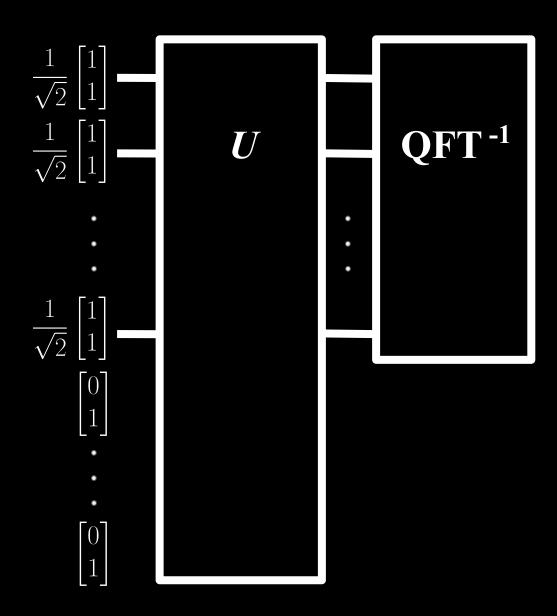
Adiabatic Quantum Computing Lecture 2

Nike Dattani nike@hpqc.org



Largest number factored with Shor's algorithm?



Number factored	<u>Year</u>
15	2001
	2007
	2007
	2009
	2012
21	2012

Number factored	<u>Year</u>
15	2001
	2007
	2007
	2009
	2012
21	2012

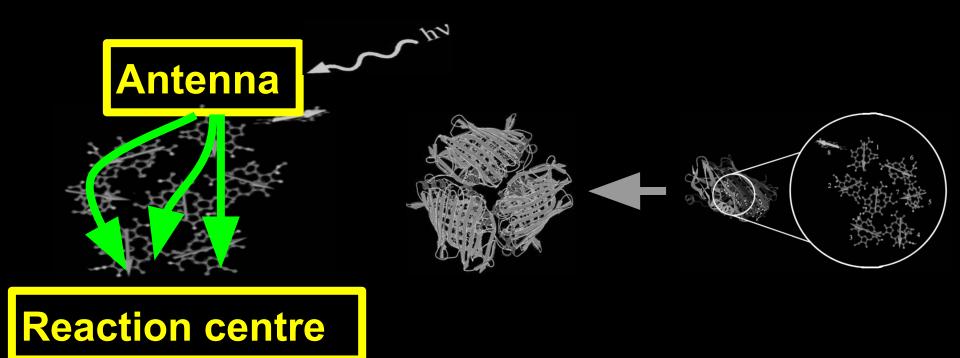
None of these used more than 7 qubits!

Number factored	<u>Year</u>
15	2001
	2007
	2007
	2009
	2012
21	2012

None of these used more than 7 qubits!

At around the same time...

Quantum effects in photosynthesis



Approximate quantum dynamics for the FMO:

```
2008 Jang et. al: Small polaron
2008 Piilo, Maniscalco, Härkönen, Suominen: NMQJ
2009 Palmieri, Abramavicius, Mukamel: Extended Lindblad approach
2009 Ishizaki & Fleming: Redfield equation
2009 Ishizaki & Fleming: Doctor equations
2009 Roden, Eisfeld, Strunz: Quantum state diffusion
2009 Rebentrost & Aspuru-Guzik: NMOJ
2010 Huo & Coker: Linearized Feynman integral
2010 Huo & Coker: Iterative Linearized Feynman integral
2010 Tao & Miller: Semi-classical Feynman integral
2010 Prior, Chin, Huelga, Plenio: t-DMRG - for 2 site sub-system
2010 Wu, ..., Silbey: generalized Bloch-Redfield
2011 Zhu, Kais, Rebentrost, Aspuru-Guzik: Scaled doctor equations
2011 Lloyd: time non-local quantum master equation
2011 Nalbach & Thorwart: Quasiadiabatic Feynman integral – for 7 site sub-system
2011 Ritschel, Roden, Strunz, Eisfeld: NMQSD-ZOFE, 7-level, arb. Temp., arb. J(w)
2011 Pachon & Brumer: NIBA, 2-level, ohmic J(w)
2011 Alicki & Miklaszewski: Wigner-Weisskopf-type model (not a typical model)
2012 Reichman, Markland, Berkelbach: RDM-hybrid
2012 Markland, Berkelbach, Reichman: Ehrenfest Trajectories
```

....... and more (stochastic Liouville equations, generalized master equations, etc.)

