



Quantum Simulation with Nuclear Spins

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Outline:

- 1. Introduction**
- 2. Quantum Digital Simulation Of Tunelling**
- 3. Nonadiabatic Holonomic Quantum Computing**
- 4. Superfast Evolution In 'PT' Systems**
- 5. Summary**

Quantum computer was proposed from two fronts:

1.The need to reduce heat dissipation---
Benioff 1980

2.The need to simulate quantum systems

Quantum Computer can Solve certain important mathematical problems

Factorization problem, Shor (1994).

Classical Computer: exponential in N
Quantum Comput: polynomial in N



P. Shor, in *Proceedings of the 35th Annual Symposium on the Foundations of Computer Science*, edited by S. Goldwasser ~IEEE Computer Society, Los Alamitos, 1994!, p. 124.

Experimental demonstration:

L. M. K. Vandersypen *et al.*, *Nature*, **414**, 883 (2001).

Search problem, Grover (1995).

Classical computer: $O(N)$

Quantum Comput: $O(\sqrt{N})$

L. K. Grover, Phys. Rev. Lett. **79**, 325 (1997).

Experimental demonstration:

J.A. Jones et al., Nature 393 (1998) 344.

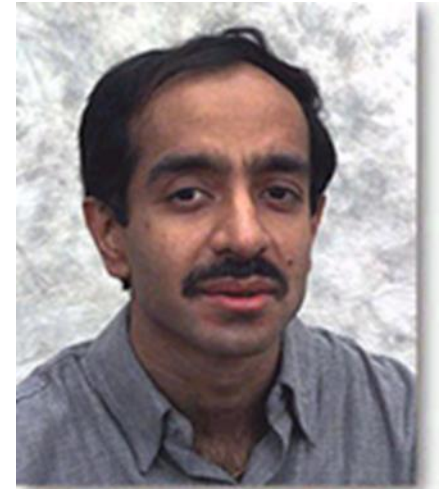
I.L. Chuang et al., Phys. Rev. Lett. 80 (1998) 3408.

Improved Grover Algorithm

G L Long, Phys. Rev. A64 (2001) 022307

Experimental demonstration:

Spreeuw et al., **Phys. Rev. Lett.** 88 (2002) 137901



Quantum Simulations

- **Quantum simulation—use a quantum system that is easy to control to simulate dynamical properties of another that is difficult to control or unknown.**

- **Two kinds of quantum simulations: *digital vs analog*.**

Analog: The hamiltonians are similar

Digital: No special requirement, just a universal quantum computer

- **QS has attracted much interests in recent years:**

Quantum many-body physics

C. Negrevergneet al., Phys. Rev. A 71, 032344 (2005).

J. Zhang, T.-C. Wei and R. Laflamme, Phys. Rev.Lett. 107, 010501 (2011).

Chemical reactions

D. W. Lu et al., Phys. Rev. Lett. 107, 020501 (2011).

2. Digital Quantum Simulation of Tunneling

G.R. Feng, Y. Lu, L. Hao, F.H. Zhang, and G.L. Long,
Scientific Reports 3, 2232 (2013).

The digital simulation algorithm

- In Schrödinger picture, the evolution of the wave function with time

$$|\psi(x, t + \Delta t)\rangle = e^{-i[\frac{\hat{P}^2}{2m} + V(\hat{X})]\Delta t} |\psi(x, t)\rangle ,$$

C. Zalka, Proc. Roy. Soc. Lond. A. 1998, 454, 313-322 1998
A. T. Sornborger, 1202.15036

Discretizing time

- Using Trotter Formula

$$e^{t(\hat{A}+\hat{B})} = e^{t\hat{A}}e^{t\hat{B}} + O(t^2)$$

$$|\psi(x, t + \Delta t)\rangle = e^{-i[\frac{\hat{P}^2}{2m} + V(\hat{X})]\Delta t} |\psi(x, t)\rangle,$$



$$|\psi(x, t + \Delta t)\rangle = \left[e^{-i\frac{\hat{P}^2}{2m}\Delta t} e^{-iV(\hat{X})\Delta t} + O(\Delta t^2) \right] |\psi(x, t)\rangle$$

Discretizing coordinate degree

- Suppose $\psi(x, t)$ is the wave function, and it is continuous on the region $0 < x < L$, with a periodic boundary condition $\psi(x + L, t) = \psi(x, t)$.
- x is discretized into a lattice with spacing Δl and the wave function is stored in an n -qubit quantum register:

$$|\psi(x, t)\rangle \rightarrow \sum_{k=0}^{2^n-1} \psi(x_k, t) |k\rangle, \quad x_k = k\Delta l, \quad \Delta l = \frac{L}{2^n}$$

- The 2-qubit simulation:

$$|k\rangle: |00\rangle, |01\rangle, |10\rangle \text{ and } |11\rangle \quad |k\rangle \equiv |k \Delta l\rangle$$

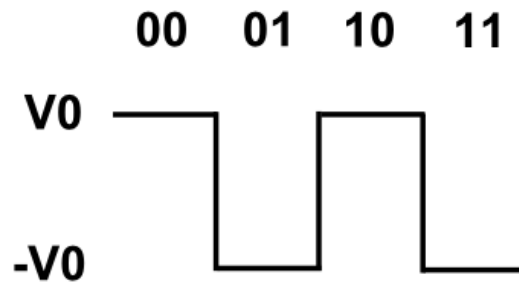
Discretizing the potential operator $V(\hat{X})$

- Because the potential operator $V(\hat{X})$ is a function of the coordinate operator \hat{X} , it is diagonal in the coordinate representation.
- In a n-qubit discretized grid, $V(\hat{X})$ can be decomposed as:

$$V = \sum_{i_1, i_2, \dots, i_n=3}^4 c_{i_1 i_2 \dots i_n} \otimes_{k=1}^n \sigma_{i_k}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \text{ and } \sigma_4 = I$$

Discretizing the potential operator $V(\hat{X})$

- In a 2-qubit system $V = V_0 I \otimes \sigma_z$, corresponds to a double well potential of amplitude V_0



- This double-well potential can be implemented using only a single qubit gate

$$Q = e^{-iV(\hat{X})\Delta t} = I \otimes e^{-iV_0\sigma_z\Delta t}$$

Discretizing momentum degree

- In the momentum representation, the eigen state $|j\rangle$ of the momentum operator \hat{P}_p can be expressed using the eigen states $|k\rangle$ of \hat{X} in the coordinate representation.

$$|j\rangle = \frac{1}{2^n} \sum_{k=0}^{2^n-1} e^{-\frac{2\pi}{2^n} i\pi jk} |k\rangle, j = 0, 1, \dots, 2^n - 1.$$

- This is obtained with the help of quantum Fourier transformation (QFT)

Discretizing momentum degree

- The eigen values of momentum

$$p_j = \begin{cases} \frac{2\pi}{2^n} j & 0 \leq j \leq 2^{n-1} \\ \frac{2\pi}{2^n} (2^{n-1} - j) & 2^{n-1} < j < 2^n \end{cases}$$

Discretizing momentum degree

- In the momentum representation, the \hat{P}_p operator is diagonal

$$\hat{P}_p = \sum_{j=0}^{2^n-1} \frac{2\pi}{2^n} j |j\rangle \langle j| + \sum_{j=2^{n-1}+1}^{2^n-1} \frac{2\pi}{2^n} (2^{n-1} - j) |j\rangle \langle j|$$

- For a 2-qubit simulation:

$$\hat{P}_p = \frac{2\pi}{4} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Discretizing momentum degree

- The kinetic energy operator can be obtained via QFT

$$\frac{\hat{P}^2}{2m} = \mathbf{F}^{-1} \frac{\hat{P}_p^2}{2m} \mathbf{F} = \mathbf{F}^{-1} \frac{\pi^2}{4} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \mathbf{F}$$

- Here we have taken $m=1/2$, \mathbf{F} is the discrete QFT operator.

$$e^{-i \frac{\hat{P}^2}{2m} \Delta t} = \mathbf{F}^{-1} e^{-i \frac{\hat{P}_p^2}{2m} \Delta t} \mathbf{F}$$

Realization of Quantum Fourier Transform

- F (qubits exchanged) can be implemented in quantum circuits via

$$F = H_2 R_{\frac{\pi}{2}} H_1$$

- H_1 and H_2 are Hadamard gates on the first and second qubits. $R_{\frac{\pi}{2}} = \text{diag} [1, 1, 1, i]$ is the controlled phase gate.

The Discretized Schrödinger Eq.

