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Experimental quantum simulations: towards exotic quantum many-body physics with nuclear spins

Xinhua Peng Univ. of Sci. & Tech of China (USTC) CAS Key Laboratory of Microscale Magnetic Resonance



Frontier Lecture Sunday, 21th Oct. from 9:00 to 10:00

Outline

I. Motivation

- Quantum simulation: Why? What?
- Spin-based Quantum information processing
- II. NMR quantum simulators
 - Our platform & basic principles
- III. Recent experimental QS results
 - Detecting topological quantum phase transition
 - Identifying Z2 topological order and its breakdown
 - Measuring out-of-time correlation
 - Controlling quantum dynamics based on QS

IV. Conclusion and Outlook

Quantum simulation: Why?

Simulating of quantum systems with computers



The Puzzle: Feynman's main thesis was quantum systems could not be efficiently imitated on classical systems.

Quantum simulation: What?

Controllable Quantum Systems As Simulators

Quantum computers - Universal quantum simulators



1982 Richard P. Feynmann

"Simulating Physics with Computers", Int. J. Theor. Phys. <u>21</u>, 467-488, 1982

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



Quantum simulation: Targets



I. M. Georgescu et al., Rev. Mod. Phys., Vol. 86, No. 1, January–March 2014

Quantum simulation: Implementation





- Nuclear spins have long decoherence time
- Electronic spins have the fast operation time
- Spins can be easily manipulated by mature magnetic resonance techniques (NMR, EMR, ODMR, FMR)

Spin-based QIP is one of most successful physical implementations, and provides inspired technology for others solid systems, as an important testbed for developing quantum control methods.

Spin-based quantum information processing







Our platform: NMR QIP

Liquid state NMR is an excellent system for small quantum registers.





NMR Quantum simulators



I. M. Georgescu et al., Rev. Mod. Phys., Vol. 86, No. 1, January–March 2014

Quantum simulation: How?

Main steps



Digital vs. Analog QS

Digital QS

- State $|\psi\rangle$ to be encoded using the computational basis (qubits)
- Quantum circuit model:
 Evolution is
 implemented through
 single- and two-qubit
 gates
- DQS is universal
- Example: Quantum chemistry

Analog QS

- The system and simulator are sufficiently similar
- Map the evolution of the system to be simulated onto the controlled evolution of the quantum simulator

$$H_{\rm sys} \leftrightarrow H_{\rm sim}$$

- Robustness
- Example: Adiabatic
 quantum simulation (the
 dynamics or ground state)

DQS: Quantum chemistry

• First-quantized Hamiltonian:

$$H = T + V = \frac{p^2}{2m} + V(x)$$

Particle's wavefunction (position representation)

$$|\psi\rangle = \sum_{x=0}^{2^n - 1} a_x |x\rangle$$

Quantum evolution

$$U(\delta t) = e^{-i(T+V)\delta t} \approx U_{\rm QFT} e^{-iT\delta t} U_{\rm QFT}^{\dagger} e^{-iV\delta t}$$

• Example: chemical dynamics

$$H = \sum_{i} \frac{p_i^2}{2m_i} + \sum_{i < j} \frac{q_i q_j}{r_{ij}}$$

DQS: Simulating chemical reaction

Simulation of Chemical Isomerization Reaction Dynamics



DQS: Quantum chemistry

• Second-quantized Hamiltonian:

$$\hat{H} = \sum_{p,q} h_{pq} \hat{a}_p^+ \hat{a}_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} \hat{a}_p^+ \hat{a}_q^+ \hat{a}_r \hat{a}_s$$
$$[\hat{a}_i, \hat{a}_j^+]_+ = \delta_{ij} \text{ and } [\hat{a}_i, \hat{a}_j]_+ = 0$$

- ✓ O(N⁴) terms, N is the num- ber of single-electron basis functions (i.e. spin-orbitals)
- ✓ Coefficients are classically evaluated by a preliminary Hartree-Fock procedure
- ✓ Straightforward mapping to qubits

