Quantum Computing with NMR

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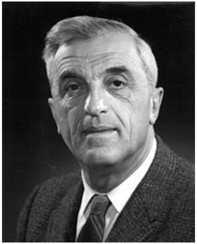
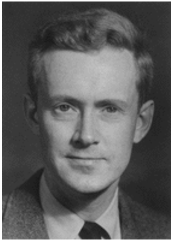
History of NMR

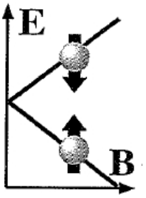
- nuclear magnetic resonance discovered by Rabi in 1938
- Nobel prize 1952 for Purcell and Bloch "for their development of new methods for nuclear magnetic precision measurements and discoveries in connection therewith"
- various applications
  - chemistry: examination of molecule structures
  - medicine: magnetic resonance imaging
  - solid state physics: stucture of different materials

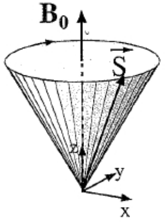




Principles of NMR

- charged particle with spin has magnetic moment $\vec{\mu}$
- external magnetic field $\vec{B_0} = B_0 \vec{e}_z$
  $\Rightarrow$ depending on the spin orientation energy levels split up with $V = -\mu_z B_0$
  $\Rightarrow$ Zeeman Effect
- spin precesses around magnetic field with lamor frequency $\omega_L = \gamma B_0$
- resonant electromagnetic pulses can excite transition between spin states
- averaging over 10^{18} spins $\Rightarrow$ resulting magnetization



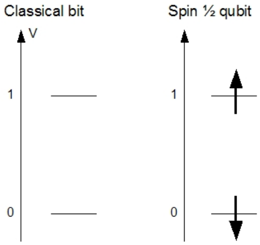


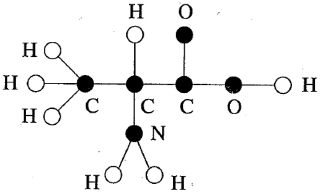
Di Vincenzo's Requirements

1. Well defined qubits
2. Initializiation to a pure state
3. Universal set of quantum gates
4. Long decoherence times
5. Qubit specific measurement

Qubits

- two level system equals two states of a particle with spin $s = \frac{1}{2}$
- logical 0 represented by $|m_s = +1/2>$, logical 1 represented by $|m_s = -1/2>$
- nuclear spin of atoms in molecules
  - freely floating $\rightarrow$ liquid state NMR
  - ordered in a lattice $\rightarrow$ solid state NMR
- suitable nuclei: ^{1}H, ^{13}C, ^{19}F



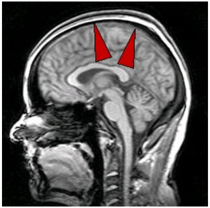


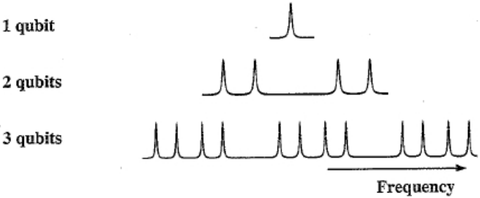
Initialization

- relaxation to the ground state by cooling in principle possible (optical pumping...)
- problem: the cooled liquid crystallizes $\Rightarrow$ structure of the system changes
- alternative at room temperature: pseudo pure states
- pseudo pure states = mixed states that behave in respect to the unitary transformations like pure states

