

# Quantum Algorithms in NMR Experiments

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# Introduction to Shor's algorithm

- Given an integer  $N$ , find its prime factors.
- Classically, prime factorization takes  $O(\exp[1.9(\log N)^{1/3}(\log \log N)^{2/3}])$  operations.
- On a quantum computer, it runs in polynomial time, taking only  $O((\log N)^3)$  operations. Much faster!
- With a sufficient number of qubits, Shor's algorithm can be used to break public-key cryptography schemes such as the widely used RSA scheme.
- Shor's algorithm consists of two parts:
  - Classical part:  
A reduction of the factoring problem to the order-finding problem, which can be done on a classical computer.
  - Quantum part:  
A quantum algorithm is used to solve the order-finding problem.

# Shor's algorithm (classical part)

- Task:
  - Given an integer  $N$ , find its prime factors
  - Calculate  $a^x \bmod N = 1$ ; find period  $r$  (order of  $a$ ) of  $f_{N,a}(x) = a^x \bmod N$
- Procedure:
  - $a^2 \bmod N = 1 \iff (a + 1)(a - 1) = 0 \bmod N$
  - If neither  $(a + 1)$  nor  $(a - 1)$  multiple of  $N$ , then at least one factor of  $N$  is in  $(a + 1)$  and also in  $(a - 1)$
- Algorithm:
  - Choose  $a \in \{2, \dots, N - 1\}$
  - $y := \gcd(a, N)$ , check  $y = 1$
  - $r := \text{ord}(a)$ , check  $r = 2k$
  - $z := \max\{\gcd(ar/2 - 1, N), \gcd(ar/2 + 1, N)\}$

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Example: to factorize 21:

Choose  $a=13$

$\gcd(13,21)=1$  ok.

$\text{ord}(13): 13^2 \bmod 21 = 1 \implies r=2$  ok.

$\gcd(12,21)=3, \gcd(14,21)=7$

$\implies 21=3*7$

# Shor's algorithm (quantum part)

## 1. Initialization

$$Q^{-1/2} \sum_{x=0}^{Q-1} |x\rangle |0\rangle$$

## 2. Construction

$$Q^{-1/2} \sum_{x=0}^{Q-1} |x\rangle |f(x)\rangle$$

## 3. Transformation

$$Q^{-1} \sum_x \sum_y \omega^{xy} |y\rangle |f(x)\rangle$$

$$\sum_{x:f(x)=f(x_0)} \omega^{xy} = \sum_b \omega^{(x_0+r_b)y} = \omega^{x_0y} \sum_b \omega^{rby}$$

# Shor's algorithm (quantum part)

## 1. Initialization

$$Q^{-1/2} \sum_{x=0}^{Q-1} |x\rangle |0\rangle$$

a superposition of Q states

## 2. Construction

$$Q^{-1/2} \sum_{x=0}^{Q-1} |x\rangle |f(x)\rangle$$

f(x) as a quantum function and apply it to the above state

## 3. Transformation

$$Q^{-1} \sum_x \sum_y \omega^{xy} |y\rangle |f(x)\rangle$$

apply the quantum Fourier transform, and leads to the final state

$$\sum_{x:f(x)=f(x_0)} \omega^{xy} = \sum_b \omega^{(x_0+r_b)y} = \omega^{x_0y} \sum_b \omega^{rby}$$

# Shor's algorithm (quantum part)

## 4. Measurement

$$\left| Q^{-1} \sum_{x:f(x)=f(x_0)} \omega^{xy} \right|^2 = Q^{-2} \left| \sum_b \omega^{(x_0+r_b)y} \right|^2 = Q^{-2} \left| \sum_b \omega^{rby} \right|^2$$



# Shor's algorithm (quantum part)

## 4. Measurement

$$\left| Q^{-1} \sum_{x:f(x)=f(x_0)} \omega^{xy} \right|^2 = Q^{-2} \left| \sum_b \omega^{(x_0+r_b)y} \right|^2 = Q^{-2} \left| \sum_b \omega^{rby} \right|^2$$