- The kinetic evolution operator

$$\begin{aligned}
 e^{-i\frac{\hat{P}^2}{2m}\Delta t} &= F^{-1} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} e^{-i\frac{\hat{P}_p^2}{2m}\Delta t} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} F \\
 &= F^{-1}\Phi_\pi Z_1 Z_2 F
 \end{aligned}$$

Here $\Phi_\pi = \exp[-i\frac{3\pi^2}{4} R_\pi \Delta t]$, $Z_1 = \exp[i\frac{\pi^2}{4} \sigma_z \otimes I \Delta t]$,

$$Z_2 = \exp[i\frac{3\pi^2}{4} I \otimes \sigma_z \Delta t]$$

- The potential evolution operator

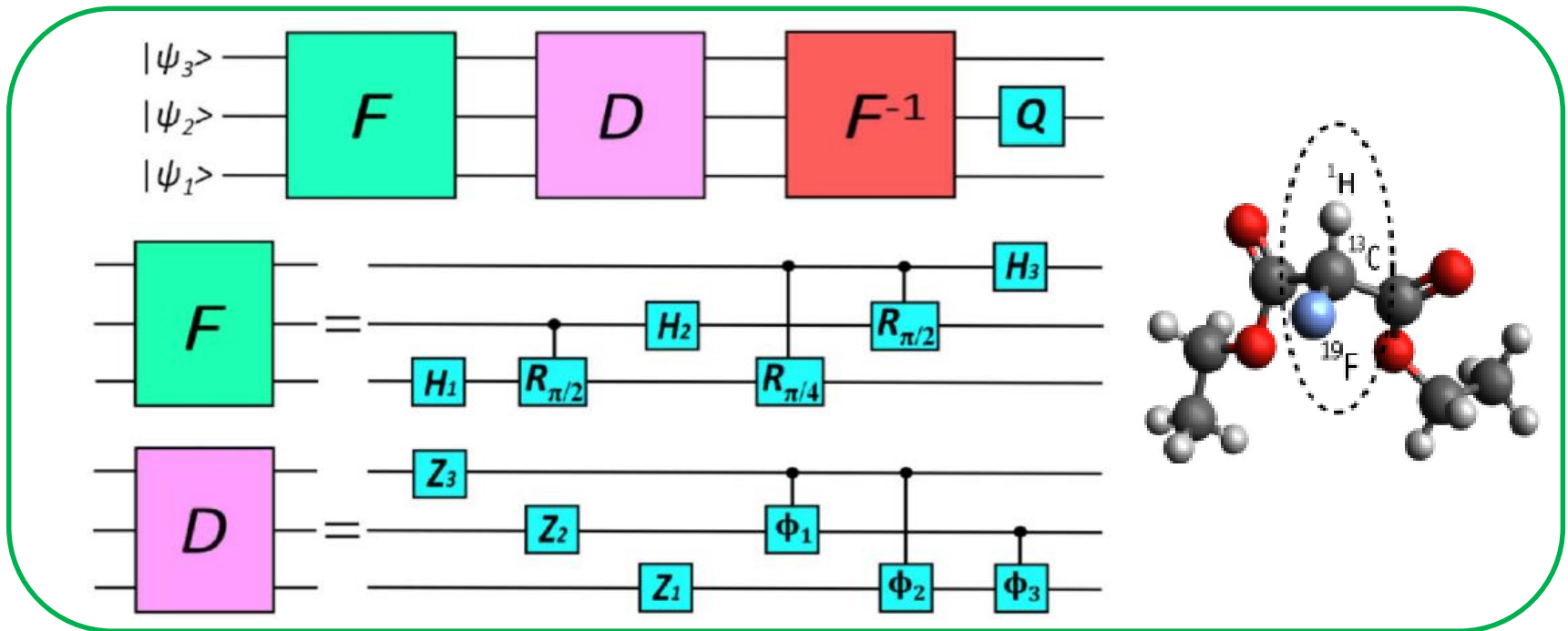
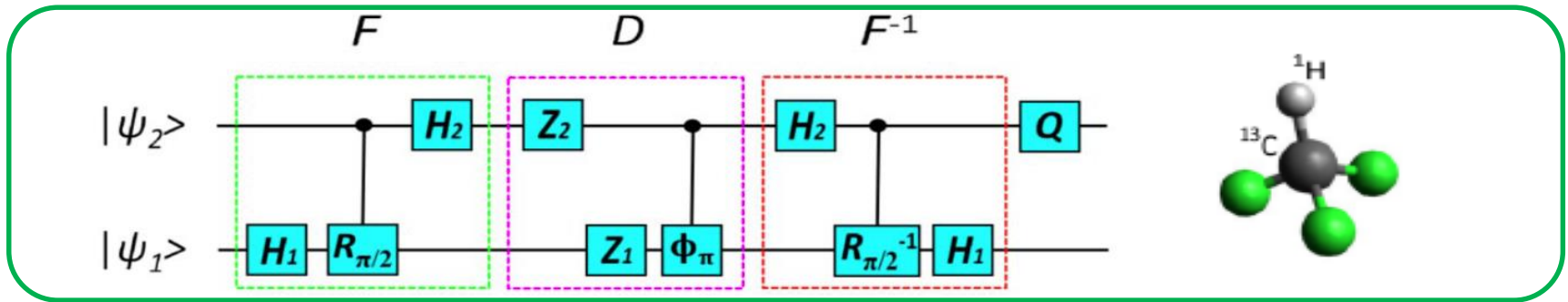
$$e^{-iV(\hat{X})\Delta t} = I \otimes e^{-iV_0\sigma_z\Delta t} = Q$$

The Discretized Schrödinger Eq.

- The time-dependent Schrödinger Eq. can be rewritten as:

$$\sum_{k=0}^3 \psi(x_k, t + \Delta t) |k\rangle = F^{-1} \Phi_{\pi} Z_1 Z_2 F Q \sum_{k=0}^3 \psi(x_k, t) |k\rangle$$

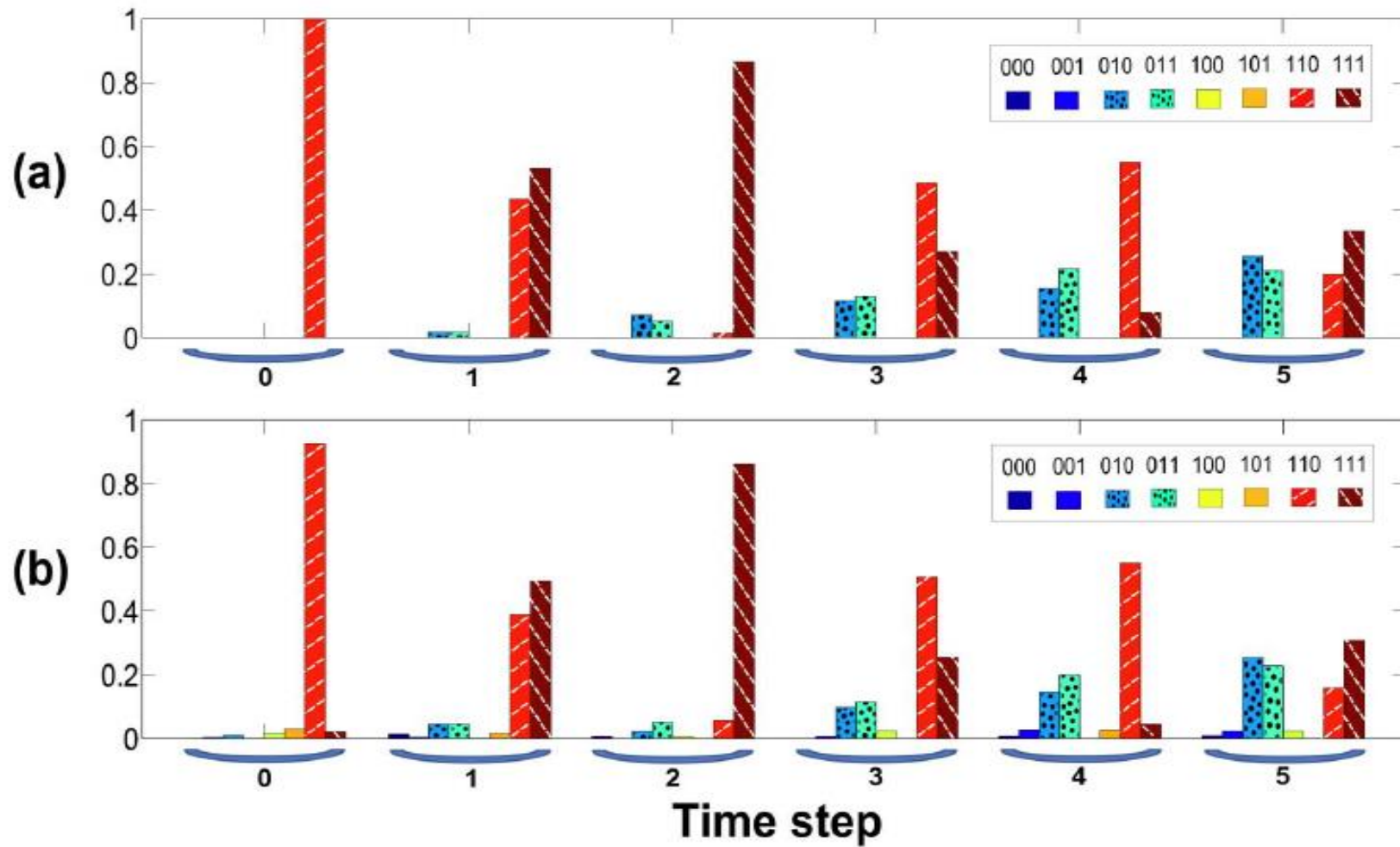
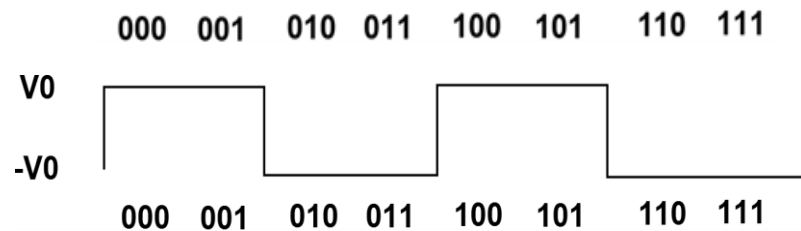
Circuits for QS of Tunneling



D : evolution of kinetic energy in k-rep, F : QFT, Q : evolution with potential.

G.R. Feng, Y. Lu, L. Hao, F.H. Zhang, and G.L. Long, Scientific Reports 3, 2232 (2013).