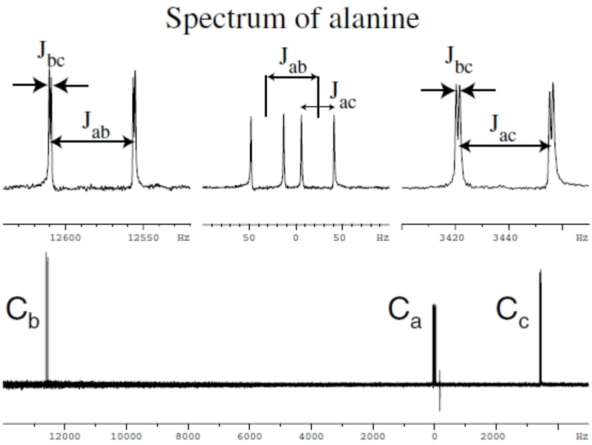
Gates I

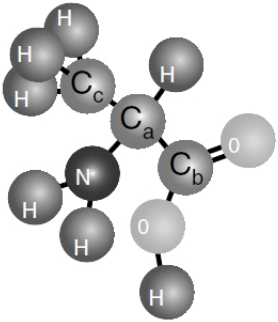
- qubits are selectively adressable because of different resonance frequencies $\omega_L = \gamma B$
  - heteronuclear: different gyromagnetic ration
  - homonuclear: chemical shift
- complete set of unitary transformations available (RF pulses, spin-spin coupling)





Gates II


Spectrum of alanine
J bc
J ab
J ab
J ac
J bc
J ac
12600
12550
Hz
50
0
50
Hz
3420
3440
Hz
C b
C a
C c
12000
10000
8000
6000
4000
2000
0
2000
Hz


H
H
H
C c
H
C a
0
C b
N
H
H
0
H

Decoherence Time

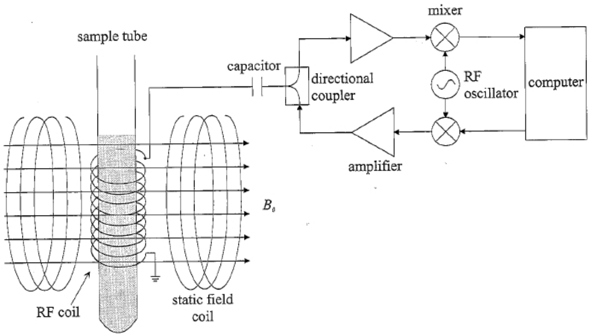
- reason for decoherence: spins interact with environment
- typical decoherence time ≈ 1 s
- typical gate times $\approx$ several ms
  $\Rightarrow$ number of feasible gates in order of 100

Measurement

- weak measurement instead of projective measurement
  $\Rightarrow$ no collaps of the wavefunction
  $\Rightarrow$ continuous measurement possible
- averaging over 10^{15} to 10^{20} spins $\Rightarrow$ "ensemble quantum computing"
- classical description:
  - measurement of the induction voltage (free induction decay = FID)
  - different qubits have different precession frequency
  - Fourier transformation separates qubits in frequency space

Experimental setup

- superconducting coil
  $\Rightarrow$ homogeneous B_0 field in z direction (10 to 15 T)
- RF coils
  $\Rightarrow$ exitation of nuclear spins in x-y plain and measurement of induced magnetisation



Hamiltonian

- Molecule with nuclear spins
- Interaction with external magnetic field
- Indirect spin coupling through electrons
- Dipolar interaction between molecules averaged to zero because of molecular motion

$$H = \frac{1}{2}\sum_i \omega_i \sigma_z^{(i)} + \frac{\pi}{2}\sum_{i \neq j} J_{ij}\sigma_z^{(i)}\sigma_z^{(j)}$$

Thermal Equilibrium Density Matrix

- macroscopic spin ensemble (10^{18} - 10^{20} spins!)
- $\Rightarrow$ mixed state
- use pseudo pure states
- density matrix at thermal equilibrium describes initial state:

$$\rho = \frac{1}{Z} e^{-\beta H}$$

- for one spin ($H = \frac{1}{2}\hbar\omega_0\sigma_z$):

$$\rho = \frac{1}{\exp(-\frac{1}{2}\beta\hbar\omega_0) + \exp(\frac{1}{2}\beta\hbar\omega_0)} \begin{pmatrix} \exp(-\frac{1}{2}\beta\hbar\omega_0) & 0 \\ 0 & \exp(\frac{1}{2}\beta\hbar\omega_0) \end{pmatrix}$$