-Perform Continued Fraction Expansion on  $y/Q$  to make an approximation, and produce some  $c/r'$  by it that satisfies two conditions:

A:  $r' < N$

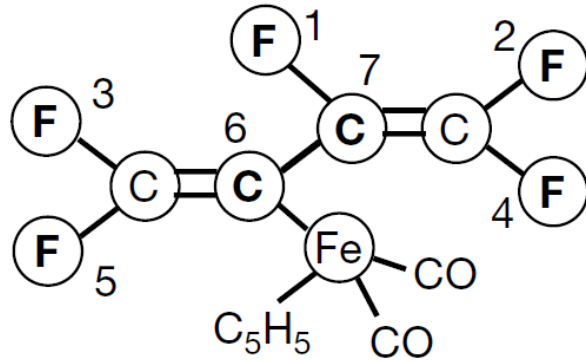
B:  $|y/Q - c/r'| < 1/2Q$

$r'$  would be the appropriate period  $r$  with high probability.

-Check if  $f(x) = f(x + r') \iff a^{r'} = 1 \pmod{N}$ ; if so, done.

-Otherwise, obtain more candidates for  $r$  near  $y$ .

# Qubit system: nuclear spins in a molecule



Perfluorobutadienyl molecule with 7 nuclear spins

- $^{19}\text{F}$  and  $^{13}\text{C}$  are spin half nuclei
- 2 level system due to Zeeman splitting in static magnetic field

$$H = -\sum_i^n \bar{h} \omega_{0i} I_{iz} \quad \omega_{0i} = \frac{g\mu_i B_0}{\bar{h}}$$

- $\omega_{0i}$  Transition frequency between  $|0\rangle$  &  $|1\rangle$

$$11.7 \text{ T} \rightarrow \begin{array}{l} {}^{13}\text{C} \ \omega_{0i} = 125 \text{ MHz} \\ {}^{19}\text{F} \ \omega_{0i} = 470 \text{ MHz} \end{array}$$

# Spin properties

- Chemical shifts in molecule causes inhomogenities in magnetic field, well separated frequencies for each qubit

$$\omega_{0i} = (1 - \sigma_i) \frac{g\mu_i B_0}{\hbar}$$

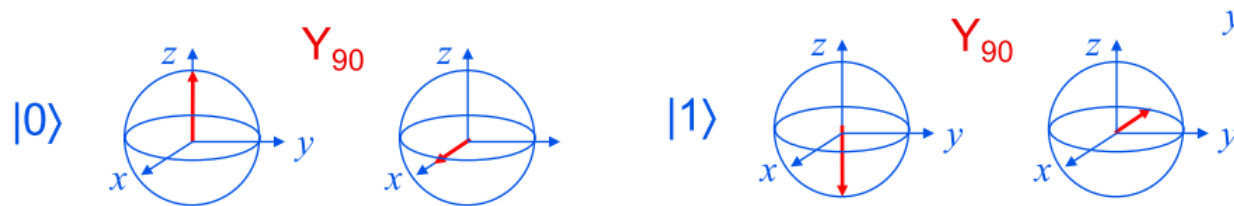
- Longitudinal and transvers coherence times  $T_1$  and  $T_2$  in order of seconds
- Pairwise J coupling between spins

$$H_J = \sum_{i < j} 2\pi\hbar J_{ij} I_{iz} I_{jz}$$

$i$	$\omega_i/2\pi$	$T_{1,j}$	$T_{2,j}$	$J_{7i}$	$J_{6i}$	$J_{5i}$	$J_{4i}$	$J_{3i}$	$J_{2i}$
1	-22052.0	5.0	1.3	-221.0	37.7	6.6	-114.3	14.5	25.16
2	489.5	13.7	1.8	18.6	-3.9	2.5	79.9	3.9	
3	25088.3	3.0	2.5	1.0	-13.5	41.6	12.9		
4	-4918.7	10.0	1.7	54.1	-5.7	2.1			
5	15186.6	2.8	1.8	19.4	59.5				
6	-4519.1	45.4	2.0	68.9					
7	4244.3	31.6	2.0						

