Quantum
Physics & Quantum Information

Towards simulating many-body physics on a NMR quantum simulator

Xinhua Peng

Univ. of Sci. & Tech of China (USTC)

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Outline

I. Introduction

– Why quantum simulation (QS)
– Basic principle of QS

II. Operations Interpreted for Experimental QS

– Mapping the system
– Initialization
– Hamiltonian engineering
– Measurement

III. Towards Simulating Many-Body Physics

– Quantum magnets: Quantum “baby” phase transition
– Thermal systems: Lee-Yang zeros
– Non-equilibrium systems: Dynamical quantum Hall effect

V. Conclusion

Why QS?

Simulating of quantum systems

- **Classical computers**

  Exponential growth of Hilbert space

Computational basis

n

$$|\Psi\rangle = \sum_{i_1=1}^{2} \cdots \sum_{i_n=1}^{2} c_{i_1 \ldots i_n} \,|\, i_1 \ldots i_n \rangle$$

System with 50 qubits

$2^{50} \approx 10^{15}$ complex amplitudes ~ 32 x 10^{15} bytes of information

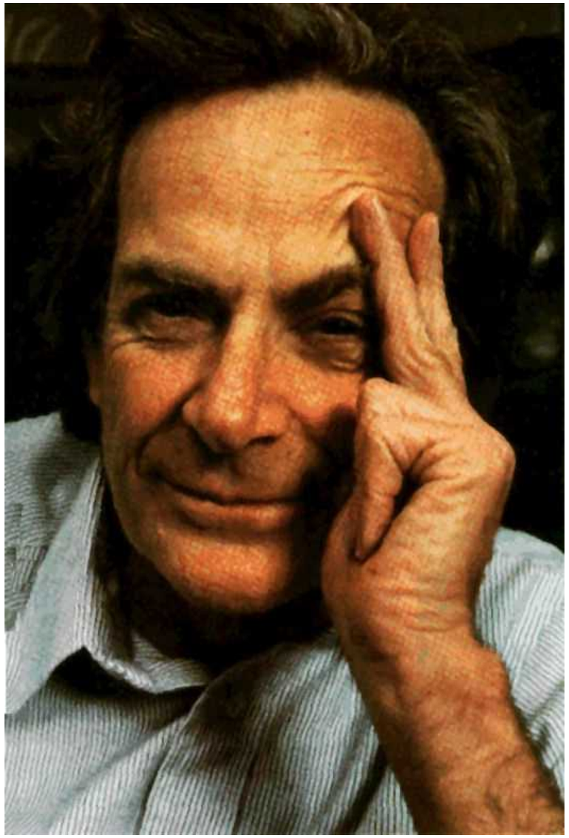
well beyond the capacity of existing computers

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

Why QS?

Simulating of quantum systems

- **Quantum computers - Universal quantum simulators**



1982 Richard P. Feynmann

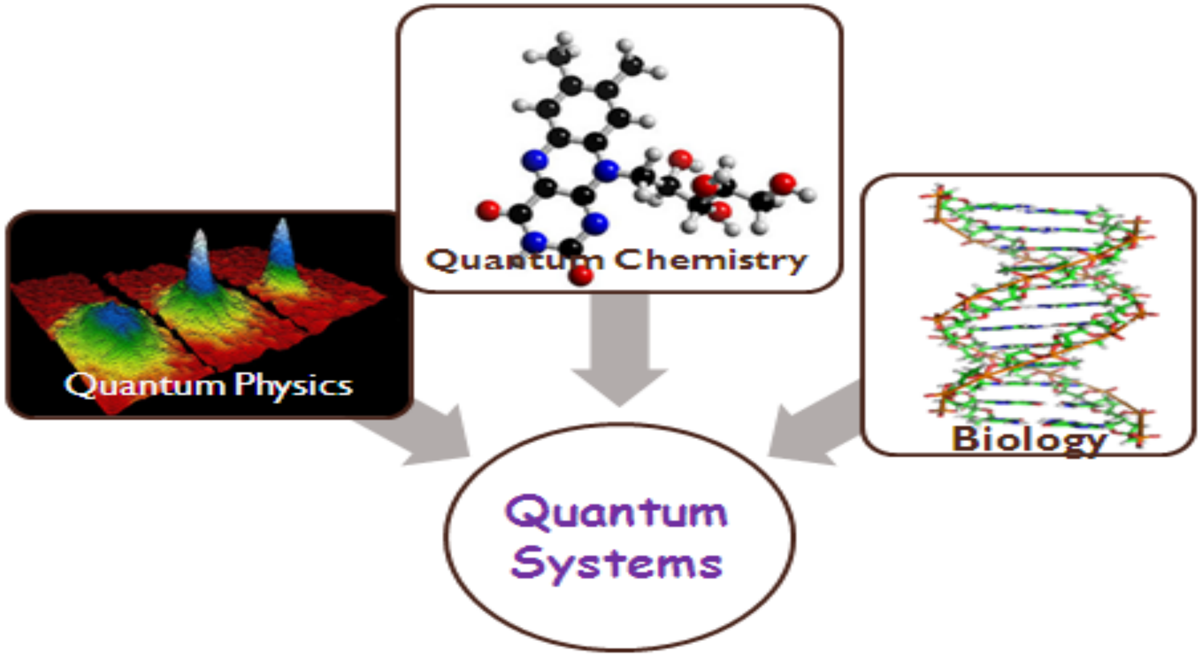
R.P. Feynman, "Simulating Physics with Computers", *Int. J. Theor. Phys.* **21**, 467-488, 1982

Can we do it with a new kind of computer – a quantum computer? Now it turns out, as far as I can tell, that you can simulate this with a quantum system, with quantum computer elements. […] I therefore believe it's true that with a suitable class of quantum machines you can imitate any quantum system, including the physical world.

What is QS?

- Quantum simulation: simulating a quantum system by quantum mechanical means.

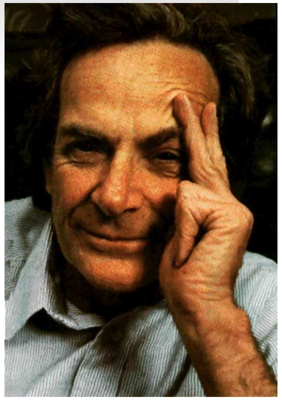
- Quantum simulator: a controllable quantum system used to simulate or emulate other quantum systems



量子计算

主要应用

经典难题
量子算法



量子系统
量子模拟

N = p*q

分解一个300位的整数所需时间比较

	经典计算机	量子计算机
算法	二次筛法	Shor算法
步数	10^{24}	10^{10}
CPU频率	1 THz	1 THz
时间	15万年	1秒

$$|\Psi\rangle = \sum_{i_1=1}^{2} \cdots \sum_{i_n=1}^{2} c_{i_1 \ldots i_n} \, |i_1 \ldots i_n\rangle$$

n= 50

~ 32 x 10^{15} 字节经典信息

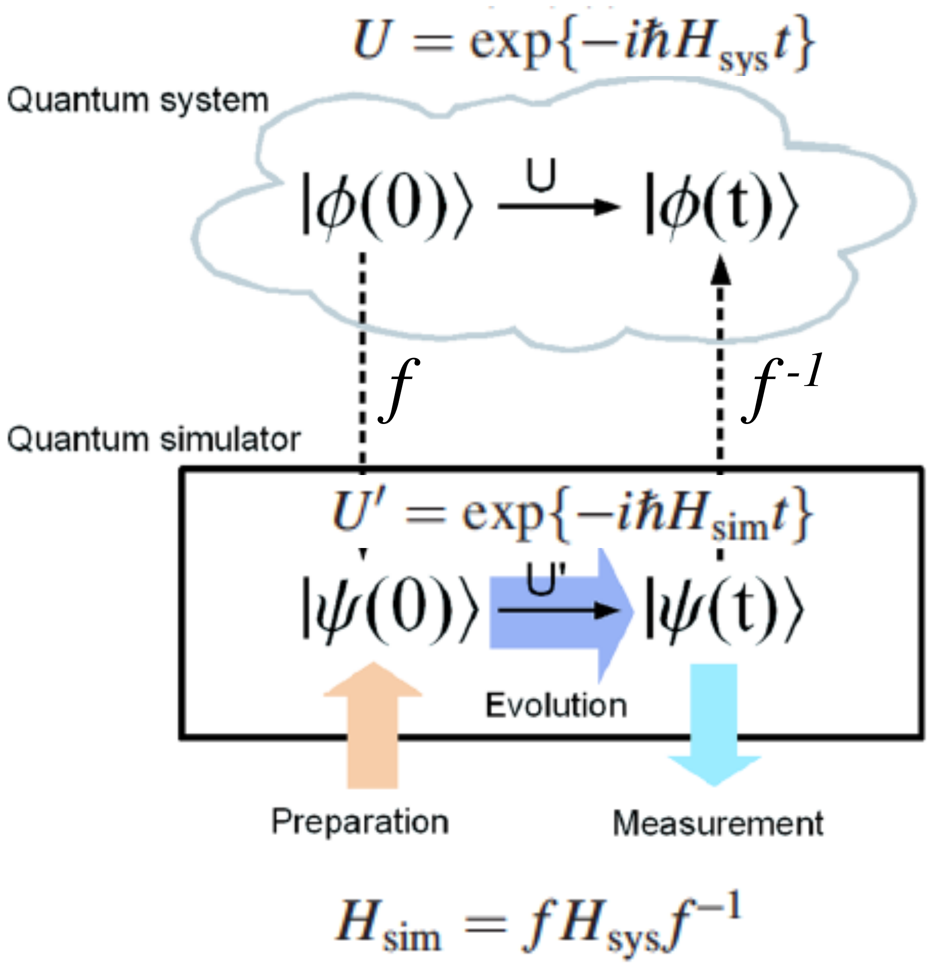
50位量子比特信息

<u>中等规模的量子仿真即有可能超越经典计算的极限，在实际问题的解决中展现量子计算的优势！</u>

<u>Quantum simulator ≠ Universal quantum computer</u>

Basic principle of QS

QS: a controllable quantum system used to simulate or emulate other quantum systems



Two types:

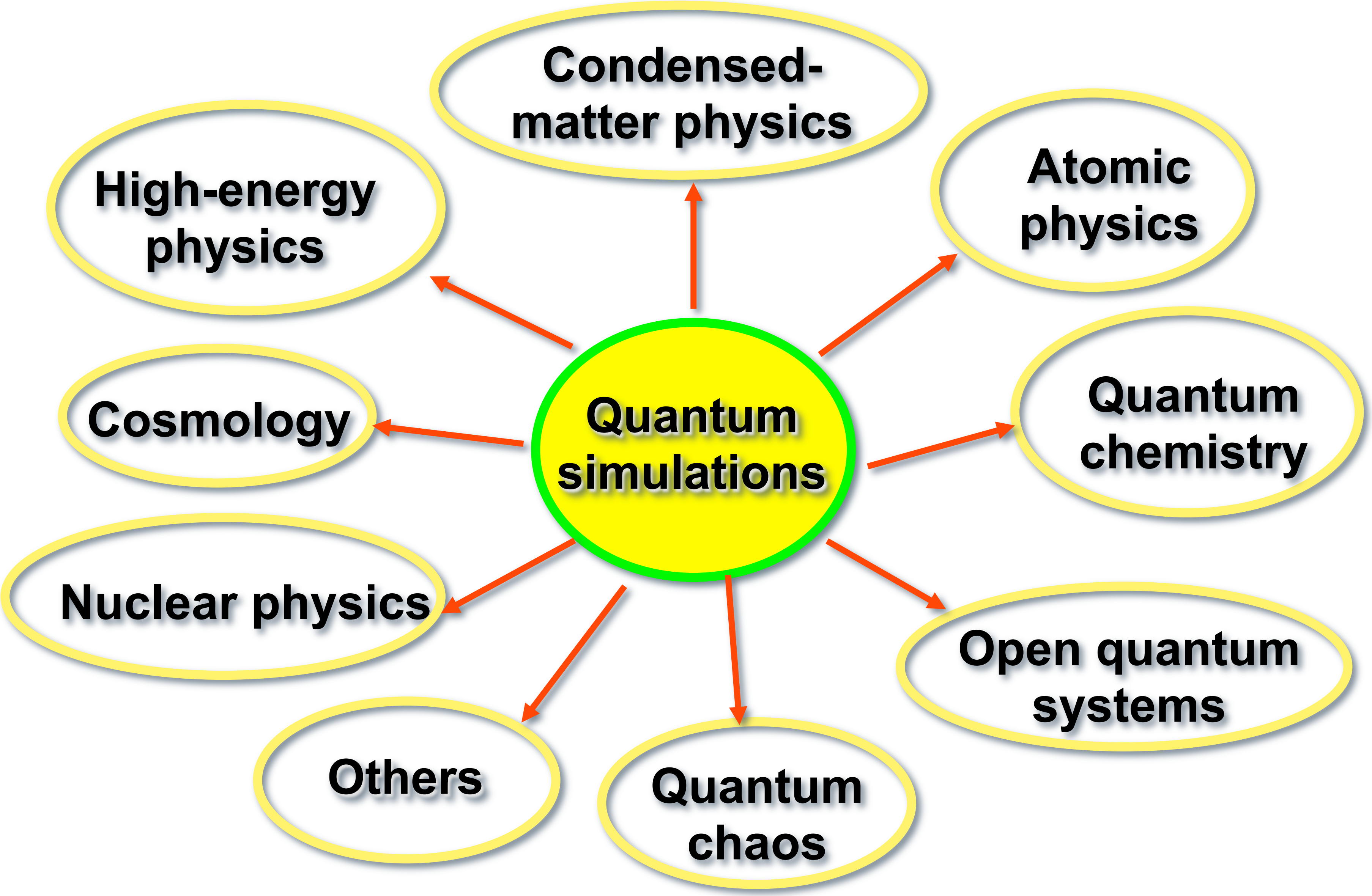
Digital quantum simulation: to use qubits to encode the state of the quantum system, "translate" its unitary evolution in terms of elementary quantum gates, and implement them in a circuitbased quantum computer.

