## Quantum Simulation

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### Outline LECTURE 1:

- A Brief History of Computing
- Pioneers of Quantum Computing and Quantum Simulation
- Classical and Quantum Simulations of Quantum Spin Systems **LECTURE 2**:
- High-Temperature Superconductors versus QCD
- The Nature of the Sign Problem
- From Wilson's Lattice Gauge Theory to Quantum Link Models **LECTURE 3**:
- Quantum Simulators for Abelian Lattice Gauge Theories
- Non-Abelian Quantum Link Models
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#### The first "digital computer" in Babylonia about 2400 b.c.



The first "analog computer": Antikythera for determining the position of celestial bodies, Crete, about 100 b.c.





The first programmable computer: Charles Babbagge's (1791-1871) "difference engine" was realized by his son.





#### The first software developer: Ada Lovelace (1815-1852).





## Konrad Zuse's (1910-1992) relay-driven computer Z3





#### From the vacuum-tube ENIAC to the IBM Blue Gene





#### Pioneers of theoretical computer science: John von Neumann (1903-1992) and Alan Turing (1912-1954)





#### Model of a universal Turing machine



RSA encryption: multiplication is easy, factorization is hard. RSA decryption challenge in 1991: factorize the following 174-digit number with 576 bits

RSA576 = 18819881292060796383869723946165043980716356 33794173827007633564229888597152346654853190 60606504743045317388011303396716199692321205734031879550656996221305168759307650257059

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- RSA576 = 18819881292060796383869723946165043980716356 33794173827007633564229888597152346654853190 60606504743045317388011303396716199692321205 734031879550656996221305168759307650257059
  - = 39807508642406493739712550055038649119906436 2342526708406385189575946388957261768583317
  - \* 47277214610743530253622307197304822463291469 5302097116459852171130520711256363590397527

This problem was solved only in 2003 by two mathematicians in Bonn using very large computer resources.

Only in 2009, when the challenge was no longer active, the 232-digit number RSA768 with 768 bits has finally been factorized.

Moore's law: "Every two years the number of transistors per area increases by a factor of 2."



Modern micro chips consist of several billions of transistors, each about  $10^{-8}$  m in size. This is already close to the quantum mechanical limit set by the size of individual atoms.

From bits to qubits

$$|\Psi
angle=a|1
angle+b|0
angle, \quad |a|^2+|b|^2=1$$

Entangled state of two qubits

$$|\Psi
angle=rac{1}{\sqrt{2}}\left(|10
angle+|01
angle
ight)$$



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### Richard Feynman's vision of 1982



"I'm not happy with all the analyses that go with just the classical theory, because 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." A universal quantum computer (David Deutsch's quantum analog of a classical Turing machine) could use Peter Shor's algorithm to solve the factorization problem.



David Deutsch



Peter Shor

A universal quantum computer (David Deutsch's quantum analog of a classical Turing machine) could use Peter Shor's algorithm to solve the factorization problem.





David Deutsch Peter Shor Until today, only  $15 = 3 \cdot 5$  has been correctly factorized by a quantum computer, at least in about 50 % of all trials.



### lon traps as a digital quantum computer?





#### Franklin Medal 2010: I. Cirac, D. Wineland, P. Zoller



#### Bose-Einstein condensation in ultra-cold atomic gases



#### Eric Cornell, Carl Wieman, Wolfgang Ketterle, 1995



# Ultra-cold atoms in optical lattices as analog quantum simulators



#### Transition from a superfluid to a Mott insulator



Theodor Hänsch

Immanuel Bloch

Can one understand high- $T_c$  superconductivity in this way?

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### Richard Feynman, Int. J. Theor. Phys. 21 (1982) 467



"Can quantum systems be probabilistically simulated by a classical computer? This is the hidden variable problem: it is impossible to represent the results of quantum mechanics with a classical universal device."