Experiment with 3-qubits



That should open the floodgates for more digital quantum simulations in future. It's significant because this approach has the potential to simulate much more complex quantum phenomenon than is currently possible

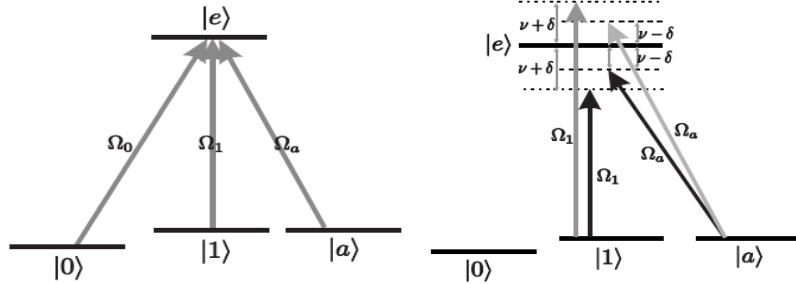
quantum computers. Such a demonstration would be the first example of a digital quantum simulation.

And today Guan Ru Feng and pals at Tsinghua University in Beijing say they've done it. To simulate tunnelling, these guys used a quantum computer that relies on nuclear magnetic resonance to manipulate qubits in encoded in the carbon and hydrogen atoms that make up chloroform molecules. They say this is the first demonstration of a quantum tunnelling simulation using an NMR quantum computer.

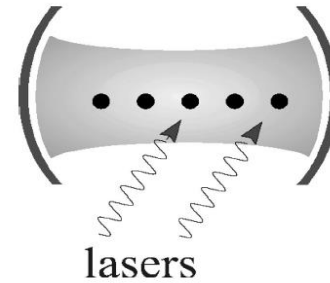
3. Nonadiabatic Holonomic Quantum Computation

G. R. Feng, G. F. Xu, and G. L. Long, Phys. Rev. Lett. 110, 190501 (2013).

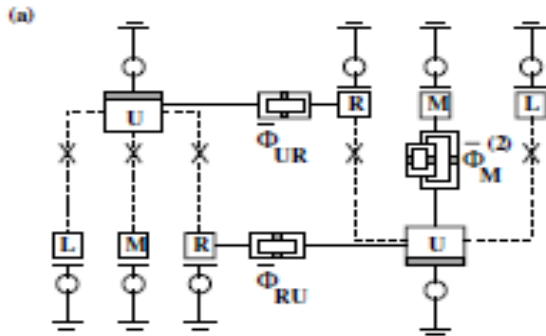
HQC proposals



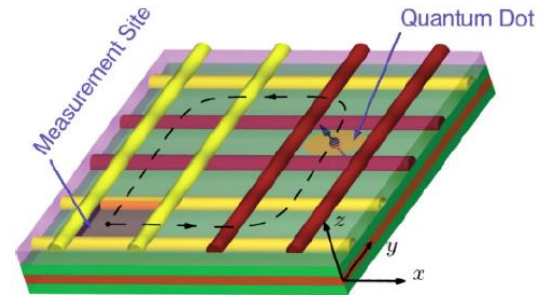
L. M. Duan et al., Science 292, 1695 (2001).
(离子阱系统)



A. Recati et al., Phys. Rev. A 66, 032309 (2002).
(原子-微腔系统)



L. Faoro et al., Phys. Rev. Lett. 90, 028301 (2003).
(超导比特系统)



Vitaly N. Golovach et al., Phys. Rev. A 81, 022315 (2010).
(量子点系统)

L.-A. Wu, P. Zanardi, and D. A. Lidar, Phys. Rev. Lett. 95, 130501 (2005).

X. D. Zhang, Phys. Rev. A 74, 034302 (2006).



AHQC & DFS
combined

- **NHQC: subspace spanned by $\{|\phi_k(0)\rangle\}_{k=1}^L$ $\{|\phi_k(t)\rangle\}_{k=1}^L$, satisfying**

$$(i) \quad \sum_{k=1}^L |\phi_k(\tau)\rangle\langle\phi_k(\tau)| = \sum_{k=1}^L |\phi_k(0)\rangle\langle\phi_k(0)|, \quad (1)$$

$$(ii) \quad \langle\phi_k(t)|H(t)|\phi_l(t)\rangle = 0, \quad k, l = 1, \dots, L. \quad (2)$$

After cycle τ , the evolution $U(\tau)$ is a holonomy matrix

[1] E. Sjöqvist et al., New Journal of Physics 14, 103035 (2012). [2] G. F. Xu et al., Phys. Rev. Lett. 109, 170501 (2012).



Reduce dec

Nonadiabatically



Theoretical protocol

- One-qubit NHQC gates: $|0\rangle_L = |10\rangle$ $|1\rangle_L = |11\rangle$
- In the basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$

$$H_1(\phi_1) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & e^{i\frac{\phi_1}{2}} & -e^{-i\frac{\phi_1}{2}} \\ 0 & e^{-i\frac{\phi_1}{2}} & 0 & 0 \\ 0 & -e^{i\frac{\phi_1}{2}} & 0 & 0 \end{pmatrix}$$

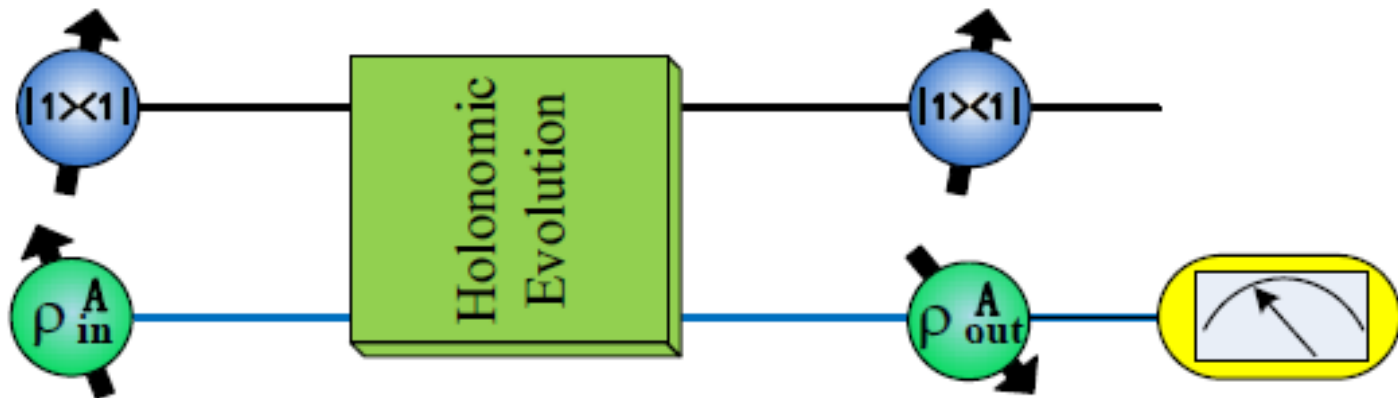
$$= \frac{1}{2}(a(X_1X_2 + Y_1Y_2) + b(X_1Y_2 - Y_1X_2) - aX_1(I_2 - Z_2) - bY_1(I_2 - Z_2))$$

$$a_1 = J_1 \cos(\phi_1/2) \quad b_1 = J_1 \sin(\phi_1/2)$$



$$H_2(\phi_2) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i \sin \frac{\phi_2}{2} & -\cos \frac{\phi_2}{2} \\ 0 & i \sin \frac{\phi_2}{2} & 0 & 0 \\ 0 & -\cos \frac{\phi_2}{2} & 0 & 0 \end{pmatrix}$$
$$= \frac{1}{2}(a_2(Y_1X_2 - X_1Y_2) - b_2X_1(I_2 - Z_2)),$$

$$a_2 = J_2 \sin(\phi_2/2) \quad b_2 = J_2 \cos(\phi_2/2)$$



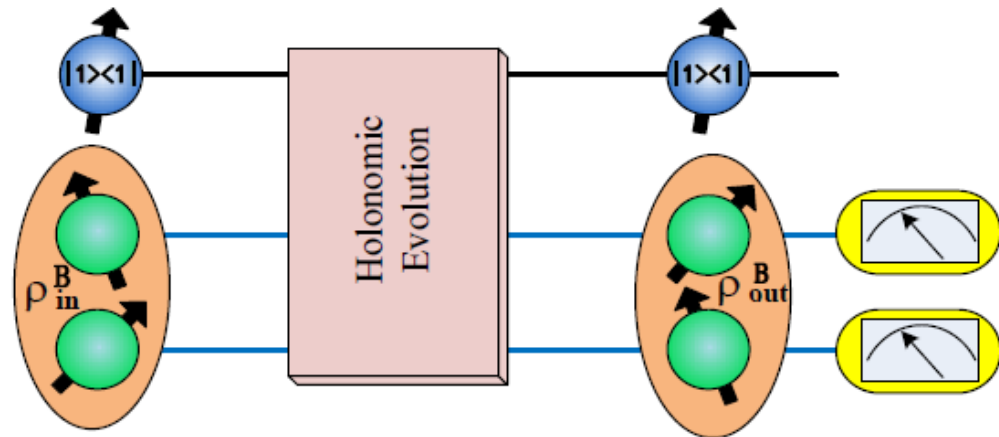
- NHQC CNOT gate

$$|00\rangle_L = |100\rangle \quad |01\rangle_L = |101\rangle \quad |10\rangle_L = |110\rangle \quad |11\rangle_L = |111\rangle$$