Analog quantum simulation: to map the evolution of the system to be simulated onto the controlled evolution of the quantum simulator

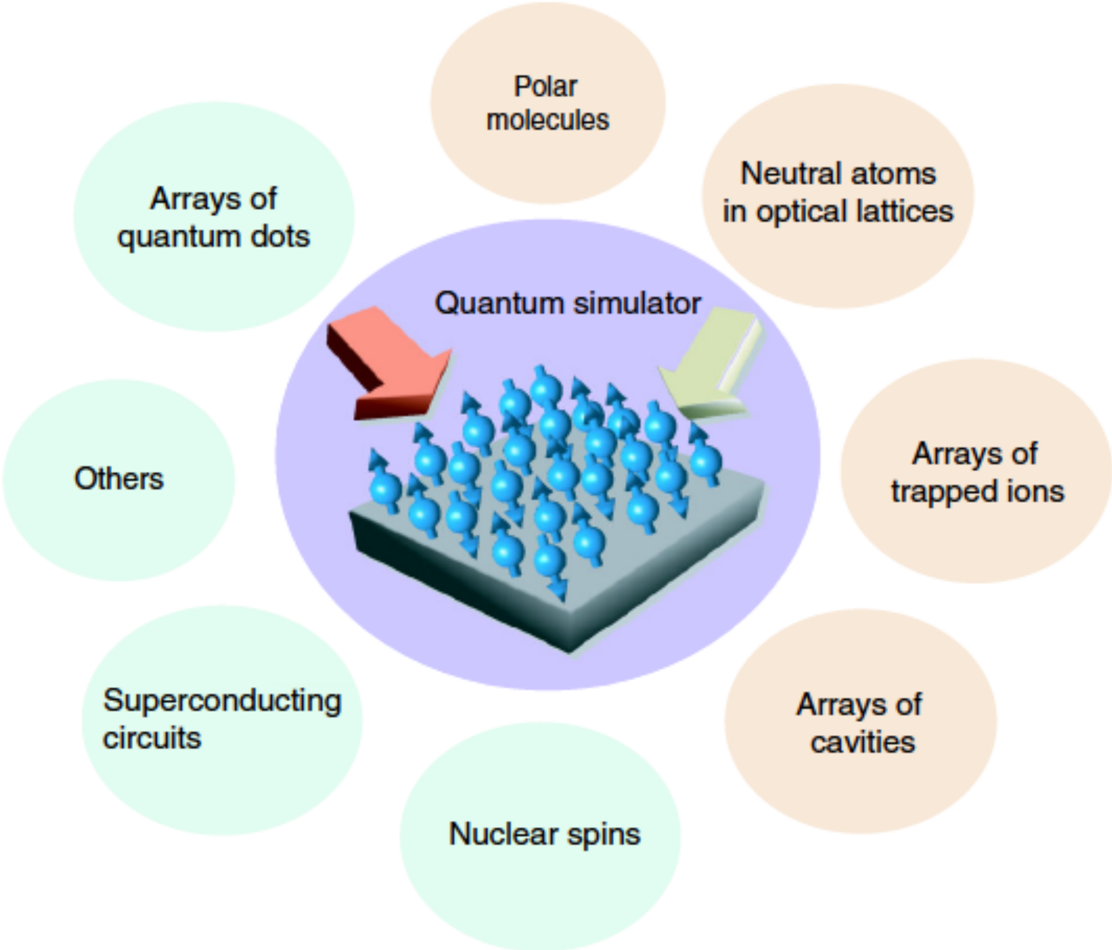
$$H_{sys} \leftrightarrow H_{sim}.$$

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

Applications of QS



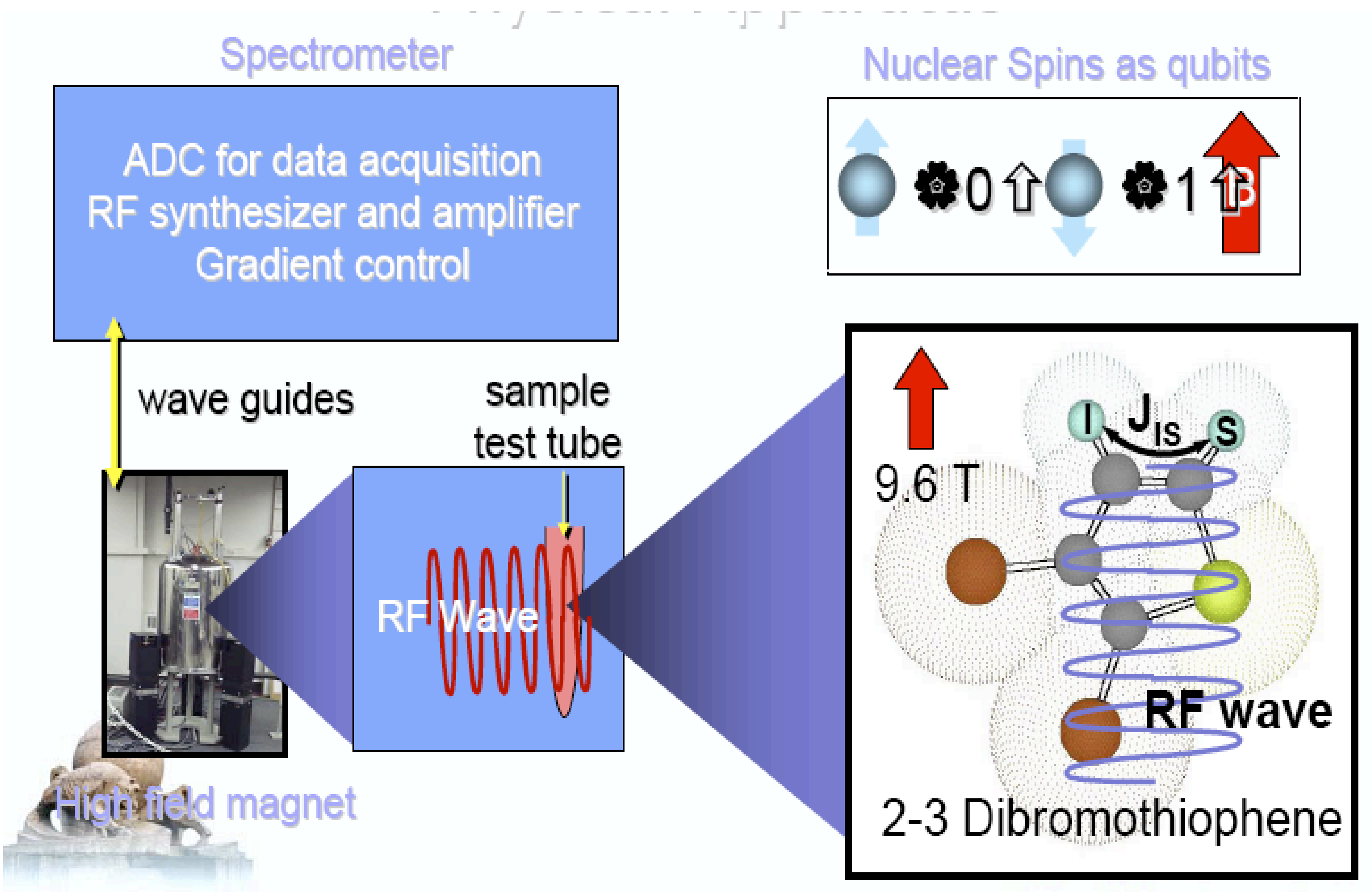
Physical implementations of QS



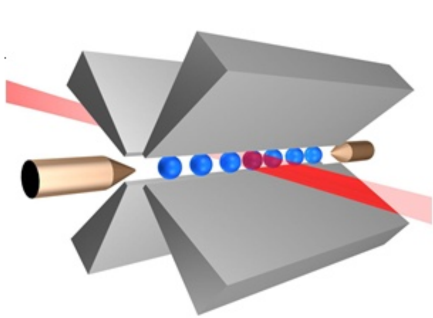
核自旋体系

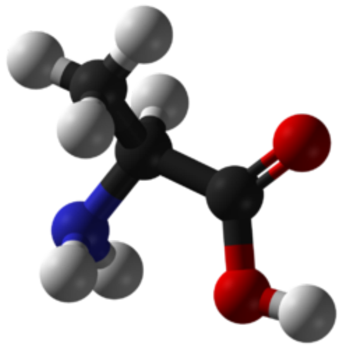
- 核自旋具有较长的消相干时间
- 相当成熟的磁共振技术
- 很好的测试平台

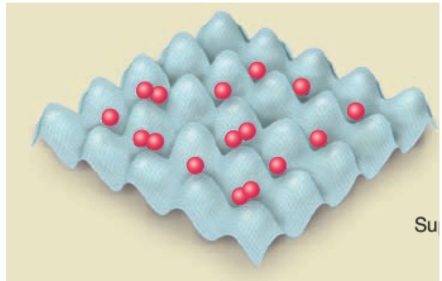
NMR QIP

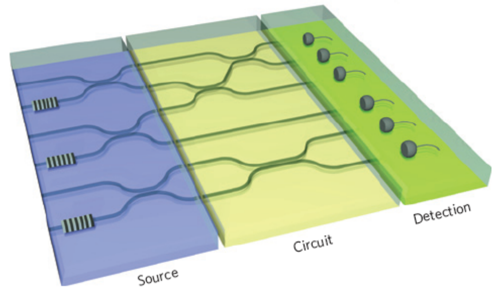

Spectrometer
ADC for data acquisition
RF synthesizer and amplifier
Gradient control
wave guides
sample
test tube
RF Wave
High field magnet
Nuclear Spins as qubits
0
1
9.6 T
I
J_{IS}
S
RF wave
2-3 Dibromothiophene

Different classes of quantum simulations









- **explore new physics (perhaps even trackable classically)**
- **outperform classical computation (address the classically non-trackabkle)**

Quantum harmonic and anharmonic oscillators

Many-fermion system

Quantum spin model (quantum phase transition)

Localization effects by decoherence

Quantum walk

Quantum chemistry

Quantum chaos

Paring Hamiltonian

Quantum Tunneling

Entropy 2010, *12*, 2268-2307

Basic principle of QS

Main steps

- ***Mapping***
- ***Initialization***
  - Direct state construction
  - Adiabatic quantum state preparation
- ***Hamiltonian engineering***
  - Lloyd’s method (Average Hamiltonian theory)
  - Quantum network
- ***Measurement***
  - Quantum state tomography (full characterization)
  - Phase estimation algorithm (Energy spectrum and eigenstates)
  - Specialized measurement scheme to extract the desired observables (e.g., correlation functions)

