Quantum simulation with cold atoms An experimental and theoretical challenge

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First vs. second quantum revolution

The first quantum revolution

Paradigm: macroscopic objects are classical elementary constituents obey new laws (quantum mechanics)



Macroscopic quantum effects



Superconductivity (1913)



Lasers (1960)



Superfluidity of He-4 (1938)

etc....

Quantum matter: the 2nd quantum revolution

Design of (meta-)materials dominated by quantum effects

Complex oxides: novel superconductors/ quantum magnets (~1987)



chemical synthesis



nanotechnologies

Nano-patterned superconductors (~1980)



quantum-dot arrays on a surface (~2000)







Optical lattices: artificial solids of light (~2000)



Ultra-cold atoms: Bose-Einstein condensates (1995)

The complexity of quantum matter

Quantum matter = quantum fields



operator-valued field (field of matrices)

Fermions: 2x2 matrix

Bosons: $\infty \times \infty$ matrix

$$\hat{\psi} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \qquad \hat{\psi} = \begin{pmatrix} 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}$$

 $\hat{\psi}_i^{\dagger}\hat{\psi}_i = \text{particle number at site } i$ $\hat{\psi}_i^{\dagger}\hat{\psi}_i \neq \hat{\psi}_i\hat{\psi}_i^{\dagger}$

Quantum matter = quantum fields



interacting quantum fields: energy is also an operator (Hamiltonian)

$$\hat{\mathcal{H}} = \sum_{ij} \left(J_{ij} \ \hat{\psi}_i^{\dagger} \hat{\psi}_j + \text{h.c.} \right) + \sum_{ij} V_{ij} \ \hat{\psi}_i^{\dagger} \hat{\psi}_i \ \hat{\psi}_j^{\dagger} \hat{\psi}_j$$

Quantum many-body problem: condensed matter

quantum chemistry quantum field-theory and particle physics nuclear physics etc..

Numerics: matrix diagonalization

$$\hat{\mathcal{H}} = \sum_{ij} \left(J_{ij} \ \hat{\psi}_i^{\dagger} \hat{\psi}_j + \text{h.c.} \right) + \sum_{ij} V_{ij} \ \hat{\psi}_i^{\dagger} \hat{\psi}_i \ \hat{\psi}_j^{\dagger} \hat{\psi}_j$$

Time-independent Schrödinger's equation

$$\hat{\mathcal{H}}|\Psi\rangle = E|\Psi\rangle$$



(written with atoms in optical lattices)



You just have to solve a simple **linear** eigenvalue problem!

That's easy!

My **F=ma** is a set of **coupled nonlinear partial differential equations!** (now, that's hard...)



Numerics: matrix diagonalization

Then just take the biggest supercomputers and crunch numbers...



Tianhe-2 (China) (> 3 million cores)



"The Hilbert space is a big place"

Take the simplest quantum field: the S=1/2 spin (two values on each site)



Hamiltonian describing a system of N interacting spins: $2^N \times 2^N$ matrix

 $N = 250: 2^{250} >$ number of atoms in the universe







"Things we know we don't know"

http://en.wikipedia.org/wiki/List_of_unsolved_problems_in_physics



We do not know the **mechanism of superconductivity** of *most* superconducting materials

(in particular, of materials with a high critical temperature)

We do not know the phase diagram of nuclear matter (Quantum Chromodynamics)



We do not know the ground state of "frustrated" quantum spin systems

We do not know how a closed quantum system relaxes towards its equilibrium state







The big idea: use quantum machines...

different worlds and every arrangement of configurations are all there just like our arrangement of configurations, we just happen to be sitting in this one. It's possible, but I'm not very happy with it.

So, I would like to see if there's some other way out, and I want to emphasize, or bring the question here, because the discovery of computers and the thinking about computers has turned out to be extremely useful in many branches of human reasoning. For instance, we never really understood how lousy our understanding of languages was, the theory of grammar and all that stuff, until we tried to make a computer which would be able to understand language. We tried to learn a great deal about psychology by trying to understand how computers work. There are interesting philosophical questions about reasoning, and relationship, observation, and measurement and so on, which computers have stimulated us to think about anew, with new types of thinking. And all I was doing was hoping that the computer-type of thinking would give us some new ideas, if any are really needed. I don't know, maybe physics is absolutely OK the way it is. The program that Fredkin is always pushing, about trying to find a computer simulation of physics, seem to me to be an excellent program to follow out. He and I have had wonderful, intense, and interminable arguments, and my argument is always that the real use of it would be with quantum mechanics, and therefore full attention and acceptance of the quantum mechanical phenomena—the challenge of explaining quantum mechanical phenomena -has to be put into the argument, and therefore these phenomena have to be understood very well in analyzing the situation. And 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. Thank you.

9. DISCUSSION

Question: Just to interpret, you spoke first of the probability of A given B, versus the probability of A and B jointly—that's the probability of one observer seeing the result, assigning a probability to the other; and then you brought up the paradox of the quantum mechanical result being 3/4, and this being 2/3. Are those really the same probabilities? Isn't one a joint probability, and the other a conditional one?