Approximate quantum dynamics for the FMO:

```
2008 Jang et. al: Small polaron
2008 Piilo, Maniscalco, Härkönen, Suominen: NMQJ
2009 Palmieri, Abramavicius, Mukamel:
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2011 Lloyd: time non-local quantum master equation
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2011 Ritschel, Roden, Strunz, Eisfeld: NMQSD-ZOFE, 7-level, arb. Temp., arb. J(w)
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....... and more (stochastic Liouville equations, generalized master equations, etc.)

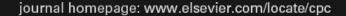
Numerically exact quantum dynamics:

Feynman Dynamics on GPUs (https://github.com/ndattani)



Contents lists available at ScienceDirect

Computer Physics Communications





FeynDyn: A MATLAB program for fast numerical Feynman integral calculations for open quantum system dynamics on GPUs*



Nikesh S. Dattani*

Physical and Theoretical Chemistry, Laboratory, Department of Chemistry, Oxford University, Oxford, OX1 3QZ, UK

Why Quantum Coherence Is Not Important in the Fenna–Matthews–Olsen Complex

David M. Wilkins*,

Physical and Theoretical Chemistry Laboratory, Oxford University, South Parks Road, Oxford, OX1 3QZ, United Kingdom Nikesh S. Dattani*

Quantum Chemistry Laboratory, Department of Chemistry, Kyoto University, 606-8502, Kyoto, Japan School of Materials Science and Engineering, Nanyang Technological University, Block N4.1, Nanyang Avenue, Singapore 639798

J. Chem. Theory Comput., 2015, 11 (7), pp 3411-3419

