

NMR Quantum Computation

C/CS/Phys 191:

Quantum Information Science and
Technology

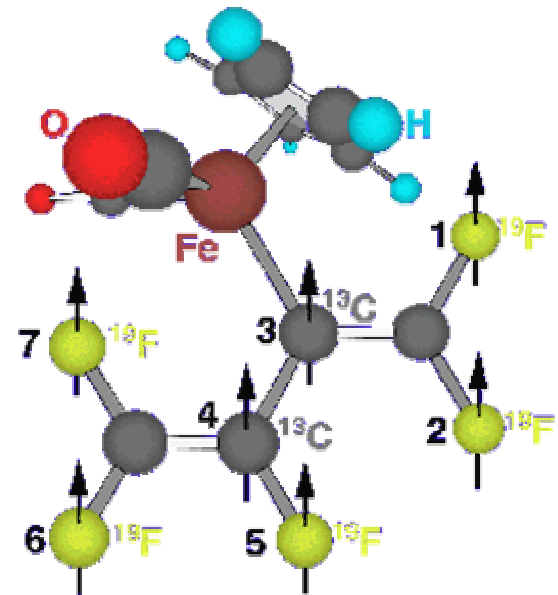
11/13/2003

Thaddeus Ladd

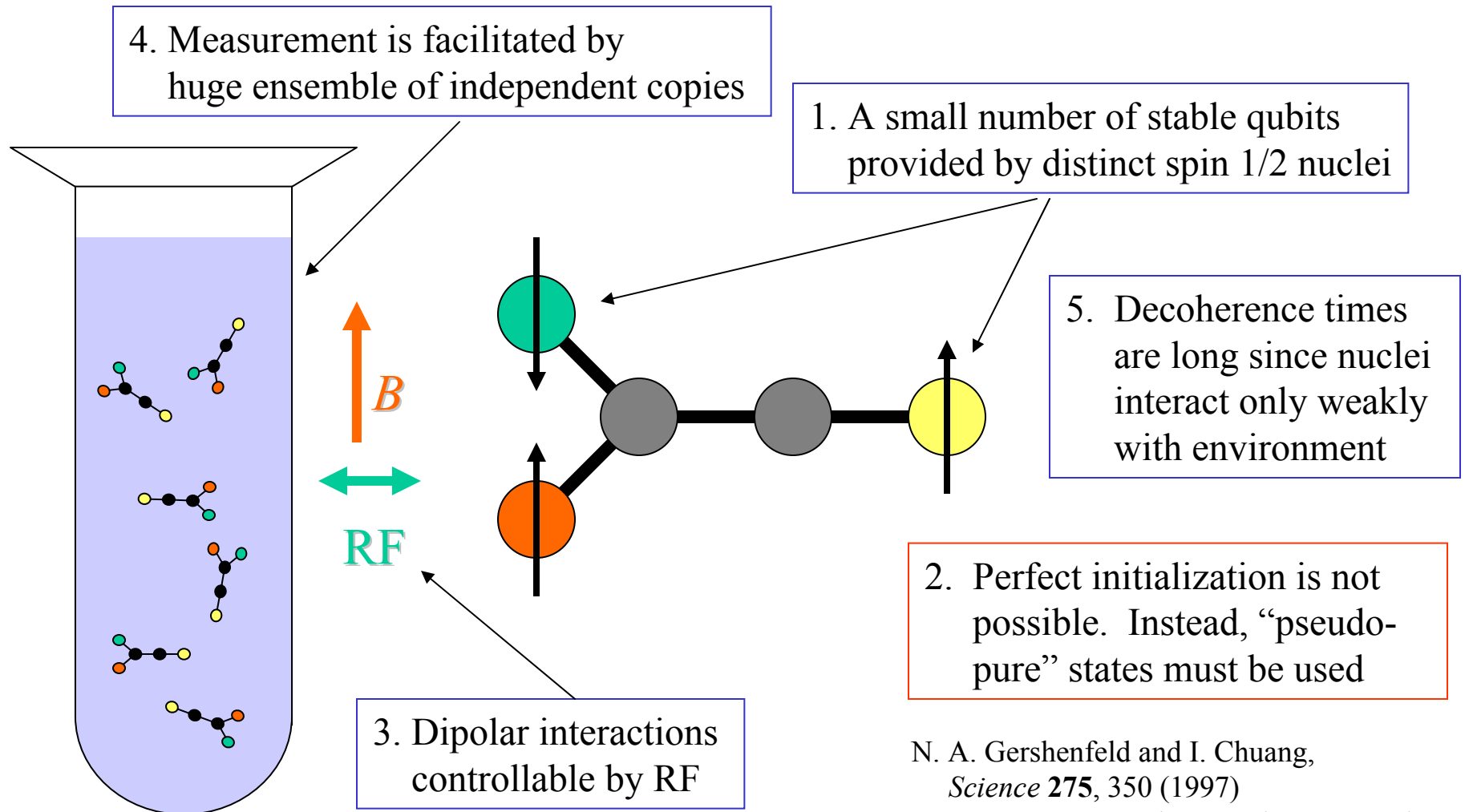
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Solution NMR Quantum Computation



N. A. Gershenfeld and I. Chuang,
Science **275**, 350 (1997)

D. G. Cory, A. F. Fahmy, and T. F. Havel,
Proc. Natl. Acad. Sci. USA **94**, 1634 (1997)

Solution NMR QC: Why Bother?

- From the start (1997), researchers knew solution NMR would not surpass the 10-qubit level.
- Why bother going through the trouble of making solution NMR quantum computers then?

Because classical computers are too slow to factor 15 and decide whether 3-bit functions are constant or balanced. These problems will soon to be solved by “coffee cup” NMR quantum computers in every home!

Right answer:

NMR is “easy,” due to the 50+ year history and extensive commercial engineering of the technique. If we cannot do quantum computing with this “plug and play,” high- Q system, then our chances with atoms, semiconductor electrons, etc. are slim! NMR gives us a “head start” on solving the problems in quantum control that we will face with other architectures.

Outline

- Why bother with solution NMR quantum computing?
- Basic physics of NMR and ingredients for QC
 - Nuclear magnetic moments in static and RF magnetic fields
 - Nuclear-nuclear couplings
 - Weak ensemble measurement
 - Experimental Overview
- Initialization
 - Physical polarization
 - Algorithmic cooling
 - Pseudo-pure states
 - Scaling
- Quantum logic
 - RF implementations of the universal gate set
 - Refocussing
- Survey of results
- The future of NMR quantum computing

Definitions and Units

$\hat{\mathbf{I}}_n$ is unitless spin operator for n^{th} nuclear species.
For example, assuming spin-1/2, $I_n^z = \frac{1}{2}\hat{\sigma}^z$.

Gaussian electromagnetic units are used throughout. Remember to include factor of $\mu_0/4\pi$ when converting a magnetization to a field in SI units!

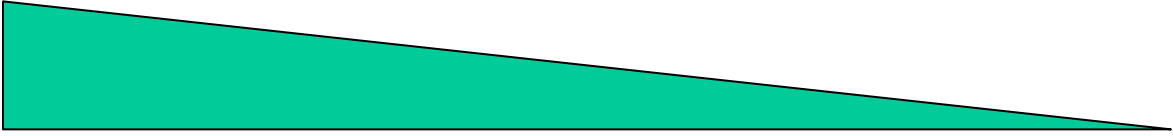
$$\hat{\boldsymbol{\mu}}_n = \hbar\gamma_n\hat{\mathbf{I}}_n$$

Subscripts indicate nuclei from different atoms of the molecule.

$$\frac{\gamma_n}{2\pi} = \frac{g_n e}{4\pi m_p c} = g_n \times 7.6 \text{ MHz/T}$$

$$\hat{\mathcal{H}} = \hat{H}/\hbar \quad (\text{All Hamiltonians in units of angular frequency})$$

The Hamiltonian

Bigger  smaller

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\text{motion}} + \underbrace{\hat{\mathcal{H}}_Z + \hat{\mathcal{H}}_{\text{HF}} + \hat{\mathcal{H}}_{\text{RF}} + \hat{\mathcal{H}}_{\text{D}}}_{\text{All of form } -\gamma\hat{\mathbf{I}} \cdot \mathbf{B}}$$

↑
Independent of spin

Term	Size	Role
Motion	$kT \gg 6 \text{ THz}$	Bath for thermal relaxation. Affects decoherence.
Zeeman	$\omega_0 \gg 100 \text{ MHz}$	Allows polarization. Establishes resonance. SNR.
HyperFine	$A \gg 1 \text{ MHz}$	Chemical shielding and J -coupling.
RadioFrequency	$\omega_1 \gg 10 \text{ kHz}$	The “knob.” Allows spin rotations.
Dipolar	$D \gg 1 \text{ kHz}$	Decoherence source.