Answer: No, they are the same. P_{OO} is the joint probability that both you



es <u>itself</u>



 $V_{ij} \ \hat{\psi}_i^\dagger \hat{\psi}_i \ \hat{\psi}_j^\dagger \hat{\psi}_j$

Exquisite experimental control on cold atoms



Control on the **nature of the quantum fields** (bosons/fermions, spinful/spinless)



Is a quantum machine going to solve it all?





Is a quantum machine going to solve it all?

"Never make a calculation until you know the answer"



John Wheeler

Never make a quantum simulation until you know the answer

The D-Wave machine



512 superconducting qubits



Feb. 17, 2014

How "Quantum" is the D-Wave Machine?

Seung Woo $\mathrm{Shin}^*,$ Graeme Smith †, John A. Smolin †, and Umesh Vazirani *

^{*}Computer Science division, UC Berkeley, USA. [†]IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA.

arXiv:1401.7087v1 [quant-ph] 28 Jan 2014

Distinguishing Classical and Quantum Models for the D-Wave Device

Walter Vinci,^{1,2,*} Tameem Albash,^{3,4,*} Anurag Mishra,^{3,4} Paul A. Warburton,^{1,5} and Daniel A. Lidar^{3,4,6,7}

arXiv:1403.4228v1 [quant-ph] 17 Mar 2014

Quantum simulators need "classical simulators" (and viceversa)

"Classical simulators" can test the experimental Hamiltonians



Quantum simulators can test approximate theories (and approx. classical simulation methods)

"Quantum stimulators" for the study of complex quantum phenomena (A. Aspect)

Quantum simulation in practice: *extension of theory*





Quantum simulation in practice: extension of theory



Quantum simulation in practice: *test of theory*

theory: numerical resummation of a non-simply convergent infinite series



K. van Houcke et al., Nat. Phys. 2012

exp: ultracold gas of K-40 fermions

"Calibrating" quantum simulators (and learning new physics while doing so)

Quantum simulation of complex phase diagrams





quantum chromodynamics





All condensed matter experiments are performed in a **heat bath**

Thermometry in a cold-atom quantum simulator

Where's the heat bath here?

The system is its own heat bath (microcanonical setting)

Temperature has to be measured



Thermometer = "gentle probe" whose thermodynamics is perfectly known

Atomic physic quantum simulators: ~100,000 particles at *T* ~ 10 nK !!

Idea: use the noise!



Brownian motion: Einstein's relation (1905)



 $\mu_{\gamma} = 1/\gamma \quad \mathbf{F}_{\mathrm{frict}} = -\gamma \mathbf{v}$



R. Kubo

Fluctuation-dissipation relation (~1950's) (*R. Kubo*)

$$D = \int_0^\infty dt \, \left\langle \delta \mathbf{v}(0) \cdot \delta \mathbf{v}(t) \right\rangle = |\delta \tilde{\mathbf{v}}(\omega = 0)|^2 = \frac{k_B T}{\gamma}$$

fluctuation of the particle's velocity

dissipation term

Noise thermometry

Thermal noise in a resistor: Johnson-Nyquist noise (1928)



$$|\tilde{V}(\omega)|^2 = \int dt \ e^{-i\omega t} \langle V(0) \ V(t) \rangle$$





J. B. Johnson

H. Nyquist

noise power spectrum

(classical) Nyquist theorem

 $4|R|k_BT$

fluctuation

dissipation

Johnson-noise thermometer

THE REVIEW OF SCIENTIFIC INSTRUMENTS

VOLUME 17, NUMBER 7

JULY, 1946

The Measurement of Thermal Radiation at Microwave Frequencies

R. H. DICKE* Radiation Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts** (Received April 15, 1946)





cosmic black-body radiation

Thermal vs. quantum noise

$$|\tilde{V}(\omega)|^{2} = 4 R k_{B}T \qquad \text{(classical) Nyquist theorem}$$

$$|\tilde{V}(\omega)|^{2} = 4 R \hbar\omega \left(n(\omega) + \frac{1}{2}\right) \qquad \text{quantum Nyquist theorem}$$

$$\frac{1}{\left|\tilde{V}(\omega)\right|^{2}} = 4 R \hbar\omega \left(n(\omega) + \frac{1}{2}\right) \qquad \text{quantum Nyquist theorem}$$

$$\frac{1}{noise} \qquad noise \qquad h\omega \ll k_{B}T \qquad \text{classical limit}$$

$$\frac{1}{k_{B}} = \frac{1}{k_{B}} = \frac$$

What noise in a cold atom experiment?



measurements in cold atoms are generally destructive

temporal fluctuations cannot be monitored



only single snapshots -> frequency-integrated noise

What noise in a cold atom experiment?