DOI: 10.1021/ct501066k

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Why Quantum Coherence Is Not Important in the Fenna–Matthews–Olsen Complex

David M. Wilkins*,

Physical and Theoretical Chemistry Laboratory, Oxford University, South Parks Road, Oxford, OX1 3QZ, United Kingdom Nikesh S. Dattani*



pan nyang Avenue, Singapore

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Accepting PhD Students

Feynman dynamics

Feynman (1959)

Leggett & Caldeira (1983): 2 levels

Makri *et. al.* (1995): 3 levels

Sim & Kim (2006): 5 levels

Kim & Sim (2010): 10 levels

Wilkins, Dattani (2011): 24 levels - FMO (quantum effects in photosynthesis)

Strumpfer, Schulten (2012): 50 levels

Tsuchimoto, Tanimura (2014): 512 levels

Jones, Dattani (2014): 600 levels

Dattani, Chen, Gelin, Domcke (2014): 800 levels

Dattani, Bryans (2014): 1024 levels - 10 qubit quantum computer

Number factored	<u>Year</u>
15	2001
	2007
	2007
	2009
	2012
21	2012

None of these used more than <u>7 qubits!</u>

At around the same time...

Methods developed for numerically exact quantum dynamics could simulate up to 10 qubits with decoherence.

Factoring 143

	b_7	b_6	b_5	b_4	b_3	b_2	b_1	b_0
Multiplier					1	p_2	p_1	1
					1	q_2	q_1	1
Binary-multiplication					1	p_2	p_1	1
				q_1	p_2q_1	p_1q_1	q_1	
		1	$q_2 \\ p_2$	$p_2q_2 \\ p_1$	p_1q_2 1	q_2		
Carry	z_{67}	Z56	Z45	Z34	z_{23}	z_{12}		
	Z57	Z46		z_{24}				
Product	1	0	0	0	1	1	1	1

<u>Factoring 143</u>

	b_7	b_6	b_5	b_4	b_3	b_2	b_1	b_0	
Multiplier					1	p_2	p_1	1	
					1	q_2	q_1	1	X