- In the basis

$$\{|000\rangle, |001\rangle, |010\rangle, |011\rangle, |100\rangle, |101\rangle, |110\rangle, |111\rangle\}$$

$$H_3 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \end{pmatrix}$$



$$= \frac{1}{4}(X_1(I_2 - Z_2)X_3 + Y_1(I_2 - Z_2)Y_3 - X_1(I_2 - Z_2)(I_3 - Z_3))$$

- The evolution operators and one-qubit gates

$$J_1\tau_1 = \frac{\pi}{\sqrt{2}}, \quad U_1^{\phi_1}(\tau_1) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & e^{-i\phi_1} \\ 0 & 0 & e^{i\phi_1} & 0 \end{pmatrix} \xrightarrow{\text{Basis: } \{|0\rangle_L, |1\rangle_L\}} U_{xz}(\phi_1) = \begin{pmatrix} 0 & e^{-i\phi_1} \\ e^{i\phi_1} & 0 \end{pmatrix}.$$

$$J_2\tau_2 = \pi, \quad U_2^{\phi_2}(\tau_2) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & \cos \phi_2 & i \sin \phi_2 \\ 0 & 0 & -i \sin \phi_2 & -\cos \phi_2 \end{pmatrix} \xrightarrow{\text{Basis: } \{|0\rangle_L, |1\rangle_L\}} U_{zx}(\phi_2) = \begin{pmatrix} \cos \phi_2 & i \sin \phi_2 \\ -i \sin \phi_2 & -\cos \phi_2 \end{pmatrix}$$

$$U_{xz}(0)U_{xz}(-\theta/2) = e^{-i\frac{\theta}{2}Z_L}$$

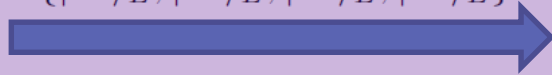
$$U_{zx}(0)U_{zx}(-\varphi/2) = e^{-i\frac{\varphi}{2}X_L}$$

- The evolution operator and CNOT gate.

$$J_3\tau_3 = \frac{\pi}{\sqrt{2}}, \quad U_3(\tau_3) = \text{Diag}[1, 1, 1, -1, 1, 1, X]$$

Basis:

$\{|00\rangle_L, |01\rangle_L, |10\rangle_L, |11\rangle_L\}$



U_{cnot}^L

CNOT gate in the
logical space

- By using $H_1(\phi_1)$, $H_2(\phi_2)$ and H_3

$$R_z^L(\theta) = U_{xz}(0)U_{xz}\left(-\frac{\theta}{2}\right) \rightarrow U_1^0(\tau_1)U_1^{-\frac{\theta}{2}}(\tau_1),$$

$$R_x^L(\phi) = U_{zx}(0)U_{zx}\left(-\frac{\phi}{2}\right) \rightarrow U_2^0(\tau_2)U_2^{-\frac{\phi}{2}}(\tau_2).$$

Experimental output state fidelities

$$R_z^L\left(\frac{\pi}{2}\right)$$

$$f_{aver} = 97.6\%$$

$$R_z^L(\pi)$$

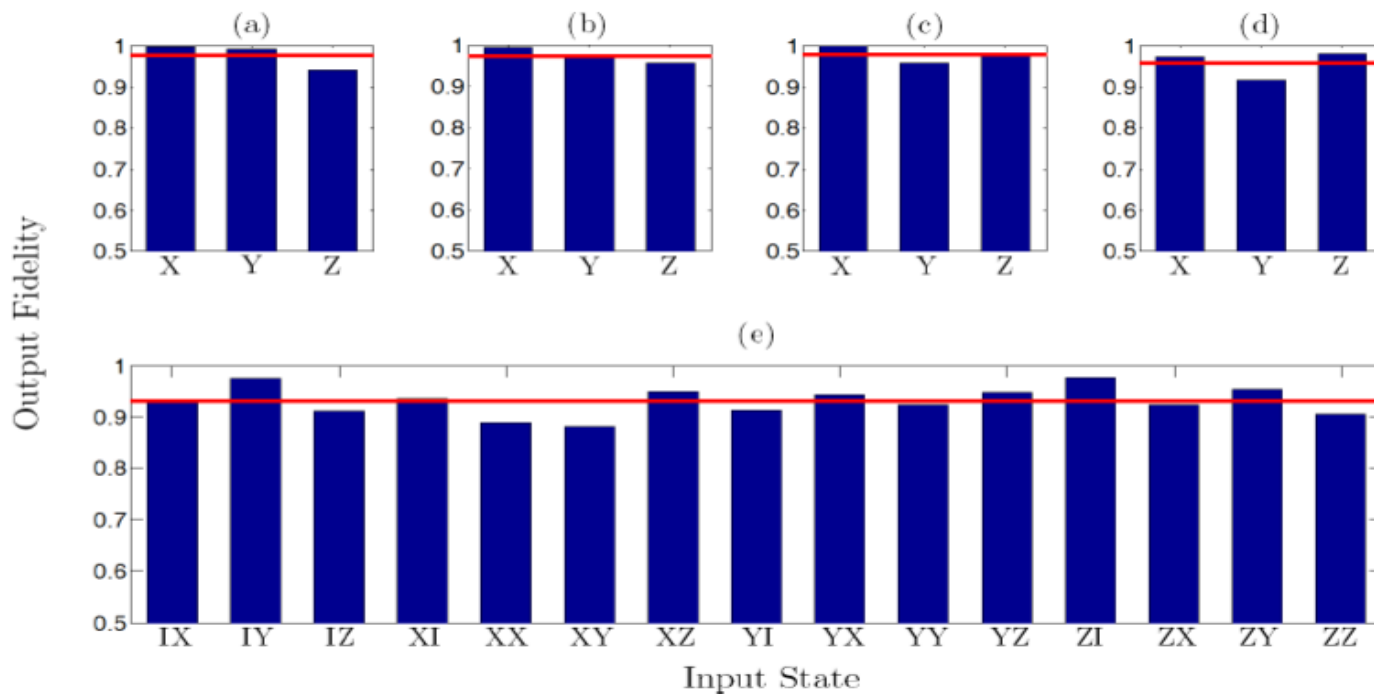
$$f_{aver} = 97.3\%$$

$$R_x^L\left(\frac{\pi}{2}\right)$$

$$f_{aver} = 97.9\%$$

$$R_x^L(\pi)$$

$$f_{aver} = 95.7\%$$

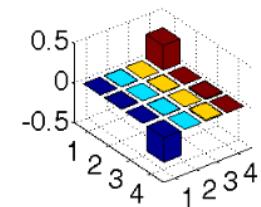
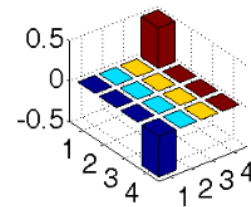
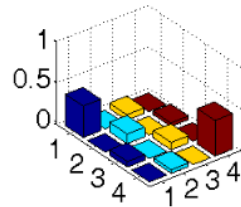
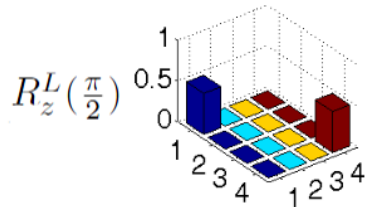


$$U_{cnot}^L \quad f_{aver} = 93.12\%$$

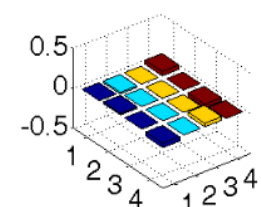
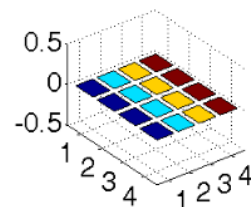
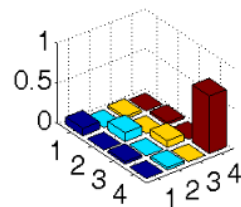
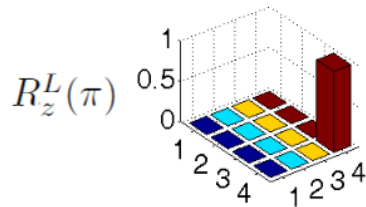
$$f = \text{Tr}(\rho_{exp}\rho_{th}) / \sqrt{\text{Tr}(\rho_{exp}\rho_{exp})\text{Tr}(\rho_{th}\rho_{th})}$$

Experimental χ matrices

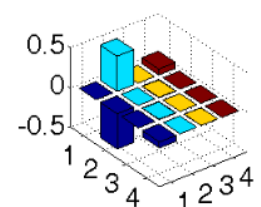
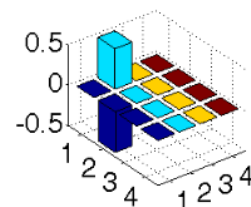
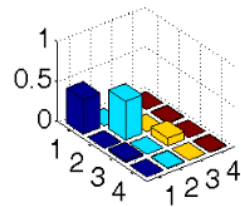
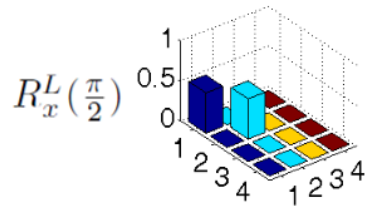
$F= 95.9\%$



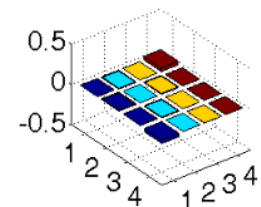
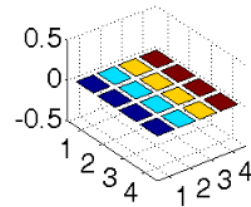
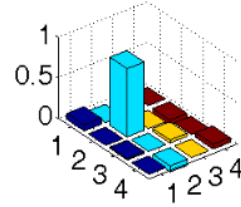
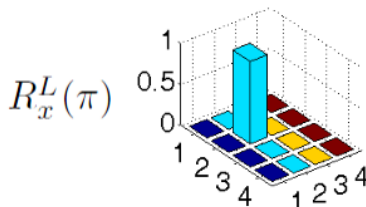
$F= 95.9\%$