S. Fölling et al., Nature 2005

in-situ microscopy image



W. Bakr et al., Nature 2009

 $G(\mathbf{k}, \mathbf{k}') = \langle \delta n(\mathbf{k}) \delta n(\mathbf{k}') \rangle$

$$C(\mathbf{r},\mathbf{r}') = \langle \delta n(\mathbf{r}) \delta n(\mathbf{r}') \rangle$$

Correlation functions for fluctuations

Fluctuation-dissipation relations

 $\mathcal{H} = \mathcal{H}_0 - hA$

static perturbation



 $\langle \delta^2 A \rangle = \chi_{AA} \ k_B T$

thermal noise

but if
$$[A, \mathcal{H}_0] \neq 0$$

$$\langle (\delta A)^2 \rangle = \langle (\delta A)^2 \rangle_T + \langle (\delta A)^2 \rangle_Q \ge \chi_{AA} k_B T$$

thermalquantumnoisenoise

Momentum-noise thermometry



 $[\hat{\mathcal{H}}, \hat{P}_n] = 0$

 $[\hat{\mathcal{H}}, \hat{P}_n] \neq 0$

$$\hat{P}_n = \sum_{\mathbf{k}} (\hbar k_n) \, \hat{n}(\mathbf{k}) \qquad \begin{array}{c} t \\ \mathbf{a} \\ \mathbf{k} \\ \hat{P}_n \end{pmatrix} = 0 \qquad \qquad \left\langle \hat{P}_n^2 \right\rangle \neq 0$$

otal momentum long n

$$\langle P_n^2 \rangle \neq 0$$

$$\frac{\langle \hat{P}_n^2 \rangle}{2mN} = \frac{1}{2}k_BT$$

kinematic def. of T beyond equipartition

$$\langle \delta^2 \hat{P}_n \rangle = N \langle \hat{p}_n^2 \rangle \qquad \frac{\langle p_n^2 \rangle}{2m} = \frac{1}{2} k_B T$$

ideal classical gas (equipartition)

$$\frac{\langle \hat{P}_n^2 \rangle}{2mN} = \frac{\langle \hat{P}_n^2 \rangle_T + \langle \hat{P}_n^2 \rangle_Q}{2mN} \ge \frac{1}{2} k_B T$$

In an optical lattice



 $\hat{P}_n \rightarrow \hat{\mathcal{J}}_n$

current along the *n*-direction







non-interacting fermions in an optical lattice

 $[\hat{\mathcal{H}}, \hat{\mathcal{J}}_n] \neq 0$

quantum fluctuations of the current due to the parabolic trap

Thermal vs. quantum fluctuations

$$\frac{\langle (\delta \mathcal{J}_n)^2 \rangle}{\partial_{\phi} \langle \mathcal{J}_n \rangle} = \frac{k_B T_{\mathcal{J}_n}}{J} \ge \frac{k_B T}{J}$$









Conclusions

. . . .

1) Asking how a quantum simulator works / might work, we can learn interesting things

2) Hamiltonian engineering needs design engineers! (= theoreticians)

3) Novel quantum many-body phenomena are within reach, but they must be predicted/understood

- out-of-equilibrium phenomena
- interaction between matter and (artificial) fields beyond QED/QCD/etc.
- quantum information processing

"Classical machines"









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How can theory deal with an exponentially big Hilbert space?



Simulating Physics with Computers

Richard P. Feynman

5. CAN QUANTUM SYSTEMS BE PROBABILISTICALLY SIMULATED BY A CLASSICAL COMPUTER?

YES: Monte Carlo methods

Stochastic sampling of statistical sums

$$\langle A \rangle_T = \frac{\sum_{\alpha} A_{\alpha} \ e^{-E_{\alpha}/(k_B T)}}{\sum_{\alpha} e^{-E_{\alpha}/(k_B T)}} = \sum_{\alpha} A_{\alpha} P_{\alpha}$$



random walk in configuration space



Quantum Monte Carlo

Quantum fields: statistical sums are traces of operators

$$\langle \hat{A} \rangle_T = \frac{1}{\mathcal{Z}} \operatorname{Tr} \left[\hat{A} \ e^{-\hat{\mathcal{H}}/(k_B T)} \right] \qquad \mathcal{Z} = \operatorname{Tr} \left[e^{-\hat{\mathcal{H}}/(k_B T)} \right]$$

Formally analogous to
$$\langle A \rangle_T = \frac{\sum_{\alpha} A_{\alpha} e^{-E_{\alpha}/(k_B T)}}{\sum_{\alpha} e^{-E_{\alpha}/(k_B T)}} = \sum_{\alpha} A_{\alpha} P_{\alpha}$$

Bootstrap problem: to know P_{α} one needs to diagonalize $\hat{\mathcal{H}}$!!



- Douglas Adams, The Hitchhiker's Guide to the Galaxy

"The Answer to the Great Question... Of Life, the Universe and Everything... Is...

Forty-two,' said Deep Thought, with infinite majesty and calm."

"It was a tough assignment," said Deep Thought mildly... "I think that the problem, to be quite honest with you, is that you've never known what the question is."...

"Once you do know what the question actually is, you'll know what the answer means."

"Can you just please tell us the question?"

"No..." "But I'll tell you who can... A computer whose merest operational parameters I am not worthy to calculate ... a computer of such infinite an subtle complexity that organic life itself shall form part of its operational matrix... And it shall be called ... **the Earth**."

"Never make a calculation until you know the answer"



John Wheeler