Binary-multiplication					1	p_2	p_1	1	Α,
				q_1	p_2q_1	p_1q_1	q_1		
		1	$q_2 \\ p_2$	$p_2q_2 p_1$	p_1q_2 1	q_2			
Carry	z_{67}	Z56	Z45	Z34	z_{23}	z_{12}			
	Z57	Z46	Z35	Z24					
Product	1	0	0	0	1	1	1	1	14

$$p_1 + q_1 = 1 + 2z_{12}$$

$$p_2 + p_1q_1 + q_2 + z_{12} = 1 + 2z_{23} + 4z_{24}$$

$$1 + p_2q_1 + p_1q_2 + 1 + z_{23} = 1 + 2z_{34} + 4z_{35}$$

$$q_1 + p_2q_2 + p_1 + z_{34} + z_{24} = 0 + 2z_{45} + 4z_{46}$$

$$q_2 + p_2 + z_{45} + z_{35} = 0 + 2z_{56} + 4z_{57}$$

$$1 + z_{56} + z_{46} = 0 + 2z_{67}$$

$$z_{67} + z_{57} = 1.$$

Deductions!!!

$$a + b = 1 + 2c$$

What is c?

Compile your code before you run it:

$$p_{1} + q_{1} = 1 + 2z_{12}$$

$$p_{2} + p_{1}q_{1} + q_{2} + z_{12} = 1 + 2z_{23} + 4z_{24}$$

$$1 + p_{2}q_{1} + p_{1}q_{2} + 1 + z_{23} = 1 + 2z_{34} + 4z_{35}$$

$$q_{1} + p_{2}q_{2} + p_{1} + z_{34} + z_{24} = 0 + 2z_{45} + 4z_{46}$$

$$q_{2} + p_{2} + z_{45} + z_{35} = 0 + 2z_{56} + 4z_{57}$$

$$1 + z_{56} + z_{46} = 0 + 2z_{67}$$

$$z_{67} + z_{57} = 1.$$

$$p_{1} + q_{1} = 1$$

$$p_{2} + q_{2} = 1$$

$$p_{2}q_{1} + p_{1}q_{2} = 1$$

$$(p_1 + q_1 - 1)^2$$

The solution to:

$$p_1 + q_1 = 1$$

Is the same as the input that minimizes the function:

$$(p_1 + q_1 - 1)^2$$

The solution to:

$$p_1 + q_1 = 1$$

$$p_2 + q_2 = 1$$

$$p_2q_1 + p_1q_2 = 1$$

Is the same as the minimum of the function:

$$(p_1 + q_1 - 1)^2 + (p_2 + q_2 - 1)^2 + (p_2q_1 + p_1q_2 - 1)^2$$

The solution to:

$$p_1 + q_1 = 1$$

$$p_2 + q_2 = 1$$

$$p_2q_1 + p_1q_2 = 1$$

Is the same as the minimum of the function:

$$(p_1 + q_1 - 1)^2 + (p_2 + q_2 - 1)^2 + (p_2q_1 + p_1q_2 - 1)^2 5 - 3p_1 - p_2 - q_1 + 2p_1q_1 - 3p_2q_1 + 2p_1p_2q_1 - 3q_2 + p_1q_2 + 2p_2q_2 + 2p_2q_1q_2$$

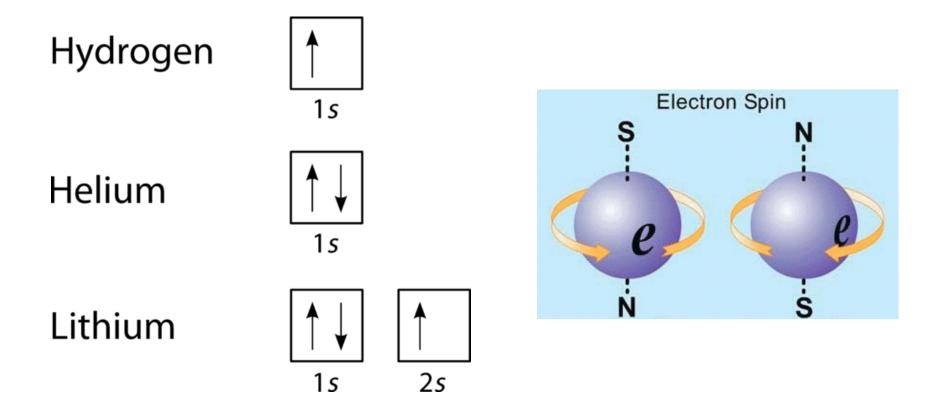
Search through 2⁴ possibilities

Search through 2⁵⁰⁰⁰ possibilities

 $5 - 3p_1 - p_2 - q_1 + 2p_1q_1 - 3p_2q_1 + 2p_1p_2q_1 - 3q_2 + p_1q_2 + 2p_2q_2 + 2p_2q_1q_2$ $5 - 3b_1 - b_2 - b_3 + 2b_1b_3 - 3b_2b_3 + 2b_1b_2b_3 - 3b_3 + b_1b_4 + 2b_2b_4 + 2b_2b_3b_4$

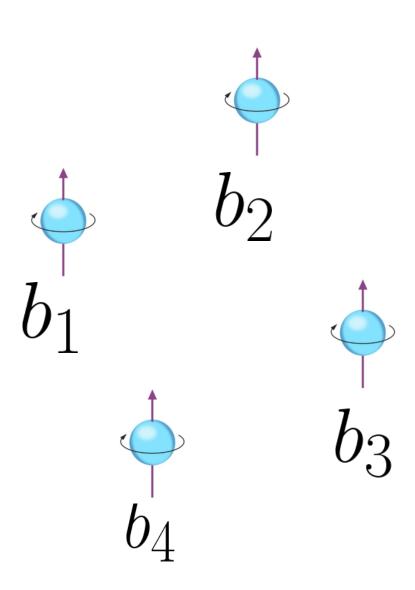
$$5 - 3p_1 - p_2 - q_1 + 2p_1q_1 - 3p_2q_1 + 2p_1p_2q_1 - 3q_2 + p_1q_2 + 2p_2q_2 + 2p_2q_1q_2$$

$$5 - 3b_1 - b_2 - b_3 + 2b_1b_3 - 3b_2b_3 + 2b_1b_2b_3 - 3b_3 + b_1b_4 + 2b_2b_4 + 2b_2b_3b_4$$



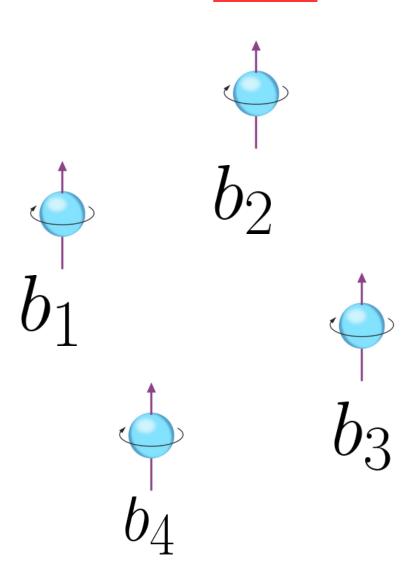
$$5 - 3p_1 - p_2 - q_1 + 2p_1q_1 - 3p_2q_1 + 2p_1p_2q_1 - 3q_2 + p_1q_2 + 2p_2q_2 + 2p_2q_1q_2$$

$$5 - 3b_1 - b_2 - b_3 + 2b_1b_3 - 3b_2b_3 + 2b_1b_2b_3 - 3b_3 + b_1b_4 + 2b_2b_4 + 2b_2b_3b_4$$



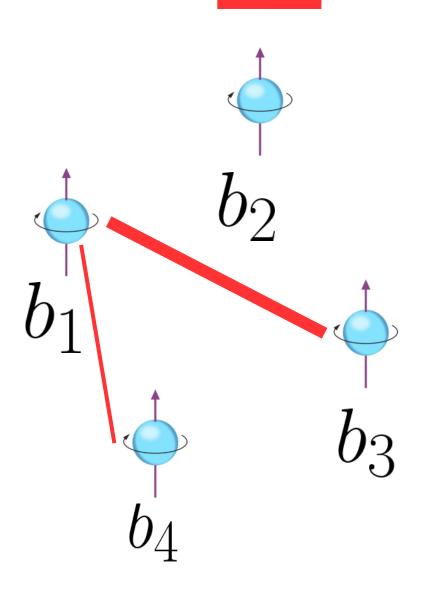
$$5 - 3p_1 - p_2 - q_1 + 2p_1q_1 - 3p_2q_1 + 2p_1p_2q_1 - 3q_2 + p_1q_2 + 2p_2q_2 + 2p_2q_1q_2$$

$$5 - 3b_1 - b_2 - b_3 + 2b_1b_3 - 3b_2b_3 + 2b_1b_2b_3 - 3b_3 + b_1b_4 + 2b_2b_4 + 2b_2b_3b_4$$



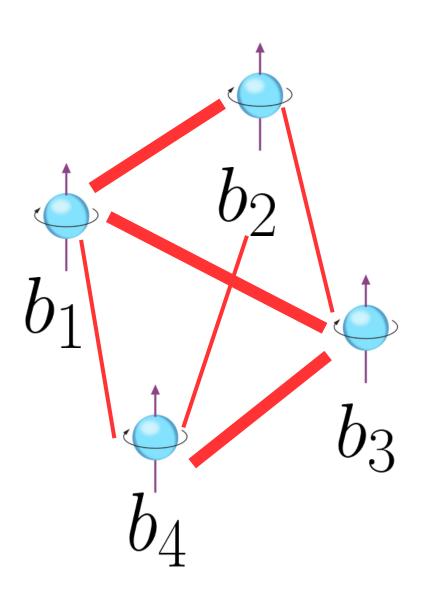
$$5 - 3p_1 - p_2 - q_1 + 2p_1q_1 - 3p_2q_1 + 2p_1p_2q_1 - 3q_2 + p_1q_2 + 2p_2q_2 + 2p_2q_1q_2$$

$$5 - 3b_1 - b_2 - b_3 + 2b_1b_3 - 3b_2b_3 + 2b_1b_2b_3 - 3b_3 + b_1b_4 + 2b_2b_4 + 2b_2b_3b_4$$



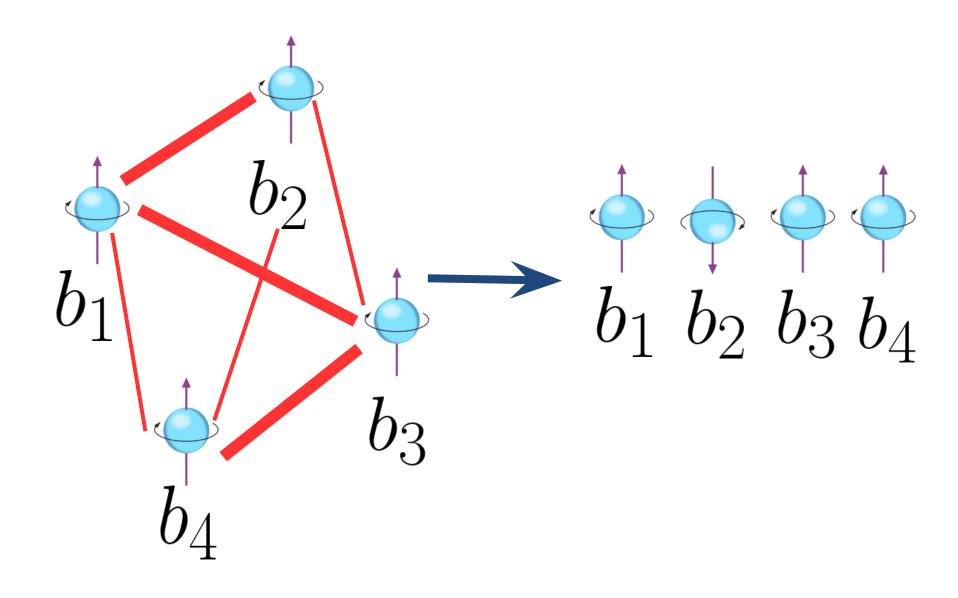
$$5 - 3p_1 - p_2 - q_1 + 2p_1q_1 - 3p_2q_1 + 2p_1p_2q_1 - 3q_2 + p_1q_2 + 2p_2q_2 + 2p_2q_1q_2$$

