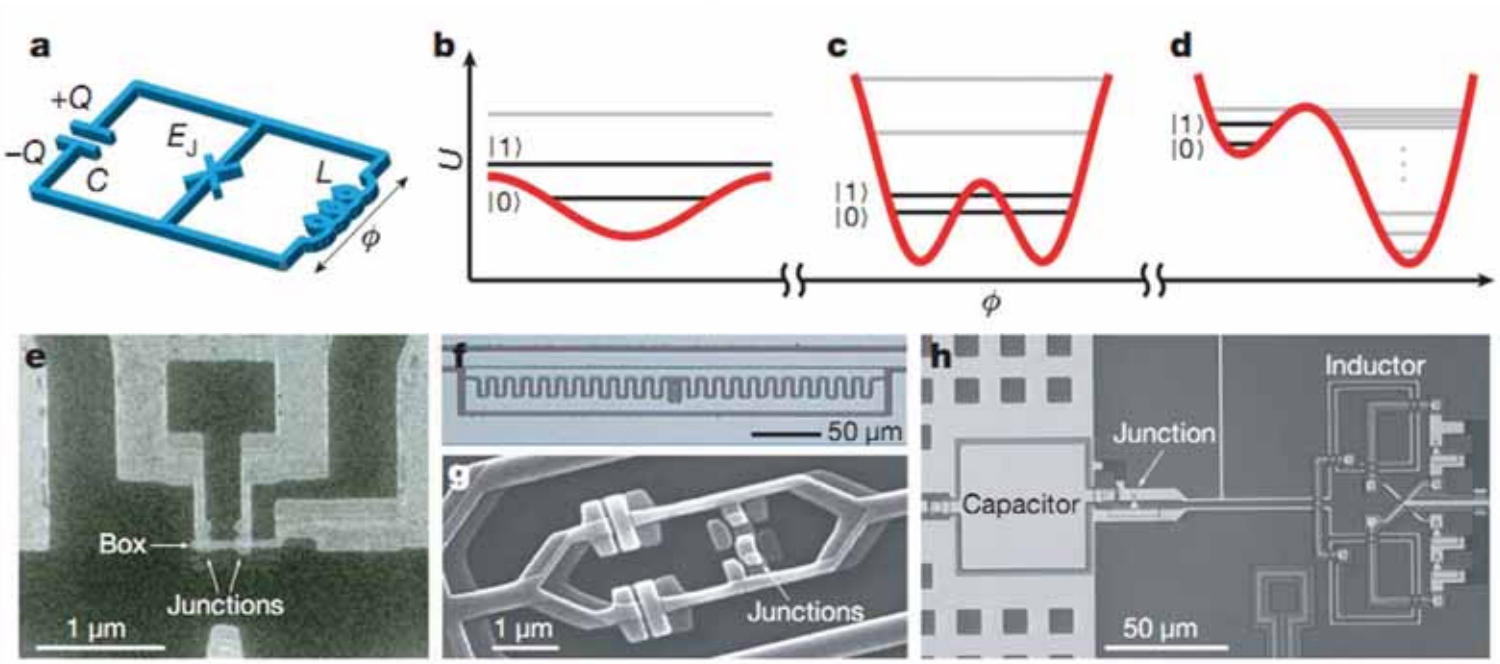
Anderson and Kondo Models

Garcia-Ripoll et al., Phys. Rev. B 77, 024522 (2008)

Tunable Metamaterials

A. Rakhmanov et al., Phys. Rev. B 77, 144507 (2008)

Superconducting Circuits



T. Ladd et al., Nature 464, 45 (2010)

Nuclear Magnetic Resonance

- ✓ **Qubits: Nuclear spins**
- ✓ **Single-qubit gate: Resonant radio-frequency pulse**
- ✓ **Two-qubit gate: Indirect couplings through molecular electrons**
- ✓ **Initialize: Pseudo pure state**
- ✓ **Measure: Observing the induce current in the coil**

D. Cory et al., PNAS 94, 1634 (1997)
L. Vandersypen and I. Chuang, Rev. Mod. Phys. 76, 1037 (2004)

Harmonic and Anhamonic Oscillators

S. Somaroo et al., Phys. Rev. Lett. 82, 5381 (1999)

Many-body interactions

C. Tseng et al., Phys. Rev. A 61, 012302 (2000)

Pairing Hamiltonian

X. Yang et al., Chem. Phys. Lett. 422, 20 (2006)

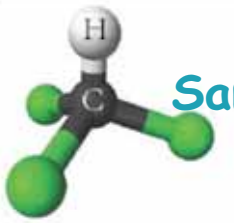
Quantum Chaos

Y. Weinstein et al., Phys. Rev. Lett. 89, 157902 (2002)

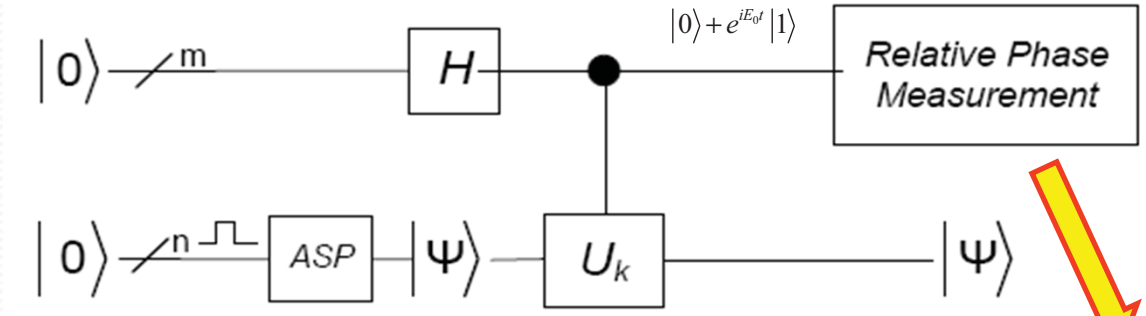
Nuclear Magnetic Resonance

Simulating Energy of Hydrogen Molecule in NMR

Target: Hydrogen



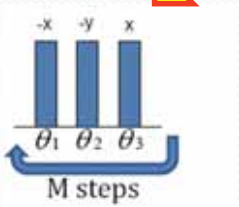
Sample: CHCl3

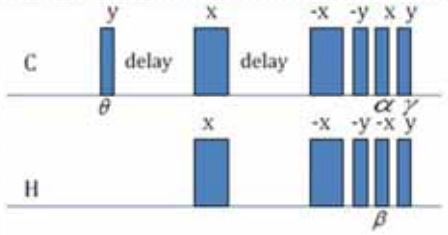


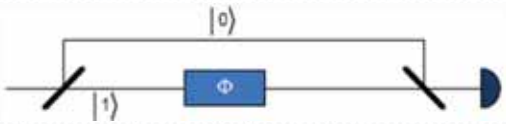
Adiabatic

Evolution

NMR interferometer







J. Du et al., Phys. Rev. Lett. 104, 030502 (2010)

Comparison

Table 1 | Current performance of various qubits

Type of qubit	T_2	Benchmarking (%)		References
		One qubit	Two qubits	
Infrared photon	0.1 ms	0.016	1	20
Trapped ion	15 s	0.48†	0.7*	104–106
Trapped neutral atom	3 s	5		107
Liquid molecule nuclear spins	2 s	0.01†	0.47†	108
e^- spin in GaAs quantum dot	3 μs	5		43, 57
e^- spins bound to ^{31}P:^{28}Si	0.6 s	5		49
^{29}Si nuclear spins in ^{28}Si	25 s	5		50
NV centre in diamond	2 ms	2	5	60, 61, 65
Superconducting circuit	4 μs	0.7†	10*	73, 79, 81, 109

Measured T_2 times are shown, except for photons where T_2 is replaced by twice the hold-time (comparable to T_1) of a telecommunication-wavelength photon in fibre. Benchmarking values show approximate error rates for single or multi-qubit gates. Values marked with asterisks are found by quantum process or state tomography, and give the departure of the fidelity from 100%. Values marked with daggers are found with randomized benchmarking[110]. Other values are rough experimental gate error estimates. In the case of photons, two-qubit gates fail frequently but success is heralded; error rates shown are conditional on a heralded success. NV, nitrogen vacancy.

T. Ladd et al., Nature 464, 45 (2010)

- What is Quantum Computer and Quantum Simulation?
- Categories, Resources and Errors
- Possible Physical Realization
- **Applications of Quantum Simulation**

Condensed Matter Physics (A)

Phenomena	System	Paper
Quantum Phase Transition	Neutral Atoms	M. Greiner et al., Nature 415, 39 (2002)
	Polar Molecules	B. Capogrosso et al., PRL 104, 125301 (2010) L. Pollet et al., PRL 104, 125302 (2010)
	Trapped Ions	G. Giorgi et al., PRA 81, 052118 (2010) A. Retzker et al., PRL 101, 260504 (2008) A. Friedenauer et al., Nat. Phys. 4, 757 (2008)
	NMR	X. Peng et al., PRA 71, 012307 (2005) G. Roumpos et al., PRB 75, 094415 (2007) J. Zhang et al., PRL 100, 100501 (2008)
	Superconducting	A. Van Oudenaarden et al., PRL 76, 4947 (1996)
Hubbard Models	Neutral Atoms	D. Jaksch et al., PRL 81, 3108 (1998)
	Polar Molecules	M. Ortner et al., NJP 11, 055045 (2009)
	Trapped Ions	X. Deng et al., PRA 77, 033403 (2008)
	Quantum Dots	T. Byrnes et al., PRB 78, 075320 (2008)

Condensed Matter Physics (B)

Phenomena	System	Paper
Hubbard Models	Cavities	A. Greentree et al., Nat. Phys. 2, 856 (2006) M. Hartmann et al., Nat. Phys. 2, 849 (2006)
Spin Models	Neutral Atoms	Garcia-Ripoll et al., PRL 93, 250405 (2004) E. Jane et al., QIC 3, 15 (2003)
	Trapped Ions	D. Porras et al., PRL 92, 207901 (2004) E. Edwards et al., PRB 82, 060412 (2010) A. Bermudez et al., PRA 79, 060303 (2009) X. Deng et al., PRA 72, 063407 (2005)
	Superconducting	D. Tsokomos et al., PRA 82, 052311 (2010)
	Cavities	Z. Chen et al., PRA 81, 022303 (2010) J. Cho et al., PRA 78, 062338 (2008)
	Electrons on He	S. Mostame et al., PRL 101, 220501 (2010)
Spin Glasses	DQS	D. Lidar et al., PRE 56, 3661 (1997)
	Superconducting	D. Tsokomos et al., NJP 10, 113020 (2008)

Condensed Matter Physics (C)

Phenomena	System	Paper
High Tc Superconductivity	DQS	F. Yamaguchi et al., Superlattices and Microstructures, 32, 343 (2002)
	Quantum Dots	E. Manousakis, J. Low Temp. Phys. 126, 1501 (2002)
BCS Pairing	NMR	X. Yang et al., Chem. Phys. Lett. 422, 20 (2006)
BCS-BEC Crossover	Neutral Atoms	M. Zwierlein et al., Nature 435, 1047 (2005)
Metamaterials	Superconducting	A. Rakhmanov et al., PRB 77, 144507 (2008)
Disordered Systems	Neutral Atoms	L. Fallani et al., PRL 98, 130404 (2007) T. Schulte et al., PRL 95, 170411 (2005) J. Billy et al., Nature 453, 891 (2008)
	Trapped Ions	A. Bermudez et al., arXiv: 1002.3748 (2010)
	NMR	G. Alvarez et al., PRL 104, 230403 (2010) C. Negrevergne et al., PRA 71, 032344 (2005)
	Superconducting	J. Garcia-Ripoll et al., PRL 93, 250405 (2008)

Condensed Matter Physics (D)

Phenomena	System	Paper
Frustrated Systems	Photons	X. Ma et al., Nat. Phys. 7, 399 (2011)
	Trapped Ions	D. Porras et al., PRL 96, 250501 (2006) K. Kim et al., Nature 465, 590 (2010)
Tonks-Girardeau Gas	Neutral Atoms	B. Paredes et al., Nature 429, 277 (2004)
Time-Symmetry Breaking	Superconducting	J. Koch et al., PRA 82, 043811 (2010)
Topological Order	Photons	A. Bermudez et al., arXiv 1002.3748 (2010) C. Lu et al., PRL 102, 030502 (2009)
	Polar Molecules	A. Micheli et al., Nat. Phys. 2, 341 (2006)
	Neutral Atoms	M. Aguado et al., PRL 101, 260501 (2008)
	Superconducting	J. You et al., PRB 81, 014505 (2010)

High-Energy Physics

Phenomena	System	Paper
Lattice Gauge Theories	DQS	T. Byrnes et al., PRA 73, 022328 (2006)
	Neutral Atoms	H. Buchler et al., PRL 95, 040402 (2005)
Dirac Particles	Neutral Atoms	J. Cirac et al., PRL 105, 190403 (2010) N. Goldman et al., PRL 103, 035301 (2009) J. Hou et al., PRA 79, 043621 (2009)
	Trapped Ions	L. Lamata et al., PRL 98, 253005 (2007) T. Rusin et al., arXiv 1003.5504 (2010) R. Gerritsma et al., Nature, 463, 68 (2010) J. Casanova et al., PRA 82, 020101 (2010) J. Casanova et al., arXiv 1102.1651v1 (2011)
Nucleons	Photons	F. Semiao et al., arXiv 1005.2775 (2010)

Cosmology

Phenomena	System	Paper
Unruh Effect	Trapped Ions	P. Alsing et al., PRL 94, 220401 (2005)
Hawking Radiation	Neutral Atoms	S. Giovanazzi, PRL 94, 061302 (2005)
	Trapped Ions	B. Horstmann et al., PRL 104, 250403 (2010)
	Superconducting	P. Nation et al., PRL 103, 087004 (2009)
Universe Expansion	BEC	U. Fischer et al., PRA 70, 063615 (2004)
	Trapped Ions	N. Menicucci et al., NJP 12, 095019 (2010) R. Schutzold et al., PRL 99, 201301 (2007)

Atomic Physics

Phenomena	System	Paper
Cavity QED	Superconducting	L. Zhou et al., PRA 78, 063827 (2008) J. Fink et al., Nature 454, 315 (2008)
Cooling	Superconducting	M. Grajcar, Nat. Phys. 4, 612 (2008) F. Nori, Nat. Phys. 4, 589 (2008)

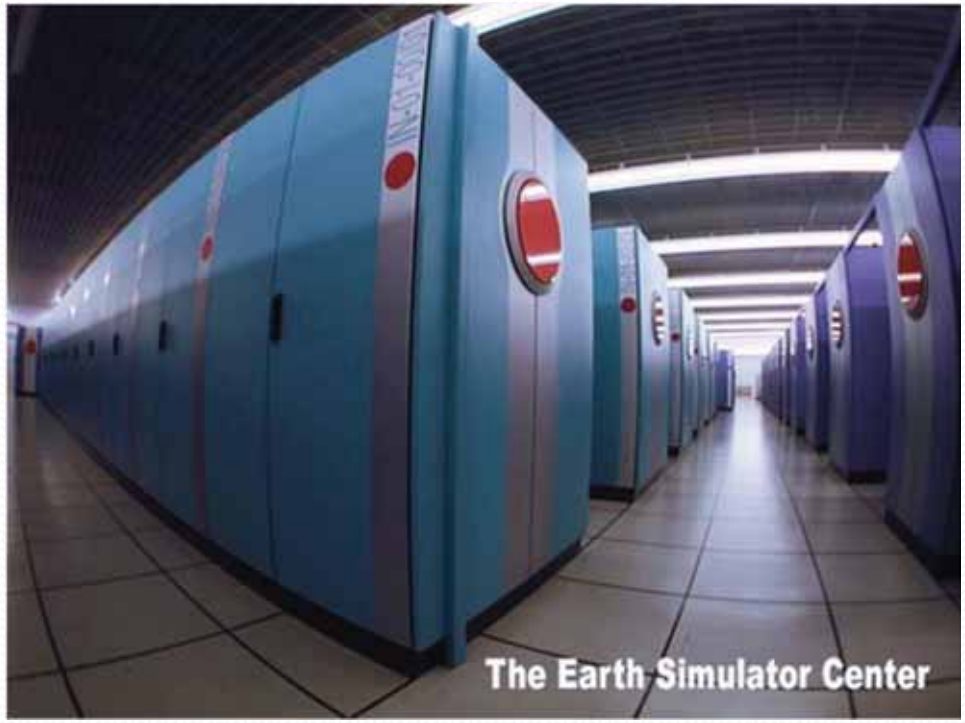
Chemistry

Phenomena	System	Paper
Thermal Rate Calculations	DQS	D. Lidar et al., PRE 59, 2429 (1999)
Molecular Energies	DQS	A. Aspuru-Guzik et al., Science 309, 1704 (2005)
	Photons	B. Lanyon et al., Nat. Chem. 2, 483 (2010)
	NMR	J. Du et al., PRL 104, 030502 (2010)
Chemical Reactions	DQS	I. Kassal et. al., PNAS 105, 18681 (2008)
	NMR	D. Lu et al., PRL 107, 020501 (2011)
	Quantum Dots	A. Smirnov et al., EPL 80, 67008 (2007)

Other

Phenomena	System	Paper
Open System	Trapped Ions	J. Piilo et al., PRA 74, 032303 (2006)
	NMR	C. Tseng et al PRA 62, 032309 (2002)
Quantum Chaos	Photons	J. Howell et al., PRA 61, 012304 (2000)
	NMR	Y. Weinstein et al., PRL 89, 157902 (2002)
Schrodinger Equation	DQS	B. Boghosian et al., Physica D 120, 30 (1998)
Quantum Thermodynamic	Superconducting	H. Quan et al., PRE 76, 031105 (2006)
Nonlinear Interferometers	Trapped Ions	D. Leibfried et al., PRL 89, 247901 (2002)

Perspective: Earth Simulator?



NEC Super Computer

It is said that PS3 can simulate the earth…

Only Quantum Simulators Do!

D-Wave's quantum computer

$ 10,000,000 !!!!!!!

Thank you !

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Hefei, Anhui, P.R.China

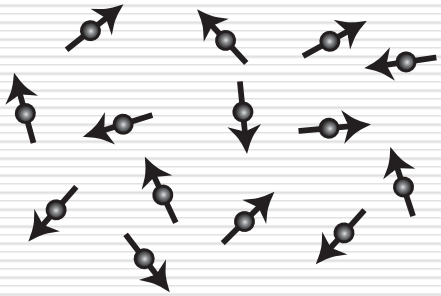
NMR Quantum Computation

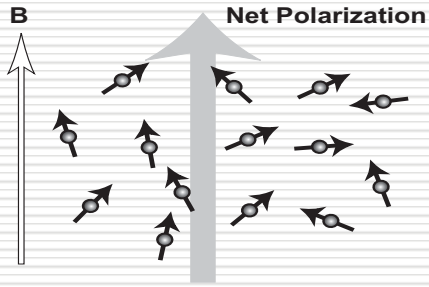
Nuclear Spin

The spins of nuclei are formed by combining together the spins of the protons and the neutrons.

nuclei	spin	Natural abundance(%)	NMR frequency
^{1}H	1/2	99.98	100
^{2}D	1	0.015	15.351
^{13}C	1/2	1.11	25.144
^{15}N	1/2	0.37	10.133
^{19}F	1/2	100	94.077
^{23}Na	3/2	100	26.451
^{31}P	1/2	100	40.481

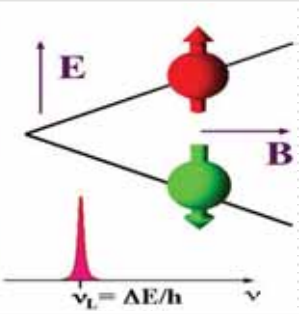
Nuclear magnetic resonance





In the absence of a magnetic field, the distribution of magnetic moments is completely *isotropic* ,i.e. all possible directions are equally represented.

If the external is turned on, net polariazation appear .



Physical Realization of QCs

Requirements for Quantum Computers[1]:

- A quantum system with qubits
- Individually addressable qubits
- Two qubit interactions (universal set of quantum gates)
- Long coherence times
- Initialize quantum system to known state
- Extract result from quantum system

Meeting all of these requirements *simultaneously* presents a significant experimental challenge.

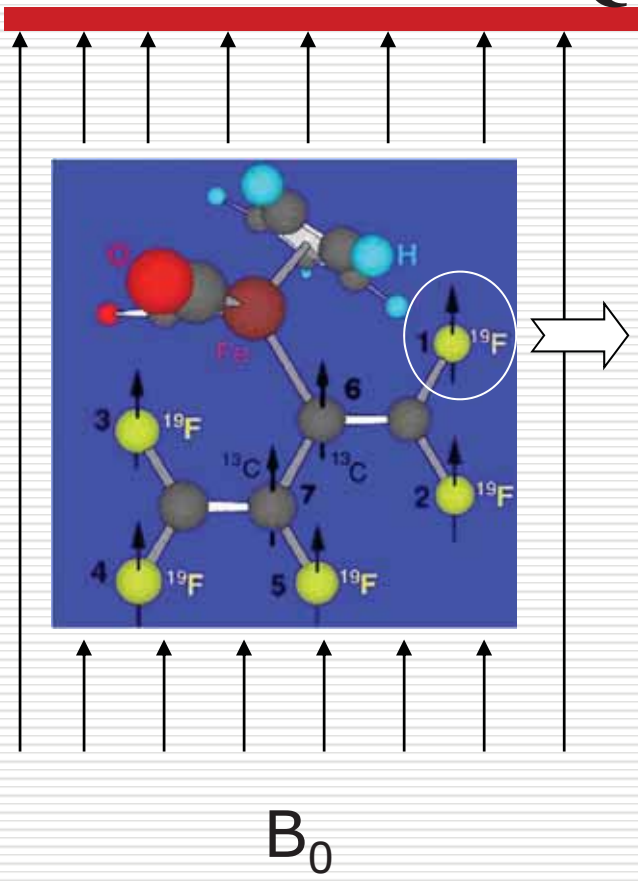
$\Rightarrow$ Nuclear Magnetic Resonance (NMR) techniques largely satisfies these requirements and have enabled experimental exploration of small-scale quantum computers

[1] DiVincenzo D.P., *Fortschr. Physik*, **48** (9-11), 771 – 783 (2000)

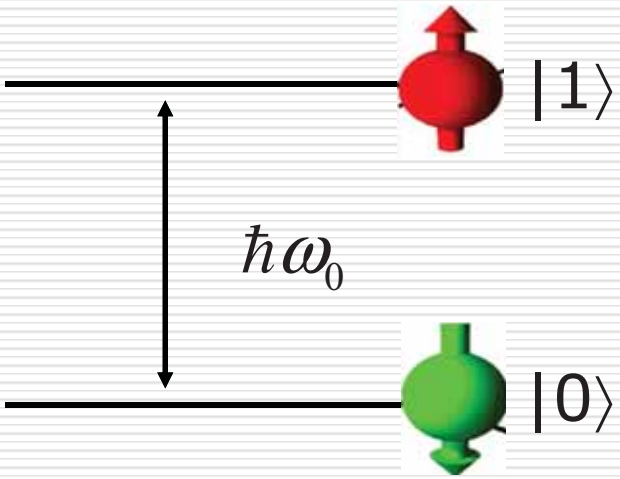
Physical Realization of QCs

System	τ_Q	τ_{op}	$n_{op} = \lambda^{-1}$
Nuclear spin	$10^{-2} - 10^{8}$	$10^{-3} - 10^{-6}$	$10^{5} - 10^{14}$
Electron spin	10^{-3}	10^{-7}	10^{4}
Ion trap (In^{+})	10^{-1}	10^{-14}	10^{13}
Electron – Au	10^{-8}	10^{-14}	10^{6}
Electron – GaAs	10^{-10}	10^{-13}	10^{3}
Quantum dot	10^{-6}	10^{-9}	10^{3}
Optical cavity	10^{-5}	10^{-14}	10^{9}
Microwave cavity	10^{0}	10^{-4}	10^{4}

Quantum qubit



B_0



$$H_0 = -\frac{\hbar\gamma B_0\sigma_z}{2} = \frac{\hbar\omega_0\sigma_z}{2} = \frac{\hbar\omega_0}{2}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$$

[1] Gershenfeld, N. et al., *Science,* **275**, 350 – 356 (1997)

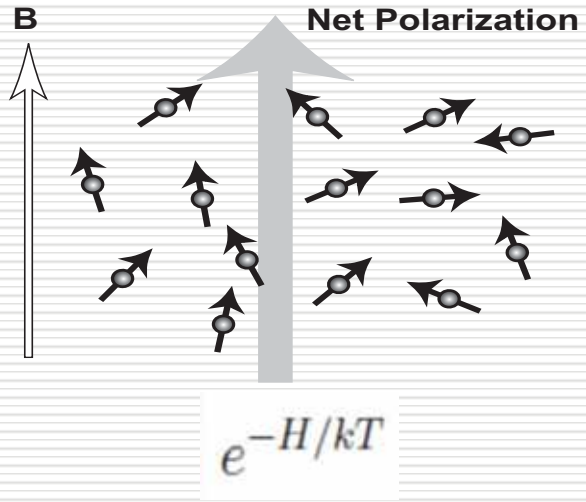
[2] Cory D. et al., *Proc. Natl. Acad. Sci.*, **94**, 1634 – 1639 (1997)

State initialization

Thermal Equilibrium: $\rho_{eq} = \frac{1}{2^n} E + \frac{1}{2^n}(\sum_i \varepsilon_i I_z^i)$

Pseudopure state： $\rho_{pps} = \frac{1-\epsilon}{2} I + \epsilon |0\rangle\langle 0|$

deviation density matrix： $\delta = \epsilon |0\rangle\langle 0|$



$$U\rho_{pps}U^{+} = (1-\varepsilon)/2 + U\delta U^{+}$$

With respect to scale-independent NMR observations and unitary evolution, a PPS **is equivalent to** the corresponding pure state.

One-qubit gates

An arbitrary one-qubit gate:

$$U(\delta,\alpha,\beta,\theta) = e^{i\delta}\begin{bmatrix} e^{i(\alpha+\beta)/2}\cos\frac{\theta}{2} & ie^{i(\alpha-\beta)/2}\sin\frac{\theta}{2} \\ ie^{-i(\alpha-\beta)/2}\sin\frac{\theta}{2} & e^{-i(\alpha+\beta)/2}\cos\frac{\theta}{2} \end{bmatrix}$$

$$= e^{i\delta}\begin{bmatrix} e^{-i\alpha/2} & 0 \\ 0 & e^{i\alpha/2} \end{bmatrix}\begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}\begin{bmatrix} e^{-i\beta/2} & 0 \\ 0 & e^{i\beta/2} \end{bmatrix}$$

$$= e^{i\delta}R_z(\alpha)R_y(\theta)R_z(\beta) \equiv Z(\alpha)Y(\theta)Z(\beta),$$

Specific one-qubit gates

NOT gate: |0> → |1>; |1> → |0>

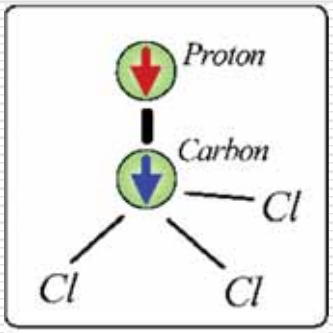
$$\mathrm{NOT}=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\square\, R_x(\pi)$$

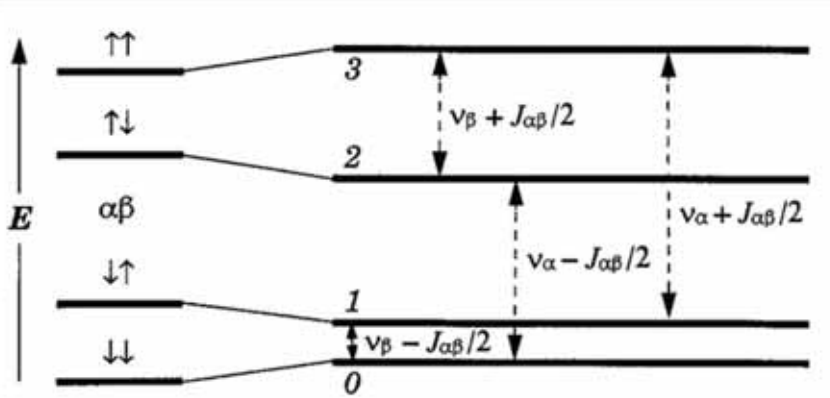
Hardamard gate: to create the superposition state

$$|0\rangle \rightarrow \frac{1}{\sqrt{2}}(|0>+|1>);|1\rangle \rightarrow \frac{1}{\sqrt{2}}(|0>-|1>)$$

$$H=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\square\, R_x(\pi)R_y\left(-\frac{\pi}{2}\right)$$

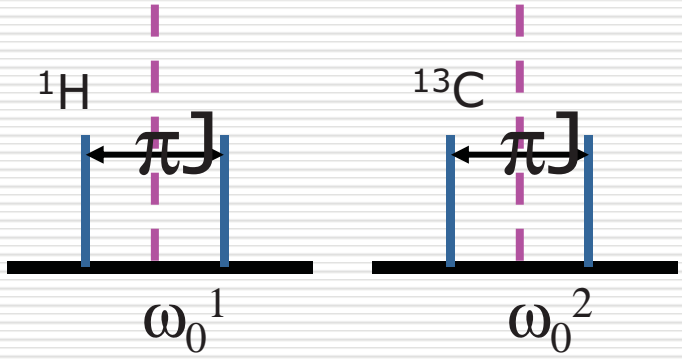
Multiple spin nuclei





$$\mathcal{H}_{sys} = -\sum_i \hbar\omega_0^i I_z^i + \hbar\sum_{i<j} 2\pi J_{ij} I_z^i I_z^j .$$

（**weakly coupled**）



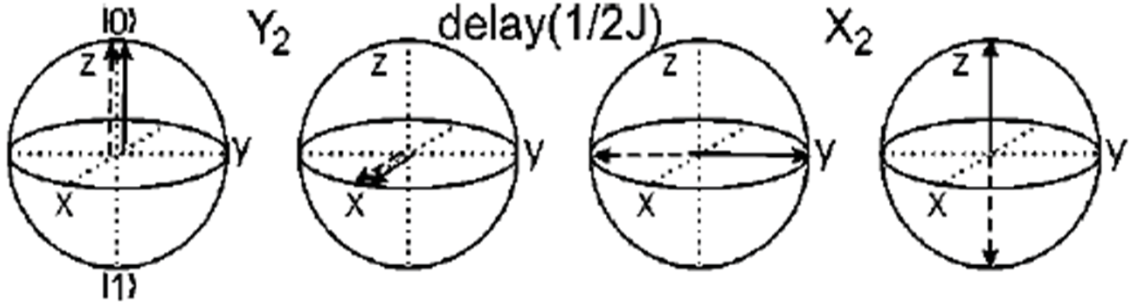
Two qubit gates

Lamour frequency of spin *i* shifts by $-J_{ij}/2$ if spin *j* is in $|0\rangle$ and by $+J_{ij}/2$ if spin *j* is in $|1\rangle$

2-bit CNOT

Y_2 - 1/2J - X_2

input	output
00	00
01	01
10	11
11	10



$$U_{\mathrm{CNOT}} = iZ_1^2\bar{Y}_2 U_{\mathrm{CPHASE}} Y_2$$

$$= \sqrt{i}Z_1\bar{Z}_2 X_2 U_J(1/2J) Y_2$$

Readout : Quantum state tomography

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} \\ \rho_{21} & \rho_{22} & \rho_{23} & \rho_{24} \\ \rho_{31} & \rho_{32} & \rho_{33} & \rho_{34} \\ \rho_{41} & \rho_{42} & \rho_{43} & \rho_{44} \end{pmatrix}$$

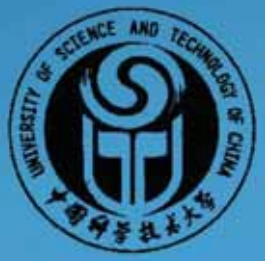
Observable

$$\rho^{+} = \rho$$

Different readout pulses: e.g., XE, EX, XX etc.

