

量子模拟多体物理

Heng Fan (范桁) Institute of Physics Chinese Academy of Sciences

2020年5月14日

Outline

- 1. 量子计算模拟多体物理主要进展
- 2. 量子计算优势(经典难)体现在什么地方?
- 3. 量子计算模拟多体物理适用于哪些问题?
- 4. 量子计算模拟怎样超越经典计算(量子优势)?
- 5. 量子计算实用化展望







量子计算机可有效模拟物理过程

"Nature isn't classical, dammit, and if you want to make a simulation of Nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem because it doesn't look so easy."

R. P. Feynman, 1981

two parts.

Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

4. QUANTUM COMPUTERS—UNIVERSAL QUANTUM SIMULATORS

The first branch, one you might call a side-remark, is, Can you do it with a new kind of computer—a quantum computer? (I'll come back to the other branch in a moment.) Now it turns out, as far as I can tell, that you can simulate this with a quantum system, with quantum computer elements.

Int.J.Theor.Phys. 1982

物理基础

1

量子计算机实现

数字式量子模拟动力学相变: 分解为量子逻辑门操作

横场lsing模型
$$H(g) = -\sum_{j}^{L} \sigma_{j}^{z} \sigma_{j+1}^{z} + g \sigma_{j}^{x}.$$



一个例子:量子模拟动力学相变

		R.x 🖉	Rx 🖉 Rx 🦉	Rx 🕗 - Rx 🕗 -
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	+ Rx - + Rz + Rx - + Rz + Rx		+ R2 + RX	+ Rz + Rx
6				
				Rz ++ + Rx -+ Rz ++ + Rx -+ Rx
	+ Rx - + Rz + Rx - + Rz +		+ RZ + RX	+ RZ + RX
12		Ree 🕜		
13 - + Rz + + + Rz + Rz + + + Rz + Rz +		Rx 🕜 - + Rz + + + Rx 🔗 - + Rz + + Rz + Rx 🔗 - + Rz +		Rz + + Rx - + Rz + + Rx -
14 + Rz + Rx 🖉 + Rz + Rx 🖉 + Rz + Rx	+ Rx 🖉 - + Rz + Rx 🖉 - + Rz +	Rx 🔼 + Rz + Rx 🖉 + Rz + Rx 🖉	+ Rz + Rx 🖉	+ Rz + Rx 🕗 + Rz + Rx 🖉

			Rx Rz Rz Rx	RZ + RZ RX				RZ + RX RX
+ R2 + RX + R2 + RX	+ RZ + RX + RX + RZ + RZ +		Rx + R2 + Rx Rx + Rz + Rx	+ Rz + Rx		x + Rz + Rx x + Rz + Rz + Rx	+ RZ + RX RX	
+ Rz + Rx		RZ + RX A RZ + RZ +	$\begin{array}{c} Rx \\ \hline & \\ Rx \\ \hline & \\ \hline \\ \hline$	A RZ + RZ + RX		x 2 + Rz + Rz + Rx		
Rz + Rz + Rx		Rz ++ Rx	Rx - Rz + Rz + Rx Rx - Rx - Rx			x 2 + Rz + Rz + Rx x 2 - + Rz + Rz + Rx		
+ R2 + R2 + Rx		R2 + RX + R2 +	Rx 2 + Rz + Rx Rx 2 + Rz + Rx			x 2 + Rz + Rz + Rx		
RZ + RZ + RX		Rz + Rx	Rx + Rz + Rx			x 2 + Rz + Rz + Rx		RX RX
Rz + Rx		Rz ++ Rz ++ Rz ++		Rz + Rz		x		
+ R2 + Rx 2	+ Rz	Rz + Rx	RX + RZ + RX Rx + Rz + Rx	+ R2 + Rz + Rx	Rz +	x + RZ + RZ + RX	+ R2 + R2 + Rx	+ Rz + Rx





g=0->4 , 通过相变点 有动力学相变点(QtVM)





g=0->0.5,没通过相变点 没有动力学相变点

量子模拟动力学相变:与精确对角化的对比

1



Analog Quantum Simulator





Martinis group, Nature 2016.