$F= 98.1\%$



$F= 96.3\%$



(a)

(b)

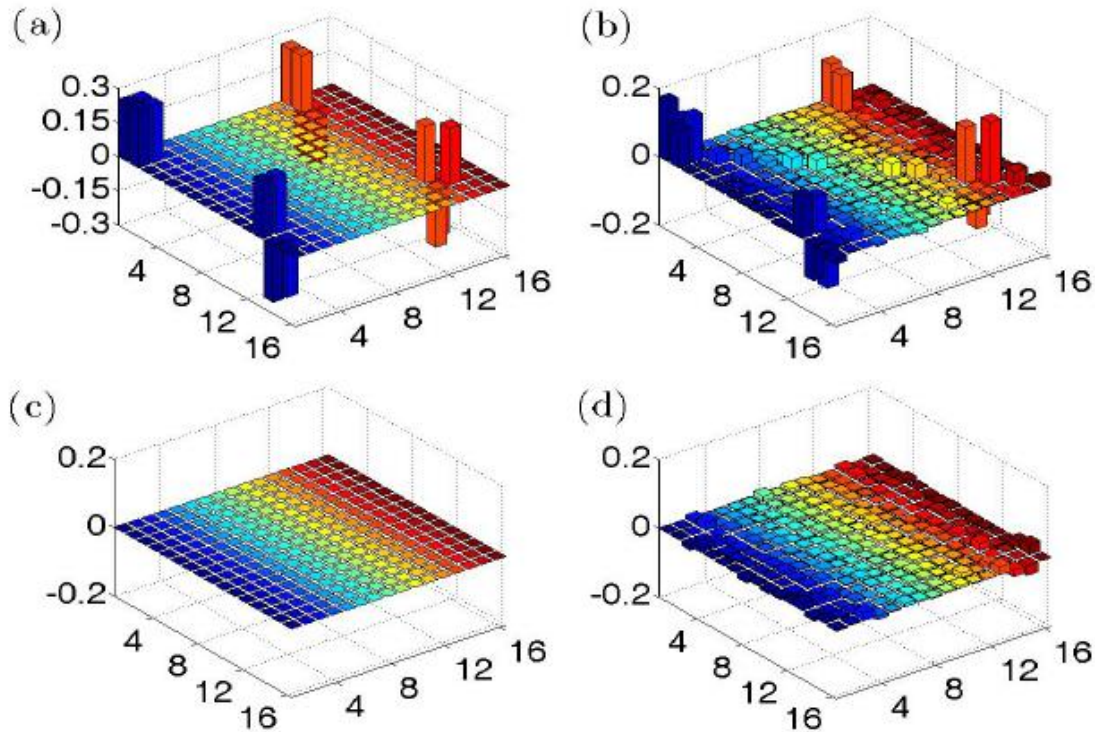
(c)

(d)

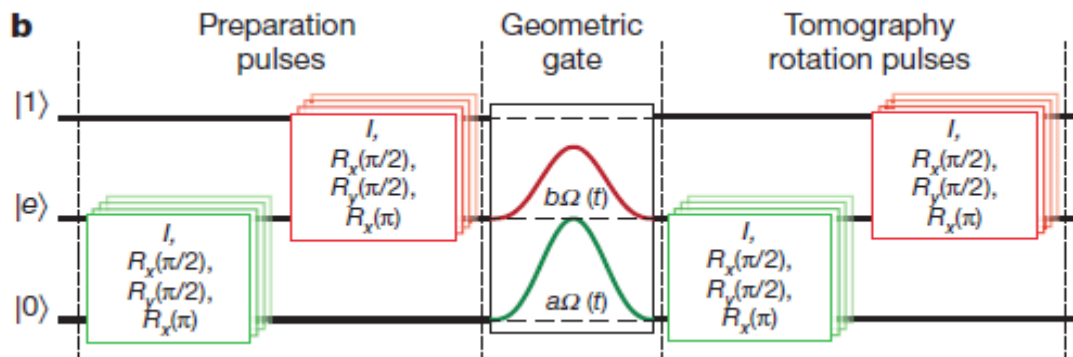
Experimental χ matrix

U_{cnot}^L

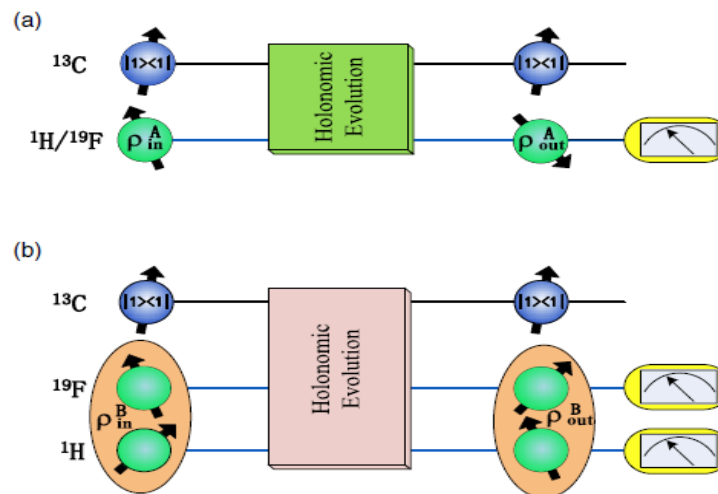
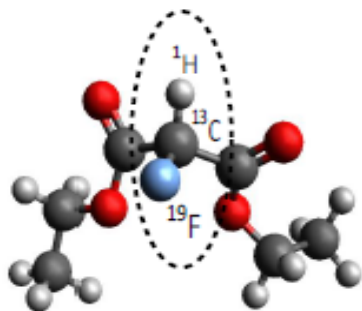
$F = 91.43\%$



$$F_{\chi} = |\text{Tr}(\chi_{exp}\chi_{th}^{\dagger})| / \sqrt{\text{Tr}(\chi_{exp}\chi_{exp}^{\dagger})\text{Tr}(\chi_{th}\chi_{th}^{\dagger})}$$



瑞士研究组：A. A. Abdumalikov Jr, J. M. Fink, K. Juliusson, M. Pechal, S. Berger, A. Wallraff & S. Filipp, Nature 496, 482 (2013) . (超导比特系统)



我们小组：G. R. Feng, G. F. Xu, and G. L. Long, Phys. Rev. Lett. 110, 190501 (2013). (核磁共振系统)

ARTICLE

Received 10 Jul 2014 | Accepted 31 Jul 2014 | Published 12 Sep 2014

DOI: 10.1038/ncomms5870

OPEN

Room temperature high-fidelity holonomic single-qubit gate on a solid-state spin

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At its most fundamental level, circuit-based quantum computation relies on the application of controlled phase shift operations on quantum registers. While these operations are generally compromised by noise and imperfections, quantum gates based on geometric phase shifts can provide intrinsically fault-tolerant quantum computing. Here we demonstrate the high-fidelity realization of a recently proposed fast (non-adiabatic) and universal (non-Abelian)

Experimental realization of universal geometric quantum gates with solid-state spins

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Nature **514**, 72–75 (02 October 2014) | doi:10.1038/nature13729

Received 06 May 2014 | Accepted 31 July 2014 | Published online 01 October 2014



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Experimental realization of a universal set of quantum logic gates is the central requirement for the implementation of a quantum computer. In an ‘all-geometric’ approach to quantum computation^{1, 2}, the quantum gates are implemented using Berry phases³ and their non-Abelian extensions, holonomies⁴, from geometric transformation of quantum states in the Hilbert space⁵. Apart from its fundamental interest and rich mathematical structure, the geometric approach has some built-in noise-resilience features^{1, 2, 6, 7}. On the experimental side, geometric phases and holonomies have

4. Superfast Evolution in ‘PT’ Systems

Chao Zheng; Liang Hao; Gui-Lu Long, Observation of a fast evolution in a parity-time-symmetric system,
Phil. Trans. Royal Soc. A- Math. Phys. Eng. Sci., 371, 20120053 (2013).



Process

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \xrightarrow{e^{-i\frac{t}{\hbar}H}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Minimum time:

$$\tau = \frac{\pi\hbar}{E}$$

Minimal time:

$$\tau = (2\alpha + \pi) \frac{\hbar}{E}$$

Bender CM, et al. Faster than Hermitian quantum mechanics. 2008, *Phys. Rev. Lett.* **98**, 040403

Parity-time-symmetric whispering-gallery microcavities

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Optical systems combining balanced loss and gain provide a unique platform to implement classical analogues of quantum systems described by non-Hermitian parity-time (PT)-symmetric Hamiltonians. Such systems can be used to create synthetic materials with properties that cannot be attained in materials having only loss or only gain. Here we report PT-symmetry breaking in coupled optical resonators. We observed non-reciprocity in the PT-symmetry-breaking phase due to strong field localization, which significantly enhances nonlinearity. In the linear regime, light transmission is reciprocal regardless of whether the symmetry is broken or unbroken. We show that in one direction there is a complete absence of resonance peaks whereas in the other direction the transmission is resonantly enhanced, a feature directly associated with the use of resonant structures. Our results could lead to a new generation of synthetic optical systems enabling on-chip manipulation and control of light propagation.

