Quantum Information Processing using Nuclear Magnetic Resonance (NMR): What can be done and How to do it?

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Quantum Information Processing: School
HRI-Allahabad- Feb 15, 2011

Centre for Quantum Information and Quantum Computing (CQIQC)

(At Indian Institute of Science, Bangalore)

Investigators:

Prof. Anil Kumar
Prof. Vasant Natarajan
Dr. P.S. Anil Kumar
Dr. Arindam Ghosh
Prof. K.V. Ramanathan
Prof. Apoorva Patel
Prof. Rahul Pandit
Prof. H.R. Krishnamurthy
Prof. N.D. Hari Dass
Prof. C.E. Veni Madhavan
Dr. Subroto Mukerjee
Prof. Diptiman Sen

Funded by Department of Science and Technology, New Delhi

June-2010- June-2015

Activities of the Centre

1. **Bring the experimentalists and the theorists working in the area of Quantum Information, Quantum Computation and Foundations of Quantum Mechanics together. We have already organized about a dozen lectures (nearly one per month).**

2. **Exchange of information, collaboration and cross-fertilization of ideas leading to consolidation of efforts in this important area.**

3. **Invite National and International experts and have colloquia, seminars and lectures, with the aim of exchanging information, ideas and collaboration. We have provision for Visiting Scientists, Post-Docs and Project Assistants positions.**

4. **Organize schools and workshops to train young researchers in the field.**

5. **Channelize/assist/expedite/inspire and focus research in different experimental areas of Quantum Information and Computation, such as (a) quantum dots, (b) NMR, (c) superconducting devices, (d) lasers and (e) trapped ions, with added experimental facilities.**

The Centre for QIQC has the unique feature of combining experimental and theoretical work under one umbrella.

The various areas in which the Centre is consolidating its efforts are:

Experimental Investigations

1. **Nuclear Magnetic Resonance:**
   Prof. Anil Kumar and Prof. K.V. Ramanathan

2. **Ion Trap:**
   Prof. Vasant Natarajan

3. **Superconducting Qubits:**
   Dr. P.S. Anil Kumar

4. **Quantum Dots:**
   Dr. Arindam Ghosh

Theoretical Investigations

1. **Quantum Algorithms**:
   Prof. Apoorva Patel
2. **Study of entanglement in quantum many body systems:**
   Prof. Rahul Pandit and Dr. Subroto Mukerjee
3. **Theoretical support to experimental efforts:**
   Prof. H.R. Krishnamurthy
4. **Foundational aspects of quantum theory:**
   Prof. Hari Dass
5. **Computer science effort:**
   Prof. Veni Madhavan

Liquid-State Room-Temperature NMR: Using spins in molecules as qubits:

- -- Pseudo-Pure States (PPS)
- -- One qubit Gates
- -- Multiqubit Gates
- -- Implementation of DJ and Grover's Algorithms
- -- How to increase the number of Qubits
  - -- Quadrupolar Nuclei as multiqubits
    - -- Spin 1 as qudit
  - -- Dipolar Coupled spin ½ Nuclei- up to 8 qubits
- -- Geometric Phase and its use in Quantum Algorithms
- -- Quantum Games
- -- Adiabatic Algorithms

Acknowledgements

Former QC- IISc-Associates/Students

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Dr. K.V.R.M.Murali - IBM, Bangalore
Dr. Ranabir Das - NCIF/NIH USA
Dr. Rangeet Bhattacharyya - IISER Kolkata
Dr.Arindam Ghosh - NISER-Bhubaneswar
Dr. Avik Mitra - Varian Pune
Dr. T. Gopinath - Univ. Minnesota
Dr. Pranaw Rungta - IISER Mohali
Dr. Tathagat Tulsi – IIT Bombay

This lecture is dedicated
to the memory of
Ms. Jharana Rani Samal*
(*Deceased, Nov., 12, 2009)

Current QC IISc - Students

Mr. Rama K. Koteswara Rao
Mr. V.S. Manu

Other IISc Collaborators

Prof. Apoorva Patel
Prof. K.V. Ramanathan
Prof. N. Suryaprakash

Other Collaborators

Prof. Malcolm H. Levitt - UK
Prof. P.Panigrahi IISER Kolkata
Dr. Arun K. Pati IOP +HRI
Mr. Ashok Ajoy BITS-Goa-MIT

Funding: DST/DAE/DBT

NMR Research Centre, IISc

Field/Frequency stability = 1:10 ^{9}

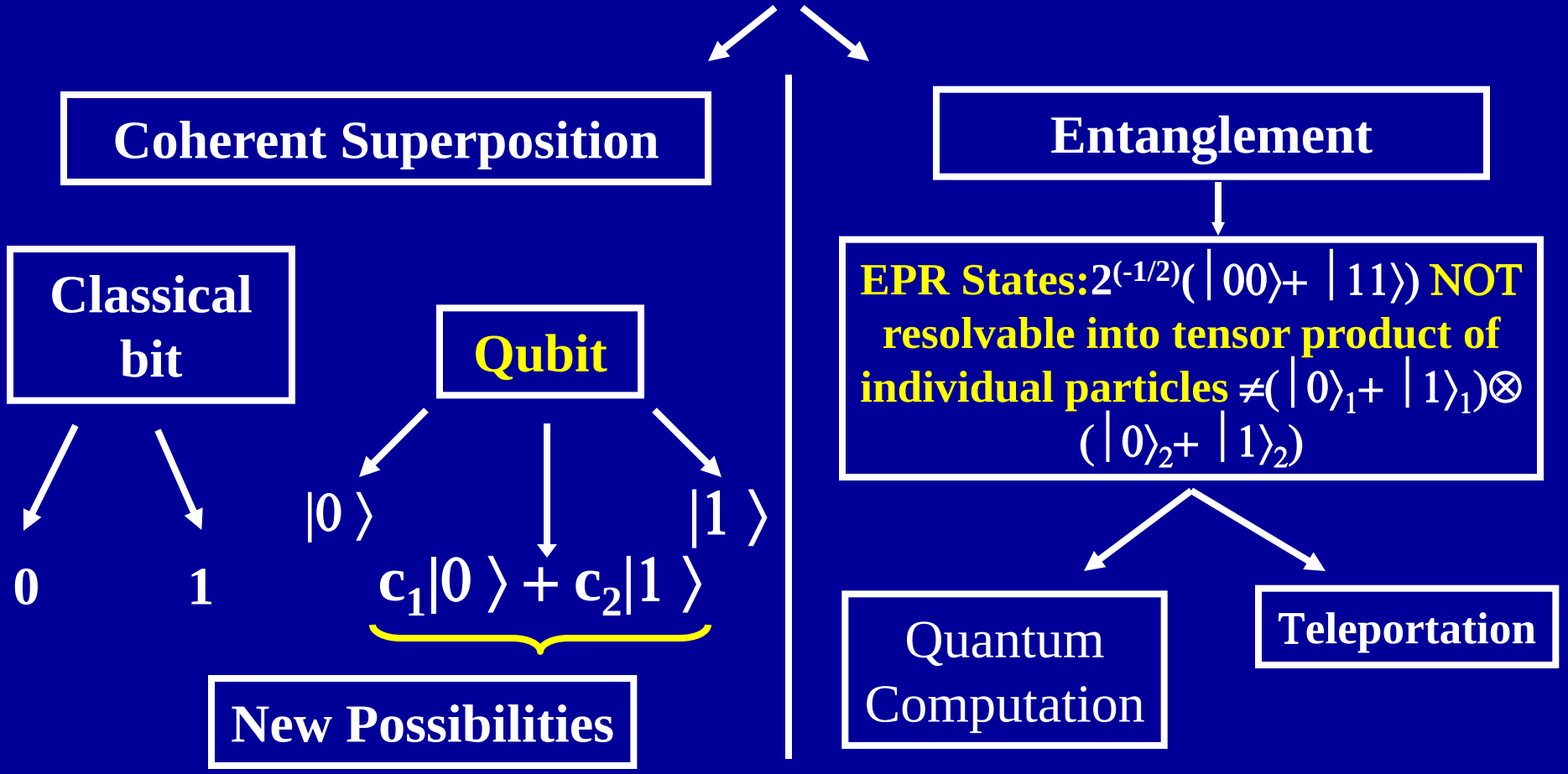
1 ppb

Introduction to QC/QIP

All present day computers (classical computers) use binary (0,1) logic, and all computations follow this Yes/No answer.

Feynman (1982) suggested that it might be possible to simulate the evolution of quantum systems efficiently, using a quantum simulator

What is Special about Quantum Systems?



Quantum Algorithms

1. **PRIME FACTORIZATION**

Classically :
exp $[2(\ln c)^{1/3}(\ln \ln c)^{2/3}]$ — **400 digit**

10^{10}years (Age of the Universe)

Shor's algorithm : **(1994)**
$(\ln c)^3$ — **3 years**

2. **SEARCHING 'UNSORTED' DATA-BASE**

Classically : $N/2$ **operations**
Grover's Search Algorithm : (1997) $\sqrt{N}$ **operations**

3. **DISTINGUISH CONSTANT AND BALANCED FUNCTIONS:**

Classically : $(2^{N-1} + 1)$ **steps**
Deutsch-Jozsa(DJ) Algorithm : (1992) . **1 step**

4. **Quantum Algorithm for Linear System of Equation:**

A.W. Harrow, A. Hassidim and Seth Lloyd; PRL, 103, 150502 (2009).

Exponential speed-up

Recent Developments

5. Simulating a Molecule: Using Aspuru-Guzik Algorithm

(i) J.Du, et. al, Phys. Rev. letters 104, 030502 (2010).

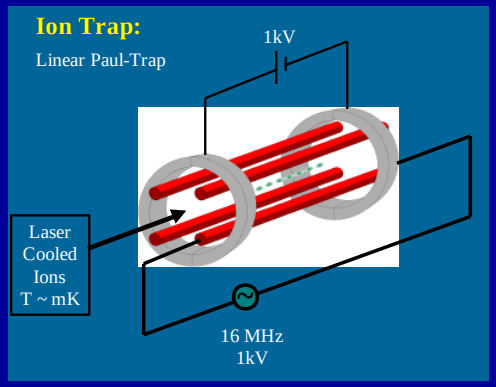
Used a 2-qubit NMR System ($^{13}CHCl_3$) to calculated the ground state energy of Hydrogen Molecule up to 45 bit accuracy.

(ii) Lanyon et. al, Nature Chemistry 2, 106 (2010).

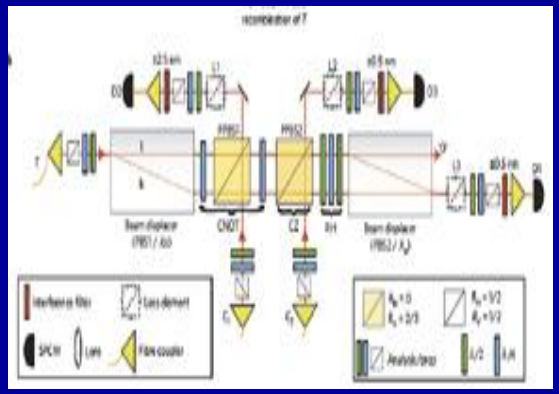
Used Photonic system to calculate the energies of the ground and a few excited states up to 20 bit precision.

Experimental Techniques for Quantum Computation:

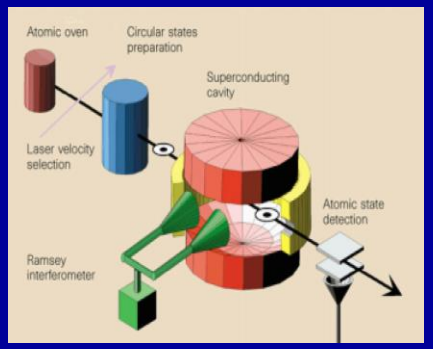
1. Trapped Ions



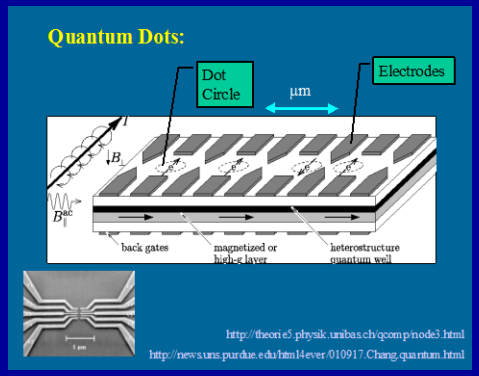
2. Polarized Photons Lasers



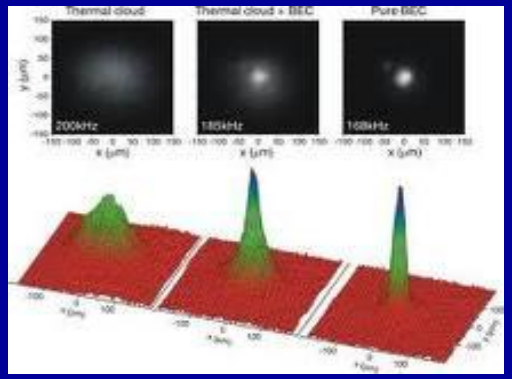
3. Cavity Quantum Electrodynamics (QED)



4. Quantum Dots



5. Cold Atoms



6. NMR

7. Josephson junction qubits

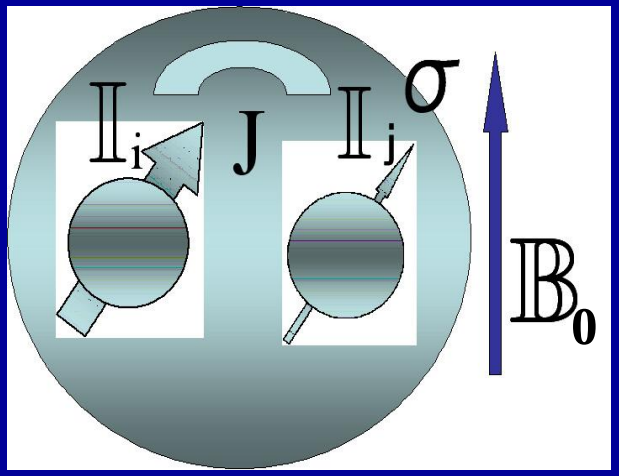
8. Fullerence based ESR quantum computer

Introduction to NMR QIP

Nuclear Magnetic Resonance (NMR)

1. Nuclear spins have small magnetic moments (I) and behave as tiny quantum magnets.

2. When placed in a large magnetic field B_0 , they oriented either along the field ($|0\rangle$ state) or opposite to the field ($|1\rangle$ state) .



3. A transverse radiofrequency field (B_1) tuned at the Larmor frequency of spins can cause transition from $|0\rangle$ to $|1\rangle$ (NOT Gate by a 180^0 pulse).
Or put them in coherent superposition (Hadamard Gate by a 90^0 pulse).

Single qubit gates.

4. Spins are coupled to other spins by indirect spin-spin (J) coupling, and controlled (C-NOT) operations can be performed using J-coupling.

Multi-qubit gates

SPINS ARE QUBITS

NMR sample has ~ 10^{18} spins.

↓

Do we have 10^{18} qubits?

No - because, all the spins can't be individually addressed.

↓ **Progress so far**

Spins having different Larmor frequencies can be individually addressed in the Frequency Space.

As many Larmor Frequencies → as many "qubits"

↓

One needs resolved couplings between the spins in order to encode information as qubits.

NMR Hamiltonian

$$\mathcal{H} = \mathcal{H}_{\text{Zeeman}} + \mathcal{H}_{\text{J-coupling}}$$

$$= \sum_i \omega_i I_{zi} + \sum_{i<j} J_{ij}\, \mathbf{I}_i \cdot \mathbf{I}_j$$

Weak coupling Approximation

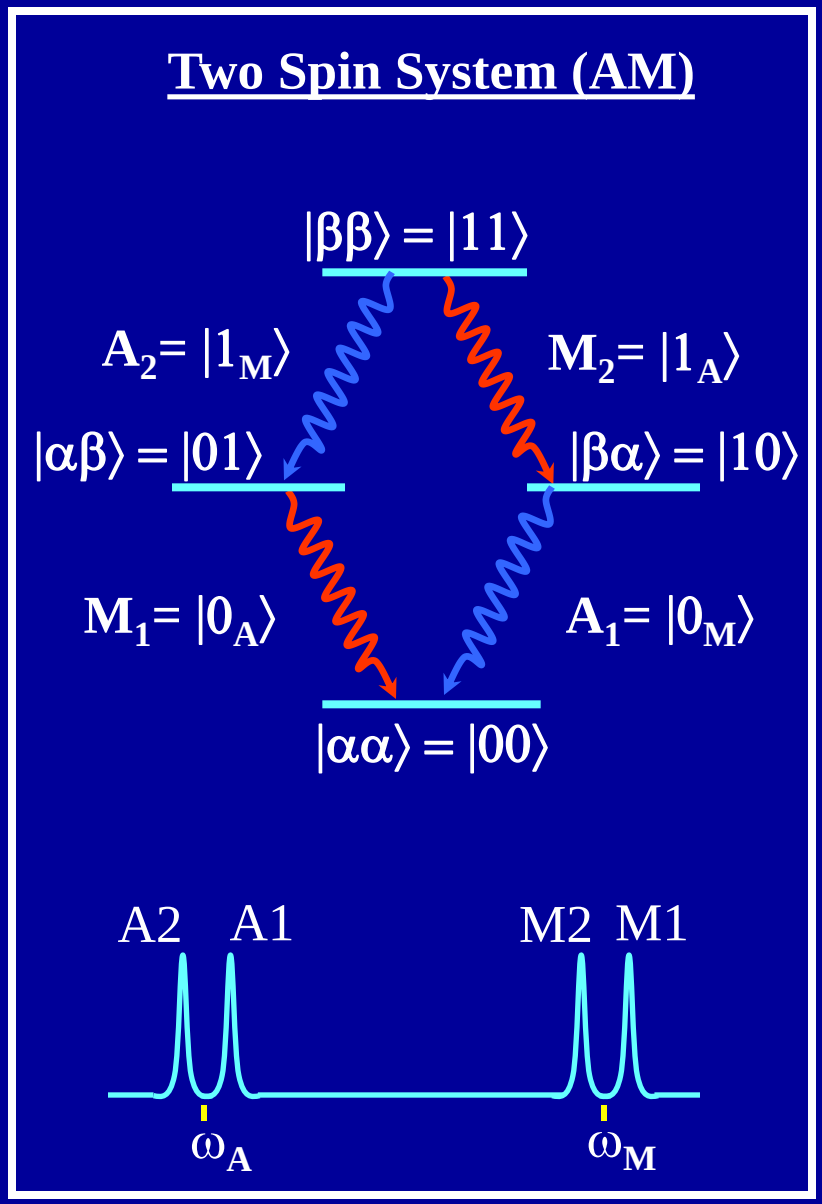
$$|\omega_i - \omega_j| >> J_{ij}$$

$$\mathcal{H} = \underbrace{\sum_i \omega_i I_{zi} + \sum_{i<j} J_{ij}\, I_{zi}\, I_{zj}}$$

Spin Product States are Eigenstates

Under this approximation all spins having same Larmor Frequency can be treated as one Qubit.

Different Larmor frequencies = Different Qubits

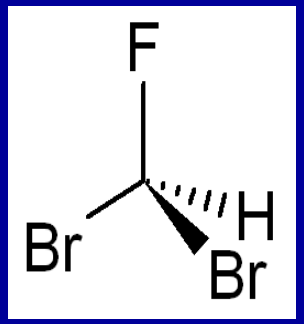


An example of a three qubit system.

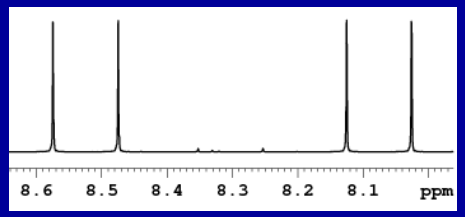
A molecule having three different nuclear spins having different Larmor frequencies all coupled to each other

forming a 3-qubit system

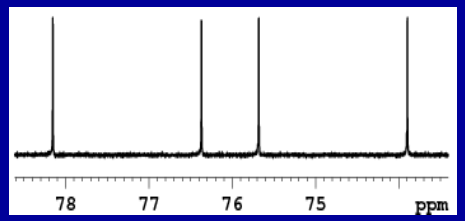
$^{13}CHFBr_2$



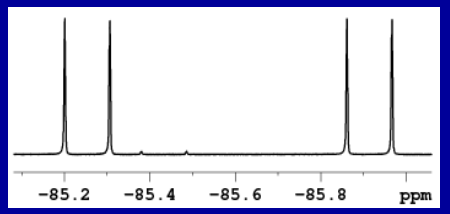
^{1}H = 500 MHz



^{13}C = 125 MHz



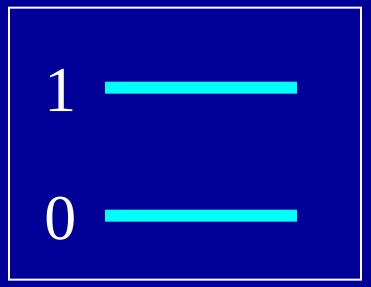
^{19}F = 470 MHz

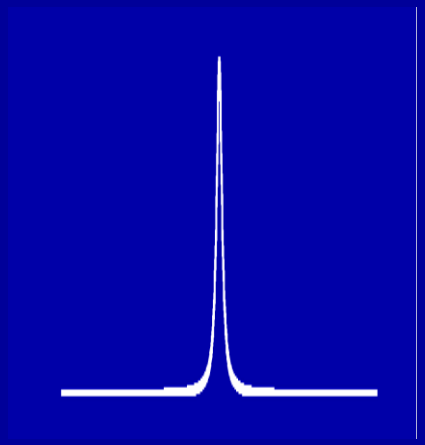


Homo-nuclear spins having different Chemical shifts (Larmor frequencies) also form multi-qubit systems

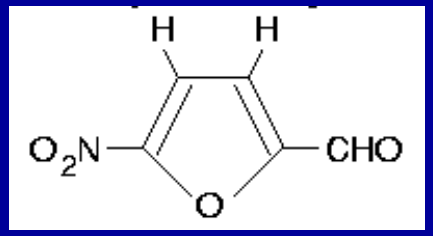
1 Qubit

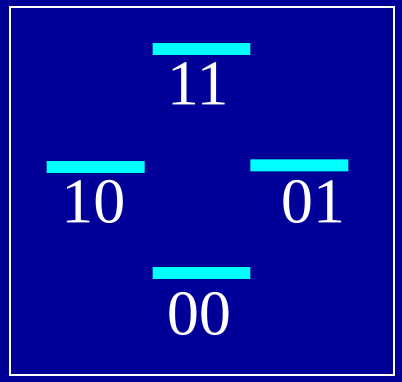
$CHCl_3$

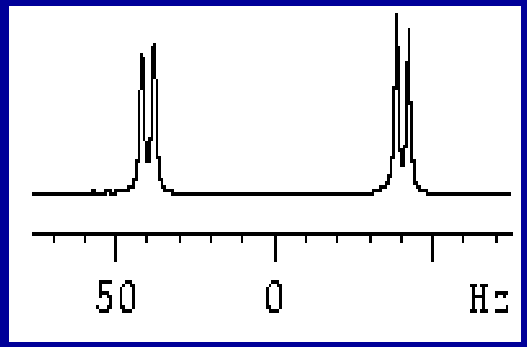




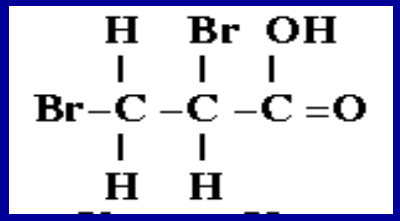
2 Qubits

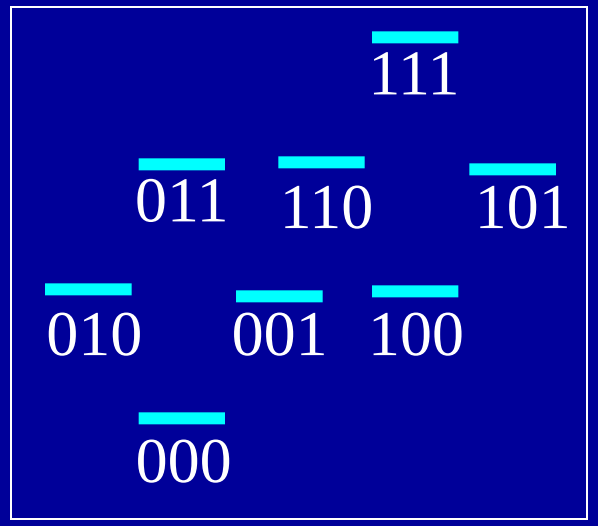


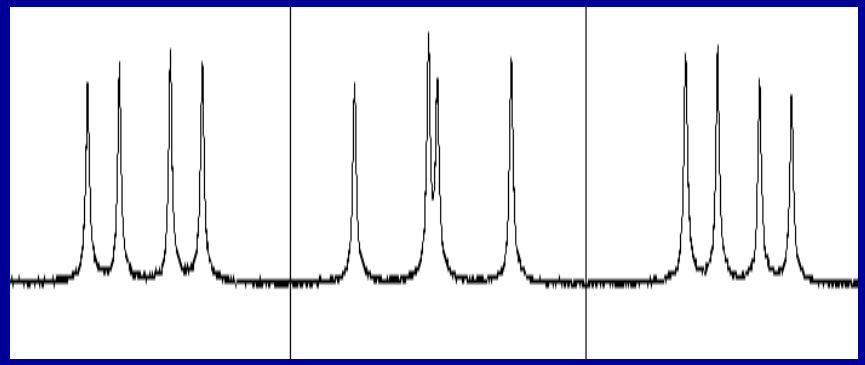




3 Qubits







Achievements of NMR - QIP

√ 1. Preparation of Pseudo-Pure States

√ 2. Quantum Logic Gates

√ 3. Deutsch-Jozsa Algorithm

√ 4. Grover's Algorithm

√ 5. Hogg's algorithm

√ 6. Berstein-Vazirani parity algorithm

√ 7. Quantum Games

√ 8. Creation of EPR and GHZ states

√ 9. Entanglement transfer

√ 10. Quantum State Tomography

√ 11. Geometric Phase in QC

√ 12. Adiabatic Algorithms

√ 13. Bell-State discrimination

14. Error correction

15. Teleportation

16. Quantum Simulation

17. Quantum Cloning

18. Shor's Algorithm

√ 19. No-Hiding Theorem

√ Also performed in our Lab.