10-qubit GHZ PRL119, 2017.

Time dependent wave function can be readout by state tomography, physical quantities can then be obtained

$$H_{l} = -B_{x,l} \sum_{i} \sigma_{x}^{i}$$

$$H_{P} = -\sum_{i} \left(B_{z}^{i} \sigma_{z}^{i} + B_{x}^{i} \sigma_{x}^{i} \right) - \sum_{i} \left(J_{zz}^{i,i+1} \sigma_{z}^{i} \sigma_{z}^{i+1} + J_{xx}^{i,i+1} \sigma_{x}^{i} \sigma_{x}^{i+1} \right)$$

$$H = \sum_{i=1}^{9} \delta_{i} \hat{n}_{i} + \frac{\eta_{i}}{2} \hat{n}_{i} (\hat{n}_{i} - 1) + \sum_{i=1}^{8} g_{i} \left(\hat{a}_{i}^{\dagger} \hat{a}_{i+1} + \hat{a}_{i} \hat{a}_{i+1}^{\dagger} \right)$$

$$\frac{H}{\hbar} = \sum_{i < j} J_{ij} (\sigma_{i}^{+} \sigma_{j}^{-} + \sigma_{i}^{-} \sigma_{j}^{+}) + \sum_{i} (h_{i} + \delta h_{i}) \sigma_{i}^{+} \sigma_{i}^{-},$$

量子模拟进展: Analog Simulation



Quantum Simulator: Rydberg atoms, Ising型



Trapped ions quantum simulator: 横场Ising型



Time-crystal: trapped ions and NV (含时调控)



量子机器学习



Supervised learning with quantum-enhanced feature spaces

Nature 567, 209 (2019)

Many-body localization

(c) r_{P12} r_{Z} r_{Z} r_{Z









能谱读出

Google Martinis group, Science '17.

Many-body localization



Many-body localization with a 10 qubits quantum processor, PRL 120, 050507 (2018).

Many-body localization



Many-body localization:不同平台测量不同观测量



离子阱系统:热化/局域化,参数 Aj

冷原子光晶格:热化/局域化,参数W

1. Probing entanglement in a many-body–localized system, A. Lukin et al., Science 364, 256 (2019).

2. Probing Rényi entanglement entropy via randomized measurements, Tiff Brydges...P. Zoller, R. Blatt, C. F. Roos, Science 364, 260 (2019).

有噪音中等规模量子计算与量子模拟

利用19个超导量子比特模拟不同系统能量mobility edge现象



Q. Guo et al., arXiv:1912.02818.

5 Device with 24 qubits in a ladder configuration

Simulation of Bose-Hubbard ladder model



Phys. Rev. Lett. 123, 050502 (2019)

5 Device with 24 qubits in a ladder configuration

Simulation of Bose-Hubbard ladder model



有噪音中等规模量子计算与量子模拟





K. Xu et al., arXiv:1912.05150.





Fig. 5 | Dynamics of a hole defect in the Mott insulator. a, To explore

A dissipatively stabilized Mott insulator of photons, Ruichao Ma... David I. Schuster, Nature 566, 51 (2019).

Background: quantum walks(归入量子态演化)



Nature (2012),Gross, Bloch... optical lattice Nature (2014),Blatt, Roos... trapped ions Science (2015), Greiner, ...optical lattice





Science

REPORTS

Cite as: Z. Yan *et al.*, *Science* 10.1126/science.aaw1611 (2019).