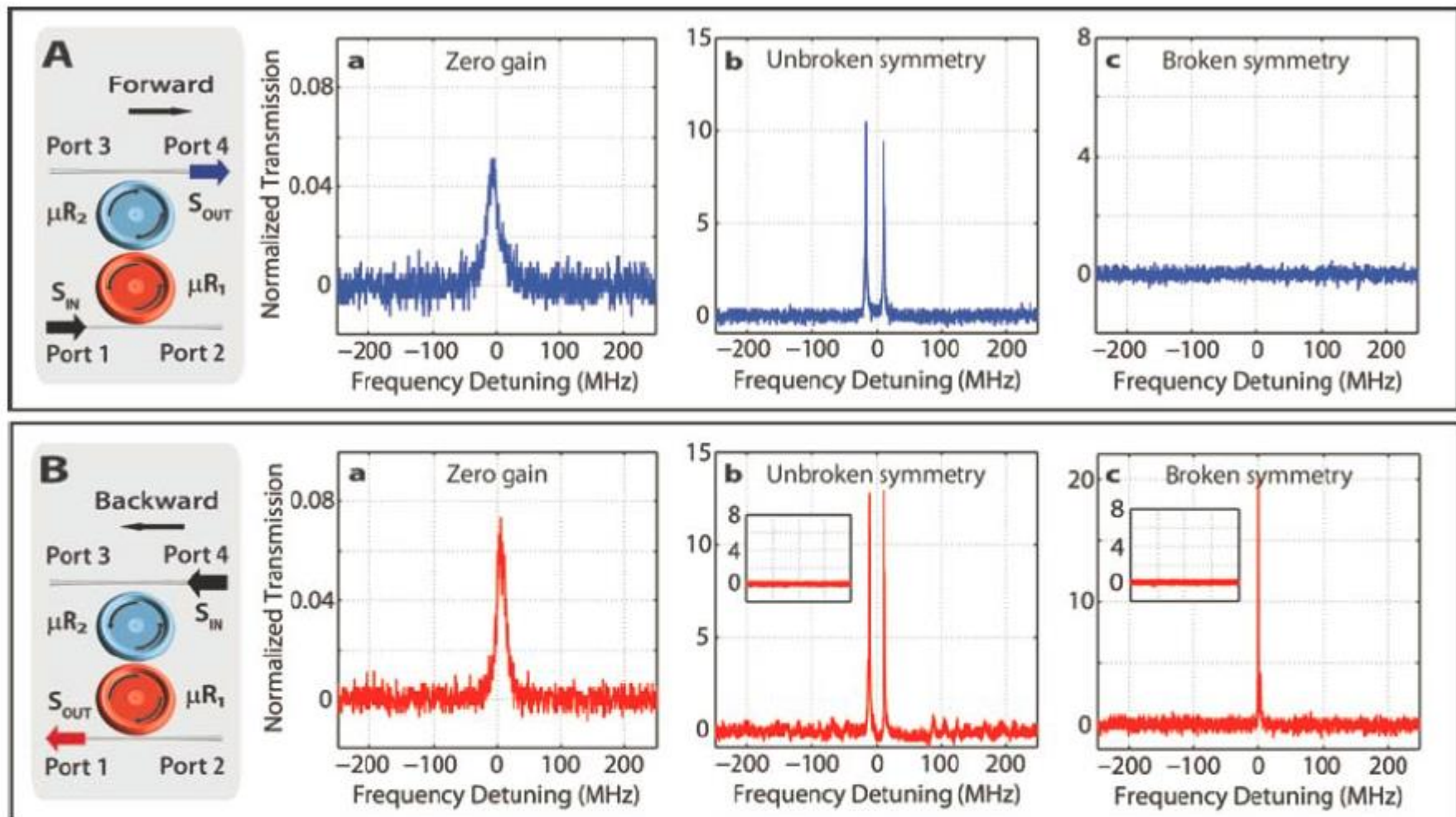


Fig.5. Experimentally observed unidirectional transmission for PT -symmetric WGM microresonators in the nonlinear regime. When both resonators are passive (no gain), the transmission is bi-directional (reciprocal), and light is transmitted in both forward (**A(a)**) and backward directions (**B(a)**). In the unbroken-symmetry region, where the coupling exceeds the critical value and gain and loss are balanced, the transmission is still bi-directional (**A(b)** & **B(b)**). Mode splitting due to coupling is now resolved because gain compensates loss leading to narrower linewidths. In the broken-symmetry region (**A(c)** & **B(c)**), transmission becomes

Non-Hermitian PT symmetric Case: (CM Bender)

$$H = \begin{pmatrix} re^{i\theta} & s \\ s & re^{-i\theta} \end{pmatrix} \quad s, r, \alpha \text{ real}$$

$$E_{\pm} = r \cos \theta \pm \sqrt{s^2 - r^2 \sin^2 \theta}$$

Real if

$$s^2 > r^2 \sin^2 \theta$$

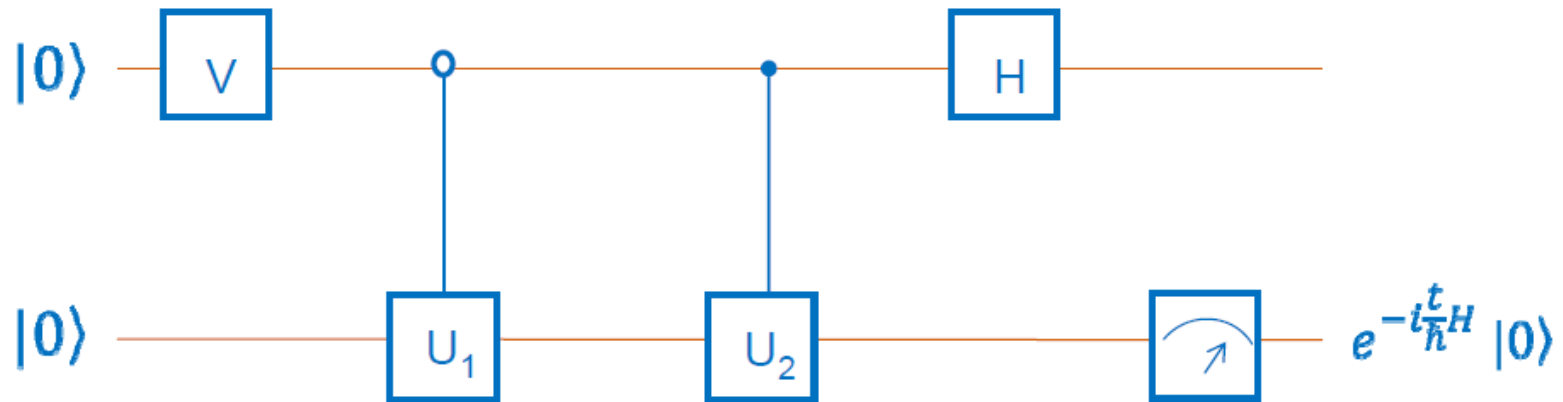
The time needed from $|0\rangle$ to $|1\rangle$ is

$$t = \frac{2\hbar\pi}{\omega} \left(\alpha + \frac{\pi}{2} \right)$$

If $\alpha = -\pi/2$, the time needed from $|0\rangle$ to $|1\rangle$ is **Zero!**

C.M.Bender, D.C.Brody, H.F.Jones, B.K.Meister. Faster than Hermitian quantum mechanics. *Phys. Rev. Lett.* **98**, 040403 (2007)

Constructing a PT-symmetric System



1. G. L. Long, Quantum computation using nonlinear quantum optics, an abstract (5111-53) (Tracking No. FN03-FN02-32) submitted to SPIE conference "Fluctuations and Noise in Photonics and Quantum Optics" in 18 Oct 2002.
2. G L Long, General Principle of Quantum Interference and the Duality Computer, Commun.Theor. Physics, 45, 825-844 (2006). quant-ph /0512120.
3. Gudder S. Mathematical theory of duality quantum computers. Quantum Inf Process, 2007, 6:37-48.
4. Long G L,Int.J.Theor. Phys.50: 1305-1318(2011).

本文证明了利用Long的duality quantum computer[G.L.Long, Commun. Theor. Phys. 45(5): 825-844 (2006)],可以更有效的对Hamiltonian体系进行模拟。图1和图3在文献[G. L. Long, Y.Liu and C. Wang, Commun. Theor. Phys. 51,65-67 (2009)]给出。图1的 $V_k=H$ 的情况在文献G. L. Long, Y.Liu,Commun. Theor. Phys. 50,1303-1306]给出。

Hamiltonian Simulation Using Linear Combinations of Unitary Operations

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We present a new approach to simulating Hamiltonian dynamics based on implementing linear combinations of unitary operations rather than products of unitary operations. The resulting algorithm has superior performance to existing simulation algorithms based on product formulas and, most notably, scales better with the simulation error than any known Hamiltonian simulation technique. Our main tool is a general method to nearly deterministically implement linear combinations of nearby unitary operations, which we show is optimal among a large class of methods.

本文正式发表在Quantum Information and Computation 12, 901-924 (2012)。

I. INTRODUCTION

Simulating the time evolution of quantum systems is a major potential application of quantum computers. While quantum simulation is apparently intractable using classical computers, quantum computers are naturally suited to this task. Even before a fault-tolerant quantum computer is built, quantum simulation techniques can be used to prove equivalence between Hamiltonian-based models of quantum computing (such as adiabatic quantum computing [1] and continuous-time quantum walks [2]) and to develop novel quantum algorithms [3–7].