 $|0\rangle = \text{occupied}, |1\rangle = \text{unoccupied}$

✓ Jordan-Wigner transformation to spins

 $\hat{a}_j \rightarrow \mathbf{1}^{\otimes j-1} \otimes \hat{\sigma}^+ \otimes (\hat{\sigma}^z)^{\otimes N-j} \quad \hat{a}_j^+ \rightarrow \mathbf{1}^{\otimes j-1} \otimes \hat{\sigma}^- \otimes (\hat{\sigma}^z)^{\otimes N-j}$

DQS: Quantum chemstry



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

DQS: Simulating hydrogen molecule

We achieve a 45-bit estimation of the ground-sate energy



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

AQS: Quantum phase transition

Quantum spin model (Quantum magnets)

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

External fields Heisenberg couplings

Heisenberg isotropic, Ising, XX, XY, XYZ model

Mapping: A more realistic model in that it treats the spins quantummechanically, by replacing the spin by a quantum operator (<u>Pauli</u> <u>spin-1/2 matrices</u> at spin 1/2).



Quantum phase transition (QPT)



Adiabatic quantum simulations



Adiabatic quantum simulations

Our experiments for many-body systems on QPT:



Recent work1: Detecting topological quantum phase transition

Exotic quantum many-body physics

New Physics: Topological orders (new quantum orders)

Kitaev's toric code model

$$H = -\sum_{s} A_{s} - \sum_{p} B_{p}$$
$$A_{s} = \sigma_{sa}^{x} \sigma_{sb}^{x} \sigma_{sc}^{x} \sigma_{sl}^{x}$$
$$B_{p} = \sigma_{ij}^{z} \sigma_{jk}^{z} \sigma_{kl}^{z} \sigma_{li}^{z}$$

Wen-plaquette model

$$\begin{split} H &= -J\sum_{i}\hat{F}_{i},\\ \hat{F}_{i} &= \sigma_{i}^{x}\sigma_{i+\hat{e}_{x}}^{y}\sigma_{i+\hat{e}_{x}+\hat{e}_{y}}^{x}\sigma_{i+\hat{e}_{y}}^{y} \end{split}$$



Topologic orders = pattern of quantum entanglements A. Kitaev, Ann. Phys. 303, 2 (2003); X. G. Wen, PRL. 90, 016803 (2003)

Z2 topological orders

Experiments?

Great Challenge in experimental study for TOs:

Difficult to realize topological orders directly in real systems

A possible solution: Quantum simulation

Quantum computers provide an alternative way to investigate TOs in experiments (artificial states of matter).

Most previous experiments for the toric-code model:

Photon systems [Nature 482, 489-494 (2012), PRL 102, 030502 (2009), New. J. Phys 11, 083010 (2009)]

NMR systems [PRA 88, 022305 (2013); New J. Phys. 18, 043043 (2016)]

State-based approaches, rather than attempting to realize the Hamiltonian

Hamiltonian Engineering

Quantum Control Model

$$U = e^{-iH_IT} \xleftarrow{\overline{H}_p = \phi H_I \phi^{-1}} V_T = e^{-i\overline{H}_pT} = \prod_k e^{-iH_pt_k} V_k$$

• Lloyd's method $\hat{H} = \sum_{j=1}^{n} \hat{H}_j$

Trotter-Suzuki formula

$$\hat{U}(t) = e^{-iHt} = (e^{-iH_1(t/m)}e^{-iH_2(t/m)}\cdots e^{-iH_k(t/m)})^m + \sum_{i< j} [H_i, H_j] \frac{t^2}{2m} + \dots$$
(

the number of operations $Op_{\text{Lloyd}} \propto t^2 ng^2/\epsilon$ Polynomial scaling

S. Lloyd. Universal Quantum Simulators. Science, 273(5278):1073–1078, 1996.

Hamiltonian Engineering

Many-body interactions **Physical** Simulated $H_{nmr} = \sum_{i=1}^{n} \omega_i \sigma_{iz} + \sum_{\substack{i < j=1 \\ i \neq j}}^{n} J_{ij} \vec{\sigma}_i \cdot \vec{\sigma}_j$ $\hat{\sigma}_z^1 \hat{\sigma}_z^2 \hat{\sigma}_z^3 \hat{\sigma}_z^4$ **(b) -y -y** 6 $e^{-i\,2J\,\sigma_z^{\rm l}\sigma_z^2\sigma_z^3\sigma_z^4}$ -X Ż $2 au_1$ $2\tau_2$ τ_3 τ_2 $2 au_1$ $\pi/2 \quad = \pi \quad \Theta_0 \quad \Theta_1 \quad \Theta_2 \quad \Theta_3$ Note:

Phase diagram

Transverse Wen-plaquette model



The transition region depends on the value of |J/g|:

- The transition
- becomes narrower and sharper as g decreases.

