NMR Quantum Computing

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with some annotations by Andreas Wallraff.
How to factor 15 with NMR?

perfluorobutadienyl iron complex

red nuclei are qubits: F, $^{13}$C
Goals of this lecture

Survey of NMR quantum computing

Principles of NMR QC
Techniques for qubit control
State of the art
Future of spins for QIPC
Example: factoring 15
NMR largely satisfies the DiVincenzo criteria

- **Qubits**: nuclear spins $\frac{1}{2}$ in $B_0$ field (↑ and ↓ as 0 and 1)
- **Quantum gates**: RF pulses and delay times
- **Input**: Boltzman distribution (room temperature)
- **Readout**: detect spin states with RF coil
- **Coherence times**: easily several seconds

(Gershenfeld & Chuang 1997, Cory, Havel & Fahmi 1997)
Nuclear spin Hamiltonian
Single spin

\[ \mathcal{H}_0 = -\hbar \gamma B_0 I_z = -\hbar \omega_0 I_z = \begin{bmatrix} -\hbar \omega_0 /2 & 0 \\ 0 & \hbar \omega_0 /2 \end{bmatrix} \]

\[ |0\rangle \]
\[ |1\rangle \]
\[ \hbar \omega_0 \]
\[ \frac{|0\rangle + i |1\rangle}{\sqrt{2}} \]
\[ \frac{|0\rangle + |1\rangle}{\sqrt{2}} \]

angular momentum: \[ \hat{L} = \hbar \hat{\mathbf{I}} \]
magnetic moment: \[ \hat{\mathbf{M}} = \gamma \hbar \hat{\mathbf{I}} \]
energy: \[ \mathcal{H}_0 = -\mathbf{M} \cdot \mathbf{B}_0 \]
gyromagnetic (g-)factor: \[ \gamma \]
Nuclear spin Hamiltonian

Multiple spins

\[ \mathcal{H}_0 = - \sum_{i=1}^{n} \hbar (1 - \tilde{\sigma}_i) \gamma_i B_0 I_z^i = - \sum_{i=1}^{n} \hbar \omega_0^i I_z^i \]

chemical shifts
of the five F qubits

MHz

\begin{align*}
{^1}_H & \quad 500 \quad \sim 25 \text{ mK} \\
{^{13}}_C & \quad 126 \\
{^{15}}_N & \quad -51 \\
{^{19}}_F & \quad 470 \\
{^{31}}_P & \quad 202 \\
\end{align*}

(at 11.7 Tesla)

qubit level separation
Hamiltonian with RF field

single-qubit rotations

\[ \mathcal{H} = -\hbar \omega_0 I_z - \hbar \omega_1 \left[ \cos(\omega_{rf} t + \phi) I_x + \sin(\omega_{rf} t + \phi) I_y \right] \]

\[ |\psi\rangle^{rot} = \exp(-i\omega_{rf} t I_z) |\psi\rangle \]

\[ \mathcal{H}^{rot} = -\hbar (\omega_0 - \omega_{rf}) I_z - \hbar \omega_1 \left[ \cos \phi I_x + \sin \phi I_y \right] \]

rotating wave approximation

typical strength \( I_x, I_y : \text{up to } 100 \text{ kHz} \)

Lab frame

Rotating frame
Nuclear spin Hamiltonian

Coupled spins $J > 0$: antiferro mag.

$J < 0$: ferro-mag.