Approximation

- β typically $\sim 10^{-5}$, approximation of density matrix:

$$\rho = \frac{1}{2}\mathbf{1} + \frac{1}{2}\beta\hbar\omega_0\sigma_z$$

- Generalization for n qubits:

$$\rho = \frac{1}{2^n}(\mathbf{1} - \beta H)$$

- ρ is diagonal
- signal $\propto \frac{1}{2^n}$

Temporal Averaging I

Assume a mixed 2 qubit system:

Initial state

$$\rho_1 = a|00\rangle\langle 00| + b|01\rangle\langle 01| + c|10\rangle\langle 10| + d|11\rangle\langle 11| = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & c & 0 \\ 0 & 0 & 0 & d \end{pmatrix}$$

where $a + b + c + d = 1$ ($\Rightarrow Tr\{\rho_1\} = 1$)

Temporal Averaging II

- combination of CNOT operations $\rightarrow$ similar initial states:

$$\rho_2 = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & c & 0 & 0 \\ 0 & 0 & d & 0 \\ 0 & 0 & 0 & b \end{pmatrix}, \quad \rho_3 = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & d & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & 0 & c \end{pmatrix}$$

- time evolution in three seperate experiments:

$$\rho_i(t) = U(t)\rho_i U^\dagger(t)$$

Temporal Averaging III

- time evolution is a linear operator:

$$\rho(t) = \rho_1(t) + \rho_2(t) + \rho_3(t) = U(t)(\rho_1 + \rho_2 + \rho_3)U^\dagger(t)$$

- pseudo pure state can be obtained:

$$U(t)\left((1-a)\mathbf{1} + (4a-1)\underbrace{\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}}_{|00\rangle\langle 00|}\right)U^\dagger(t)$$

Temporal Averaging IV

- Measurement of $\sigma_z^{(k)}$ (linearity of Trace):

$$\sum_i Tr\{\rho_i(t)\sigma_z^{(k)}\} = Tr\{\rho(t)\sigma_z^{(k)}\}$$

- $Tr\{\mathbf{1}\sigma_z^{(k)}\} = 0 \Rightarrow$

$$Tr\{U(t)\left((1-a)\mathbf{1} + (4a-1)|00\rangle\langle 00|\right)U^\dagger(t)\sigma_z^{(k)}\}$$
$$= Tr\{U(t)|00\rangle\langle 00|U^\dagger(t)\sigma_z^{(k)}\}$$

- same result as for initial pure state $|00\rangle\langle 00|$

RF Field

- RF field of the coil as superposition of counter-rotating fields:

$$B_{RF} = 2B_1 \begin{pmatrix} \cos(\omega t) \\ 0 \\ 0 \end{pmatrix} = B_1 \begin{pmatrix} \cos(\omega t) \\ \sin(\omega t) \\ 0 \end{pmatrix} + B_1 \begin{pmatrix} \cos(\omega t) \\ -\sin(\omega t) \\ 0 \end{pmatrix}$$

- switch to a rotating frame:

$$x' = \begin{pmatrix} \cos(\omega t) & \sin(\omega t) & 0 \\ -\sin(\omega t) & \cos(\omega t) & 0 \\ 0 & 0 & 1 \end{pmatrix} x$$

Rotating frame

- B_{RF} in rotating frame:

$$B_{RF} = B_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + B_1 \begin{pmatrix} \cos(2\omega t) \\ -\sin(2\omega t) \\ 0 \end{pmatrix}$$

- only the static term has an effect
- quantum computing experiments use rotating frame

Transformation of the State

$$|\psi'\rangle = U^{-1}|\psi\rangle \text{ with } U(t) = e^{i\frac{\omega}{2}t\sigma_z}$$

Hamiltonian

- transformation of the Hamiltonian:

$$H' = U^{-1}HU + i\hbar\dot{U}^{-1}U = -\frac{\hbar}{2}\Delta\omega_L\sigma_z + \frac{\hbar}{2}\omega_1\sigma_x$$