Applied Magnetic Fields and the Rotating Frame

- RF frequency ω is chosen to be different from resonant frequency $\omega_0 = \gamma B_0$ by $\delta\omega$.

$$\begin{aligned}\hat{\mathcal{H}}_Z + \hat{\mathcal{H}}_{\text{RF}} &= -\gamma \hat{\mathbf{I}} \cdot \{B_0 \hat{\mathbf{z}} + 2B_1(t) \cos[\omega t + \phi(t)] \hat{\mathbf{x}}\} \\ &= -(\omega - \delta\omega) \hat{I}^z + 2\omega_1(t) \cos[\omega t + \phi(t)] \hat{I}^x\end{aligned}$$

$\underbrace{\qquad\qquad\qquad}_{\gamma B_0 = \omega_0 = \omega - \delta\omega}$

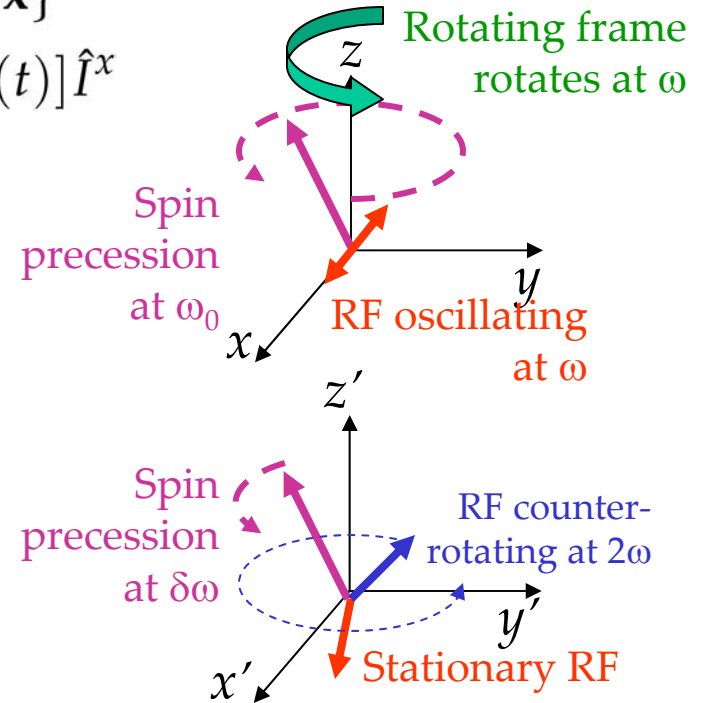
To Rotating Frame

- New frame rotates at ω in spin subspace.
- Fastest, uninteresting motion (rotation about z-axis at ω) removed.
- Terms oscillating at 2ω are neglected.

$$\begin{aligned}\hat{\mathcal{H}}_Z^* + \hat{\mathcal{H}}_{\text{RF}}^* &= \delta\omega \hat{I}^z + \omega_1 \cos \phi \hat{I}^x + \omega_1 \sin \phi \hat{I}^y \\ &= \mathbf{\Omega} \hat{\mathbf{I}} \cdot \hat{\mathbf{n}}\end{aligned}$$

$$\mathbf{\Omega} = \sqrt{\omega_1^2 + \delta\omega^2}$$

Change $\delta\omega$, ω_1 , and ϕ to achieve arbitrary rotation angle and axis!



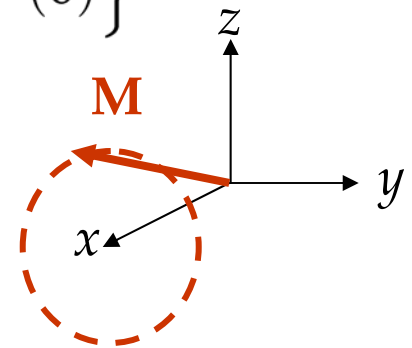
Single Spin Rotations with the Density Matrix

- Consider example of a spin $\frac{1}{2}$ in pure state

$$\hat{\rho}^*(t) = \frac{1}{2}\hat{\mathbf{1}} + \mathbf{M}(t) \cdot \hat{\mathbf{I}} \quad \mathbf{M}(t) = 2\langle \hat{\mathbf{I}}(t) \rangle = 2\text{Tr} \{ \hat{\rho}^*(t) \hat{\mathbf{I}} \}$$

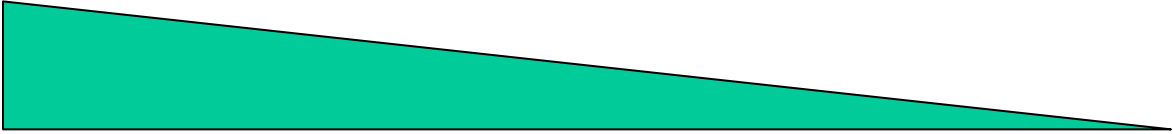
- Suppose we apply on-resonant RF ($\delta\omega=0$) with phase $\phi=0$ for time τ .

$$\begin{aligned} \mathbf{M}(\tau) &= 2\text{Tr} \left\{ e^{-i\hat{\mathcal{H}}_{\text{RF}}^* \tau} \hat{\rho}^*(0) e^{i\hat{\mathcal{H}}_{\text{RF}}^* \tau} \hat{\mathbf{I}} \right\} = 2\text{Tr} \left\{ e^{i\Omega\tau \hat{I}^x} \hat{\mathbf{I}} e^{-i\Omega\tau \hat{I}^x} \hat{\rho}^*(0) \right\} \\ &= 2\text{Tr} \left\{ e^{i\Omega\tau \hat{I}^x} \hat{\mathbf{I}} e^{-i\Omega\tau \hat{I}^x} \hat{\mathbf{I}} \cdot \mathbf{M}(0) \right\} \\ &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\Omega\tau) & -\sin(\Omega\tau) \\ 0 & \sin(\Omega\tau) & \cos(\Omega\tau) \end{pmatrix} \cdot \begin{pmatrix} M^x(0) \\ M^y(0) \\ M^z(0) \end{pmatrix} \end{aligned}$$



- The last step is the result of some simple matrix algebra; it is worth deriving in your spare time. (Result is independent of representation.)
- End result is standard rotation of a vector!
- Thus we write: $U(\tau) = e^{-i\Omega\tau \mathbf{I} \cdot \hat{\mathbf{n}}} = R_{\hat{\mathbf{n}}}(\Omega\tau)$
- Of particular importance are “ π -pulses,” corresponding to $\Omega\tau=\pi$, which invert \mathbf{M} , and “ $\pi/2$ pulses,” corresponding to $\Omega\tau=\pi/2$, which are Hadamard gates.

The Hamiltonian

Bigger  smaller

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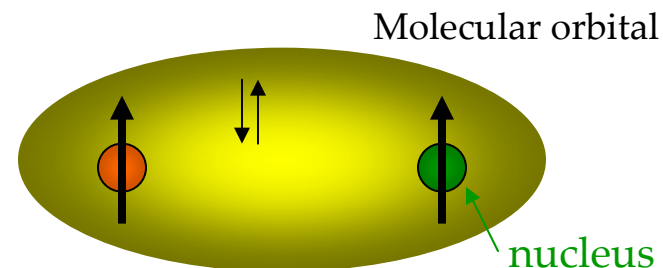
↑
Independent of spin

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Zeeman	$\omega_0 \gg 100$ MHz	Allows polarization. Establishes resonance. SNR.
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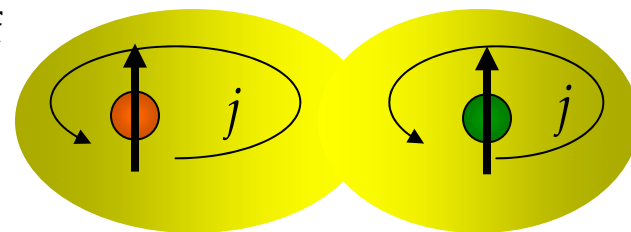
The Chemical Shift

$$\hat{\mathcal{H}}_{\text{HF}} = \gamma g \mu_{\text{B}} \hat{\mathbf{I}} \cdot \sum_k \left[\frac{\hat{\mathbf{L}}_k}{r_k^3} - \hat{\mathbf{S}}_k r_k^3 + 3 \frac{\mathbf{r}_k (\hat{\mathbf{S}}_k \cdot \mathbf{r}_k)}{r_k^5} + \frac{8\pi}{3} \hat{\mathbf{S}}_k \delta(\mathbf{r}_k) \right]$$

- Although the hyperfine coupling constants can be large (~MHz), this term ends up small because the sums over spin (\mathbf{S}_k) and orbital (\mathbf{L}_k) angular momentum of electrons vanish in molecular orbital ground states.
- The chemical shift arises as a first order perturbation of the ground state wave function due to the magnetic field
- Tiny electron currents oppose magnetic fields
- Magnetic field seen by nucleus is reduced by a few parts per million, depending on the molecular orbital state
- Varies from nucleus to nucleus according to symmetry of molecule
- Gives quantitative information about molecular structure;
- Allows qubits of same nuclear species to be distinguished.



No magnetic field:
 $\langle \hat{\mathcal{H}}_{\text{HF}} \rangle = 0$

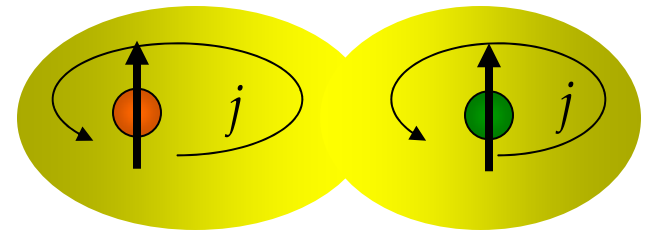


Magnetic field:
 $\langle \hat{\mathcal{H}}_{\text{HF}} \rangle \sim 10^{-6} \hat{\mathcal{H}}_Z$

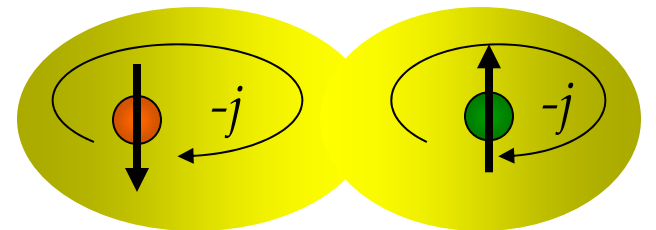
$$\hat{\mathcal{H}}_{\text{CS}}^* = \langle \psi_e | \hat{\mathcal{H}}_{\text{HF}}^* | \psi_e \rangle = -\sigma_n \gamma_n B_0 \hat{I}_n^z$$

The J -Coupling

- The J -coupling arises as a second order perturbation to the ground state wavefunction as a result of the effective field due to the nuclei.
- Magnetic field of one nucleus distorts electron orbital
- Tiny electron currents change magnetic field at second nucleus
- The matrix J gives quantitative information about molecular structure.
- Nonlinear term used for quantum logic.