$$5 - 3b_1 - b_2 - b_3 + 2b_1b_3 - 3b_2b_3 + 2b_1b_2b_3 - 3b_3 + b_1b_4 + 2b_2b_4 + 2b_2b_3b_4$$



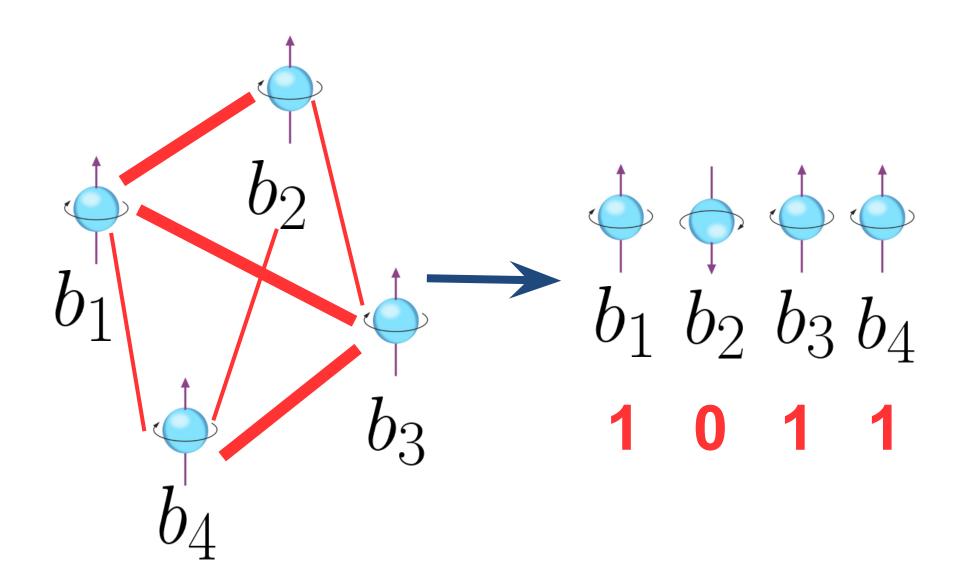
$$5 - 3p_1 - p_2 - q_1 + 2p_1q_1 - 3p_2q_1 + 2p_1p_2q_1 - 3q_2 + p_1q_2 + 2p_2q_2 + 2p_2q_1q_2$$

$$5 - 3b_1 - b_2 - b_3 + 2b_1b_3 - 3b_2b_3 + 2b_1b_2b_3 - 3b_3 + b_1b_4 + 2b_2b_4 + 2b_2b_3b_4$$



$$5 - 3p_1 - p_2 - q_1 + 2p_1q_1 - 3p_2q_1 + 2p_1p_2q_1 - 3q_2 + p_1q_2 + 2p_2q_2 + 2p_2q_1q_2$$

$$5 - 3b_1 - b_2 - b_3 + 2b_1b_3 - 3b_2b_3 + 2b_1b_2b_3 - 3b_3 + b_1b_4 + 2b_2b_4 + 2b_2b_3b_4$$

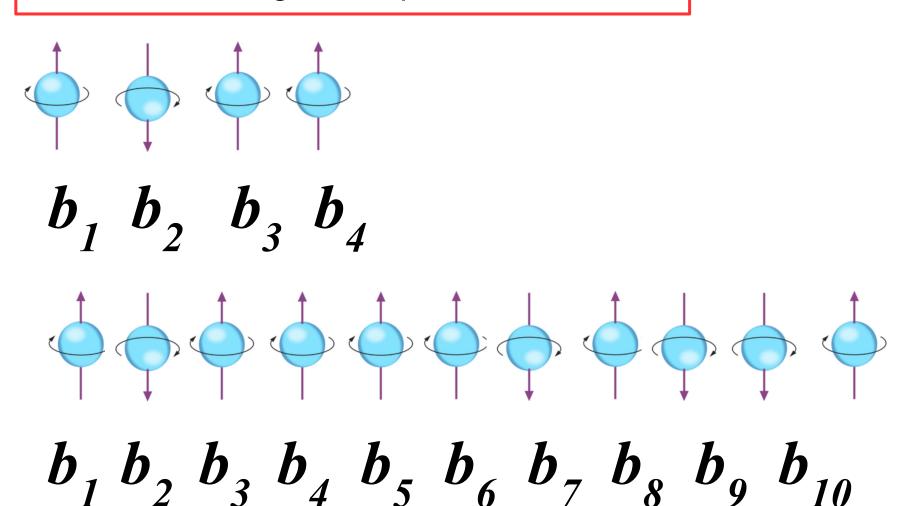


4 variables:

Search through 2⁴ possibilities

5000 variables:

Search through 2⁵⁰⁰⁰ possibilities



Adiabatic Quantum Computing

- Encode the solution to your problem in the ground state of a Hamiltonian.
- Find the ground state of that Hamiltonian

Quantum Chemistry

$$H = \sum_{p,q} h_{pq} a_p^{\dagger} a_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} a_p^{\dagger} a_q^{\dagger} a_r a_s$$

Jordan-Wigner Transform

$$a_{j} \Leftrightarrow \mathbf{1}^{\otimes j-1} \otimes \sigma^{+} \otimes \sigma^{z \otimes N-j-1}$$

$$a_{j}^{\dagger} \Leftrightarrow \mathbf{1}^{\otimes j-1} \otimes \sigma^{-} \otimes \sigma^{z \otimes N-j-1}$$

$$\sigma^{y} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \sigma^{x} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\sigma^{+} \equiv \frac{\sigma^{x} + i\sigma^{y}}{2} \quad \sigma^{-} \equiv \frac{\sigma^{x} - i\sigma^{y}}{2}$$

H₂ molecule