Maximum number of qubits achieved in our lab: 8

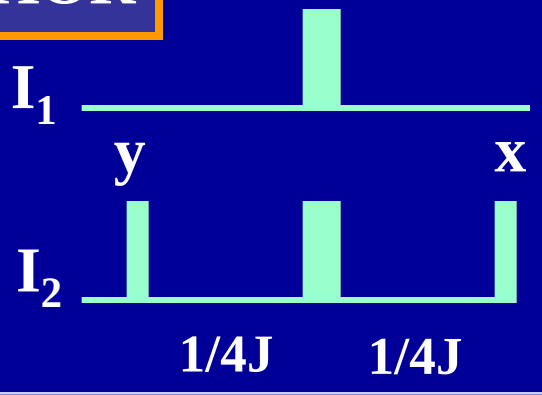
The two methods

Coupling (J) Evolution

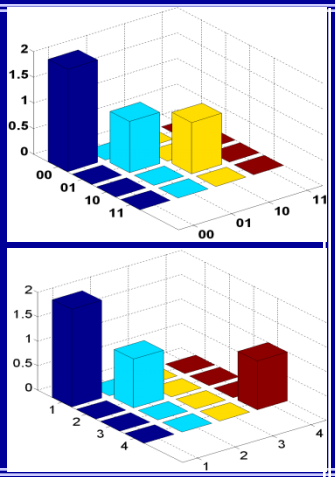
Transition-selective Pulses

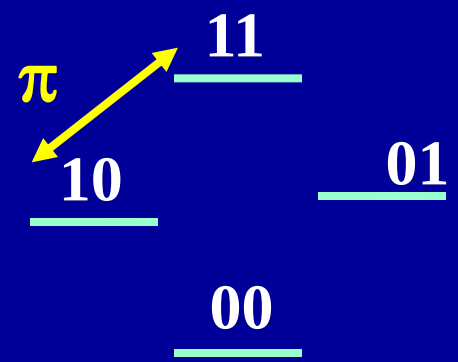
Examples

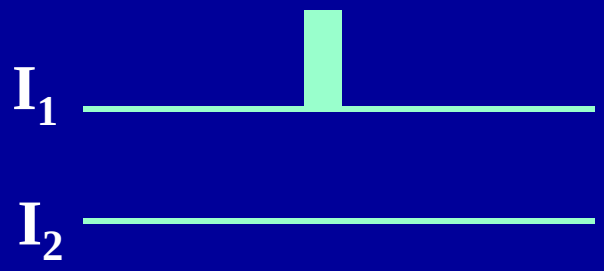
XOR



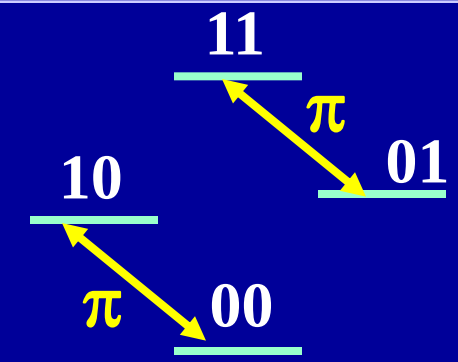
$I_{1z}+I_{2z}$ →
y↓
$I_{1z}+I_{2x}$
(1/2J)↓
$I_{1z}+2I_{1z}I_{2y}$
x↓
$I_{1z}+2I_{1z}I_{2z}$ →

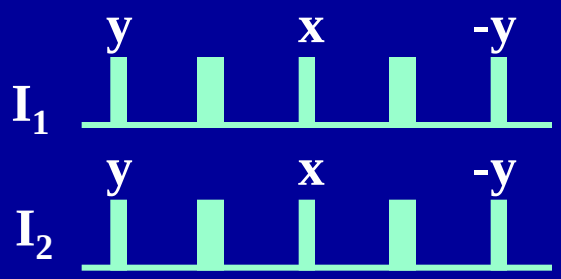




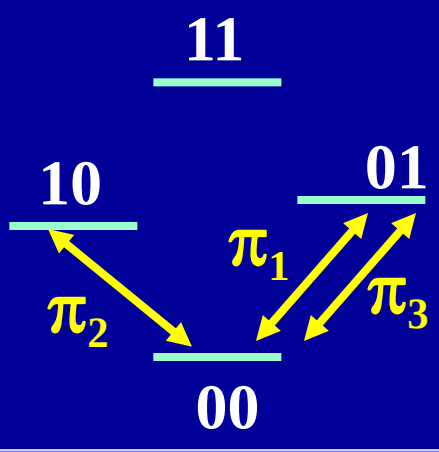


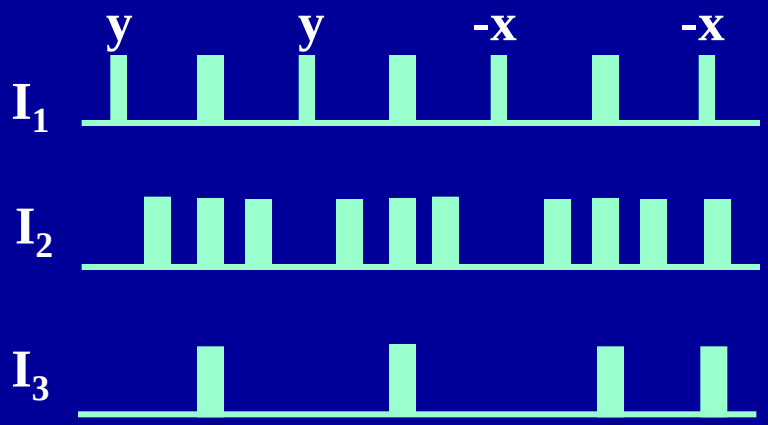
NOT1



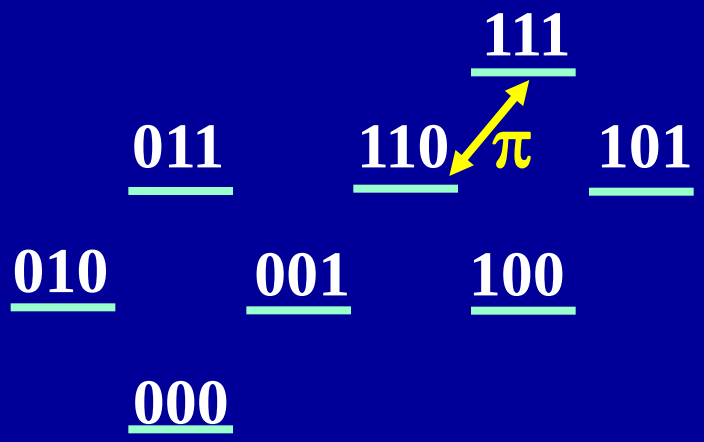


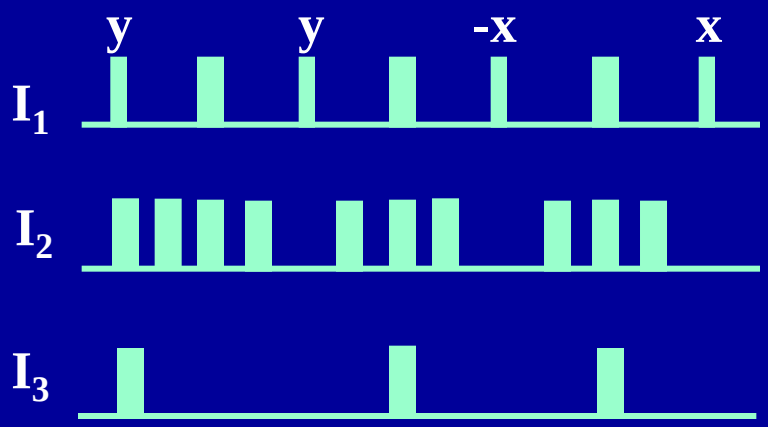
SWAP





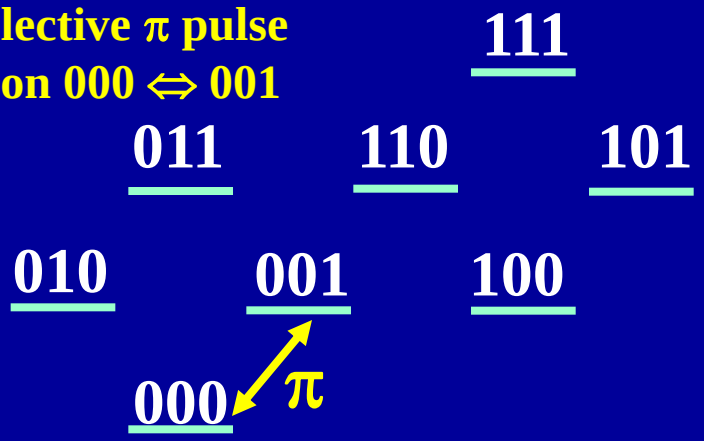
Toffoli





OR/NOR

non-selective π pulse
+ a π on 000 ⇔ 001



Pure States:

$$Tr(\rho) = Tr(\rho^2) = 1$$

For a diagonal density matrix, this condition requires that all energy levels except one have zero populations.

Such a state is difficult to create in NMR

Pseudo-Pure States

Under High Temperature Approximation

$\rho = 1/N (\alpha 1 - \Delta\rho)$ Here $\alpha = 10^5$ and $U\ 1\ U^{-1} = 1$

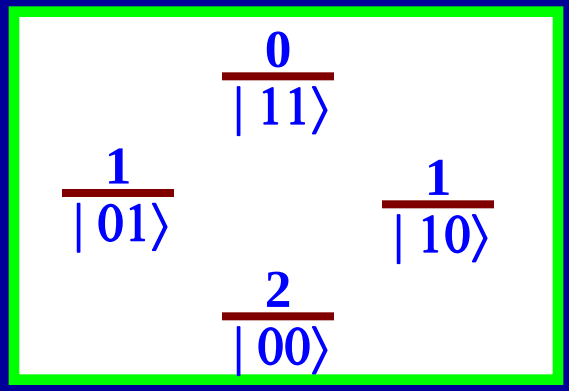
We create a state in which all levels except one have EQUAL populations. Such a state mimics a pure state.

Pseudo-Pure State

In a two-qubit Homo-nuclear system:

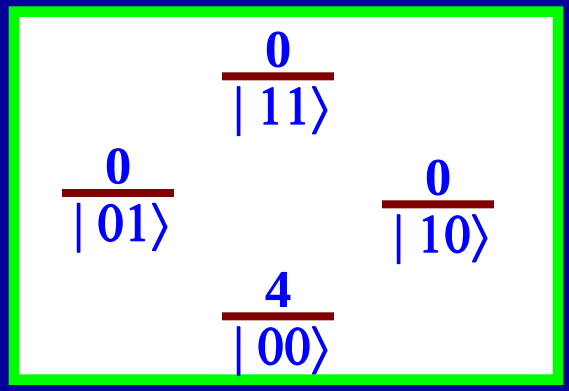
(i) Equilibrium:

$$\rho = 10^5 + \Delta\rho = \{2, 1, 1, 0\}$$



(ii) Pseudo-Pure

$$\Delta\rho = \{4, 0, 0, 0\}$$



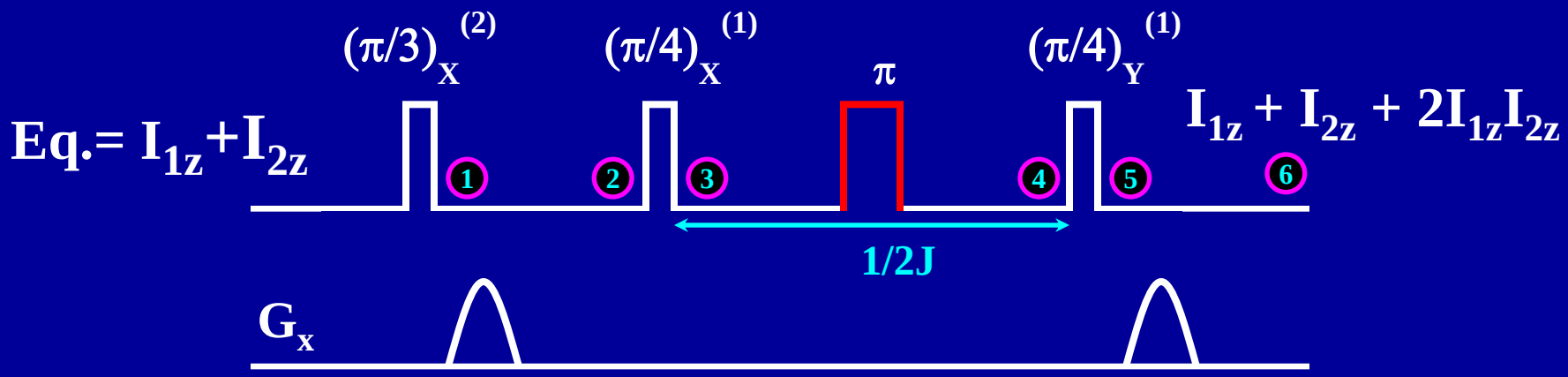
Preparation of Pseudo-pure states

- Spatial Averaging — Cory, Price, Havel, PNAS, 94, 1634 (1997)
- Logical Labeling — N. Gershenfeld et al, Science, 275, 350 (1997); Kavita, Arvind, Anil Kumar, PRA 61, 042306 (2000)
- Temporal Averaging — E. Knill et al., PRA, 57, 3348 (1998)
- Pairs of Pure States (POPS) — B.M. Fung, Phys. Rev. A **63**, 022304 (2001)
- Spatially Averaged Logical Labeling Technique (SALLT) — T. S. Mahesh and Anil Kumar, PRA 64, 012307 (2001)
- Using long lived Singlet States — S.S. Roy and T.S. Mahesh, PRA, (in press) 2010.

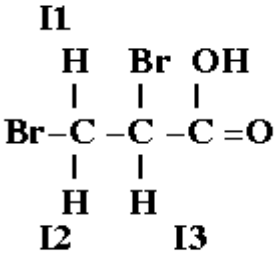
1 **Spatial Averaging:** Cory, Price, Havel, PNAS, 94, 1634 (1997)

$$I_{1z} = 1/2 \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad I_{2z} = 1/2 \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad 2I_{1z}I_{2z} = 1/2 \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

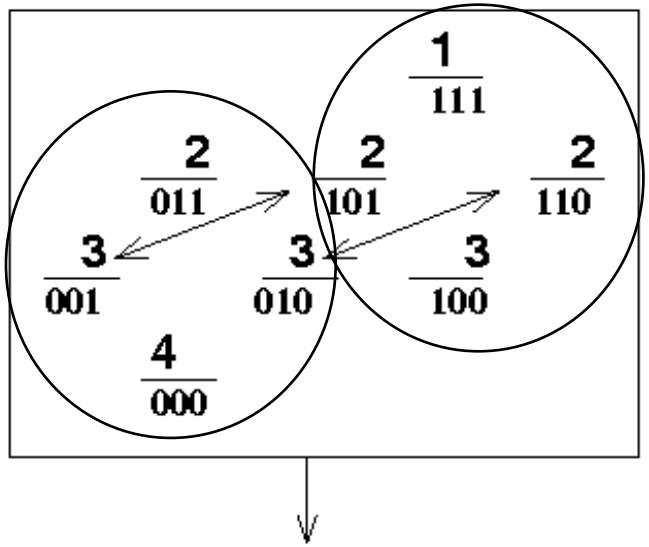
$$I_{1z} + I_{2z} + 2I_{1z}I_{2z} = 1/2 \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \leftarrow \textbf{Pseudo-pure state}$$

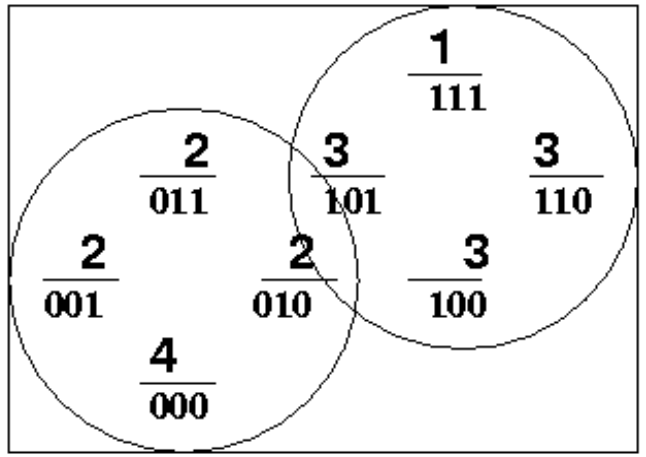


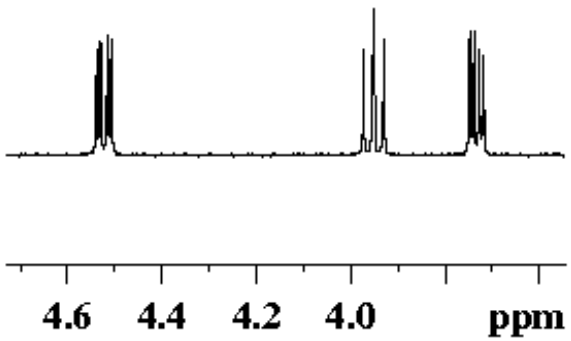
2. Logical Labeling

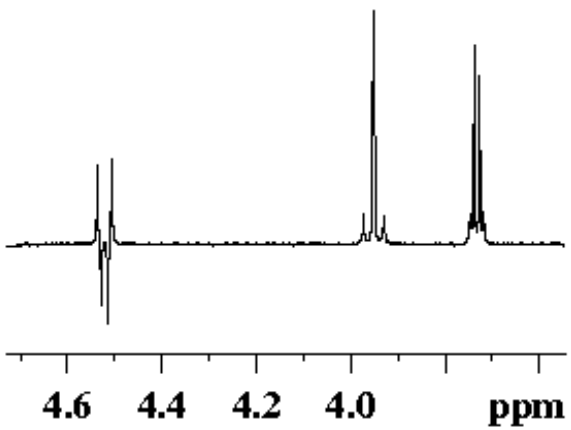


2,3–dibromo propionic acid







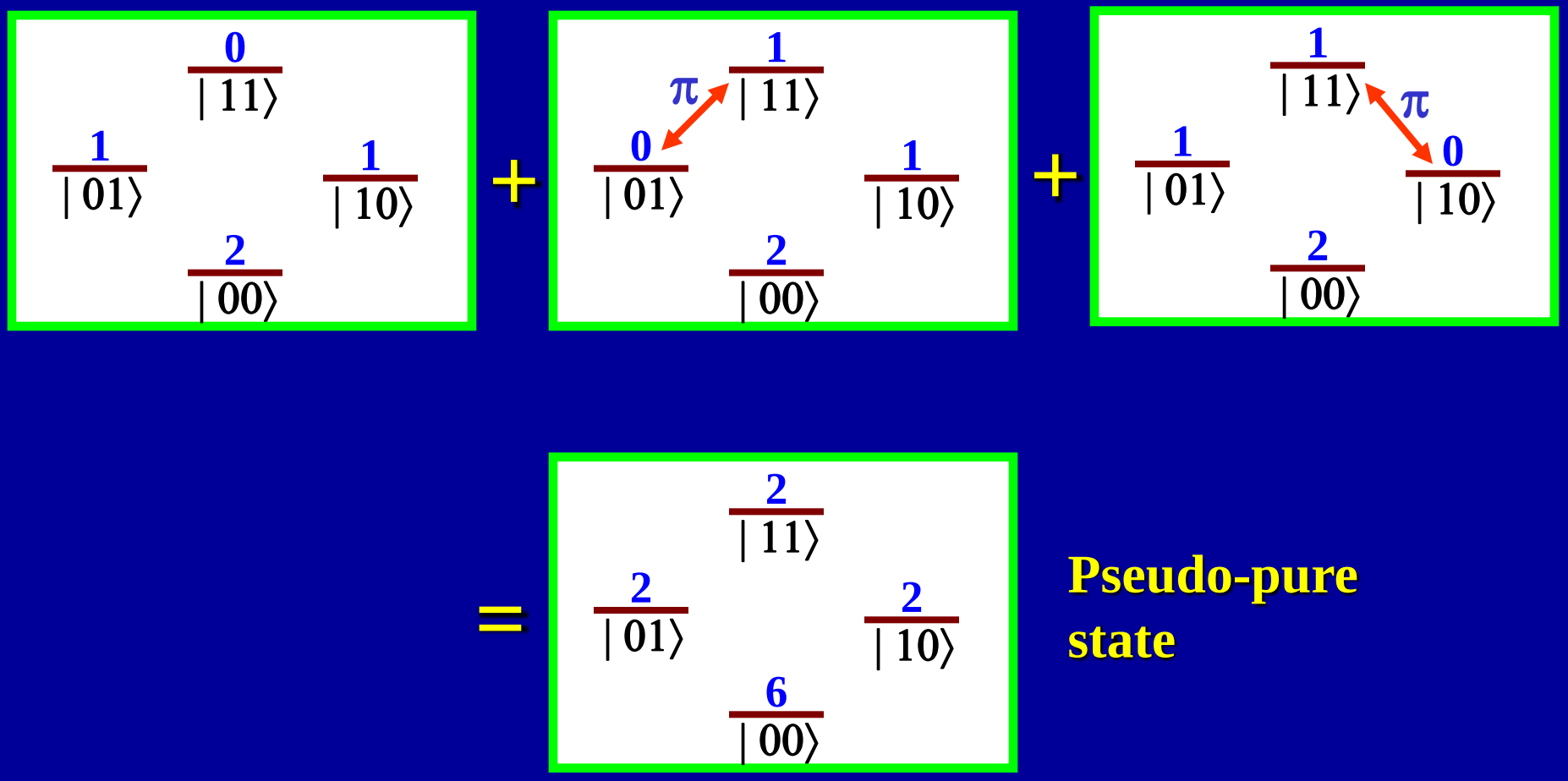


•N. Gershenfeld et al, **Science, 1997, 275, 350**

Kavita, Arvind, and Anil Kumar **Phys. Rev. A, 2000, 61, 042306**

DRX-500
SIF

3. Temporal Averaging

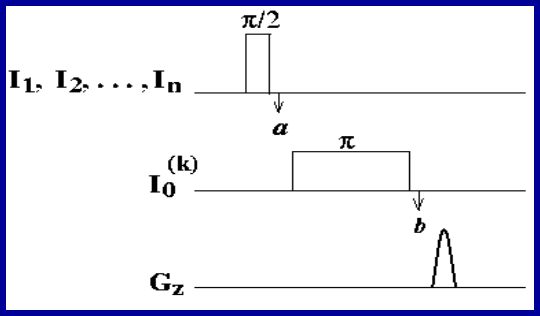


E. Knill et al., PRA, 57, 3348 (1998)

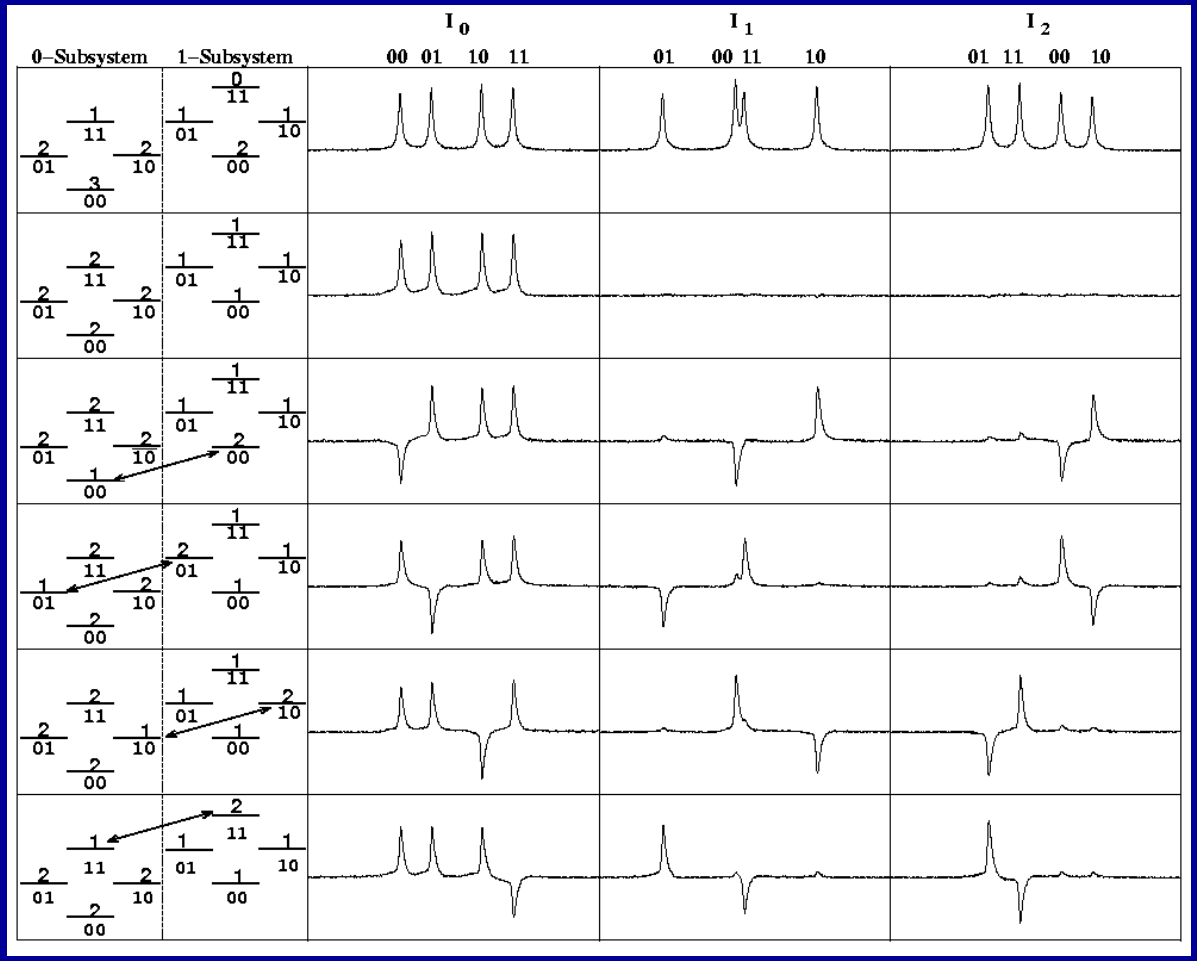
4. Pseudo Pure State by SALLT:

(Spatially Averaged Logical Labeling Technique)

This method does not scale with number of qubits

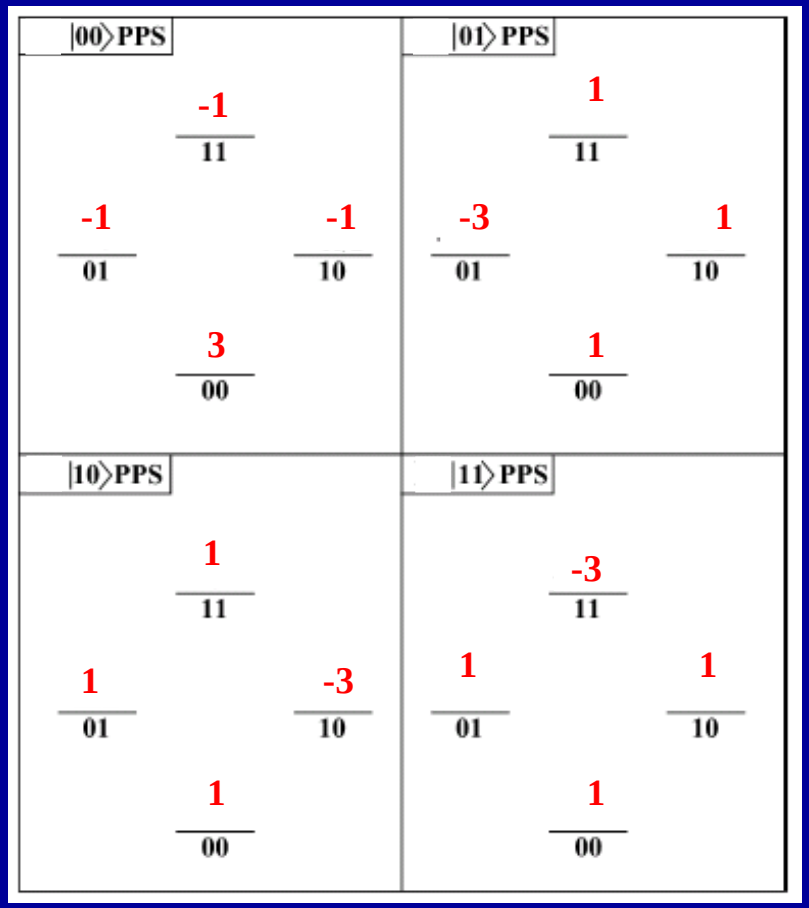


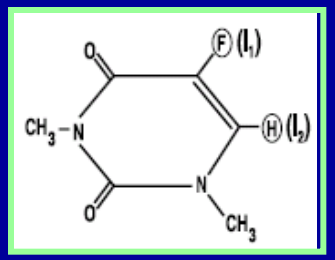
Subsystem Pseudo-pure states of 2 qubits