$$B_{\text{eff}} |j| I^z > 0$$



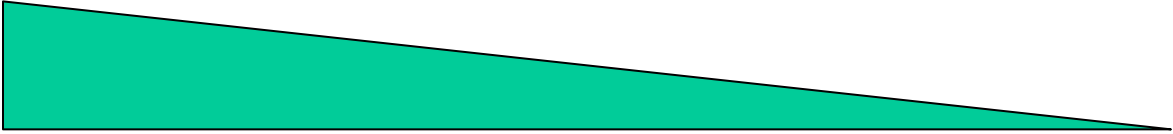
$$B_{\text{eff}} |j| I^z < 0$$

$$\hat{\mathcal{H}}_J = \frac{\langle \psi_e | \hat{\mathcal{H}}_{\text{HF}} | \psi'_e \rangle \langle \psi'_e | \hat{\mathcal{H}}_{\text{HF}} | \psi_e \rangle}{E - E'} = \hat{\mathbf{I}}_n \cdot J_{nm} \cdot \hat{\mathbf{I}}_m$$

- Components of effective magnetic field due to J -coupling not in z -direction time-average to zero due to rapid Larmor rotation of nuclei in large applied magnetic field.

$$\hat{\mathcal{H}}_J^* = J_{nm} \hat{I}_n^z \hat{I}_m^z$$

The Hamiltonian

Bigger  smaller

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\text{motion}} + \underbrace{\hat{\mathcal{H}}_Z + \hat{\mathcal{H}}_{\text{HF}} + \hat{\mathcal{H}}_{\text{RF}} + \hat{\mathcal{H}}_D}_{\text{All of form } -\gamma \hat{\mathbf{I}} \cdot \mathbf{B}}$$

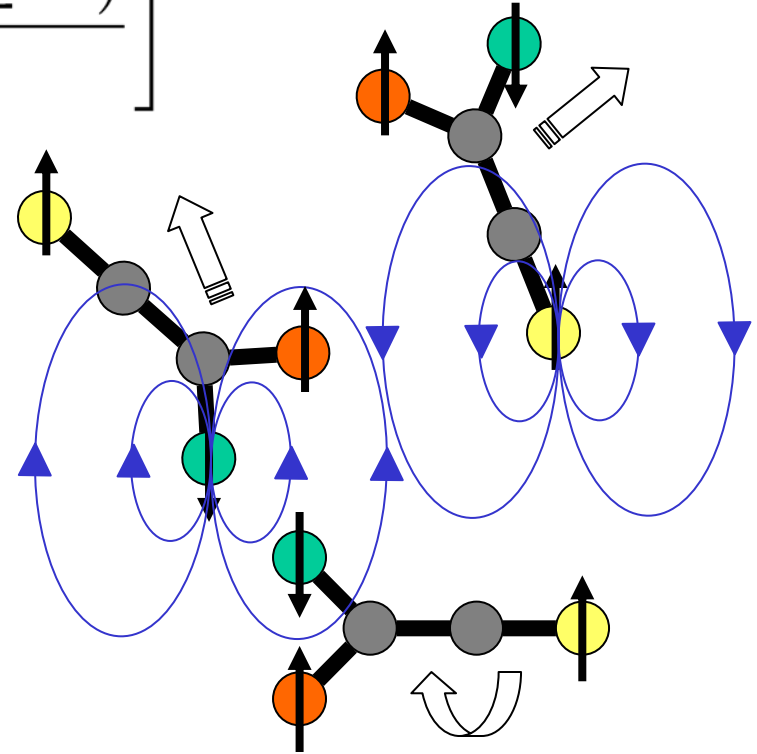
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The Dipolar Coupling: The Advantage of Liquids

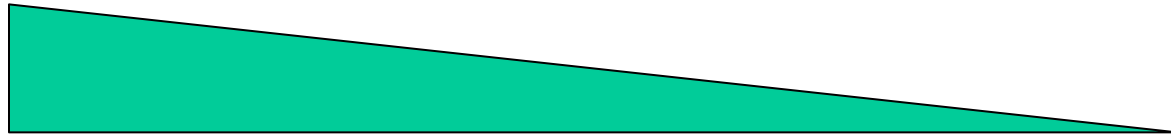
$$\hat{\mathcal{H}}_D = \hbar \frac{\gamma_1 \gamma_2}{\hat{r}^3} \left[\hat{\mathbf{I}}_1 \cdot \hat{\mathbf{I}}_2 - 3 \frac{(\hat{\mathbf{I}}_1 \cdot \hat{\mathbf{r}})(\hat{\mathbf{I}}_2 \cdot \hat{\mathbf{r}})}{\hat{r}^2} \right]$$

- Couples nuclear spins. Coupling strength is ~ 1 kHz.
- Includes relative distance \mathbf{r} between nuclear spins,.
- The advantage of liquids is that, due to the thermal motion of the molecules in the liquid, the dipolar coupling averages to zero in first order.
- Residual dipolar coupling is leading cause of
 - Decoherence, T_2 :
 - Random magnetic fields due to nuclear dipoles on other molecules apply random z-rotations
 - Initially parallel spins go out of phase due to random rotations
 - Nuclear magnetization from different molecules destructively interferes
 - Thermal relaxation, T_1 :
 - Sometimes, moving molecules interact for timescale of order $1/\omega_0$ (Larmor period)
 - Such a random interaction is like a random, resonant RF applied field
 - Tips spins with energy compensated by motional bath



The Hamiltonian in the Rotating Frame

Bigger



smaller

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\text{motion}} + \hat{\mathcal{H}}_Z + \hat{\mathcal{H}}_{\text{HF}} + \hat{\mathcal{H}}_{\text{RF}} + \hat{\mathcal{H}}_D$$

$$\hat{\mathcal{H}}^* = \left[(\hat{\mathcal{H}}_Z^* + \hat{\mathcal{H}}_{\text{CS}}^*) + \hat{\mathcal{H}}_{\text{RF}}^* \right] + \hat{\mathcal{H}}_J^* + \hat{\mathcal{H}}_D^*(t)$$

$$= \sum_j \Omega_j(t) \hat{\mathbf{n}}_j \cdot \hat{\mathbf{I}}_j + \sum_{j \neq k} J_{jk} I_j^z I_k^z + \hat{\mathcal{H}}_D^*(t)$$

We have complete control over single spin rotations. Spin couplings and relaxation are always present.

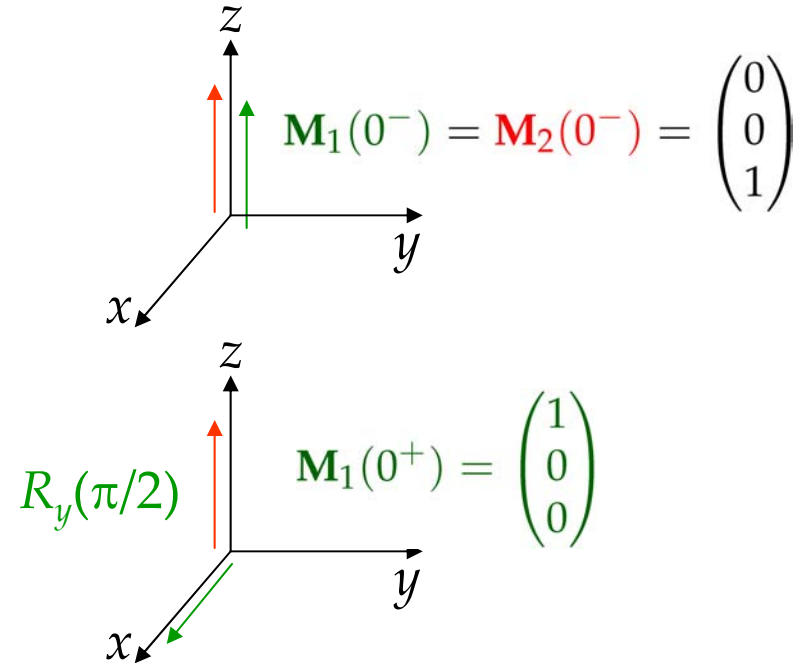
Select spin with RF frequency $\delta\omega_j = \omega - \gamma_j B_0 (1 - \sigma_j)$

Select angle with RF amplitude $\Omega_j = \sqrt{\omega_1^2 + \delta\omega_j^2}$

Select axis with RF phase $\hat{\mathbf{n}}_j = \frac{1}{\Omega_j} \begin{pmatrix} \omega_1 \cos \phi \\ \omega_1 \sin \phi \\ \delta\omega_j \end{pmatrix}$

Free Induction Decay (FID)

- Consider a two spin molecule.
(Neglect T_1).
- Suppose spins begin in ground state
(parallel to field)
- Set $\delta\omega_1=0$ by choosing RF frequency
to match chemical shifted Larmor
frequency of first nucleus.
- Apply $\pi/2$ pulse about y -axis.
- Remove RF.
- J -coupling causes precession about z -
axis in rotating frame, at frequency
 $J\hbar I_2^z \mathbf{i} = J/2$.
- Due to dephasing from the random
dipolar coupling, the different spins
of the ensemble start to interfere, and
the magnetization shrinks.



$$\hat{\mathcal{H}}^* = J_{12} \hat{I}_1^z \hat{I}_2^z + \hat{\mathcal{H}}_D^*(t)$$