Simulation of Quantum Physics on an NMR Quantum Computer

Jiangfeng Du



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Outline

- Quantum Phase Transition
  - 1) Heisenberg spin model
  - 2) Triangular spin chain
  - 3) Ground state geometric phase
- Quantum Factoring
  - 1) Factoring 21
  - 2) Factoring 143
- Quantum Annealing

- **Quantum Phase Transition**
  - 1) Heisenberg spin model
  - 2) Triangular spin chain
  - 3) Ground state geometric phase
- Quantum Factoring
- Quantum Annealing

Quantum Phase Transition

- *Quantum phase transition of ground-state entanglement in a Heisenberg spin chain simulated in an NMR quantum computer*

1). Why quantum phase transition and Heisenberg spin model

2). Theory

3). Experiments in an NMR system

4). Summary and Outlook

X.H. Peng et al, *PRA* **71**, 012307, 2005

Why Quantum Phase Transition

– *A quantum critical phenomenon*

- Quantum phase transition (QPT) occurs at absolute zero temperature when a suitable control parameter in its Hamiltonian is varied.
  - Conductivity in the Mott-insulator transition and quantum Hall effect
  - Magnetization in the external-field-induced phase transition
- The transition describes an abrupt change in the ground state of the system.
- It is believed that the ground-state entanglement plays a crucial role in QPTs.

Why Heisenberg Spin Model

- *Importance of Heisenberg Spin Model (HSM)*
  - ***A central model both to condensed-matter physics and quantum information theory***

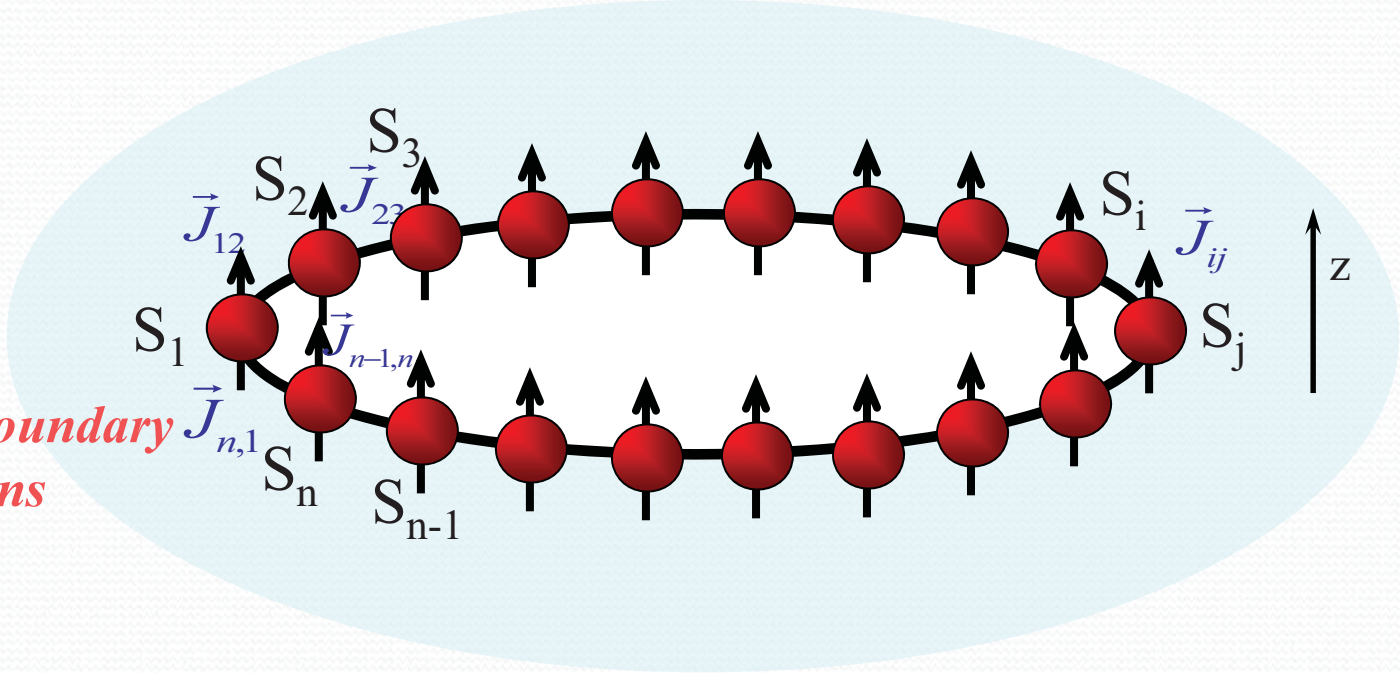
    - Solid-state quantum computer (universal fault-tolerant quantum computation)
      - Advantages: scalability, silicon compatibility, microfabrication (and nanofabrication), possibility of 'engineering' structures, interaction with light
      - Realizations: quantum dots, donor-atom in silicon, quantum Hall system, electrons on helium
    - Quantum communication (avoiding interfacing problem)

Heisenberg Spin Model

- *Hamiltonian (spin-1/2):*

$$H = \sum_{i=1}^{n} B_i \sigma_{iz} + \sum_{i<j=1}^{n} \left(J_{ij}^{x} \sigma_{ix} \sigma_{jx} + J_{ij}^{y} \sigma_{iy} \sigma_{jy} + J_{ij}^{z} \sigma_{iz} \sigma_{jz} \right)$$

External fields — Heisenberg couplings



Cyclic boundary conditions

Theory

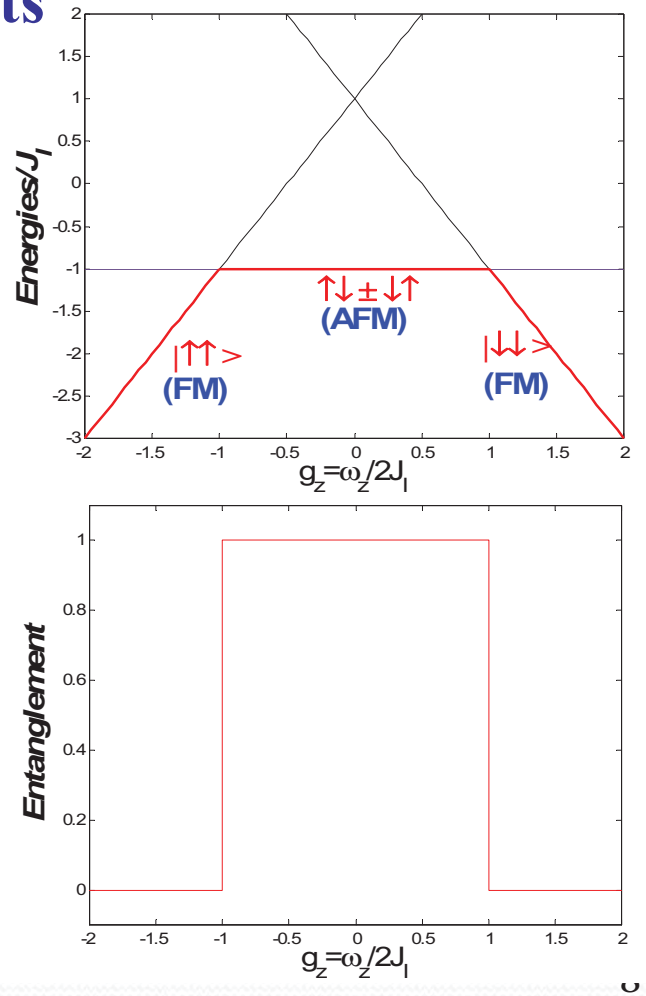
Heisenberg Ising Model of two qubits

$$H_I = \frac{\omega_z}{2}\left(\sigma_z^1 + \sigma_z^2\right) + J_I \sigma_z^1 \sigma_z^2$$

Its ground state

$$|\psi_g\rangle = \begin{cases} |\uparrow\uparrow\rangle & g_z < -1 \quad \text{Ferromagnetic} \\ |\Psi^+\rangle = \left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)/\sqrt{2} & \\ & -1 < g_z < 1 \quad \text{Antiferromagnetic} \\ |\downarrow\downarrow\rangle & g_z > 1 \quad \text{Ferromagnetic} \end{cases}$$

$$g_z = \frac{\omega_z}{2J_I}$$



System and Hamiltonian

- *Hamiltonian of the studied system*

$$H_I = J_I g_z\left(\sigma_z^1 + \sigma_z^2\right) + J_I g_x\left(\sigma_x^1 + \sigma_x^2\right) + J_I \sigma_z^1 \sigma_z^2, \quad |g_x| \ll 1, \quad J_I > 0$$

H' **a perturbation**

The ground state and its energy

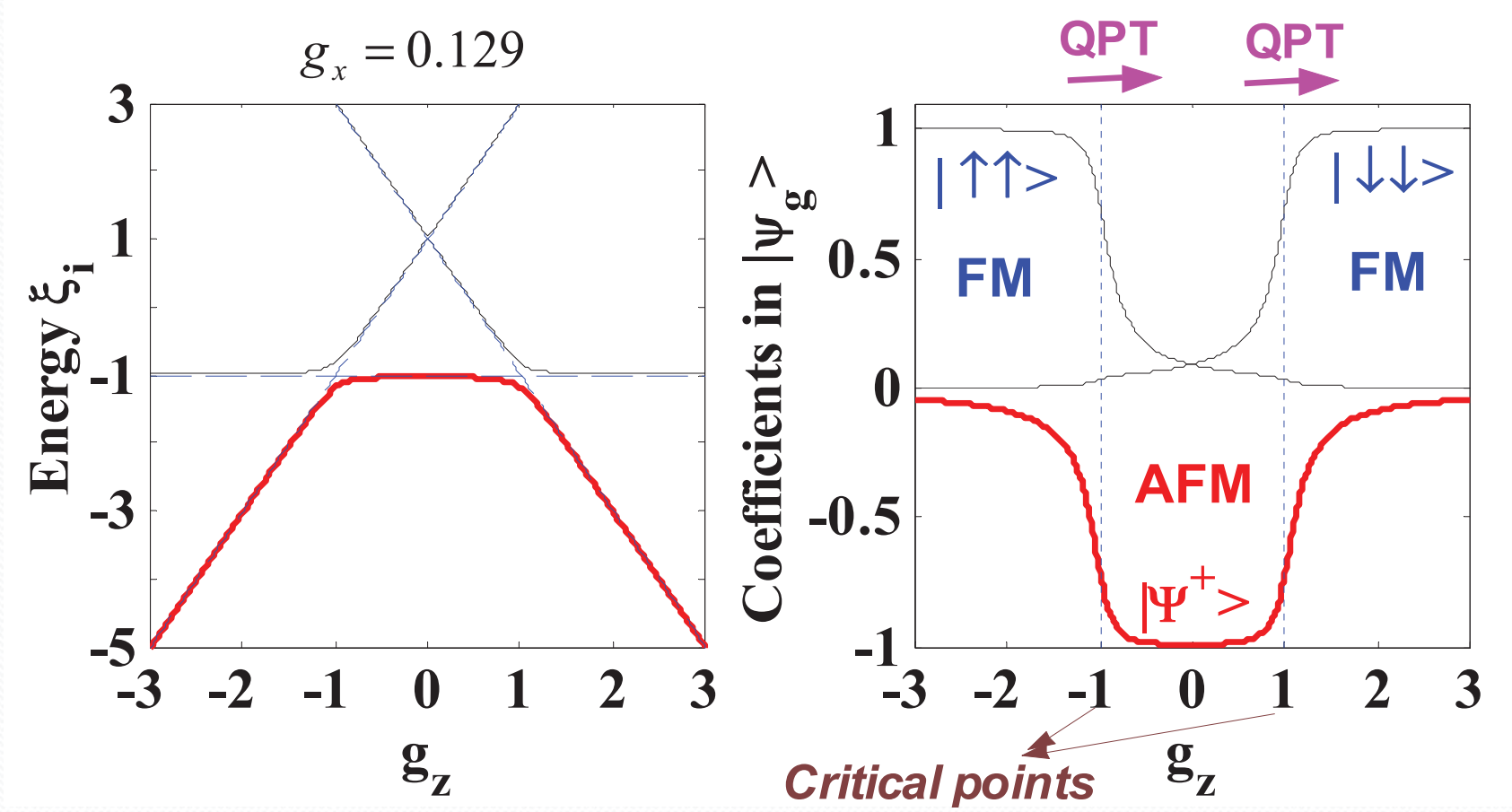
$$|\psi_g\rangle \cong \begin{cases} |\uparrow\uparrow\rangle \\ |\Psi^+\rangle = \left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)/\sqrt{2} \\ |\downarrow\downarrow\rangle \end{cases}$$

$g_z < -1$ **Ferromagnetic**

$-1 < g_z < 1$ **Antiferromagnetic**

$g_z > 1$ **Ferromagnetic**

The ground state and its energy



Quantum Simulation

- An NMR system

$$H_p = \frac{\omega_L^1}{2}\sigma_z^1 + \frac{\omega_L^2}{2}\sigma_z^2 + \frac{J_{12}}{4}\sigma_{1z}\sigma_{2z}$$

Natural Hamiltonian

$$+$$

$$H_{rf} = \frac{\omega_{rf}}{2}\left(\sigma_x^1 + \sigma_x^2\right)$$

Available external Hamiltonian

Simulating

$$\omega_L^1 = \omega_L^2 = \frac{\tau}{\tau_{prec}} J_I g_z, \tau_{prec} = \frac{J_I}{J_{12}}\tau, \tau_p = \frac{J_I g_x}{\omega_{rf}}\tau$$

$$U = e^{-iH_I\tau} = e^{-iH_{rf}\frac{\tau_p}{2}} e^{-iH_p\tau_{prec}} e^{-iH_{rf}\frac{\tau_p}{2}} + O(\tau^2)$$

$$\tau \to 0$$

Average Hamiltonian Theory

$$H_I = J_I g_z\left(\sigma_z^1 + \sigma_z^2\right) + J_I g_x\left(\sigma_x^1 + \sigma_x^2\right) + J_I\sigma_z^1\sigma_z^2$$

Simulated system

Adiabatic condition

- **Adiabatic theorem**: Given a H(t) (0≤ t ≤T) , we start in the ground state of H(0). By varying H(t) slowly, the quantum system stays always in its instantaneous ground state of H(t).
- **Adiabatic condition**:

$$\left|\frac{\left\langle \psi_g(t)\middle|\dot{\psi}_e(t)\right\rangle}{\varepsilon_e-\varepsilon_g}\right| << 1$$

$$\Rightarrow \quad \left|\frac{dg_z}{dt}\right| << J_I^2\chi = J_I^2\left|\frac{\left(\xi_{1e}(t)-\xi_g(t)\right)^2}{\left\langle \psi_g(t)\middle|\frac{\partial H_I}{\partial g_z}\middle|\psi_{1e}(t)\right\rangle}\right|$$

$$\Rightarrow \quad \gamma=\left|\frac{\left\langle \psi_g(t)\middle|\dot{\psi}_{1e}(t)\right\rangle}{\varepsilon_{1e}-\varepsilon_g}\right| \approx \begin{cases} \left|\dfrac{\dot{g}_z g_x}{\sqrt{2}J_I(g_z+1)^3}\right|, & g_z<-1,-1<g_z<0 \\ \left|\dfrac{\dot{g}_z}{8J_I g_x{}^2}\right|, & g_z=\pm 1 \\ \left|\dfrac{\dot{g}_z g_x}{\sqrt{2}J_I(g_z-1)^3}\right|, & 0<g_z<1, g_z>1 \end{cases} << 1$$

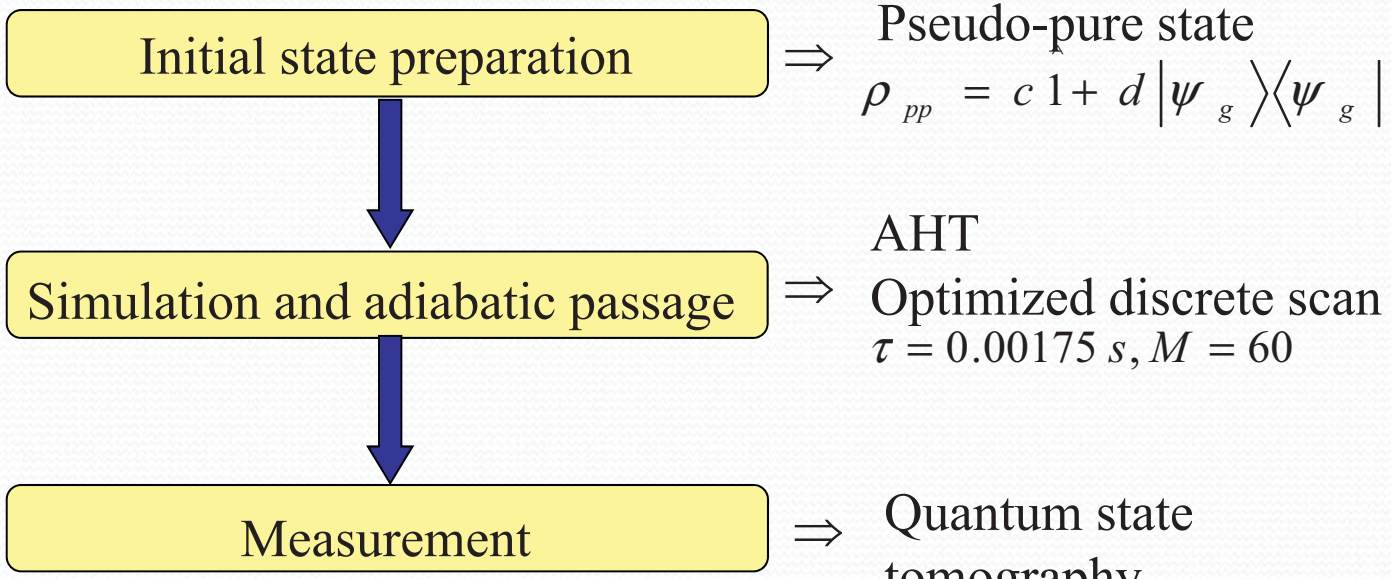
Critical points of QPT

Experiment

- ***Sample***

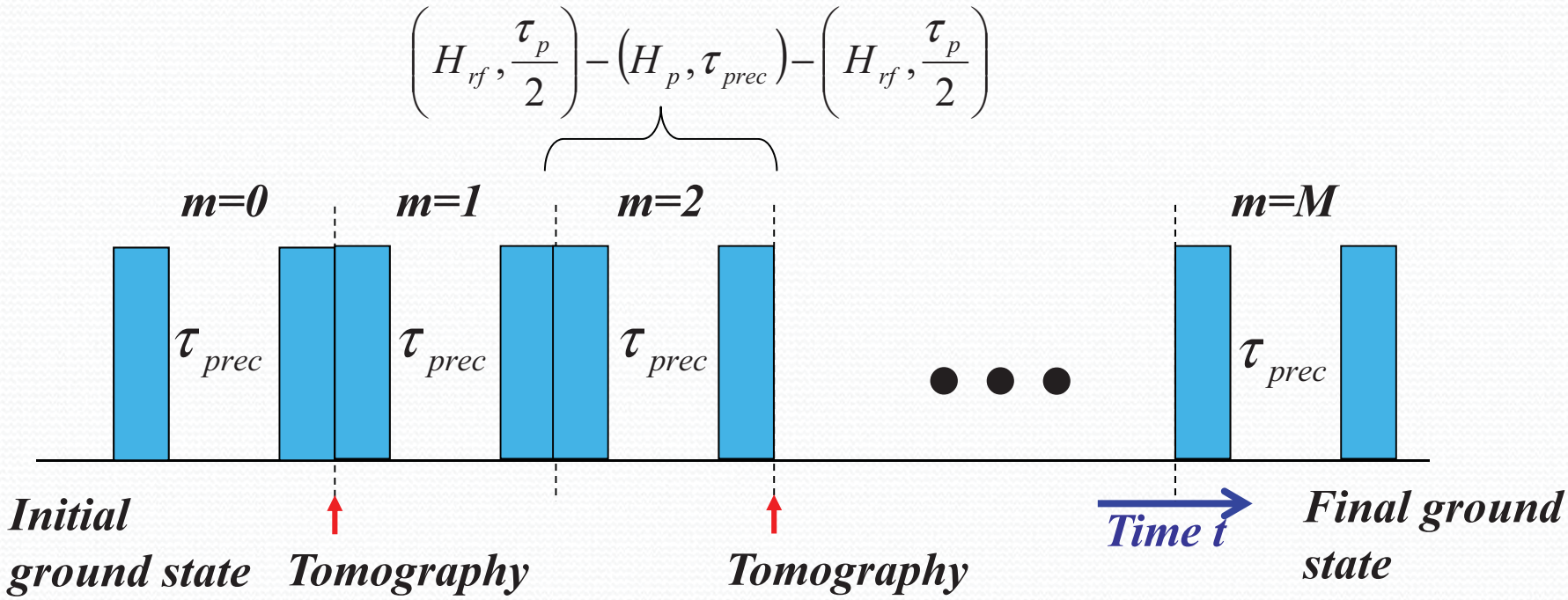
  Carbon-13 labeled chloroform $^{13}CHCl_3$

- ***Procedure***



Pulse Sequence

Adiabatic passage



Results

- Concurrence C: measurement of entanglement

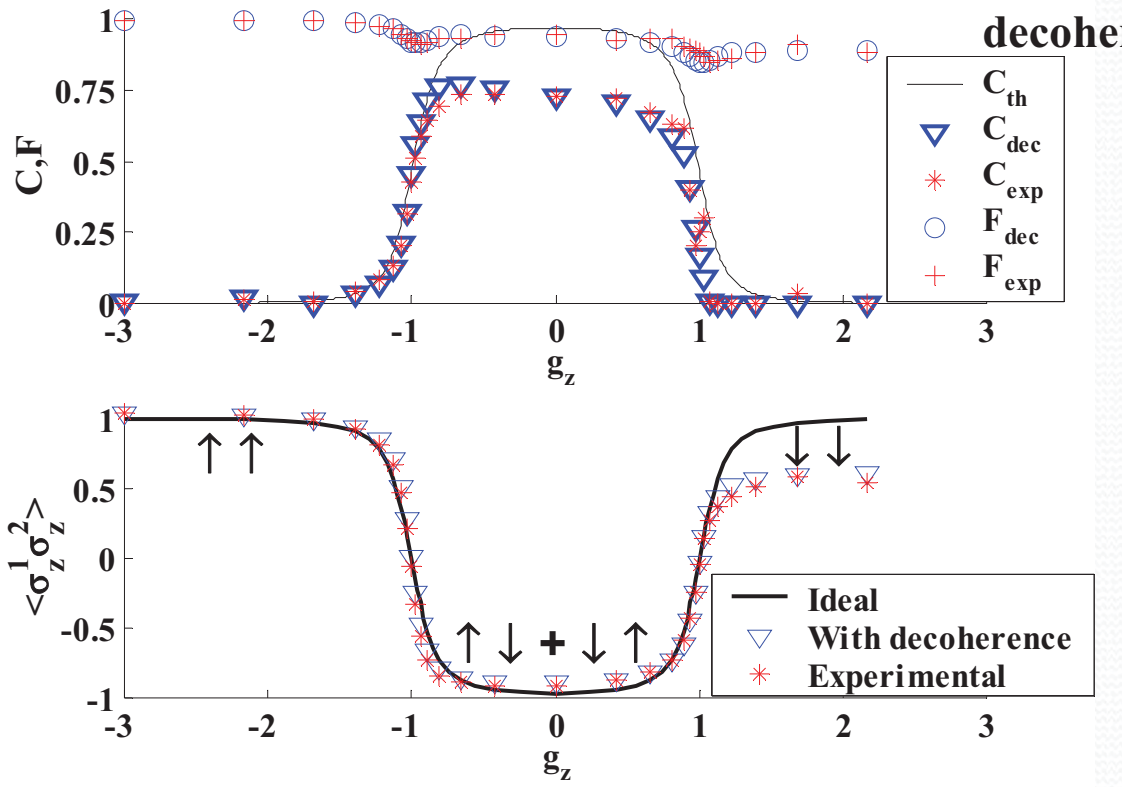
$$C_{12} = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\}$$

$\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ are the square roots of the eigenvalues of $\rho_{12}(\sigma_y \otimes \sigma_y)\rho_{12}^*(\sigma_y \otimes \sigma_y)$

- Spin-spin correlation:

$$\left\langle \sigma_z^1 \sigma_z^2 \right\rangle = Tr\left(\rho_{12}\sigma_z^1\sigma_z^2\right)$$

F > 0.84 due to decoherence



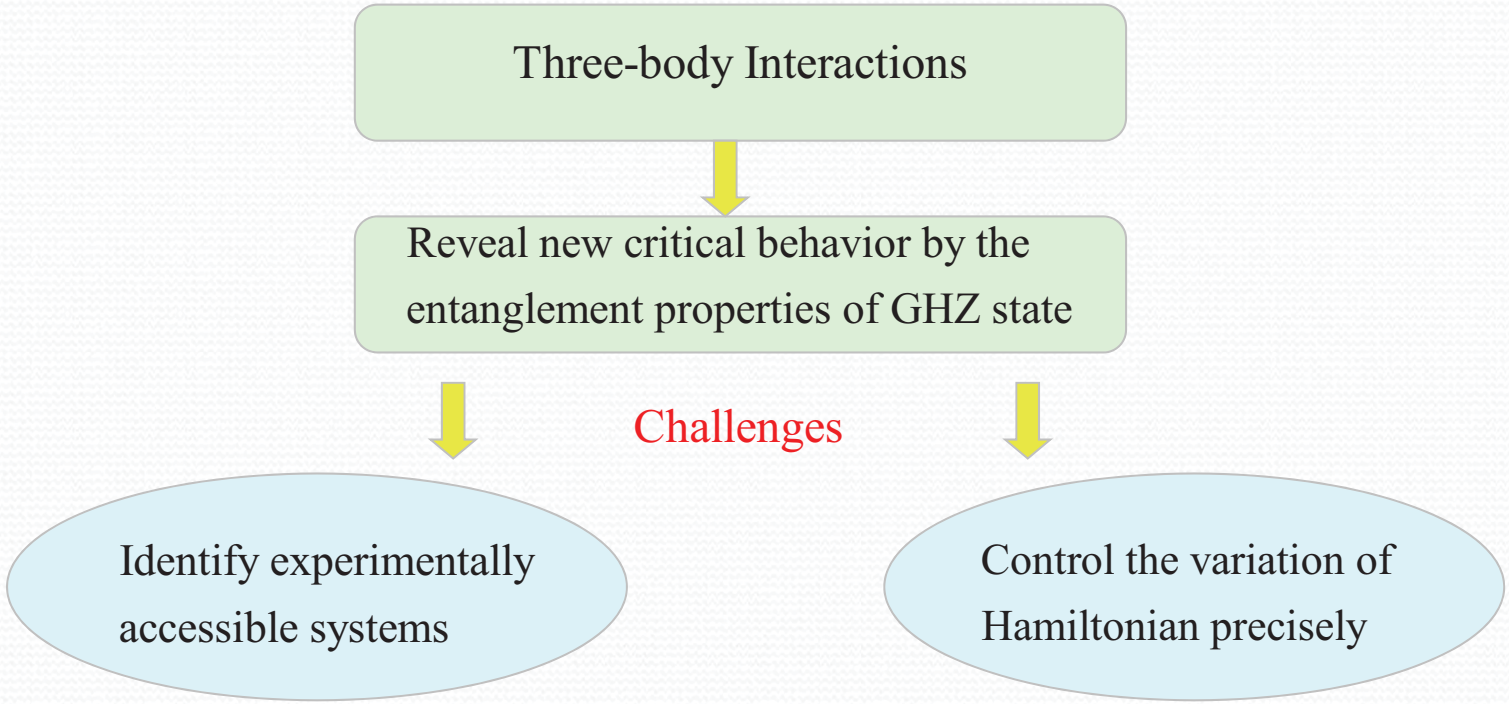
Summary

- The first experimental proof of principle for a QPT of ground-state entanglement in the Heisenberg Ising Model
- The simulation of the HSM by combining average Hamiltonian techniques with adiabatic passage
- The analysis of the results by quantum state tomography, including the decoherence effect
- If extending into three-body interactions...