# Experimental realization

- RF coil in  $xy$  plane for applying RF pulses to manipulate spins
- Spin state is detected by rotating about  $y$ -axis by  $90^\circ$ 
  - $10^{23}$  nuclei produce measurable RF field in the coil (ensemble measurement)



- Qubit system of the molecule fulfills the DiVincenzo criteria
  - For proper initialization temporal averaging can be used
  - Long enough coherence times
  - Pairwise  $J$  coupling of spins allows to implement gates
  - Readout of spin states possible

# Shor's algorithm applied to 15

For  $N=15$  have to consider 3 cases:

*i.*  $a = 3, 5, 6, 10 \rightarrow \gcd(a, 15) = 3 \text{ or } 5$   
no quantum computation step needed

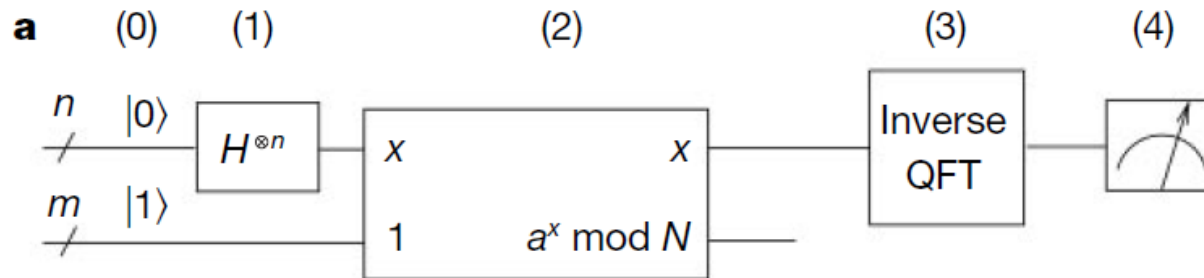
*ii.*  $a = 4, 11, 14 \rightarrow \gcd(a, 15) = 1$   
 $f(2) = a^2 \bmod 15 = 1$

*iii.*  $a = 2, 7, 8, 13 \rightarrow \gcd(a, 15) = 1$   
 $f(4) = a^4 \bmod 15 = 1$

Periodicity is either  $r=2$  or  $4$   
 $r$  is even  
 $a^{r/2} \neq -1 \bmod 15$

- First register has  $n=3$  qubits to hold the periode  $r$   
(two would be sufficient to represent 2 and 4, but there is one additional for possible higher periods)
- Second register has  $m=4$  qubits to hold  $f(x) = a^x \bmod 15$

# Quantum circuit



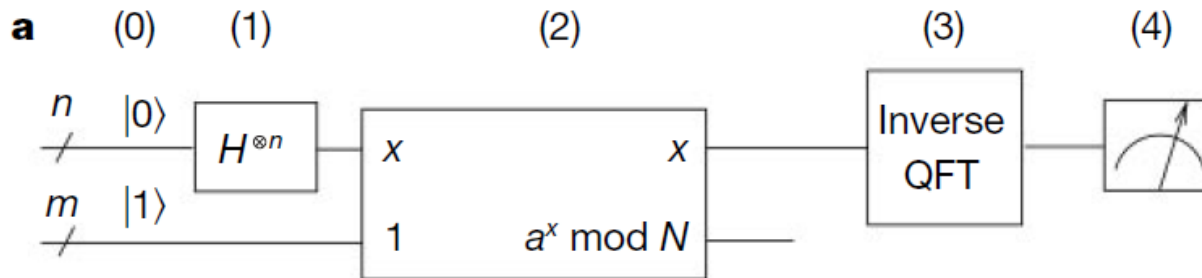
- 0) Initialize first register to  $|0\rangle = |000\rangle$  and the second to  $|1\rangle = |0001\rangle$   
 1) Hadamard gate on first register creates superposition

$$|\Psi_1\rangle = \sum_{x=0}^7 \frac{1}{\sqrt{8}} |x\rangle |1\rangle$$

- 2) Multiply second register with  $f(x) = a^x \bmod N$

$$|\Psi_2\rangle = \sum_{x=0}^7 \frac{1}{\sqrt{8}} |x\rangle |1\rangle \langle a^x \bmod N|$$