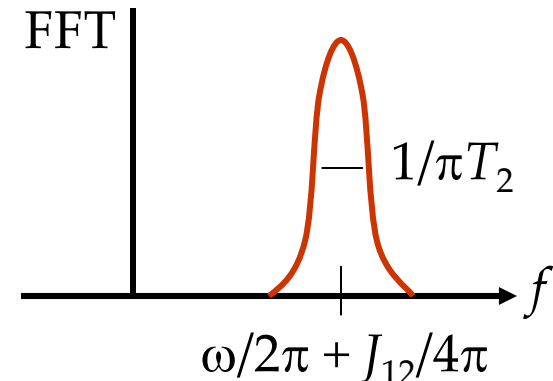
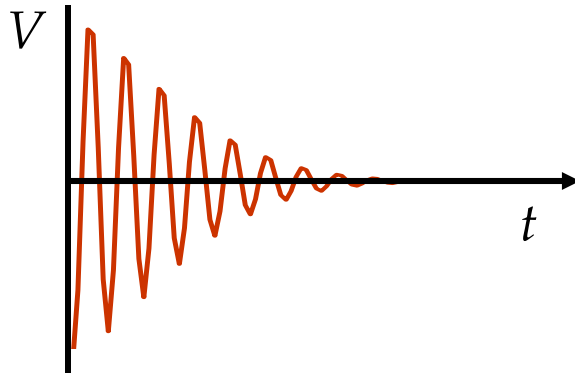
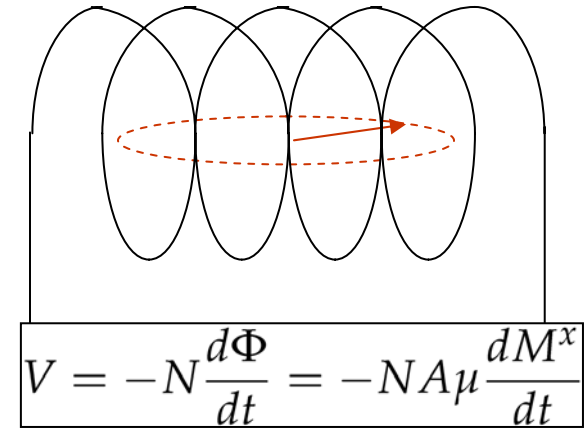
$$\mathbf{M}_1(t) = \begin{pmatrix} \cos(J_{12}t/2)e^{-t/T_2} \\ \sin(J_{12}t/2)e^{-t/T_2} \\ 0 \end{pmatrix}$$

Free Induction Decay in Laboratory Frame

- That was the rotating frame. In the laboratory frame,

$$\mathbf{M}_1(t) = \begin{pmatrix} \cos(\omega t + J_{12}t/2)e^{-t/T_2} \\ \sin(\omega t + J_{12}t/2)e^{-t/T_2} \\ 0 \end{pmatrix}$$

- Rotating magnetization in coil of wire causes an EMF due to Faraday's law of induction.

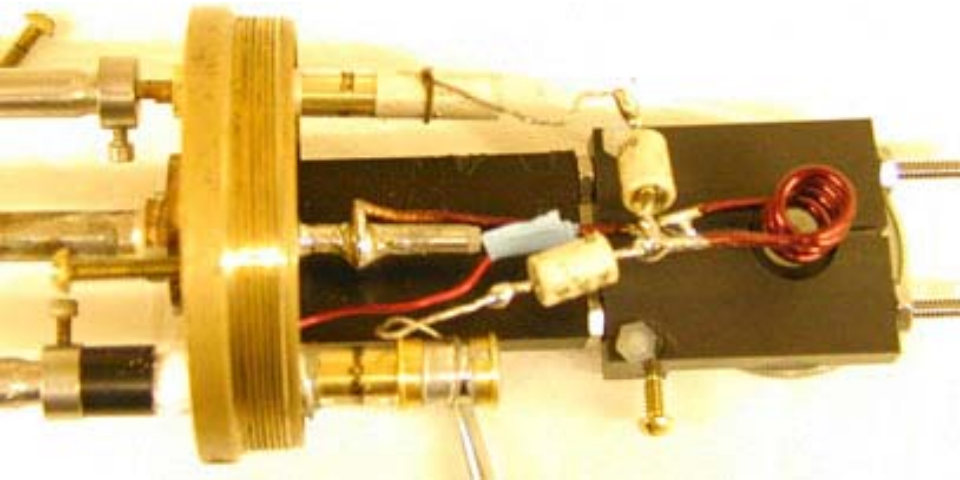


Weak Ensemble Measurement

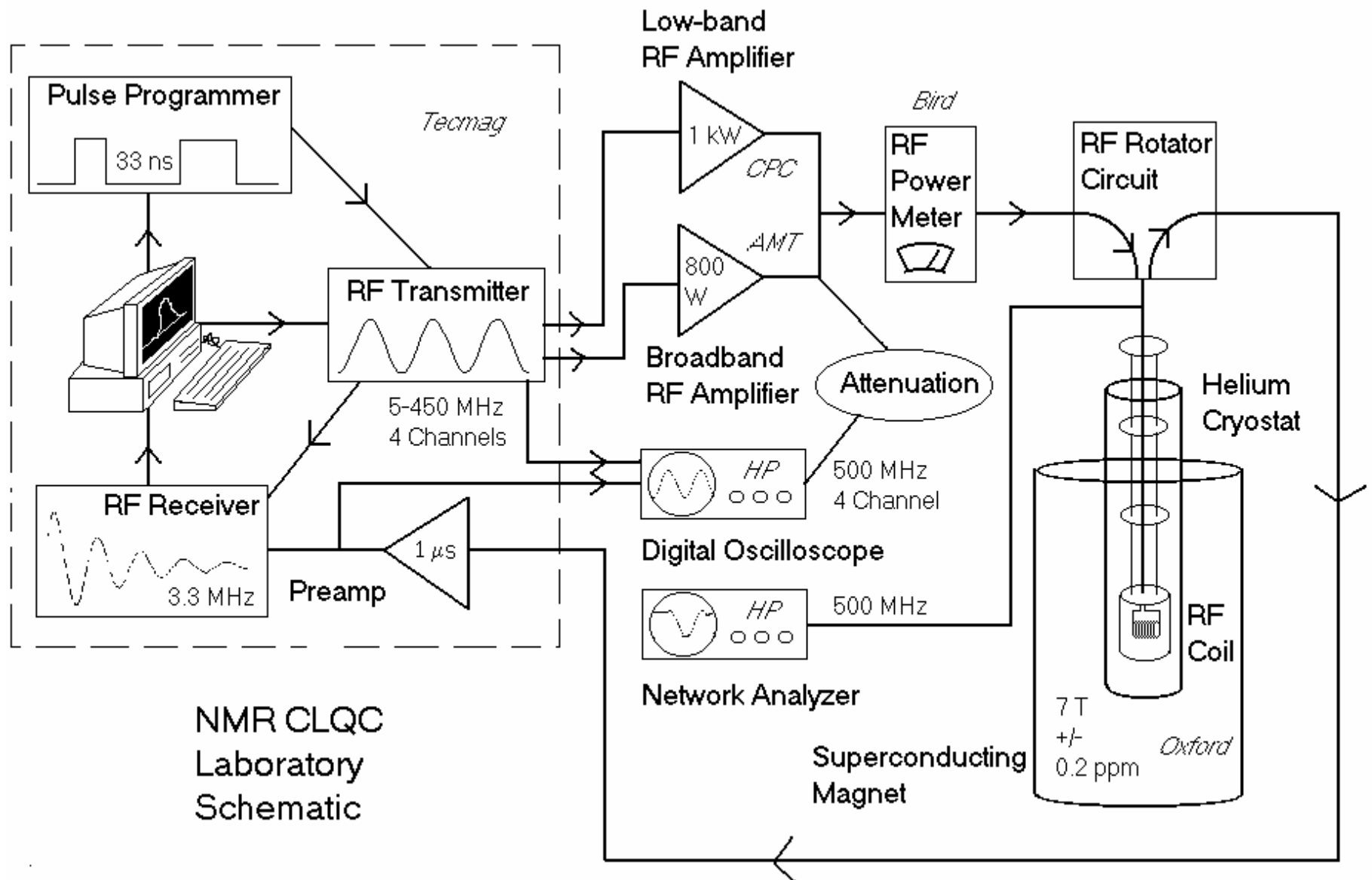
- Wait a minute!!!
 - What happened to quantum mechanics?!?
 - Why doesn't measurement affect the spins? Why can we measure all the components of the spin at once?
 - Why can we treat the spins as classical precessing magnetization?!?
1. The measurement is very weak
 - The interaction of one nucleus with a macroscopic coil of wire is extremely small
 - The inductive emf from one nucleus gives very little information about that nucleus.
 - This is **good**, because it means that the measurement circuit (the coil) does not cause much decoherence.
 - Decoherence due to measurement circuitry is a big problem in many quantum computing architectures, but *not* solution NMR.
 - However, it requires a very, very large ensemble of nuclei in order to get enough signal to measure anything
 2. The ensemble averages of quantum observables behave classically under *macroscopic forces* as the ensemble gets very large.
 - Known as *Ehrenfest's Theorem*.
 - Same theorem clarifies that large ensembles may act "quantum" under microscopic forces (e.g. the J -coupling)

Experimental Overview

- Key experimental aspect is RF engineering
- Commercial equipment is readily available
- Key issues:
 - Homogeneity of magnetic field
 - Homogeneity of RF field
 - Efficiency of probe

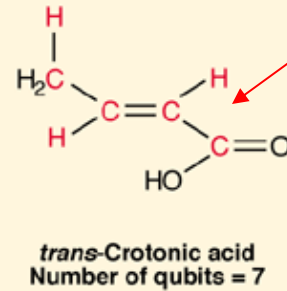
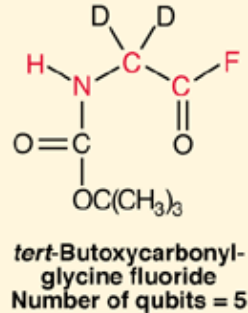
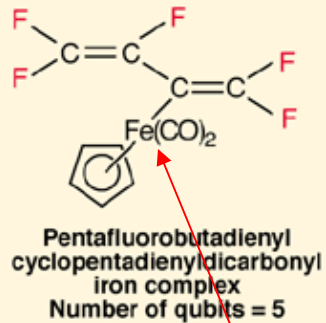
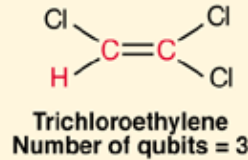
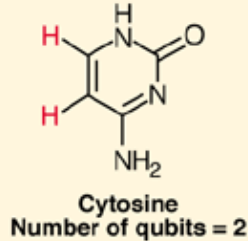
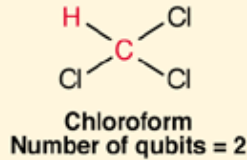


Experimental Overview



Sample Molecules

Molecules used in NMR quantum computers

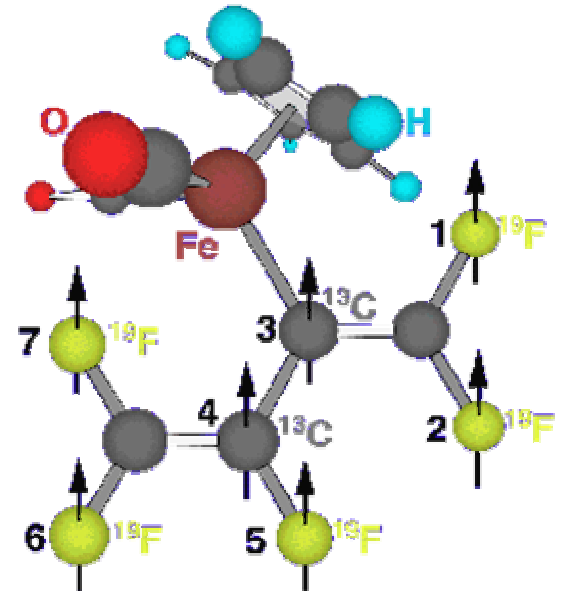


Note: Color indicates nuclei serving as qubits.