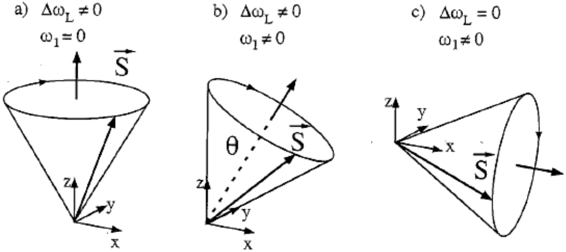
  with $\Delta\omega_L = \omega_L - \omega$ and $\omega_1 = \gamma B_1$

- effective field:

$$\omega = (\omega_1, 0, \Delta\omega_L)$$

Evolution

- spins precess around the static field in the rotating frame



- Rabi flopping:
  - apply resonant RF field (effective field in xy plane)
  - spins precess around effective field
  - spin moves to xy plane and then to -z
- possible effective Field in x or y direction by shift of RF phase
- used to implement quantum gates.

Spin Coupling

- spins of the qubits are coupled
- causes unintended time evolution
- has to be removed to gain controll
- can be achieved by refocusing method

Time Evolution

- example: two qubit interaction.

Interaction Hamiltonian

$$H_I = \alpha \sigma_z^{(1)} \sigma_z^{(2)}$$

where α determines the strength of the coupling.

Time evolution

$$U_I(t) = e^{-i\alpha t \sigma_z^{(1)} \sigma_z^{(2)}}$$

Refocusing

- RF-Pulse that rotates the first spin around the x-axis (rotating frame):

π pulse

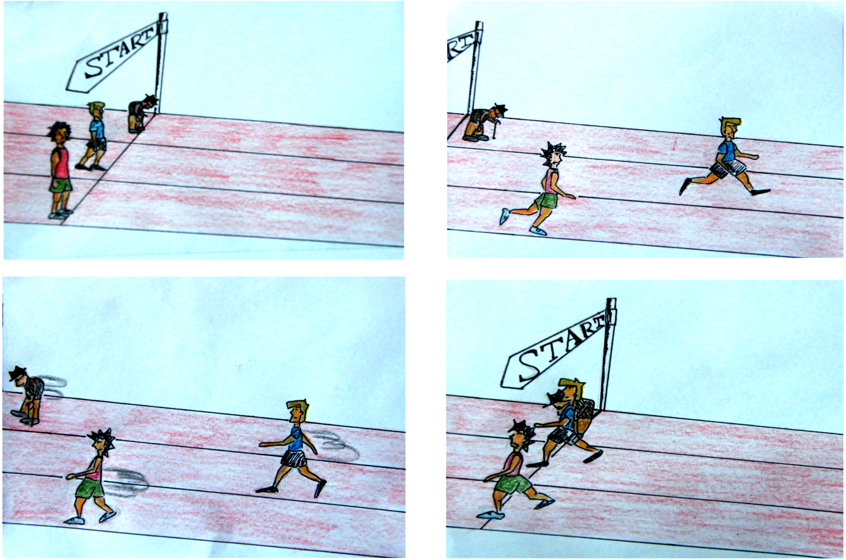
$$R_{x1}(\pi) = e^{-i\frac{\pi}{2}\sigma_x^{(1)}} = -i\sigma_x^{(1)}$$

- series of RF pulses $\rightarrow$ suppress the evolution after a time t:

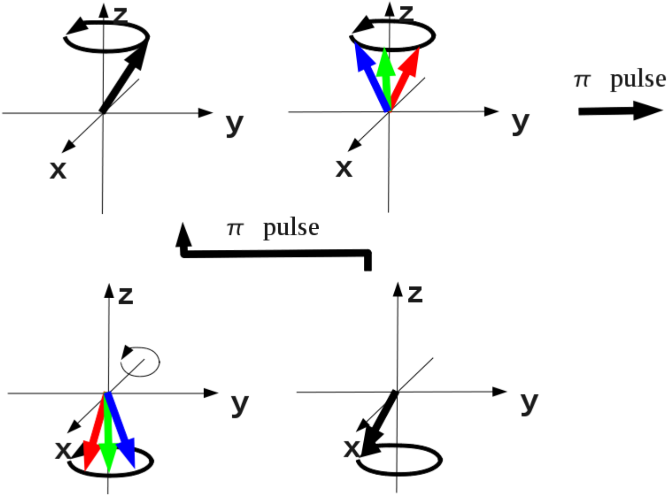
$$U_I\left(\frac{t}{2}\right)R_{x1}(\pi)U_I\left(\frac{t}{2}\right)R_{x1}(\pi) = \mathbf{1}$$