Strongly correlated quantum walks with a 12-qubit superconducting processor

Zhiguang Yan^{1,2*}, Yu-Ran Zhang^{3,4,5*}, Ming Gong^{1,2*}, Yulin Wu^{1,2}, Yarui Zheng^{1,2}, Shaowei Li^{1,2}, Can Wang^{1,2}, Futian Liang^{1,2}, Jin Lin^{1,2}, Yu Xu^{1,2}, Cheng Guo^{1,2}, Lihua Sun^{1,2}, Cheng-Zhi Peng^{1,2}, Keyu Xia^{6,7,4}, Hui Deng^{1,2}, Hao Rong^{1,2}, J. Q. You^{8,3}, Franco Nori^{4,9}, Heng Fan^{5,10+}, Xiaobo Zhu^{1,2}†, Jian-Wei Pan^{1,2}



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Comparison between theory and experiments

Science 364, 753 (2019)









Two-particle QWs show similar density distributions

Science 364, 753 (2019)



$\Gamma_{ij} = \langle \hat{a}_i^{\dagger} \hat{a}_j^{\dagger} \hat{a}_i \hat{a}_j \rangle$

Corresponding there are two particles at sites (i,j)

Strong on-site interaction

(theoretical and experimental), without on-site interaction

Science 364, 753 (2019)



Simulation of dynamical quantum phase transition

$$\begin{split} H_{\text{lsing}} &= -\sum_{i=1}^{N} \left(\sigma_{i}^{x} \sigma_{i+1}^{x} + g \sigma_{i}^{z} \right) \qquad H = \sum_{k} \Psi_{k}^{\dagger} h(k) \Psi_{k} \\ h(k) &= d_{0}(k) + \mathbf{d}(k) \cdot \sigma, \\ \rho_{i}(k) &= |\phi_{i}(k)\rangle \langle \phi_{i}(k)| = \frac{1}{2} \left[1 - \hat{\mathbf{d}}_{i}(k) \cdot \sigma \right] \\ \rho(k,t) &= |\phi(k,t)\rangle \langle \phi(k,t)| = \frac{1}{2} \left[1 - \hat{\mathbf{d}}(k,t) \cdot \sigma \right], \\ \hat{\mathbf{d}}(k,t) \cdot \sigma &= e^{-it\mathbf{d}_{f}(k) \cdot \sigma} \left(\hat{\mathbf{d}}_{i}(k) \cdot \sigma \right) e^{it\mathbf{d}_{f}(k) \cdot \sigma} \\ f(t) &= -\frac{1}{N} \sum_{k} \log |\langle \phi_{i}(k)| e^{-ith_{f}(k)} |\phi_{i}(k)\rangle|^{2}. \end{split}$$

Xue-Yi Guo, Chao Yang,…Shu Chen, Dongning Zheng,

Heng Fan, Phys. Rev. Applied 11, 044080 (2019).

Simulation of dynamical quantum phase transition



Here $g_i = 0.2$ is fixed, cases with $g_f = 1.5$ are presented in (a)-(g) in upper panel, cases of $g_f = 0.5$:

Xue-Yi Guo, Chao Yang,...Shu Chen, Dongning Zheng, Heng Fan, Phys. Rev. Applied 11, 044080 (2019).

Simulation of quantum dynamical phase transition



PHYSICAL REVIEW APPLIED 11, 044080 (2019)

Observation of a Dynamical Quantum Phase Transition by a Superconducting Qubit Simulation

Xue-Yi Guo,^{1,2} Chao Yang,^{1,2} Yu Zeng,^{1,2} Yi Peng,^{1,2} He-Kang Li,^{1,2} Hui Deng,³ Yi-Rong Jin,^{1,4} Shu Chen,^{1,2,*} Dongning Zheng,^{1,2,4,5,†} and Heng Fan^{1,2,4,5,‡}

Criterion of genuine multipartite entanglement

Table 1

Results on local decompositions of different entanglement witnesses for different states.