Experimental realization of an
order-finding algorithm with an NMR QC
L. Vandersypen et al., PRL **85**, 5452 (2000)

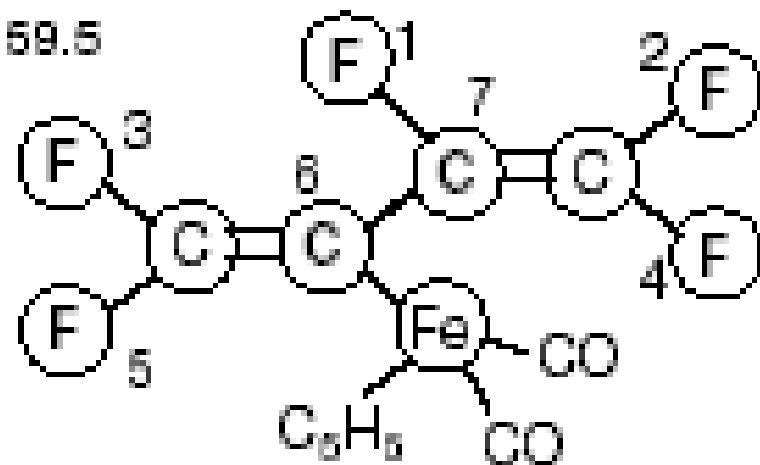
7-qubit molecule used to factor 15 by
Shor's algorithm:
I. Chuang et al., *Nature* **414**, 883 (2001)

A Cat-State Benchmark on
Seven Bit QC
E. Knill et al.,
quant-ph/9908051



Real Timescales

i	$\omega_i/2\pi$	$T_{1,i}$	$T_{2,i}$	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						



7-qubit molecule used to factor 15 by Shor's algorithm:

I. Chuang et al., *Nature* **414**, 883 (2001)

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- Survey of results
- The future of NMR quantum computing

Physical Polarization

$$p_0 = \tanh \frac{\hbar \gamma B_0}{2kT} \approx 10^{-5}$$

$$\begin{array}{l} \downarrow \text{---} \bullet \text{---} \\ \uparrow \text{---} \bullet \text{---} \end{array} \quad \begin{array}{l} P_{\downarrow} = \frac{1+p_0}{2} \\ P_{\uparrow} = \frac{1+p_0}{2} \end{array}$$

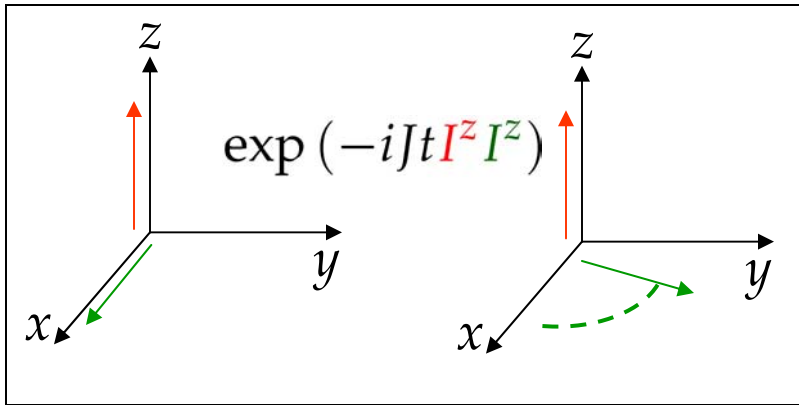
- In thermal equilibrium, density matrix is

$$\hat{\rho}_{\text{eq}} = \frac{1}{Z} e^{-\hat{\mathcal{H}}/kT} \approx \frac{1}{2^n} \left(1 - \frac{\hat{\mathcal{H}}_Z}{kT} \right) \approx \frac{1}{2^{n-1}} \left(\frac{1}{2} + p_0 \sum_{j=1}^n \hat{I}_j^z \right)$$

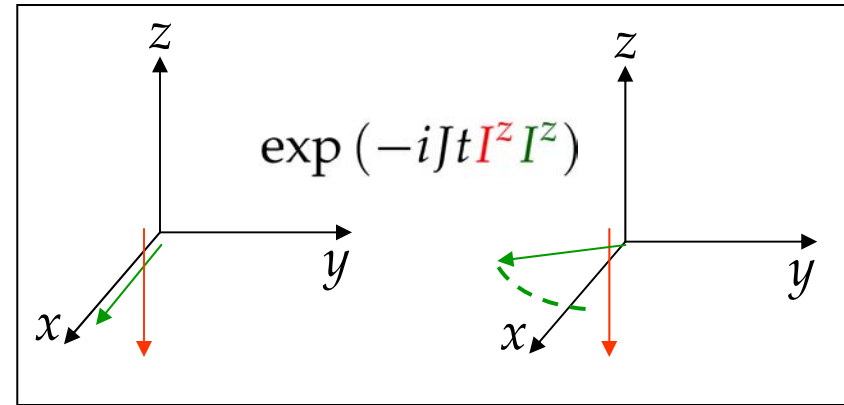
- For single spin, effectively equivalent to spin in pure state with \mathbf{M} scaled down by factor p_0 .
 - In this approximation, all the spins that are up and down cancel out and have no effect on the excess pointing up.
- For multiple spins, equilibrium state is *not* like pure state.

$$\hat{\rho}_{\text{pure}} = \frac{1}{4} \hat{1} + \frac{1}{4} \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad \hat{\rho}_{\text{eq}} = \frac{1}{4} \hat{1} + \frac{p_0}{4} \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix} \quad \begin{array}{l} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{array}$$

The FID Revisited



+

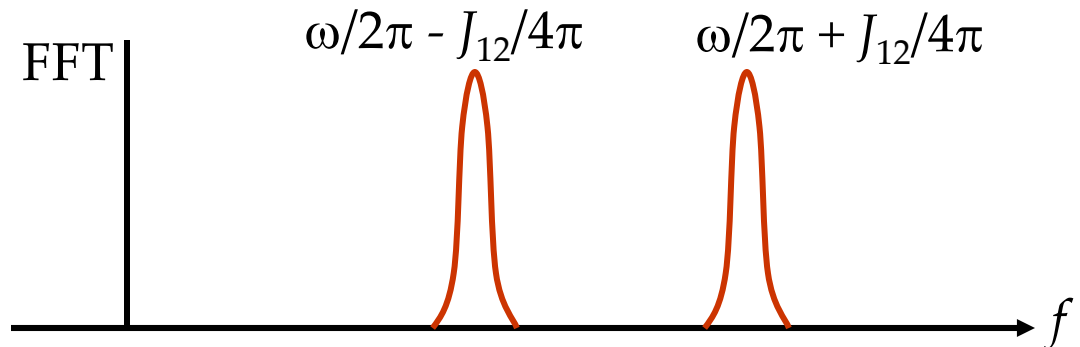


$$M_1^x(t) = \text{Tr} \left\{ \hat{I}_1^x e^{-i\hat{H}^*t} e^{-i(\pi/2)I^y} \hat{\rho} e^{i(\pi/2)I^y} e^{i\hat{H}^*t} \right\} = \frac{p_0}{2} \text{Tr} \left\{ \hat{I}_1^x e^{-i\hat{H}^*t} [\hat{I}_1^x + \hat{I}_2^z] e^{i\hat{H}^*t} \right\}$$

$$= \frac{p_0}{4} \left[\cos(Jt/2) e^{-t/T_2} + \cos(-Jt/2) e^{-t/T_2} \right]$$

$$V(t) \propto \frac{dM_{1,\text{lab}}^x}{dt} \approx \frac{\omega_0 p_0}{4} \left[\cos(\omega_0 t + Jt/2) e^{-t/T_2} + \cos(\omega_0 t - Jt/2) e^{-t/T_2} \right]$$

For a pure state, we saw one peak.
For the mixed state, we see 2^{n-1} peaks.



Is it practical to increase p_0 ?

- Maybe lowering the temperature, raising the field?
 - Largest reasonable laboratory static field: 12 T.
 - Highest γ nucleus: protons at 43 MHz/T.
 - What temperature is needed for $p_0=50\%$?

$$T = \frac{\hbar\gamma B_0}{2k \tanh^{-1} 0.5} = 20 \text{ mK}$$

Only helium is liquid at this low temperature!

- Cross relaxation with cold paramagnetic electrons?
 - Those same electrons lead to short T_1 .
- Exotic methods to polarize nuclei:
 - Chemical reaction with para-hydrogen
 - Cross relaxation with hyperpolarized Xenon
 - These have been done; they are not sufficient to bring nuclei close to ground state
- Efficient methods of dynamic nuclear polarization work in solids, though . . .