Typical values: $J$ up to few 100 Hz

$H_J = \hbar \sum_{i<j} n 2\pi J_{ij} I_i^z I_j^z$

solid (dashed) lines are (un)coupled levels
Controlled-NOT in NMR

A target bit
B control bit

Before        After
A  B         A  B

| 0 ⟩ + | 1 ⟩
\[
\frac{\sqrt{2}}
\]

” flip A if B ↓”

if spin B is ↑

if spin B is ↓

different rotation direction depending on control bit

wait
Delay
1/2J_{AB}

Y^A_{90}

X^A_{90}
Making room temperature spins look cold

- (Cool to mK)
- Optical pumping
- DNP, …

Effective pure state
(Gershenfeld & Chuang, Science '97,
Cory, Havel & Fahmi, PNAS '97)

Look exactly like cold spins!
Effective pure state preparation

(1) Add up \(2^N - 1\) experiments (Knill, Chuang, Laflamme, PRA 1998)

\[ \begin{array}{cccccccc}
\uparrow\uparrow & \uparrow\downarrow & \downarrow\uparrow & \downarrow\downarrow & + & \uparrow\uparrow & \uparrow\downarrow & \downarrow\uparrow & \downarrow\downarrow & + & \uparrow\uparrow & \uparrow\downarrow & \downarrow\uparrow & \downarrow\downarrow & = & \uparrow\uparrow & \uparrow\downarrow & \downarrow\uparrow & \downarrow\downarrow
\end{array} \]

Later \(\approx (2^N - 1) / N\) experiments (Vandersypen et al., PRL 2000)

prepare equal population (on average) and look at deviations from equilibrium.

(2) Work in subspace (Gershenfeld & Chuang, Science 1997)

\[ \begin{array}{cccccccccc}
\uparrow\uparrow\uparrow & \uparrow\uparrow\downarrow & \uparrow\downarrow\uparrow & \uparrow\downarrow\down\down & \down\down\down\down & \down\down\down\down & \down\down\down\down & \down\down\down\down & \down\down\down\down & \down\down\down\down & \down\down\down\down & \down\down\down\down & \down\down\down\down & \down\down\down\down
\end{array} \]

compute with qubit states that have the same energy and thus the same population.
Read-out in NMR

Phase sensitive detection

|0\rangle

Positive signal for |0\rangle (in phase)

|1\rangle

Negative signal for |1\rangle (out of phase)
Measurements of single systems versus ensemble measurements

|                        | Quantum state | |00⟩ + |11⟩ |
|------------------------|---------------|----------------|
| Single-shot bitwise    | |0⟩ and |0⟩ | |0⟩ or |1⟩ |
| Single-shot “word”wise | |00⟩ | |00⟩ or |11⟩ |
| Bitwise average        | |0⟩ and |0⟩ | Each bit average of |0⟩ and |1⟩ |
| “Word”wise average     | |00⟩ | Average of |00⟩ and |11⟩ |

Adapt algorithms if use ensemble
Quantum state tomography

Look at qubits from different angles

no pulse  after $X_{90}$  after $Y_{90}$
Outline

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- Principles of NMR QC
- Techniques for qubit control
- Example: factoring 15
- State of the art
- Outlook
Off-resonance pulses and spin-selectivity

\[ \mathcal{H}^{\text{rot}} = -\hbar (\omega_0 - \omega_{rf}) I_z - \hbar \omega_1 \left[ \cos \phi I_x + \sin \phi I_y \right] \]

Off-resonant pulses induce eff. \( \sigma_z \) rotation in addition to \( \sigma_{x,y} \) may induce transitions in other qubits
Pulse shaping for improved spin-selectivity

Less cross-talk
Missing coupling terms: Swap

How to couple distant qubits with only nearest neighbor physical couplings?

Missing couplings: swap states along qubit network

$$\text{SWAP}_{12} = \text{CNOT}_{12} \text{CNOT}_{21} \text{CNOT}_{12}$$

as discussed in exercise class

“only” a linear overhead ...
Undesired couplings: refocus
remove effect of coupling *during delay times*

opt. 1: act on qubit B

opt. 2: act on qubit A

• There exist efficient extensions for arbitrary coupling networks
• Refocusing can also be used to remove unwanted Zeeman terms
Composite pulses

Example: $Y_{90}X_{180}Y_{90}$

corrects for under/over-rotation

corrects for off-resonance

However: doesn’t work for arbitrary input state
But: there exist composite pulses that work for all input states
A quantum computer is a *known* molecule. Its desired properties are:

- spins $1/2$ (\(^{1}H, \, ^{13}C, \, ^{19}F, \, ^{15}N, \ldots\))
- long T\(_1\)'s and T\(_2\)'s
- heteronuclear, or large chemical shifts
- good J-coupling network (clock-speed)
- stable, available, soluble, ...

required to make spins of same type addressable
Quantum computer molecules (1)

red nuclei are used as qubits:

Grover / Deutsch-Jozsa

Q. Error correction

Logical labeling / Grover

Teleportation

Q. Error Detection
Quantum computer molecules (2)

Deutsch-Jozsa

7-spin coherence

Order-finding

$\text{Fe} \ (\text{CH})^5 \ (\text{CO})^2$
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{ State of the art
Outlook }
The good news

- Quantum computations have been demonstrated in the lab.
- A high degree of control was reached, permitting hundreds of operations in sequence.
- A variety of tools were developed for accurate unitary control over multiple coupled qubits.
  - useful in other quantum computer realizations
- Spins are natural, attractive qubits.
Scaling

We do not know how to scale liquid NMR QC

Main obstacles:
• Signal after initialization \( \sim \frac{1}{2^n} \) [at least in practice]
• Coherence time typically goes down with molecule size
• We have not yet reached the accuracy threshold ...
Main sources of errors in NMR QC

Early on (heteronuclear molecules)
  inhomogeneity RF field

Later (homonuclear molecules)
  $J$ coupling during RF pulses

Finally
  decoherence
Solid-state NMR?

molecules in solid matrix

Cory et al

Yamaguchi & Yamamoto, 2000

\[
\mathcal{H}_J = \hbar \sum_{i<j} 2\pi J_{ij} \vec{I}_i \cdot \vec{I}_j = \hbar \sum_{i<j} 2\pi J_{ij} (I_i^i I_j^j + I_i^x I_j^x + I_i^y I_j^y + I_i^z I_j^z)
\]

\[
\mathcal{H}_D = \sum_{i<j} \frac{\mu_0 \gamma_i \gamma_j \hbar}{4\pi |\vec{r}_{ij}|^3} \left[ \vec{I}_i \cdot \vec{I}_j - \frac{3}{|\vec{r}_{ij}|^2} (\vec{I}_i \cdot \vec{r}_{ij})(\vec{I}_j \cdot \vec{r}_{ij}) \right]
\]
Electron spin qubits

Kane, Nature 1998

Loss & DiVincenzo, PRA 1998
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Quantum Factoring

Find the prime factors of $N$: chose $a$ and find order $r$.

$$f(x) = a^x \mod N$$

Results from number theory:

- $f$ is periodic in $x$ (period $r$)
- $\gcd(a^{r/2} \pm 1, N)$ is a factor of $N$

Quantum factoring: find $r$

Complexity of factoring numbers of length $L$:

Classically: $\sim e^{L/3}$

Quantum: $\sim L^3$ P. Shor (1994)

Widely used crypto systems (RSA) would become insecure.
Factoring 15 - schematic

\[ |x\rangle = |0\rangle + |1\rangle + \ldots + |2^{2L}-1\rangle \]

\[ \sum_k |k2L/r\rangle \quad \text{Interference} \]

2 \( L \) bits
3 qubits

\( L = \log_2(15) \)
4 qubits

\[ x = \ldots + x_2 2^2 + x_1 2^1 + x_0 2^0 \]

\[ a^x = \ldots a^{4x_2} a^{2x_1} a^{x_0} \]

\[ a = 4, 11 \quad \Rightarrow \quad a^2 \mod 15 = 1 \quad \Rightarrow \quad \text{"easy" case period 2} \]

\[ a = 2, 7, 8, 13 \quad \Rightarrow \quad a^4 \mod 15 = 1 \quad \Rightarrow \quad \text{"hard" case period 4} \]

\[ a = 14 \quad \Rightarrow \quad \text{fails} \]
Quantum Fourier transform and the FFT