• When $g \rightarrow 0$, Z2B \rightarrow Z2A topological order @ J = 0.

Analogy quantum simulation

Experiment for TQPT



Recent work2: Identifying Z2 topological order and its breakdown

Characterizing Topological orders

One of the most important questions in condensed matter physics is the description and the classification of different phases of matter.

How to classify different topological orders (TOs)?

old question \rightarrow new objects

Landau's theory

Direct-product states "short-range entanglement" Symmetry Topologically ordered states

Quantum many-body states "long-range entanglement".

?

an especially challenging task!

Characterizing topological order

Topological order characterization



How to identify the topological phase uniquely and purely by experimental means ?

Modular Matrices

- Non-Abelian geometric phases of degenerate ground state
- All the information of quasiparticles statistics and their fusion
- A complete and one-to-one description of TOs
- Non-local order parameter



braiding and fusion of two anyons self-statistics of all anyons (multual statistics)

TOs and modular matrices

Z2 toric code

of two

Doubled semion

Doubled Fibonacci

Measure modular matrices?

Obtain elements of S/T matrices in standard basis

 $\langle \phi_i^{\rm std} | S | \phi_j^{\rm std} \rangle \qquad \langle \phi_i^{\rm std} | T | \phi_j^{\rm std} \rangle$

A solution: Interferometry method



$$\left|\phi_{i}^{std}\right\rangle = S^{+}U\left|\psi_{0}\right\rangle, \left|\phi_{j}^{std}\right\rangle = V\left|\psi_{0}\right\rangle$$

R. Somma et al., Phys. Rev. A, 65, 042323, (2002)

Experimental scheme



Initialization

How to prepare a set of linearly independent states in the degenerated ground-state subspace?

Random adiabatic method

$$\hat{H}(t) = [1 - s(t)]\hat{H}_{rd} + s(t)\hat{H}_{T}^{4}$$
$$s(t): 0 \rightarrow 1 \qquad \qquad \hat{H}_{rd} = \sum_{i}^{4} \sum_{\alpha \in x, y, z} C_{i}^{\alpha} \hat{\sigma}_{i}^{\alpha}$$

 C_i^{α} are randomly generated coefficients between [-1, 1]

Without the information of string operators $|\psi^{rd}\rangle \rightarrow \sum_{i=1}^{4} c_i |\psi_g^i\rangle$ Different $\hat{H}_{rd} \longrightarrow \{|\psi_1^{rd}\rangle, |\psi_2^{rd}\rangle, \cdots, |\psi_n^{rd}\rangle\}$

Initialization

• Check $\{|\psi_1^{\rm rd}\rangle, |\psi_2^{\rm rd}\rangle, \cdots, |\psi_n^{\rm rd}\rangle\}$ are linearly independent



If $a_k^k \ge |\xi|$ (ξ is the readout error in the experiment) $|\psi_k^{\text{rd}}\rangle$ is linearly independent from $|\psi_{k'}^{\text{rd}}\rangle$

S, T operations



S, T operations

A NxN square lattice of Kitaev toric code model



a series of permutations with length 4 and N

- S: $\#(SWAP) = 3(n^2 1) + 3(n 1) + 1 = 3n^2 + 3n + 5$
- T: $\#(\text{SWAP}) = N^2 N \sum_{j=-n+1}^{n-1} \gcd(n+j, N)$

polynomial SWAP gates! n = [(N+1)/2]

Measurement

How to experimentally measure the elements of S, T?



Note that the S and T matrices obtained in the random basis are not in their standard forms.

Data processing

How to recover the representation of S, T in the standard basis?

• Standard basis: diagonalize the T matrix.