- **Quantum Phase Transition**
  - 1) Heisenberg spin model
  - 2) Triangular spin chain
  - 3) Ground state geometric phase
- Quantum Factoring
- Quantum Annealing

QPT in a Triangular Spin Chain

- *Experimental Detection of Quantum Criticality in a Triangular Spin Chain*



X.H. Peng et al, Phys. Rev. Lett. 103, 140501 (2009)

Hamiltonian and Ground State

- ***Hamiltonian of the studied system***

$$H_I = \omega_z \sum_i \sigma_z^i + \omega_x \sum_i \sigma_x^i + J_2 \sum_i \sigma_z^i \sigma_z^{i+1} + J_3 \sum_i \sigma_z^i \sigma_z^{i+1} \sigma_z^{i+2}, |\omega_x| \ll 1, \omega_z \geq 0$$

***H'* a perturbation**

The ground state

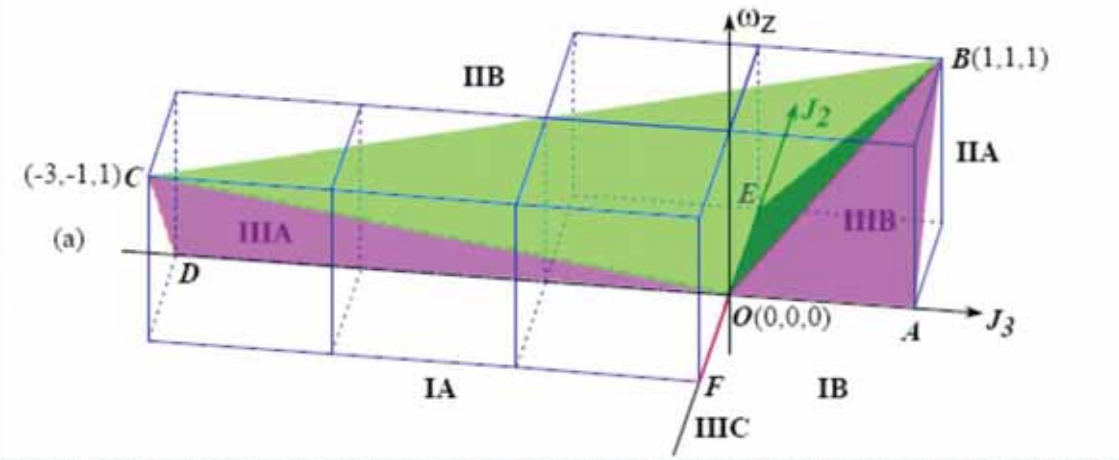
Phase	Parameter range	Ground state
Phase I	A: $J_2 < -\omega_z, J_3 < -3\omega_z$	$\|000\rangle$
	B: $\begin{cases} J_2 < \omega_z, J_3 > \omega_z \\ J_2 < \frac{J_3+\omega_z}{2}, -3\omega_z < J_3 < \omega_z \end{cases}$	$\|111\rangle$
Phase II	A: $J_2, J_3 > \omega_z$	$\|W_{001}\rangle$
	B: $\begin{cases} J_2 > -\omega_z, J_3 < -3\omega_z \\ J_2 > \frac{J_3+\omega_z}{2}, -3\omega_z < J_3 < \omega_z \end{cases}$	$\|W_{110}\rangle$
Phase III	A: $J_2 = -\omega_z, J_3 < -3\omega_z$	$\|\overline{GHZ}_+\rangle$
	B: $J_2 = \omega_z, J_3 > \omega_z$	$\|\overline{GHZ}_-\rangle$
	C: $\omega_z = J_3 = 0, J_2 < 0$	$\|GHZ_-\rangle$

Retain maximal bipartite entanglement

Entanglement vanishes

Quantum Phase Transition

Phase diagram with 3-dimensional parameter space (J_3, J_2, ω_z)

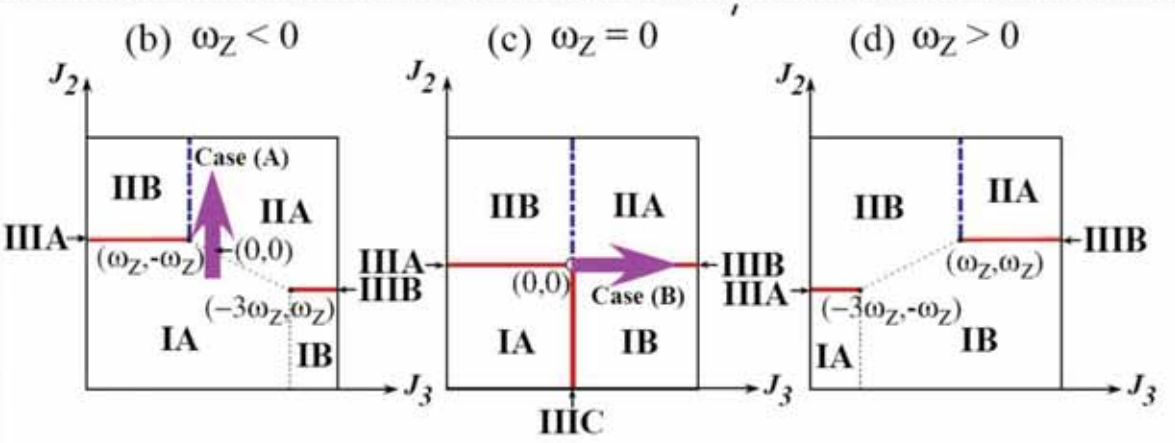


$(b)\ \omega_z = -2, \omega_x = 0.99, J_3 = 0$

$J_2(0) = 0 \rightarrow J_2(T) = 2$

$(c)\ \omega_z = 0, \omega_x = 0.12, J_2 = 0$

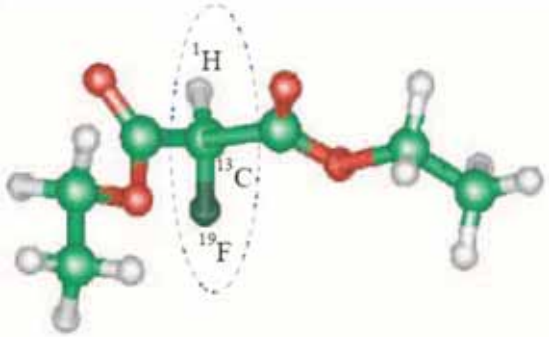
$J_3(0) = 0 \rightarrow J_3(T) = 2$



Quantum Simulation

Diethyl-fluoromalonate

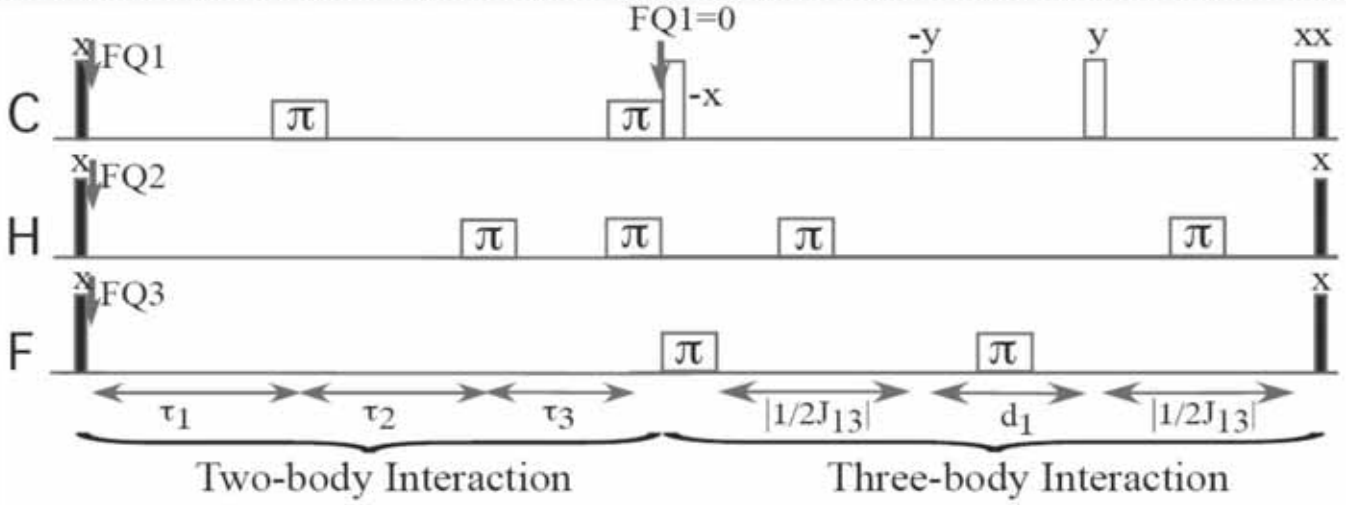
$$H_{NMR} = \sum_{i=1}^{3} \frac{\omega_i}{2} \sigma_z^i + \sum_{i<j,=1}^{3} \frac{\pi J_{ij}}{2} \sigma_z^i \sigma_z^j$$



	^{13}C	^{1}H	^{19}F	T_1(s)	T_2(s)
^{13}C	125 MHz			3.2	1.3
^{1}H	161.3 Hz	500 MHz		3.3	1.0
^{19}F	-192.2 Hz	47.6 Hz	470 MHz	3.2	1.7

$$e^{-iH\tau} = e^{-iH_x\tau/2} e^{-iH_z\tau} e^{-iH_x\tau/2} + O(\tau^3), H_x = \omega_x \sum \sigma_x^i, H_z = H - H_x$$

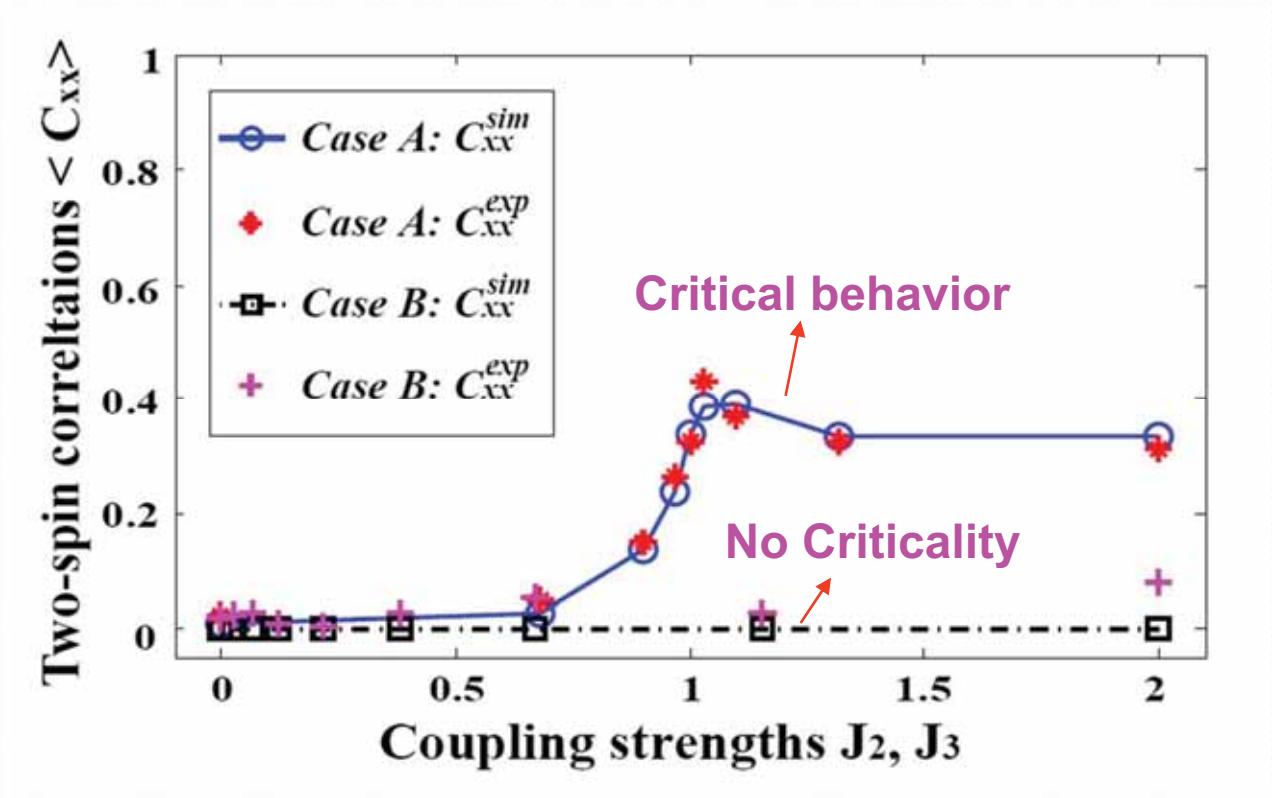
AHT



Criticality Detection (1)

- Two-spin correlation

$$C_{xx} = \sum_{i \neq j} \left| \left\langle \sigma_x^i \sigma_x^j \right\rangle \right| / 3$$

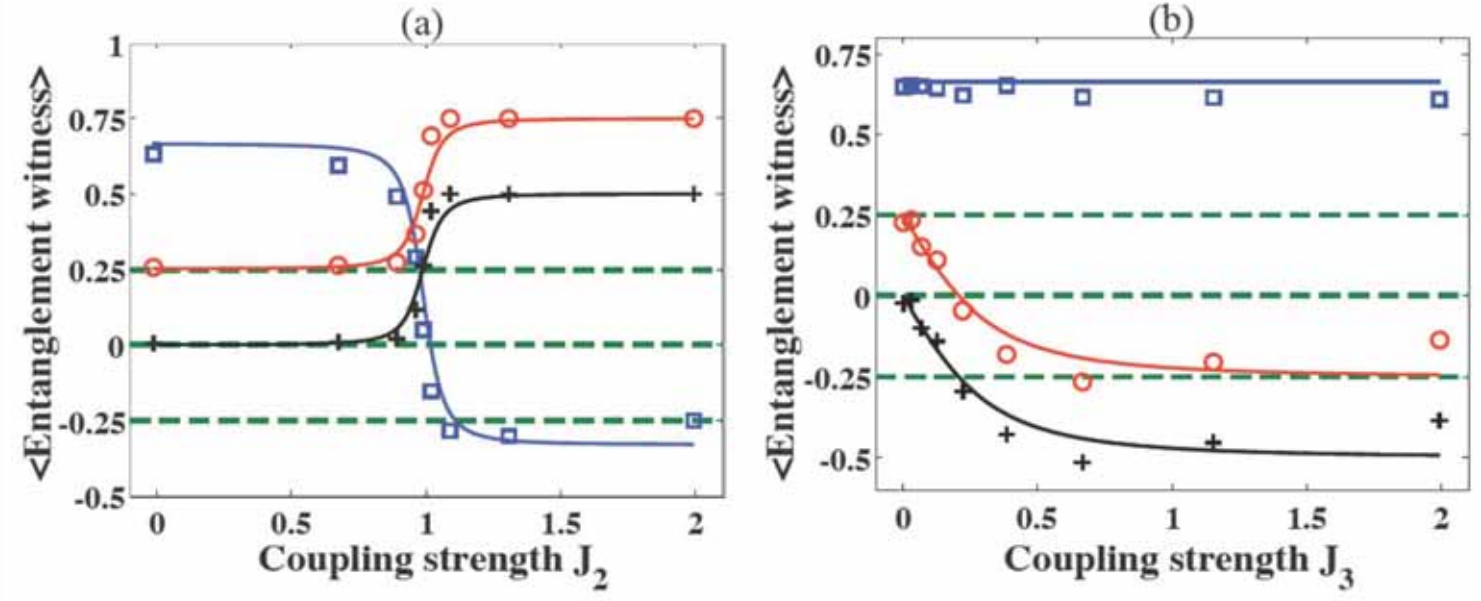


Criticality Detection (2)

Entanglement witness operators

$\mathcal{W}_d$	$\mathcal{W}_{\mathrm{GHZ}}$	$\mathcal{W}_{\mathrm{W}_1}$	$\mathcal{W}_{\mathrm{W}_2}$	
$Tr(\rho\mathcal{W}_d)$	<0	<0	$[0,-1/4]$	$\leq -1/4$
Class	GHZ	GHZ, W	GHZ, W	GHZ

$$\mathcal{W}_{\mathrm{GHZ}} = \tfrac{3}{4}\mathbf{1} - |\mathrm{GHZ}_-\rangle\langle\mathrm{GHZ}_-|$$
$$\mathcal{W}_{\mathrm{W}_1} = \tfrac{2}{3}\mathbf{1} - |\mathrm{W}_{001}\rangle\langle\mathrm{W}_{001}|$$
$$\mathcal{W}_{\mathrm{W}_2} = \tfrac{1}{2}\mathbf{1} - |\mathrm{GHZ}_-\rangle\langle\mathrm{GHZ}_-|.$$



Summary

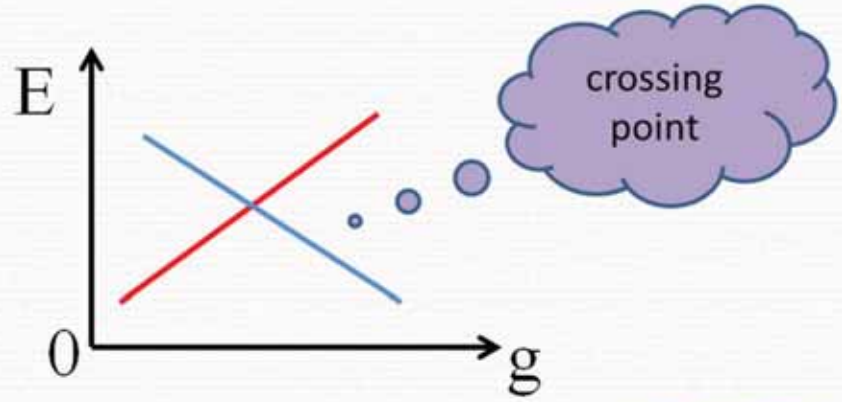
- Experimentally detect two different kinds of QPTs in a triangular spin chain
- The adiabatic evolution can provide an alternative method to generate entangled states with robustness against errors
- Extending into a triangular ladder in multi-spin systems, we expect the entanglement witnesses still remain helpful

- **Quantum Phase Transition**
  - 1) Heisenberg spin model
  - 2) Triangular spin chain
  - 3) Ground state geometric phase
- Quantum Factoring
- Quantum Annealing

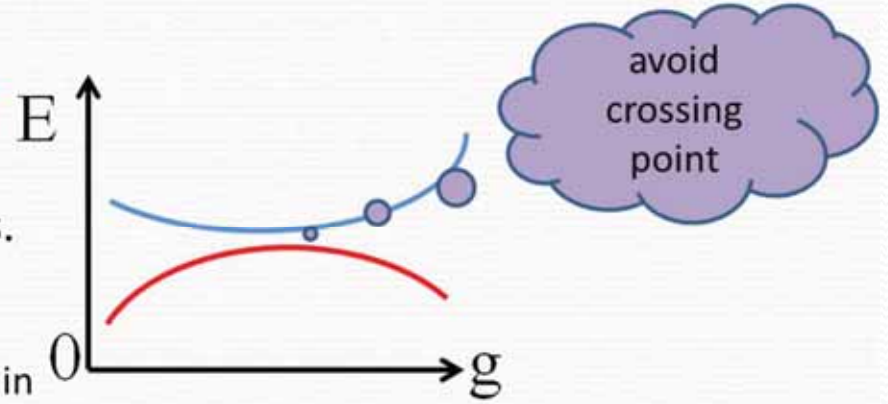
Quantum Phase Transition

a Hamiltonian, *H(g)*, varies as a function of a dimensionless coupling, *g*.

- By pure quantum fluctuations.
  the systems undergo phase transitions at zero temperature when *H(g)* is varied ;



- At the critical point , the QPT occurs, then the ground state of the system undergoes a critical change in some of its properties.



QPT is certainly one of the major interests in condensed matter physics. such as topological order, quantum entanglement, geometric phases and some other geometric quantities.

X.H. Peng et al, Phys. Rev. Lett., 105, 240405 (2010)

What is Berry's phase?

In 1984,Berry made this surprising discovery:

When a quantum system is subjected to a cyclic adiabatic evolution, it returns to its original state but may acquire a geometric phase factor in addition to the dynamical one.

For this phase reflects the geometrical properties of the parameter space of the Hamiltonian, we also call it GP

generalization → noncyclic evolution, nonadiabatic evolution

applications →
- molecular dynamics
- many-body systems
- quantum computation

GP and QPT

Recently ,the GP of many-body systems has been shown to be closely connected to quantum phase transitions (QPTs),

In the following papers：

- A.C. M. Carollo and J. K. Pachos, Phys. Rev. Lett. 95,157203 (2005).
- S.-L. Zhu, Phys. Rev. Lett. 96, 077206 (2006).
- S. Oh, Phys. Lett. A 373, 644 (2009)

conclusion

the GP difference between the ground state and the first excited state encounters a singularity when the system undergoes a QPT in the XY spin chain.

GP could be used to detect level crossings for a two-qubit system with XY interaction

Observation of the ground-state-geometric phase in a Heisenberg XY model

Ground-State Geometric Phase

$$H = -1/2 * g * (\sigma_z^1 + \sigma_z^2) - (1+\gamma)/2 * \sigma_x^1 \sigma_x^2 - (1-\gamma)/2 * \sigma_y^1 \sigma_y^2$$

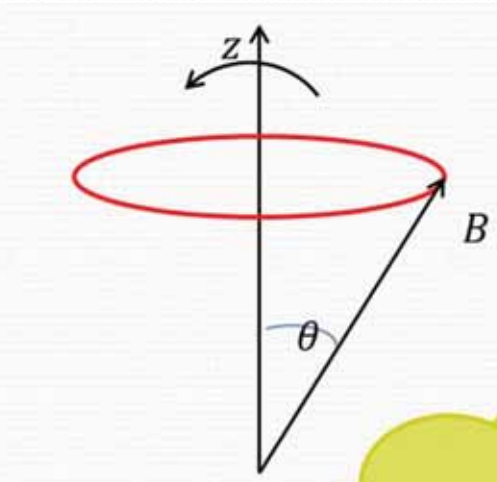
We found that when

$$\lambda^2 + \gamma^2 = 1$$

the level crossing point between ground state and first excited state

- the ground state changes discontinuously.
- the GP associated with the ground state changes discontinuously

Berry phase generated in NMR



the Hamiltonian rotates around the z-axis

$$\tilde{H}(\lambda,\gamma,\phi) = U_z^{+}(\phi)\ H(\lambda,\gamma)U_z(\phi)$$

$$U(\phi) = \Pi_k e^{-i\phi\sigma_z^k/2}$$

$$\beta_g = i\oint_{0\to\pi}\langle\Psi_g|\partial_\phi|\Psi_g\rangle$$

$$\beta_g = \begin{cases} 0 \\ \pi(1-\cos\theta) \end{cases}$$

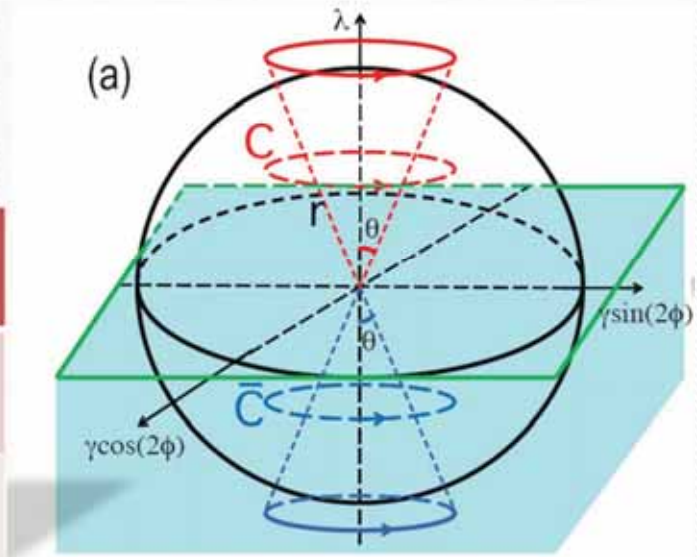
$$|\psi_g\rangle = \begin{cases} \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \quad \lambda^2+\gamma^2<1 \\ \cos\frac{\theta}{2}|00\rangle + \sin\frac{\theta}{2}e^{-i2\phi}|11\rangle \quad \lambda^2+\gamma^2>1 \end{cases}$$

Problem

When the system undergoes the cyclic adiabatic evolution along trajectory , there will also be an additional dynamic phase generated, besides the GP . How can we acquire the pure GP in experiment?

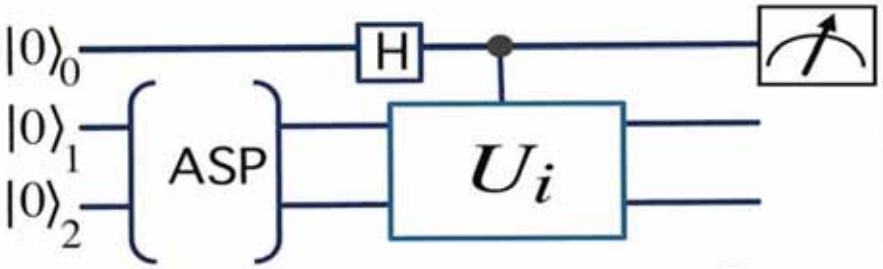
To eliminate the dynamical part, we combine two experiments with the closed paths: C and $\tilde{C}$

	Dynamical phase	Geometric phase
path C	opposite	same
path $\tilde{C}$		

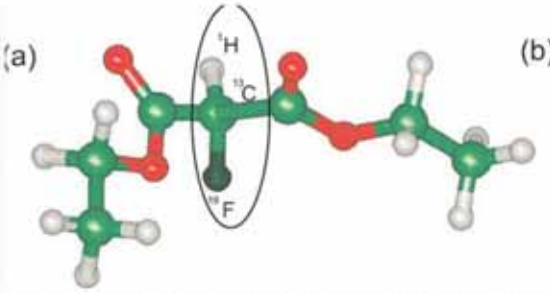


Experiment

- Adiabatic state preparation(ASP)
- Generate the pure geometric phase (GP) on one of the two paths where an auxiliary spin is introduced
- Phase measurement via quadrature detection in NMR



(a)



(b)

	^{1}H	^{13}C	^{19}F	T_1(s)	T_2(s)
^{1}H	400MHz			2.8	1.2
^{13}C	161.3Hz	100MHz		2.9	1.1
^{19}F	47.6Hz	-192.2Hz	376MHz	3.1	1.3

Adiabatic State Preparation

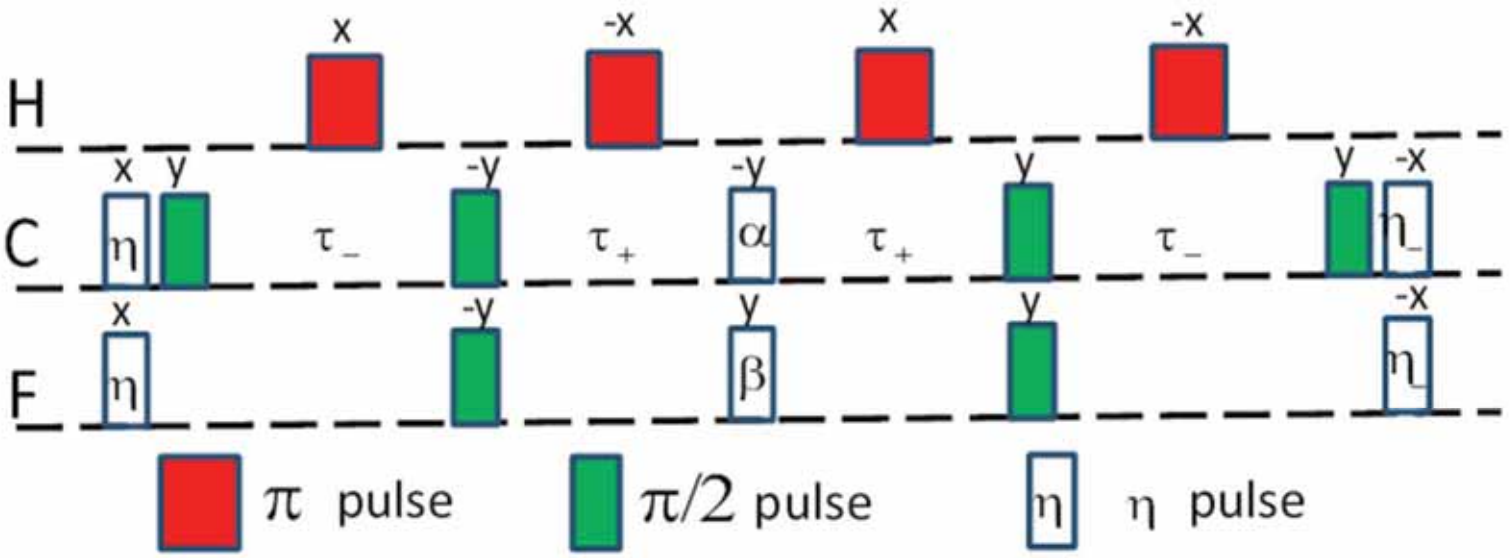


FIG. 6: The pulse sequence for a step of adiabatic state preparation. Here, $\tau_\pm = |\frac{\theta \pm \frac{\pi}{4}}{\pi J_{12}}|$, $\eta = (1 - s_m)\delta$, $\eta_- = \frac{\pi}{2} - \eta$, $\alpha = (-r - 1)s_m\delta$, $\beta = (-r + 1)s_m\delta$.