The FFT (and QFT)
- Inverts the period
- Removes the off-set

\[ a = 11 \]

\[ |\psi_3\rangle = |0\rangle |0\rangle + |1\rangle |2\rangle + |2\rangle |0\rangle + |3\rangle |2\rangle + |4\rangle |0\rangle + |5\rangle |2\rangle + |6\rangle |0\rangle + |7\rangle |2\rangle \]
\[ = ( |0\rangle + |2\rangle + |4\rangle + |6\rangle ) |0\rangle + ( |1\rangle + |3\rangle + |5\rangle + |7\rangle ) |2\rangle \text{ after mod exp} \]

\[ |\psi_4\rangle = ( |0\rangle + |4\rangle ) |0\rangle + ( |0\rangle - |4\rangle ) |2\rangle \text{ after QFT} \]
Experimental approach

- 11.7 Tesla Oxford superconducting magnet; room temperature bore
- 4-channel Varian spectrometer; need to address and keep track of 7 spins
  - phase ramped pulses
  - software reference frame
- Shaped pulses
- Compensate for cross-talk
- Unwind coupling during pulse

Larmor frequencies
- 470 MHz for $^{19}$F $\sim 25$ mK
- 125 MHz for $^{13}$C

$J$ - couplings: 2 - 220 Hz

coherence times: 1.3 - 2 s
Thermal Equilibrium Spectra

- line splitting due to $J$-coupling
- all lines present

Qubit 1: Line splitting and all lines present.

Qubit 2: Uncoupled qubit states indicated by arrows.

Qubit 3: Uncoupled qubit states indicated by arrows.
Spectra after state initialization

- only the $|00 \ldots 0\rangle$ line remains
- the other lines are averaged away by adding up multiple experiments

RT spins appear cold!
Pulse sequence \((a=7)\)

\(\pi/2\) \(X\)- or \(Y\)-rotations (H and gates)
\(\pi\) \(X\)-rotations (refocusing)
\(Z\) - rotations

> 300 pulses, \(\approx 720 \text{ ms}\)
"Easy" case ($a=11$)

| Ideal prediction | Qubit 1: up → $|0\rangle$ | Real prediction |
|-------------------|-----------------------------|----------------|
| $|000\rangle$      | 0                           | 8 / $r = 4$    |
| $|100\rangle$      | 4                           | $r = 2$        |

$\gcd(11^{2/2} - 1, 15) = 5$
$\gcd(11^{2/2} + 1, 15) = 3$

$15 = 3 \times 5$

Qubit 2: up/down → $|0\rangle, |1\rangle$

Qubit 3: recall read-out scheme

Qubit 1: Ideal prediction

Qubit 2: Ideal prediction

Qubit 3: Ideal prediction
"Hard" case \((a=7)\)

- \(|000\rangle\): 0
- \(|010\rangle\): 2
- \(|100\rangle\): 4
- \(|110\rangle\): 6

\[
\gcd(7^{4/2} - 1, 15) = 3
\]
\[
\gcd(7^{4/2} + 1, 15) = 5
\]

\[15 \cong 3 \times 5\]

**Qubit 1:**
- Up \(\rightarrow |0\rangle\)

**Qubit 2:**
- Up/down \(\rightarrow |0\rangle, |1\rangle\)

**Qubit 3:**
- Up/down \(\rightarrow |0\rangle, |1\rangle\)

Real part [arb. units]

Imag part [arb. units]
Model quantum noise (decoherence)

Spins interact with the environment

Decoherence

The decoherence model for 1 nuclear spin is well-described.

We created a workable decoherence model for 7 coupled spins. The model is parameter free.
Simulation of decoherence (1)

fundamental limit

decoherence can be understood and modeled

hard case
Simulation of decoherence (2)

fundamental limit

easy case
decoherence can be understood and modeled