Mapping

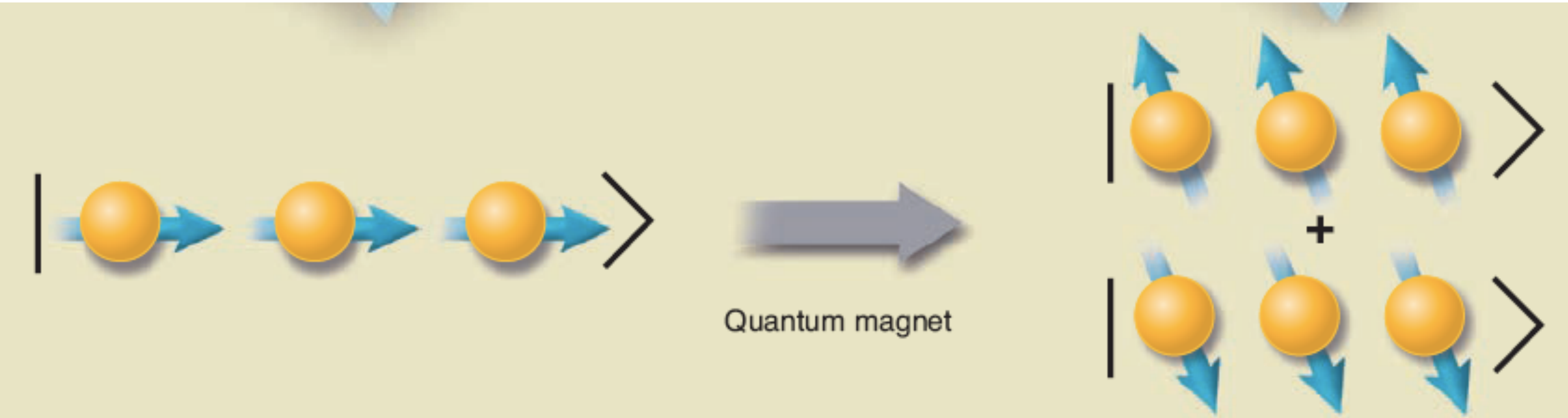
Quantum spin model (Quantum magnets)

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

External fields Heisenberg couplings

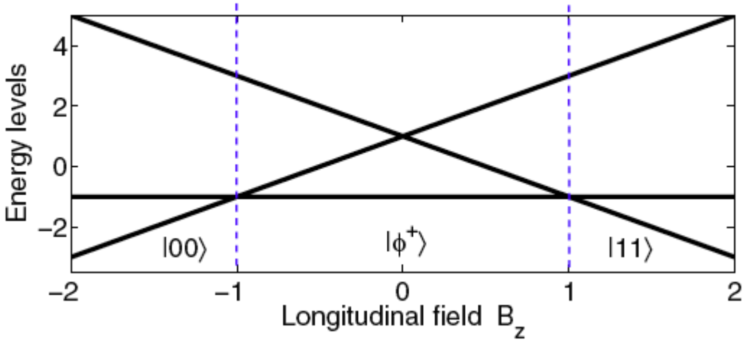
Heisenberg isotropic, Ising, XX, XY, XYZ model

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



Simulating quantum-spin-systems

$$H = B^z \sum_i \sigma_i^z + J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z$$



<u>First-order phase transition</u>

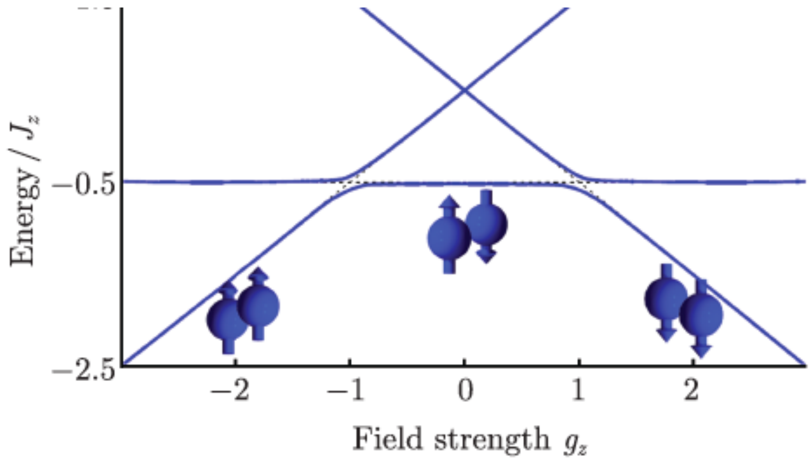
<u>how to simulate</u>

<u>Ising model</u>

- ➔ **spin σ**
- ➔ **magnetic field B**
- ➔ **Spin-spin interaction J**
- ➔ **ground state**
- ➔ **detection**

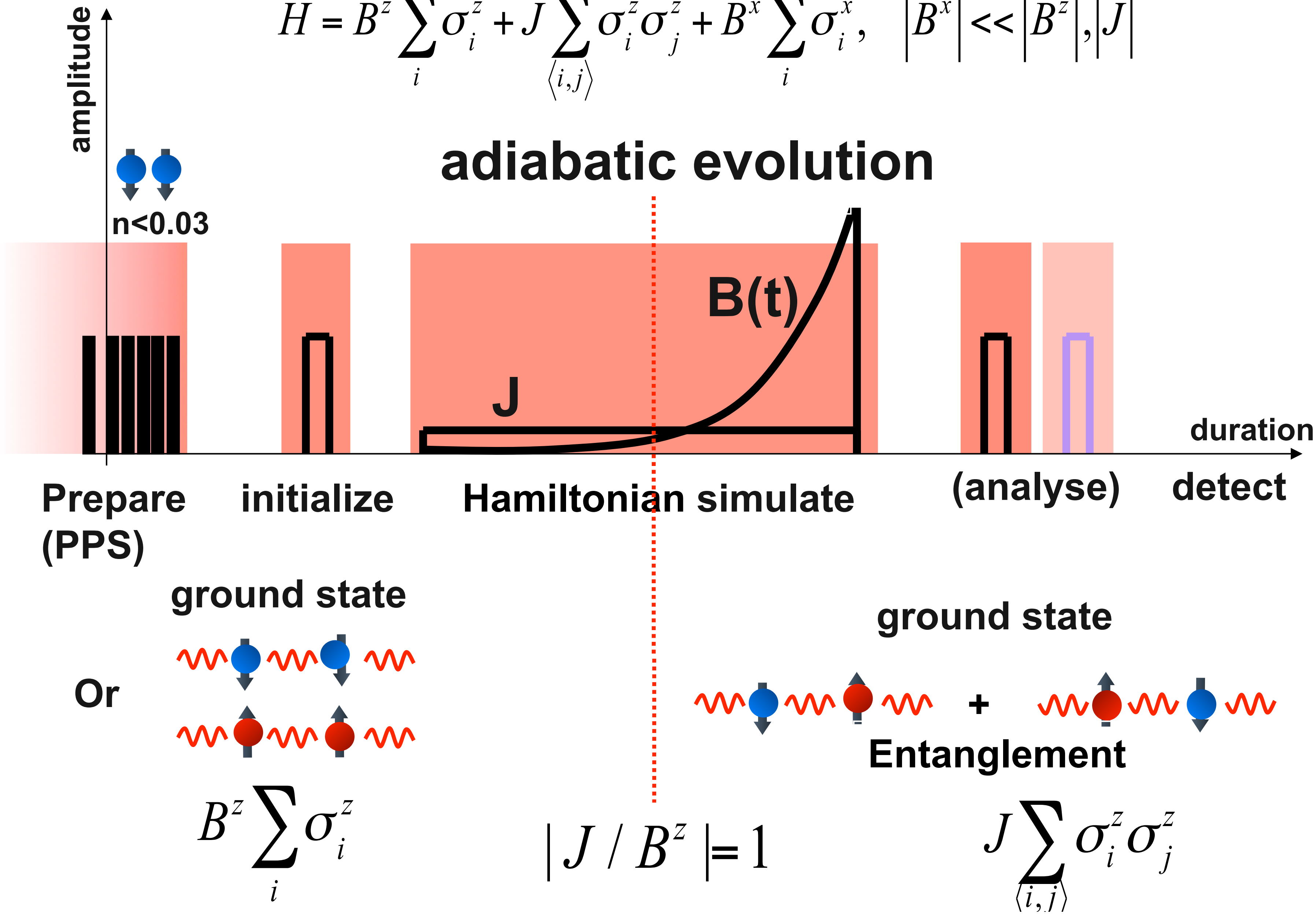
$$H = B^z \sum_i \sigma_i^z + J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z + B^x \sum_i \sigma_i^x, \quad \left|B^x\right| << \left|B^z\right|, \left|J\right|$$

- ➔ ***Nuclear spins***
- ➔ ***Average Hamiltonian theory***
- ➔ ***Use pseudo-pure states***
  & Adiabatic evolution
- ➔ ***Landau-Zener anticrossing***



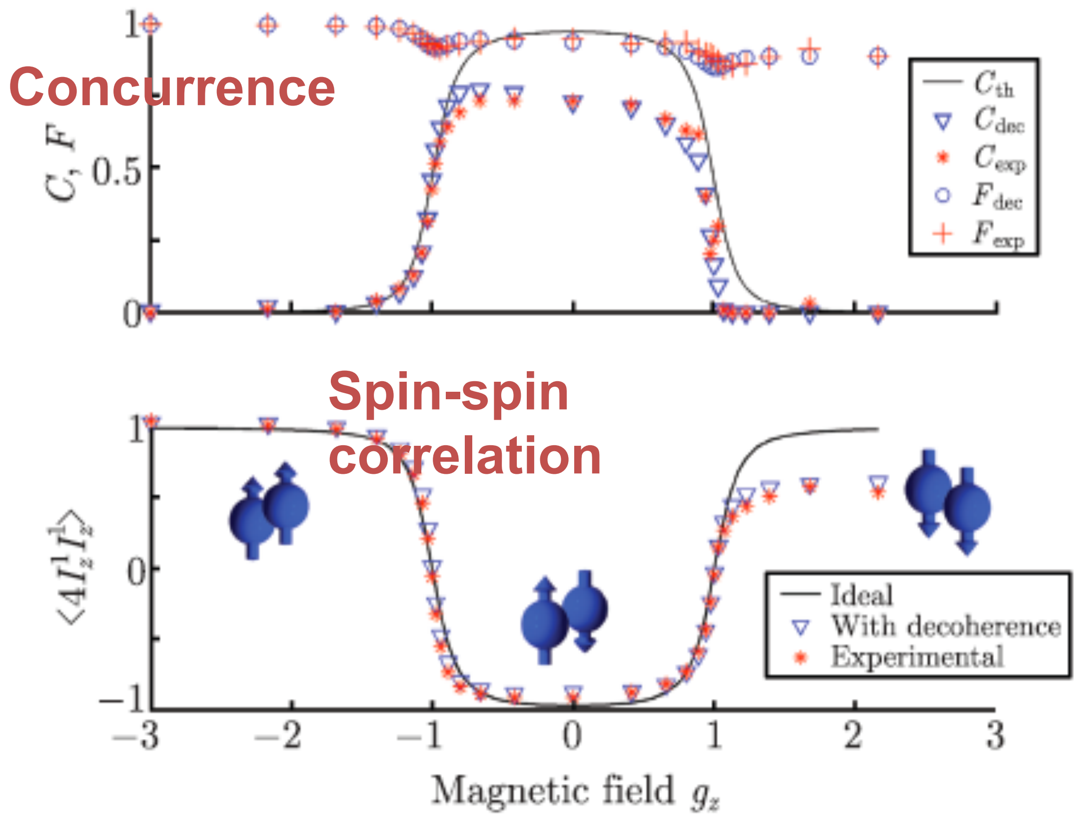
Quantum "baby" phase transition

$$H = B^z \sum_i \sigma_i^z + J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z + B^x \sum_i \sigma_i^x, \quad |B^x| << |B^z|, |J|$$



Entanglement and QPTs

Change in the ground-state wavefunction in the critical region: the concurrence as a function of **λ.**



XH Peng et al., PRA 72, 052109 (2005)

simulating a quantum magnet

2008年德国研究小组在离子阱中的类似实现

LETTERS

Simulating a quantum magnet with trapped ions

两个离子

A. FRIEDENAUER*, H. SCHMITZ*, J. T. GLUECKERT, D. PORRAS AND T. SCHAETZ†
Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany

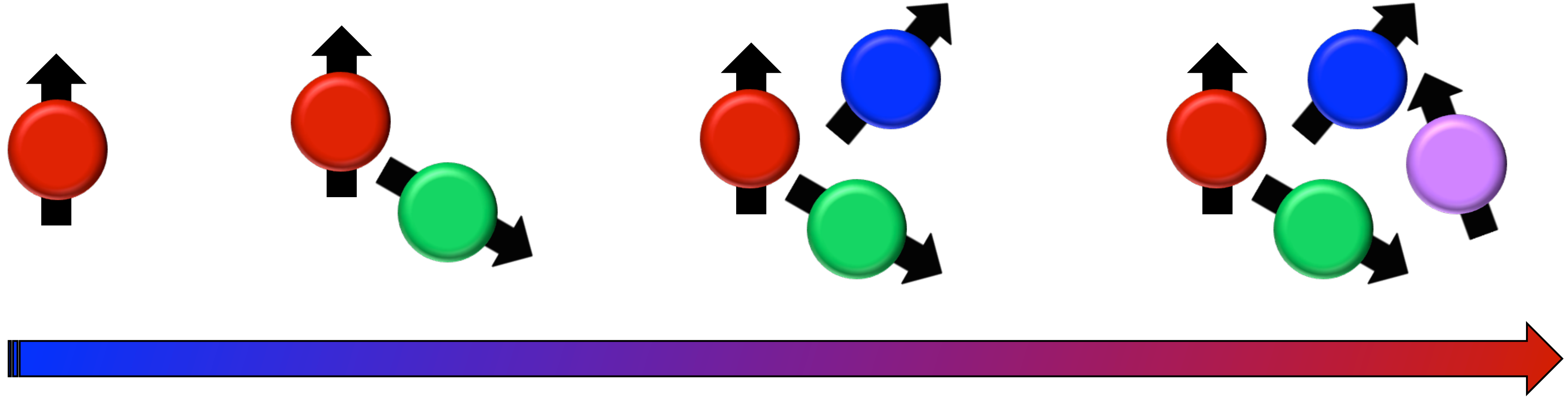
nature physics | VOL 4 | OCTOBER 2008 |

Here we study the building blocks for simulating quantum spin Hamiltonians with trapped ions[2]. We experimentally simulate the adiabatic evolution of the smallest non-trivial spin system from paramagnetic into ferromagnetic order with a quantum magnetization for two spins of 98%. We prove that the transition is not driven by thermal fluctuations but is of quantum-mechanical origin (analogous to quantum fluctuations in quantum phase transitions[3]). We observe a final superposition state of the two degenerate spin configurations for the ferromagnetic order ($|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle$), corresponding to deterministic entanglement achieved with 88% fidelity. This method should allow for scaling to a higher number of coupled spins[2], enabling implementation of simulations that are intractable on conventional computers.

译注：实验模拟了最小非平凡的两自旋体系从顺磁序到铁磁序的绝热演化。……我们观察到铁磁序的两个简并组态的叠加态，取得了88%保真度的确定性纠缠。

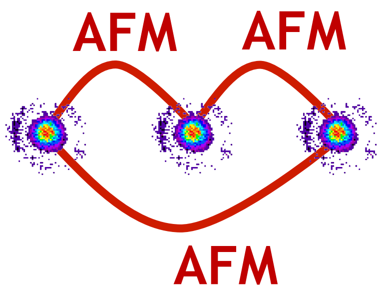
Exotic quantum many-body physics

Spin Chain (complex interaction)

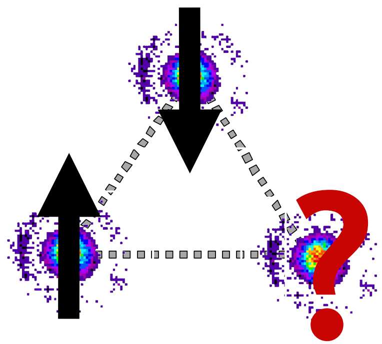


Many-body interaction

New Physics?



$J_{12}=J_{13}=J_{23} > 0$



Degenerated ground state

Frustration

Entanglement

多自旋系统的绝热量子模拟

2005	2009	2014	2014
2自旋	3自旋	4自旋	5自旋
PRA	PRL	PRL	PRL
首次的尝试 绝热量子模拟	三体相互作用 新的相变类型	四体相互作用 拓扑量子相变	32自旋体系 压缩量子模拟

2002年关于“多体系统中纠缠和量子相变”的研究引发了这一领域一系列重要的理论工作，然而，没有任何的实验验证。

Phys. Rev. A 72, 052109 (2005)

Phys. Rev. Lett. 103, 140501 (2009)

Phys. Rev. Lett. 113, 080404(2014)

Phys. Rev. Lett. 112, 220501 (2014)

What about thermal systems?

Previous experiments:

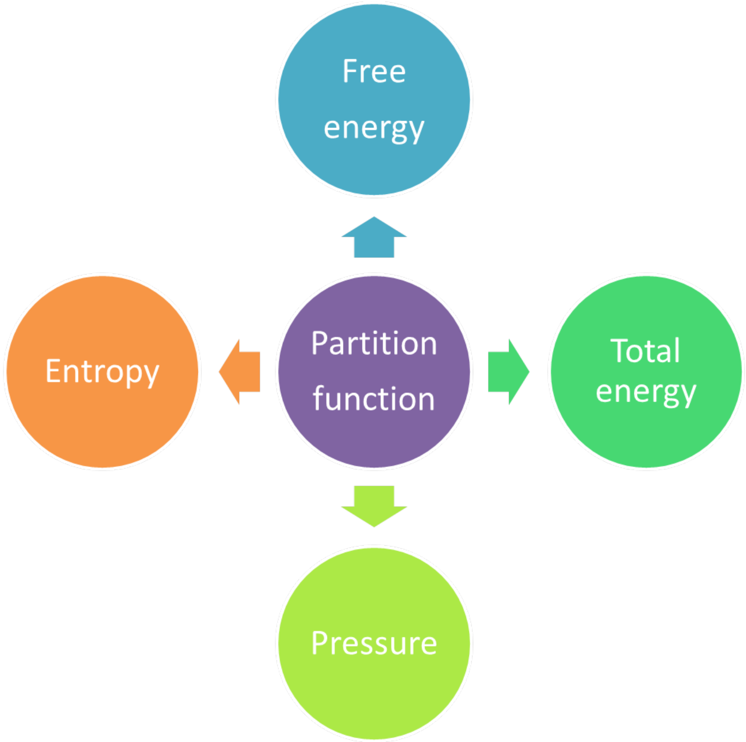
QPT $\Longleftrightarrow$ **Simulating ground states (T = 0)**

Thermal systems (T > 0)?

Partition functions

$$Z(\beta, h) = \mathrm{Tr}[e^{-\beta H}]$$

describe the statistical properties of a system in thermodynamic equilibrium and play a central role in statistical mechanics.



Thermal systems: Lee-Yang Zeros

1952, T. D. Lee and C. N. Yang:

Phys. Rev. 87, 410–419 (1952)

Lee Yang Zeros: Partition functions of thermal systems vanish at certain points on the complex plane of fugacity or a magnetic field.

Unit-circle theorem: All zeros of a general Ising ferromagnet are purely imaginary and located on the unit circle.

$$Z(\beta,h)=p_0 e^{\beta N h}\Pi_{n=1}^{N}(z-z_n) \qquad z_n = e^{i\theta}$$

Imaginary → not physical

$$z=e^{-2\beta h}$$

Wick rotation

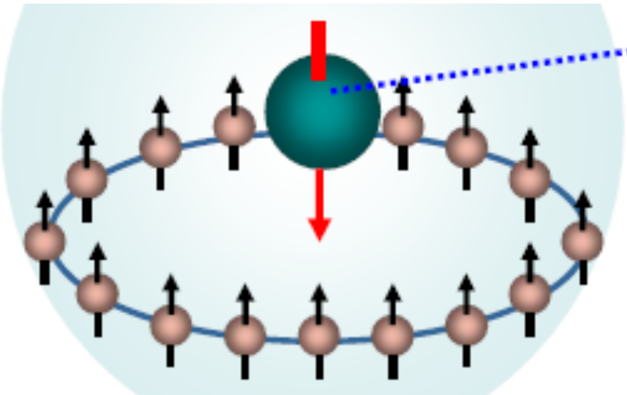
imaginary inverse temperature → time → Observable

Lee-yang zeros and spin coherence

arbitrary Ising model: $H(h) = -\sum J_{ij}\sigma_i\sigma_j - h\sum\sigma_j$

probe-bath coupling: $H_I = -2\lambda S_z\sum\sigma_j \equiv -2\lambda S_z H_1 \equiv -S_z B$

$$[H(h), H_I] = 0$$



Lee-Yang Zeros:

$$Z(\beta,h) = p_0 e^{\beta N h}\Pi_{n=1}^{N}(z - z_n) \qquad z_n = e^{i\theta}$$

Spin Coherence: $L(t) = e^{-2iN\lambda t}\dfrac{Z(\beta,\ h - i2t\lambda/\beta,)}{Z(\beta,\ h)}$

$$= e^{-2iN\lambda t}\frac{\prod_{n=1}^{N}(e^{-2\beta h}e^{4i\lambda t} - z_n)}{\prod_{n=1}^{N}(e^{-2\beta h} - z_n)}$$

由于辅助比特和系统之间存在的相互作用，相当于在该热力学系统上附加一个虚数磁场偏移，这使得实验探测复参数空间中的李-杨零点成为可能。

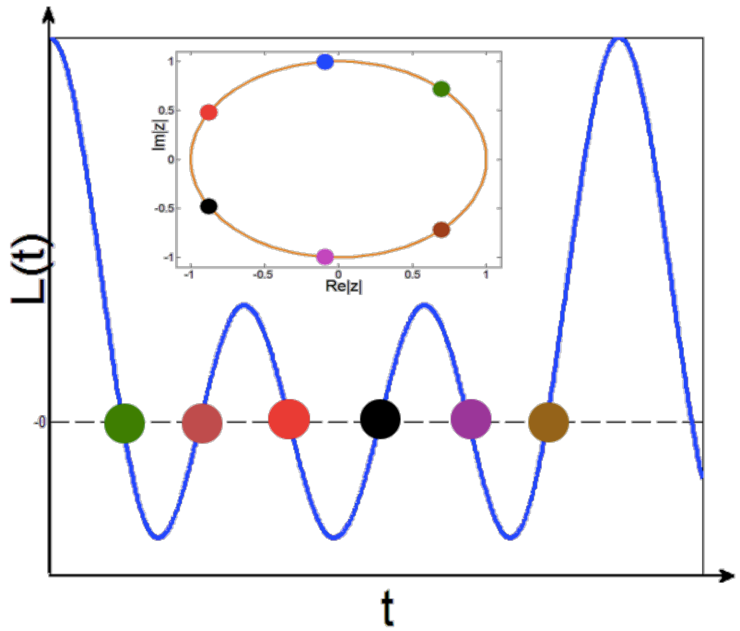
B.-B. Wei & R.-B. Liu. PRL 109, 185701 (2012)

• Lee-yang zeros and spin coherence

探测自旋的相干项包含了该系统的李-杨零点信息,尤其是在外磁场为零情况下:

$$h = 0 \Rightarrow 4\lambda t_n = \arg\left(z_n\right)$$

- ➢ **Imaginary Lee-Yang zeros now accessible**
- ➢ **Coherence zeros @ Lee-Yang zeros**



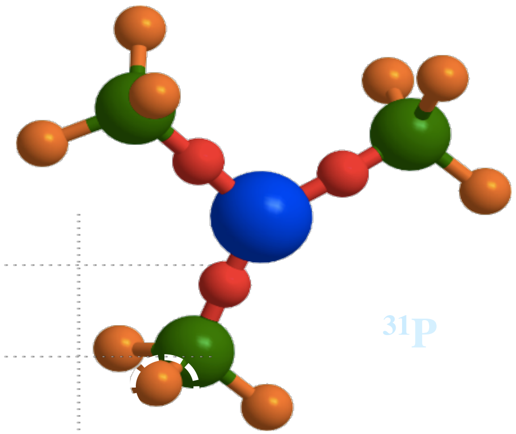
B.-B. Wei & R.-B. Liu. PRL 109, 185701 (2012)