- can be considered a single-qubit "NO" gate
- used to decouple certain spins

Runners Analogy I



Runners Analogy II



z-rotation

- only rotations around x- and y-axis by RF pulse
- no z-axis rotation
- implementation by a series of x,y rotations:

ϕ rotation around z-axis

$$e^{-i\frac{\phi}{2}\sigma} = \begin{pmatrix} e^{-i\frac{\phi}{2}} & 0 \\ 0 & e^{i\frac{\phi}{2}} \end{pmatrix} = e^{-i\frac{\pi}{4}\sigma_x} e^{-i\frac{\phi}{2}\sigma_y} e^{i\frac{\pi}{4}\sigma_x}$$

NOT and Hadamard Gate

- NOT gate implemented using a π-rotation:

NOT gate

$$e^{-i\frac{\pi}{2}\sigma_x} = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} = e^{-i\frac{\pi}{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

(The global phase can be neglected since it has no observable effect.)

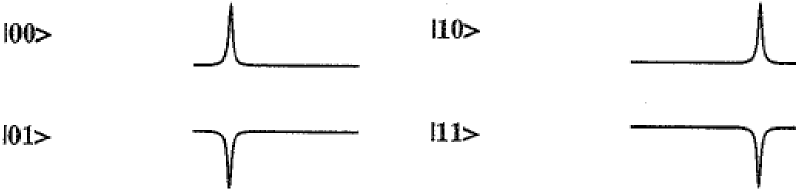
- Hadamard gate implemented by a combination of rotations:

Hadamard gate

$$\mathbf{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = e^{i\frac{\pi}{2}\sigma_z} e^{i\frac{\pi}{4}\sigma_y}$$

CNOT with Resonance Frequency

- CNOT gate inverts the second qubit if the first one is in state $|1\rangle$
- possible implementation: the resonace frequencies for the second qubit depends on the state of the first one
  - apply an RF pulse with the correct resonance frequenzy for the $|10\rangle$ and $|11\rangle$ state
  - this flips the second spin to $|11\rangle$ resp. $|10\rangle$
  - it does not change the $|00\rangle$ and $|01\rangle$ state



spectrum of second qubit

CNOT with RF Pulses I

- alternative implementation without using selective RF pulses
- non-selective rotations and precission (spin-coupling $e^{-i\alpha t\sigma_z^{(1)}\sigma_z^{(2)}}$)
- Start with a $|00\rangle$ state
- apply $e^{-i\frac{\pi}{4}\sigma_y^{(2)}}$ (flips the spin to the x-axis):

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle \otimes (|0\rangle + |1\rangle)\right)$$

- precission of the spin (rotating frame!):

$$|0\rangle_{(1)} \Rightarrow U_I(t) = e^{-i\alpha t\sigma_z^{(1)}\sigma_z^{(2)}} = e^{-i\alpha t(+1)\sigma_z^{(2)}}$$

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle \otimes (|0\rangle e^{-i\alpha t} + |1\rangle e^{i\alpha t})\right)$$

CNOT with RF Pulses II

- $t = \frac{\pi}{4\alpha} \longrightarrow$ spin has moved to y-axis:

$$|\psi(0)\rangle = \frac{1}{2}\left(|0\rangle \otimes ((1-i)|0\rangle + (1+i)|1\rangle)\right)$$

- final rotation $e^{-i\frac{\pi}{4}\sigma_x^{(2)}} \longrightarrow$ spin returns to its initial state $|00\rangle$.