Pulse Sequence

- Generate the pure geometric phase (GP) on one of the two paths where an auxiliary spin is introduced

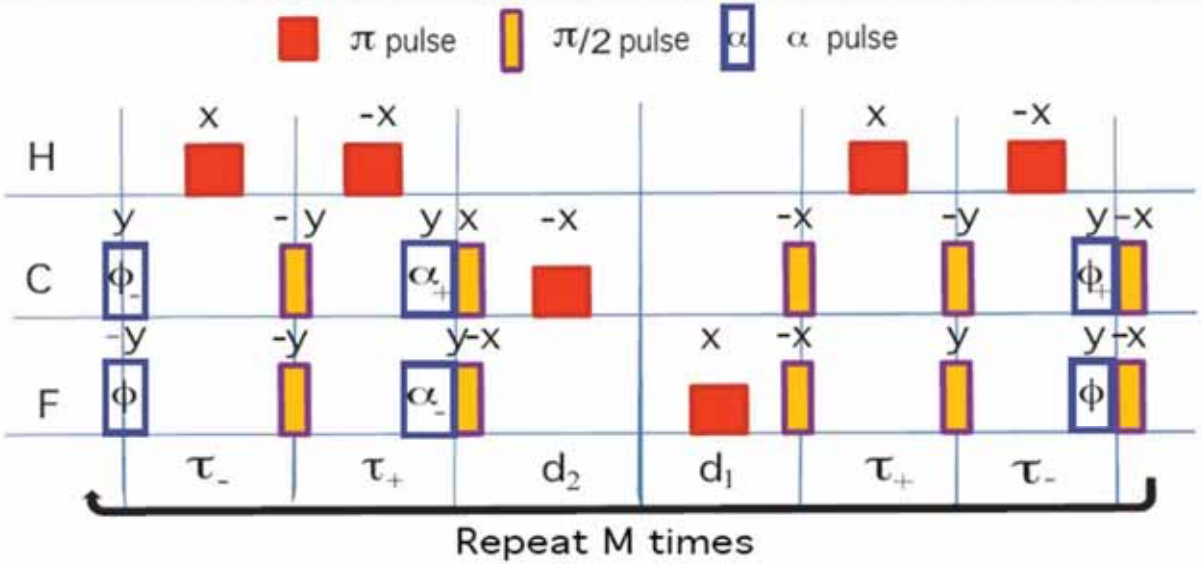
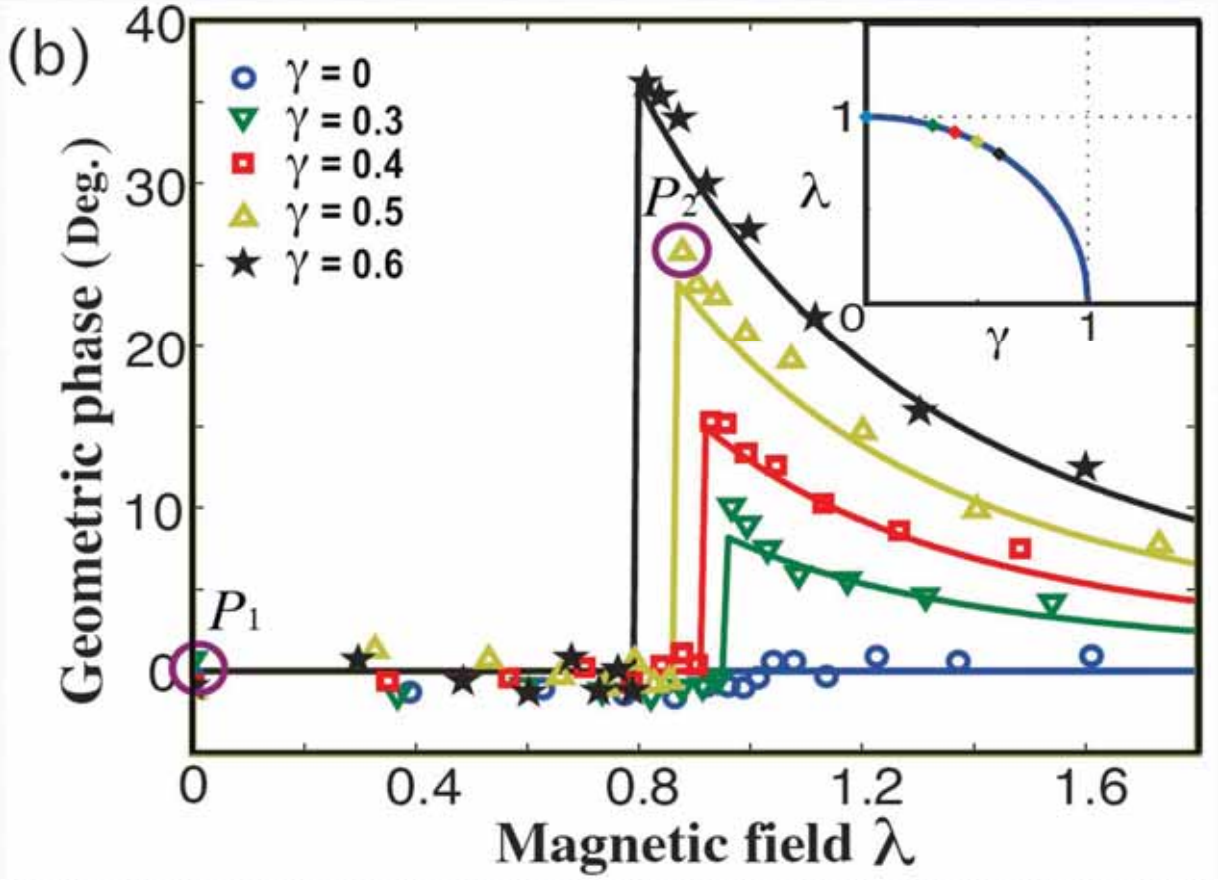


FIG. 8: Pulse sequence for implementing the control operation $\mathcal{U}_C$ for the adiabatic path C. Here $\tau_\pm = |\frac{\theta \pm \frac{\pi}{4}}{\pi J_{12}}|$, $d_i = |\frac{T(1-(-1)^i r)}{2M\pi J_{ai}}|$ $(i = 1, 2)$, $\phi_\pm = \frac{\pi}{2} \pm \phi$, and $\alpha_\pm = \frac{T(r\pm 1)}{2M}$.

Result

- Phase measurement via quadrature detection in NMR



- Quantum Phase Transition
- **Quantum Factoring**
  1) Factoring 21
  2) Factoring 143
- Quantum Annealing

Quantum Simulation for Factorizaion

- Quantum Adiabatic Algorithm for Factorization and Its Experimental Implementation

  Problem: Given an integer N=pxq, how to find its nontrival prime factors p and q?

  N = ? x ?

  Classical algorithms:

  $$O(\exp(l^{1/3}\log l^{2/3}))$$ **In sub-exponential time**

  Shor's algorithm:

  $$O(l^3)$$ **In polynmial time**

  X.H. Peng et al, Phys. Rev. Lett., **101**, 220405 (2008).

Basic Adiabatic Procedure

- (i) Design the problem Hamiltonian H_P to encode the solution.
- (ii) Choose H(0) whose ground state is easy to construct.
- (iii) Perform a suitable interpolation H(t) between H(0) and H(t) = H_P.

$$H(t) = [1 - s(t)]H_0 + s(t)H_P$$

- (iv) Adiabatically drive the system from H(0) to H(t).
- (v) Measure the final state.

Problem Hamiltonian

Optimized Function:

When $x=p, y=q$, $xy = N$, $f_{min} = 0$.

$$f(x,y) = (N - xy)^2, 1 \le x \le N, 1 \le y \le N$$

Problem Hamiltonian:

f(x,y) are the eigenvalues;
|x,y> are the corresponding eigenvectors.

$$H_P = \sum_{x,y} f(x,y) |x,y\rangle\langle x,y|$$

$$H_P |x,y\rangle = (N - xy)^2 |x,y\rangle$$

First register: n_x qubits

Second register: n_y qubits

$f_{min}(p,q)=0 \Leftrightarrow$ *Ground state* $|p,q\rangle \Rightarrow$ *Factors p and q*

Initial and final Hamiltonian

Initial Hamiltonian

$$H(0) = g(\sigma_x^1 + \sigma_x^2 + \cdots + \sigma_x^n)$$

Ground state

$$|\psi_g(0)\rangle = \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right)^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{j=0}^{2^n-1} (-1)^{b(j)} |j\rangle$$

Final Hamiltonian

$$H_P = \{NI - (2^{n_x-1}\frac{I-\sigma_z^1}{2} + \cdots + 2\frac{I-\sigma_z^{n_x-1}}{2} + I) \times$$

Variable x

$$(2^{n_y-1}\frac{I-\sigma_z^{n_x}}{2} + \cdots + 2\frac{I-\sigma_z^{n}}{2} + I)\}^2.$$

Variable y

$$\frac{I-\sigma_z}{2}|0\rangle = 0|0\rangle \quad \frac{I-\sigma_z}{2}|1\rangle = |1\rangle$$

Spatial Complexity

- 1) N is odd, x and y must also be odd
  the last bits for both registers are always 1 (omitted)

- 2) We choose $3 \le x \le \sqrt{N}, \sqrt{N} \le y \le N/3$

First register: $n_x = m\left(\left\lfloor \sqrt{N} \right\rfloor_o\right) - 1 \le \left\lfloor \frac{l+1}{2} \right\rfloor - 1$

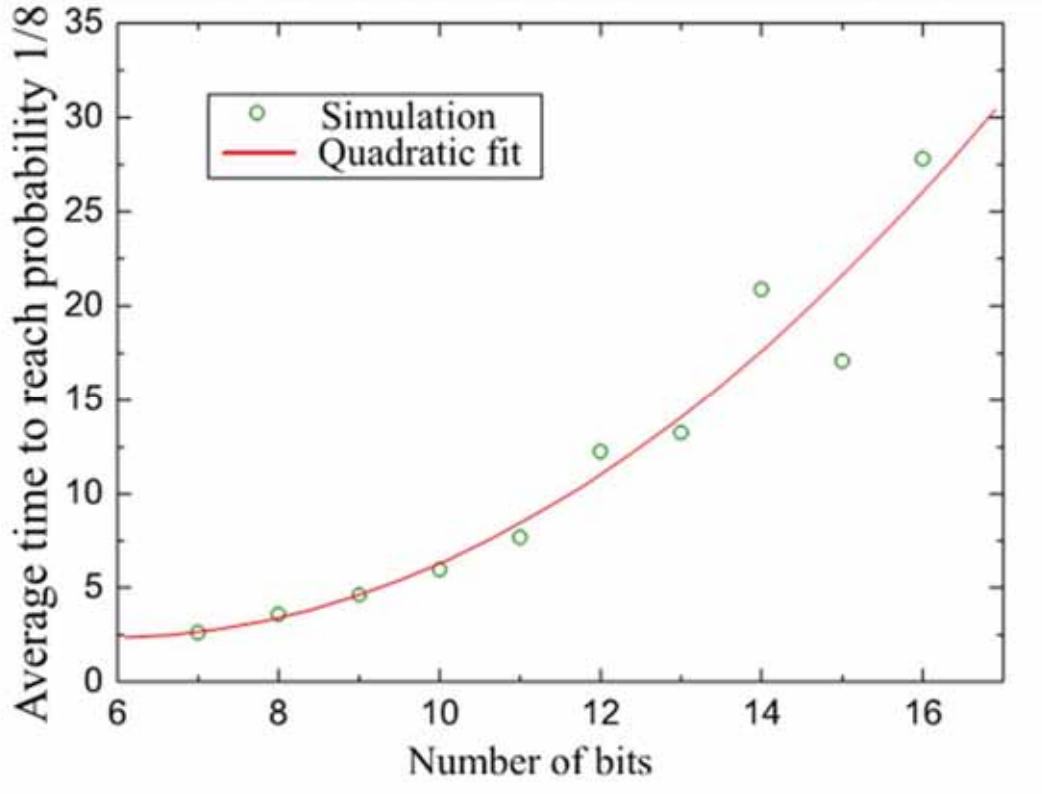
Second register: $n_y = m\left(\left\lfloor \frac{N}{3} \right\rfloor\right) - 1 \le l - 2$

Total Qubits: **Shor's:** $O(2l)$

$$n = n_x + n_y \le \left\lfloor \frac{l+1}{2} \right\rfloor + l - 3 \sim O(3l/2)$$

Time Complexity

Average evolution time: Quadratic behavior



To achieve the probability 1/8 for 50 instances.

Experimentally Factorizing 21

First register: $n_x = m\left(\left\lfloor \sqrt{21} \right\rfloor_o\right) - 1 = 1$

Second register: $n_y = m\left(\left\lfloor 7 \right\rfloor\right) - 1 = 2$

Initial Hamiltonian: $H(0) = g(\sigma_x^1 + \sigma_x^2 + \sigma_x^3)$

Problem Hamiltonian:

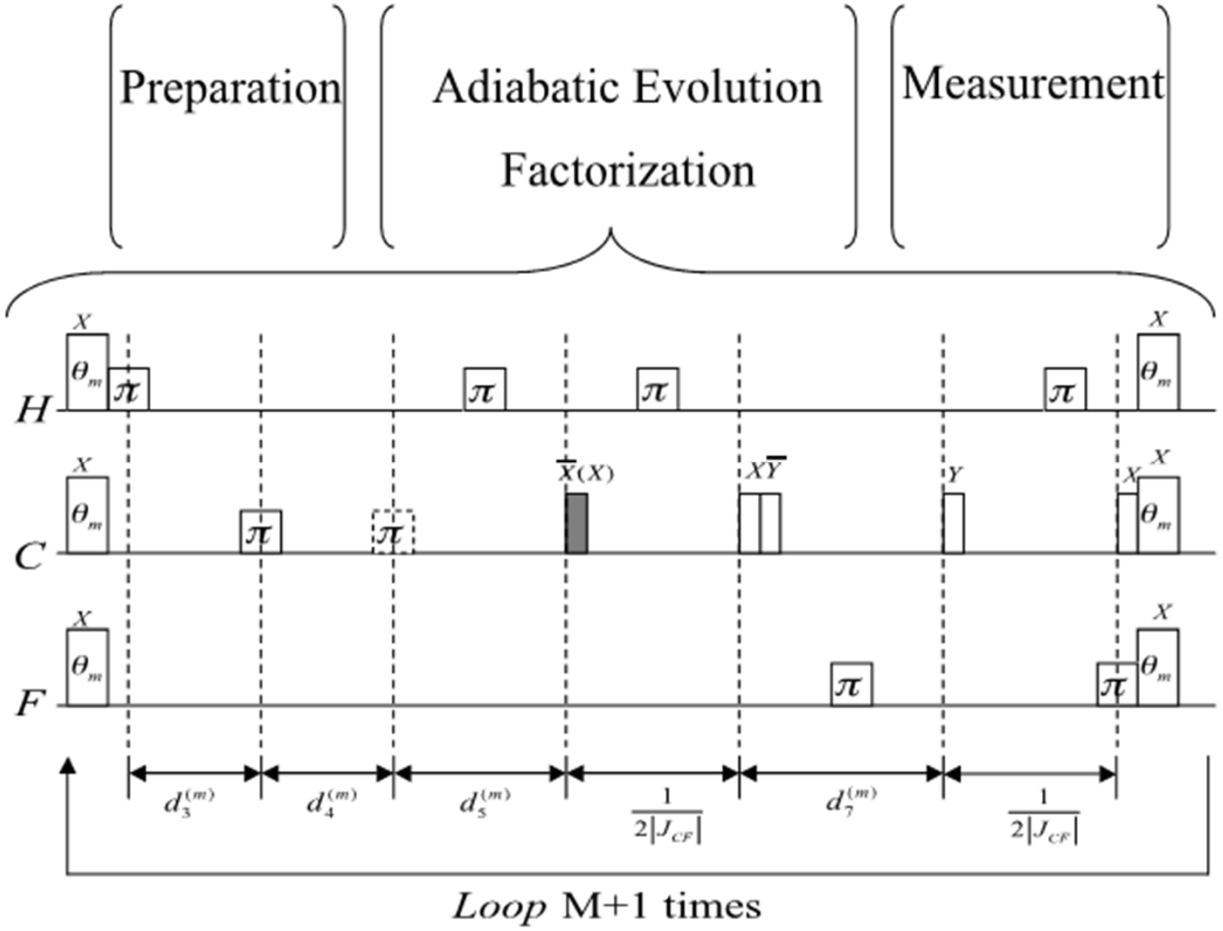
$$H_P = 210I + 84\sigma_z^1 + 88\sigma_z^2 + 44\sigma_z^3 - 20\sigma_z^1\sigma_z^2 - 10\sigma_z^1\sigma_z^3 + 20\sigma_z^2\sigma_z^3 - 16\sigma_z^1\sigma_z^2\sigma_z^3.$$

Task: to find its ground state $H_P|111\rangle = 0\,|111\rangle$

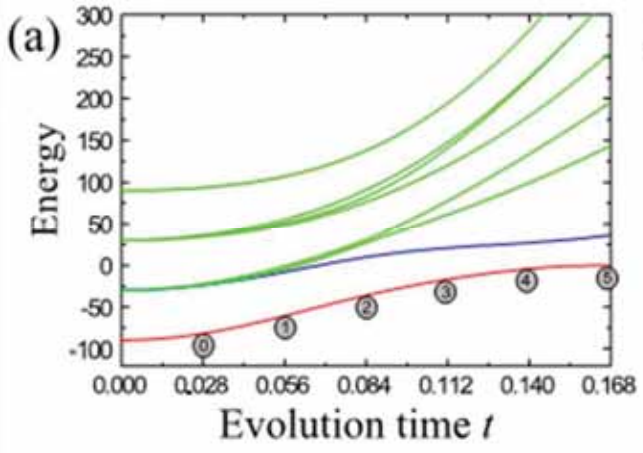
NMR Implementation

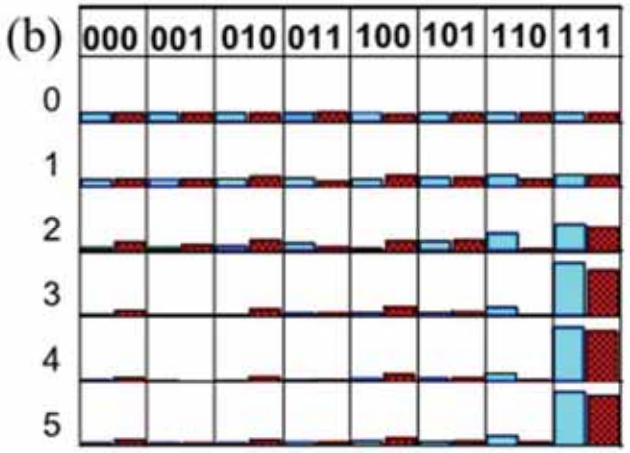
Diethyl-fluoromalonate

$$g = 30, r = 2, M = 5, \tau = 0.028$$



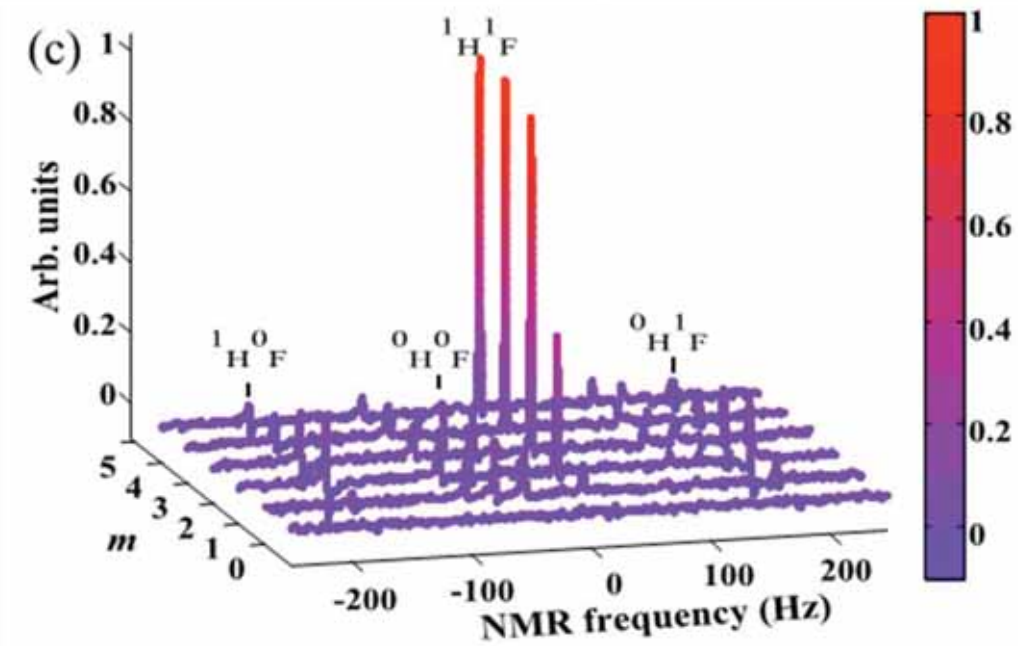
Results





$F_{the} = 0.91$

$F_{exp} = 0.87$



Final state: close to |111>
First register: |1>
Second register: |11>
Adding the last bit 1
First register: |11>=3,
Second register: |111> =7

21 = 3 x 7

- Quantum Phase Transition
- **Quantum Factoring**
  - 1) Factoring 21
  - **2) Factoring 143**
- Quantum Annealing

New Challenge: 143

- **Theory: Improve the adiabatic factoring algorithm**

  Energy gap of the Hamiltonian

  $$N^2 \rightarrow \log_2 N$$

- **Experiment: Dipolar coupling system**

  1. **Less qubits**
  2. **Control of the liquid-crystal sample, which has a more complicated Hamiltonian with dipolar couplings.**

N. Y. Xu et al, submitted to Phys. Rev. Lett.

Improvement

- **Old algorithm**

  Based on the equation $(N-ab)^2=0$

- **New algorithm**

  Based on the equation set

				1	p_2	p_1	1
				1	q_2	q_1	1
				1	p_2	p_1	1
			q_1	p_2q_1	p_1q_1	q_1	
		q_2	p_2q_2	p_1q_2	q_2		
	1	p_2	p_1	1			
z_{67}	z_{56}	z_{45}	z_{34}	z_{23}	z_{12}		
z_{57}	z_{46}	z_{35}	z_{24}				
1	0	0	0	1	1	1	1

$$
\begin{aligned}
p_1+q_1 &= 1+2z_{12}\\
p_2+p_1q_1+q_2+z_{12} &= 1+2z_{23}+4z_{24}\\
1+p_2q_1+p_1q_2+1+z_{23} &= 1+2z_{34}+4z_{35}\\
q_1+p_2q_2+p_1+z_{34}+z_{24} &= 0+2z_{45}+4z_{46}\\
q_2+p_2+z_{45}+z_{35} &= 0+2z_{56}+4z_{57}\\
1+z_{56}+z_{46} &= 0+2z_{67}\\
z_{67}+z_{57} &= 1.
\end{aligned}
$$

Theoretical Hamiltonian

- **Simplification of the equation set**

$$\begin{cases} p_1 + q_1 = 1 \\ p_2 + q_2 = 1 \\ p_2 q_1 + p_1 q_2 = 1 \end{cases}$$

- **Adiabatic Hamiltonian**

$$H_p^1 = (\hat{p}_1 + \hat{q}_1 - 1)^2$$
$$H_p^2 = (\hat{p}_2 + \hat{q}_2 - 1)^2$$
$$H_p^3 = (p_2 q_1 + p_1 q_2 - 1)^2$$

$$H_p = \sum_{i=1}^{3} H_p^i = 5 - 3\hat{p}_1 - \hat{p}_2 - \hat{q}_1 + 2\hat{p}_1\hat{q}_1 - 3\hat{p}_2\hat{q}_1 + 2\hat{p}_1\hat{p}_2\hat{q}_1 - 3\hat{q}_2 + \hat{p}_1\hat{q}_2 + 2\hat{p}_2\hat{q}_2 + 2\hat{p}_2\hat{q}_1\hat{q}_2,$$

Evolution and Results

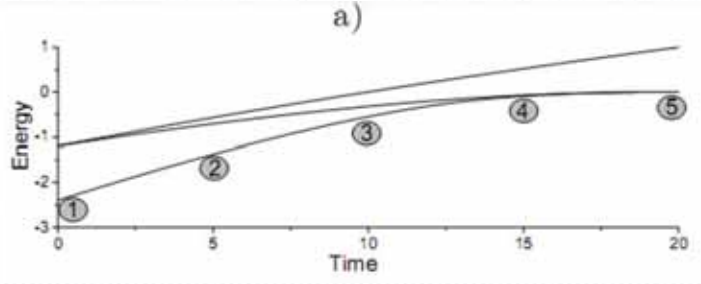
- **Initial Hamiltonian:** $H_i = g(\sigma_x^1 + \sigma_x^2 + \cdots + \sigma_x^n)$

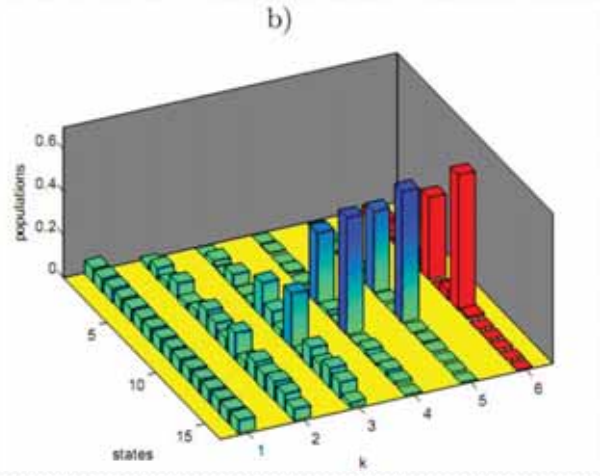
  Final Hamiltonian :

$$H_p = \sum_{i=1}^{3} H_p^i = 5 - 3\hat{p}_1 - \hat{p}_2 - \hat{q}_1 + 2\hat{p}_1\hat{q}_1 - 3\hat{p}_2\hat{q}_1 + 2\hat{p}_1\hat{p}_2\hat{q}_1 - 3\hat{q}_2 + \hat{p}_1\hat{q}_2 + 2\hat{p}_2\hat{q}_2 + 2\hat{p}_2\hat{q}_1\hat{q}_2,$$

$$\hat{p}_1 = \frac{1-\sigma_z^1}{2}, \hat{p}_2 = \frac{1-\sigma_z^2}{2}, \hat{q}_1 = \frac{1-\sigma_z^3}{2} \text{ and } \hat{q}_2 = \frac{1-\sigma_z^4}{2}$$