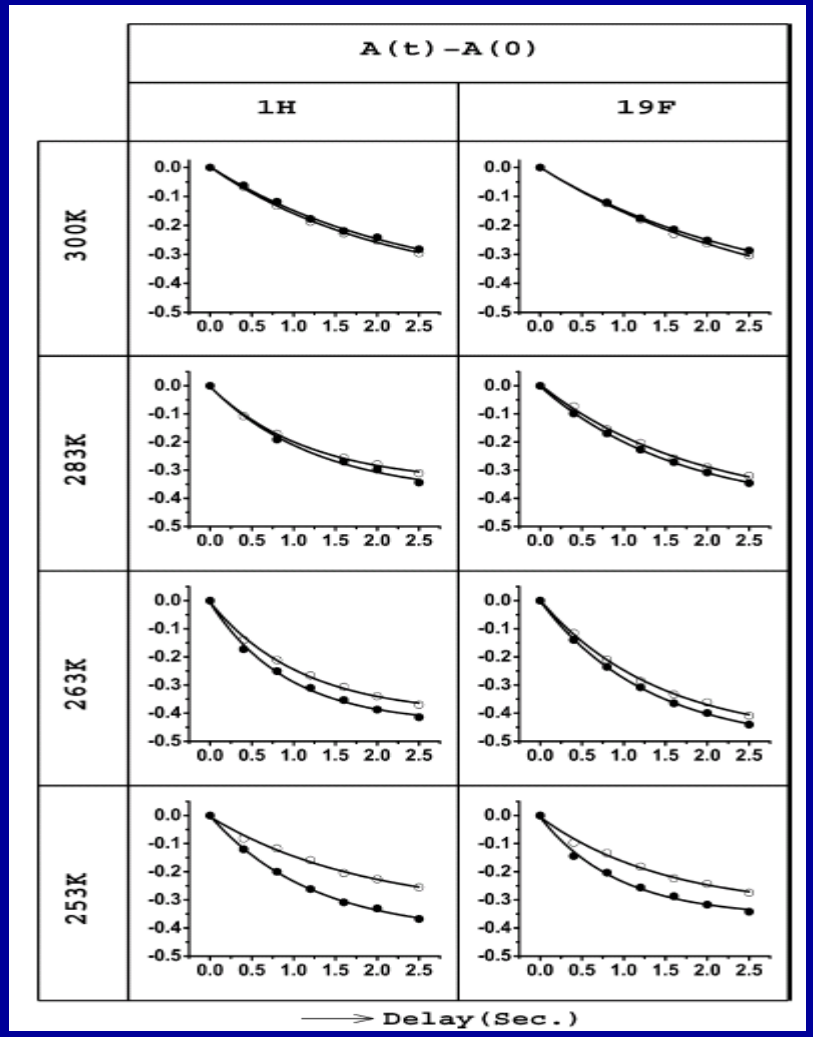
T. S. Mahesh and Anil Kumar, PRA 64, 012307 (2001)

Relaxation of Pseudopure states





Cross Correlations retard the relaxation of some PPS



Open circles 00; Filled circles 11 PPS

Arindam Ghosh and Anil Kumar, J. Magn. Reson., 173, 125 (2005).

Logic Gates using NMR

Single qubit gates

NOT gate

$$U_{NOT} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Hadamard gate

$$U_H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Phase shift gate

$$U_\Phi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$$

$$U_{NOT} = (\pi)_x = e^{-i\pi I_x} = -i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad U_H = [(\pi/2)_{-y}.(\pi)_x] = e^{i\pi/2 I_y}.e^{-i\pi I_x} = \frac{-i}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$U_\Phi = U_z(\phi) = [(\pi/2)_{-y}.\phi_x.(\pi/2)_y] = e^{i(\pi/2)I_y}.e^{-i\phi I_x}.e^{-i(\pi/2)I_y} = e^{-i\phi/2} \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$$

Composit z-pulse

Single qubit gates can be obtained by applying qubit selective pulses (spin selective pulses)

Multi-qubit gates

Quantum computing also requires the implementation of unitary operators on a qubit cont to the states of other qubits, such gates are called multi-qubit gates.

These gates can be implemented by,

(i) J-evolution method

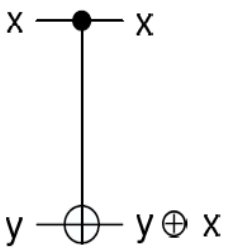
(ii) Trnasition selective pulses

J-evolution method: The evolution of J-couplings and RF pulses are used.

The Hamiltonian of J-coupling,

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

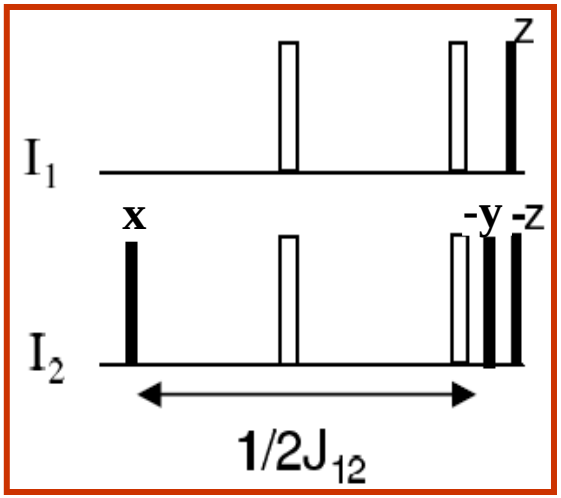
CNOT(2)



Truth table

Input $\|x,y\rangle$	Output $\|x,y\oplus x\rangle$
00	00
01	01
10	11
11	10

$$U_{CNOT(2)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

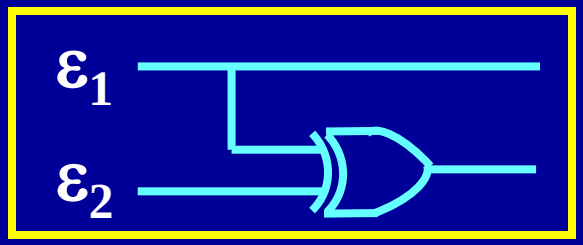


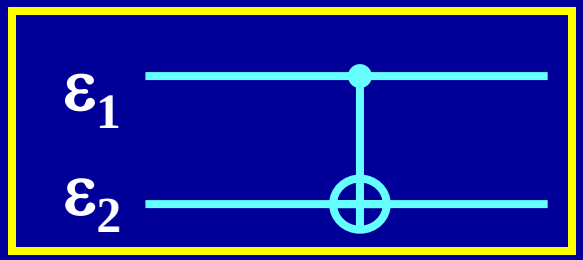
Logic Gates

XOR2

(Exclusive OR or C-NOT)

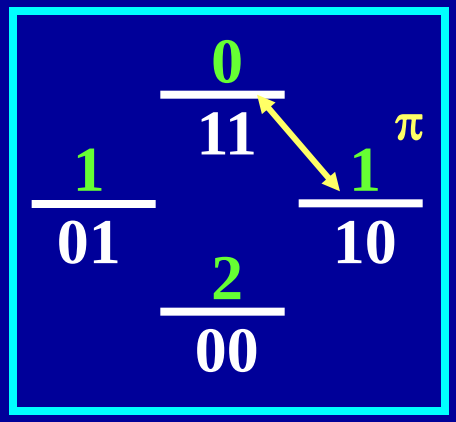
$$|\varepsilon_1, \varepsilon_2\rangle \xrightarrow{U_{XOR2}} |\varepsilon_1, \varepsilon_1 \oplus \varepsilon_2\rangle$$





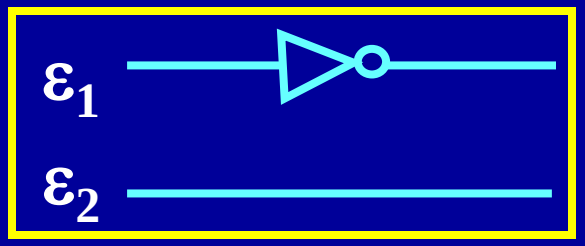
INPUT	OUTPUT
$\|0\,0\rangle$	$\|0\,0\rangle$
$\|0\,1\rangle$	$\|0\,1\rangle$
$\|1\,0\rangle$	$\|1\,1\rangle$
$\|1\,1\rangle$	$\|1\,0\rangle$

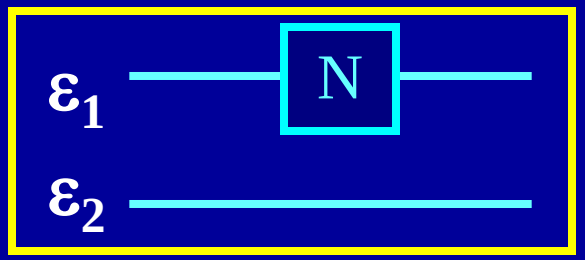
π



NOT1

$$|\varepsilon_1, \varepsilon_2\rangle \xrightarrow{U_{NOT1}} |\bar{\varepsilon}_1, \varepsilon_2\rangle$$

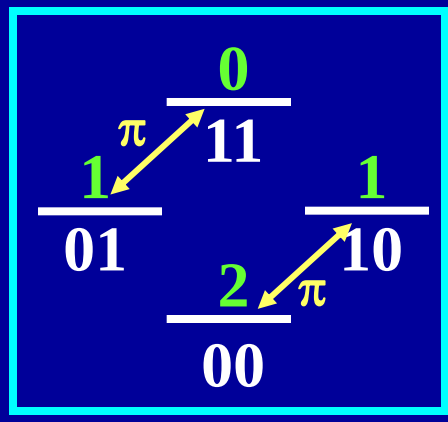




INPUT	OUTPUT
$\|0\,0\rangle$	$\|1\,0\rangle$
$\|0\,1\rangle$	$\|1\,1\rangle$
$\|1\,0\rangle$	$\|0\,0\rangle$
$\|1\,1\rangle$	$\|0\,1\rangle$

π

π

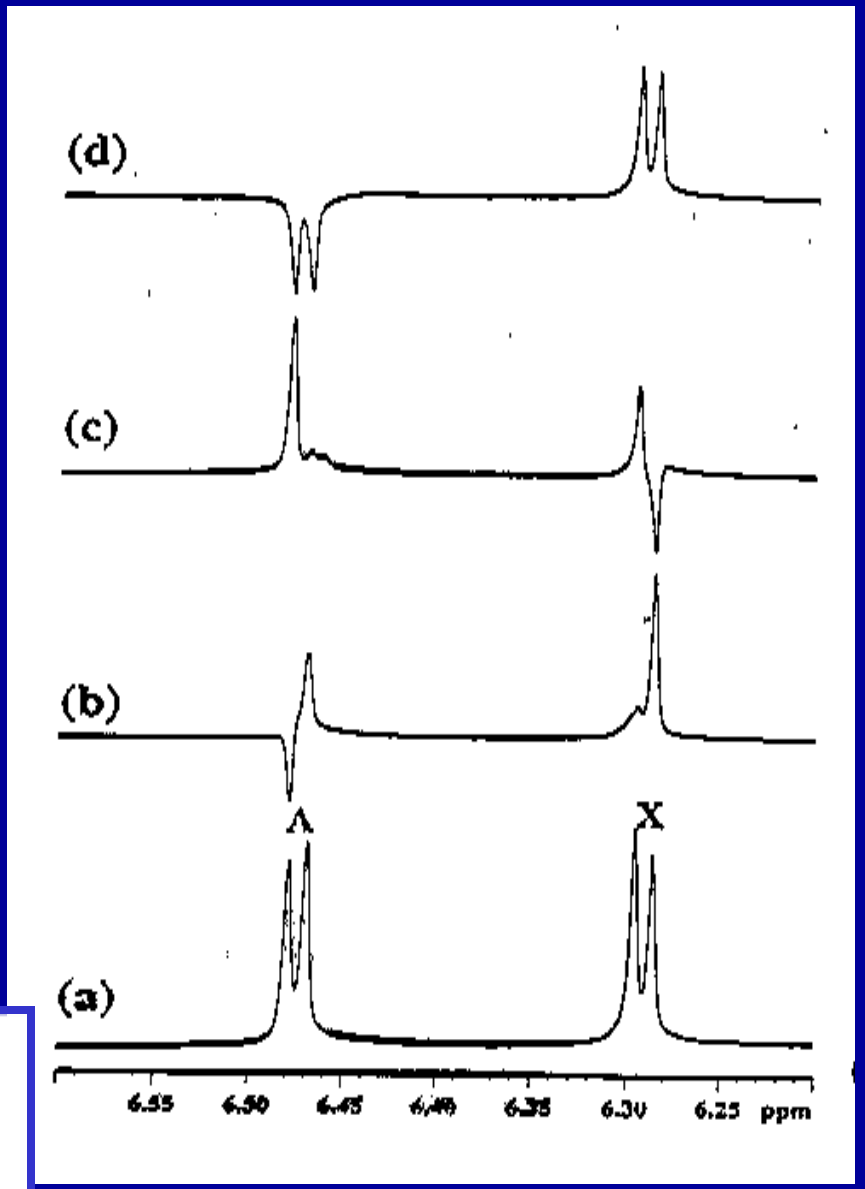


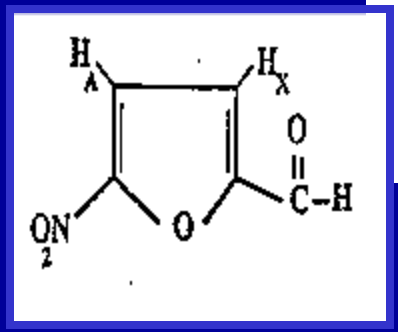
Logic Gates Using 1D NMR

NOT(I_1)

XOR2

XOR1

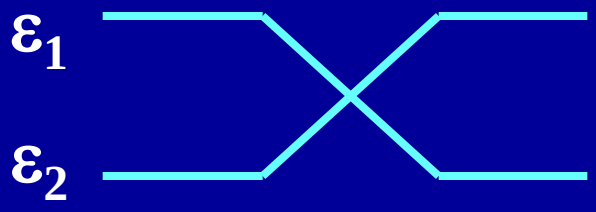


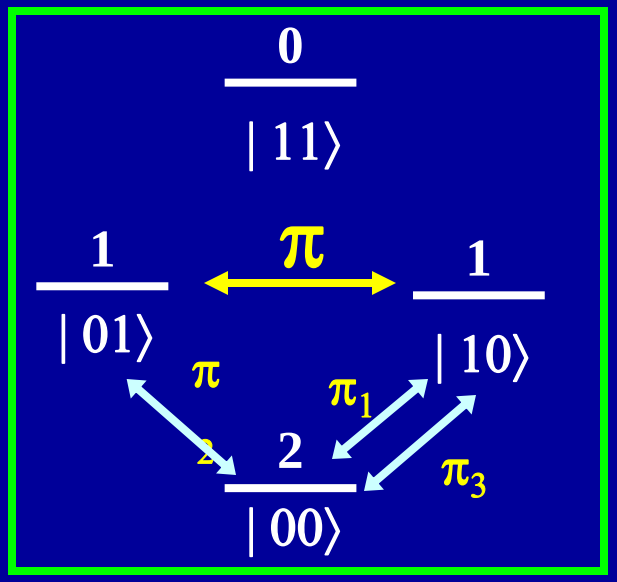


Kavita Dorai, PhD Thesis, IISc, 2000.

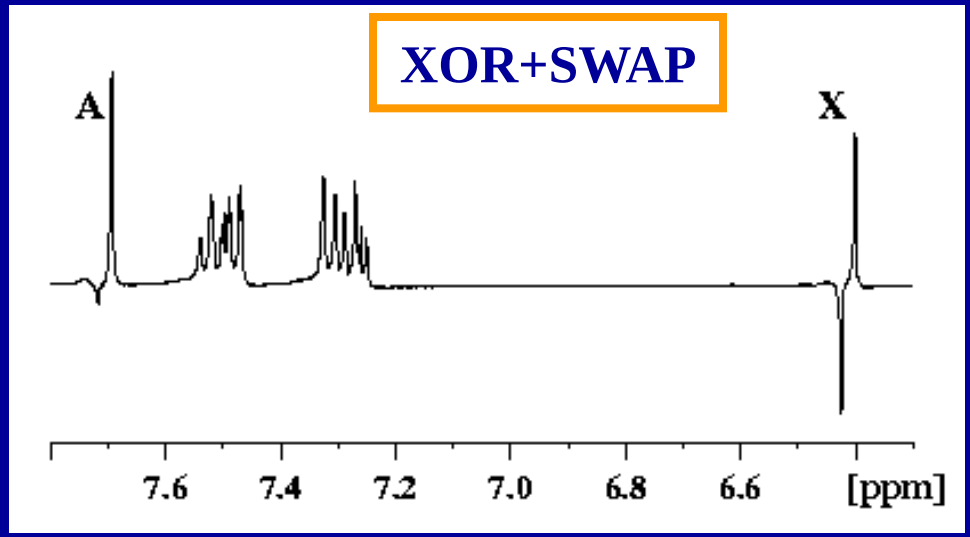
Logical SWAP

$|\varepsilon_1, \varepsilon_2\rangle \rightarrow |\varepsilon_2, \varepsilon_1\rangle$





INPUT	OUTPUT
$\|0\,0\rangle$	$\|0\,0\rangle$
$\|0\,1\rangle$] π	$\|1\,0\rangle$
$\|1\,0\rangle$] π	$\|0\,1\rangle$
$\|1\,1\rangle$	$\|1\,1\rangle$



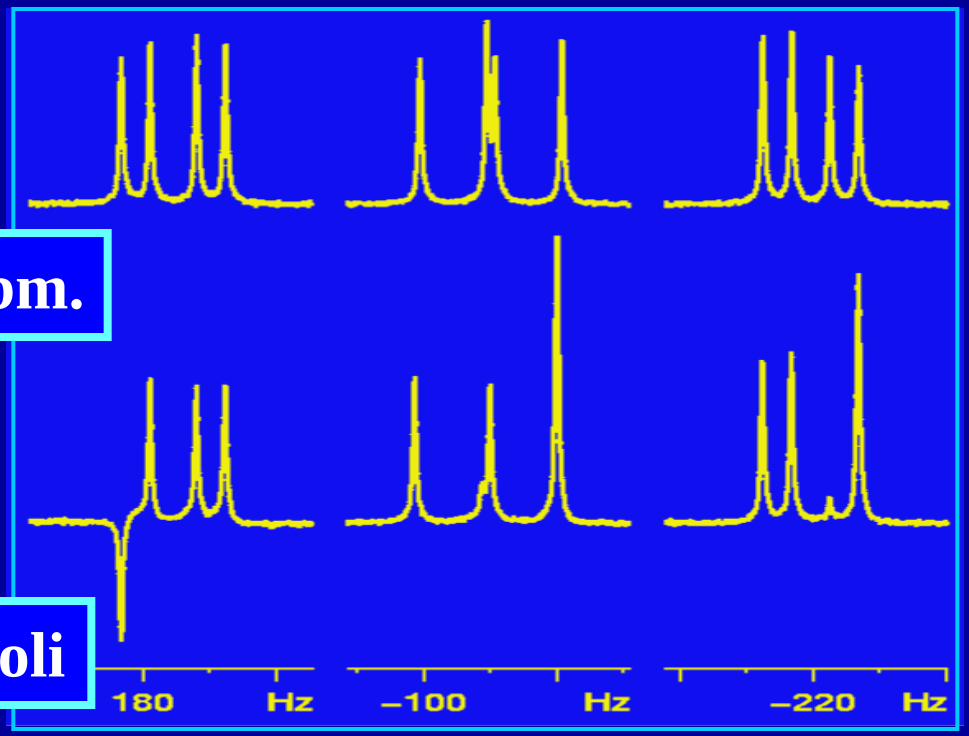
Kavita, Arvind, and Anil Kumar
Phys. Rev. A, 2000, 61, 042306

Toffoli Gate = C^2-NOT

$$|\varepsilon_1, \varepsilon_2, \varepsilon_3\rangle \rightarrow |\varepsilon_1, \varepsilon_2, \varepsilon_3 \oplus (\varepsilon_1 \wedge \varepsilon_2)\rangle$$

	Input	Output
AND	000	000
	001	001
	010	010
	011	111
NAND	100	100
	101	101
	110	110
	111	011

π



Kavita Dorai, PhD Thesis, IISc, 2000.

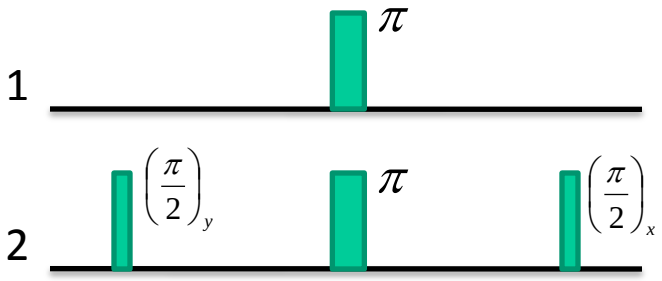
CNOT GATE

$$\rho_{eq} \propto \gamma_1 I_z^1 + \gamma_2 I_z^2$$

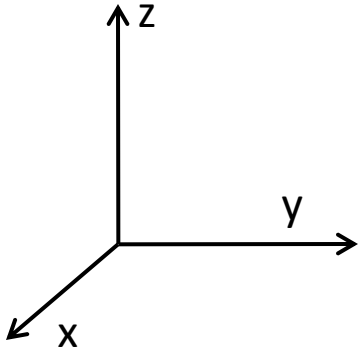
$$\rho_2 = \gamma_1 I_z^1 + \gamma_2 I_x^2$$

$$\rho_3 = \gamma_1 I_z^1 + \gamma_2 \left[-2 I_z^1 I_y^2 \right]$$

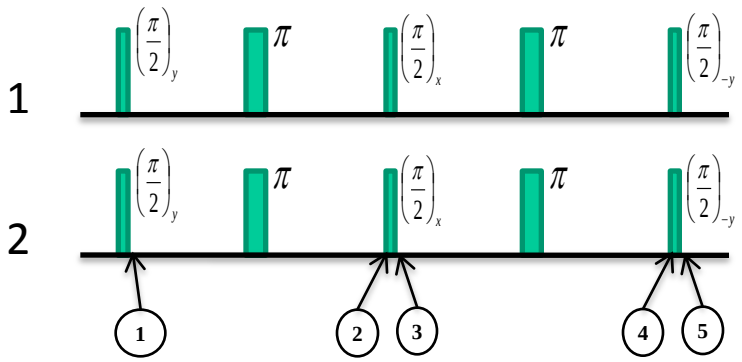
$$\rho_4 = \gamma_1 I_z^1 + \gamma_2 \left[2 I_z^1 I_z^2 \right]$$

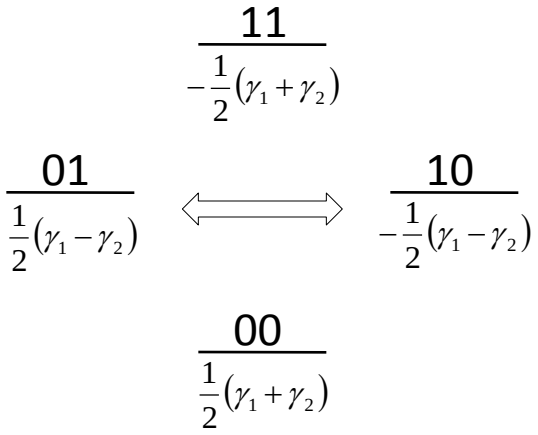


IN	ρ_{eq}	ρ_4	OUT
|00>	$\frac{1}{2}(\gamma_1+\gamma_2)$	$\frac{1}{2}(\gamma_1+\gamma_2)$	|00>
|01>	$\frac{1}{2}(\gamma_1-\gamma_2)$	$\frac{1}{2}(\gamma_1-\gamma_2)$	|01>
|10>	$-\frac{1}{2}(\gamma_1-\gamma_2)$	$-\frac{1}{2}(\gamma_1-\gamma_2)$	|11>
|11>	$-\frac{1}{2}(\gamma_1+\gamma_2)$	$-\frac{1}{2}(\gamma_1+\gamma_2)$	|10>



SWAP GATE





$$\rho_{eq} \propto \gamma_1 I_z^1 + \gamma_2 I_z^2$$

① $\rho_1 = \gamma_1 I_x^1 + \gamma_2 I_x^2$

② $\rho_2 = \gamma_1\left[-2I_y^1 I_z^2\right] + \gamma_2\left[-2I_y^1 I_z^2\right]$

$\Downarrow \left(\frac{\pi}{2}\right)_x^{1,2}$

③ $\rho_3 = \gamma_1\left[2I_z^1 I_y^2\right] + \gamma_2\left[-2I_z^1 I_y^2\right]$