CNOT with RF Pulses III

- initial state $|10\rangle \rightarrow$ precission leads to an opposite orientated rotation:

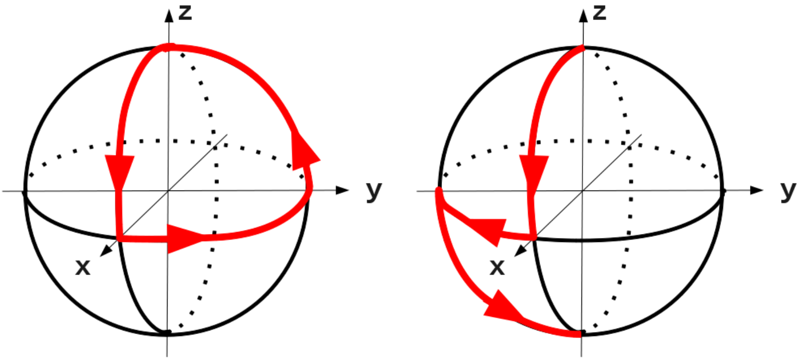
$$|1\rangle_{(1)} \Rightarrow U_I(t) = e^{-i\alpha t \sigma_z^{(1)} \sigma_z^{(2)}} = e^{-i\alpha t(-1)\sigma_z^{(2)}}$$

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle \otimes \left(|0\rangle e^{i\alpha t} + |1\rangle e^{-i\alpha t} \right) \right)$$

- final state in this case: $|11\rangle$

CNOT with RF Pulses IV

CNOT operation on the Bloch sphere



CNOT with RF Pulses V

- effect of this operation: CNOT gate:

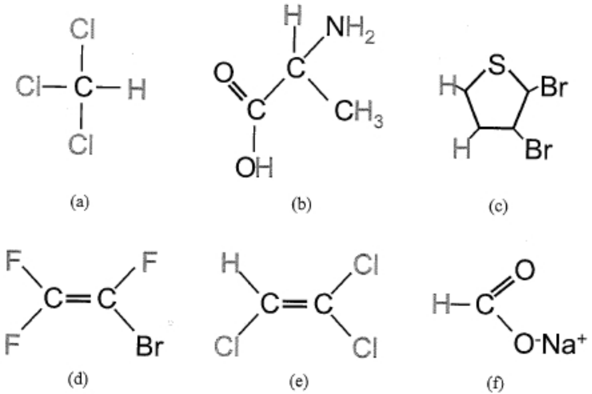
$$|00\rangle \rightarrow |00\rangle, \quad |10\rangle \rightarrow |11\rangle$$

- in the same way:

$$|01\rangle \rightarrow |01\rangle, \quad |11\rangle \rightarrow |10\rangle$$

- we have single-qubit gates and the CNOT gate.
  $\Rightarrow$ We can construct a full set of quantum gates.

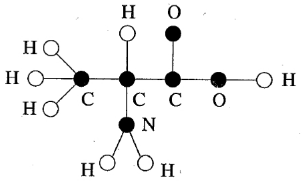
Molecules used for QC

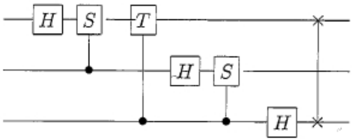


(a) (b) (c) (d) (e) (f)

Quantum Fourier-Transformation

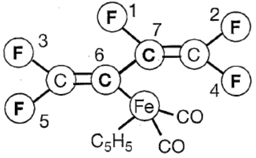
- principle of quantum Fourier transform:
  $|j> \rightarrow \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} x_j e^{2\pi ijk/N} |k>$
- implemented by Weinstein et al. 2001
- goal: find periodicity of state
  $|\Psi> = \frac{1}{2}(|000> + |010> + |100> + |110>)$
- uses gates: three Hadamard gates, three controlled phase shift gates
- accuracy of implementation: 62 to 80 %