Recovering procedure

 $\langle \psi_i^{\rm rd} | S | \psi_j^{\rm rd} \rangle \rightarrow \langle \phi_i | S | \phi_j \rangle \rightarrow \langle \phi_i^{\rm std} | S | \phi_j^{\rm std} \rangle$

random basis orthogonal basis standard basis $\langle \psi_i^{\rm rd} | T | \psi_j^{\rm rd} \rangle \rightarrow \langle \phi_i | T | \phi_j \rangle \rightarrow \langle \phi_i^{\rm std} | T | \phi_j^{\rm std} \rangle$

Constructing orthogonal basis

$$\langle \psi_i^{\rm rd} | \mathcal{O} | \psi_j^{\rm rd} \rangle = \sum_k \underbrace{A_{ik}}_{k} \langle \phi_k | \mathcal{O} | \phi_j \rangle \implies \langle \phi_i | \mathcal{O} | \phi_j \rangle$$
Measured

Recovering standard basis: Optimize, diagonalize and transform

$$T_{ab} = \exp(\mathrm{i}\theta_a)\delta_{ab} \qquad S_{1a} = 1$$

NMR Quantum simulator

1-bromo-2,4,5-trifluorobenzene

a	h							
Br	N	0	1	2	3	4	T ₂ * (ms)	T ₁ (s)
	0	-38032					40	0.8
	1	258.4	-45908				40	0.8
	2	107.3	-7.5	-48358			40	0.8
2 ^E U3	3	1454.0	1184.1	51.7	2712		100	1.5
	4	51.2	101.1	1430.3	-4.5	2736	100	1.5

Physical system $H_{\text{NMR}} = \sum_{j=1}^{5} \pi \nu_j \sigma_j^z + \sum_{1 \le j < k \le 5} \frac{\pi}{2} (J_{jk} + 2D_{jk}) \sigma_j^z \sigma_k^z$

F1+H1+H2+H3

Kitaev toric code model $\hat{H}_{Z_2}^4 = -2(\sigma_1^x \sigma_2^x \sigma_3^x \sigma_4^x + \sigma_1^z \sigma_2^z \sigma_3^z \sigma_4^z)$

Step 1. State preparation

Experimental measure				-0.3344 + 0.4432i
				0.8317 + 0.0000i
$\langle \psi_1^{ m rd} \psi_2^{ m rd} angle$	-0.3344 + 0.4432i		a_3^1	0.6932 - 0.1028i
$\langle \psi_1^{\rm rd} \psi_3^{\rm rd} \rangle$	0.6932 - 0.1028i		a_3^2	0.0495 - 0.1916i
$\langle \psi_1^{ m rd} \psi_4^{ m rd} angle$	0.1882 + 0.1908i		a_3^3	0.6854 + 0.0000i
$\langle \psi_2^{\rm rd} \psi_3^{\rm rd} \rangle$	-0.2362 - 0.4322i		a_4^1	0.1882 + 0.1908i
$\langle \psi_2^{ m rd} \psi_4^{ m rd} angle$	0.1532 - 0.0482i		a_4^2	0.1582 + 0.1190i
$\langle \psi_3^{ m rd} \psi_4^{ m rd} angle$	-0.0942 + 0.4642i		a_{4}^{3}	-0.2773 + 0.4033i
	1	L	a_4^4	0.8059 + 0.0000i

Step 2. Measuring S/T matrices

Experimental S, T matrices in randomly generated linearly independent ground states (h = 0)



Step 3. Recovering standard S/T

 $\operatorname{Re}(\langle \phi_{i} | \mathbf{T} | \phi_{i} \rangle)$

 $\operatorname{Im}(\langle \phi_{\mathbf{i}} | \mathbf{T} | \phi_{\mathbf{i}} \rangle)$

¹2₃₄

¹2₃₄



12³⁴

1234

0.5

0

-0.5

-1













What's more: Robustness

• A pertured model: Detuning and disordered Hamiltonian:

$$\hat{H}_{\mathrm{T}} = \hat{H}_{\mathbb{Z}_2} - h \sum_{i} \hat{\sigma}_{i}^{z} - \sum_{i} \epsilon_{i} \hat{\sigma}_{i}^{z},$$

detuining disordered

• Detuning the system from the Kitaev soluble point

A small enough but finite detuning

- preserve the topological nature of the phase while introducing a finite correlation length
- Phase transition: robustness of this approach / topological phase
- A small inhomogeneity: break all accidental translation symmetries to mimic more realistic situations