## The spin $\frac{1}{2}$ quantum Heisenberg model





Quantum spins  $[S_x^a, S_y^b] = i\delta_{xy}\varepsilon_{abc}S_x^c$  and their Hamiltonian

$$H = J \sum_{\langle xy 
angle} ec{S}_x \cdot ec{S}_y$$

Partition function at inverse temperature  $\beta = 1/T$ 

$$Z = \mathsf{Tr} \exp(-\beta H)$$

Low-energy effective action for antiferromagnetic magnons

$$S[\vec{e}] = \int_0^\beta dt \int d^2 x \; \frac{\rho_s}{2} \left( \partial_i \vec{e} \cdot \partial_i \vec{e} + \frac{1}{c^2} \partial_t \vec{e} \cdot \partial_t \vec{e} \right)$$

#### Fit to analytic predictions of effective theory



 $\mathcal{M}_s = 0.30743(1), \quad \rho_s = 0.18081(11)J, \quad c = 1.6586(3)Ja$ UJW, H.-P. Ying (1994); F.-J. Jiang, UJW (2010)

#### Optical lattice quantum simulation of quantum spin systems



J. Simon, W. S. Bakir, R. Ma, M. E. Tal, P. M. Preis, M. Greiner, Nature 472 (2011) 307. Homework 1: Show that the Heisenberg Hamiltonian H commutes with the total spin  $\vec{S}$ 

$$H = J \sum_{\langle xy 
angle} ec{S}_x \cdot ec{S}_y, \quad ec{S} = \sum_x ec{S}_x.$$

Show that ferromagnetic spin waves  $|p_1p_2\rangle$  are eigenstates of H and determine their energy-momentum dispersion relation,

$$|p_1p_2\rangle = \sum_x \exp(i(p_1x_1+p_2x_2))S_x^+|\uparrow\uparrow\ldots\uparrow\rangle$$

#### Some important lessons from lecture 1:

• Quantum computers or quantum simulators are potentially much more powerful than classical computers.

• The Heisenberg quantum spin model in thermal equilibrium can be simulated very efficiently using classical computers.

• The collective dynamics of discrete quantum spin degrees of freedom can give rise to an emergent quantum field theory for the low-energy spin wave Goldstone boson excitations.

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#### Antiferromagnetic precursors of high- $T_c$ superconductors



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#### Phase diagrams of QCD and of doped antiferromagnets



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#### Correspondences between QCD and Antiferromagnetism

	QCD	Antiferromagnetism
broken phase	hadronic vacuum	antiferromagnetic phase
global symmetry	chiral symmetry	spin rotations
symmetry group G	$SU(2)_L \otimes SU(2)_R$	$SU(2)_s$
unbroken subgroup H	$SU(2)_{L=R}$	$U(1)_s$
Goldstone boson	pion	magnon
Goldstone field in $G/H$	$U(x) \in SU(2)$	$ec{e}(x)\in S^2$
order parameter	chiral condensate	staggered magnetization
coupling strength	pion decay constant $F_\pi$	spin stiffness $ ho_s$
propagation speed	velocity of light	spin-wave velocity <i>c</i>
conserved charge	baryon number $U(1)_B$	electric charge $U(1)_Q$
charged particle	nucleon or antinucleon	electron or hole
long-range force	pion exchange	magnon exchange
dense phase	nuclear or quark matter	high- $T_c$ superconductor
microscopic description	lattice QCD	Hubbard or <i>t</i> - <i>J</i> model
effective description	chiral perturbation	magnon effective
of Goldstone bosons	theory	theory
effective description	baryon chiral	magnon-hole
of charged fields	perturbation theory	effective theory





$$H=-t\sum_{\langle xy
angle}(c_x^{\dagger}c_y+c_y^{\dagger}c_x)+U\sum_x(c_x^{\dagger}c_x-1)^2,\quad c_x=\left(egin{array}{c}c_{x\uparrow}\c_{x\downarrow}\end{array}
ight)$$

reduces to the Heisenberg model at half-filling for  $U \gg t$ 

$$H = J \sum_{\langle xy 
angle} ec{S}_x \cdot ec{S}_y$$

Important open question:





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$$H = J \sum_{\langle xy \rangle} \vec{S}_x \cdot \vec{S}_y$$