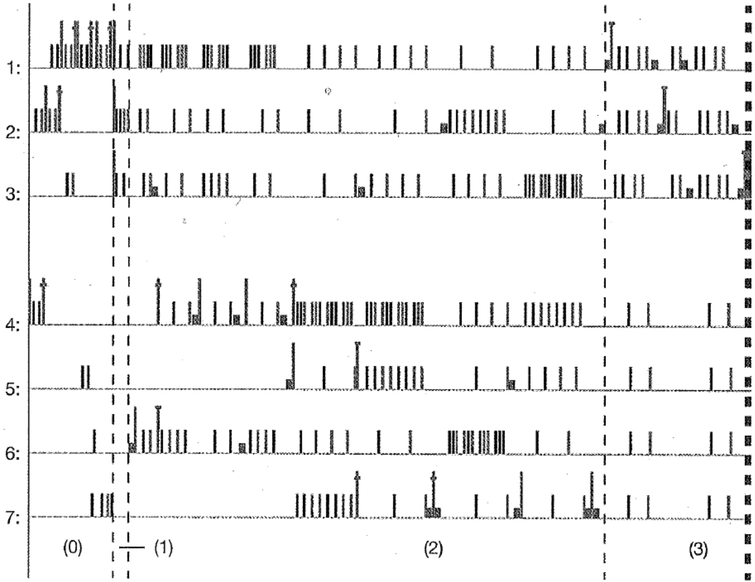


Shore Algorithm I

- group at IBM Almaden Research Center implemented Shor's factoring algorithm using a custom designed molecule with five ^{19}F and two ^{13}C spins
- number of resonance lines per spin: $2^6 = 64$
- chemical shift 1 kHz
- sequence: factorization of 15
  - sequence lasted almost 1 s (order of decoherence time)
  - group needed about 300 pulses

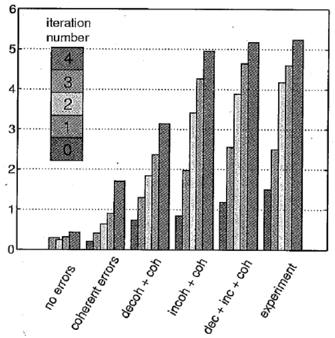


Shore Algorithm II



Errors

- coherent errors: real unitary transformations differ from ideal operators
- incoherent errors: inhomogenities across the sample
  $\Rightarrow$ different molecules evolve differently (non unitary for ensemble)
- decoherent errors: coupling between qubit and environment (non unitary for single qubits)



Strengths of liquid state NMR

Strengths

- long experimental experience
- RF excitations tunable in a wide range
- easy experimental setup
- easy implementation of gates

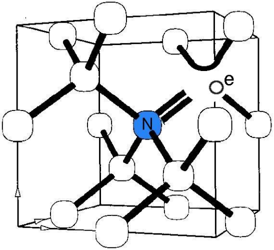
Weaknesses of liquid state NMR

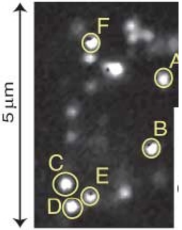
Weaknesses

- exponential signal loss in pseudo-pure states with number of qubits N
- number of resonance lines can increase with $N2^N$
  $\Rightarrow$ only molecules with strong chemical shift suitable
- when chemical shift is small
  $\Rightarrow$ bandwidth of the RF pulses must be small
  $\Rightarrow$ duration of the pulses is long
  $\Rightarrow$ decoherence

Solid-based NMR in diamand I

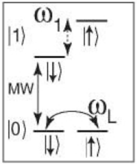
- possible advantages of solid state NMR
  - higher polarization
  - longer decoherence time
  - stronger couplings between spins $\Rightarrow$ faster gate times
- Childress, Dutt et al. (Science 2006/2007): coupled electron and nuclear spin
- electronic spin triplet of nitrogen-vacancy (NV) centers ($m_s = \pm 1, 0$) in diamond couples coherently to the nuclear spin of nearby ^{13}C nuclei





Solid-based NMR in diamand II

- NV center can be manipulated with optical and microwave excitation
- addressing and manipulating the nucleus via the electronic spin is possible
  - $m_s = 0 \Rightarrow$ no influence on nuclear spins, free lamor precession
  - $m_s = 1 \Rightarrow$ hyperfine interaction $\Rightarrow$ splitting between states $|1, \downarrow>$ and $|1, \uparrow>$, inhibited lamor precession



- quantum registers: chemical shift results from different interactions of the nuclear spins with the NV center

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