• 实验体系

我们采用使用亚磷酸三甲酯(TMP)作为量子模拟器，9个等价的^{1}H核自旋(用$s_1, s_2, \ldots, s_9$表示，在实验中模拟铁磁相互作用长程Ising模型)和一个^{31}P核自旋(s_0，在实验中模拟探测自旋)，^{1}H与^{31}P之间耦合λ=10.57Hz。

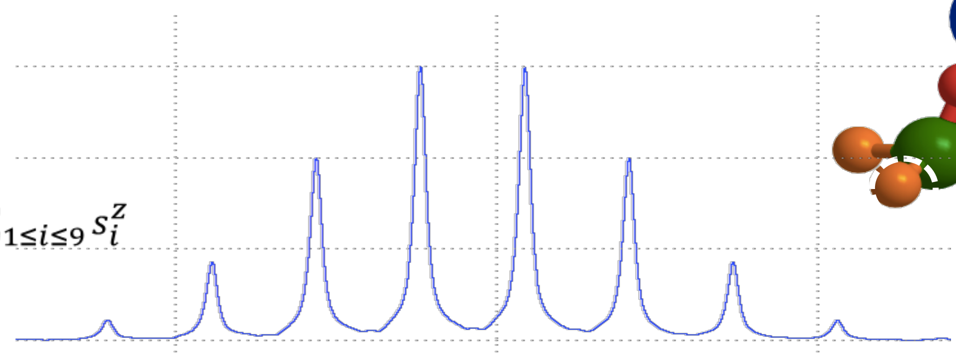
$$H_{\mathrm{TMP}} = -\nu_{\mathrm{H}} \sum_{j=1}^{9} s_j^z - \nu_{\mathrm{P}} s_0^z - \sum_{1 \le i < j \le 9} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j + \lambda s_0^z \sum_{j=1}^{9} s_j^z$$

$$H_{\mathrm{eff}} = -J \sum_{1 \le i < j \le 9} s_i^z s_j^z - h \sum_{1 \le i \le 9} s_i^z$$



在室温条件下：

$$\rho_{eq}^{TMP} \cong \varepsilon_P s_0^z + \varepsilon_H \sum_{1 \le i \le 9} s_i^z$$



• 实验过程

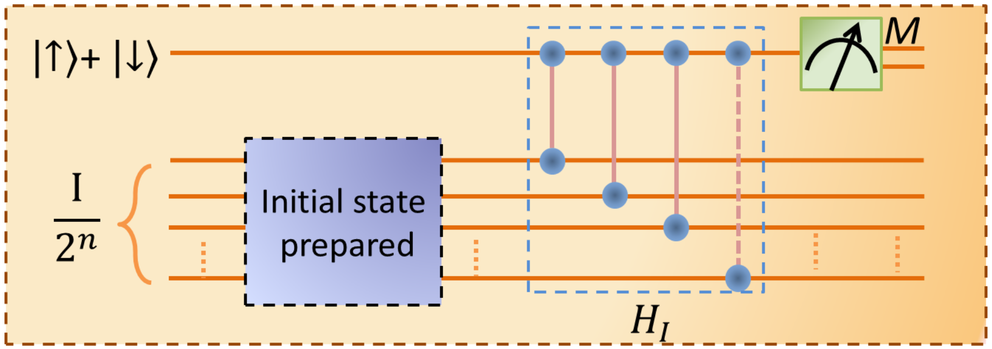
基于核磁共振量子模拟机，我们在实验上模拟探测了铁磁伊辛模型李-杨零点这一过程。

实验过程

初态制备

系统演化

测量



• 实验过程－ 有效温度模拟

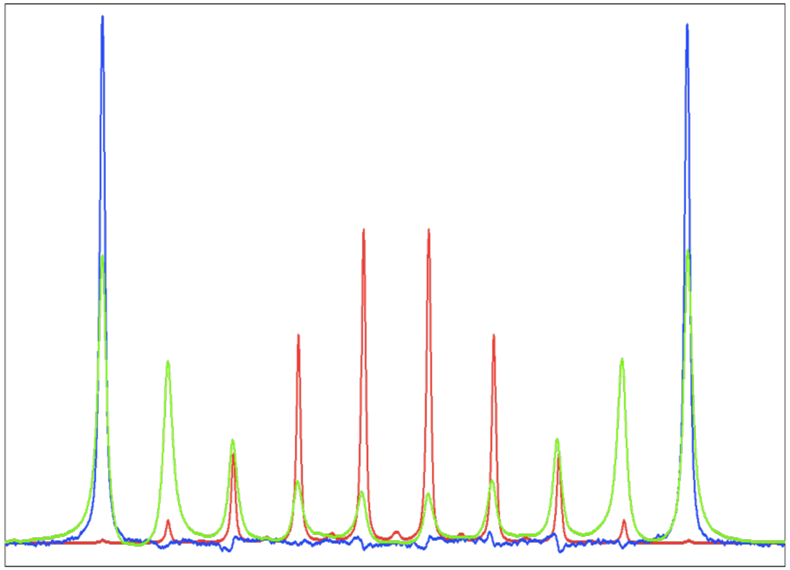
把探测自旋的初始状态一并考虑在内，我们需要制备$\rho_{in} = s_0^x \otimes \rho_{eff}$
由于ρ_m和^{31}P的每个共振谱线对应，我们可以对特定的共振谱线进行激发，并使不同谱线之间激发的强度满足不同有效初始态要求。

➢ 实验模拟实现不同有效温度系统的NMR谱线

红色→ $T_{eff} = \infty$

绿色→ $T_{eff} = 15J/8$

蓝色 → $T_{eff} = 9J/40$

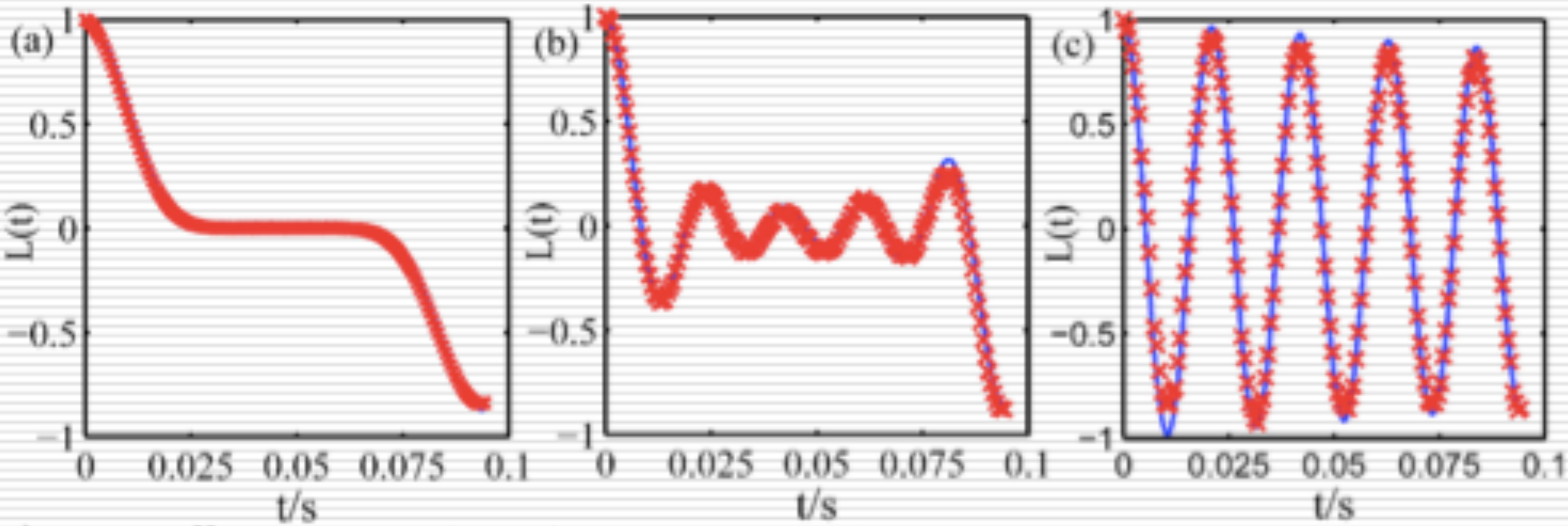


为了确定初始态制备的成功，通过部分态层析方法：

保真度$F = Tr[\rho_{exp} * \rho_{th}] / \sqrt{Tr[\rho_{exp}^2 * \rho_{th}^2]} > 0.99$

• 实验结果

探测自旋的相干$L(t)$的实验数据点可以通过^{31}P的FID直接获得。

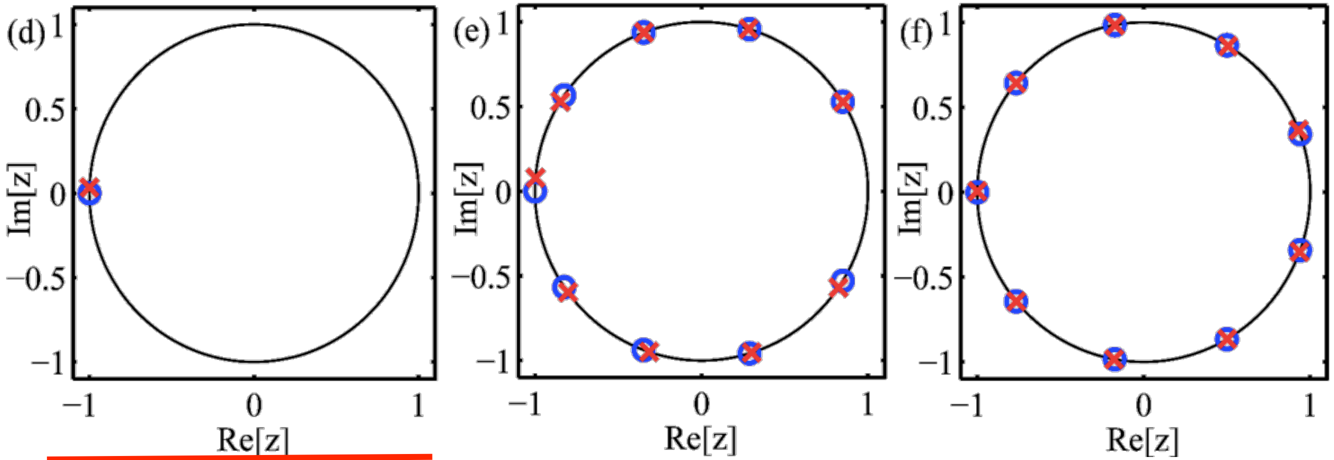


➤ 红色X号表示实验中辅助比特相干随时间的演化结果，蓝色实线表示理论预期结果。从左至右分别对应了有效温度$T_{eff} = \infty$、15J/8、9J/40

最后我们用多项式拟合对实验数据进行拟合获得相干$L(t)$的零点t_n。

• 实验结果

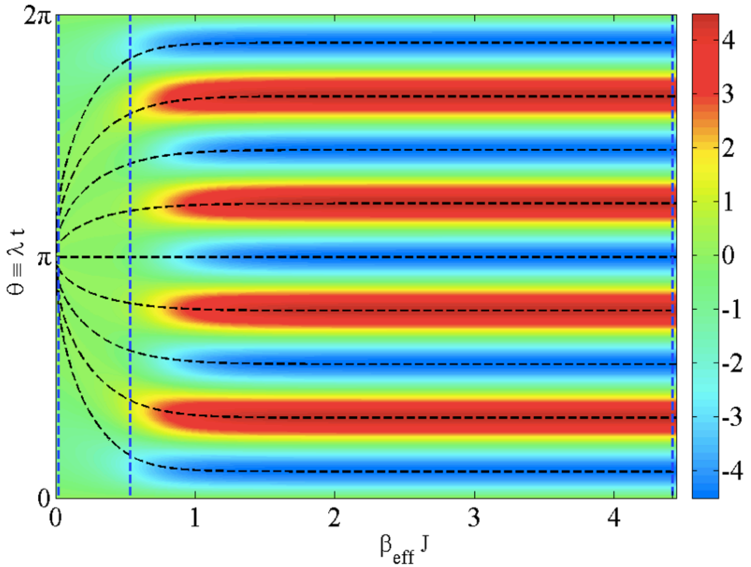
一旦知道t_n，利用公式$z_n = e^{-i\lambda t_n} = e^{-i\theta_n}$，单位圆上的李−杨零点就可以获得。