Feb 2012

Theorem 1. *Let the system Hamiltonian be $H = \sum_{j=1}^m H_j$ where each $H_j \in \mathbb{C}^{2^n \times 2^n}$ is Hermitian and satisfies $\|H_j\| \leq h$ for a given constant h . Then the Hamiltonian evolution e^{-iHt} can be simulated on a quantum computer with failure probability and error at most ϵ as a product of linear combinations of unitary operators. In the limit of large $m, ht, 1/\epsilon$, this simulation uses*

$$\tilde{O}\left(m^2 h t e^{1.6 \sqrt{\log(mht/\epsilon)}}\right) \tag{1}$$

elementary operations and exponentials of the H_j s.

Although we have not specified the method used to simulate the exponential of each H_j , there are well-known techniques to simulate simple Hamiltonians. In particular, if H_j is 1-sparse (i.e., has at most one non-zero matrix element in each row and column), then it can be simulated using $O(1)$ elementary operations [4, 9], so (1) gives an upper bound on the complexity of simulating sparse Hamiltonians.

Our simulation is superior to the previous best known simulation algorithms based on product formulas. Previous methods have scaling of the same form, but with the coefficient 1.6 replaced by 2.54 [11, Theorem 1] or 2.06 [20, Theorem 1]. Also note that Theorem 1 of [12] gives a similar scaling as in [20], except the term in the exponential depends on the second-largest $\|H_j\|$ rather than h .

Pulse sequences for the operations

V:

$$[2\phi_V]_y^a$$

C_0-U_1 :

$$[\frac{\pi}{2}]_{-y}^e \rightarrow [\frac{\phi_{U_1}}{2\pi J}] \rightarrow [\pi]_x^{a,e} \rightarrow [\frac{\phi_{U_1}}{2\pi J}] \rightarrow [\pi]_{-x}^{a,e} \rightarrow [\frac{\pi}{2}]_y^e \rightarrow [-\phi_{U_1}]_x^e,$$

C_1-U_2 :

$$[\pi]_y^e \rightarrow [\frac{1}{4J}] \rightarrow [\pi]_x^{a,e} \rightarrow [\frac{1}{4J}] \rightarrow [\pi]_{-x}^{a,e}$$

$$\rightarrow [\frac{\pi}{2}]_{-y}^e \rightarrow [\frac{\pi}{2}]_x^e \rightarrow [\frac{\pi}{2}]_{-y}^e \rightarrow [\frac{\pi}{2}]_y^a \rightarrow [\frac{\pi}{2}]_x^a \rightarrow [\frac{\pi}{2}]_{-y}^a.$$

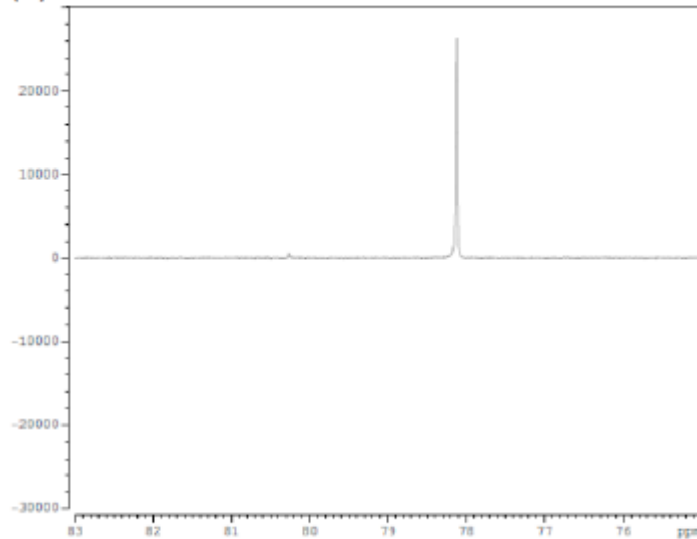
Hadamard:

$$[\frac{\pi}{2}]_y^a \rightarrow [\pi]_{-x}^a$$



$$\frac{q}{\sqrt{2}} \left[|0\rangle_a e^{-\frac{i}{\hbar} H t} |0\rangle_e + |1\rangle_a \frac{1}{q} (\cos \phi_V U_1 - \sin \phi_V U_2) |0\rangle_e \right]$$
$$\tau = \frac{2\hbar\pi}{\omega} \left(\alpha + \frac{\pi}{2} \right)$$

(a) $t = 0$



(b)

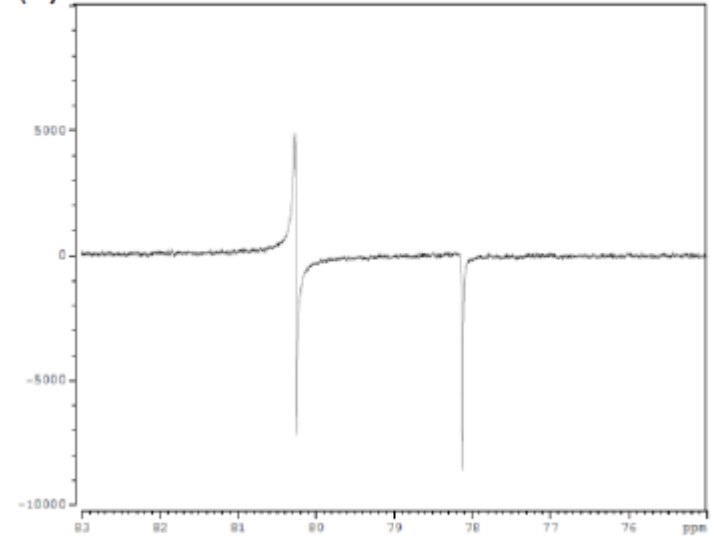
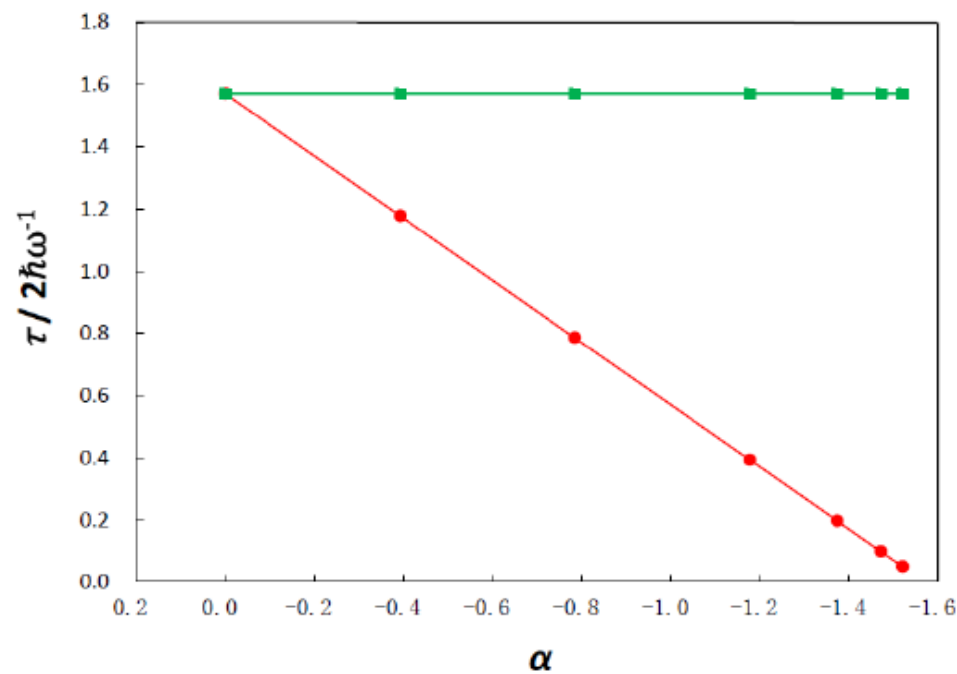
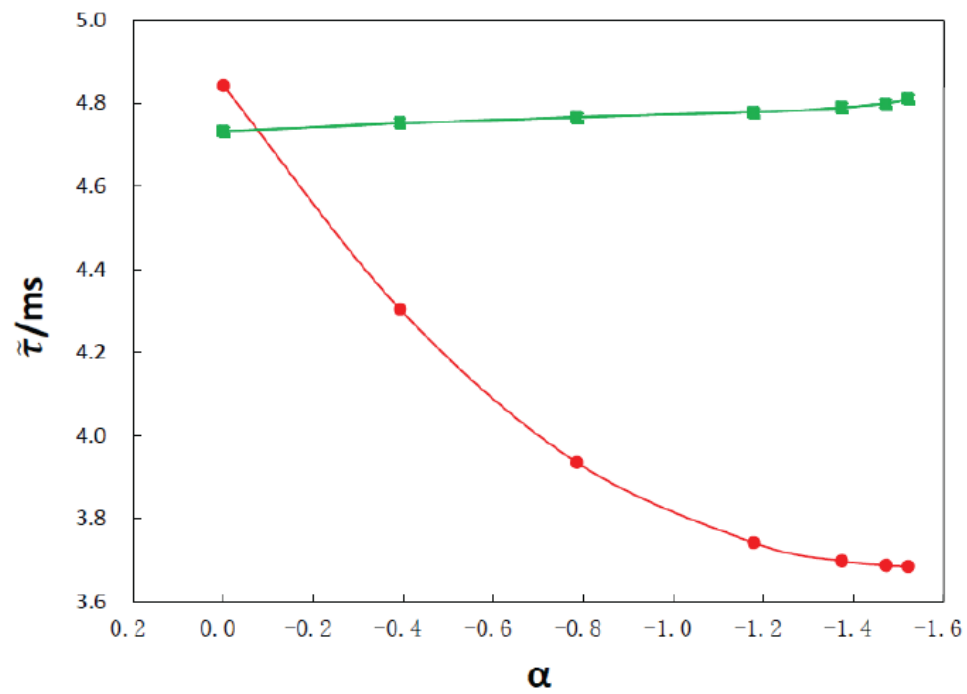
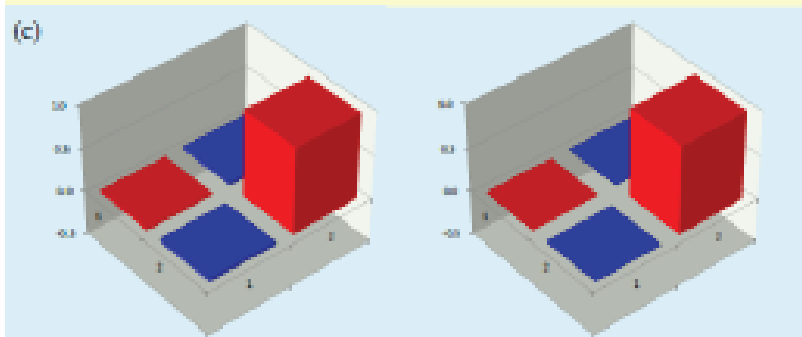
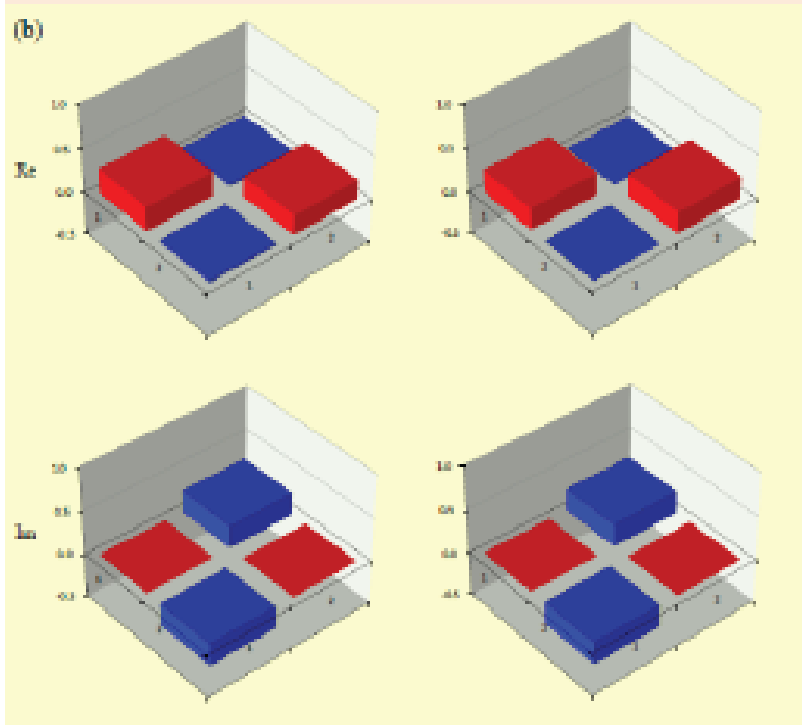
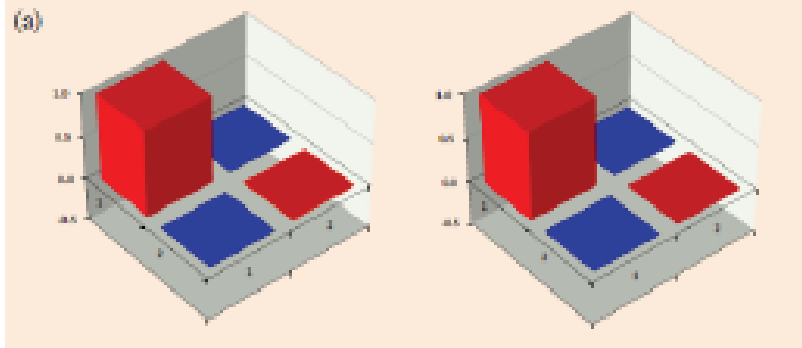