$\Downarrow$ J

④ $\rho_4 = \gamma_1\left[I_x^2\right] + \gamma_2\left[I_x^1\right]$

$\Downarrow \left(\frac{\pi}{2}\right)_{-x}^{1,2}$

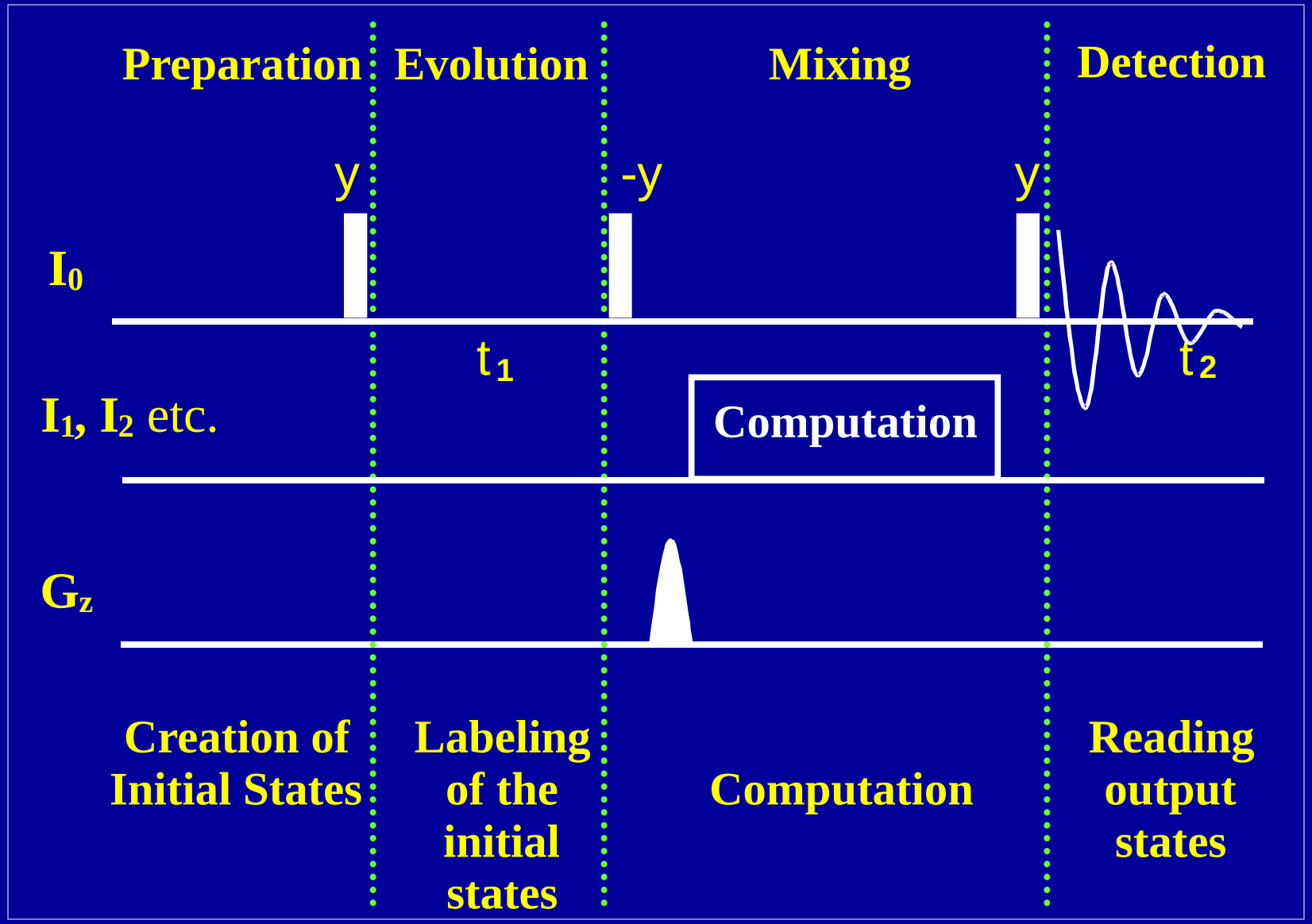
⑤ $\rho_5 = \gamma_1 I_z^2 + \gamma_2 I_z^1$

	>	
|00>	$\frac{1}{2}(\gamma_1+\gamma_2)$	$\frac{1}{2}(\gamma_1+\gamma_2)$
|01>	$\frac{1}{2}(\gamma_1-\gamma_2)$	$-\frac{1}{2}(\gamma_1-\gamma_2)$
|10>	$-\frac{1}{2}(\gamma_1-\gamma_2)$	$\frac{1}{2}(\gamma_1-\gamma_2)$
|11>	$-\frac{1}{2}(\gamma_1+\gamma_2)$	$-\frac{1}{2}(\gamma_1+\gamma_2)$

Cory et al., ~1997

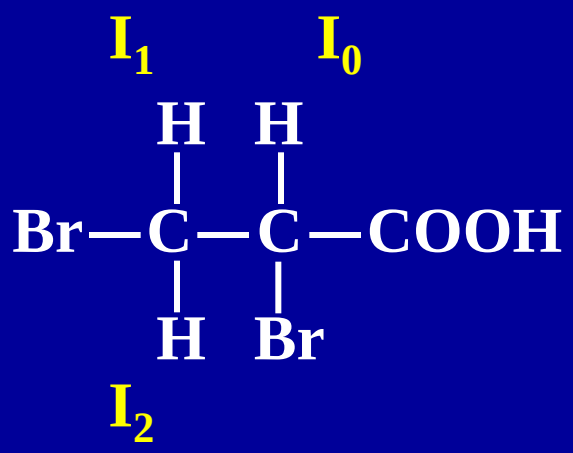
Logic Gates By 2D NMR

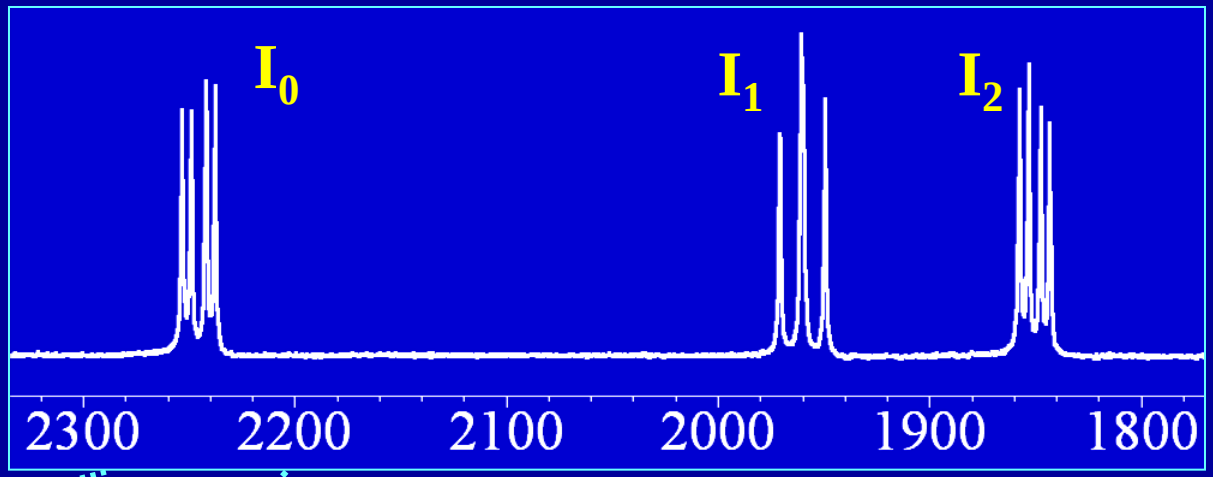
2D NMR Quantum Computing Scheme

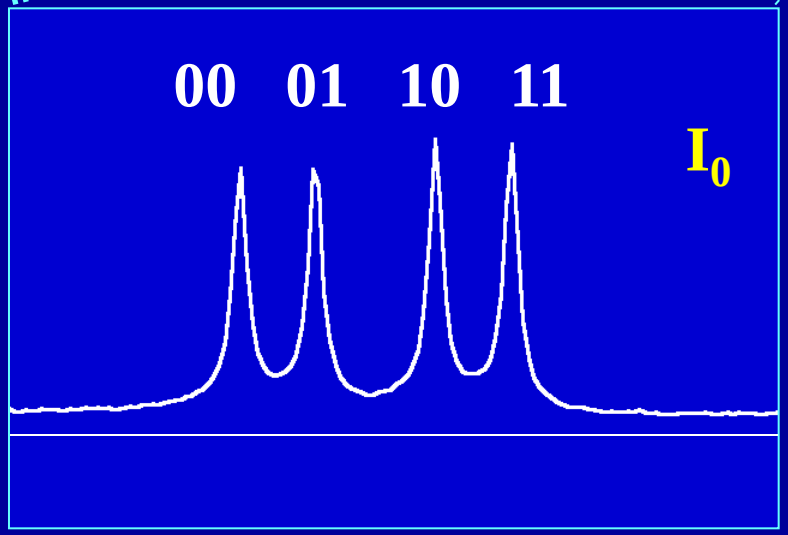


Ernst & co-workers, J. Chem. Phys., 109, 10603 (1998).

Three-spin system:



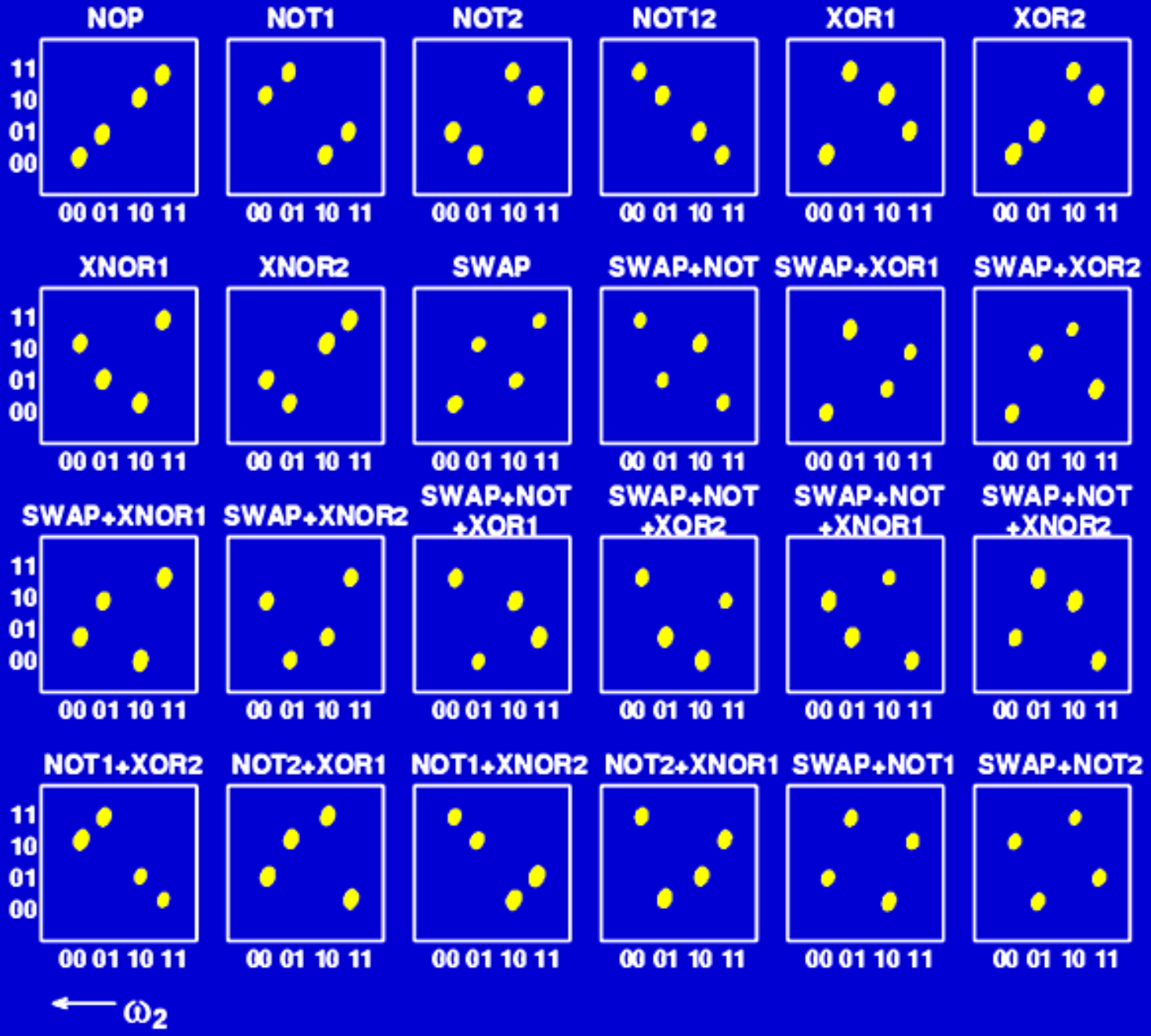




Transitions of I_0 are labeled by the states of I_1 and I_2

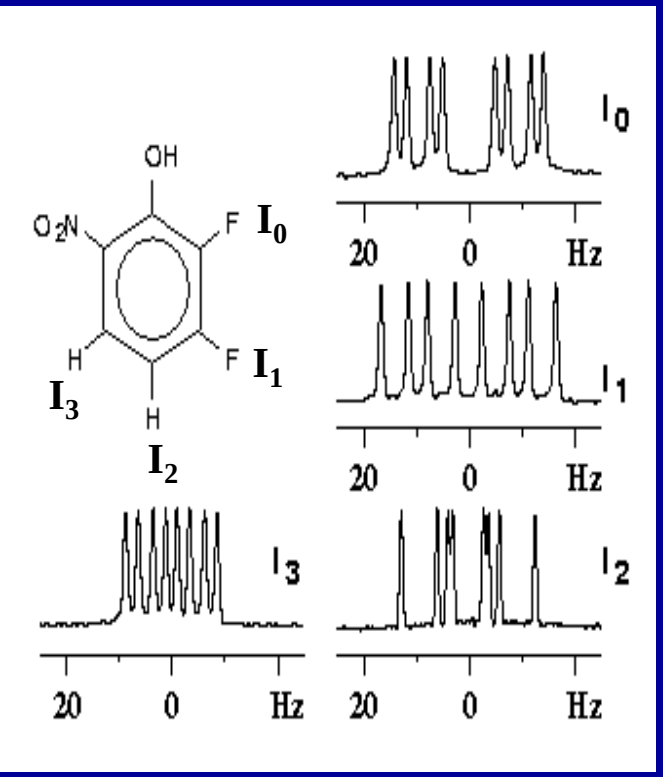
Two-Dimensional Gates

A complete set of 24 Reversible, One-to-one, 2-qubit Gates



T. S. Mahesh, Kavita Dorai, Arvind and Anil Kumar, JMR, 148, 95, (2001)

Three-qubit 2D-Gates:



NOP

NOT1

TOFFOLI

OR/NOR

INPUT

ω_1

111
110
101
100
011
010
001
000

ω_2

OUTPUT

T. S. Mahesh,et al, JMR,148, 95, 2001

Quantum Algorithms

(a) DJ

(b) Grover's Search

DJ algorithm on ONE qubit with one work bit:

x	Constant		Balanced	
	$f_1(x)$	$f_2(x)$	$f_3(x)$	$f_4(x)$
0	0	1	0	1
1	0	1	1	0

$$|x\rangle|y\rangle \xrightarrow{U_f} |x\rangle|y \oplus f(x)\rangle$$

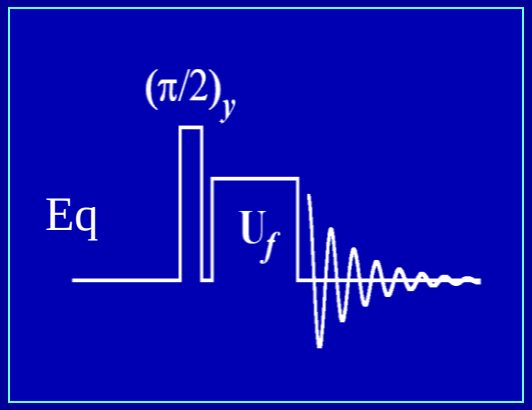
Cleve Version

$|x\rangle$ is input qubit and $|y\rangle$ is work qubit

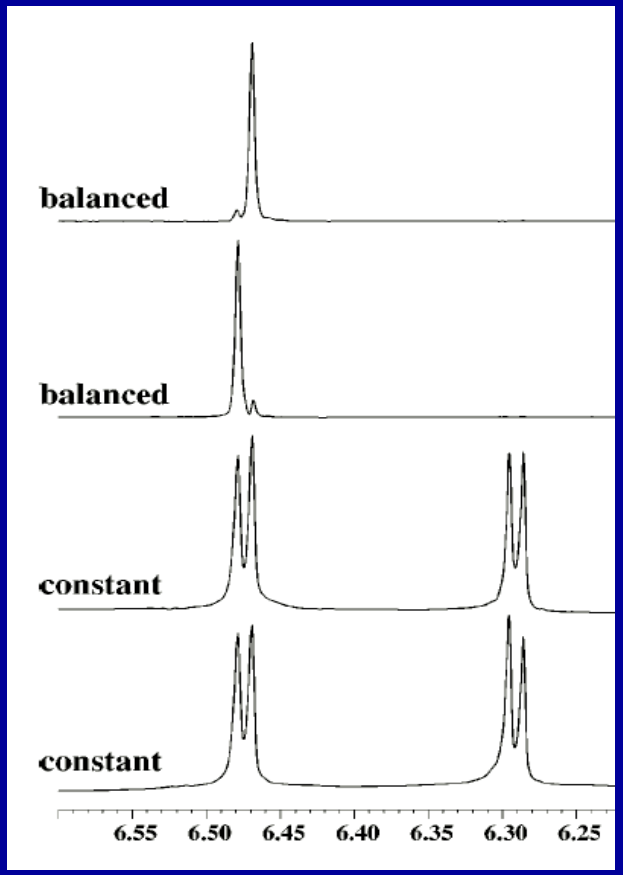
I/P		O/P							
		Constant				Balanced			
x	y	$f_1(x)$	$y \oplus f_1(x)$	$f_2(x)$	$y \oplus f_2(x)$	$f_3(x)$	$y \oplus f_3(x)$	$f_4(x)$	$y \oplus f_4(x)$
0	0	0	0	1	1	0	0	1	1
0	1	0	1	1	0	0	1	1	0
1	0	0	0	1	1	1	1	0	0
1	1	0	1	1	0	1	0	0	1
Operator	U_f	$\begin{pmatrix} 1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1 \end{pmatrix}$		$\begin{pmatrix} 0&1&0&0\\1&0&0&0\\0&0&0&1\\0&0&1&0 \end{pmatrix}$		$\begin{pmatrix} 1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0 \end{pmatrix}$		$\begin{pmatrix} 0&1&0&0\\1&0&0&0\\0&0&1&0\\0&0&0&1 \end{pmatrix}$	
U_f		1		NOT-2		C-NOT-1,2		C-NOT-2,1	

Deutsch-Jozsa Algorithm

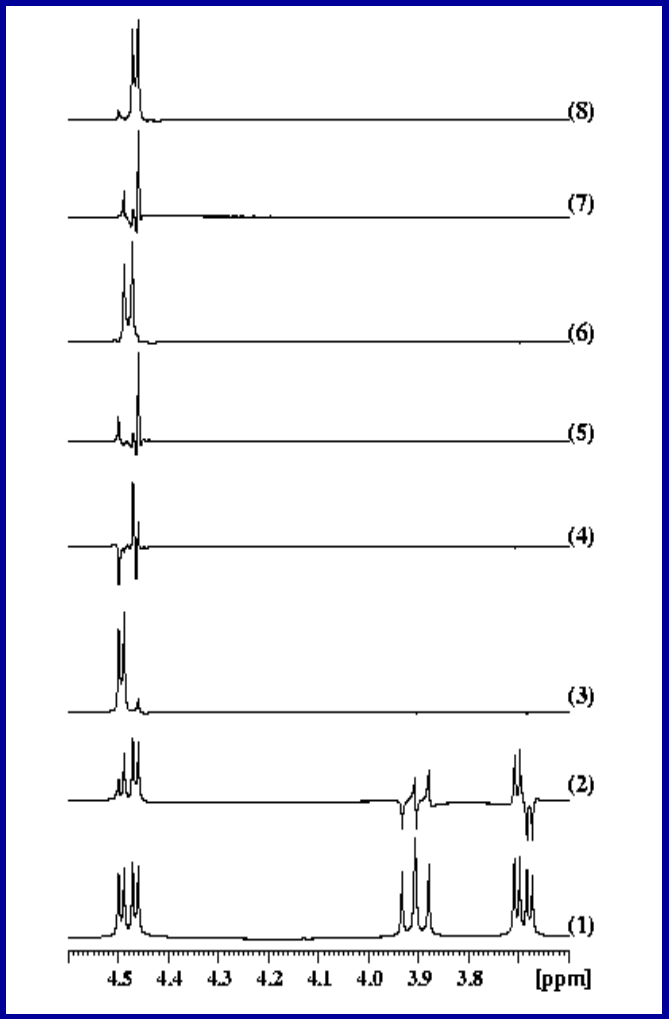
Experiment



One qubit DJ



Two qubit DJ



Kavita, Arvind, Anil Kumar,
Phys. Rev. A 61, 042306 (2000)

Grover's Algorithm

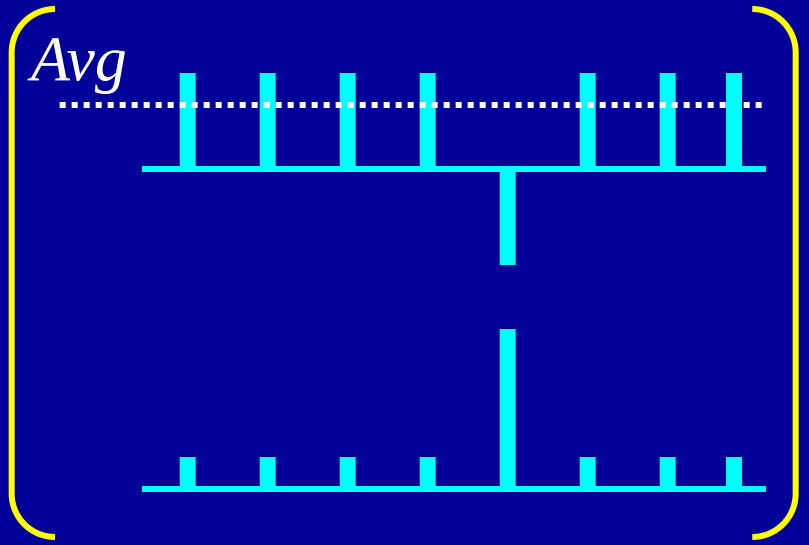
Steps:

Pure State

Superposition

Selective
Phase Inversion

Inversion about
Average



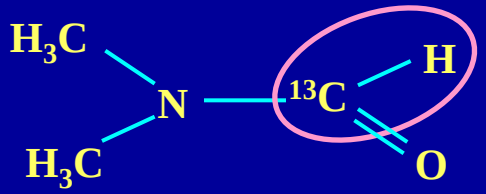
Grover iteration

√N times

Measure

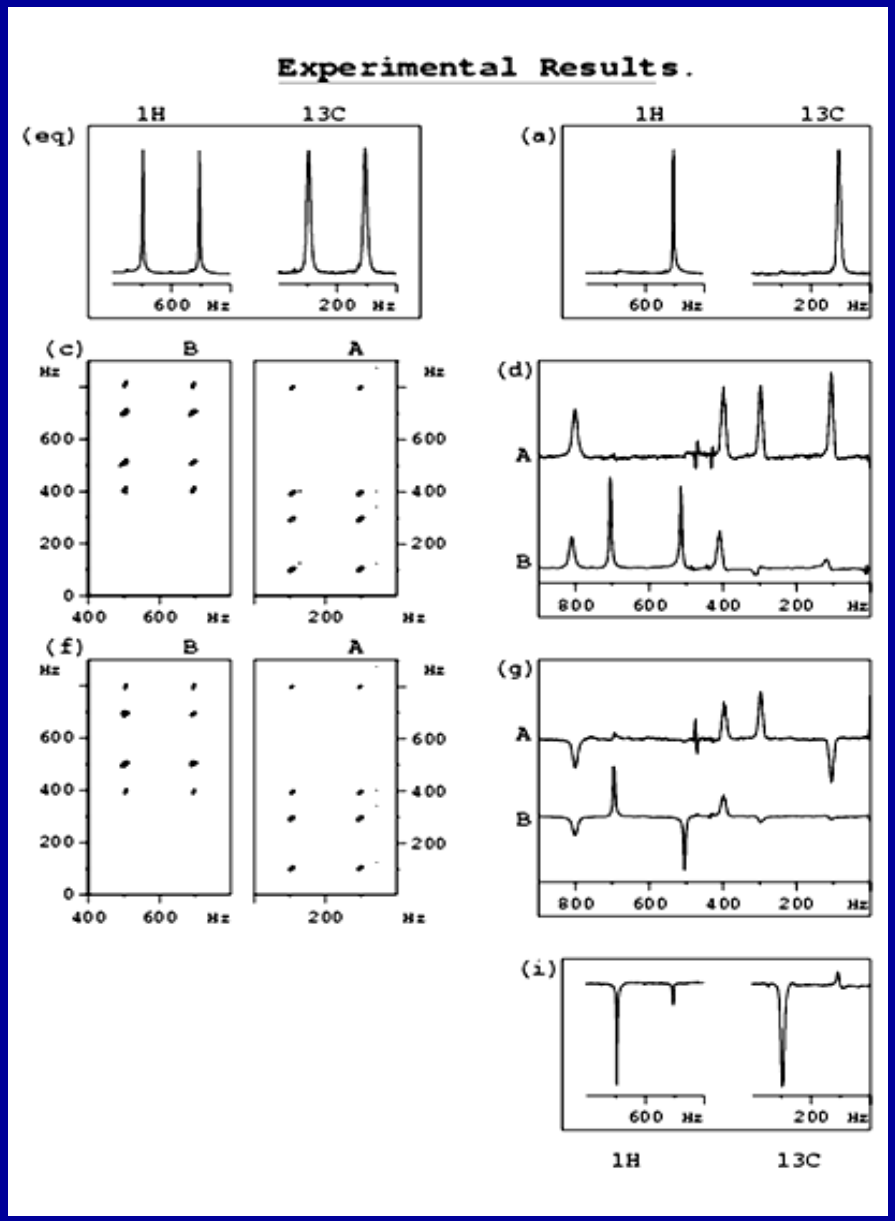
Grover's search algorithm by Tomography of the Density Matrix using 2D NMR

2-qubitComputer
(N,N-dimethyl formamide)



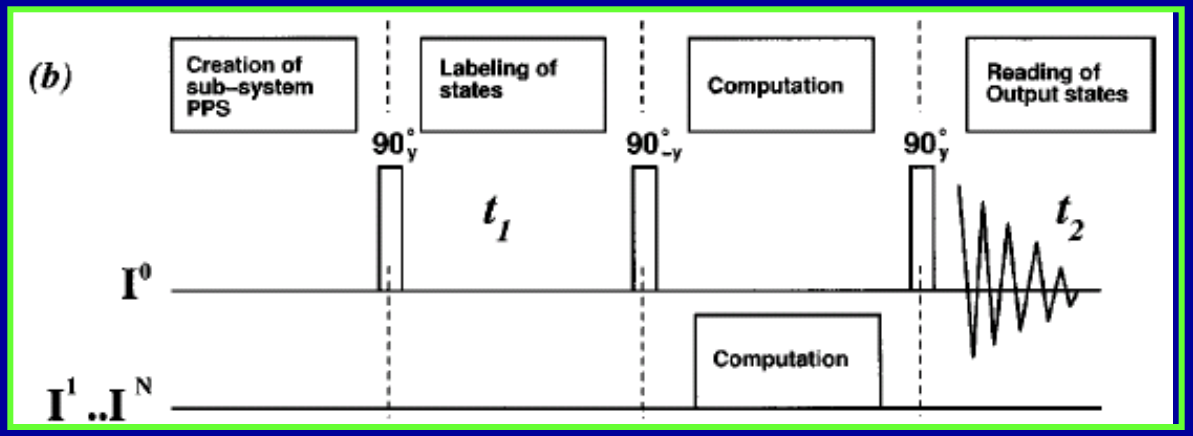
^{13}C : T_1=15s ; ^{1}H: T_1= 5s

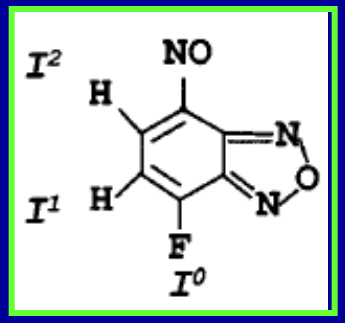
(eq)-Equilibrium spectra.
(a) - PPS (00).
(c),(d) -Uniform superposition.
(f),(g) – Conditional state flip.
(i) – Searched state (11).