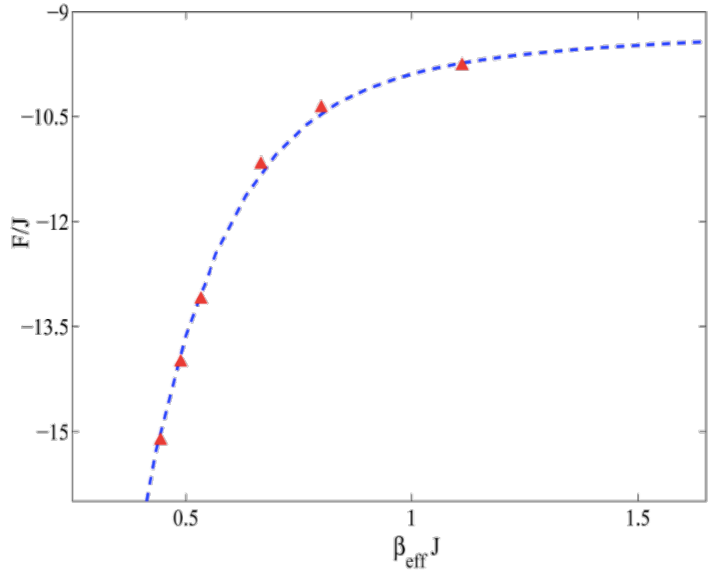


➢ 红色X号表示实验中辅助比特相干测量到的李−杨零点，蓝色圆圈表示理论预期结果。从左至右分别对应了有效温度$\mathrm{T_{eff}} = \infty$、15J/8、9J/40

在高温情况下（$T_{eff} \to \infty$），探测相干的灵敏度$\partial_\theta L(\theta, \beta_{eff}) \to 0$，这会导致零点的偏差非常大，在这种情况下，我们用用平均结果去计算相干的零点$t_n = (t_1 + t_9)/2$，其中t_1、t_2分别是在小于标准偏差η时拟合所得相干的起始点、末尾点。

• 实验结果





探测自旋相干$L(\mathrm{t})$对于演化时间t的敏感度$\partial_\theta L(\theta,\beta_{eff})$，其中$\theta=\lambda t$。黑色虚线是李-杨零点在不同等效温度$\beta_{eff}$时的位置。蓝色虚线表示我们实验上所模拟的等效温度。

通过实验上李-杨零点所计算出**Ising**模型的自由能。红色三角形是不同等效温度的实验数据，蓝色虚线是理论结果

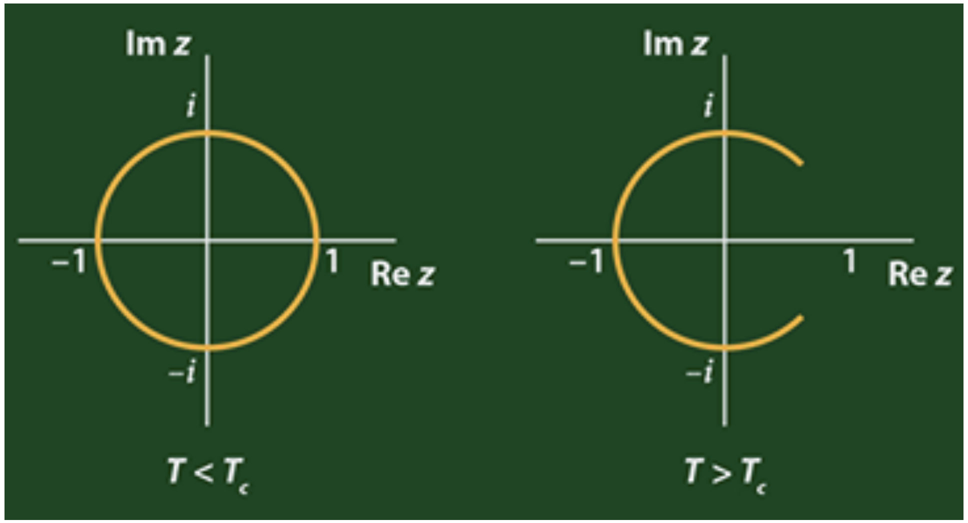
Phase transition

Phase transitions are intimately connected to the Lee-Yang zeros.

Critical temperature

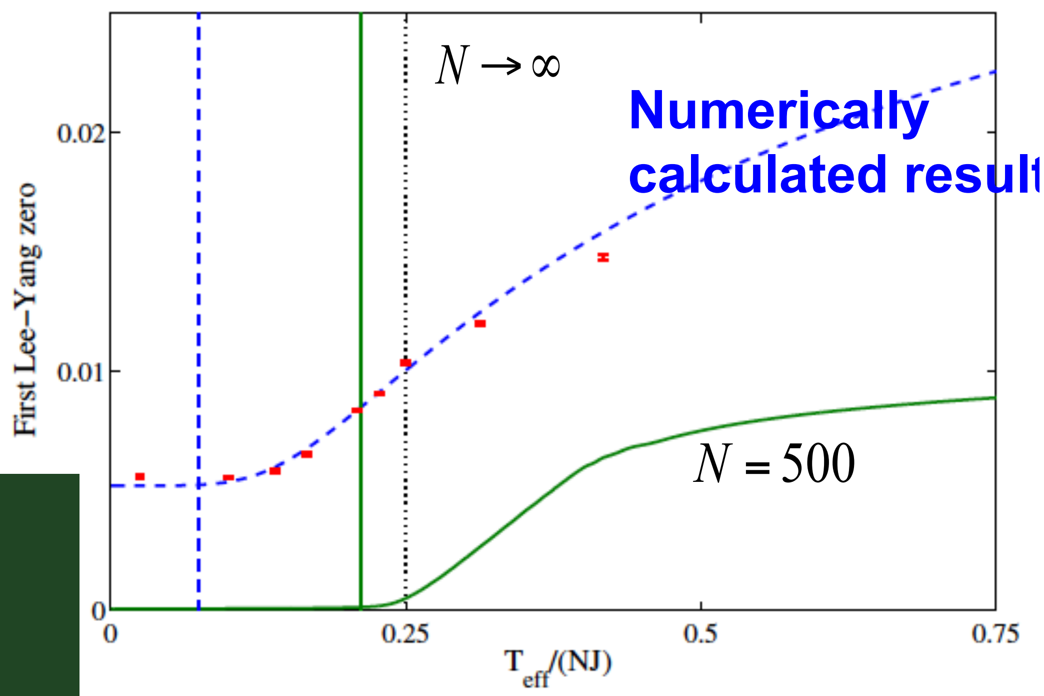
$N \to \infty$ $\quad k_B T_C / J = 1$

Evidences of onset of time-domain phase transitions (finite temperature)



$N = 9 \quad N = 500$

Finite-size effect



Phys. Rev. Lett. 114, 010601 (2015)
Collaborate with Prof. R. B. Liu

该工作发表于 Phy.Rev.Lett 后，美国物理协会（APS）的物理栏目以“Viewpoint”形式对该研究成果做了“真实世界中的虚磁场（Imaginary Magnetic Fields in the Real World）”的专题介绍。

Physics

Physics **8**, 2 (2015)

Viewpoint

Imaginary Magnetic Fields in the Real World

Nerses Ananikian
A. I. Alikhanyan National Science Laboratory, 0036 Yerevan, Armenia

Ralph Kenna
Applied Mathematics Research Centre, Coventry University, Coventry CV1 5FB, United Kingdom

Published January 5, 2015

Imaginary magnetic fields predicted by the fundamental theory of phase transitions can be realized experimentally.

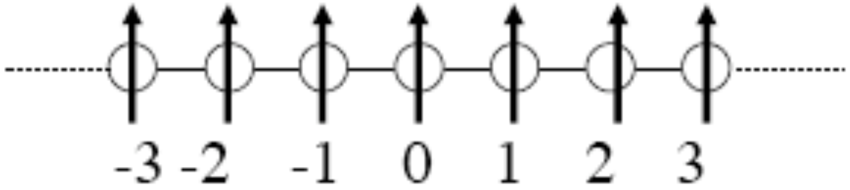
Subject Areas: **Statistical Physics**

A Viewpoint on:
Experimental Observation of Lee-Yang Zeros
Xinhua Peng, Hui Zhou, Bo-Bo Wei, Jiangyu Cui, Jiangfeng Du, and Ren-Bao Liu
Physical Review Letters ***114****, 010601 2015* – Published January 5, 2015

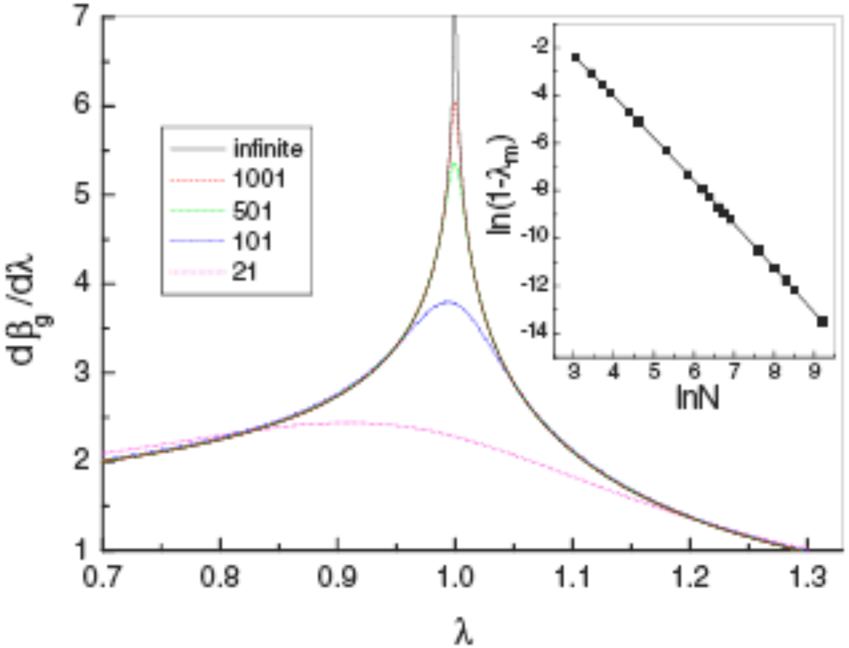
-----Physics 8, 2 (2015)

Non-equilibrium systems?

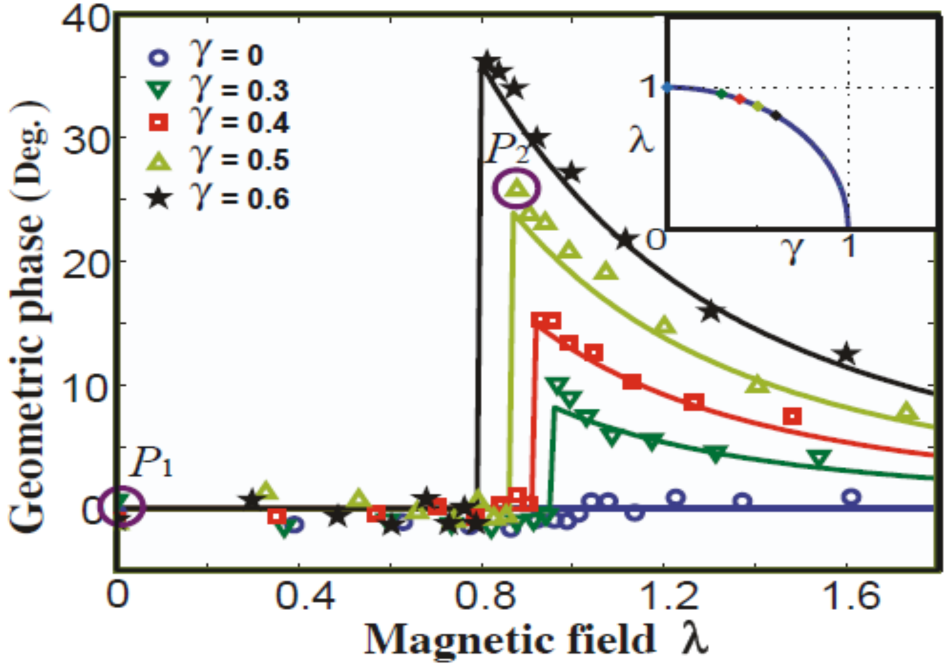
XY spin chain



Theoretical



Experimental



S.-L. Zhu, Phys. Rev. Lett. (2006)

X. H. Peng, Phys. Rev. Lett. (2010)

Ground-state geometric phase and QPT

Non-equilibrium systems

Dynamical quantum Hall effect in the parameter space

- **Non-adiabatic response:**

$$\begin{aligned}\mathcal{M}_\mu &= -\langle \psi_0(t_f)|\partial_\mu \hat{\mathcal{H}}|\psi_0(t_f)\rangle \\ &= \text{const} + \mathcal{F}_{\mu\nu} v_\nu + \mathcal{O}(v^2)\end{aligned}$$

Conditions:

(i) the velocity v_ν is turned on smoothly

(ii) the system is prepared initially in a state with a large gap

(iii) there is a weak dephasing mechanism in the system and the time of experiment is longer than the dephasing time.