Algorithmic Cooling

- Entropy in n spins with polarization p_0 ?

$$S = -\text{Tr} \{ \rho \log_2 \rho \} = nH(p_0)$$

$$H(p_0) = -\sum_{\pm} \frac{1 \pm p_0}{2} \log_2 \frac{1 \pm p_0}{2} \approx 1 - \frac{p_0^2}{2 \ln 2} \text{ bits}$$

- An algorithm cannot decrease the entropy, but it can redistribute it.
- Strategy: put all the entropy in $n-k$ spins, and keep the remaining, zero-entropy k spins.

$$nH(p_0) = kH(1) + (n-k)H(0) = (n-k) \text{ bits}$$

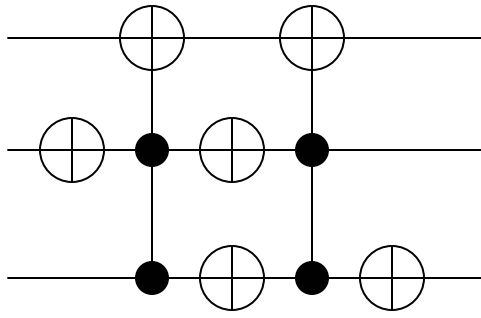
$$\rightarrow k = n(1 - H(p_0)) \approx \frac{p_0^2}{2 \ln 2} n \sim 10^{-10} n$$

- **NOT practical for solution NMR**
- Only useful if p_0 is increased substantially

Pseudo-Pure States: Logical Labeling

- Example: 3 “equivalent” spins

$$\hat{\rho}_{\text{eq}} = \frac{1}{8}\hat{1} + \frac{p_0}{8} \begin{pmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3 \end{pmatrix}, \begin{matrix} |000\rangle \\ |001\rangle \\ |010\rangle \\ |011\rangle \\ |100\rangle \\ |101\rangle \\ |110\rangle \\ |111\rangle \end{matrix}$$



$$\begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ & & & & 1 & 0 & 0 & 0 \\ & & & & 0 & 1 & 0 & 0 \\ & & & & 0 & 0 & 1 & 0 \\ & & & & 0 & 0 & 0 & -3 \end{pmatrix} \begin{matrix} \text{Pure state} \\ \text{conditioned on} \\ \text{first spin up (in} \\ \text{0 state)!} \end{matrix}$$

Scaling Issues with Pseudo-pure States

Entanglement

$$\rho(t_1) = \rho_1(t_1) \otimes \rho_2(t_1) \otimes \rho_3(t_1) \otimes \dots$$

$$U(t_1, t_2) \quad \text{[Red X over arrow]} \quad \text{[Red X over arrow]} \quad \text{[Red X over arrow]}$$

$$\rho(t_2) = \rho_1(t_2) \otimes \rho_2(t_2) \otimes \rho_3(t_2) \otimes \dots$$

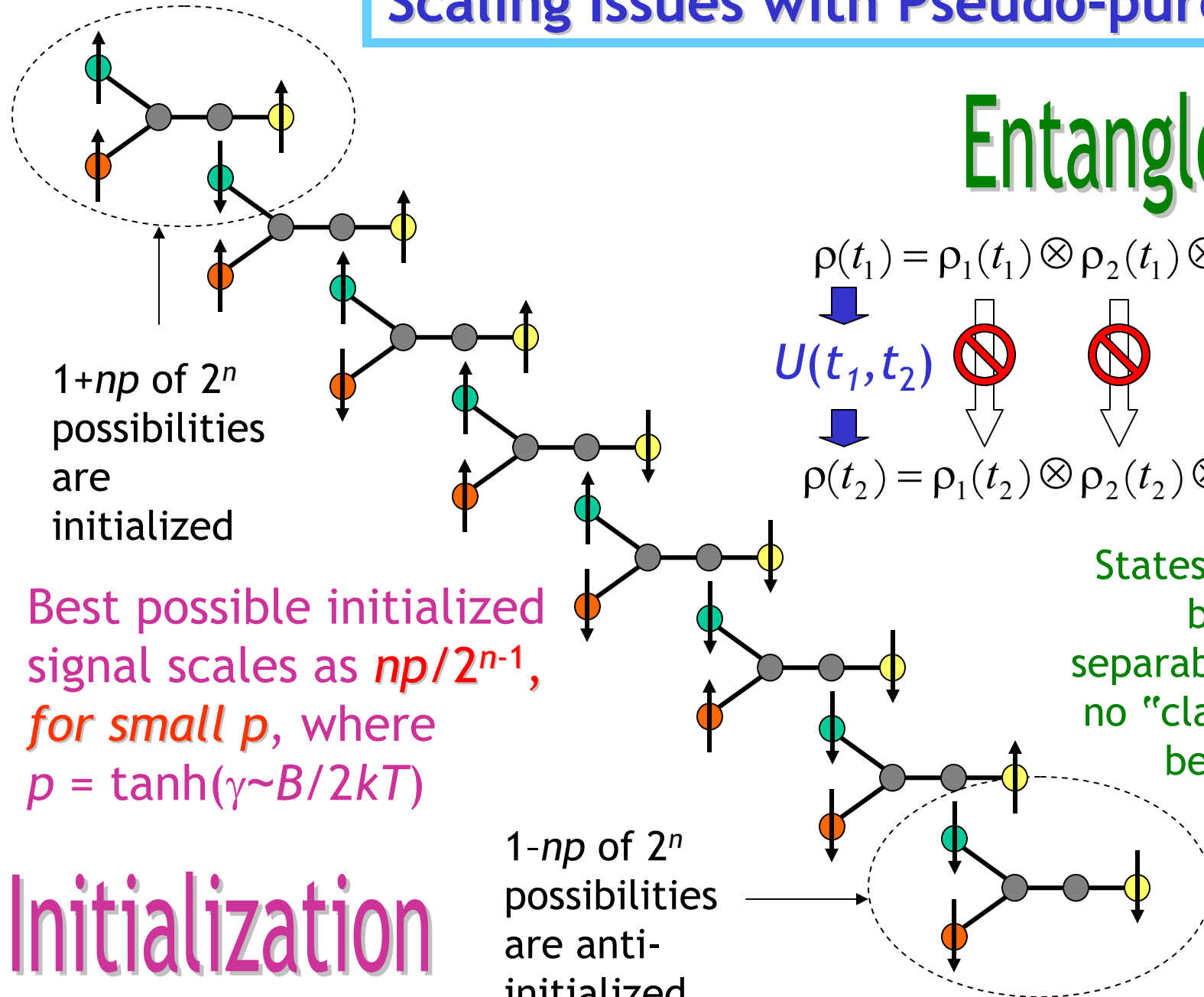
States may always be written as separable, but with no "classical" path between them

$1+np$ of 2^n possibilities are initialized

Best possible initialized signal scales as $np/2^{n-1}$, for small p , where $p = \tanh(\gamma \sim B/2kT)$

$1-np$ of 2^n possibilities are anti-initialized

Initialization



Outline

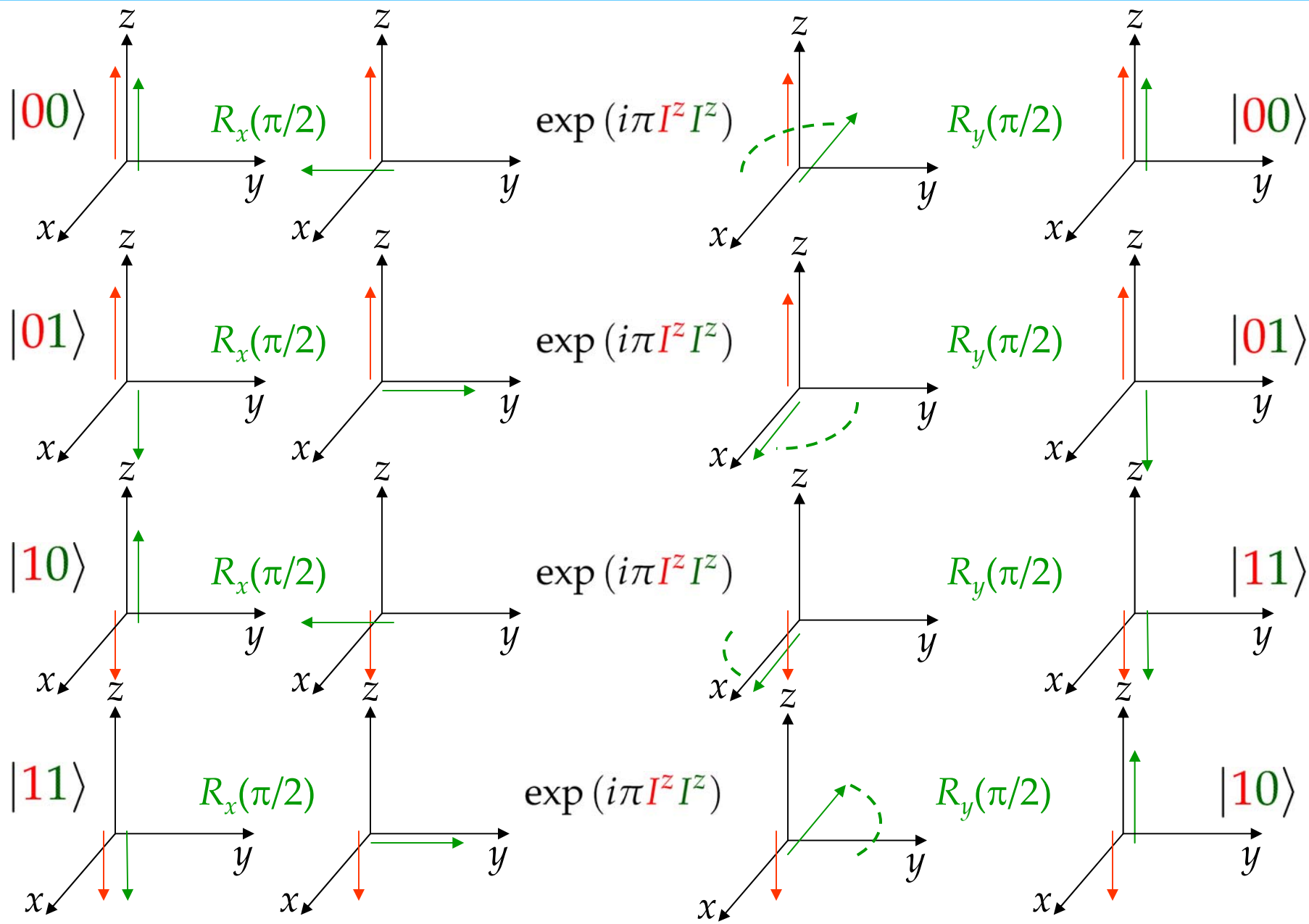
- Why bother with solution NMR quantum computing?
- Basic physics of NMR and ingredients for QC
 - Nuclear magnetic moments in static and RF magnetic fields
 - Nuclear-nuclear couplings
 - Weak ensemble measurement
 - Experimental Overview
- Initialization
 - Physical polarization
 - Algorithmic cooling
 - Pseudo-pure states
 - Scaling
- Quantum logic
 - RF implementations of the universal gate set
 - Refocussing
- Survey of results
- The future of NMR quantum computing