Figure 2: Typical spectra of the work qubit with $\alpha = -\pi/8$: (a) pseudopure state at the beginning of evolution; (b) final state after evolving for a time of τ .

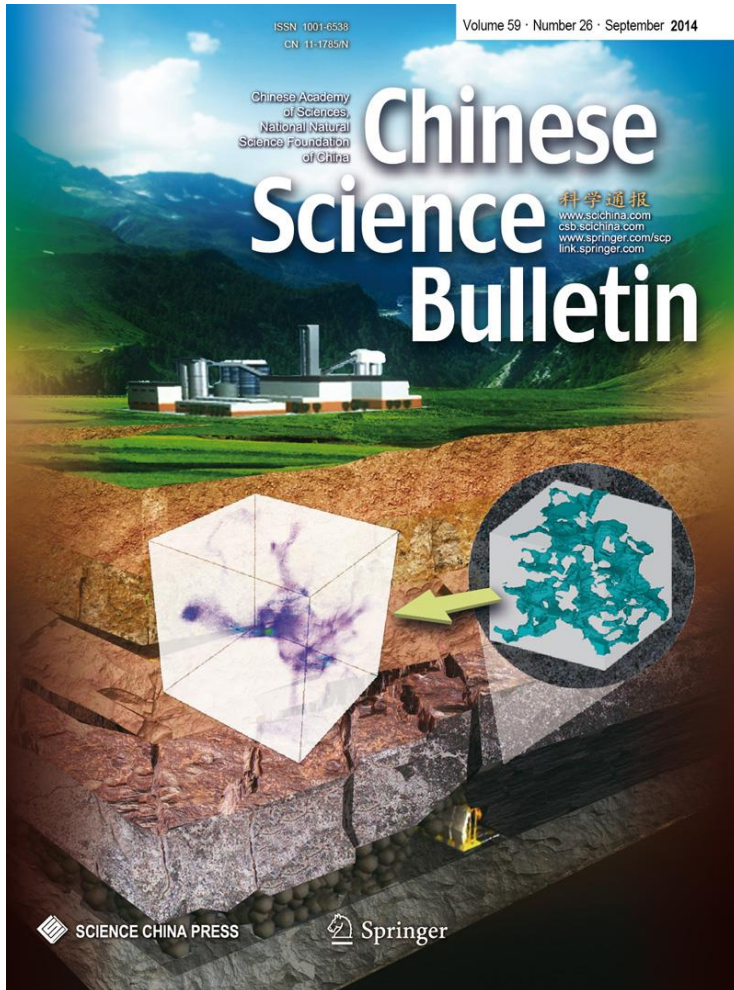


5. Summary

Summary

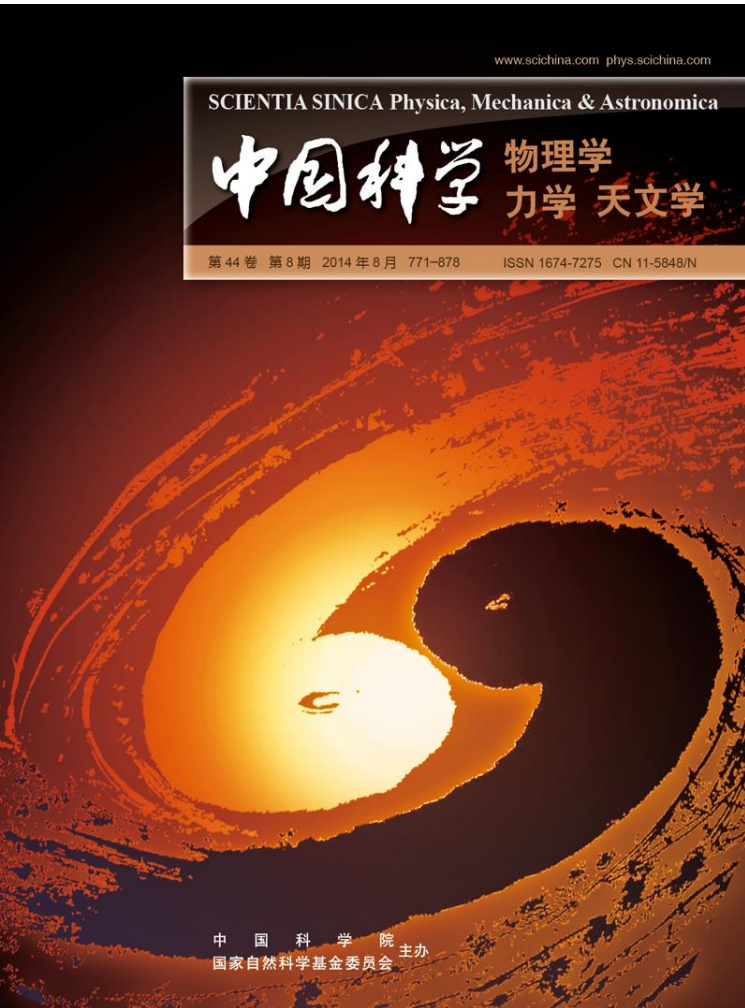
- Using NMR, digital QS of tunneling is demonstrated for the 1st time.
- Nonadiabatic HQC is first demonstrated in NMR.
- Using NMR and Duality quantum computing, superfast evolution of PT symmetric system.
- QS is an important tool in studying quantum systems. NMR is playing an important role in the experiment.

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Chinese **Science Bulletin** (CSB) is a multidisciplinary academic journal supervised by the Chinese Academy of Sciences and co-sponsored by the Chinese Academy of Sciences and National Natural Science Foundation of China. The journal aims to encourage communications of innovative research results in the fields of natural sciences and high technologies.

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organic optoelectronic materials

organic optoelectronic device



Thank you!