# Quantum circuit II



3) Perform inverse QFT on first register

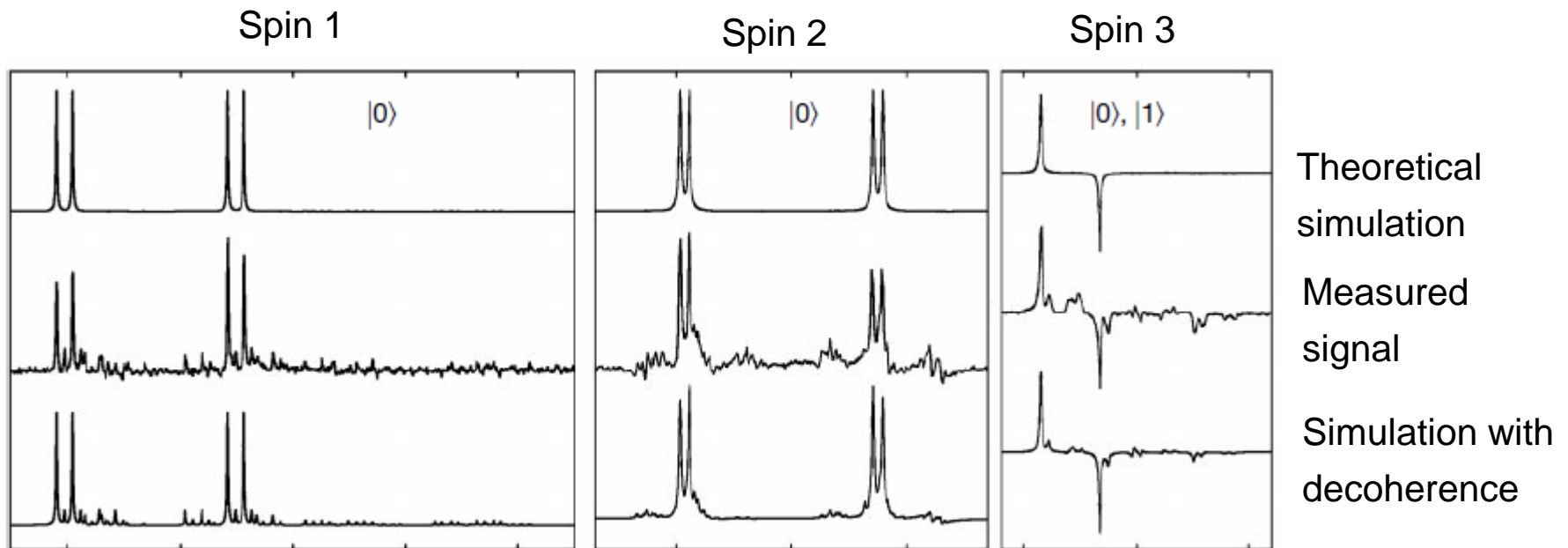
$$|\Psi_3\rangle = \sum_{y=0}^7 \sum_{x=0}^7 \frac{e^{2\pi ixy/8}}{\sqrt{8}} |y\rangle |a^x \bmod N\rangle$$

Sum over  $y$  reduces due to periodicity of  $f(x)$  to terms with  $y = \frac{2^n c}{r}$ ,  
with  $c$  a constant and  $r$  the period of  $f(x)$

4) Measuring the spin states of the first register with the pick up coil

Initialization, manipulation and the measurement processes require about 300 RF pulses within 750 ms.