Important open question:

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### Path integral

$$Z_f = \operatorname{Tr}[\exp(-\varepsilon H_1)\exp(-\varepsilon H_2)...\exp(-\varepsilon H_M)]^N$$
  
= 
$$\sum_{[n]} \operatorname{Sign}[n]\exp(-S[n])$$



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Sign problem of fermionic path integrals

$$Z_f = \operatorname{Tr} \exp(-\beta H) = \sum_{[n]} \operatorname{Sign}[n] \exp(-S[n]) , \quad \operatorname{Sign}[n] = \pm 1$$

Average sign is exponentially small

$$\langle \text{Sign} \rangle = \frac{\sum_{[n]} \text{Sign}[n] \exp(-S[n])}{\sum_{[n]} \exp(-S[n])} = \frac{Z_f}{Z_b} = \exp(-\beta V \Delta f)$$

The statistical error is exponentially large

$$\frac{\sigma_{\rm Sign}}{\langle {\rm Sign} \rangle} = \frac{\sqrt{\langle {\rm Sign}^2 \rangle - \langle {\rm Sign} \rangle^2}}{\sqrt{N} \langle {\rm Sign} \rangle} = \frac{\exp(\beta V \Delta f)}{\sqrt{N}}$$

Some very hard sign problems are NP complete M. Troyer, UJW, Phys. Rev. Lett. 94 (2005) 170201.

#### Homework 2:

Show that the anti-commutation relations

 $\{c_{x,s}^{\dagger}, c_{y,s'}\} = \delta_{xy}\delta_{ss'}$  of fermionic creation and annihilation operators imply angular momentum commutation relations

$$[S_x^a, S_y^b] = i\delta_{xy}\varepsilon_{abc}S_x^c, \quad \vec{S}_x = \sum_x c_x^\dagger \frac{\vec{\sigma}}{2}c_x, \quad c_x = \begin{pmatrix} c_{x\uparrow} \\ c_{x\downarrow} \end{pmatrix}.$$

#### Homework 3:

Show that the Hubbard Hamiltonian H commutes with the total spin  $\vec{S}$  and with the particle number N

$$H = -t \sum_{\langle xy \rangle} (c_x^{\dagger} c_y + c_y^{\dagger} c_x) + U \sum_x (c_x^{\dagger} c_x - 1)^2, \quad c_x = \begin{pmatrix} c_{x\uparrow} \\ c_{x\downarrow} \end{pmatrix}$$
$$\vec{S} = \sum_x \vec{S}_x = \sum_x c_x^{\dagger} \frac{\vec{\sigma}}{2} c_x, \quad N = \sum_x n_x = \sum_x c_x^{\dagger} c_x.$$

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# Kenneth Wilson's lattice QCD describes confinement of quarks and gluons inside protons und neutrons



#### and confirms the experimentally measured mass spectrum



Can heavy-ion collision physics or nuclear astrophysics benefit from quantum simulations in the long run?







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#### Richard Feynman's vision of 1982



"It does seem to be true that all the various field theories have the same kind of behavior, and can be simulated in every way, apparently, with little latticeworks of spins and other things."

Different descriptions of dynamical Abelian gauge fields: Maxwell's classical electromagnetic gauge fields

$$ec{
abla}\cdotec{B}(ec{x},t)=
ho(ec{x},t), \quad ec{
abla}\cdotec{B}(ec{x},t)=0, \quad ec{B}(ec{x},t)=ec{
abla} imesec{A}(ec{x},t)$$

Quantum Electrodynamics (QED) for perturbative treatment

$$E_{i} = -i\frac{\partial}{\partial A_{i}}, \quad [E_{i}(\vec{x}), A_{j}(\vec{x}')] = i\delta_{ij}\delta(\vec{x} - \vec{x}'), \quad \left[\vec{\nabla} \cdot \vec{E} - \rho\right] |\Psi[A]\rangle = 0$$