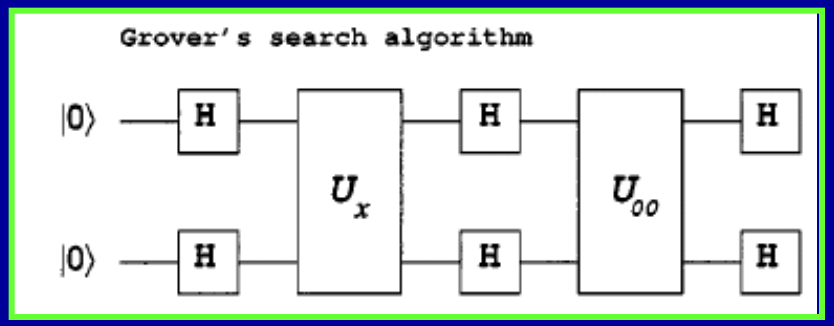


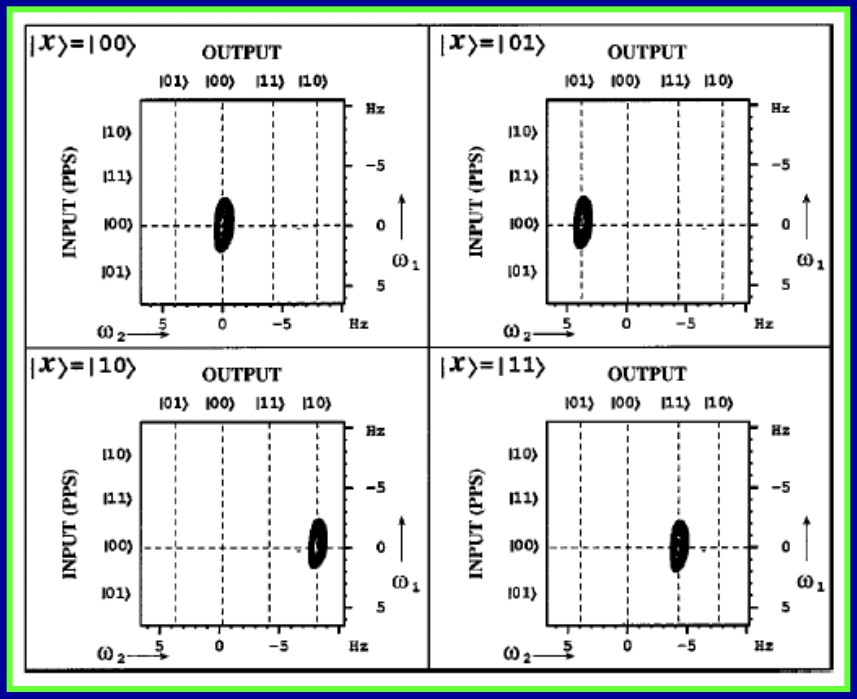
Das et al, Phys. Rev A 67, 062304 (2003)
Das et al, Chem Phys. Lett., 369, 8 (2003)

Grover search algorithm using 2D NMR





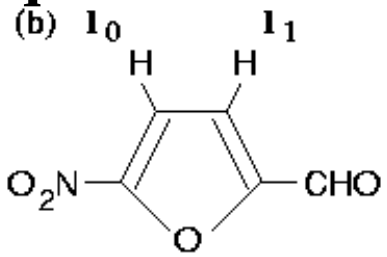




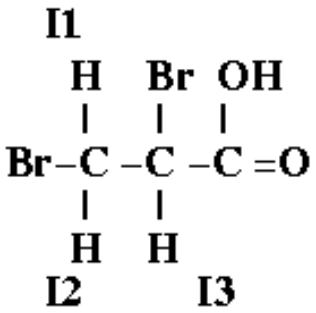
Ranabir Das and Anil Kumar, J. Chem. Phys. **121**, 7603(2004)

Typical systems used for NMR-QIP using J-Couplings

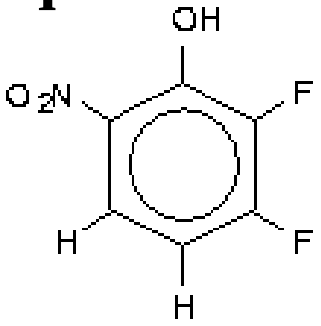
2 qubits

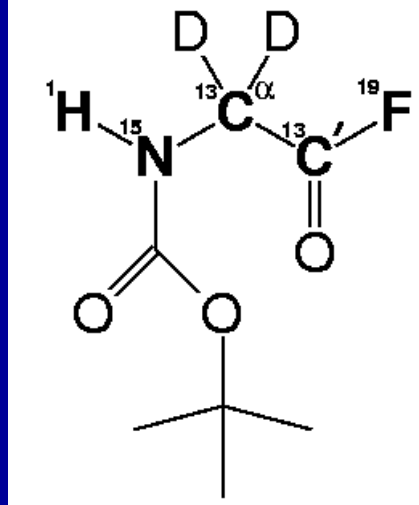


3 qubits



4 qubits

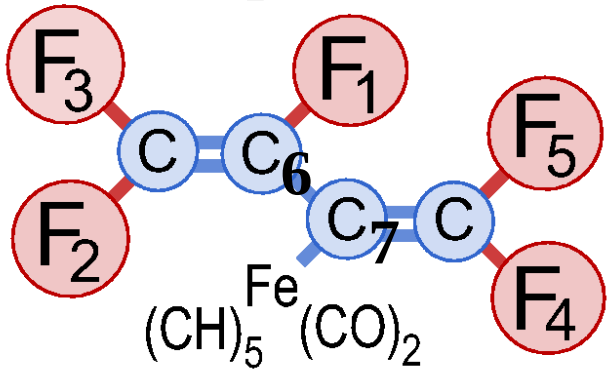




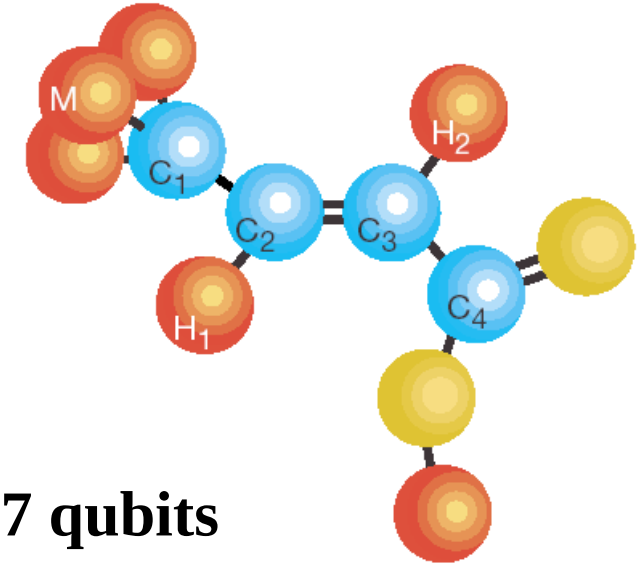
5 qubits

Chuang et al, quant-ph/0007017

7 qubits



Marx et al, Phys. Rev. A 62, 012310 (2000)



7 qubits

Knill et al, Nature, 404, 368 (2000)

How to increase the number of qubits?

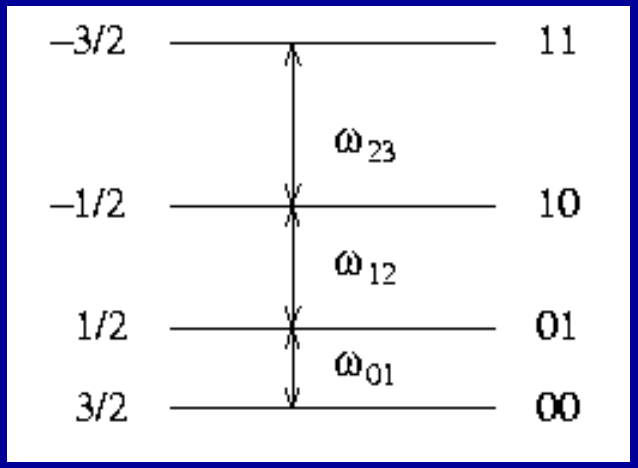
Use Molecules Partially Oriented (~ 10^{-3})
in Liquid Crystal Matrices

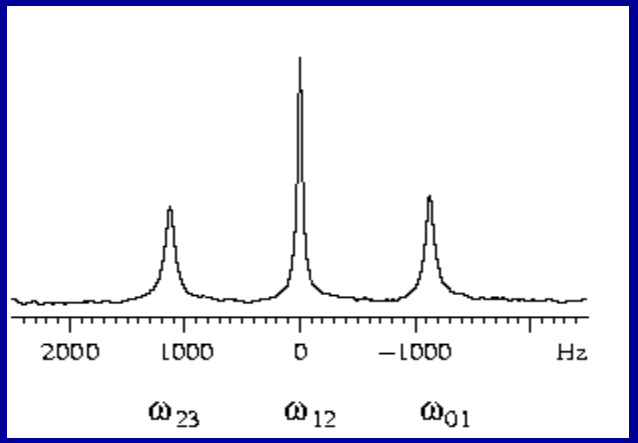
(i) Quadrupolar Nuclei (spin >1/2). Reduced Quadrupolar Couplings

(ii) Spin =1/2 Nuclei. Reduced Intramolecular Dipolar Couplings

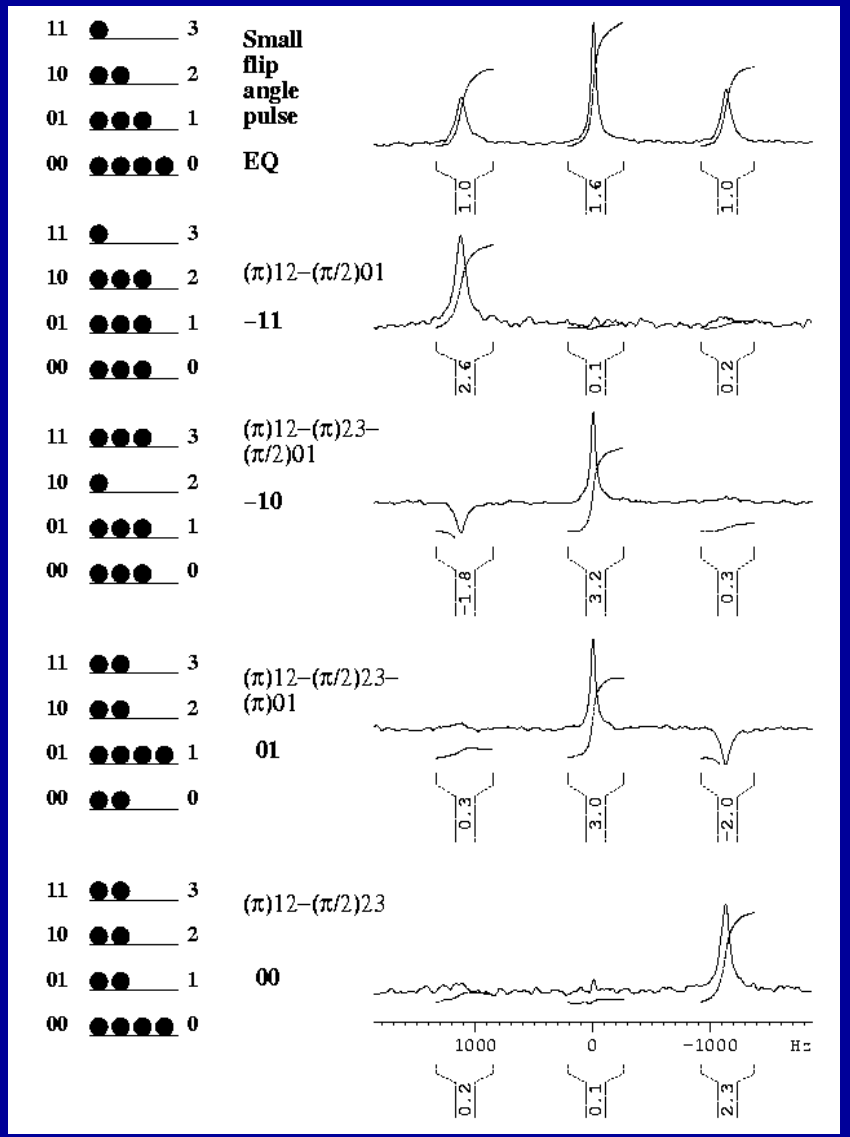
Quadrupolar Systems

Using spin-3/2 (^{7}Li) oriented system as 2-qubit system



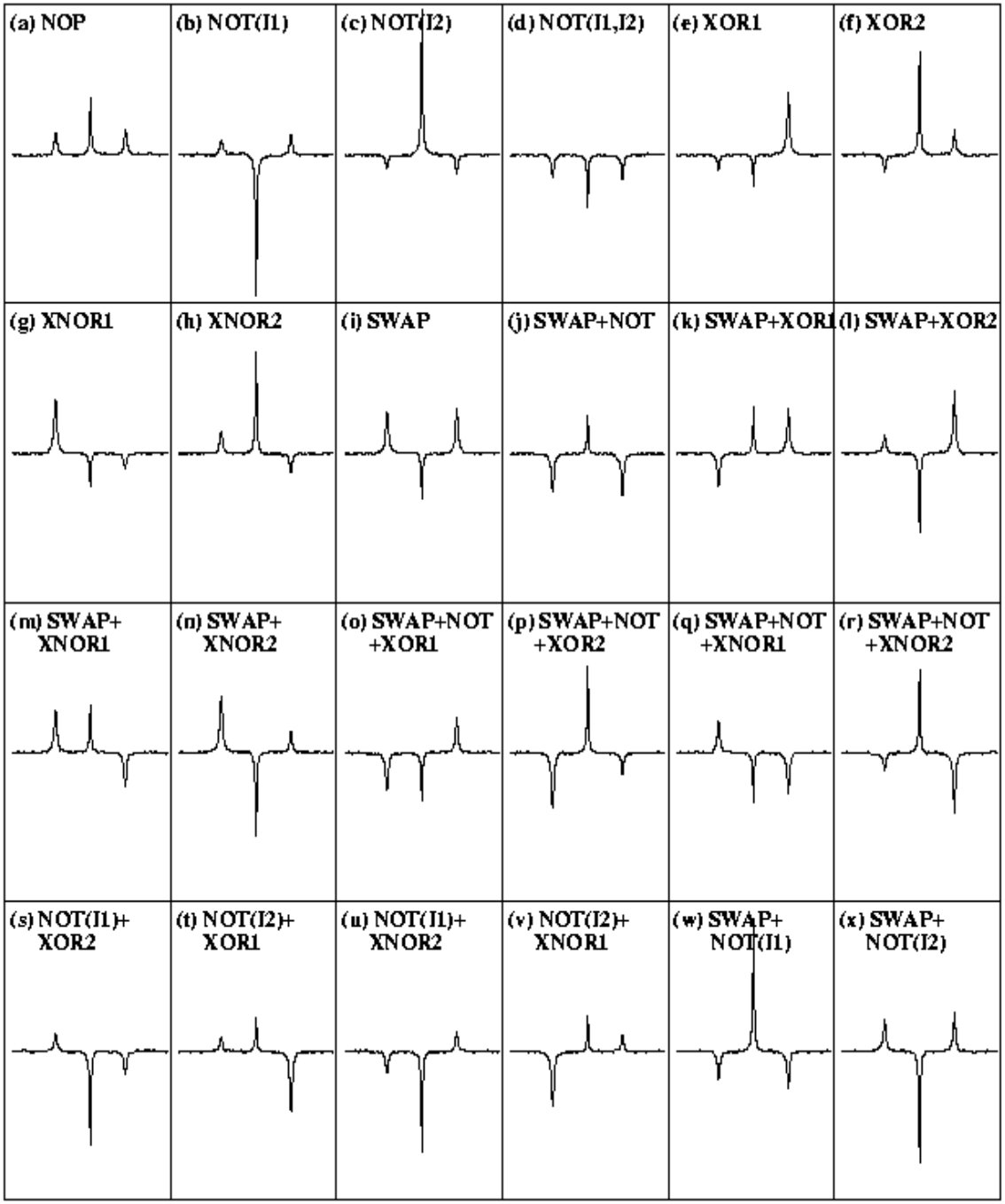


Pseudo-pure states



Neeraj Sinha,T. S. Mahesh, K. V. Ramanathan, and Anil Kumar, ***JCP, 114, 4415 (2001).***

2-qubit Gates using ^{7}Li oriented system

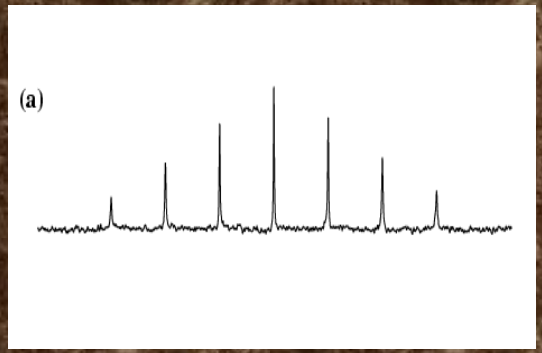


Neeraj Sinha,
T. S. Mahesh,
K. V. Ramanathan,
and Anil Kumar,
JCP, 114, 4415 (2001).

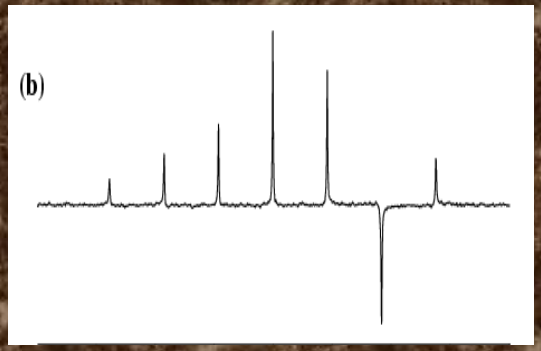
^{133}Cs system – spin 7/2 system

[Cs pentadeca-fluoro-octonate + D_2O]

Equilibrium

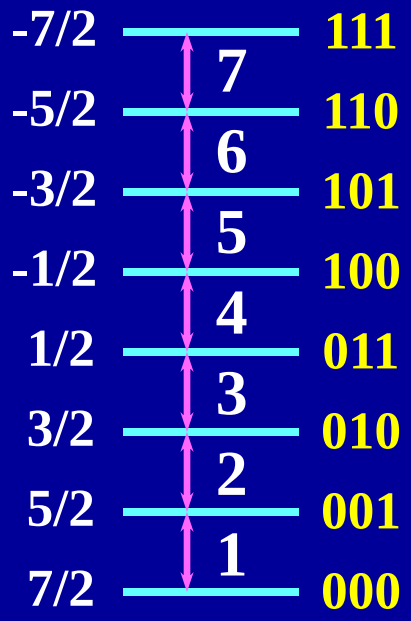


Half-Adder



Subtractor

Conventional Labeling



Half-Adder

π(5,6,5,7,6)

5-pulses

Subtractor

π(3,2,3,5,4,3,2,5,7)

9-pulses

Optimal Labeling

Half-Adder

π(1,3,2)

3-pulses

Subtractor

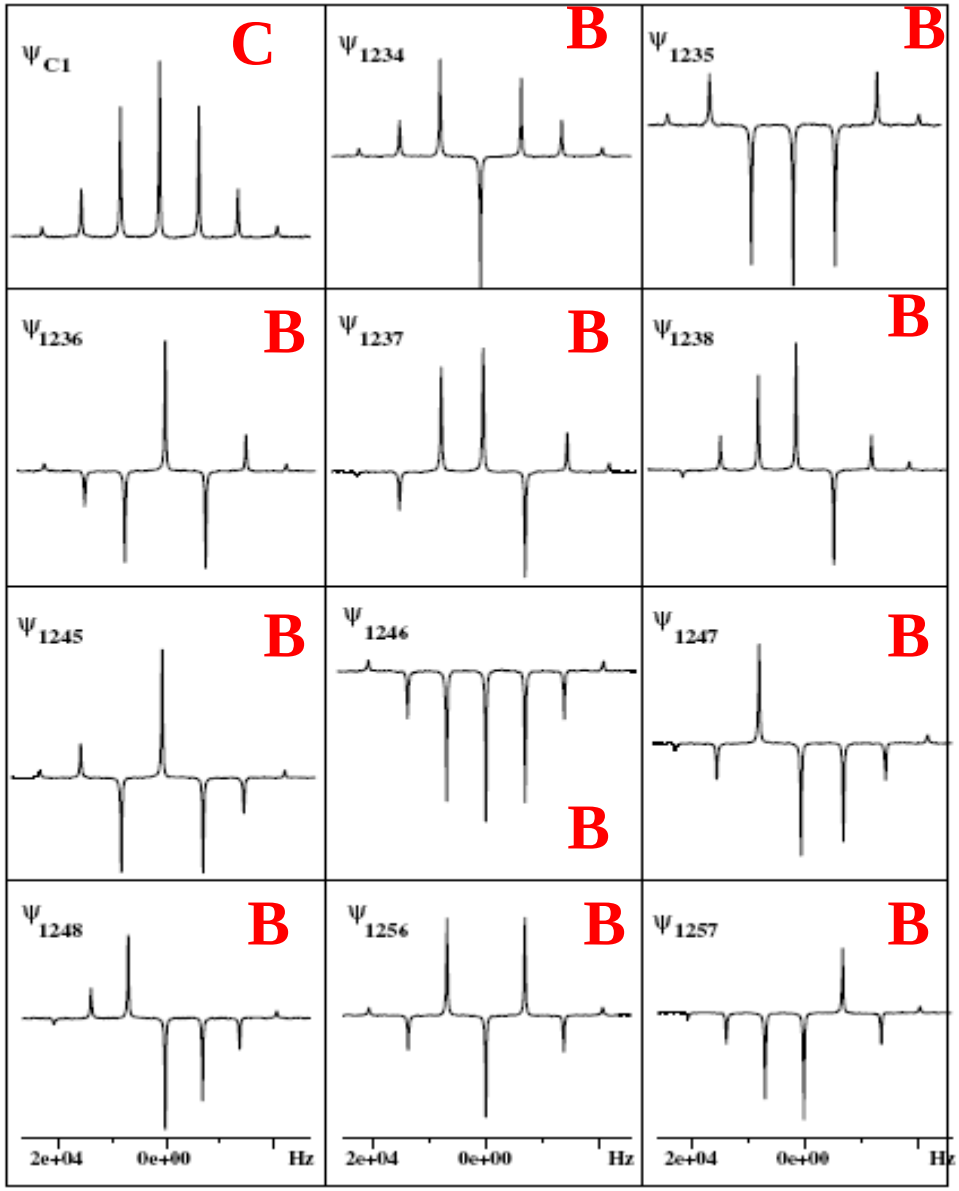
π(6,4,2)

3-pulses

Murali et.al. Phys. Rev. A. 022313 (2003)

R. Das et al, PRA 012314 (2004)

Collins version of 3-qubit DJ implemented on the 7/2 spin of Cs-133.



There are 2 constant and 70 Balanced functions. Half differ in phase of the Unitary transform.

12 are shown here.