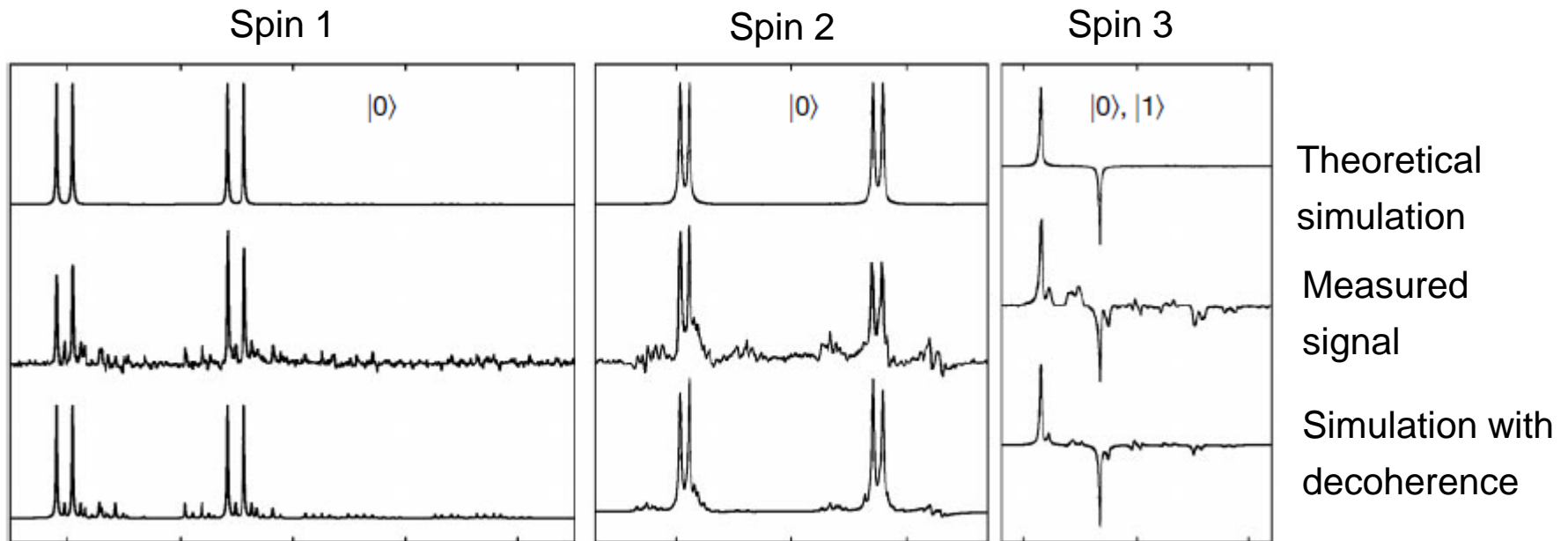
# Experimental result $a=11$ (simple case)



- Frequency vs. Phase plot for each spin
  - Positive peaks correspond to  $|0\rangle$  and negative peaks to  $|1\rangle$
- Simple case because just one qubit in a mixed state
- Multiple peaks in the spectra arise due to crosstalk of the spins