Berry curvature

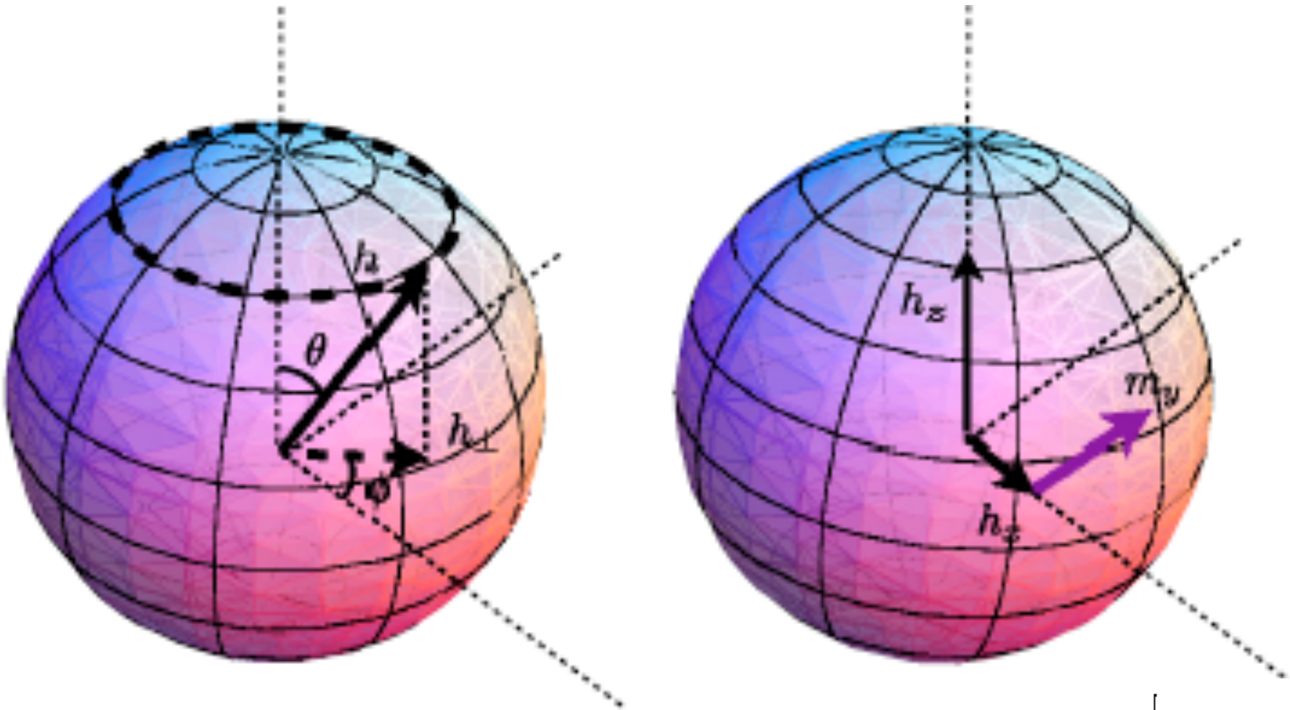
$$\mathcal{F}_{\mu\nu} = i \sum_{n \neq 0} \frac{\langle \psi_0|\partial_\mu \hat{\mathcal{H}}|\psi_n\rangle\langle \psi_n|\partial_\nu \hat{\mathcal{H}}|\psi_0\rangle - (\nu \leftrightarrow \mu)}{(\varepsilon_n - \varepsilon_0)^2}$$

The degeneracies contribute non-zero terms

V. Gritsev and A. Polkovnikov. PNAS, 109:6457 (2012)

Dynamcial QHE

Example: Single spin-1/2 particle



$$h_x(t) = h_x + v_x t$$

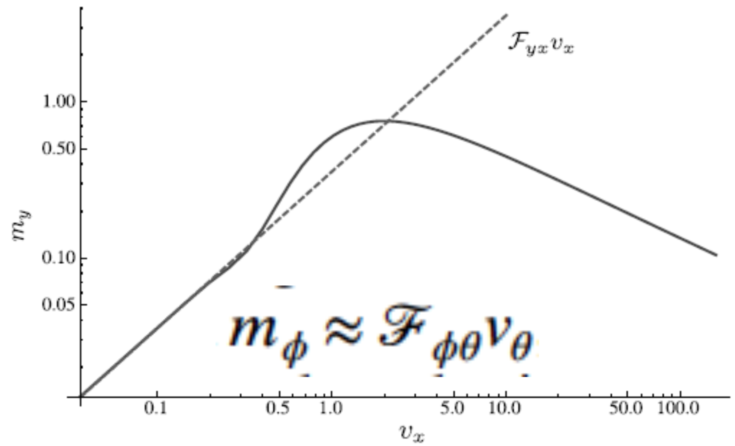
$$h_y(t) = 0$$

$$h_z(t) = 1$$

$$m_y = \langle \sigma_y \rangle$$

$$F_{yx} = h_z / 2h^3$$

$$\gamma = \pi(1 - \cos\theta) = \pi\left(1 - \frac{h_z}{h}\right)$$

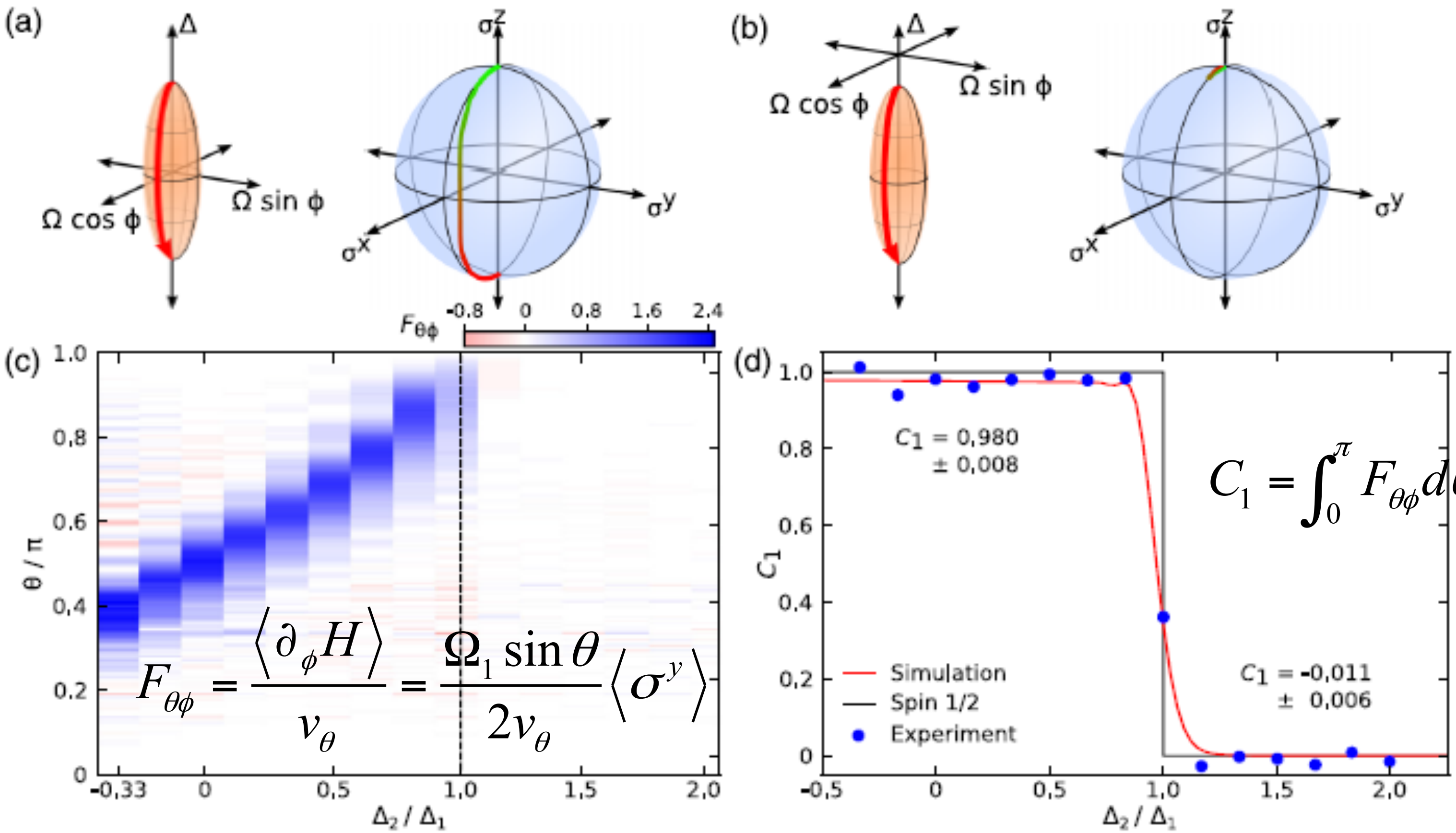


Previous experiments

- **Exp. 1:** an Artificial Spin-1/2 System PRL 113, 050402 (2014)

$$H/\mathrm{h} = \frac{1}{2}\left[\Delta\sigma_z + \Omega\sigma_x\cos\phi + \Omega\sigma_y\sin\phi\right]$$

$$\Delta = \Delta_1\cos\theta + \Delta_2 \qquad \Omega = \Omega_1\sin\theta$$



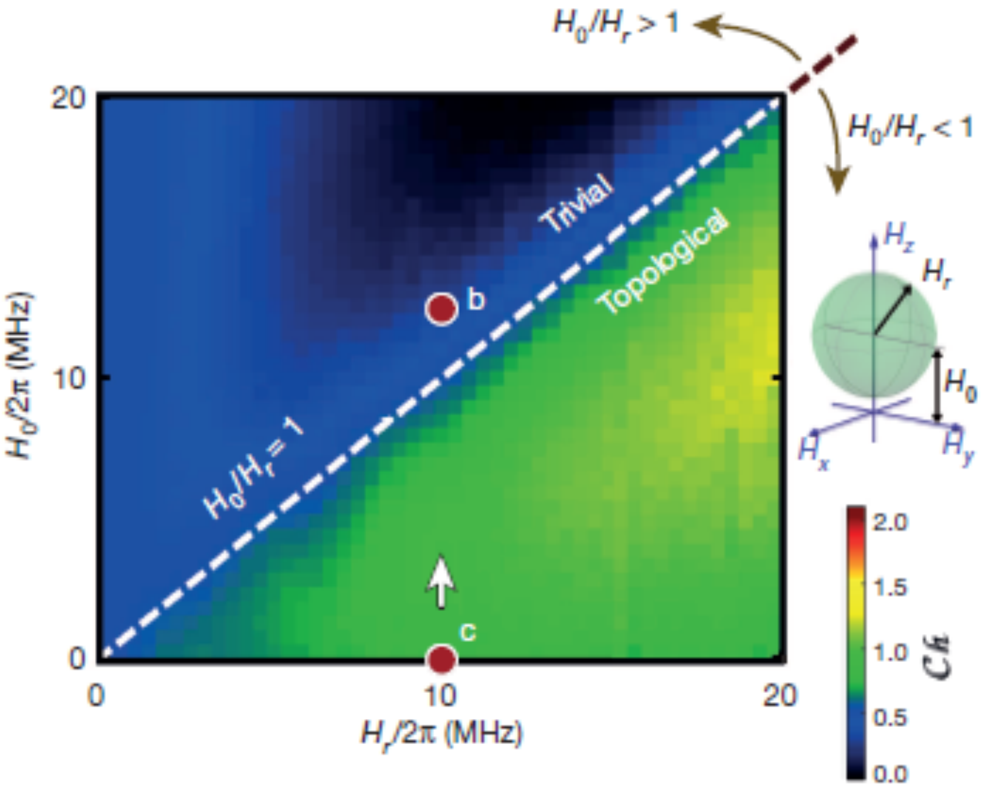
$$F_{\theta\phi} = \frac{\langle \partial_\phi H\rangle}{v_\theta} = \frac{\Omega_1 \sin\theta}{2v_\theta}\langle \sigma^y\rangle$$