- **|0110> and |1001>** ➡ **11*13 or 13*11**

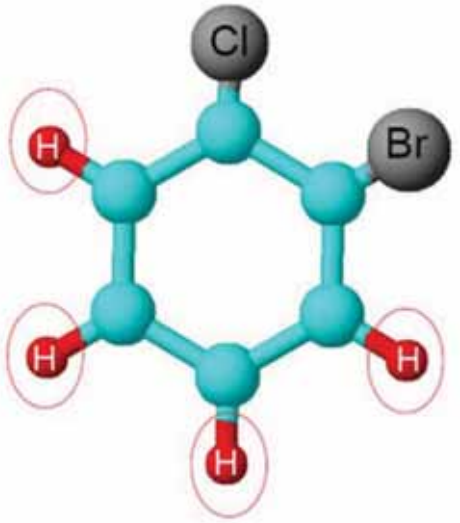




Sample

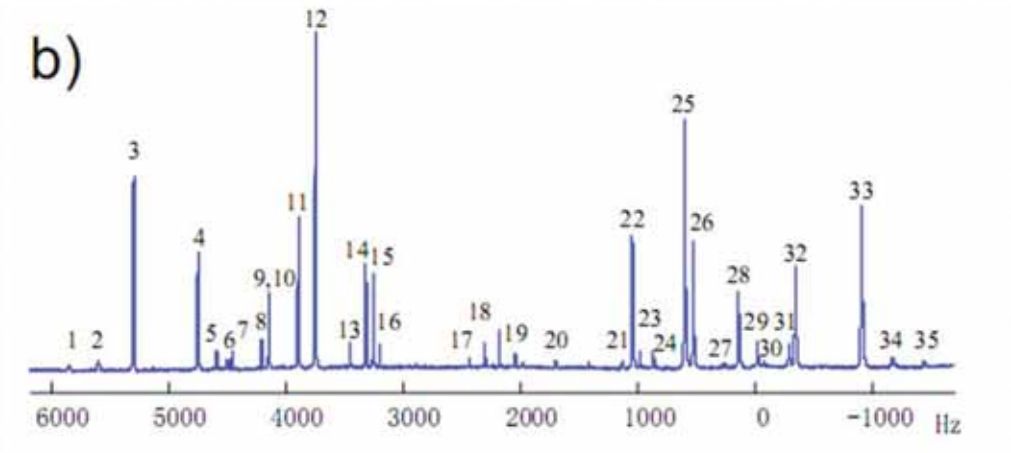
- **sample**: ortho-chlorobromobenzene

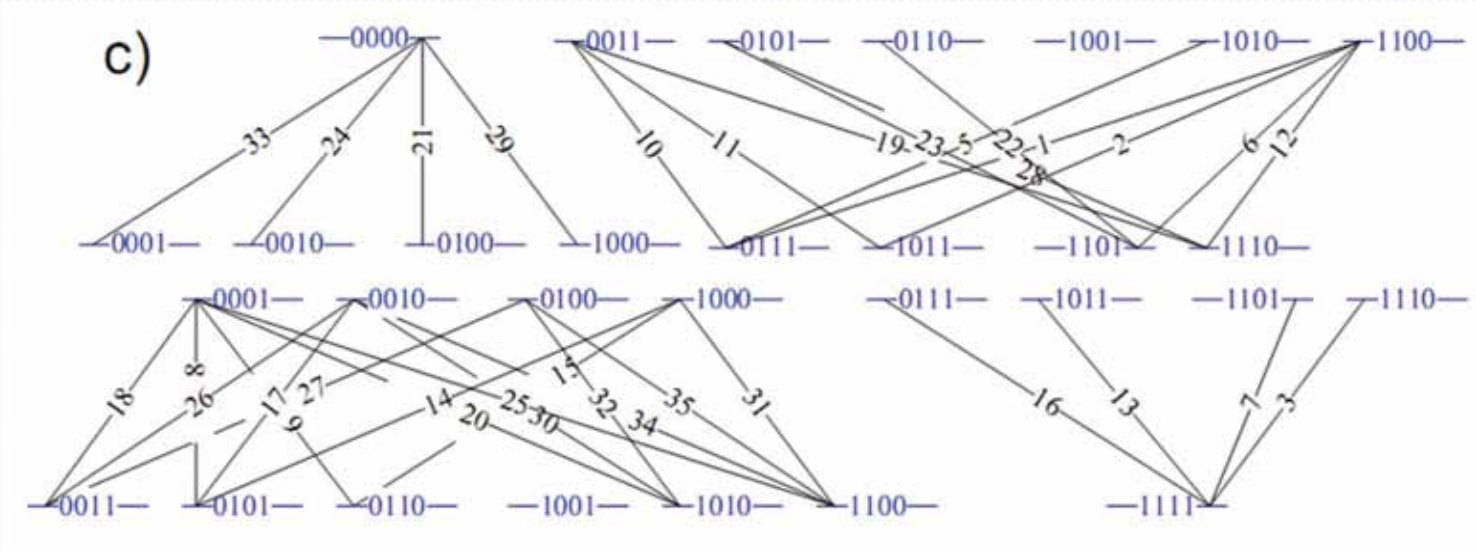
$$\mathcal{H} = 2\pi \sum_i \nu_i I_z^i + 2\pi \sum_{i,j,i<j} J_{ij} I_z^i I_z^j$$
$$+2\pi \sum_{i,j,i<j} D_{ij}(2I_z^i I_z^j - I_x^i I_x^j - I_y^i I_y^j)$$



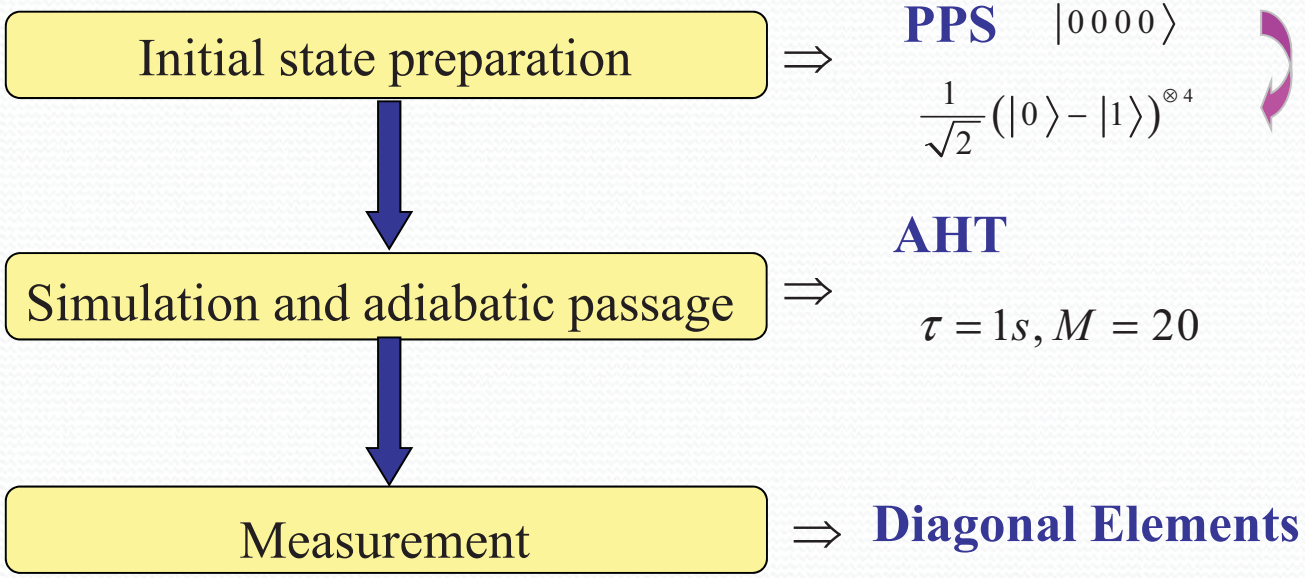
	H_1	H_2	H_3	H_4
H_1	2264.8	−706.6	−214.0	−1166.5
H_2	0	2190.4	−1553.8	−149.8
H_3	1.4	8	2127.3	−95.4
H_4	8	1.4	8	2113.5

Energy Diagram





Experimental Procedure

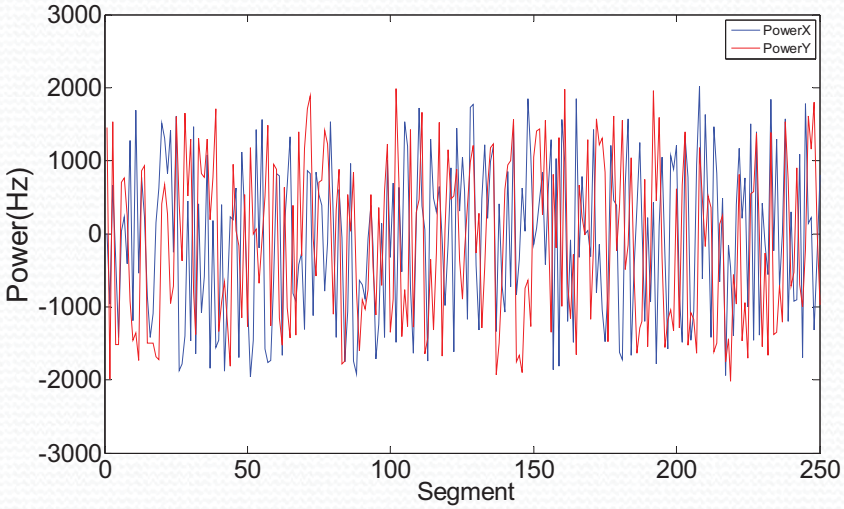


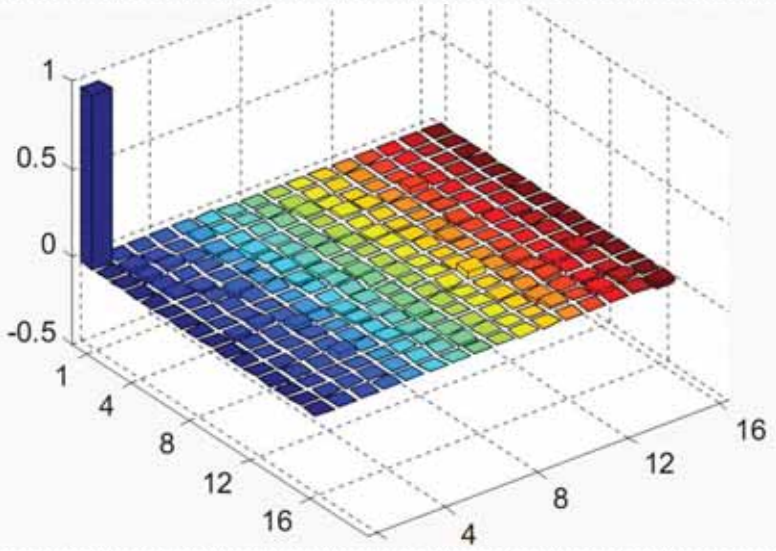
$$\rho_{0000} \rightarrow H^{\dagger\,\otimes 4} \rightarrow U_{ad} \rightarrow Measurment$$

PPS Preparation

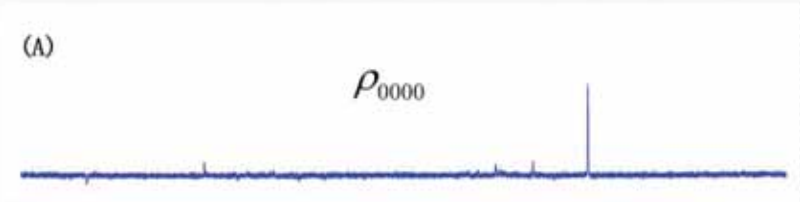
- GRAPE pulse
- Gradient pulse
- Seeking for PPS

- T = 7ms, Fidelity = 0.99



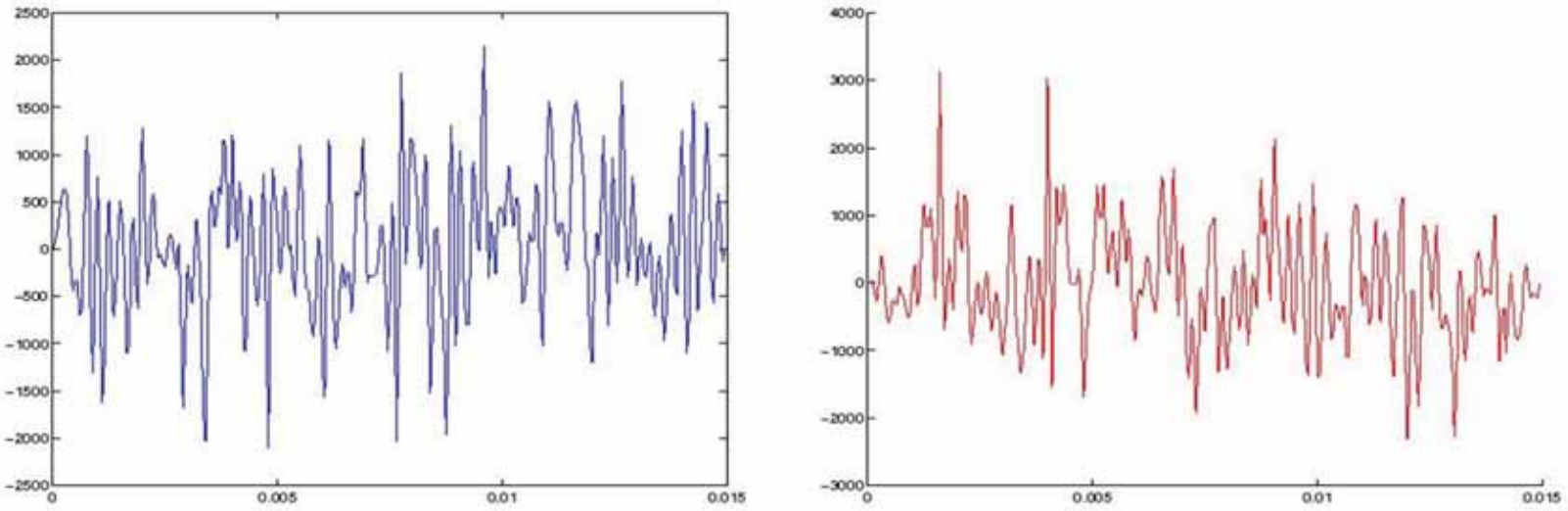


Small-Angle Flip



GRAPE Pulses

- GRAPE （GRadient Ascent Pulse Engineering）
  For every pulse: 15ms， Fidelity > 0.99



$$\rho_{0000} \rightarrow H^{\dagger \otimes 4} \rightarrow U_{ad} \rightarrow Measurment$$

4 steps and 60 ms

Result

- Adding $[\pi]^{2,3}$ after the final state

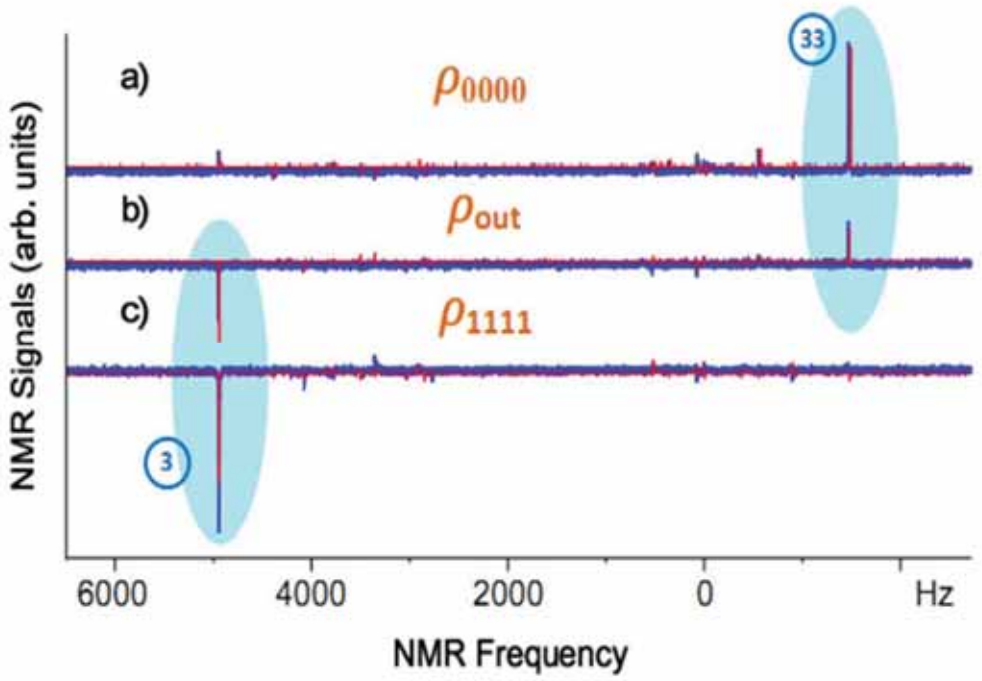
0110 + 1001

↓

0000 + 1111

$$P_{out} \approx P_{0000} + P_{1111}$$

$$P_{0000} = 0.201 \quad P_{1111} = 0.273$$



- T = 60ms, T2* = 102ms

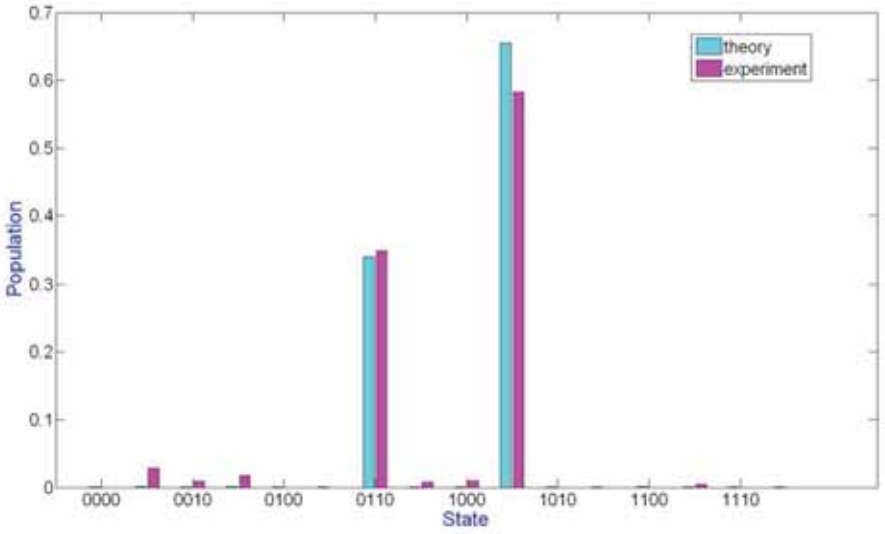
Considering decoherence

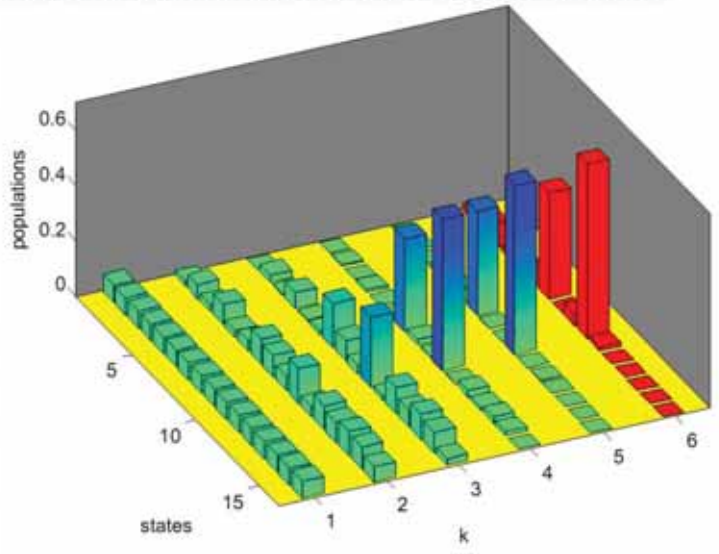
$$P_{0000} = 0.362 \,\&\, P_{1111} = 0.492$$

Diagonal Measurement

- **32 read out pulses**

  Each pulse is 20ms





Step 1-5: theoretical results

Step 6 (red): experimental results

- Quantum Phase Transition
- Quantum Factoring
- **Quantum Annealing**

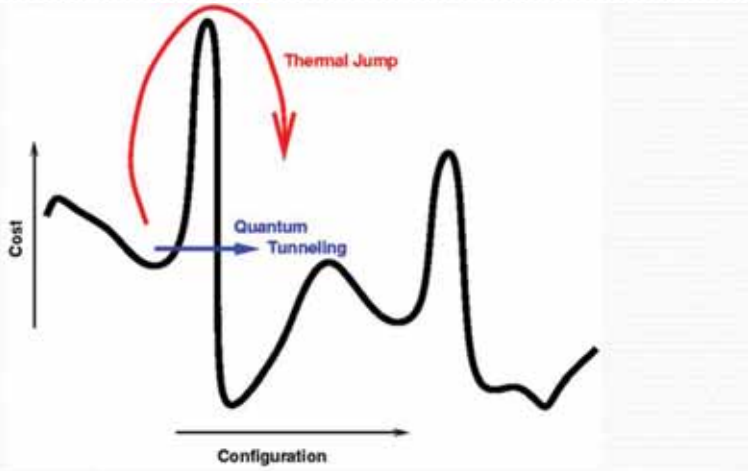
Quantum Annealing

➢ Annealing:

In materials science, annealing is a process performed by heating certain types of materials to high temperatures and then allowing them to cool down slowly, in order to improve the properties of the materials.

➢ Classical simulated annealing (SA):

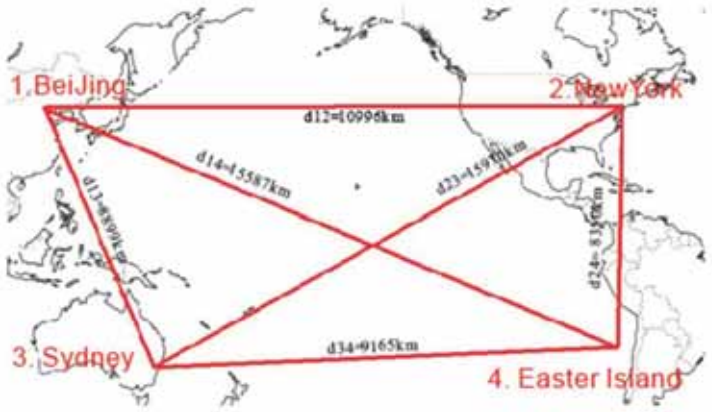
In SA, emulating thermal physics, an artificial temperature for an optimization problem is introduced and is gradually reduced to zero, this drives the system to the lowest energy state corresponding to the optimized configuration in the problem.



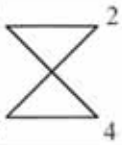
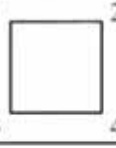
➢ Quantum Annealing (QA):

QA provides quantum fluctuations to help the search tunneling through high barriers instead of thermal fluctuations. The idea of quantum annealing is to perform optimization by a quantum adiabatic evolution which tracks the ground state of a suitable time-dependent Hamiltonian.

Traveling Salesman Problem

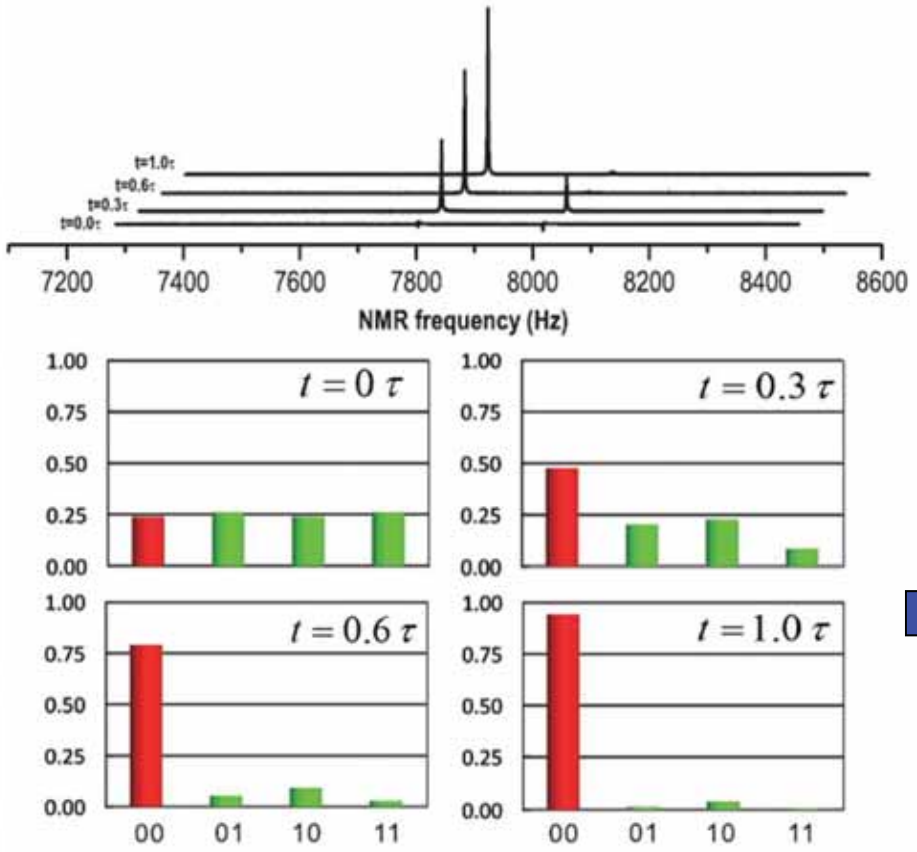


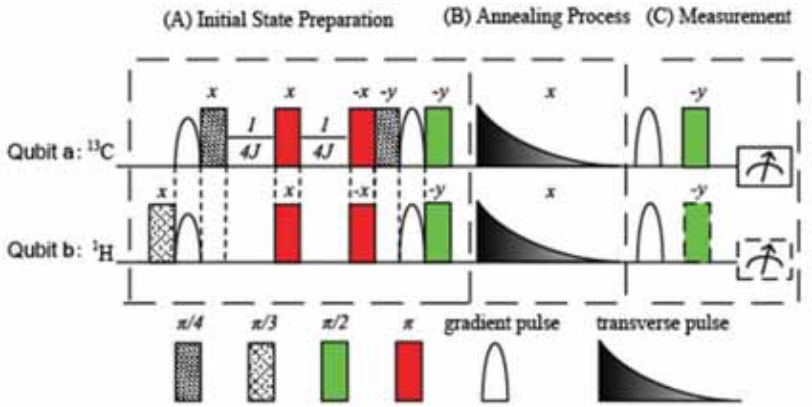
$$H(t) = \sum_{i=1}^{K} v_i \sigma_z^i + \sum_{i=1}^{K} \sum_{j=i+1}^{K} J_{ij} \sigma_z^i \sigma_z^j + \Gamma(t) \sum_{i=1}^{K} \sigma_x^i .$$

Parameters	Traveling Route	Output State	Total Length
U_{12}=1 U_{13}=0		$\|01\rangle$	51718 km
U_{12}=0 U_{13}=1		$\|10\rangle$	48806 km
U_{12}=1 U_{13}=1		$\|00\rangle$	37410 km
U_{12}=0 U_{13}=0	Invalid tour	$\|11\rangle$	Invalid

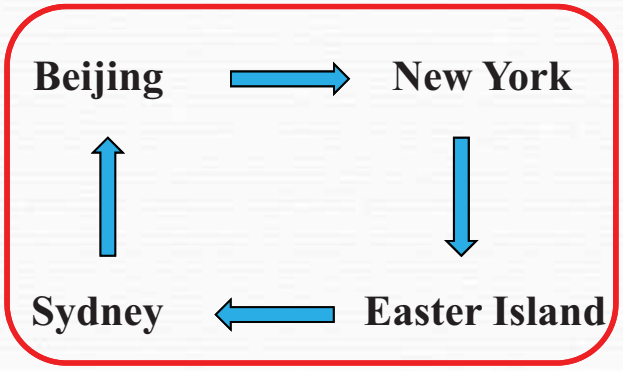
H. W. Chen, *et. al.*, Physical Review A **83**, 032314 (2011)

Experiment





Pulse Sequence



The Optimal Traveling Route

Report

RESEARCH | NEWS & VIEWS

QUANTUM PHYSICS

Keep your feet on the ground

Some complex problems in physics can be recast as finding the ground state of an interacting quantum system. Not getting excited along the way can be the challenging part. SEE LETTER P.194

To be clear, this system was not used to perform any computational algorithm. And, whereas computing algorithms based on adiabatic quantum annealing have been demonstrated with small-scale model problems in nuclear magnetic resonance systems[7], the practical benefits and scalability of quantum-annealing algorithms for large-scale problems remain unclear[8,9]. Furthermore, although

1. Johnson, M. W. *et al. Nature* **473,** 194–198 (2011).
2. Farhi, E. *et al. Science* **292,** 472–475 (2001).
3. Santoro, G. E., Martoňák, R., Tosatti, E. & Car, R. *Science* **295,** 2427–2430 (2002).
4. Clarke, J. & Wilhelm, F. K. *Nature* **453,** 1031–1042 (2008).
5. Voss, R. F. & Webb, R. A. *Phys. Rev. Lett.* **47,** 265–268 (1981).
6. Devoret, M. H., Martinis, J. M. & Clarke, J. *Phys. Rev. Lett.* **55,** 1908–1911 (1985).
7. Chen, H. *et al. Phys. Rev. A* **83,** 032314 (2011).
8. Farhi, E., Goldstone, J. & Gutmann, S. Preprint at http://arxiv.org/abs/quant-ph/0201031 (2002).
9. Matsuda, Y., Nishimori, H. & Katzgraber, H. G *N. J. Phys.* **11,** 073021 (2009).

Thank you !