# of qubits	state	witness	maximal p_{noise}	local measurements	references	remarks
3	$ GHZ_3\rangle$	$\frac{1}{2}1 - GHZ_3\rangle\langle GHZ_3 $	4/7	4 (optimal)	[387]	a
3	$ W_3 angle$	$\frac{2}{3}1 - W_3\rangle \langle W_3 $	8/21	5 (optimal)	[387]	p
4	$ CL_4 angle$	$\frac{1}{2}1 - CL_4\rangle\langle CL_4 $	8/15	9 (optimal)	[388, 391]	a
4	$ \Psi_2 angle$	$\frac{3}{4}1 - \Psi_2\rangle\langle\Psi_2 $	4/15	15	[<u>145</u> , <u>390</u>]	e
4	$ D_{2,4} angle$	$\frac{2}{3}1 - D_{2,4}\rangle\langle D_{2,4} $	16/45	21	[213]	d
N	$ GHZ_N\rangle$	$\frac{1}{2}1 - GHZ_N\rangle\langle GHZ_N $	$1/2 \cdot [1/(1 - 1/2^N)]$	N + 1	[390]	8
N	$ W_N angle$	$\frac{N-1}{N}1 - W_N\rangle\langle W_N $	$1/N \cdot [1/(1 - 1/2^N)]$	2N - 1	[<u>8</u> , <u>390</u>]	b
N	$ G_N\rangle$	$\frac{1}{2}1 - G_N\rangle\langle G_N $	$1/2 \cdot [1/(1 - 1/2^N)]$	depends on the graph	[264]	8
N	$ D_{\frac{N}{2},N}\rangle$	$\frac{N}{2N-2}1 - D_{\frac{N}{2},N}\rangle \langle D_{\frac{N}{2},N} $	$1/2 \cdot (N-2)/[(N-1)(1-1/2^N)]$	not known	[213]	

^a Witnesses that tolerate less noise but require less settings exist. See Section 6.6.1.

^b Witnesses that tolerate more noise with the same measurements exist. See Sections 6.8.2 and 8.2.

^c Witnesses that tolerate more noise and require less settings exist [190, 390].

^d For witnesses that tolerate less noise with less settings see Section 8.2, for witnesses which tolerate more noise see Ref. [190].



Physics Reports (2009)

$$\begin{aligned} \frac{H_2}{\hbar} &= \sum_{\{j,k\}\in N} \frac{g_j g_k}{\Delta} (\sigma_j^+ \sigma_k^- + \sigma_j^- \sigma_k^+) \\ &+ \sum_{j=1}^N \frac{g_j^2}{\Delta} |\mathbf{1}_j\rangle \langle \mathbf{1}_j| \\ &+ \sum_{j=1}^N \lambda_{j,j+1}^{\mathbf{c}} (\sigma_j^+ \sigma_{j+1}^- + \sigma_j^- \sigma_{j+1}^+) \end{aligned}$$



RESEARCH

QUANTUM PHYSICS

Generation of multicomponent atomic Schrödinger cat states of up to 20 qubits

Chao Song^{1*}, Kai Xu^{2,3*}, Hekang Li^{2*}, Yu-Ran Zhang^{2,4}, Xu Zhang¹, Wuxin Liu¹, Qiujiang Guo¹, Zhen Wang¹, Wenhui Ren¹, Jie Hao⁵, Hui Feng⁵, Heng Fan^{2,3}†, Dongning Zheng^{2,3}†, Da-Wei Wang^{1,3}, H. Wang^{1,6}†, Shi-Yao Zhu^{1,6} Science 365, 574 (2019).

$$H_{2}/\hbar = \sum_{\{j,k\} \in N} \frac{g_{j}g_{k}}{\Delta} \left(\sigma_{j}^{+}\sigma_{k}^{-} + \sigma_{j}^{-}\sigma_{k}^{+}\right) + \sum_{j=1}^{N} \frac{g_{j}^{2}}{\Delta} |1_{j}\rangle \langle 1_{j}|$$
$$+ \sum_{j=1}^{N} \lambda_{j,j+1}^{c} \left(\sigma_{j}^{+}\sigma_{j+1}^{-} + \sigma_{j}^{-}\sigma_{j+1}^{+}\right), \quad (2)$$
$$\mathcal{S}^{+} = \sum_{j} \sigma_{j}^{+}, \, \mathcal{S}^{-} = \sum_{j} \sigma_{j}^{-}, \qquad \mathcal{S}_{z} = \sum_{j} \sigma_{z,j}.$$
$$\sum \lambda \left(\sigma_{j}^{+}\sigma_{k}^{-} + \sigma_{j}^{-}\sigma_{k}^{+}\right) \qquad \qquad \lambda \mathcal{S}^{+} \mathcal{S}^{-} \rightarrow -\lambda \mathcal{S}_{z}^{2}$$
$$\left(|0\rangle - i |1\rangle\right) / \sqrt{2}, \qquad \left(|00...0\rangle + e^{i\varphi}|11...1\rangle\right) / \sqrt{2},$$

Science 365, 574 (2019).