Wilson's U(1) lattice gauge theory for classical simulation

$$U_{xy} = \exp\left(ie \int_{x}^{y} d\vec{l} \cdot \vec{A}\right) = \exp(i\varphi_{xy}) \in U(1), \quad E_{xy} = -i\frac{\partial}{\partial\varphi_{xy}},$$
$$[E_{xy}, U_{xy}] = U_{xy}, \quad \left[\sum_{i} (E_{x,x+\hat{i}} - E_{x-\hat{i},x}) - \rho\right] |\Psi[U]\rangle = 0$$

U(1) quantum link models for quantum simulation

$$\begin{array}{ll} U_{xy} = S_{xy}^+, & U_{xy}^\dagger = S_{xy}^-, & E_{xy} = S_{xy}^3, \\ [E_{xy}, U_{xy}] = U_{xy}, & [E_{xy}, U_{xy}^\dagger] = -U_{xy}^\dagger, & [U_{xy}, U_{xy}^\dagger] = 2E_{xy}^\dagger \end{array}$$

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Hamiltonian formulation of Wilson's U(1) lattice gauge theory

$$U=\exp(iarphi), \ U^{\dagger}=\exp(-iarphi)\in U(1)$$

Electric field operator E

$$E = -i\partial_{\varphi}, \ [E, U] = U, \ [E, U^{\dagger}] = -U^{\dagger}, \ [U, U^{\dagger}] = 0$$

Generator of U(1) gauge transformations

$$G_{x} = \sum_{i} (E_{x-\hat{i},i} - E_{x,i}), \quad [H, G_{x}] = 0$$

U(1) gauge invariant Hamiltonian

$$H = \frac{g^2}{2} \sum_{x,i} E_{x,i}^2 - \frac{1}{2g^2} \sum_{x,i\neq j} (U_{x,i}U_{x+\hat{i},j}U_{x+\hat{j},i}^{\dagger}U_{x,j}^{\dagger} + \text{h.c.})$$

operates in an infinite-dimensional Hilbert space per link

 $U(1) \text{ quantum links from spins } \frac{1}{2} \qquad \underbrace{E_{x,i}}_{x \quad U_{x,i} \quad x + \hat{i}}$  $U = S_1 + iS_2 = S_+, \ U^{\dagger} = S_1 - iS_2 = S_-$ Electric flux operator *E* 

$$E = S_3, [E, U] = U, [E, U^{\dagger}] = -U^{\dagger}, [U, U^{\dagger}] = 2E$$

Gauss law



Ring-exchange plaquette Hamiltonian



D. Horn, Phys. Lett. B100 (1981) 149

- P. Orland, D. Rohrlich, Nucl. Phys. B338 (1990) 647
- S. Chandrasekharan, UJW, Nucl. Phys. B492 (1997) 455 .

Hamiltonian with Rokhsar-Kivelson term

$$H = -J\left[\sum_{\Box}(U_{\Box} + U_{\Box}^{\dagger}) - \lambda \sum_{\Box}(U_{\Box} + U_{\Box}^{\dagger})^{2}
ight]$$

#### Phase diagram



D. Banerjee, F.-J. Jiang, P. Widmer, UJW, JSTAT (2013) P12010.

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# Energy density of charge-anti-charge pair $Q = \pm 2$ (a) 60



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#### Homework 4:

Show that the Hamiltonian of the 2-d U(1) quantum link model commutes with the local generators of gauge transformations  $G_x = \sum_i (E_{x-\hat{i},i} - E_{x,i})$ 

$$H = -\frac{1}{2g^2} \sum_{x,i\neq j} (U_{x,i}U_{x+\hat{i},j}U_{x+\hat{j},i}^{\dagger}U_{x,j}^{\dagger} + \text{h.c.}).$$

#### Some important lessons from lecture 2:

• QCD shares some qualitative features with high-temperature superconductors.

• Wilson's lattice QCD allows the precise determination of static hadron properties using Monte Carlo simulations. It also allows to simulate QCD at finite temperature. Simulations of dynamical processes or of the physics at non-zero baryon density suffer from very severe sign problems.

• Gauge theories with exact continuous gauge symmetry can be formulated in terms of discrete quantum link degrees of freedom.

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