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Department of Modern Physics,
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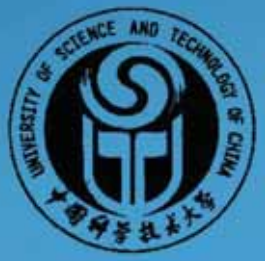
Hefei, Anhui, P.R.China

Simulation of Quantum Chemistry on an NMR Quantum Computer

Jiangfeng Du



Hefei National Laboratory for Physical Science at Micro-scale,
University of Science and Technology of China

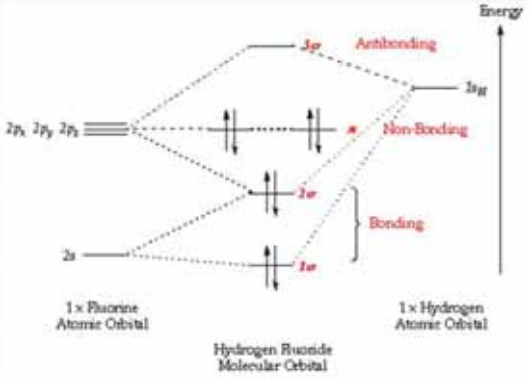
Outline

- Simulation of Hydrogen Molecular Energy
- Simulation of Chemical Reaction Dynamics
  1) How to simulate chemical reactions?
  2) An example used in our experiment
  3) NMR experimental implementation
- Simulation of 2-body Heisenberg Hamiltonian
  1) Simulate a multi-energies Hamiltonian
  2) NMR experimental implementation
     a. Eigenvalues
     b. Ground state information

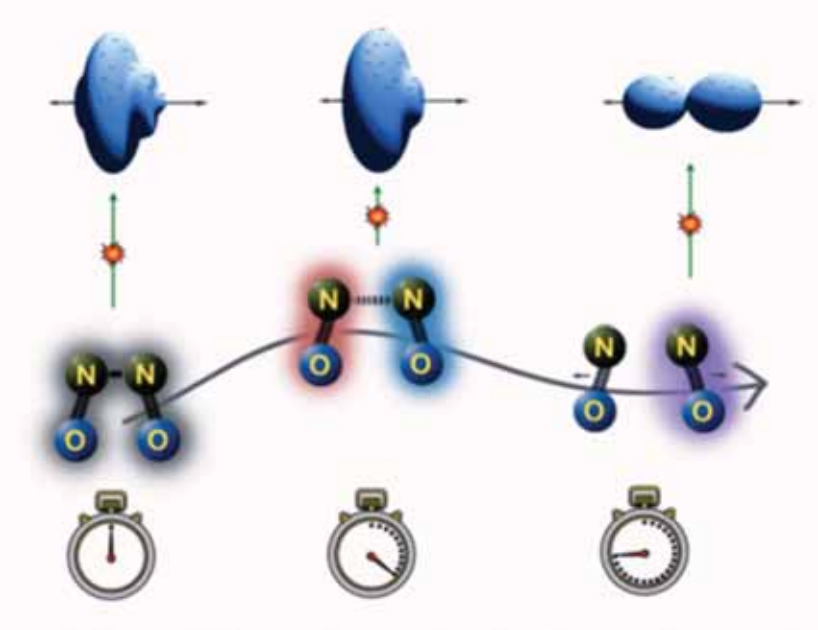
- **Simulation of Hydrogen Molecular Energy**
- Simulation of Chemical Reaction Dynamics
- Simulation of 2-body Heisenberg Hamiltonian

Simulation of Chemical Systems

Molecular static energy

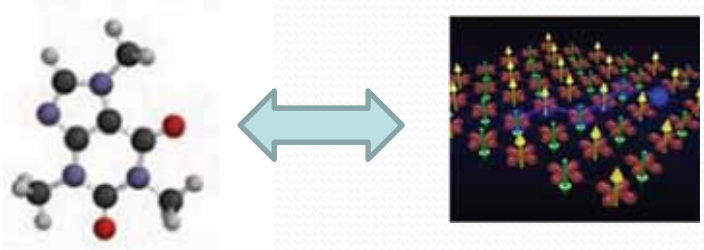


Reaction Dynamics

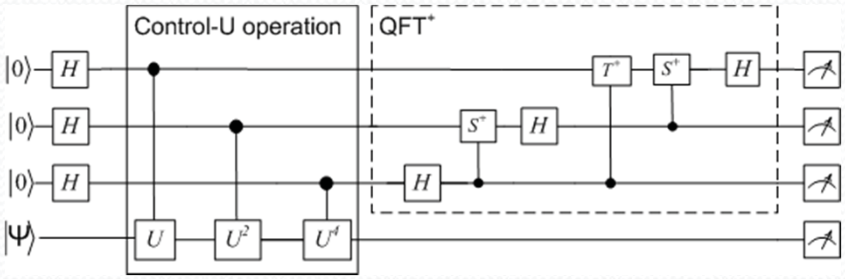


Aspuru-Guzik's Proposal

1.Molecule ➞ Qubits

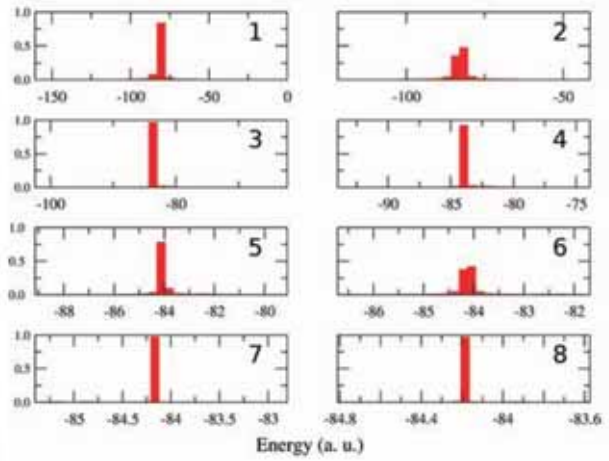


2.Phase estimation using QFT

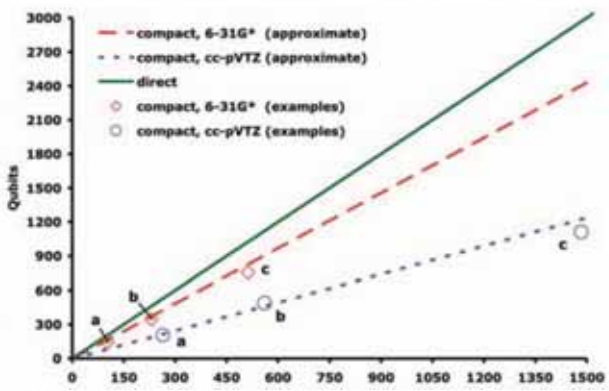


$$U\left|\psi\right\rangle = e^{-iHt}\left|\psi\right\rangle = e^{-iEt}\left|\psi\right\rangle$$

3.Improve precision through iteration



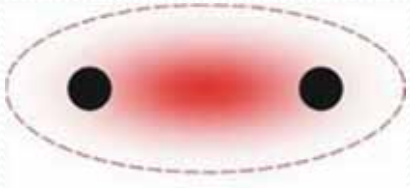
4.Polymonial in time, Linear in space



A. Aspuru-Guzik et al., Science, 309, 1704 (2005)

Hamiltonian of Hydrogen Molecule

Born-Oppenheimer Approximation : Ubiquitous in quantum chemical calculations of molecular wavefunctions



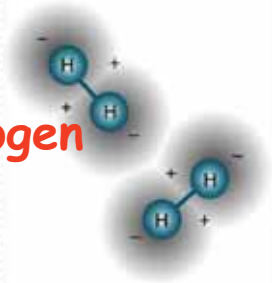
$$\mathcal{H}_{\text{elec}} = -\sum_{i=1}^{N} \frac{1}{2} \nabla_i^2 - \sum_{i=1}^{N} \sum_{A=1}^{M} \frac{Z_A}{r_{iA}} + \sum_{i=1}^{N} \sum_{j>i}^{N} \frac{1}{r_{ij}}$$

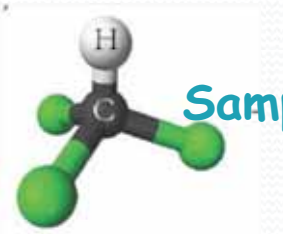
Basis Function: STO-3G

$$H = \begin{pmatrix} \langle \Psi_0 | \mathrm{H} | \Psi_0 \rangle & \langle \Psi_0 | \mathrm{H} | \Psi_{1\bar{1}}^{2\bar{2}} \rangle \\ \langle \Psi_{1\bar{1}}^{2\bar{2}} | \mathrm{H} | \Psi_0 \rangle & \langle \Psi_{1\bar{1}}^{2\bar{2}} | \mathrm{H} | \Psi_{1\bar{1}}^{2\bar{2}} \rangle \end{pmatrix} = \begin{pmatrix} -1.8310 & 0.1813 \\ 0.1813 & -0.2537 \end{pmatrix} a.u.$$

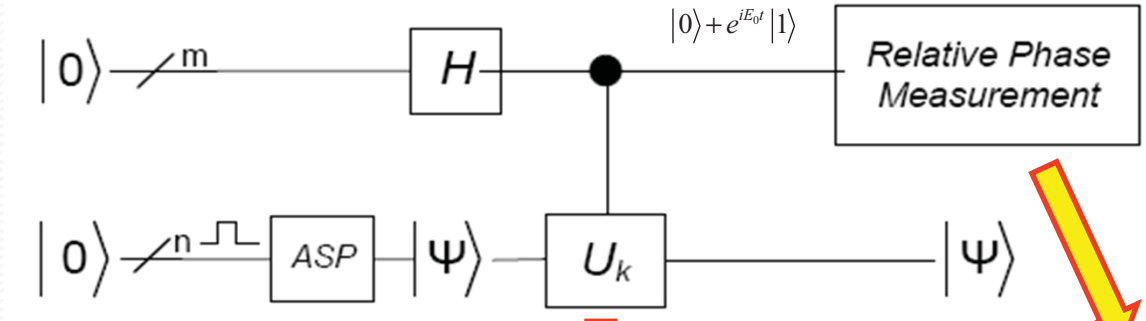
Experimental Implementation

Target: Hydrogen





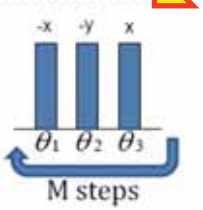
Sample: CHCl3

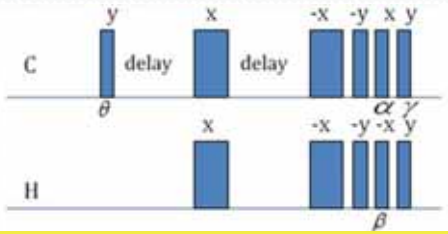


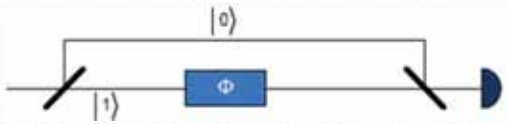
Adiabatic

Evolution

NMR interferometer





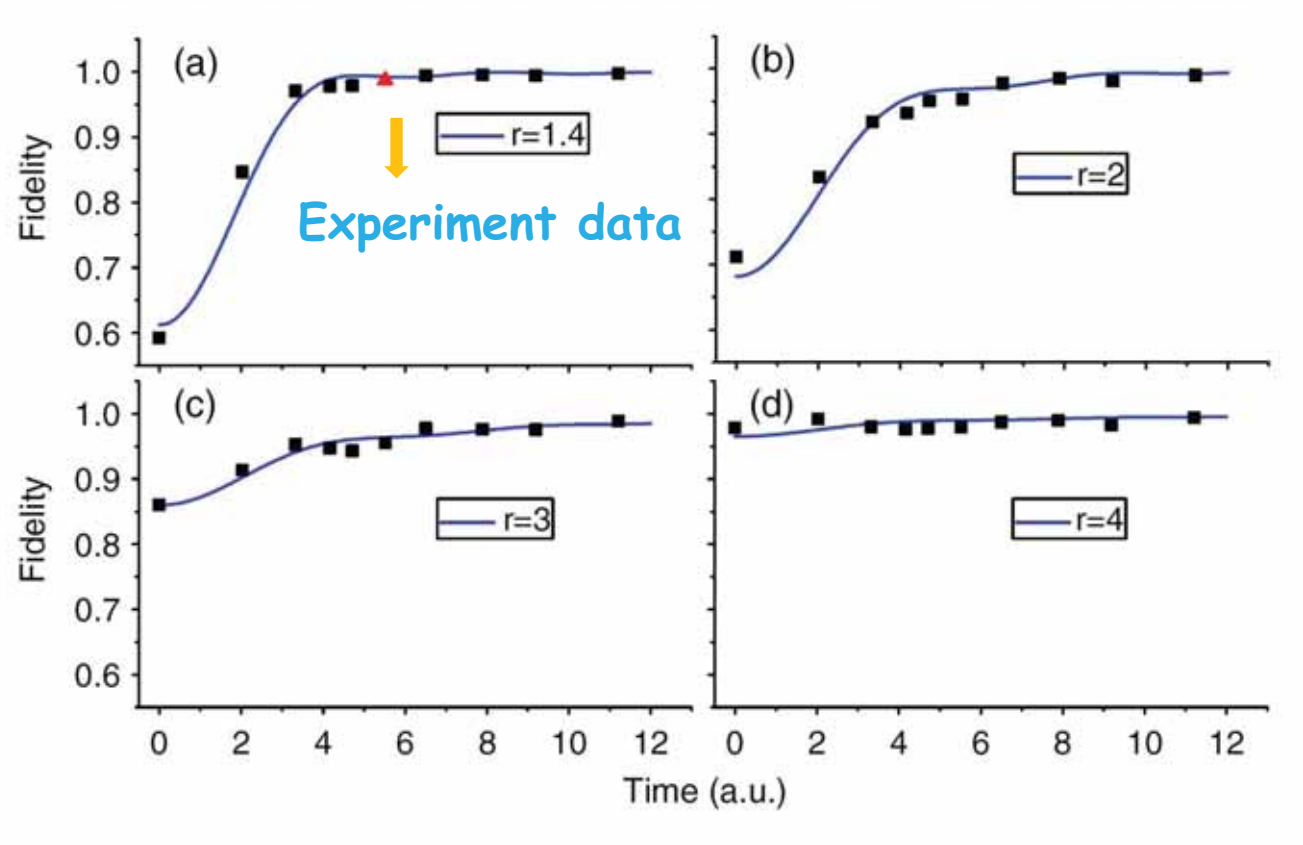


J. F. Du et al., Phys. Rev. Lett. 104, 030502 (2010)
J. F. Du et al., Phys. Rev. Lett. 91, 100403 (2003)

Adiabatic State Preparation

Hamiltonian: $\sigma_x \rightarrow H$

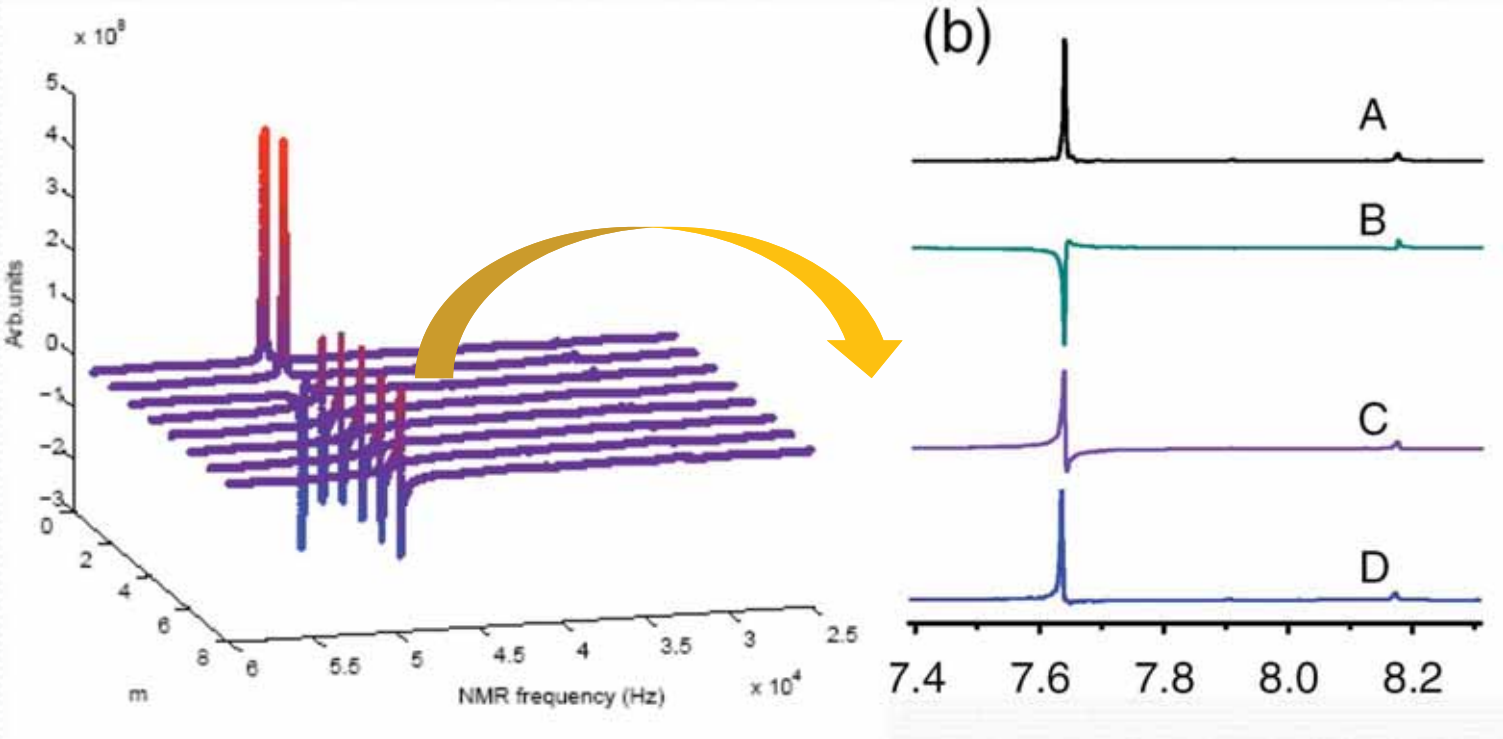
State: $|0\rangle-|1\rangle \rightarrow |\Psi\rangle$



Phase Shift Measurement

$$U|\Psi\rangle = e^{-iH\tau}|\Psi\rangle = e^{i2\pi\phi}|\Psi\rangle$$

$$E = -2\pi\,\phi/\tau$$

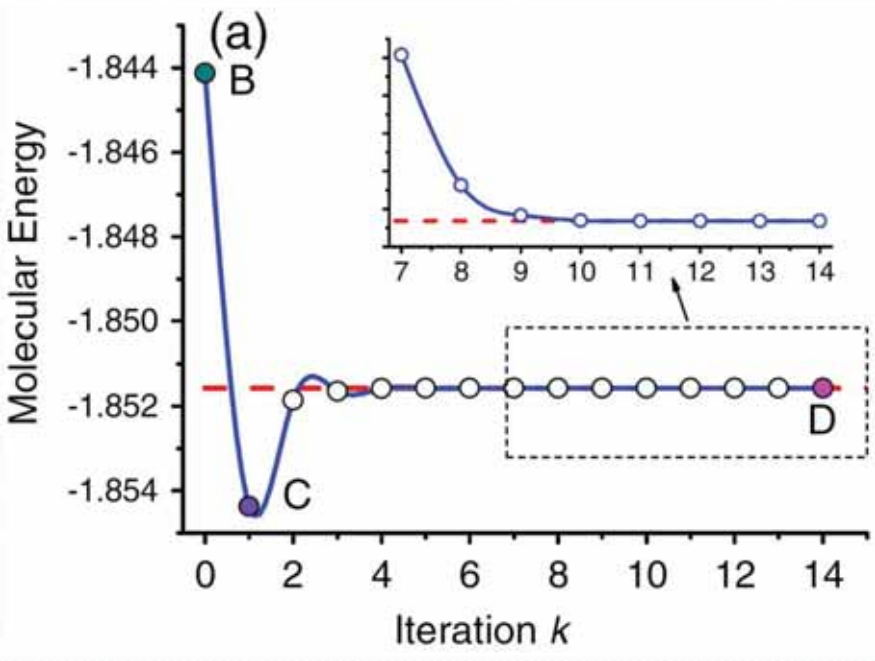


Experimental Result

	k	Binary value
ϕ_{exp}	0	**0.100**10001110110010101000011001000001111111010
	2	**0.100100100**1110101110010110100110001010010011 10
	5	**0.100100100111000000**0110100111011011110111010 01
	8	**0.100100100111000000010100001**1010001000111111 0
	11	**0.100100100111000000010100001101111001**1000000 0
	14	**0.100100100111000000010100001101111001101010110**
ϕth		0.100100100111000000010100001101111001101010110101

15 Iterations

45 Bits



Publication

PRL 104, 030502 (2010) PHYSICAL REVIEW LETTERS week ending 22 JANUARY 2010

NMR Implementation of a Molecular Hydrogen Quantum Simulation with Adiabatic State Preparation

Jiangfeng Du,* Nanyang Xu, Xinhua Peng, Pengfei Wang, Sanfeng Wu, and Dawei Lu
Hefei National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China
(Received 28 July 2009; published 22 January 2010)

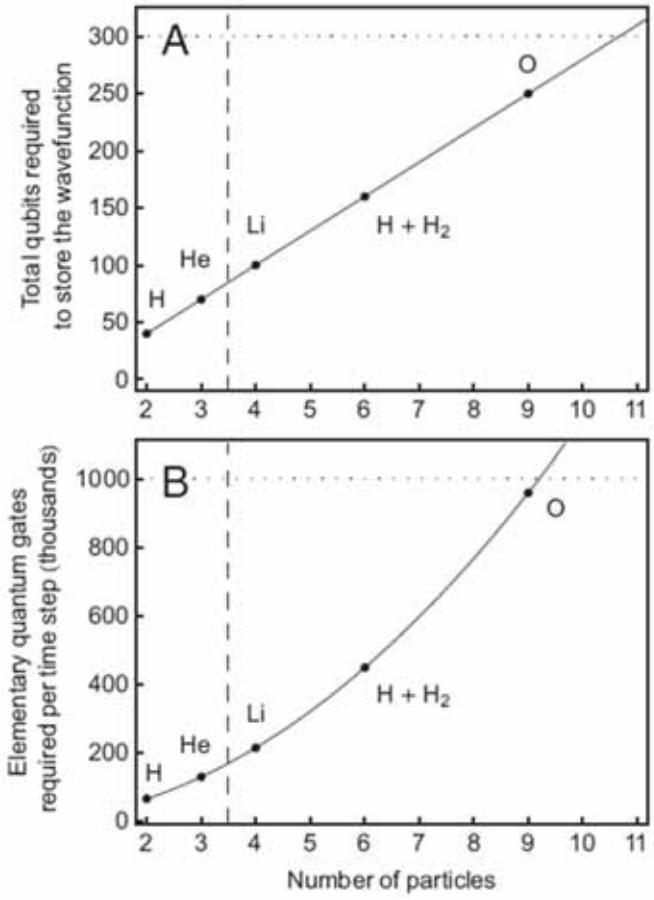
- Simulation of Hydrogen Molecular Energy
- **Simulation of Chemical Reaction Dynamics**
  - 1) How to simulate chemical reactions?
  - 2) An example used in our experiment
  - 3) NMR experimental implementation
- Simulation of 2-body Heisenberg Hamiltonian

Quantum Simulation of Molecular Dynamics

-- To Simulate Molecular Dynamics on a QC

The number of qubits scales linear with molecular size

The number of operations scales polynomial with molecular size



I. Kassala et. al., PNAS 105, 18681 (2008)

Chemical Dynamics in Position Representation

➢ Quantum Simulation Requirement:

(a) Initial wave function $|\psi(0)\rangle$

(b) System Hamiltonian H=T+V

(i) Discretization of Position with *n*-qubits:

$$|\psi(t)\rangle = \sum_{x=0}^{2^n-1} a_x(t)|x\rangle = a_0\underbrace{|0\ldots00\rangle}_{n\ qubits} + \ldots + a_{2^n-1}|1\ldots11\rangle.$$

(ii) The Propagation of Wave Function:

$$\hat{U}(\delta t) = e^{-i\hat{H}\delta t} = e^{-i\hat{T}(x)\delta t}e^{-i\hat{V}(x)\delta t} + O(\delta t^2).$$

$e^{-i\hat{V}\delta t}$:Diagonal in Position Representation

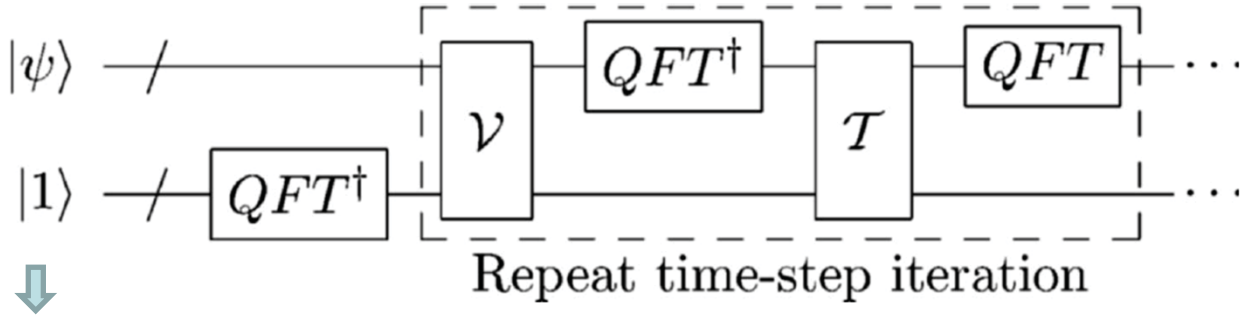
$e^{-i\hat{T}\delta t}$:Diagonal in Momentum Representation

Transformation between two Representations

- **Quantum Fourier Transform:**

$$|\psi(\delta t)\rangle = \hat{U}(\delta t)|\psi(0)\rangle \approx \mathrm{QFT} e^{-iT(p)\delta t} \mathrm{QFT}^{\dagger}\, e^{-iV(x)\delta t}|\psi(0)\rangle.$$

- **Network:**



Ancilla Register

$|0\ldots001\rangle$

$$\mathcal{V}\left(|\psi\rangle \otimes \sum_{y=0}^{M-1} \frac{e^{2\pi i y/M}}{\sqrt{M}}|y\rangle\right) = e^{-i\hat{V}\delta t}|\psi\rangle \otimes \sum_{y=0}^{M-1} \frac{e^{2\pi i y/M}}{\sqrt{M}}|y\rangle$$

I. Kassal et. al., PNAS 105, 18681 (2008)

- Simulation of Hydrogen Molecular Energy
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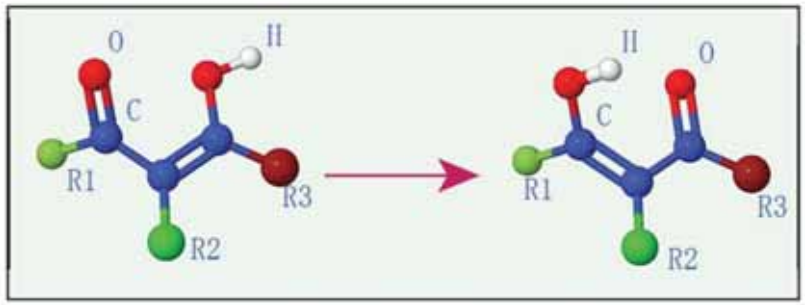
Example: Hydrogen Transfer

- **A Kind of isomerization reactions**

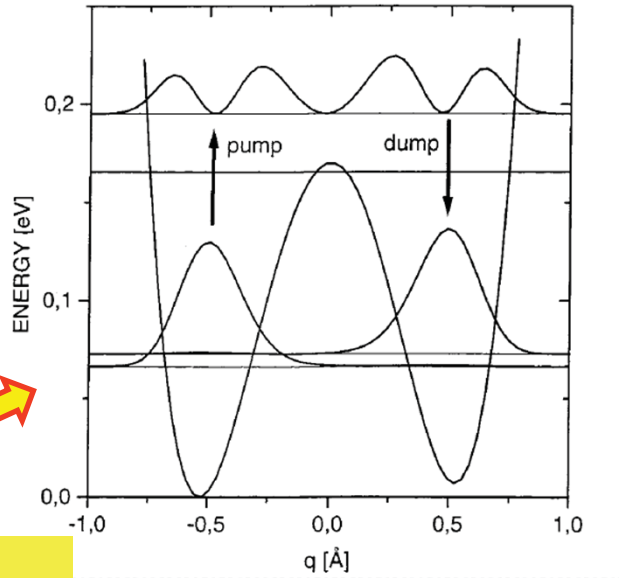


Only one degree of dynamical freedom is in this reaction

$$\hat{H}(t) = \hat{T} + \hat{V}$$

$$\begin{cases} \hat{T} = \hat{p}^2/2m \\ V(q) = \dfrac{\Delta}{2q_0}(q - q_0) + \dfrac{V^{\ddagger} - \Delta/2}{q_0^4}(q - q_0)^2(q + q_0)^2 \end{cases}$$