1-Constant and 11-Balanced

Gopinath and Anil Kumar, JMR, 193, 163 (2008)

Dipolar Systems

Advantages of Oriented Molecules

- Large Dipolar coupling - ease of selectivity - smaller Gate time
- Long-range coupling - more qubits

Disadvantage

For Homo-nuclear spin system

~~Weak coupling Approximation~~

~~$|\omega_i - \omega_j| >> D_{ij}$~~

Spins become Strongly coupled

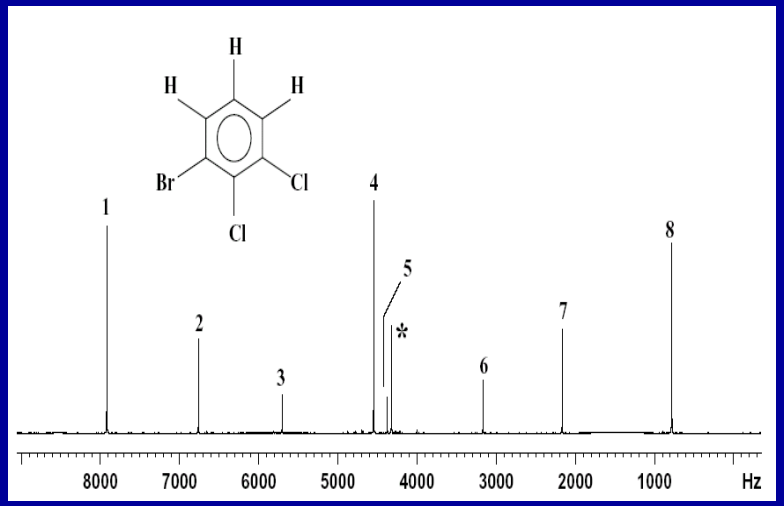
A spin can not be identified as a qubit

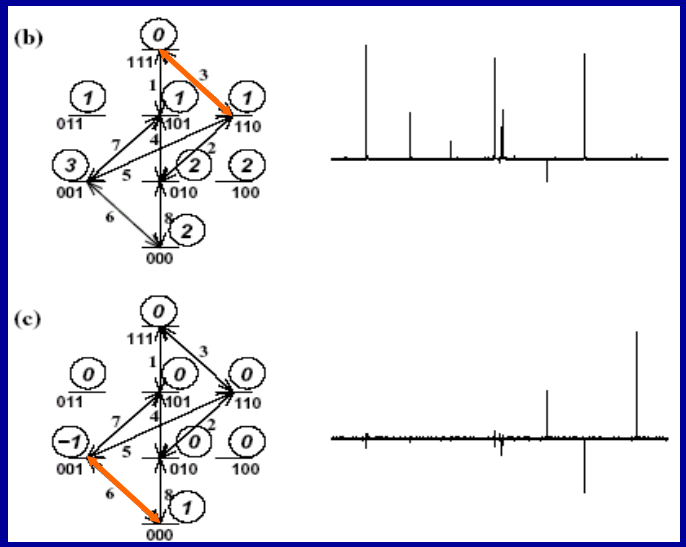
Solution

2^N energy levels are collectively treated as an N-qubit system

3-Qubit Strongly Dipolar Coupled Spin System

Bromo-di-chloro-benzene



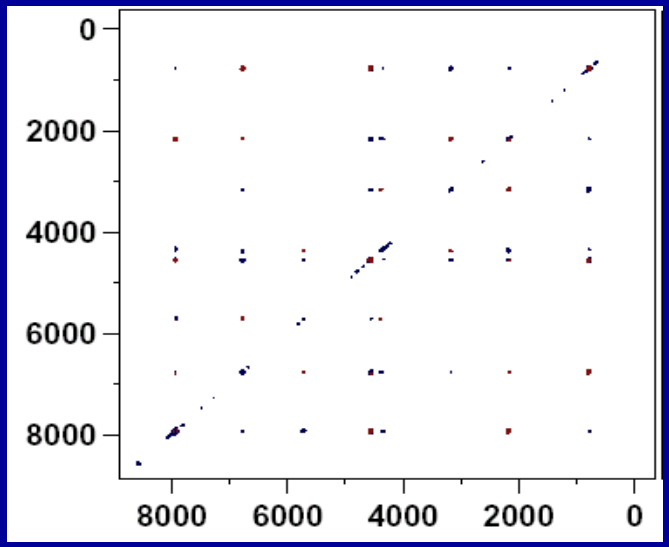


C^2-NOT gate

($|110\rangle \rightarrow |111\rangle$)

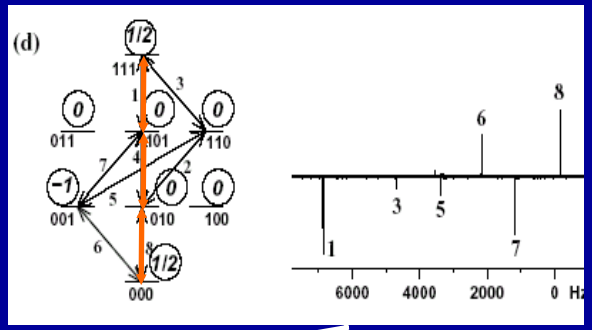
POPS

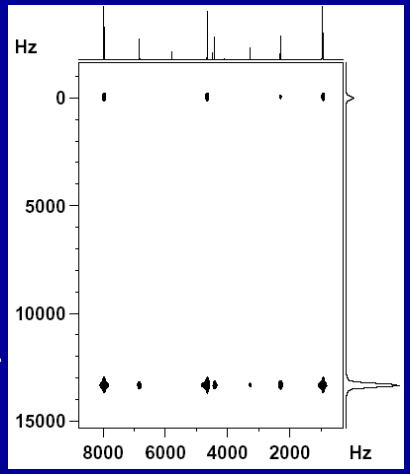
($|000\rangle\langle 000| - |001\rangle\langle 001|$)



Z-COSY ($90\text{-}t_1\text{-}10\text{-}\tau_m\text{-}10\text{-}t_2$) was used to label the various transitions

GHZ state ($|000\rangle + |111\rangle$)



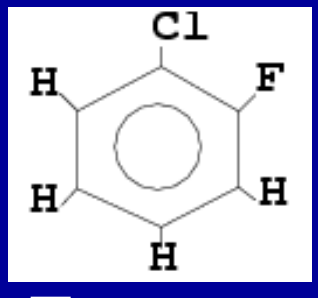


populations

coherences

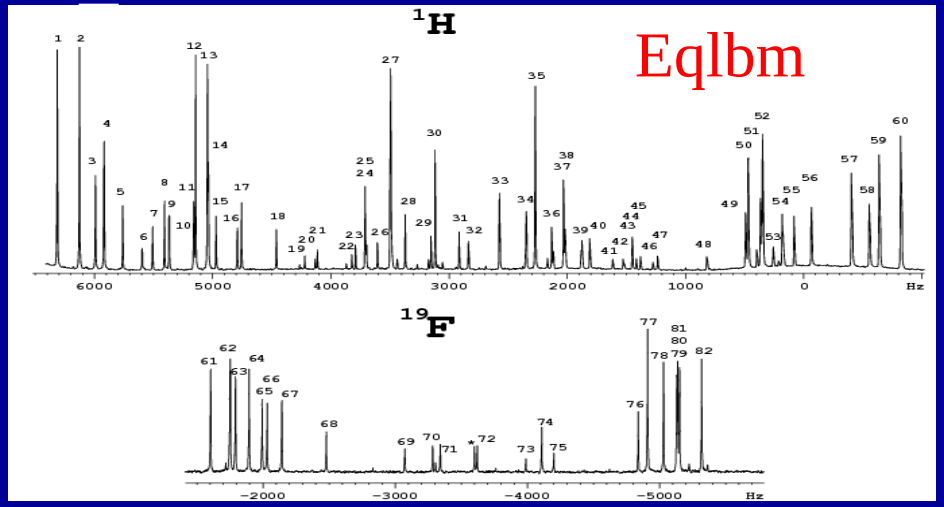
T.S. Mahesh et.al., Current Science ***85***, 932 *(2003).*

5-qubit system

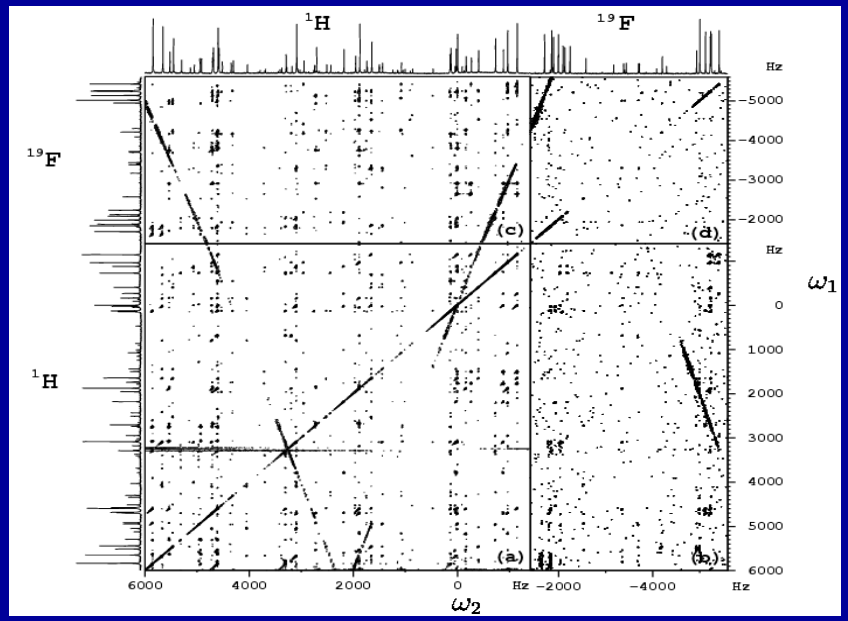


(in liquid crystal)

Eqlbm

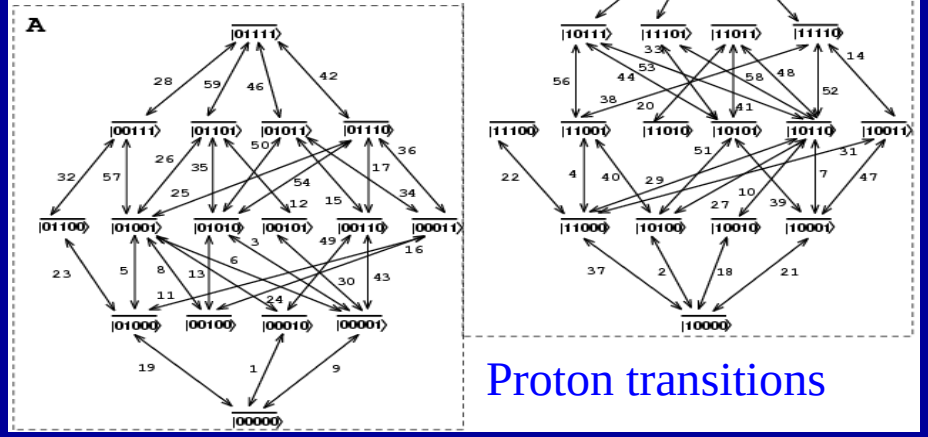


HET-Z-COSY spectrum for labeling



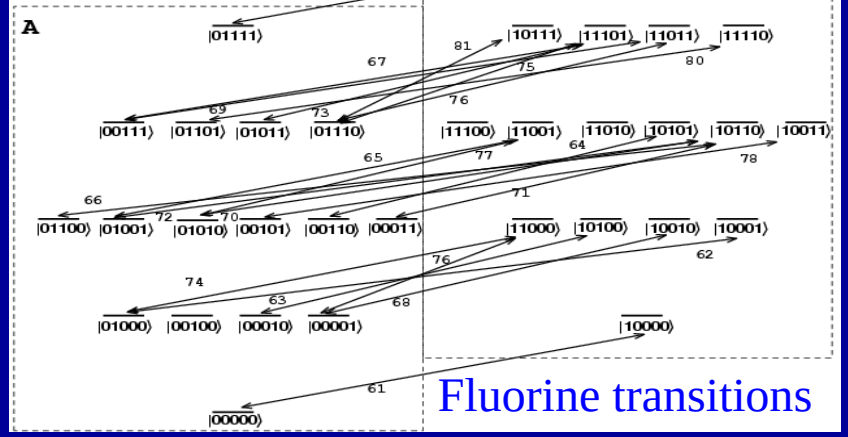
(a)

E-level diagram



Proton transitions

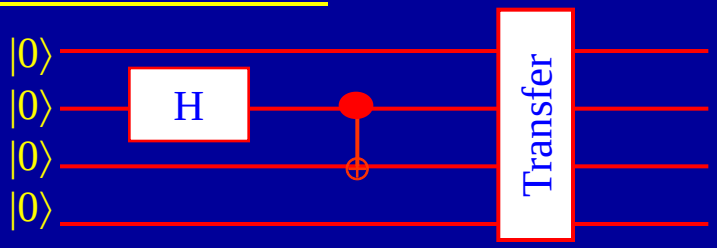
(b)



Fluorine transitions

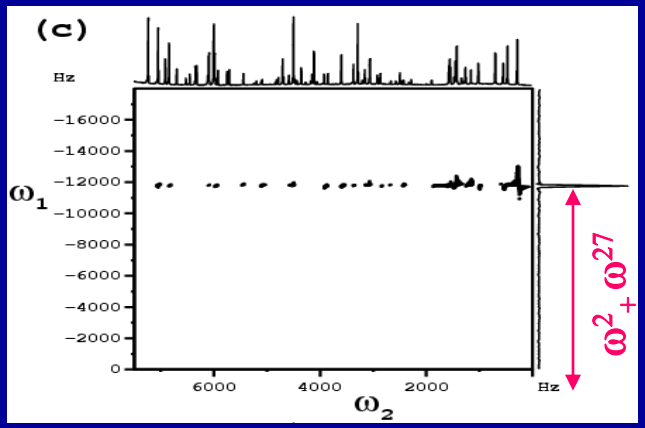
Entanglement transfer

Starting from 4-qubit PPS prepared by SAALT:



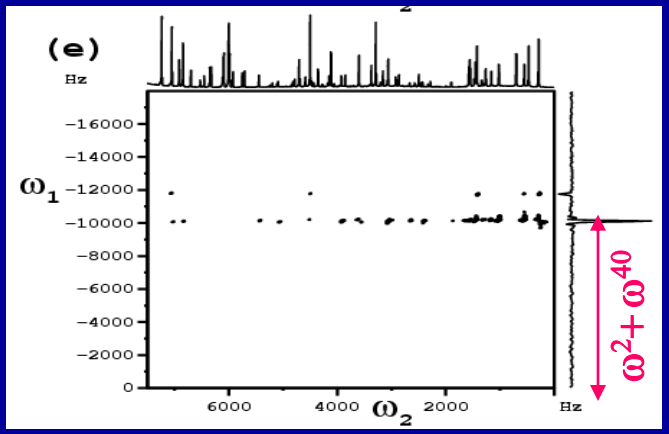
Entanglement between 2nd and 3rd qubit

|0000⟩+ |0110⟩



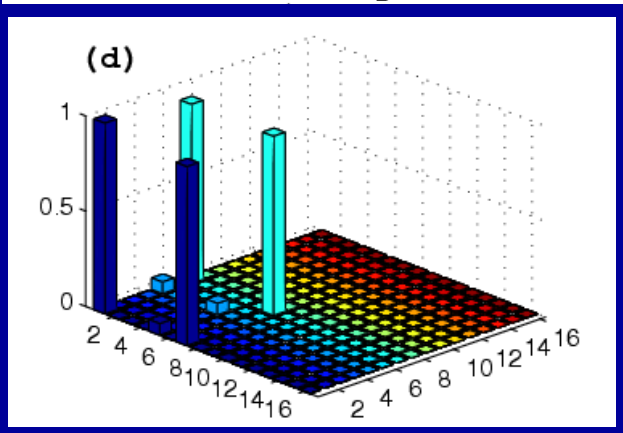
$(\pi)^{27}(\pi)^{40}$

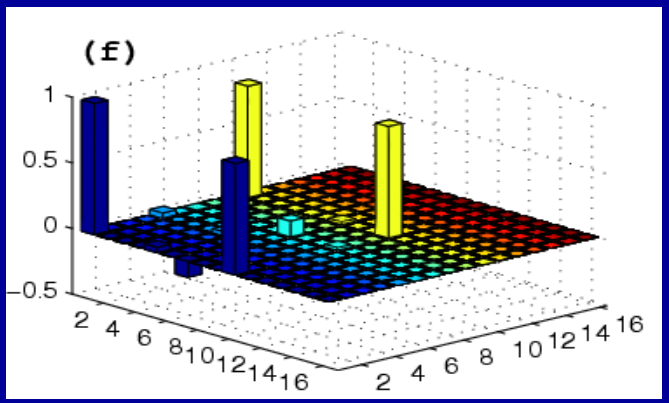
$(\pi)^{27}$



Entanglement between 1st and 4th qubit

|0000⟩+ |1001⟩

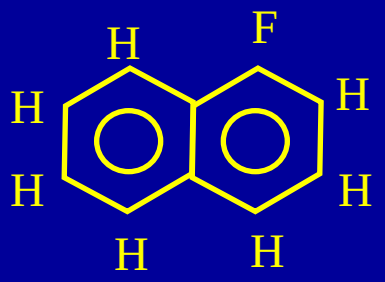




Ranabir Das , Rangeet Bhattacharya and Anil Kumar, JMR. 170, 310-321 (2004).

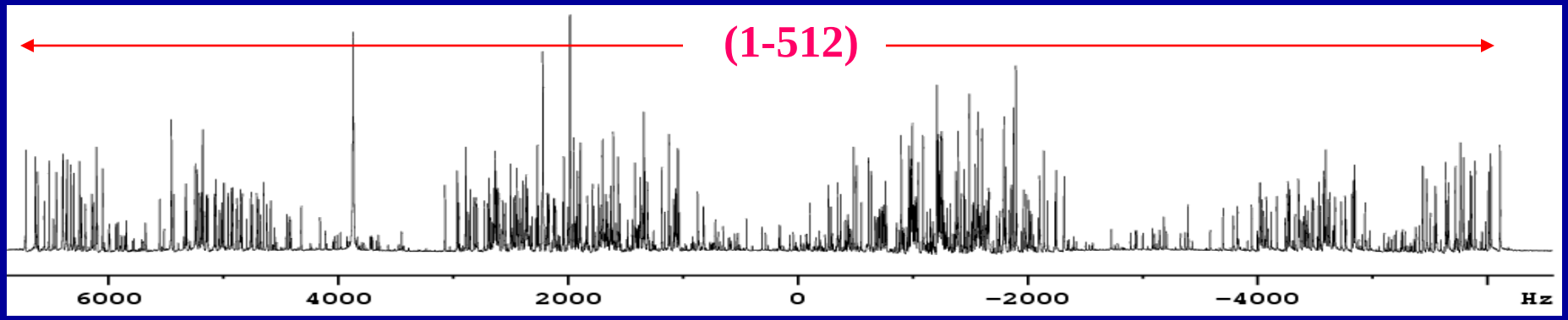
8-qubit system

Molecule: 1-floro naphthalene
(in liquid crystal ZLI1132)