Universal Gate Set with RF Pulses

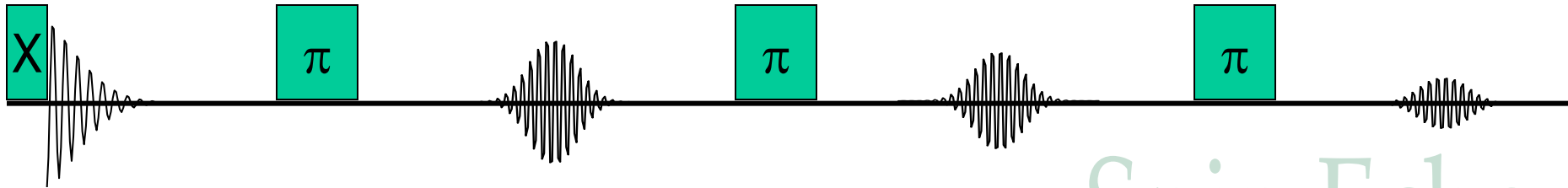
- We have already seen that arbitrary single qubit rotations are effected by appropriate choice of
 - RF phase for x and y direction
 - RF offset for z direction.
 - Note: Offset with no RF amplitude = “frame change.”
- Universal logic is present if controlled-NOT gate is available
- The J -coupling (or ZZ interaction) is sufficient. Up to single qubit phases:

$$\exp\left(-i\frac{\pi}{2}\hat{I}_1^y\right)\exp\left(i\pi\hat{I}_1^z\hat{I}_2^z\right)\exp\left(-i\frac{\pi}{2}\hat{I}_1^x\right) = \hat{U}_{CNOT}$$

Controlled-NOT gate with ZZ interaction



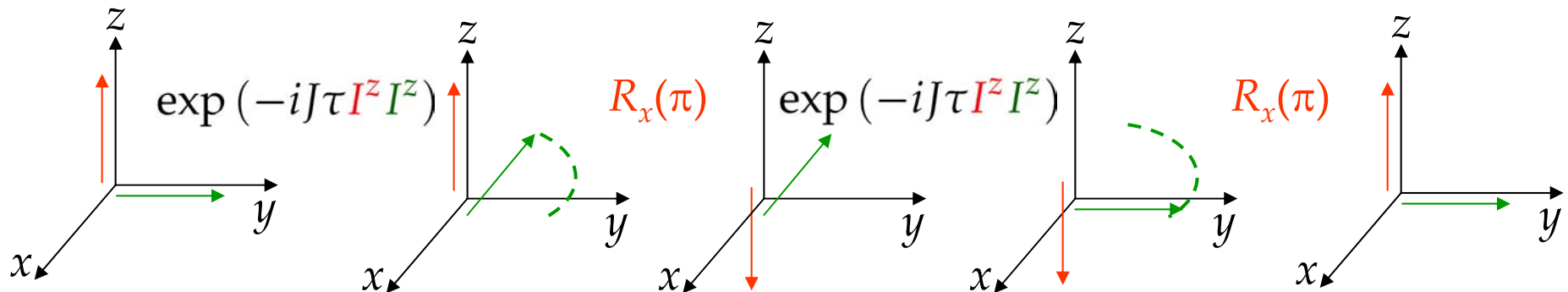
Refocussing



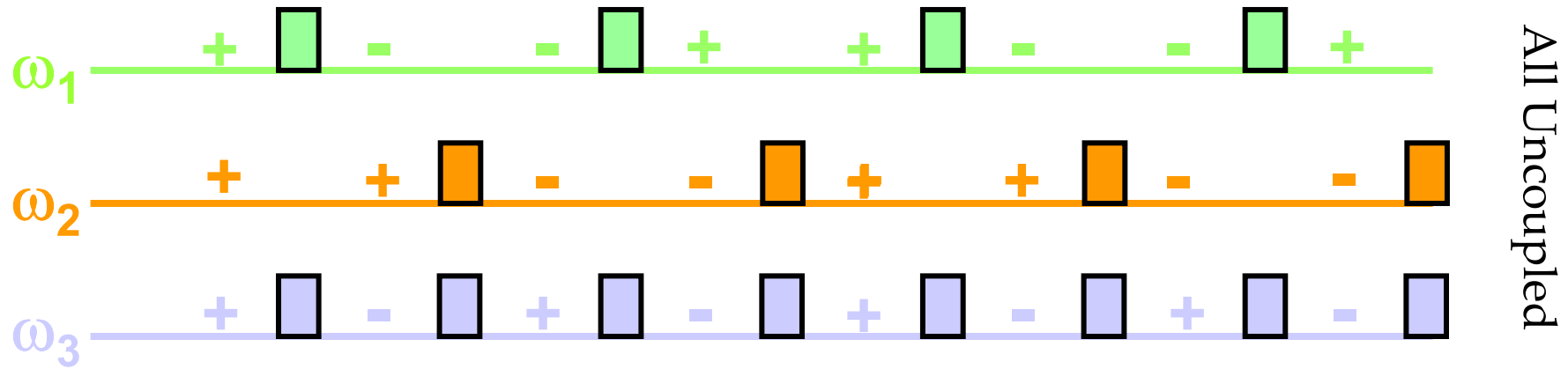
Spin Echo
Spin Echo

- The problem: the J coupling is “always on.”
- What if we want spins to be uncoupled?
- We notice:

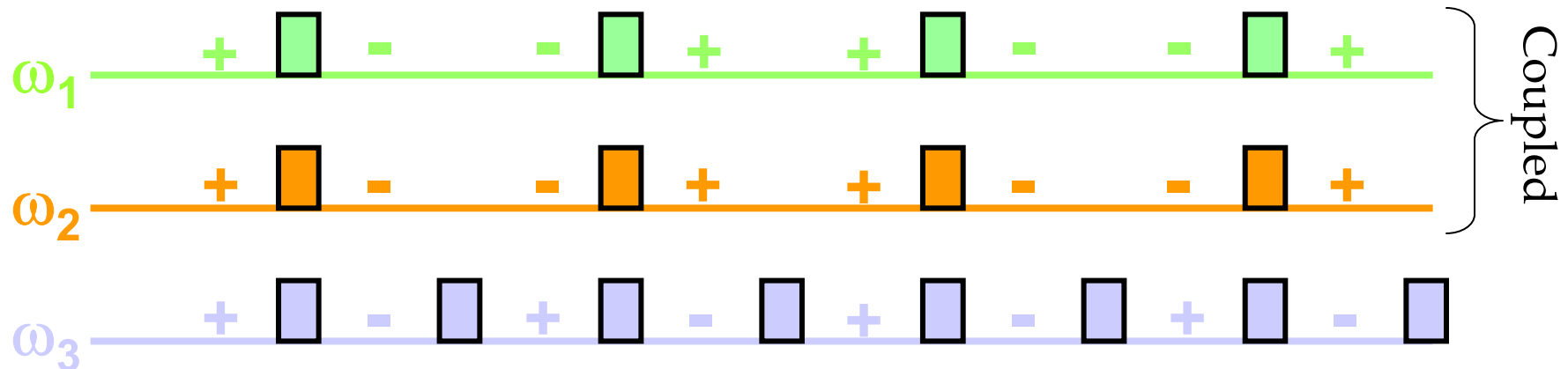
$$\begin{aligned}
 U(2\tau) &= \exp(-iJ\tau\hat{I}_1^z\hat{I}_2^z) \exp(-i\pi\hat{I}_1^x) \exp(-iJ\tau\hat{I}_1^z\hat{I}_2^z) \exp(-i\pi\hat{I}_1^x) \\
 &= \exp(-iJ\tau\hat{I}_1^z\hat{I}_2^z) \exp(-i\pi\hat{I}_1^x) \exp(-iJ\tau\hat{I}_1^z\hat{I}_2^z) \exp(i\pi\hat{I}_1^x) \exp(-2\pi i\hat{I}_1^x) \\
 &= -\exp(-iJ\tau\hat{I}_1^z\hat{I}_2^z) \exp\left(-iJ\tau e^{-i\pi\hat{I}_1^x}\hat{I}_1^z e^{i\pi\hat{I}_1^x}\hat{I}_2^z\right) \\
 &= -\exp(-iJ\tau\hat{I}_1^z\hat{I}_2^z) \exp(iJ\tau\hat{I}_1^z\hat{I}_2^z) = -1
 \end{aligned}$$



Hadamard Decoupling



- For decoupling many qubits, need to use π -pulses to alternate relative signs between all qubits
- Orthogonal “sign matrices” of size n^2 exist for most n
 - (Hadamard Conjecture, 1893)
- *Selective* recoupling can be done by putting signs in phase