```
\begin{split} H &= -0.81261\mathbf{1} + 0.171201Z_0 + 0.171201Z_1 - 0.2227965Z_2 - 0.2227965Z_3 \\ &= +0.16862325Z_1Z_0 + 0.12054625Z_2Z_0 + 0.165868Z_2Z_1 + 0.165868Z_3Z_0 \\ &= +0.12054625Z_3Z_1 + 0.17434925Z_3Z_2 - 0.04532175X_3X_2Y_1Y_0 \\ &= +0.04532175X_3Y_2Y_1X_0 + 0.04532175Y_3X_2X_1Y_0 - 0.04532175Y_3Y_2X_1X_0 \end{split}
```

```
z23
                                              z12
                                                      0 + 2z45 + 4z46 + 8z47
                                                0 + 2256 + 4257 + 8258
Solved for all carries after 31 iterations!
                    2 + q3 + z23 = 0 + 2 × z34 + 4 × z35
+ p1q3 + 1 + z34 + z24 = 0 + 2 × z45 + 4 × z46 + 8 × z47
      p3q2 + p2q3 + p1 + z45 + z35 = 0 + 2 \times z56 + 4 \times z57 + 8 \times z58
                          + 246 = 1 + 2 \times 267 + 4 \times 268
                 + 258 = 1 + 2 \times 289
```

Quantum factorization of 56153 with only 4 qubits

Nikesh S. Dattani, 1,2,* Nathaniel Bryans 3,†

¹ Quantum Chemistry Laboratory, Kyoto University, 606-8502, Kyoto, Japan, ² Physical & Theoretical Chemistry Laboratory, Oxford University, OX1 3QZ, Oxford, UK, ³ University of Calgary, T2N 4N1, Calgary, Canada. *dattani.nike@gmail.com, [†] hbryans1@gmail.com

December 1, 2014

The largest number factored on a quantum device reported until now was 143 [1]. That quantum computation, which used only 4 qubits at 300K, actually also factored much larger numbers such as 3599, 11663, and 56153, without the awareness of the authors of that work. Furthermore, unlike the implementations of Shor's algorithm performed thus far [2–8], these 4-qubit factorizations do not need to use prior knowledge of the answer. However, because they only use 4 qubits, these factorizations can also be performed trivially on classical computers. We discover a class of numbers for which the power of quantum information actually comes into play. We then demonstrate a 3-qubit factorization of 175, which would be the first quantum factorization of a triprime.

he largest number factored on a quantum device reported until now was 143 [1]. That quantum computation, which used only 4 with Shor's algorithm and no prior knowledge of qubits at 300K, actually also factored much larger numbers such as 3599, 11663, and 56153, without the awareness of the authors of that work. Fur-

Quantum factorization of 143

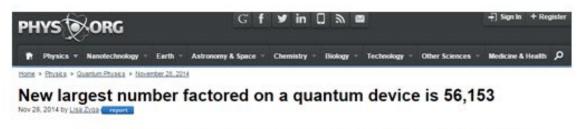
The NMR factorization of 143 in 2012 [1] began with the multiplication table:



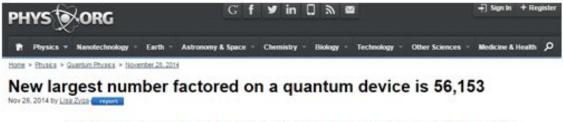
Nathaniel Bryans

Director, Artificial Intelligence at ATB Financial

Nathaniel Bryans is a Director, Artificial Intelligence at ATB Financial based in Calgary, Alberta. Previously, Nathaniel was a Test Software Deve... Read More



http://phys.org/news/2014-11-largest-factored-quantum-device.html



http://phys.org/news/2014-11-largest-factored-quantum-device.html



http://science.slashdot.org/story/14/12/03/1551239/mathematical-trick-helpssmash-record-for-the-largest-quantum-factorization



http://fizvcv.blogspot.sg/2014/11/nowy-rekord-faktoryzacji-liczb.html7.
International exchange achieved through the research

The Mathematical Trick That Helped Smash The Record For The Largest Number Ever Factorised By A Quantum Computer: 56153 = 233 x 241

https://medium.com/the-physics-arxiv-blog/the-mathematical-trick-thathelped-smash-the-record-for-the-largest-number-ever-factorised-by-a-77fde88499

NSA Plans for a Post-Quantum World

Quantum computing is a novel way to build computers — one that takes advantage of the quantum properties of particles to perform operations on data in a very different way than traditional computers. In some cases, the algorithm speedups are extraordinary.

Specifically, a quantum computer using something called Shor's algorithm can efficiently <u>factor</u> <u>numbers</u>, breaking RSA. A variant can break Diffie-Hellman and other discrete log-based cryptosystems, including those that use elliptic curves. This could potentially render all modern public-

RSA (cryptosystem)

From Wikipedia, the free encyclopedia

RSA (Rivest-Shamir-Adleman) is a public-key cryptosystem that is widely used for secure data transmission. It is also one of the oldest. The acronym RSA comes from the surnames of Ron Rivest, Adi Shamir, and Leonard Adleman, who publicly described the algorithm in 1977. An equivalent system was

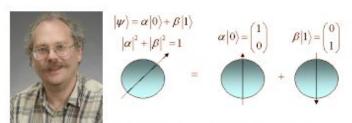
On the growth of cryptography¹

Ronald L. Rivest

Vannevar Bush Professor of EECS MIT, Cambridge, MA

Simons Institute Cryptography Program Historical Papers Seminar Series U.C. Berkeley June 3, 2015

Factoring on a Quantum Computer?



In 1994, Peter Shor invented a fast factorization algorithm that runs on a (hypothetical) *quantum computer* and works by determining multiplicative period of elements mod *n*.

- In 2001, researchers at IBM used this algorithm on a (real) quantum computer to factor 15 = 3 x 5.
- Recently (Dattani, 2014): 291311 = 557 x 523

Factoring 291311 with NMR

High-fidelity adiabatic quantum computation using the intrinsic Hamiltonian of a spin system: Application to the experimental factorization of 291311