Double Well Potential Energy



N. Doslic et al., J. Phys. Chem. A **102,** 9645 (1998)

The Laser-induced Hydrogen Transfer

➢ The Dipole Electric Field

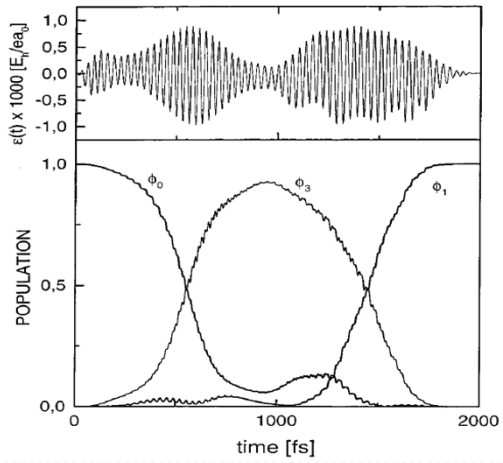
$$\hat{H}(t) = \hat{T} + \hat{V} + \hat{E}(t) \text{ with } \hat{E}(t) = -\hat{\mu}\varepsilon(t) \qquad \hat{\mu} = e\hat{q}$$

to transfer the molecular state from φ_0 to φ_1

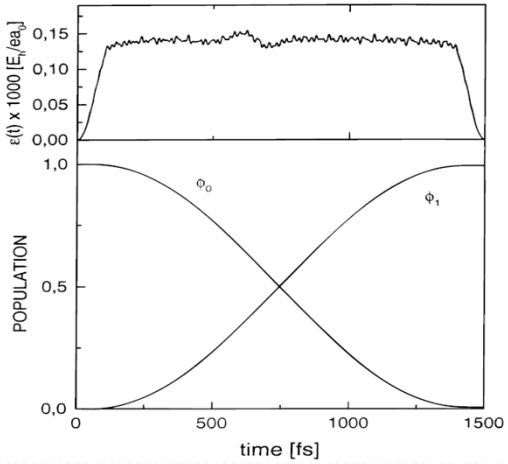
➢ Propagator

$$\hat{U}(t+\delta t, t) \approx e^{-\frac{i}{\hbar}\hat{V}\delta t/2} e^{-\frac{i}{\hbar}\hat{E}(t+\delta t)\delta t/2} e^{-\frac{i}{\hbar}\hat{T}\delta t} \times e^{-\frac{i}{\hbar}\hat{V}\delta t/2} e^{-\frac{i}{\hbar}\hat{E}(t)\delta t/2}.$$

Field 1



Field 2

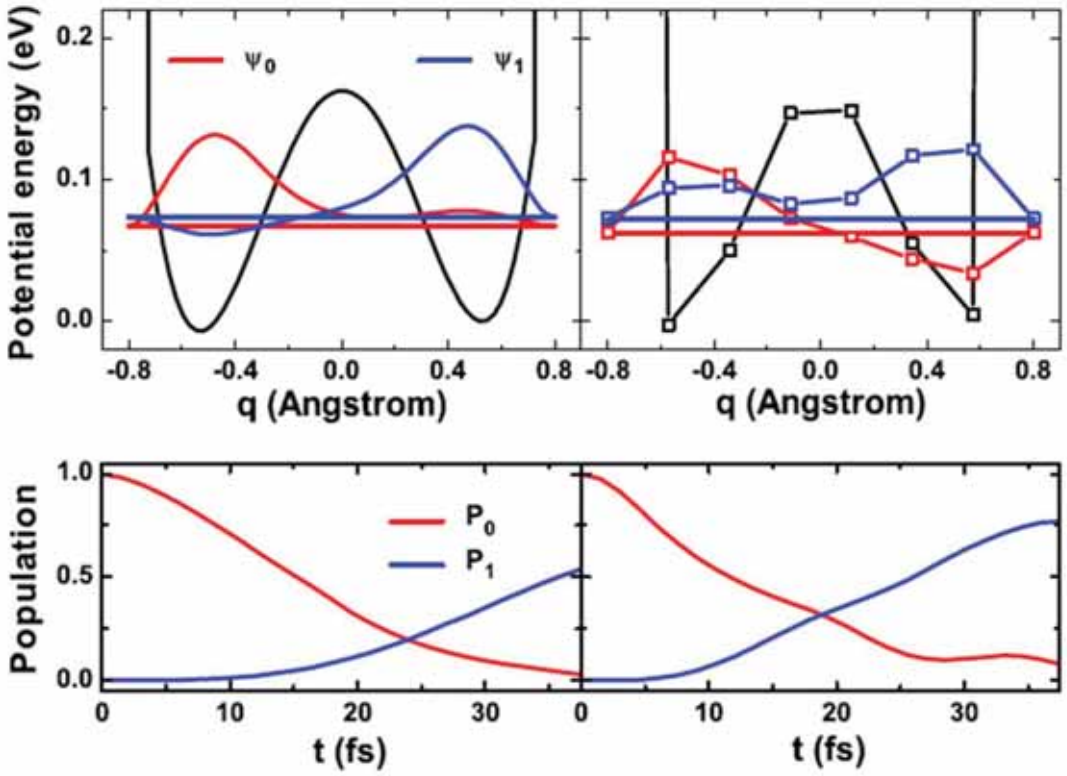


Simulation of The Example (3 Qubits)

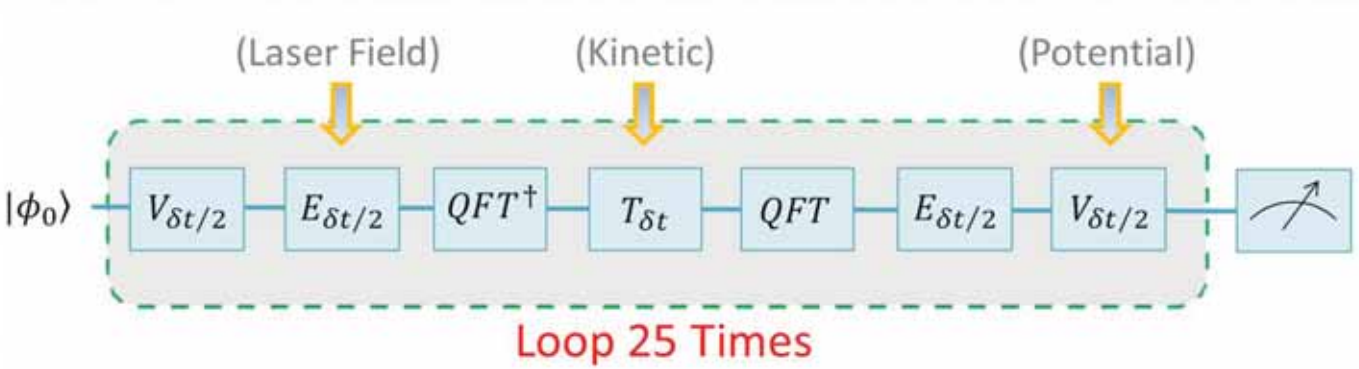
➢ Spatial Wave Function

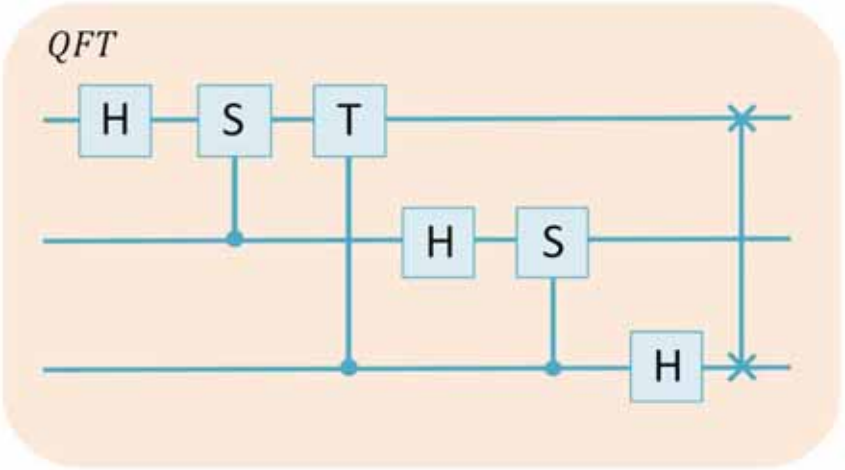
$$|\psi_t\rangle = \sum_{q=0}^{7} m_q(t)\,|q\rangle = m_0(t)\,|000\rangle + \ldots + m_7(t)\,|111\rangle\,.$$

64 points 8 points



Network





S $\begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$

T $\begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$

Parameters of Gates

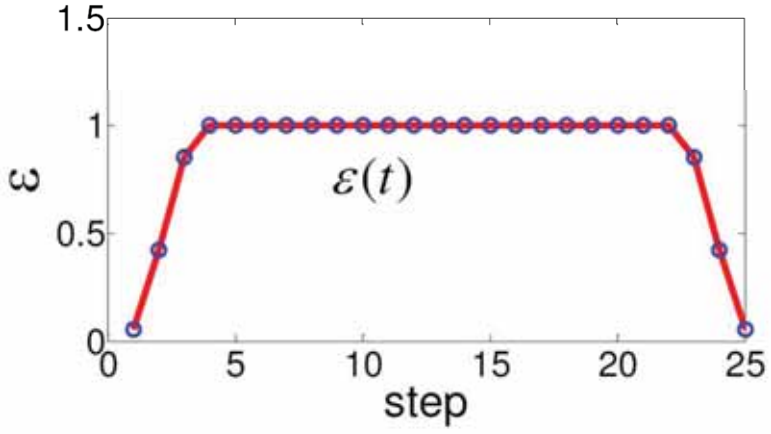
$$V_{\frac{\delta t}{2}} = e^{-i\hat{V}\frac{\delta t}{2}},$$
$$T_{\delta t} = e^{-i\hat{T}\delta t},$$
$$E_{\frac{\delta t}{2}} = e^{i\hat{q}\varepsilon(t)\frac{\delta t}{2}}.$$

$$\hat{V}_{diag} = (293.78, -0.10, 1.85, 5.41, 5.46, 2.02, 0.18, 305.44) * 10^{-3}$$
$$\hat{T}_{diag} = (0, 0.91, 3.63, 8.16, 14.51, 8.16, 3.63, -0.91) * 10^{-3}$$
$$\hat{q}_{diag} = (-1.51, -1.08, -0.65, -0.22, 0.22, 0.65, 1.08, 1.51).$$

$$\varepsilon(t) = \begin{cases} \varepsilon_0 \sin^2(\frac{\pi t}{2t_1}); & 0 \le t \le t_1 \\ \varepsilon_0; & t_1 < t < t_2 \\ \varepsilon_0 \sin^2[\frac{\pi(t_f - t)}{2(t_f - t_2)}]; & t_2 \le t \le t_f \end{cases}$$

$t_1 = 5\,\text{fs}$ and $t_2 = 32.5\,\text{fs}$

$t_f = 37.5\,\text{fs}$ $\quad \delta t = 1.5\,\text{fs}$



- Simulation of Hydrogen Molecular Energy
- **Simulation of Chemical Reaction Dynamics**
  1) How to simulate chemical reactions?
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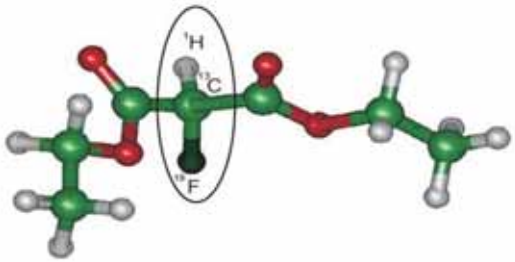
Sample

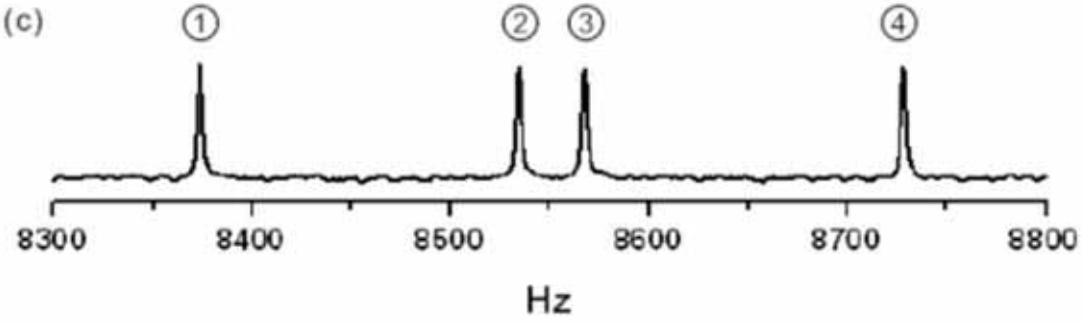
(a)



(b)

	^{1}H	^{13}C	^{19}F	T_1	T_2
^{1}H	400M			2.8	1.2
^{13}C	160.7	100M		2.9	1.1
^{19}F	47.6	−194.4	376M	3.1	1.3

(c)



$$\mathcal{H}_{int} = \sum_{j=1}^{3} 2\pi\nu_j I_z^j + \sum_{j<k,=1}^{3} 2\pi J_{jk} I_z^j I_z^k$$

Initial State Preparation

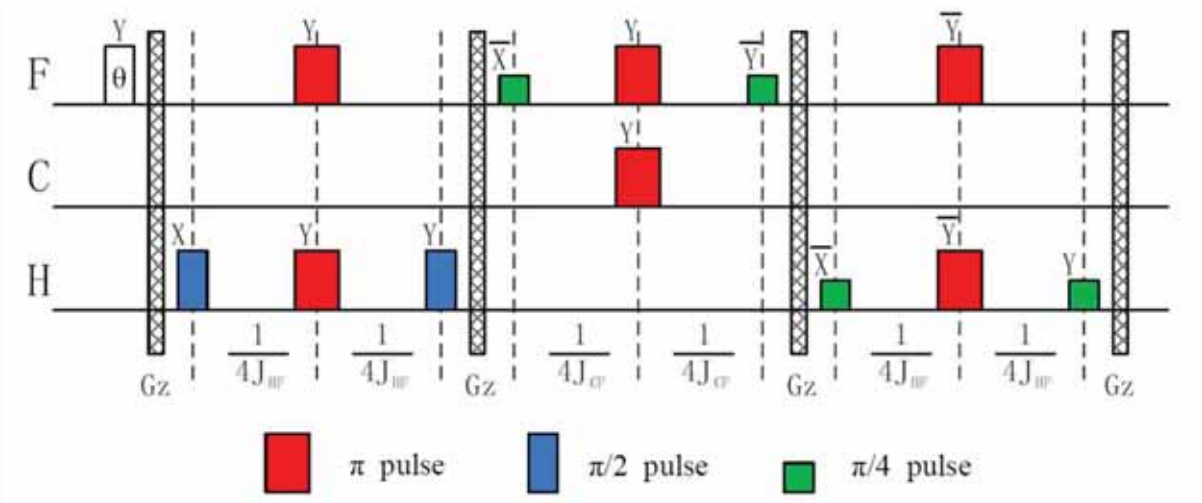
1) Thermal State $\rho = \sum_{i=1}^{3} \gamma_i I_z^i$

Spatial average technique

2) Pseudo-Pure State $\rho_{000} = \frac{1-\epsilon}{8}\mathbb{I} + \epsilon \left|000\right\rangle \left\langle 000\right|$

GRAPE technique

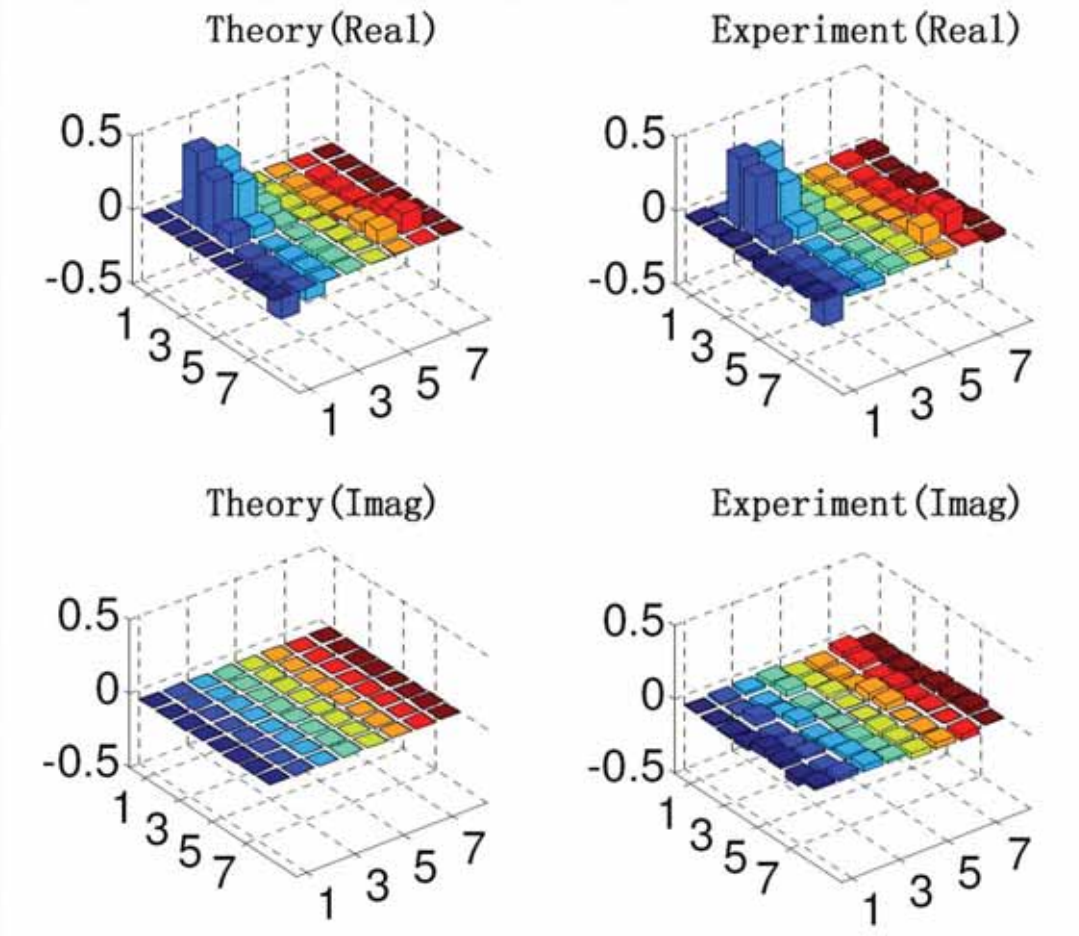
3) Initial State (reactant) $\rho_0 = \left|\phi_0\right\rangle \left\langle \phi_0\right|$



Initial State

Fidelity = 0.95

$$F = \mathrm{Tr}(\rho_{id}\rho_{expt}) / \sqrt{(\mathrm{Tr}(\rho_{id}^2)\mathrm{Tr}(\rho_{expt}^2))}$$



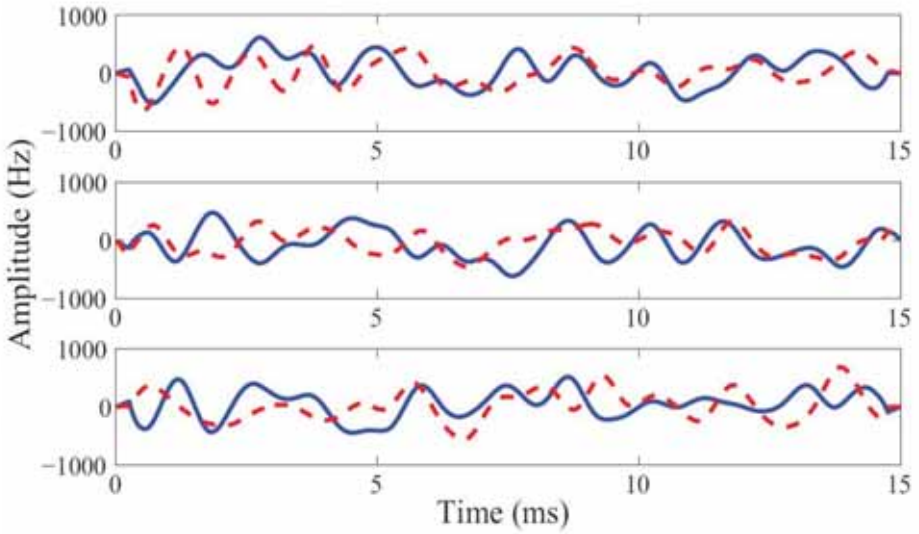
Evolution

U7 Gate: 15ms, 750 Segments, 99%

C channel

H channel

F channel



$$U = \prod_{m=1}^{25} U_m$$

Unitary Evolution

$$U_m = V_{\delta t/2} E_{\delta t/2} U_{QFT} T_{\delta t} U_{QFT}^{\dagger} E_{\delta t/2} V_{\delta t/2}.$$

Measurement

- State tomography after every step to obtain

$C(|\psi_i\rangle,|\phi_0\rangle)$ & $C(|\psi_i\rangle,|\phi_1\rangle)$

- Simplification

$$C(|\psi_i\rangle, |\phi_0\rangle) = \mathrm{Tr}(\rho_i \rho_0)$$

$$\mathrm{Tr}(\rho_i \rho_0) = \mathrm{Tr}(R\rho_i R^\dagger R\rho_0 R^\dagger) = \mathrm{Tr}(\rho_i' \rho_0'),$$

diagonalize the target density matrix — diagonal matrix

Just measure the populations of ρ_i'

Measurement of Loop 7

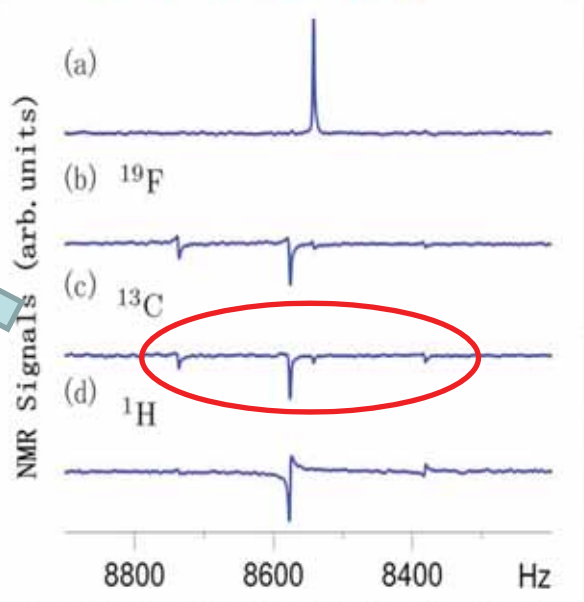
$$C(|\psi_7\rangle, |\phi_0\rangle) = \| \langle \phi_0 | \psi_7 \rangle \|^2 = \mathtt{Tr}(\rho_7 \rho_0),$$

$$\mathtt{Tr}(\rho_7 \rho_0) = \mathtt{Tr}(R \rho_i R^\dagger R \rho_0 R^\dagger) = \mathtt{Tr}(\rho_i' \rho_0').$$

$$\rho_0 = |\phi_0\rangle \langle \phi_0| \quad \rho_7 = |\psi_7\rangle \langle \psi_7|$$

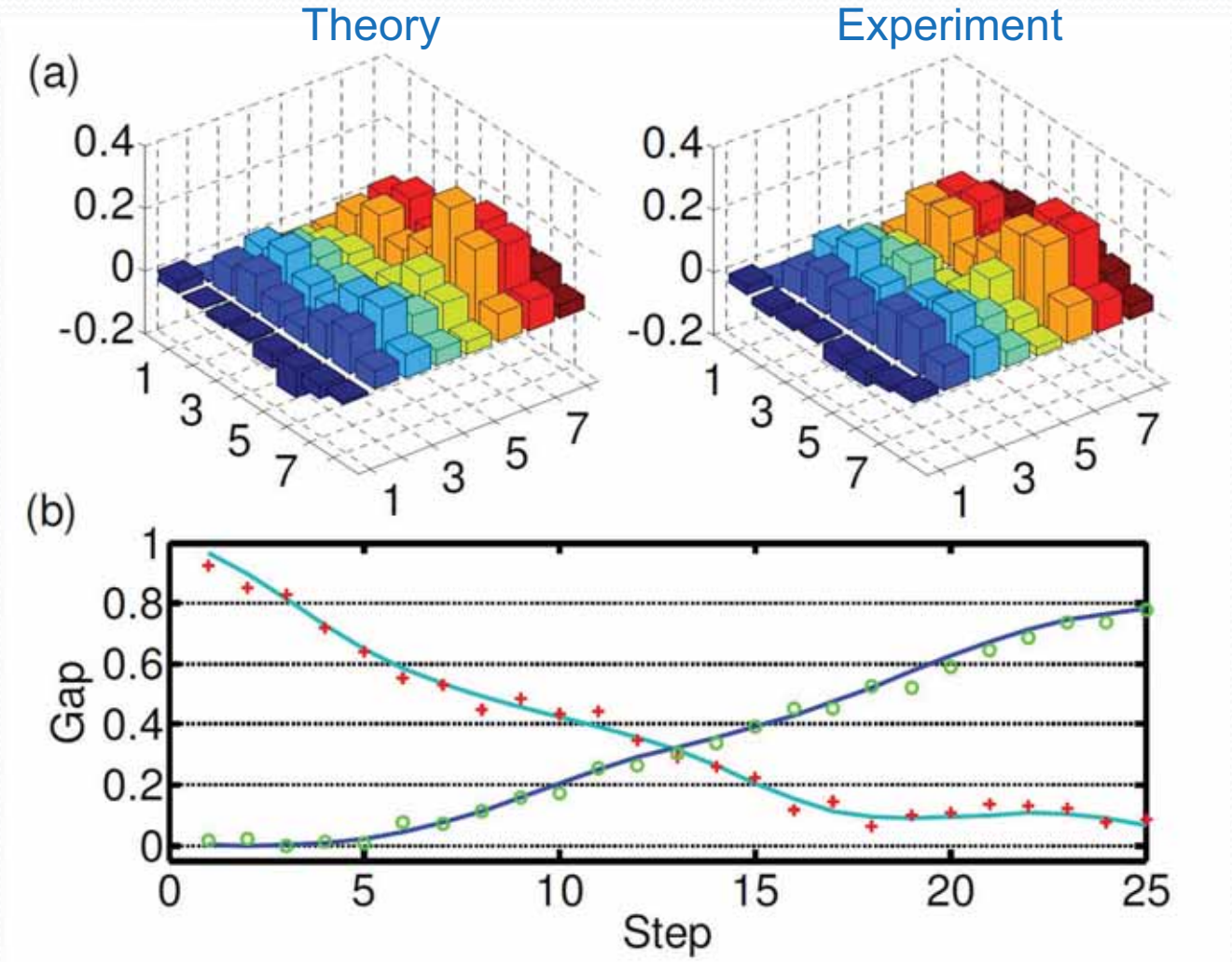
	Theo.	Exp.
P(5)-P(7)	-0.047	-0.098
P(6)-P(8)	-0.501	-0.482
P(1)-P(3)	-0.114	-0.089
P(2)-P(4)	-0.041	-0.071

Applying a $[\pi/2]_y$ Pulse



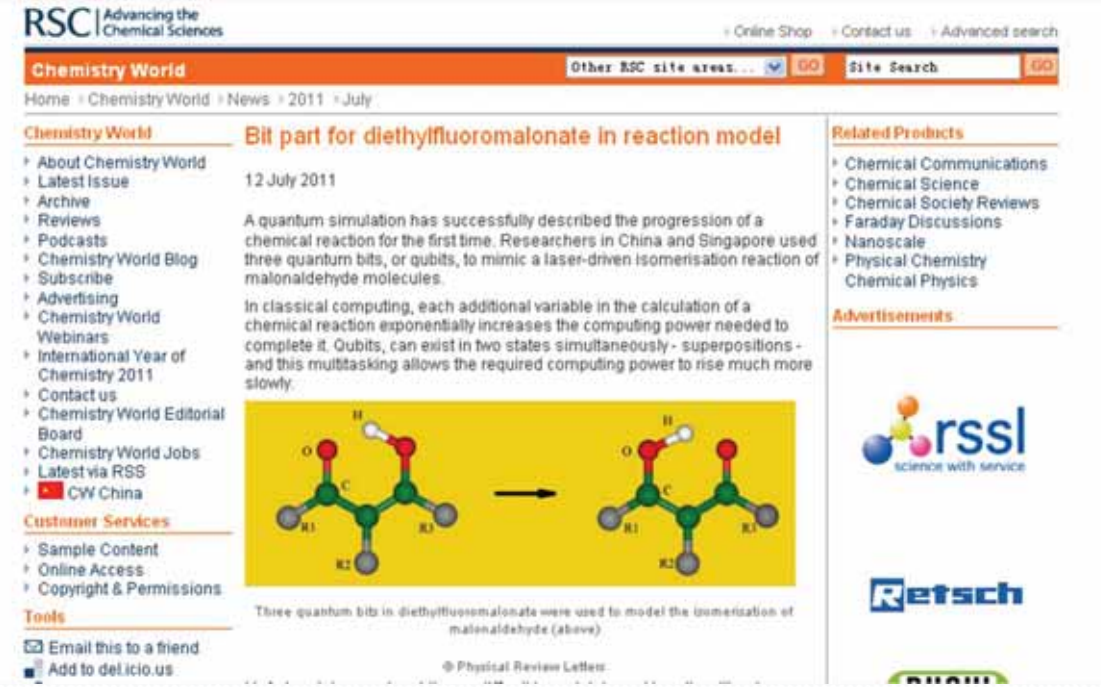
Result

Real Part of the final density matrix (0.957)



Publication

Reported by Royal Society Chemistry



Reviewing articles invited by PCCP Perspective, Phil. Trans. R. Soc. A *et al.*

D. W. Lu et al., Invited by Phys. Chem. Chem. Phys. Perspective, submitted (2011)
D. W. Lu et al., Invited by Phil. Trans. R. Soc. A, submitted (2011).

- Simulation of Hydrogen Molecular Energy
- Simulation of Chemical Reaction Dynamics
- **Simulation of 2-body Heisenberg Hamiltonian**
  1) Simulate a multi-energies Hamiltonian
  2) NMR experimental implementation
     a. Eigenvalues
     b. Ground state information

Theoretical background

In the Simulation of Hydrogen Molecular Energy,

the system qubit is prepared to ground-state.