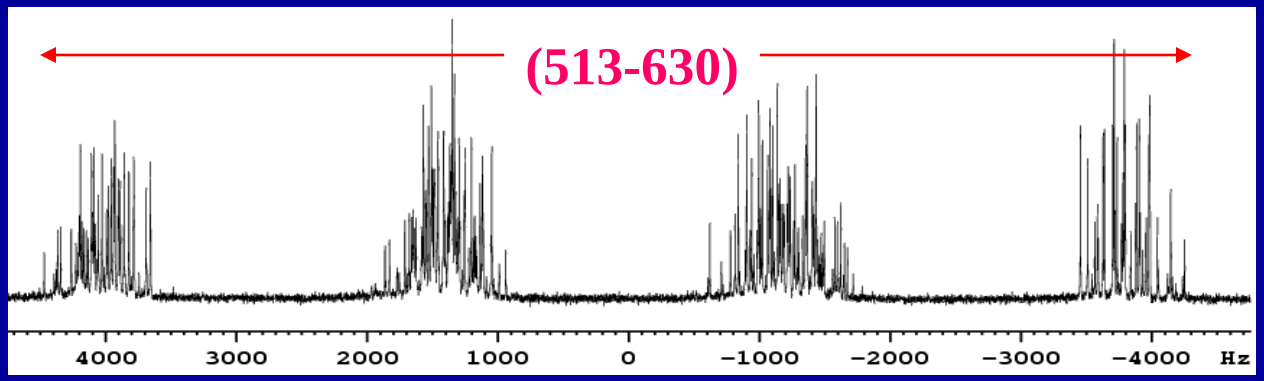


Equilibrium spectrum

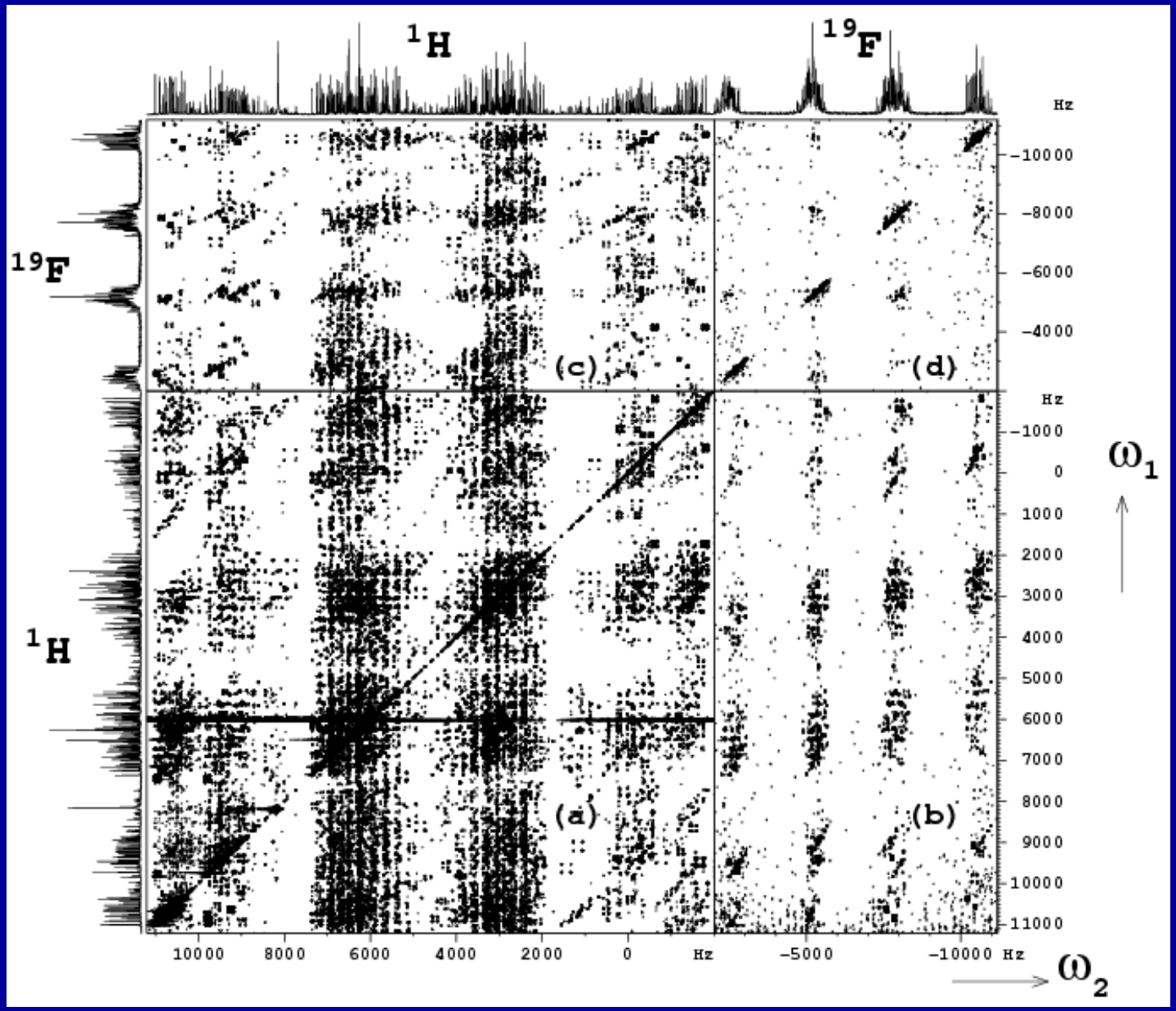
^{1}H spectrum



^{19}F spectrum



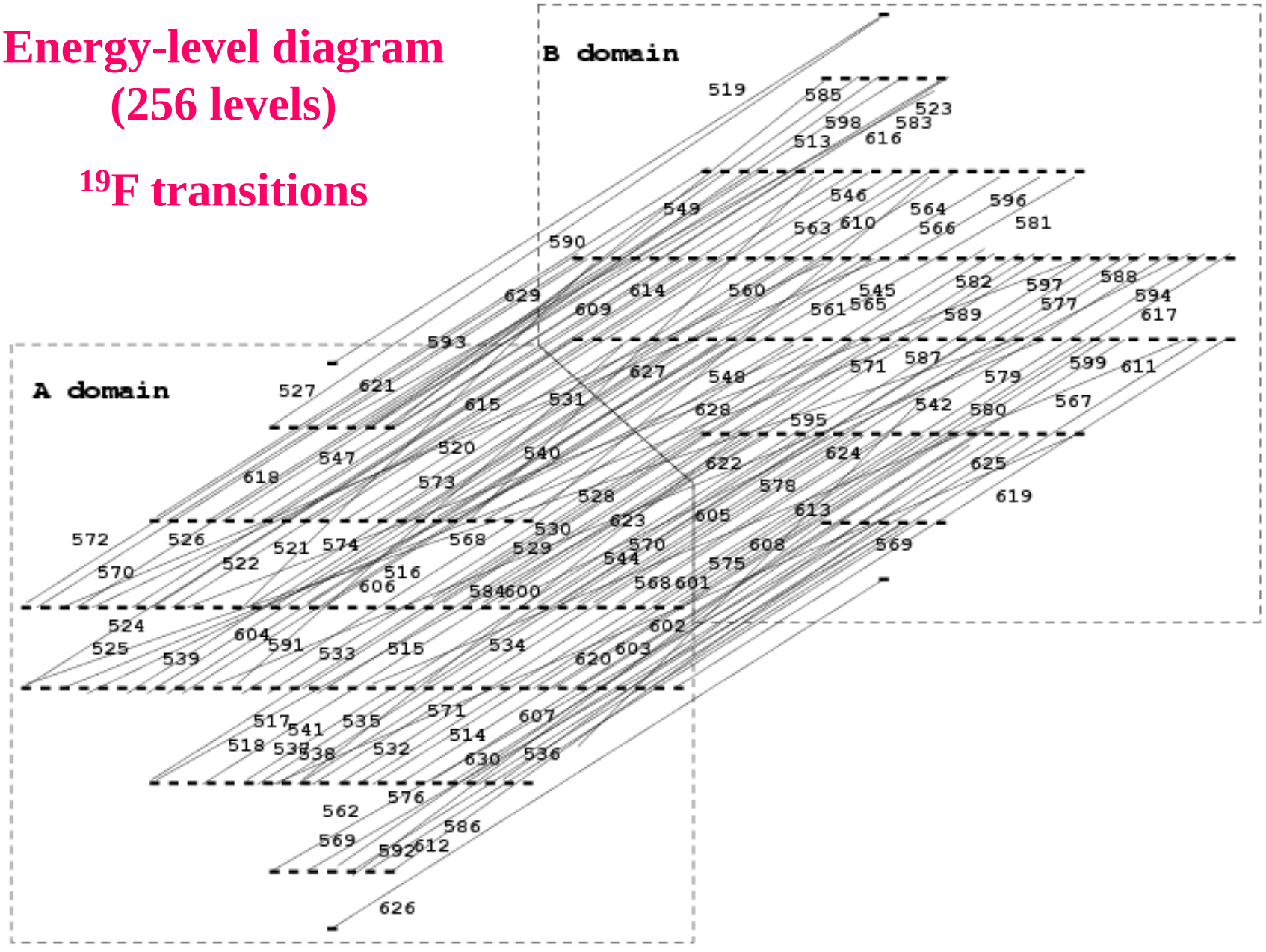
HET-Z-COSY spectrum

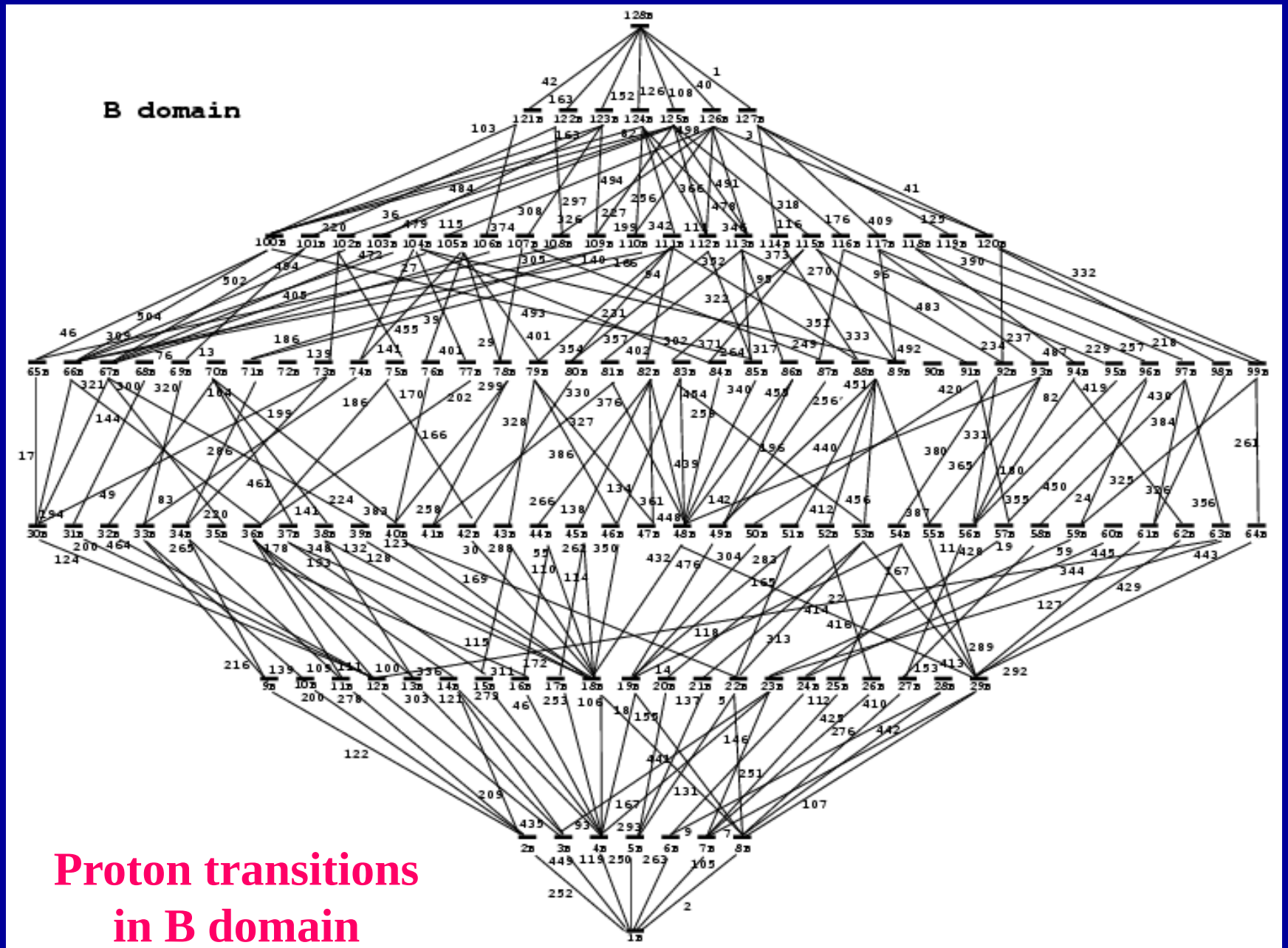


R. Das, R Bhattacharyya and Anil Kumar, Quantum Computing – Back Action, AIP Proc., 864, 313 (2006)

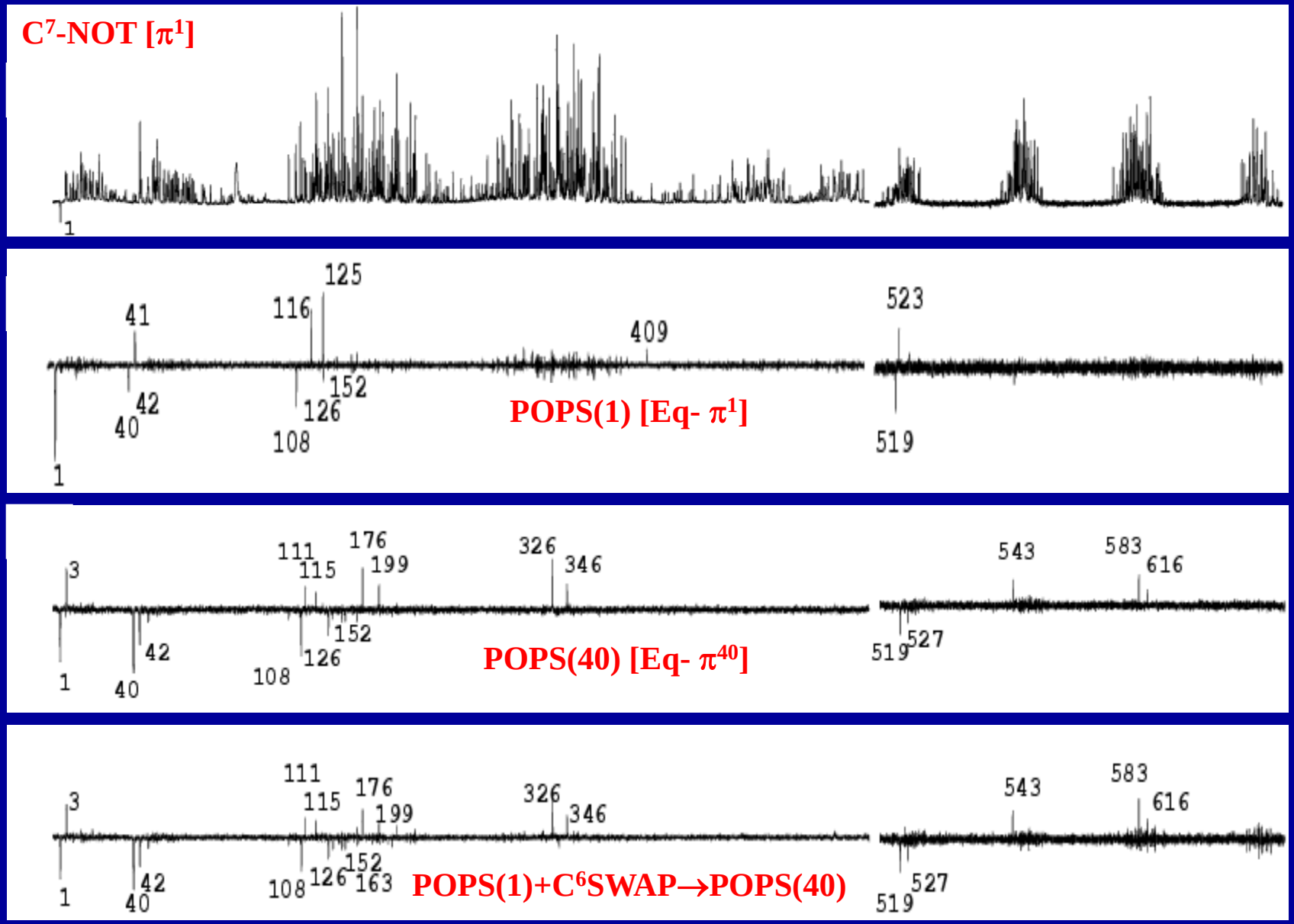
Energy-level diagram (256 levels)

^{19}F transitions





Proton transitions in B domain



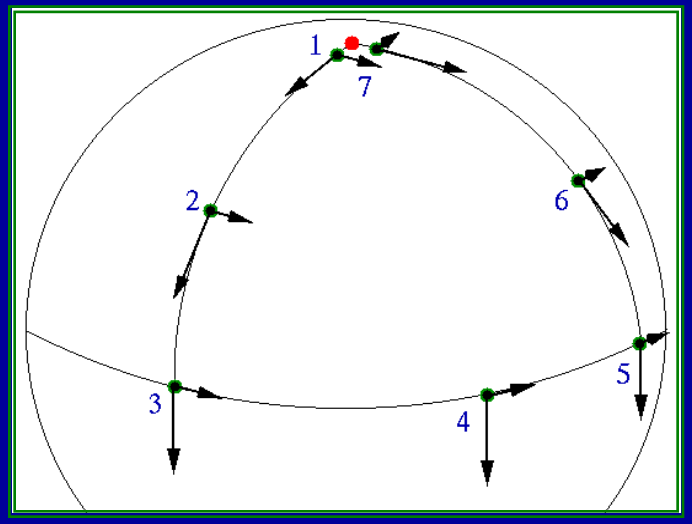
R. Das, R Bhattacharyya and Anil Kumar, Quantum Computing – Back Action, AIP Proceedings 864, 313 (2006)

Geometric Quantum Computing

- Geometrical phase is robust, since it depends only on the solid-angle enclosed by the path and is independent of the details.

- This fact can be used to perform ***fault-tolerant*** Quantum Information Processing

What is Geometric Phase ?



• When a vector is parallel transported on a curved surface, it acquires a phase. A part of the acquired phase depends on the geometry of the path.

• A state in a two-level quantum system is a vector which can be transported on a Bloch sphere. The geometrical part of the acquired phase depends on the solid angle subtended by the path at the centre of the Bloch sphere and not on the details of the path.

Adiabatic Geometric Phase

M. V. Berry, *Quantum phase factors accompanying adiabatic changes,*

Proc. R. Soc. Lond. A, 392, 45 (1984)

When a quantum system, prepared in one of the eigenstates of the Hamiltonian, is subjected to a change adiabatically, the system remains in the eigenstate of the instantaneous Hamiltonian and acquires a phase at the end of the cycle.

The phase has two parts. The dynamical and the geometric part.

$$\phi_D = \exp(-iEt/\hbar)$$ **(Dynamical Phase)**

$$\phi_g = \exp(i\gamma)$$ **(Geometric Phase)**

$$\phi = \phi_D + \phi_g$$ **(Total Phase)**

Pancharatnam, S.

***Proc. Ind. Acad. Sci. A* 44 , pp. 247-262 (1956).**

Non-Adiabatic Geometric Phase

Aharovov and Anandan later showed that adiabaticity is not a necessary condition. When the density matrix corresponding to a quantum system completes a cyclic path, in the density operator space through different intermediate stages, the system acquires the same geometric phase depending upon the geometry of the path.

Y. Aharonov and J. Anandan, *Phase change during Cyclic Quantum Evolution*, Phys. Rev. Lett. 58(16), 1593 (1987)

Non-adiabatic Geometric phases in NMR QIP using transition selective pulses

1. **Geometric phases using slice & triangular circuits.**
   - Use of above in DJ & Grover algorithms.

   Ranabir Das et al, J. Magn. Reson., **177**, 318 (2005).

2. **Experimental measurement of mixed state geometric phase by quantum interferometry using NMR.**

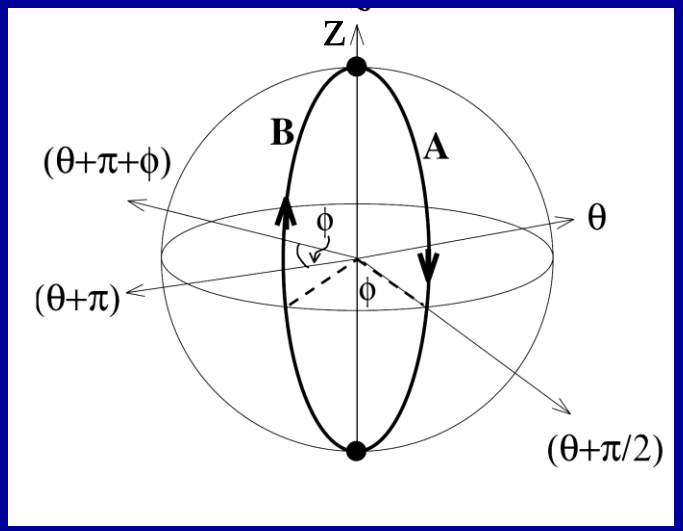
   Ghosh et al, Physics Letters **A 349**, 27 (2005).

3. **Geometric phases in strongly dipolar coupled spins.**
   - Fictitious spin- ½ subspaces.
   - Geometric phase gates in dipolar coupled $^{13}CH_3CN$.
   - Collins version of 2-qubit DJ algorithm.
   - Qubit-Qutrit parity algorithm.

   Gopinath et al, Phys. Rev **A 73**, 022326 (2006).

Geometric phase acquired by a slice circuit

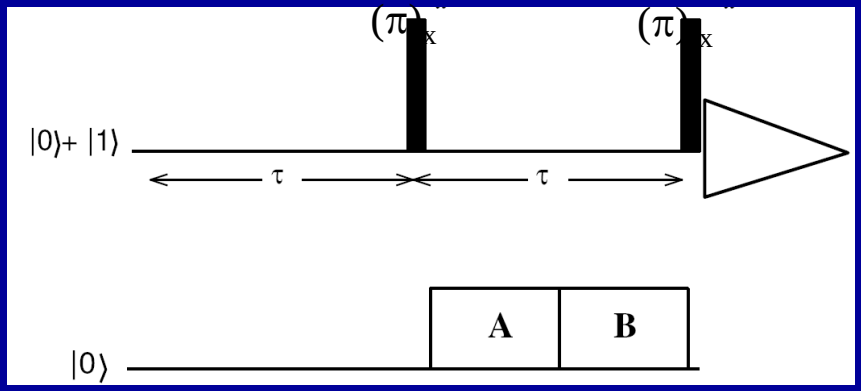
The state vector of the two level sub space cuts a slice on the Bloch sphere.



The slice circuit can be achieved by two transition selective pulses

$$A.B = (\pi)^{10 \leftrightarrow 11}_{\theta} \cdot (\pi)^{10 \leftrightarrow 11}_{\theta+\pi+\phi}$$

The resulting path encloses a solid angle $\Omega = 2\phi$.



A spin echo sequence $\tau-\pi-\tau$ is applied to refocus the evolution under internal Hamiltonian (the dynamic phase).

Second (π) pulse is applied to restore the state of the first qubit altered by the (π) pulse.

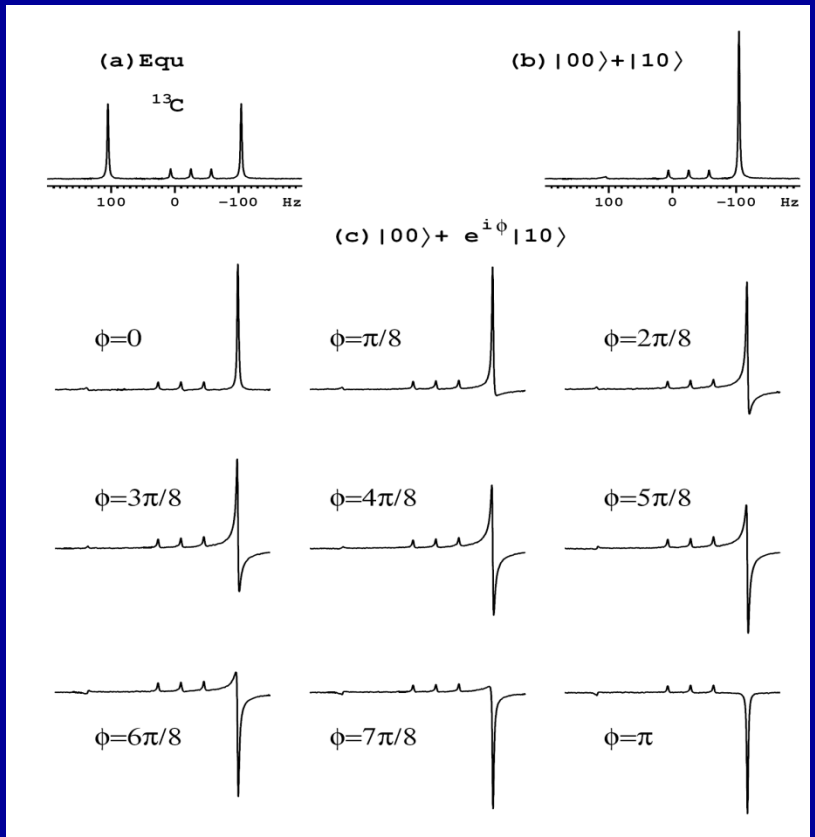
Unitary operator associated with the slice circuit:

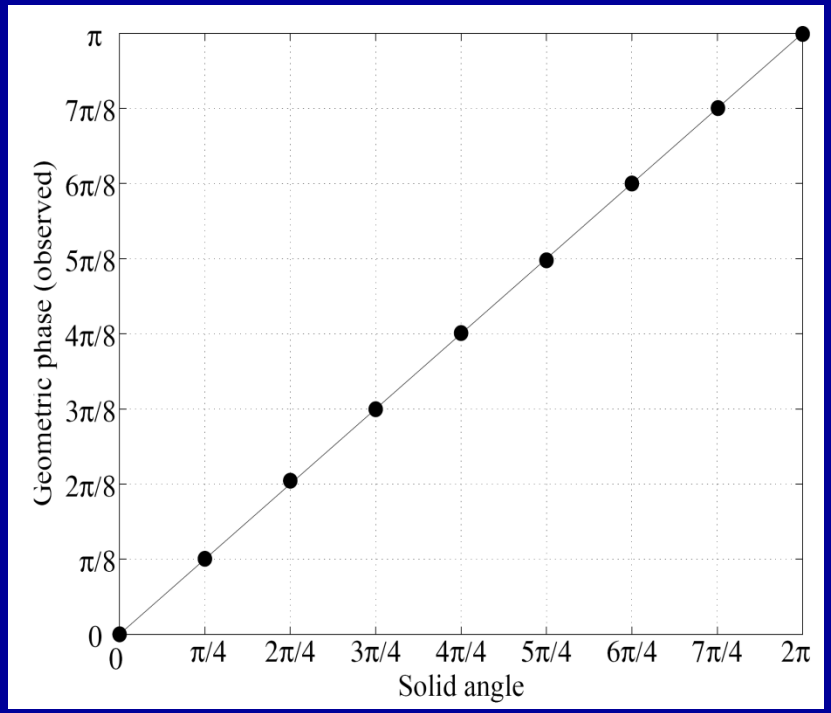
$$A.B = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{i\phi} & 0 \\ 0 & 0 & 0 & e^{-i\phi} \end{pmatrix}$$

$$\left(|0\rangle + |1\rangle\right)|0\rangle \xrightarrow{A.B} \left(|0\rangle + e^{i\phi}|1\rangle\right)|0\rangle$$

Solid angle $\Omega = 2\phi$.

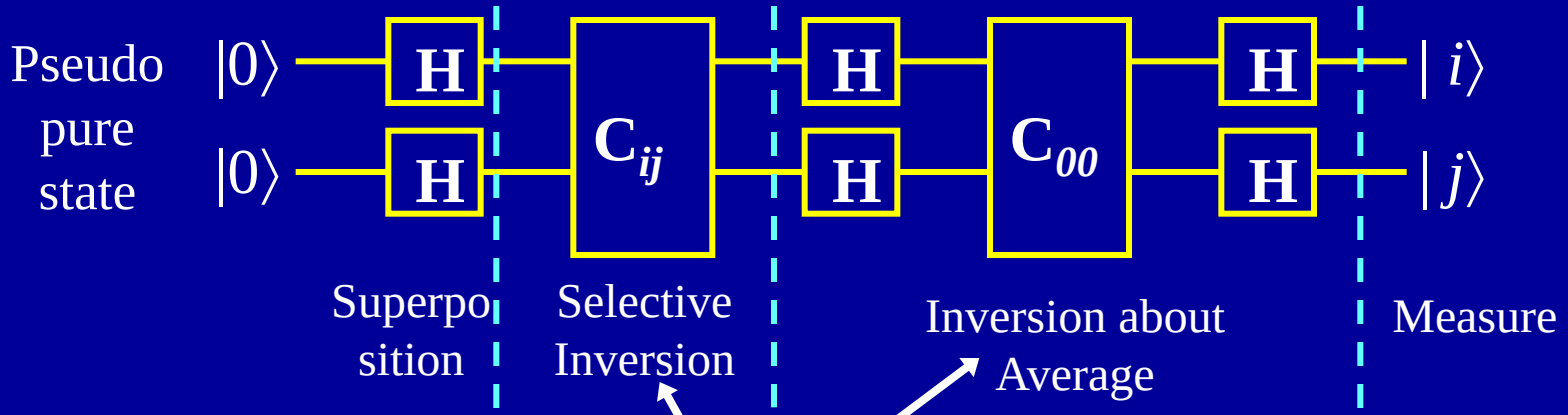
^{13}C Spectra of $^{13}CHCl3$





Ranabir Das et al, J. Magn. Reson., **177**, 318 (2005).

Grover search algorithm using geometric phases (by slice circuit):



Selective Inversion:

Using Geometric phase gates

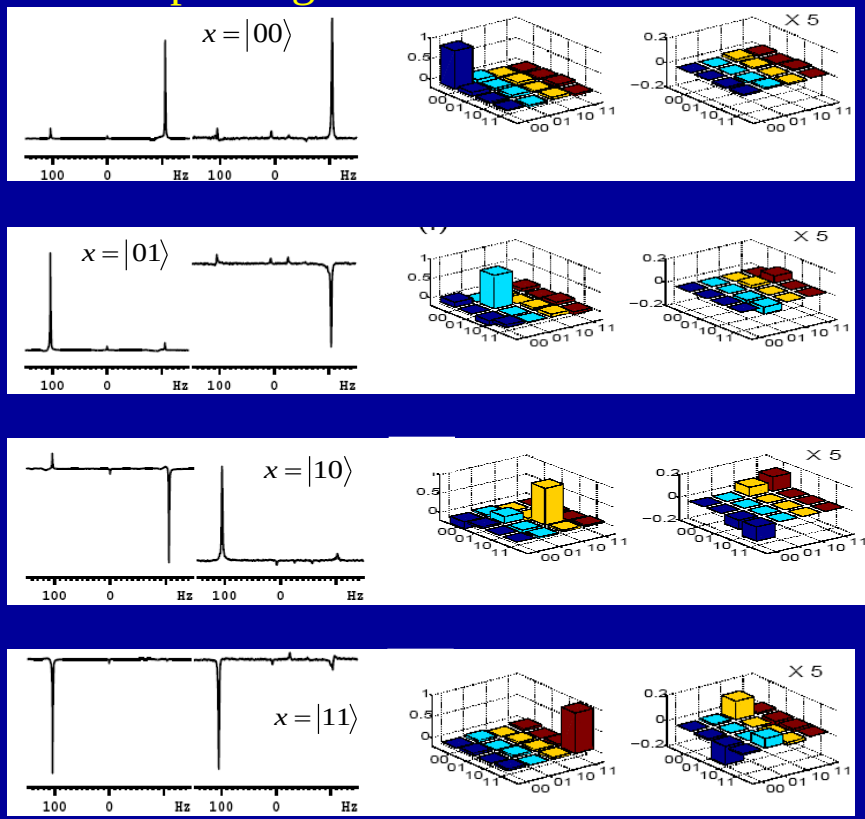
$$C_{00}(\phi) = (\pi)^1_{\theta}.(\pi)^1_{\theta+\pi+\phi/4}.(\pi)^{|10\rangle\leftrightarrow|11\rangle}_{\theta}.(\pi)^{|00\rangle\leftrightarrow|01\rangle}_{\theta+\pi+\phi/2}.$$

$$C_{01}(\phi) = (\pi)^1_{\theta}.(\pi)^1_{\theta+\pi+\phi/4}.(\pi)^{|10\rangle\leftrightarrow|11\rangle}_{\theta}.(\pi)^{|00\rangle\leftrightarrow|01\rangle}_{\theta+\pi-\phi/2}$$

$$C_{10}(\phi) = (\pi)^1_{\theta}.(\pi)^1_{\theta+\pi-\phi/4}.(\pi)^{|10\rangle\leftrightarrow|11\rangle}_{\theta}.(\pi)^{|10\rangle\leftrightarrow|11\rangle}_{\theta+\pi+\phi/2}$$

$$C_{11}(\phi) = (\pi)^1_{\theta}.(\pi)^1_{\theta+\pi-\phi/4}.(\pi)^{|10\rangle\leftrightarrow|11\rangle}_{\theta}.(\pi)^{|10\rangle\leftrightarrow|11\rangle}_{\theta+\pi-\phi/2}$$

$$\phi = \pi$$

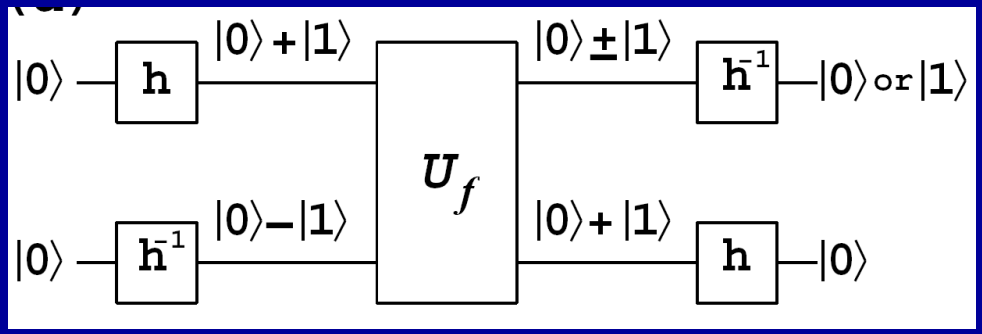


Inversion about Average C_{00} = H U_{00} H

$U_{00} = C_{00}(\pi)$

Ranabir Das et al, J. Magn. Reson., **177**, 318 (2005).