```
Zhaokai Li, <sup>1, 2</sup> Nikesh S. Dattani, <sup>3, 4</sup> Xi Chen, <sup>1</sup> Xiaomei Liu, <sup>1</sup> Hengyan Wang, <sup>1</sup> Richard Tanburn, <sup>3</sup> Hongwei Chen, <sup>5</sup> Xinhua Peng, <sup>1, 2, 6, *</sup> and Jiangfeng Du<sup>1, 2, 6, †</sup> 

<sup>1</sup> CAS Key Laboratory of Microscale Magnetic Resonance and Department of Modern Physics, University of Science and Technology of China (USTC), Hefei 230026, China 

<sup>2</sup> Synergetic Innovation Center of Quantum Information and Quantum Physics, USTC, Hefei, China 

<sup>3</sup> Oxford University, Hertford College, Oxford, OX1 3BW, UK 

<sup>4</sup> Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, 606-8103, Japan 

<sup>5</sup> High Magnetic Field Laboratory, Chinese Academy of Sciences, Hefei 230031, China 

<sup>6</sup> Hefei National Laboratory for Physical Sciences at the Microscale, USTC, Hefei, China
```

High-fidelity adiabatic quantum computation using the intrinsic Hamiltonian of a spin system: Application to the experimental factorization of 291311

Zhaokai Li, Nikesh S. Dattani, Xi Chen, Xiaomei Liu, Hengyan Wang, Richard Tanburn, Hongwei Chen, Xinhua Peng, Jiangfeng Du (Submitted on 25 Jun 2017)

High-fidelity adiabatic quantum computation using the intrinsic Hamiltonian of a spin system: Application to the experimental factorization of 291311

Zhaokai Li,^{1,2} Nikesh S. Dattani,^{3,4} Xi Chen,¹ Xiaomei Liu,¹ Hengyan Wang,¹ Richard Tanburn, Hongwei Chen,⁵ Xinhua Peng,^{1,2,6,*} and Jiangfeng Du^{1,2,6,†} ¹CAS Key Laboratory of Microscale Magnetic Resonance and Department of Modern Physics,

Article Open Access Published: 01 December 2021

Advancing mathematics by guiding human intuition with AI

<u>Alex Davies</u> [™], <u>Petar Veličković</u>, <u>Lars Buesing</u>, <u>Sam Blackwell</u>, <u>Daniel Zheng</u>, <u>Nenad Tomašev</u>,

Richard Tanburn Peter Battaglia, Charles Blundell, András Juhász, Marc Lackenby, Geordie

Williamson, Demis Hassabis & Pushmeet Kohli

Nature 600, 70-74 (2021) Cite this article

158k Accesses 4 Citations 1597 Altmetric Metrics



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PUBLIC

Breakthroughs in mathematics in 2021

Asked 2 months ago Active 1 month ago Viewed 9k times



51

Advancing mathematics by guiding human intuition with AI, Nature 600, 70 (2021), stands out because it represents the first significant advance in pure mathematics generated by artificial intelligence.

Carlo Beenakker

Article Open Access Published: 01 December 2021

Advancing mathematics by guiding human intuition with AI

Alex Davies [™], Petar Veličković, Lars Buesing, Sam Blackwell, Daniel Zheng, Nenad Tomašev,

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Nature 600 70-74 (2021) Cite this article

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15	2001
	2007
	2007
	2009
	2012
21	2012
Adiabatic Algorithm	<u>Year</u>
143	2012
56153	2014
291311	2017

Thank you!

Next lecture:

Compiling AQC algorithms to run on real hardware

nike@hpqc.org