Phase transition



Phase transition



Recent work3: Measuring out-oftime correlation



Normal correlation (accessible)

$$\langle \hat{W}^{\dagger}(t)\hat{W}(t)\hat{V}^{\dagger}(0)\hat{V}(0)\rangle_{\beta}$$

Out-of-time-order correlation (OTOC)

$$\langle \hat{W}^{\dagger}(t) \hat{V}^{\dagger}(0) \hat{W}(t) \hat{V}(0) \rangle_{\beta} \hat{W}(t) = e^{i\hat{H}t} \hat{W} e^{-i\hat{H}t}$$

H: an interacting many-body Hamiltonian W(0) and V(0): two commuting operators

$$\operatorname{Re}[F(\tau)] = 1 - \langle |[\hat{W}(\tau), \hat{V}]|^2 \rangle / 2$$

`scrambling' of quantum information inaccessible to any reasonable local measurement

Experimental scheme



 $\hat{R} = \mathbf{1}, \ \hat{R}_x(-\pi/2), \ \hat{R}_y(\pi/2) \ \text{for} \ \hat{A} = \hat{\sigma}_1^z, \ \hat{\sigma}_1^y, \ \hat{\sigma}_1^x \qquad \hat{B} = \hat{\sigma}_N^\gamma \quad \text{a local unitary}$

Experimental results



Experimental results



Experimental results

Measurement of butterfly velocity v_B



It quantifies the speed of a local operator growth in time and defines a light cone for chaos, which is also related to the Lieb-Robinson bound

The OTOC also provides a tool to determine the speed for correlation propagating

$$F(t) = a - b e^{\lambda_L(t - |x|/v_B)} + \cdots$$

|x|: distance between two operators

Measuring Out-of-Time-Order Correlators on a Nuclear Magnetic Resonance Quantum Simulator

Jun Li,¹ Ruihua Fan,^{2,3} Hengyan Wang,³ Bingtian Ye,³ Bei Zeng,^{4,5,2,*} Hui Zhai,^{2,6,†} Xinhua Peng,^{7,8,9,‡} and Jiangfeng Du^{7,8}



VIEWPOINT

Seeing Scrambled Spins

Two experimental groups have taken a step towards observing the "scrambling" of information that occurs as a many-body quantum system thermalizes.



Recent work4: Controlling quantum dynamics based on quantum simulator



Open quantum systems

Lindblad equation $\dot{\rho} = -i[H_S + H_C(t), \rho] + \sum_{j} \gamma_j \left[L_j \rho L_j^{\dagger} - \frac{1}{2} \left(L_j^{\dagger} L_j \rho + \rho L_j^{\dagger} L_j \right) \right]_{\mathcal{R}\rho: \text{relaxation part}}$ where $\{L_j\}$: Lindblad generators, γ_j : relaxation parameters.

N²-1, non-negative

More complex, uncontrollable

GRAPE (Gradient ascent pulse engineering)



Khaneja et a., J. Magn. Reson. 172, 296-305 (2005)

Two Key Challenges

Complexity: Exponential growth of Hilbert space n spin-1/2 system: 2ⁿ x 2ⁿ

Noise: irreversibly affects control performance a) Operator errors b) Relaxation effect from the environment

Difficult part: Performance (fitness), Gradients

Can they be calculated on quantum simulator?

PRL 118, 150503 (2017)

week ending 14 APRIL 2017

Hybrid Quantum-Classical Approach to Quantum Optimal Control

Jun Li,^{1,*} Xiaodong Yang,² Xinhua Peng,^{2,3,†} and Chang-Pu Sun¹



Conclusion and Outlook

Liquid state NMR is an excellent system for small quantum registers, and one can see the extraordinary achievement of NMR QIP from testing quantum theory to quantum information processing.



Outlook



Spin is among the most promising physical systems for quantum control.

Spin holds the promise of realizing various novel quantum applications.

NMR is a good testbed for QIP.

Thanks to

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- Zhengnan Zhu
- Wenjie Xu



Thanks for your attention!



CAS Key Laboratory of Microscale Magnetic Resonance (Directed by Prof. Jiangfeng Du)

E-mail: <u>xhpeng@ustc.edu.cn</u> Department of Modern Physics, University of Science and Technology of China Hefei, Anhui, P.R.China