- What should we do if this is hard to do?
- What will happen if there are more than one eigenvalues belong to the Hamiltonian been simulated?
- If the initial state is not ground state (e.g. superposition state), can we also use Phase Estimation Algorithm?
- Furthermore, if we had obtained the eigenvalues of the Hamiltonian, can we prepare the ground state by using them?

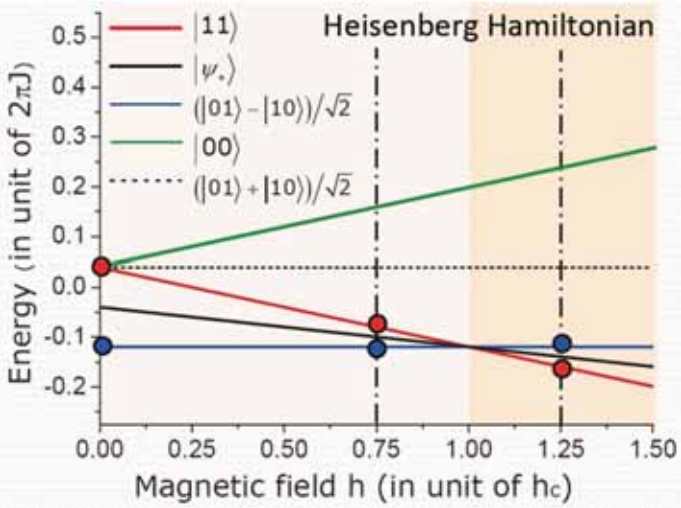
Theoretical background

- **Ground-state problem of a certain Hamiltonian H**
  - **Important in physics, chemistry, ...**
  - **Computationally hard problems**

- **Heisenberg Hamiltonian with magnetic field**

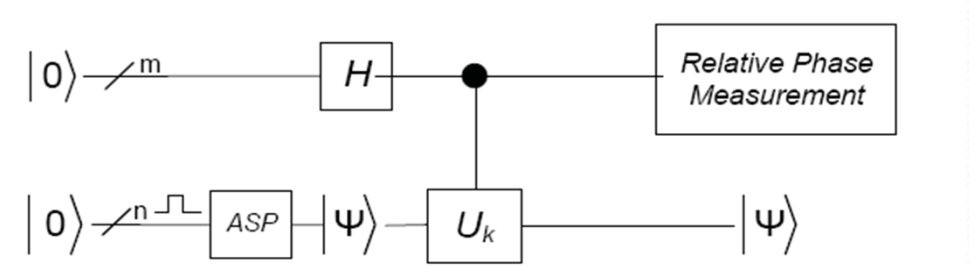
$$H = J\left(I_x^a I_x^b + I_y^a I_y^b + I_z^a I_z^b\right) + h\left(I_z^a + I_z^b\right)$$

- **Multiple eigen-energies.**
- **Ground-state is hard to prepare in some cases.**
- **Ground-state information needed.**



Difference with "Hydrogen Molecular" case

- In Hydrogen Molecular (when system qubit is on **eigenstate**)



$$|\psi_e\rangle \otimes (|0\rangle + |1\rangle)_{probe} \xrightarrow{e^{-iHt}} \Rightarrow |\psi_e\rangle \otimes (|0\rangle + e^{iE_0 t}|1\rangle)_{probe}$$

- What about **superposition state?**

$$|\Psi_{initial}\rangle = \sum_i A_i |\psi_i\rangle$$

- Final state will be:

$$\rho_{probe} = \frac{1}{2}\begin{bmatrix} 1 & \sum_i |A_i|^2 e^{iE_i t} \\ \sum_i |A_i|^2 e^{-iE_i t} & 1 \end{bmatrix}$$

Solution

➢ Simulation of Hydrogen Molecular Energy

Final state:

$$|0\rangle + e^{iE_0 t}|1\rangle$$

Detect the phase $\varphi_0 = E_0 t$

$$E_0 = \varphi_0 / t$$

➢ Simulation of Heisenberg Hamiltonian

Final state:

$$\sum_i |A_i|^2 e^{iE_i t}$$

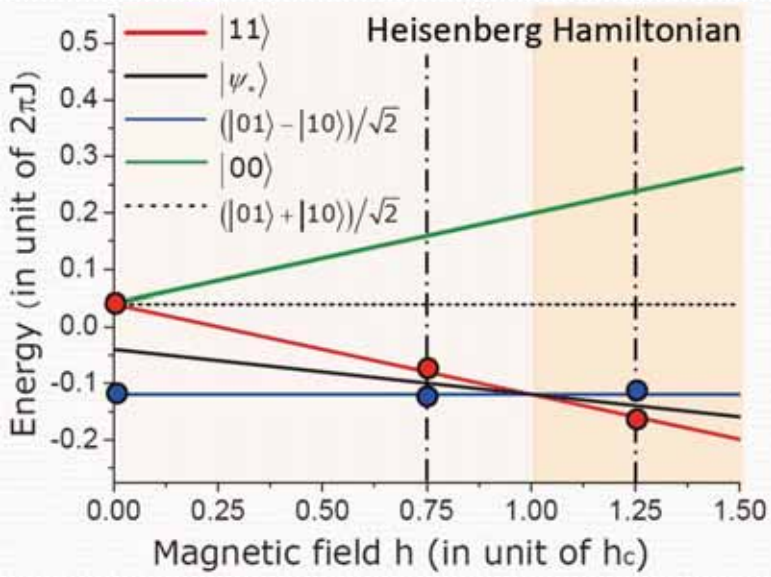
Measure $M(t) = \sum_i |A_i|^2 e^{iE_i t}$

Classical Fourier analysis

Initial state

- **A superposition of two eigenstates:**

$$|\psi_*\rangle = \frac{1}{\sqrt{2}}|\psi_1\rangle + \frac{1}{\sqrt{2}}|\psi_2\rangle$$



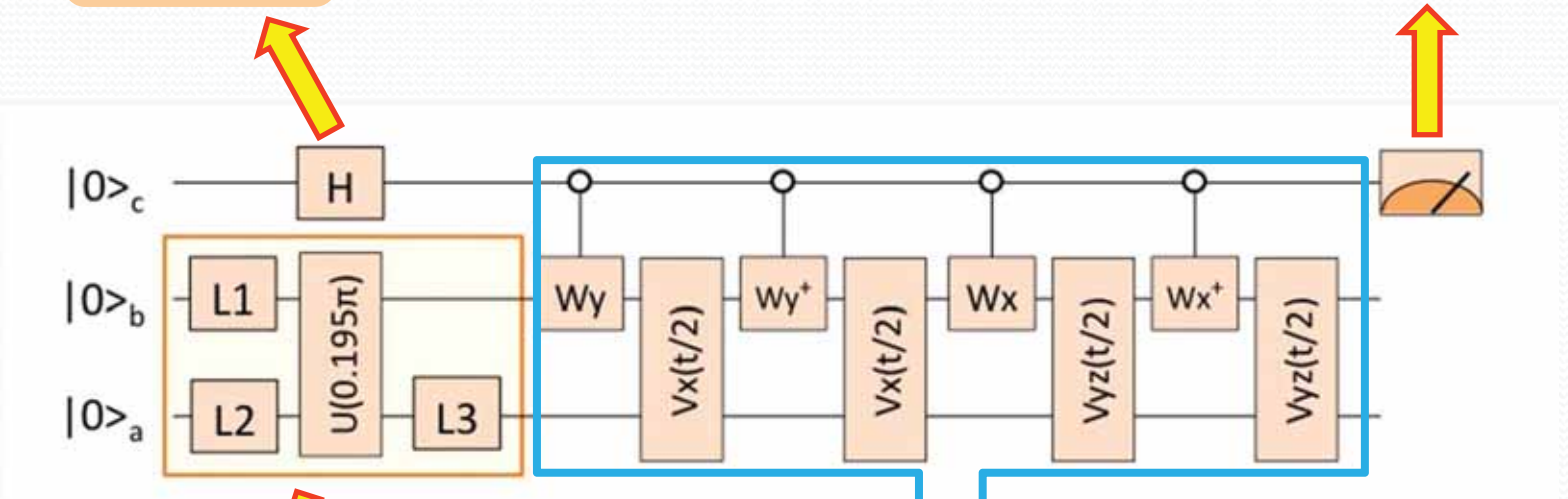
$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) \qquad (|01\rangle - |10\rangle)/\sqrt{2}$$

$$|\psi_2\rangle = |11\rangle \qquad |11\rangle$$

Evolution

$$\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$$

Measure probe qubit



$$|\psi_*\rangle=\frac{1}{\sqrt{2}}|\psi_1\rangle+\frac{1}{\sqrt{2}}|\psi_2\rangle$$

$$controlled-e^{-iHt}$$

H	Hadamard	L2	Rx(-π/2) Ry(π)	Wy	exp(-i π Iy)	Vx(t)	exp(-i J Ix Ix t)
L1	Ry(2π/3)	L3	Ry(0.195π) Rx(π/2)	Wx	exp(-i π Ix)	Vyz(t)	exp[-i J (Iy Iy + Iz Iz) t]

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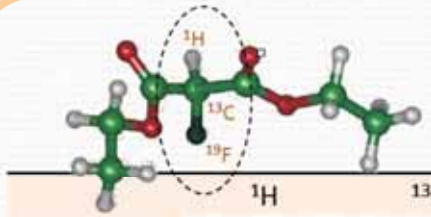
Experimental Implement

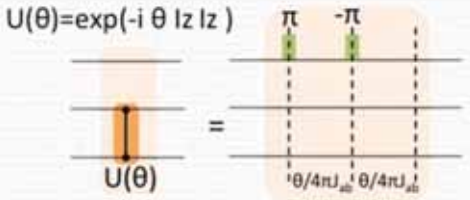
NMR Sample:



Probe Qubit : ^{19}F (qubit c)

^{13}C-labeled Diethyl-fluoromalonate

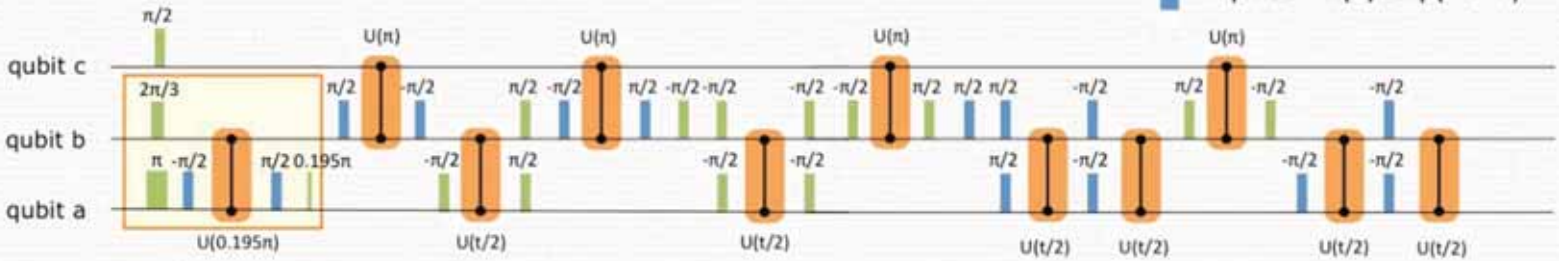
	^{1}H	^{13}C	^{19}F	T1	T2
^{1}H (qubit a)	400 MHz			2.8 s	1.2 s
^{13}C (qubit b)	160.7 Hz	100 MHz		2.9 s	1.1 s
^{19}F (qubit c)	47.6 Hz	-194.4 Hz	376 MHz	3.1 s	1.3 s



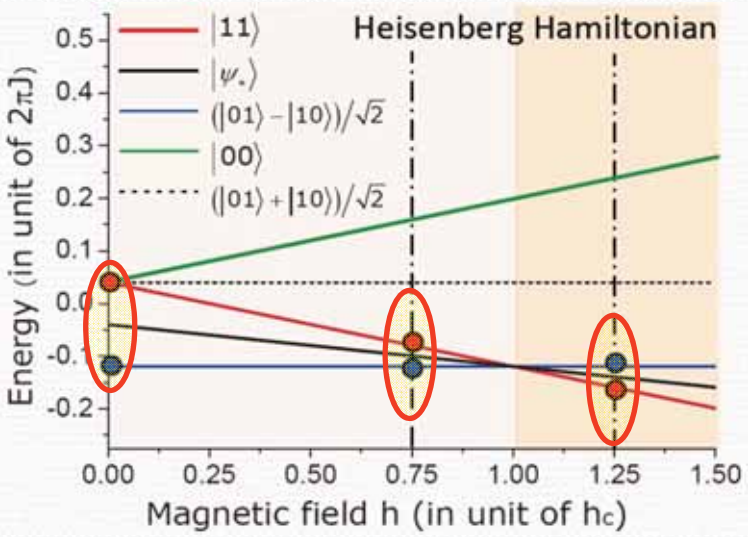
Y-pulse: Ry(θ)=exp(-i θ Iy)

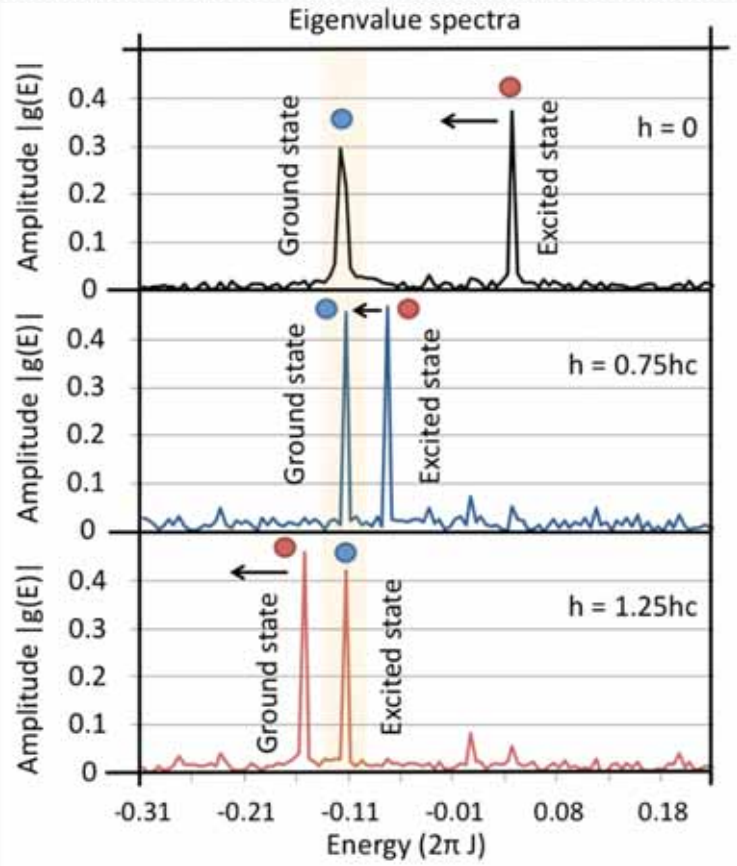
X-pulse: Rx(θ)=exp(-i θ Ix)

NMR pulse program:



Results





Three cases
(different Magnetic field)

iPEA procedure

Use iPEA procedure to improve accuracy

$E_k = 0.x_1 x_2 x_3 \ldots$ x_n : decimal digits

1) A short time evolution

Determine x_1

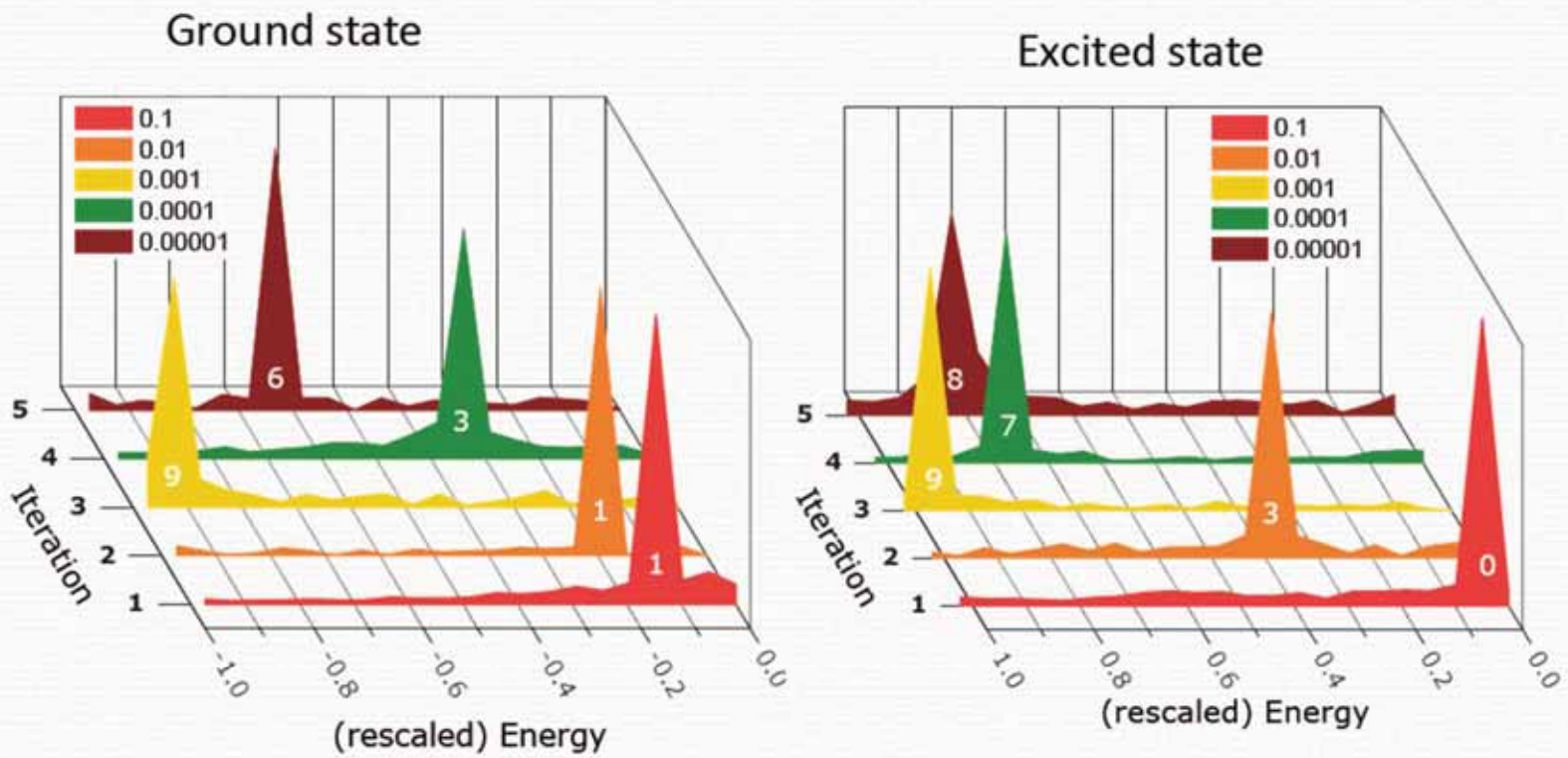
2) Evolution with Ten times longer than previous one

$$E_k(10 \times t) = (10E_k)t = x_1.x_2 x_3 \times t \ldots$$

x_2 is amplified, and can be determined now

3) Repeat this scheme iteratively for x_3 and so on

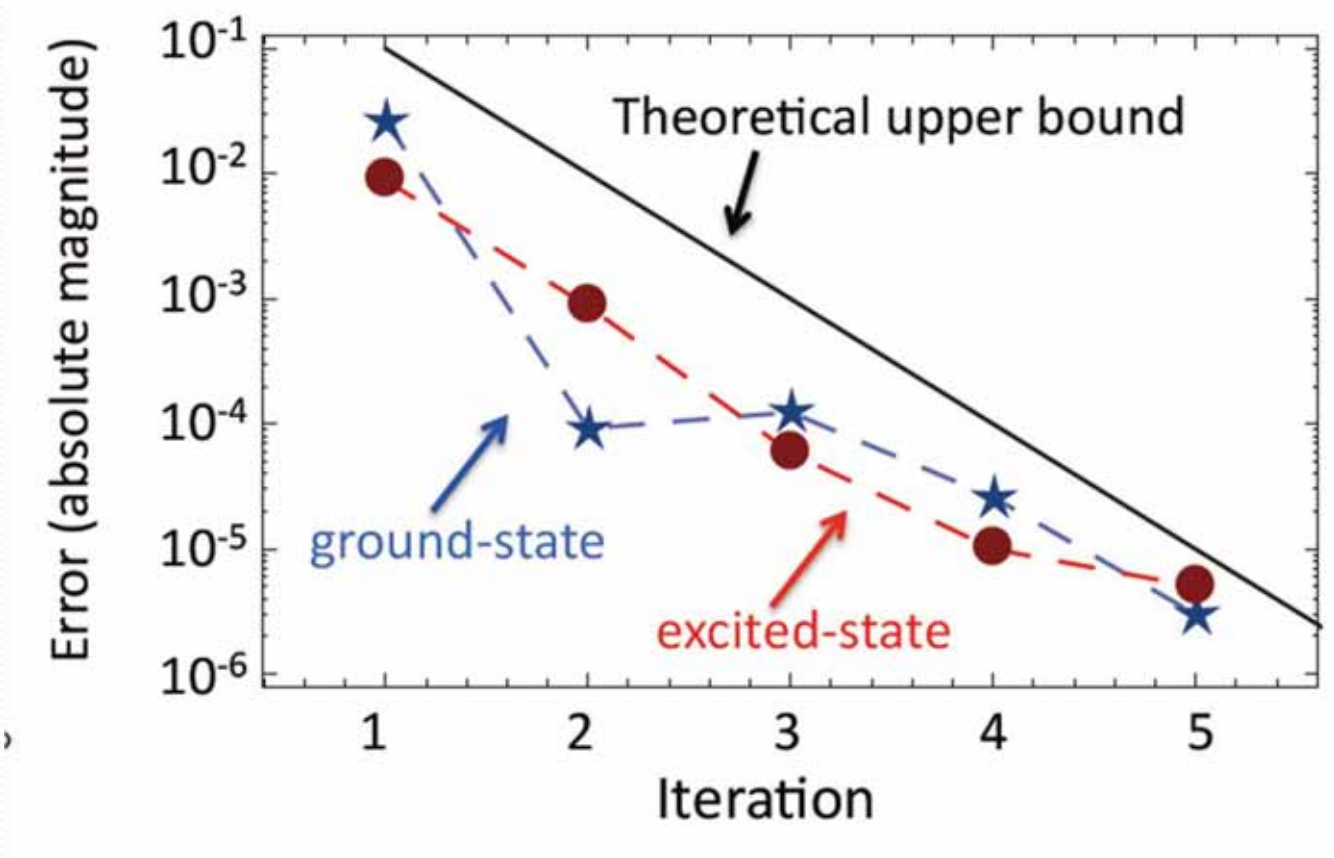
Iterative results (h=0)



Iteration	1	2	3	4	5	Theory
Ground	-0.145937	-0.119458	-0.119242	-0.119340	-0.119363	-0.119366
Excited	0.048645	0. 038916	0.039729	0.039778	0.039782	0.039788

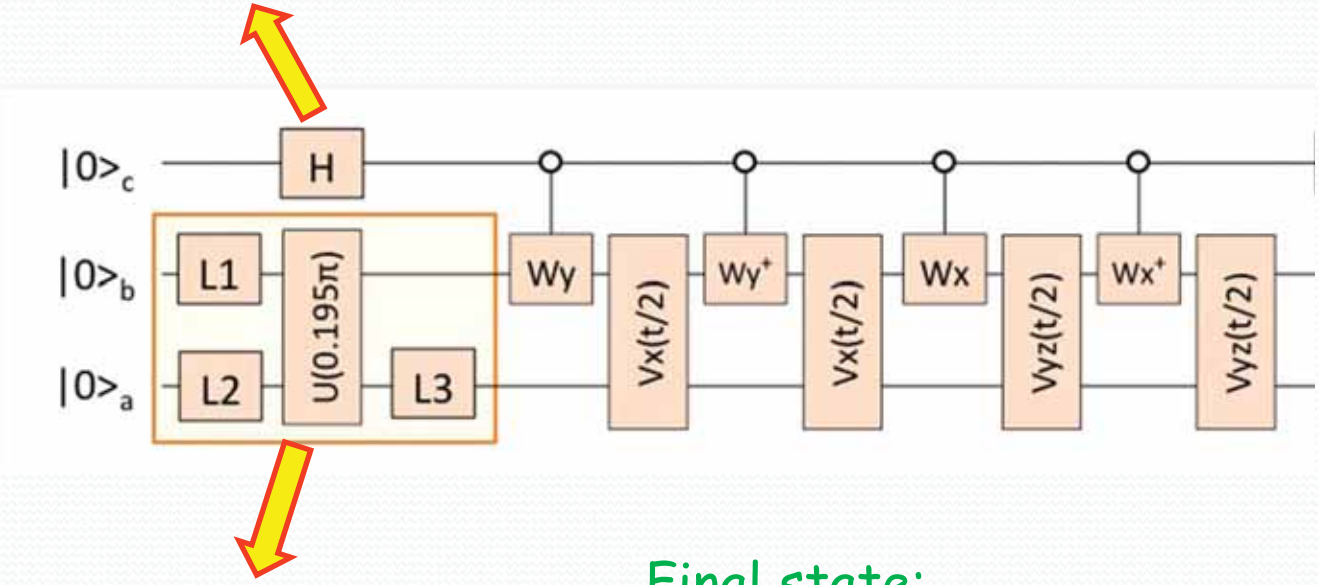
The value of ground-state energy is determined to be -0.11936(3), with a precision of 10^{-5}

Error in each iteration



Obtain ground-state information

Preload a phase : $\frac{1}{\sqrt{2}}\left(|0\rangle + e^{i\phi}|1\rangle\right)$



$$\sum_i A_i |\psi_i\rangle$$

Final state:

$$\sum_i A_i \left(|0\rangle + e^{i\phi - iE_i t}|1\rangle\right) \otimes |\psi_i\rangle$$

Obtain ground-state information

Choose ϕ and t appropriately :

g : ground state
e : exited state

$$\phi - E_g t = 0 \qquad \phi - E_e t = \pi$$

$$\sum_i A_i \left(|0\rangle + e^{i\phi - iE_i t} |1\rangle \right) \otimes |\psi_i\rangle$$

$$\Rightarrow \quad A_g \left(|0\rangle + |1\rangle \right) \otimes |\psi_g\rangle + A_e \left(|0\rangle - |1\rangle \right) \otimes |\psi_e\rangle$$

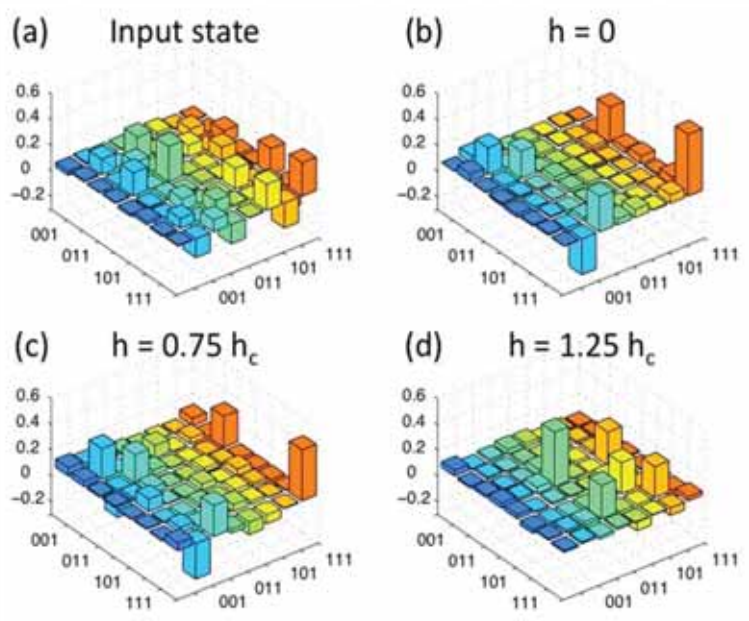
After a Hadamard gate

$$\Rightarrow \quad A_g |0\rangle |\psi_g\rangle + A_e |1\rangle |\psi_e\rangle$$

a) Projection measurement

b) State tomography

Tomography results



Theoretical Prediction:

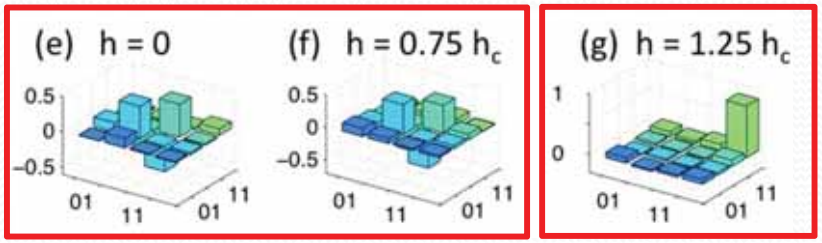
h=0 or h=0.75 hc

$$|\psi_g\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$

h=1.25 hc

$$|\psi_g\rangle = |11\rangle$$

Experimental results:



	(a)	(b)	(c)	(d)	(e)	(f)	(g)
Correlation	0.97	0.90	0.88	0.89	0.92	0.94	0.94

Publication

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Solving Quantum Ground-State Problems with Nuclear Magnetic Resonance

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Thank you !

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