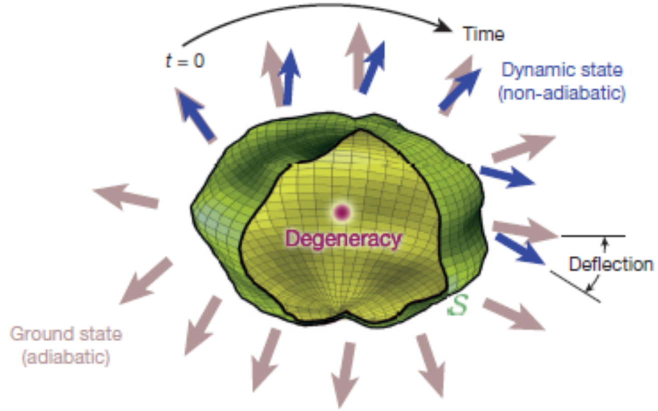
$$C_1 = \int_0^\pi F_{\theta\phi}\, d\theta$$

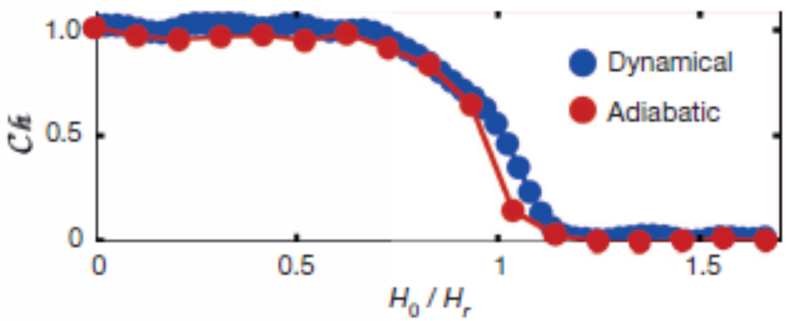
Previous experiments

- **Exp. 2: two-spin interacting quantum system**

$$H_{2Q} = -\frac{h}{2}\left[H_0\sigma_1^z + \mathbf{H_1}\cdot\boldsymbol{\sigma_1} + \mathbf{H_2}\cdot\boldsymbol{\sigma_2} - g\left(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y\right)\right]$$



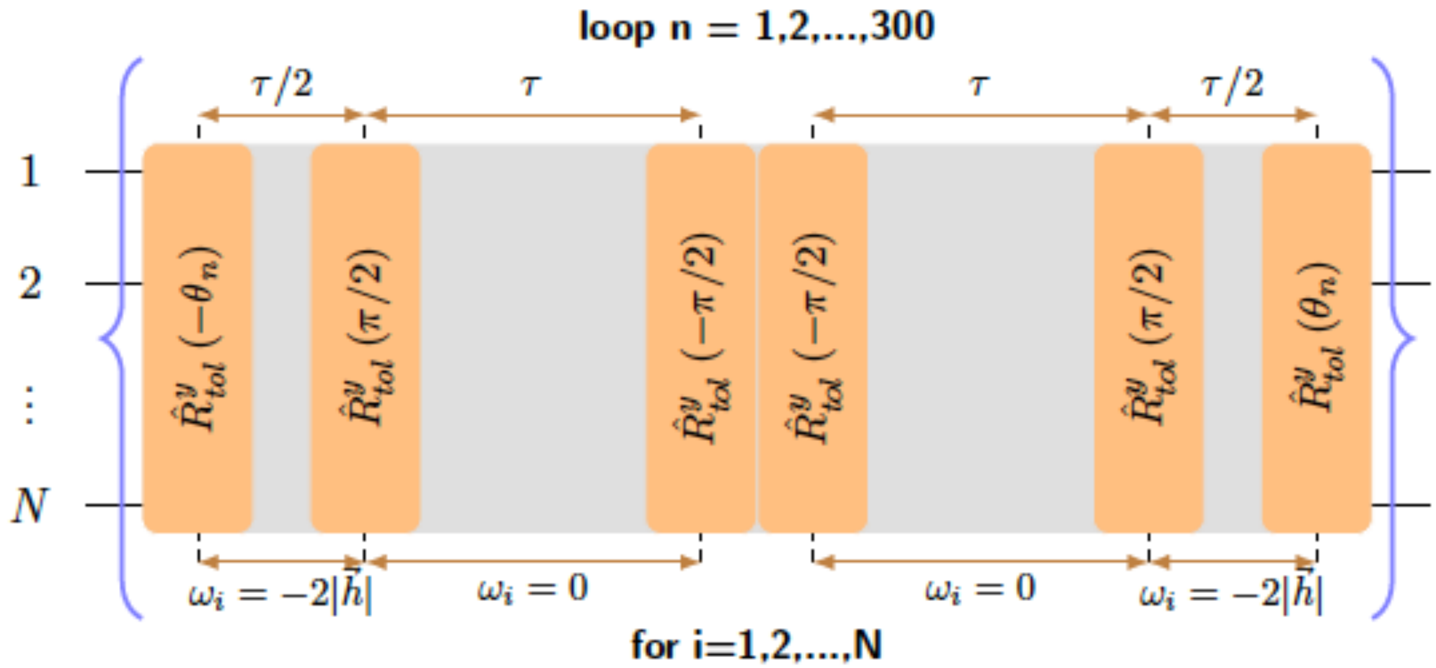




Nature. 515, 241 (2014).

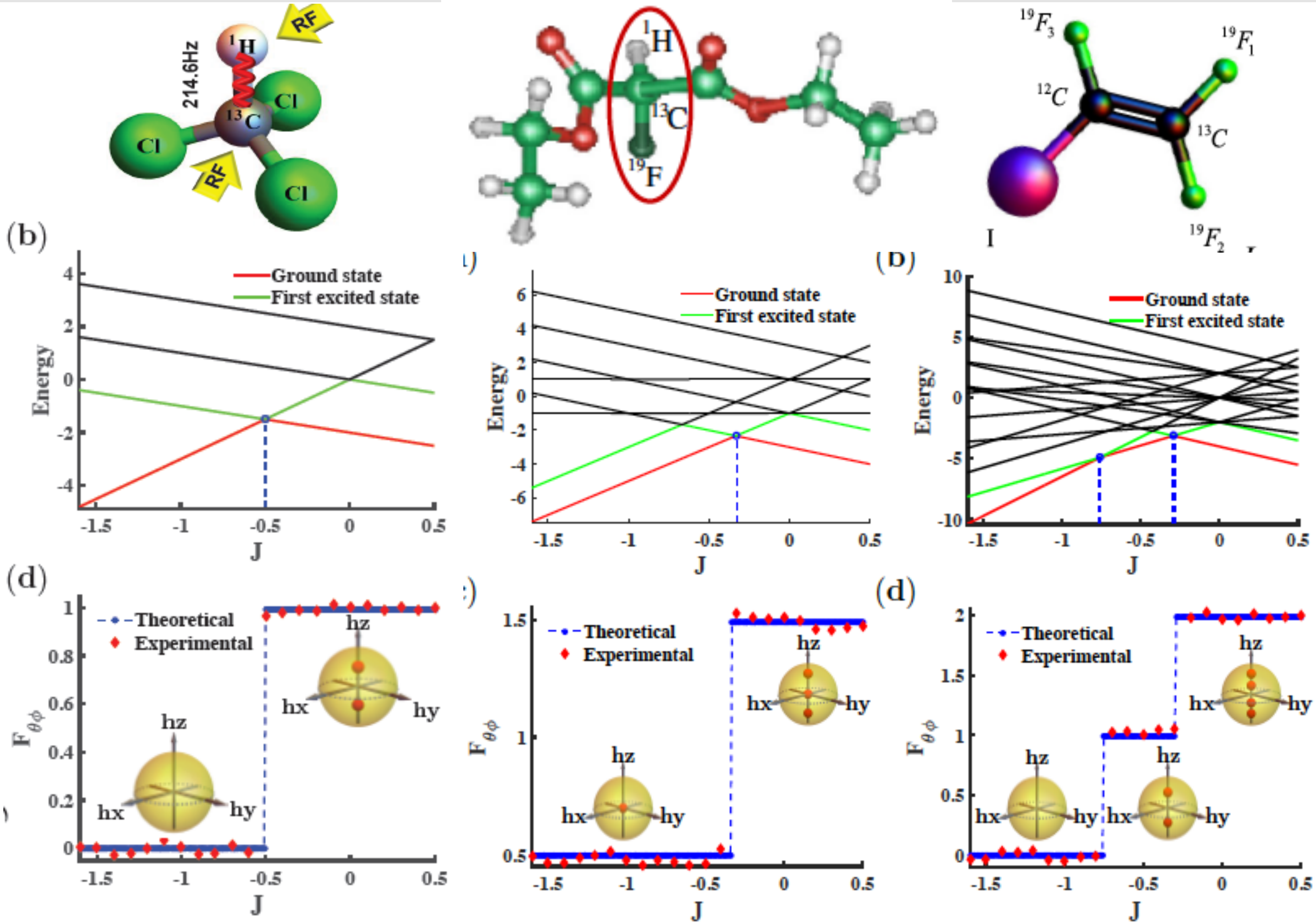
Dynamical quantum Hall effect

$$\hat{\mathcal{H}}_{\rm NMR} = \sum_{i=1}^{N} \frac{\omega_i}{2}\hat{\sigma}_i^z + \sum_{i<j,=1}^{N} \frac{\pi J_{ij}}{2}\hat{\sigma}_i^z\hat{\sigma}_j^z$$

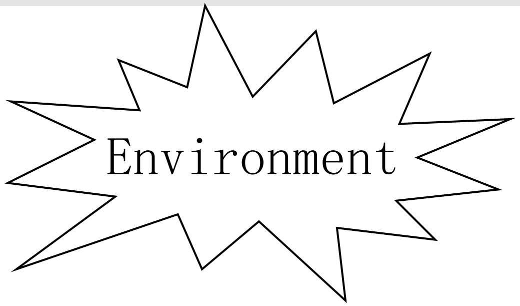


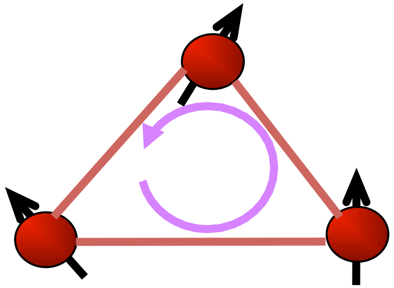
$$\hat{\mathcal{H}} = -\sum_{j=1}^{N} \vec{h}\cdot\vec{\sigma} - J\sum_{j=1}^{N-1} \vec{\sigma}_j \cdot \vec{\sigma}_{j+1}$$

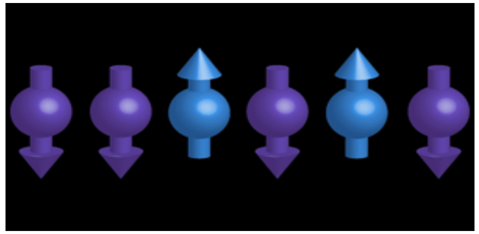
Experimental results



summary: novel physics

#1 

#2 

#3 

Decoherence ≠ error

➔ how to mitigate it
how to exploit it
(quantum control)

➔ how to investigate
(mesoscopic)
decoherence

scaling quantum simulations

➔ proof of principle on
spins

bridging the gap
(proof of principle studies and "useful" QS)

➔ outperforming classical computation
➔ deeper understanding of quantum dynamics
➔ new physical phenomena

investigate the impact on:

- Solid state physics (magnets, ferroelectrics, quantum Hall, high T_c)
  (quantum phase transitions, spin frustration, spin glasses,…)
- quantum information processing / quantum metrology
- …

Thanks to ……

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Prof. Renbao Liu
Prof. Supeng Kou
Prof. Dieter Suter
……

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Hui Zhou

Jun Li

Zhihuang Luo

Zhaokai Li

……

Funding:
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Spin Magnetic Resonance Lab
自旋共振实验室

Thanks for your attention!

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