Observation of multi-component atomic Schrödinger cat states of up to 20 qubits

Chao Song¹,* Kai Xu^{2,4},* Hekang Li²,* Yuran Zhang^{2,5}, Xu Zhang¹, Wuxin Liu¹, Qiujiang Guo¹, Zhen Wang¹, Wenhui Ren¹, Jie Hao³, Hui Feng³, Heng Fan^{2,4},[†] Dongning Zheng^{2,4},[‡] Dawei Wang^{1,4}, H. Wang^{1,6},[§] and Shiyao Zhu^{1,6}



RESEARCH

QUANTUM PHYSICS

Generation of multicomponent atomic Schrödinger cat states of up to 20 qubits

Chao Song^{1*}, Kai Xu^{2,3*}, Hekang Li^{2*}, Yu-Ran Zhang^{2,4}, Xu Zhang¹, Wuxin Liu¹, Qiujiang Guo¹, Zhen Wang¹, Wenhui Ren¹, Jie Hao⁵, Hui Feng⁵, Heng Fan^{2,3}†, Dongning Zheng^{2,3}†, Da-Wei Wang^{1,3}, H. Wang^{1,6}†, Shi-Yao Zhu^{1,6} Science 365, 574 (2019).



$$|00...0
angle + \exp(i \varphi)|11...1
angle]/\sqrt{2},$$

$$\langle \mathcal{P}(\gamma) \rangle = 2 |\rho_{00...0,11...1}| \cos(N\gamma + \varphi)$$

$$F = (P + C)/2$$

$$C = |\rho_{0...0,1...1}| +$$

 $|
ho_{1...1,0...0}|$

保真度50%对多比特系统 实际正确率很高

Science 365, 574 (2019).

in |1⟩. The amplitude of the oscillation patterns of $\langle \mathcal{P}(\gamma) \rangle$ gives $|\rho_{00...0,11...1}|$ (Fig. 2B). Using values of $\rho_{00...0}$, $\rho_{11...1}$, and $|\rho_{00...0,11...1}|$, *N*-qubit GHZ state fidelities \mathcal{F} are calculated as 0.817 ± 0.009 (N = 10), 0.775 ± 0.011 (N = 12), 0.655 ± 0.009 (N = 14), 0.579 ± 0.007 (N = 16), 0.549 ± 0.006 (N = 17), and 0.525 ± 0.005 (N = 18), all confirming genuine multipartite entanglement with $\mathcal{F} > 0.5$ (24).

IBM Graph state (arbitrary bipartition)

0.5

0.4

Negativity 50

0.1

0.0



GHZ state preparation

Three independent works about GHZ state preparation





IBM group 18 superconducting qubits GHZ state, arXiv:1905.05720.



Harvard Lukin group 20-qubit GHZ arXiv:1905.05721. Science 365, 570 (2019).

5 谷歌利用超导量子比特器件展示量子优势





谷歌宣称:最复杂的 线路,实验可以实现 准确率从随机选取的 50%上升为50.1%。 (b从1变为1.002)