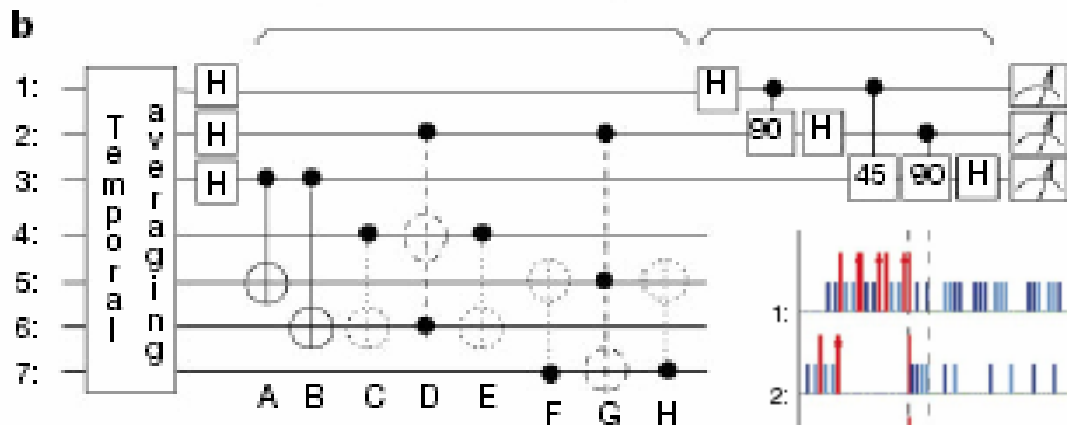
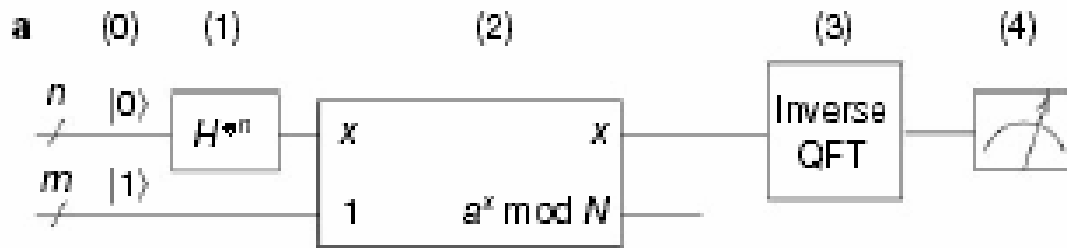
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- **The future of NMR quantum computing**

Algorithms Performed by Solution NMR

- 2-qubit Deutsch-Josza (1998) (Chuang, Jones)
- 2-qubit Grover (1998) (Chuang, Jones)
- 3-qubit Quantum Error Correction (1998) (Cory/Knill/Laflamme)
- 3-qubit Quantum Simulation (1999) (Cory)
- 3-qubit Deutsch-Josza (2000) (Knill/Laflamme)
- 3-qubit Grover (2000) (Chuang)
- 3-qubit Quantum Fourier Transform (2000) (Cory)
- 5-qubit Deutsch-Josza (2000) (Glaser)
- 5-qubit Order-Finding (2000) (Chuang)
- 5-qubit Quantum Error Correction (2001) (Knill/Laflamme)
- 7-qubit Shor's Algorithm (2001) (Chuang)

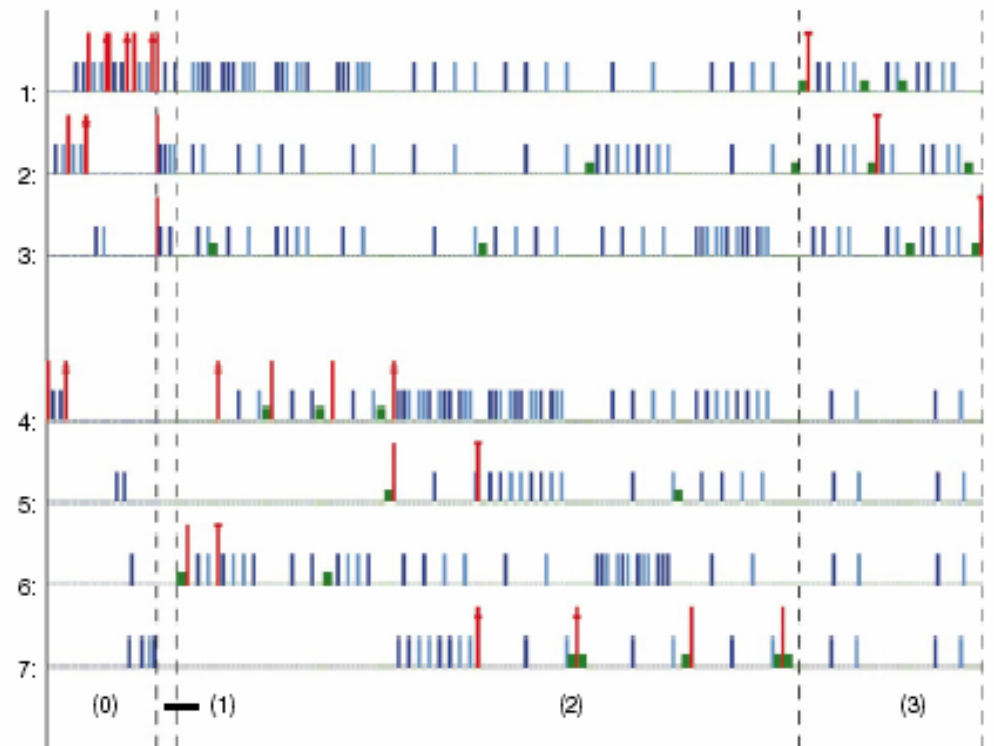
7-Qubit Shor's Algorithm: Details



| π pulse

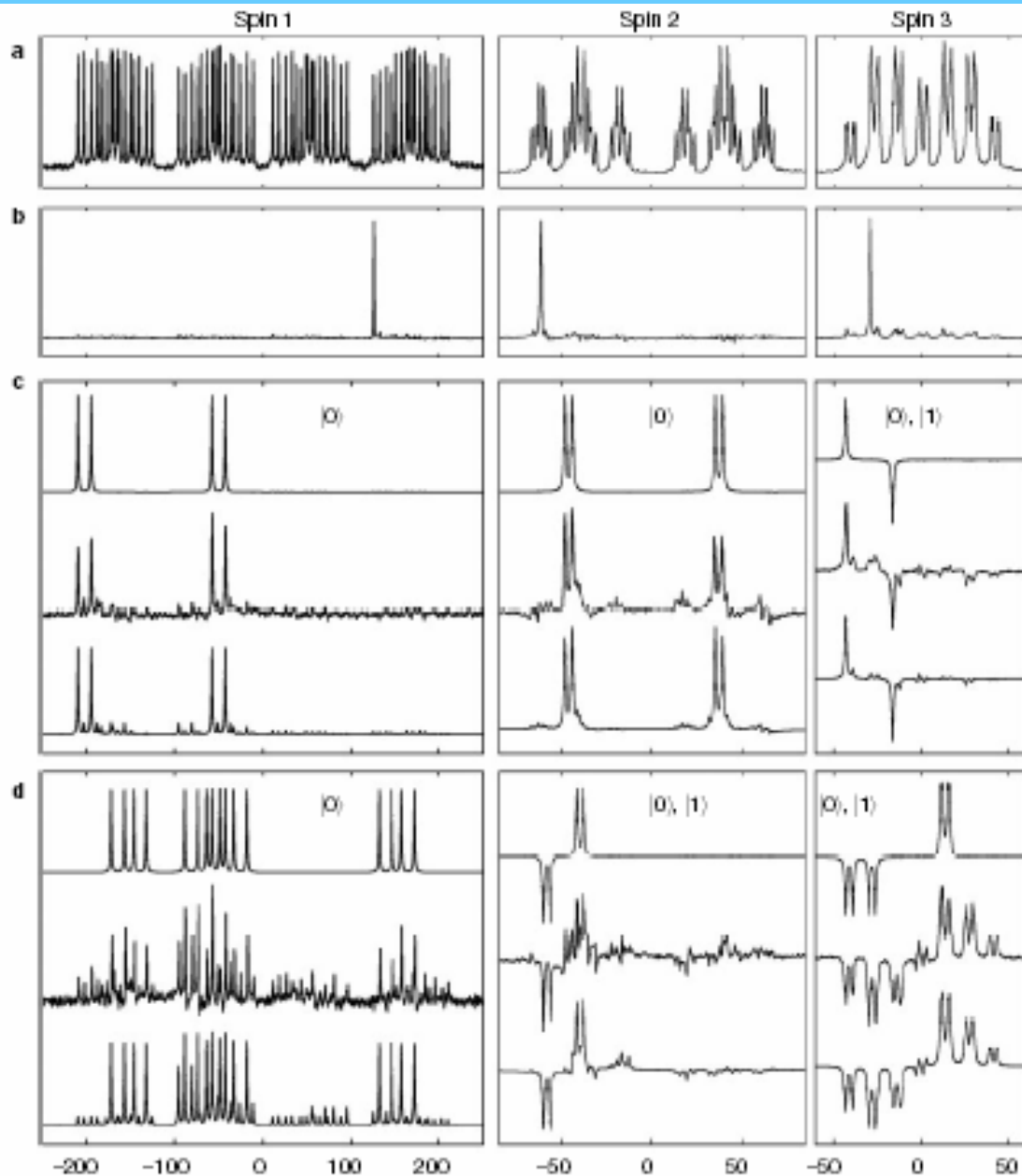
↑ $\pi/2$ pulse

■ Frame change
(z-rotation)



Pulse sequence
optimized to correct for
pulse errors.
Gate sequence
“compiled” to minimize
number of gates.

Results



Thermal FID

Pseudo-pure preparation
(Temporal Averaging)

Expected

Measured a=11

Simulated with T_1, T_2

Expected

Measured a=7

Simulated with T_1, T_2

The Future of NMR QC

- No one is seriously trying to scale solution NMR to more qubits
- Few qubit experiments are still useful for testing new ideas in quantum information theory
 - Adiabatic algorithms
 - Geometric phases for pure states
 - Algorithmic cooling
 - Quantum Random Walks
- For future improvements of NMR QC, however, we must move towards solid-state implementations
- Several bulk ensemble approaches are being pursued:
 - Dilute molecular crystals. Similar to solution, except “solid-state effect” cooling is possible. Difficult to grow good crystals of complex molecules.
 - Semiconducting or insulating crystal lattice (e.g. silicon). Ensemble. Allows optical pumping for polarization. Uses magnetic field gradient to distinguish nuclei, adding scalability. Difficult to measure nuclear spins.
- Finally, approaches using *single* spins as qubits have seen the most attention . . . (next lecture!)