# Experimental result $a=11$ (simple case)



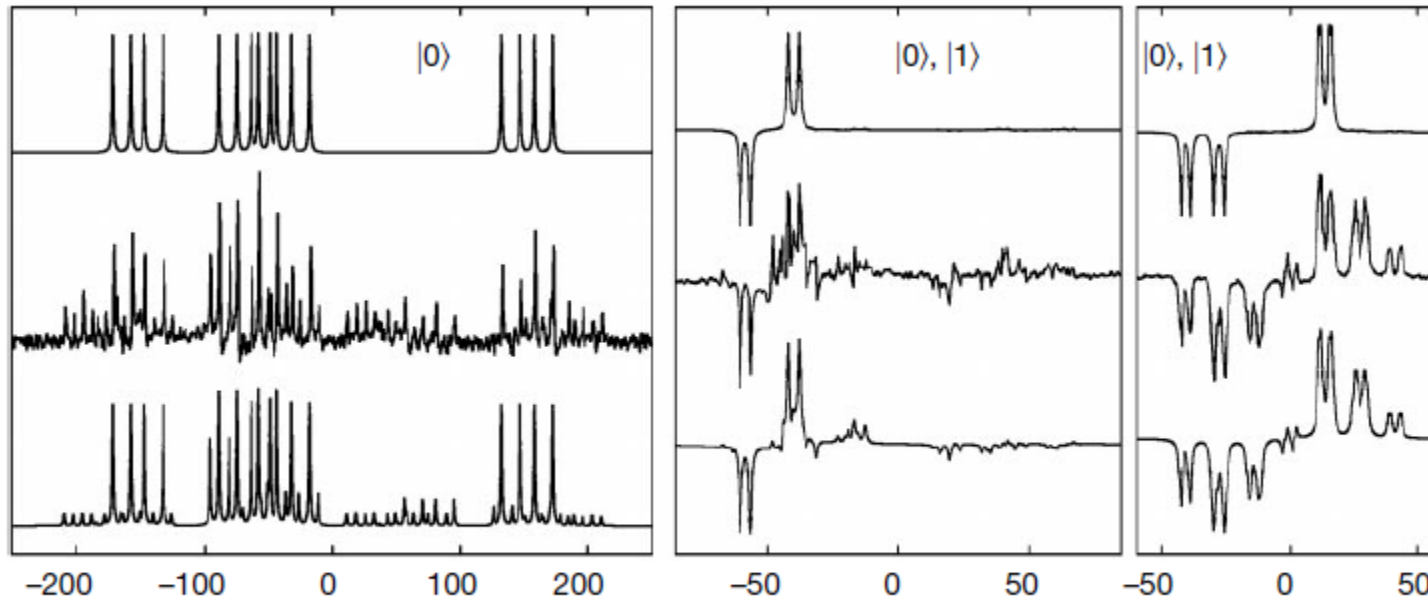
- Mixture of states  $|000\rangle$  and  $|100\rangle$  or in decimal notation  $|0\rangle$  and  $|4\rangle$
- Period of  $y$  is 4  $\rightarrow r = 2^3/4 = 2$
- $\text{gcd}(11^{2/2} \pm 1, 15) = 3 \& 5$

# Experimental result $a=7$ (difficult case)

Spin 1

Spin 2

Spin 3

Theoretical  
simulationMeasured  
signalSimulation with  
decoherence

- Mixture of states  $|000\rangle$ ,  $|010\rangle$ ,  $|100\rangle$  and  $|110\rangle$  or in decimal notation  $|0\rangle$ ,  $|2\rangle$ ,  $|4\rangle$  and  $|6\rangle$
- Period of  $y$  is 2  $\rightarrow r = 2^3/2 = 4$
- $\gcd(11^{4/2} \pm 1, 15) = 3 \& 5$

## References

- Shor Pieter W.  
Polynomial Time Algorithms for Prime Factorization and Discrete Logarithms on a Quantum Computer
- Vandersypen, LMK: et al  
Experimental realization of Shor's quantum factoring algorithm using nuclear magnetic resonance

# Conclusion

- Shor algorithm provides a solution for factoring number in polynomial time using a quantum computer
- Successful implementation of Shor's factoring algorithm in an NMR quantum computer
- Good agreement between measured and simulated spectra, discrepancies can be attributed to decoherence
- First quantum computation experiment for which decoherence is the dominant source of errors

# Outlook

- The experiment shows the limits of NMR quantum computers
  - For  $N > 15$  a molecule with more spins is needed
  - Problems of single spin accessibility, spin interactions and shorter coherence times
- Hard to find error correction schemes for quantum computers to overcome imprecision and decoherence
- Proof for powerful every day applications of quantum computers is missing
- Task of the on going research to find other qubit systems and new quantum computation algorithms