量子优势:随机量子线路采样方案



5比特,深度m的随机量子线路

$$\begin{aligned} X^{1/2} &\equiv R_X(\pi/2) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -i \\ -i & 1 \end{bmatrix}, & \text{fSim}(\theta, \phi) = e^{-i\theta(X \otimes X + Y \otimes Y)/2} e^{-i\phi(I-Z) \otimes (I-Z)/4} \\ Y^{1/2} &\equiv R_Y(\pi/2) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -i \\ 1 & 1 \end{bmatrix}, & \text{fSim}(\theta, \phi) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta) & -i\sin(\theta) & 0 \\ 0 & 0 & 0 & e^{-i\phi} \end{bmatrix} \\ W^{1/2} &\equiv R_{X+Y}(\pi/2) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -\sqrt{i} \\ \sqrt{-i} & 1 \end{bmatrix} & \theta \approx \pi/2 \text{ and } \phi \approx \pi/6 \\ & \text{iSWAP and CZ} \end{aligned}$$

single-qubit gates chosen randomly from $\{\sqrt{X}, \sqrt{Y}, \sqrt{W}\}$ on all qubits.

执行随机量子线路操作U后,我们会得到一个维度为2⁵³维希尔伯特空间的量子态 $|\Psi\rangle = U|\vec{0}\rangle$,同时对53个量子比特进行测量,得到一个53位的比特串, $x_j \in \{0,1\}^{53}$,即一次采样结果,对确定的一种线路重复测量百万次,即采样百万次,结果是百万 个比特串 $\{x_j\}_{j=1}^k$, k=10⁶,使之满足不等式,

$$\frac{1}{k} \sum_{j=1}^{k} |\langle x_j | \mathbf{U} | \vec{\mathbf{0}} \rangle|^2 \ge \frac{b}{2^{53}}, \qquad \mathbf{D} = 2^{53}$$

对一个随机量子线路,几率幅处于[p, p + dp]的比特串占比为 $Pr(p) dp = De^{-Dp} dp$,即Pr(p)是比特串密度(多少)按照其振幅p的分布函数,这个分布函数符合Porter-Thomas分布,几率幅处于[p, p + dp]的比特串总数为 $N(p)dp = D Pr(p) dp = D^2 e^{-Dp} dp$,

已知采样比特串的分布函数f(p), 需要求得 $\{p(x_j)\}_{j=1}^k$ 的平均值,可以得到 $\langle p \rangle = \int_0^1 pf(p)dp = \int_0^1 p^2 D^2 e^{-Dp}dp \approx \frac{2}{D}$

理想情况100%正确b=2;噪音无穷大,即随机选取b=1. 实验得到b=1.002,即正确率从随机的50%上升为50.1%



量子计算(态)的空间是指数增长

$$|\psi\rangle = \sum_{j_1 j_2 \dots j_N = 0}^{1} x_{j_1 j_2 \dots j_N} |j_1\rangle |j_2\rangle \dots |j_N\rangle$$

共有2^N个参数 *x*_{j1j2}...*j_N*

量子计算即是对量子态进行操作,导致2^N个参数变化, 一个53个量子比特的操作带来10¹⁶个数据的相应变化,用 经典计算机是不可能完成的!

所以, 量子计算机是不可替代的 , 如果我们先不管它做的 任务是有用还是无用



量子模拟非常适合做动力学问题,比如哈密顿量含时, 量子态在此哈密顿量作用下进行动力学演化。

量子态共含有2^N个参数,所以测量所有的参数值是不可能 做到的!

量子计算最终结果的测量应该是对某些观测量的测量,不 能涉及指数增长需求的测量方案,理想的选择是给出是和 否的答案的测量。

量子模拟一般从初态出发,初态制备不能很难,但是任意直 积态可以比较容易制备。所以量子模拟对于坐标变换一般是 容易的。

噪音预期在短期(10年)不可很小,所以现实的方案 选择也许是优化选择,正确率上升,趋势判断等问题

量子计算机解决量子问题有优势!

超过50个量子比特,动力学,含时操控,没有好的经典方 法,最终结果含有指数增长的信息(量子态),但是答案 是经典的----

好的量子优势方案!



量子优势时,量子计算机的任务不可能用经典计算机给出答案

如何知道量子计算给出的答案正确还是错误?

- 可以采取趋势标定错误率的形式:简单情况标定噪音 随比特数和时间的趋势,估计复杂情况的错误率
- 复杂计算错误率同一个简化的计算形式相差不大,类 比得到估计值。

Thank you 谢谢!