Deutsch-Jozsa algorithm using geometric phases (by slice circuit):



$U_{f(00)}$ is identity matrix

$U_{f(11)}$ is achieved by applying π pulse on the second qubit

$$U_{f10} = h - C_{11}(\pi) - h^{-1}$$

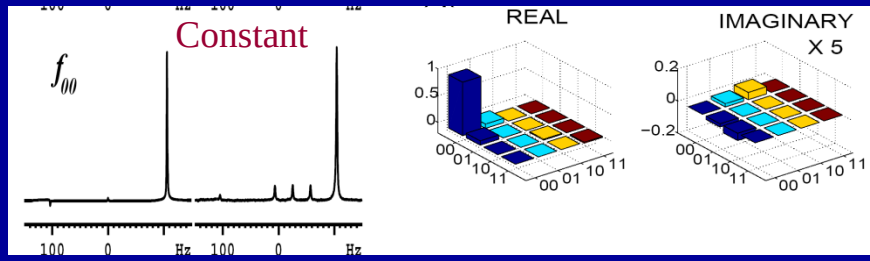
$$C_{11}(\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{pmatrix}$$

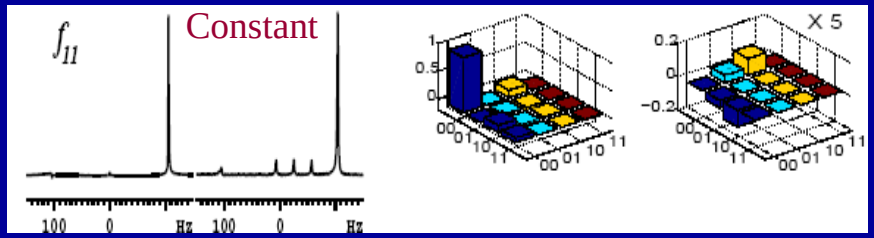
$$C_{11}(\phi) = (\pi)^{1}_{\theta}.(\pi)^{1}_{\theta+\pi-\phi/4}.(\pi)^{|10\rangle\leftrightarrow|11\rangle}_{\theta}.(\pi)^{|10\rangle\leftrightarrow|11\rangle}_{\theta+\pi-\phi/2}$$

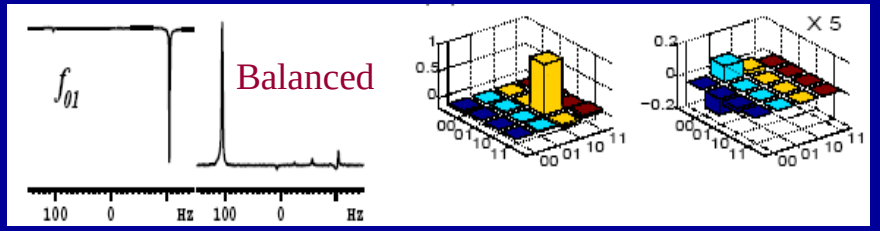
$$U_{f01} = h - C_{00}(\pi) - h^{-1}$$

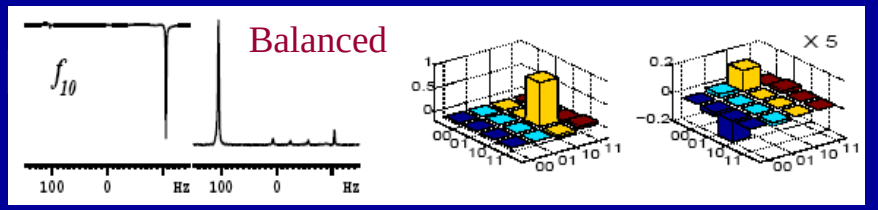
$$C_{00}(\phi) = (\pi)^{1}_{\theta}.(\pi)^{1}_{\theta+\pi+\phi/4}.(\pi)^{|10\rangle\leftrightarrow|11\rangle}_{\theta}.(\pi)^{|00\rangle\leftrightarrow|01\rangle}_{\theta+\pi+\phi/2}.$$

^{1}H ^{13}C of $^{13}CHCl_3$



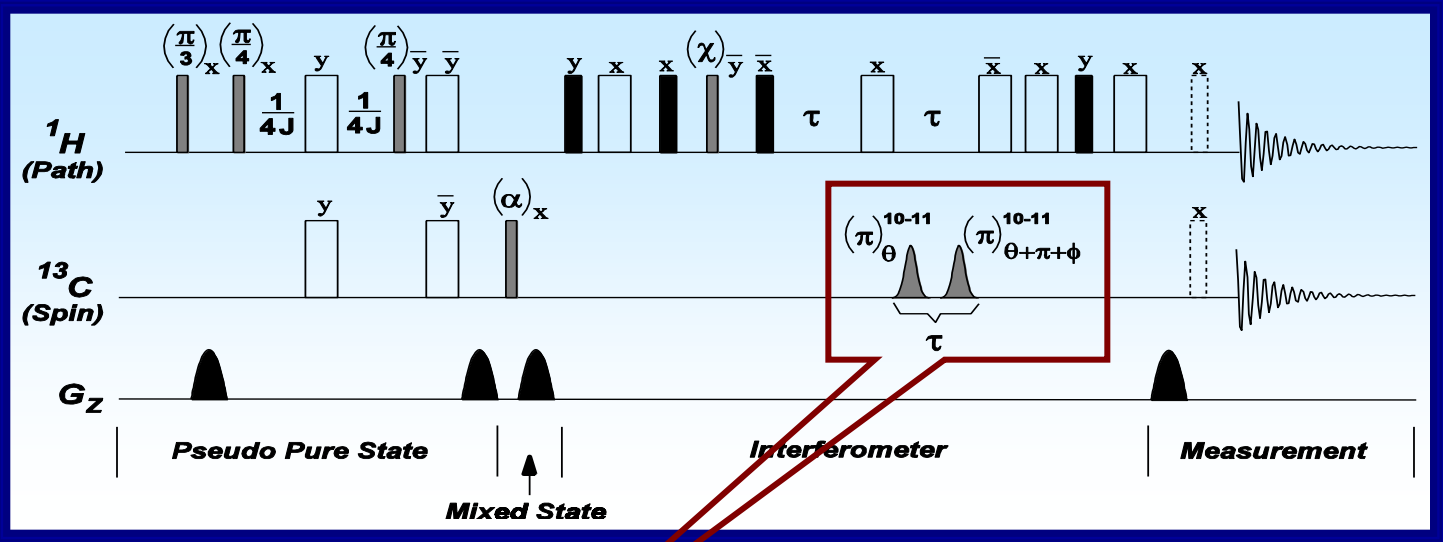


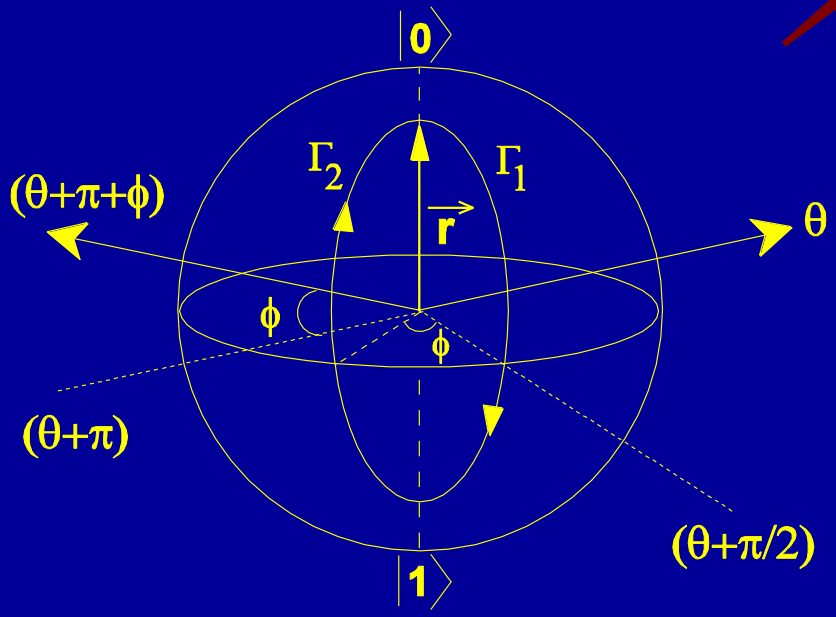




Ranabir Das et al, J. Magn. Reson., **177**, 318 (2005).

Experimental Measurement of Mixed State Geometric Phase by NMR





Creation of $|00\rangle$ PPS

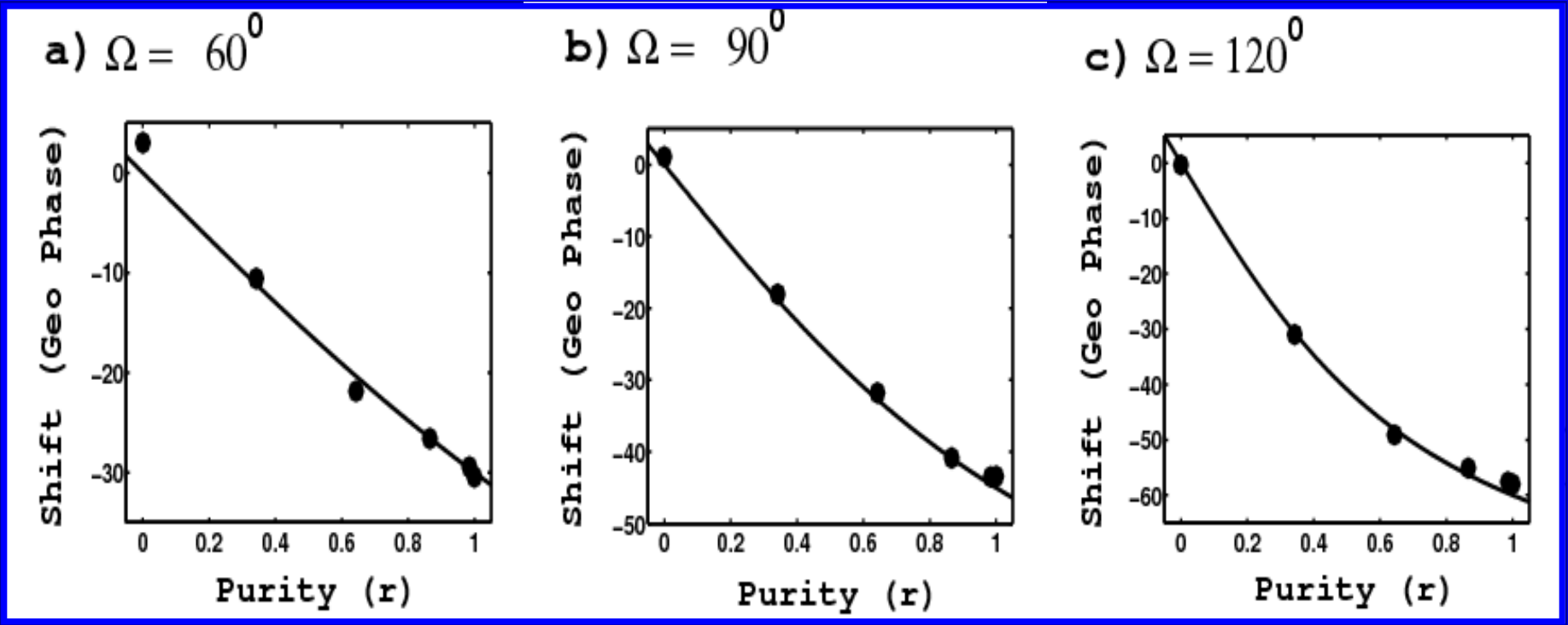
Preparation of Mixed state by the α degree pulse and a gradient.

Implementation of Slice circuit to introduce Geometric Phase.

Measurement

Results:

$$\text{Geometric Phase (Shift)} = -\tan^{-1}\left(r\tan\left(\frac{\Omega}{2}\right)\right)$$



The shift of the interference pattern as a function of Ω and r.

The shift directly gives the geometric phase acquired by the spin qubit.

Ghosh et al, Physics Letters **A 349**, 27 (2005).

Quantum Games

Game Theory

- Von Neumann and Morgenstern

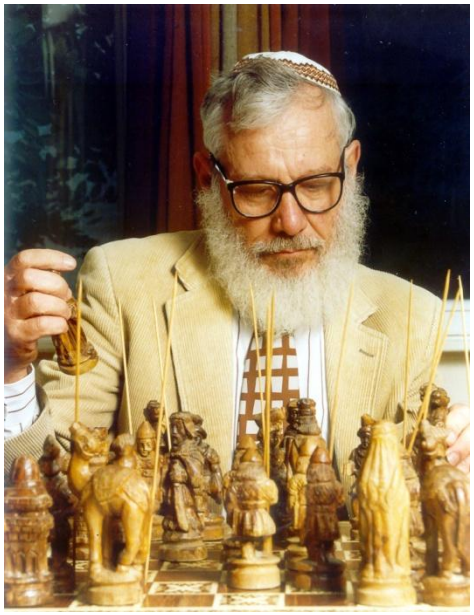
  "Theory of games and Economic behaviour"

  (Princeton University Press, 1947)

- **John F. Nash (Princeton University)**
- **Nobel Prize in Economics (1994)**

Nash Equilibrium

- **Robert Aumann (Hebrew University)**
- **Nobel Prize in Economics (2005)**



Evolutionary Games

Quantum Games by NMR

(i) Ulam's Quantum Game – Guessing a number

(ii) **Three player Dilamma Game- Optimum strategy for going to a Bar with two stool.**

Avik Mitra et al.; J. Magn. Reson., 187, 306-313 (2007).

(iii) Battle of Sexes Game – Should Bob and Alice together watch TV or go to a football game.

Avik Mitra Thesis IISc 2007

Ulam'sGame

- Two player game

- Bob thinks of a number between 1 and 2^n

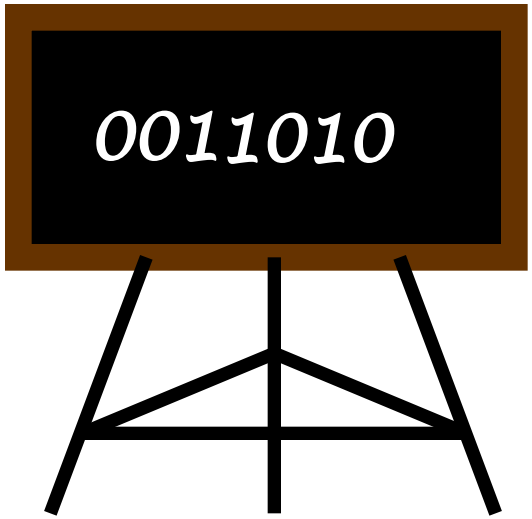
Alice tries to find out the number in minimum number of queries.

Classical: n queries
Quantum: 1 Query

Ulam'sGame

❑ Classical Algorithm

Alice



Bob

Total number of queries = $\log_2 2^n = n$

Quantum Version of Ulam'sGame

The quantum system consists of two registers.

Register A
- consists of n qubits

Register B
- consists of 1 qubit

Alice makes a superposition of all the qubits.

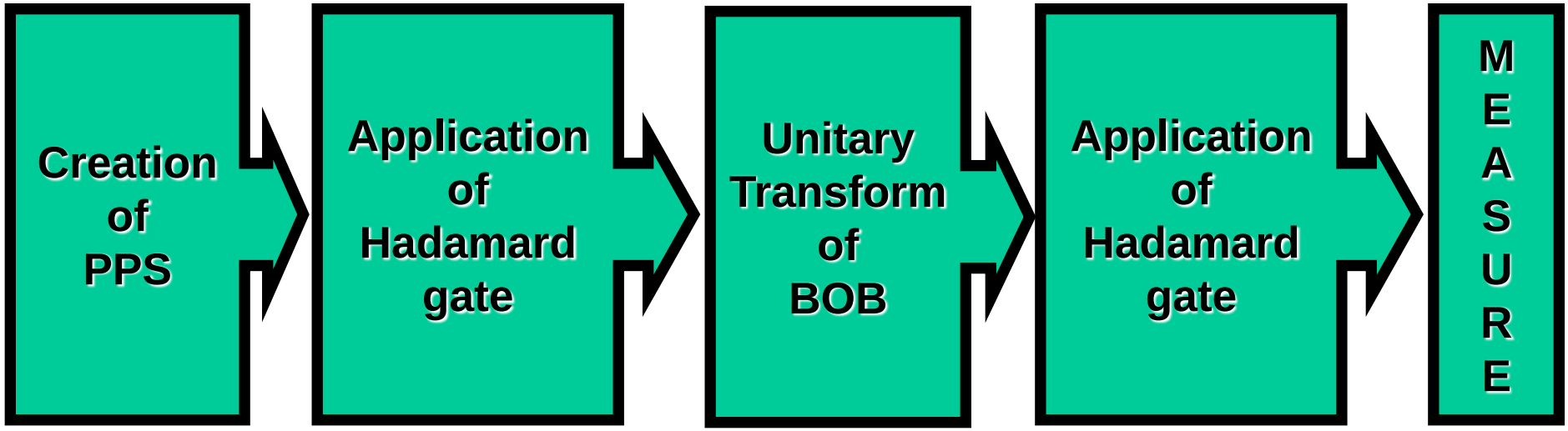
Bob performs a unitary transform and stores the result in register B.

Alice again interferes the qubits and then performs a measurement.

Total number of queries = 1

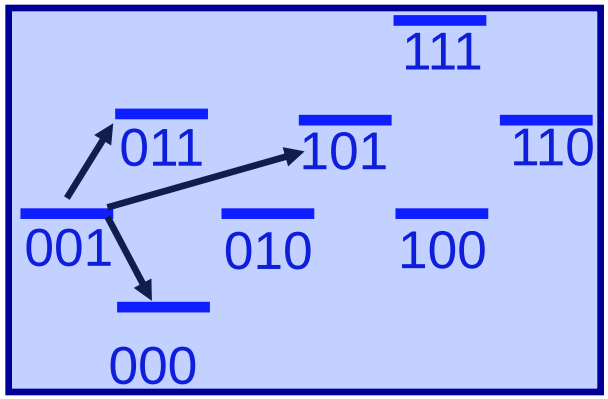
--S. Mancini and L. Maccone, quant-ph/0508156

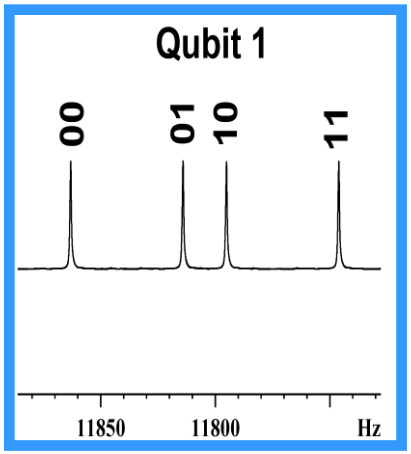
Protocol

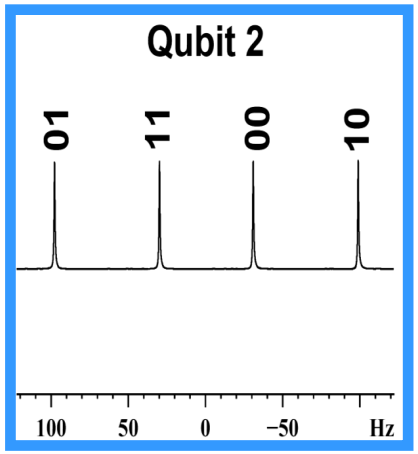

Creation of PPS
Application of Hadamard gate
Unitary Transform of BOB
Application of Hadamard gate
MEASURE

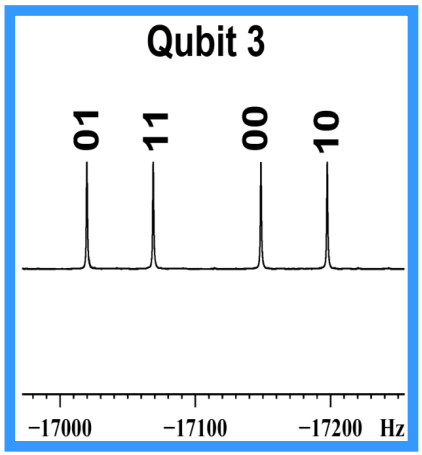
Experimental implementation

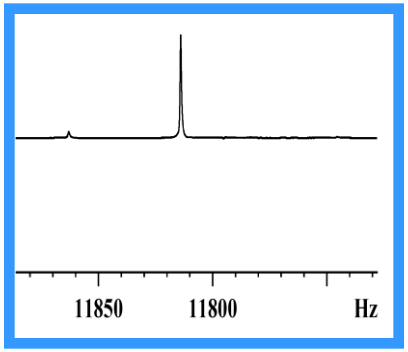
❑ Preparation of Pseudo-Pure state - PPS

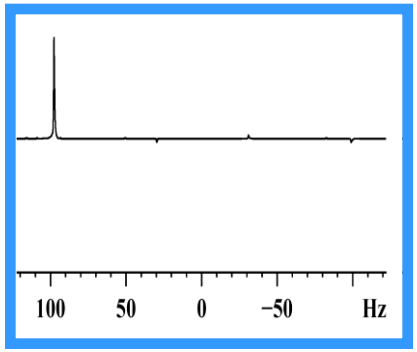


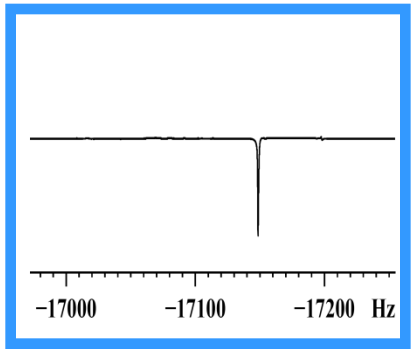




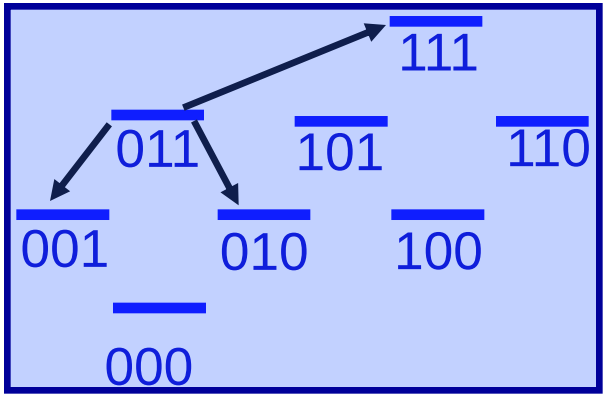


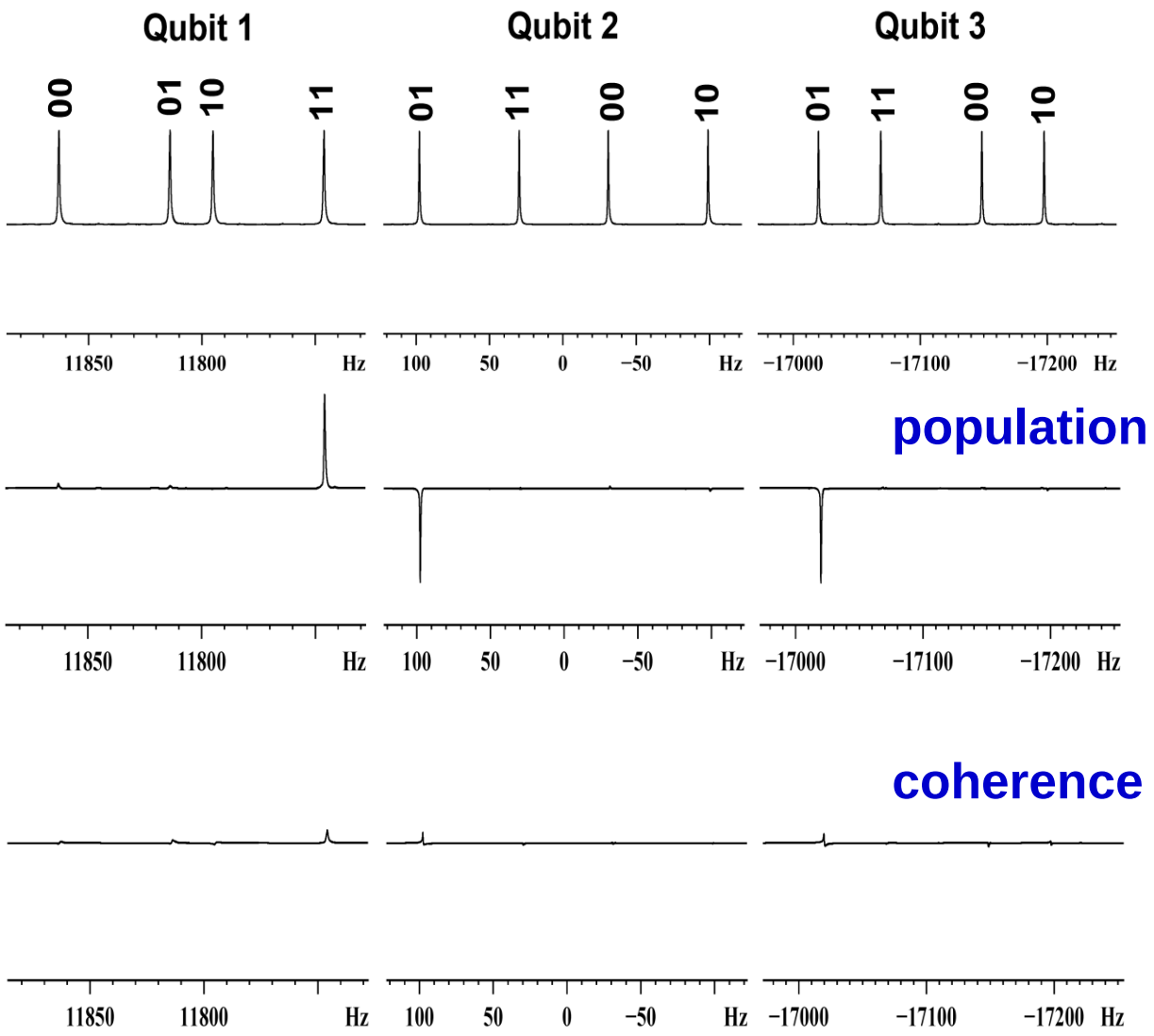






Results



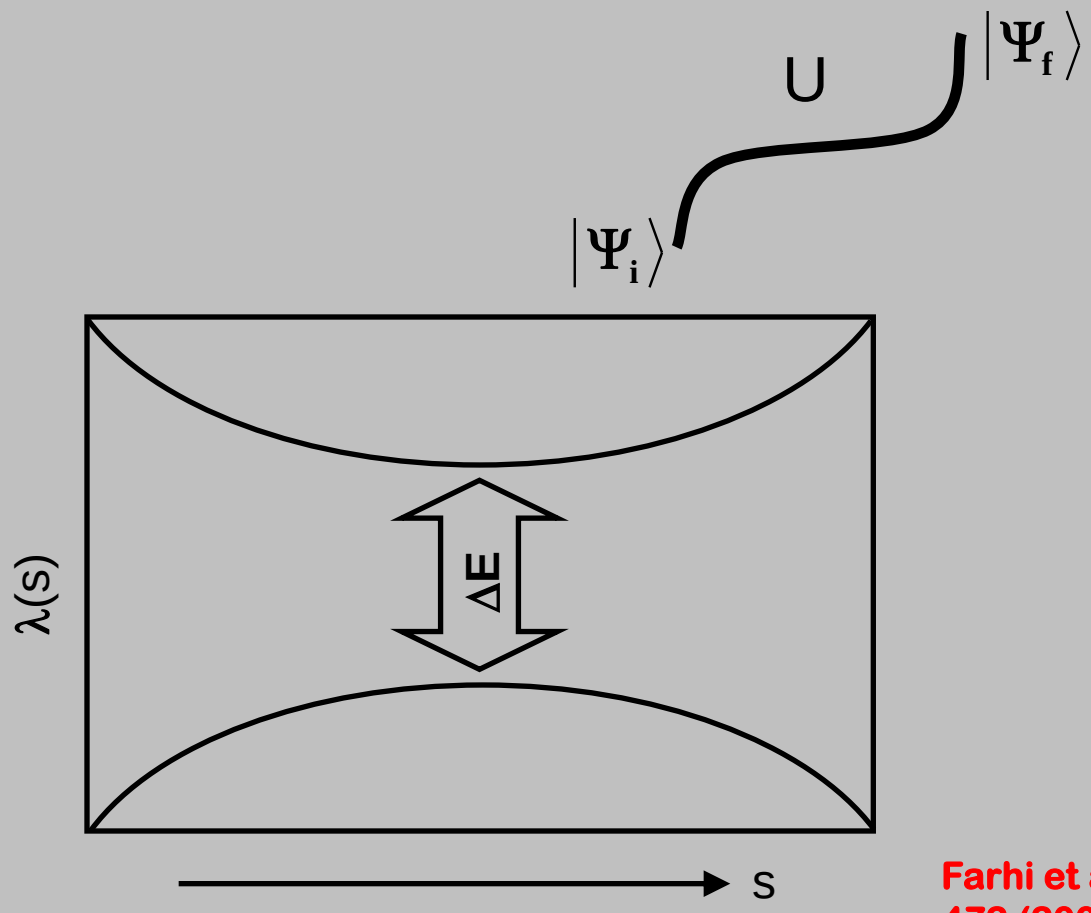


Avik et al., J. Indian Institute of Science; **89**, 309-316 (2009).

Adiabatic Quantum Algorithms

Adiabatic Quantum Computing

- Based on "*Adiabatic Theorem*" of Quantum Mechanics: A quantum system in its ground state will remain in its ground state provided that the Hamiltonian H under which it is evolved is varied slowly enough.



The system evolves from H_i to H_f with a probability $(1-\varepsilon^2)$ provided the evolution rate satisfies the condition

$$\frac{\max_{0\le s\le 1}\left|\langle 1;s|\frac{dH(s)}{dt}|0;s\rangle\right|}{g_{min}^2} \le \varepsilon$$

Where $\varepsilon << 1$

Farhi et al, PRA, 65,012322 (2002), Science, 292, 472 (2001), quant-ph/0001106; 0007071; 0208135

Adiabatic Quantum Computing

- Evolve the initial state under a slowly varying Hamiltonian so that it acts as though a unitary transformation occurred on the initial state, bringing it to a final state during some time **T**.

$H(s) = (1-s)H_B + sH_F$

$H_B \equiv$ beginning Hamiltonian

$H_F \equiv$ Final Hamiltonian

- Initialize register to desired input qubits.

- Vary the Hamiltonian towards the final Hamiltonian whose eigenstates encodes the desired final states.

$$\left|\psi_f\right\rangle = \prod_{n=0}^{N} U_n \left|\psi_i\right\rangle, where\, U_n = \exp(-iH_n t)$$

ADIABATIC ALGORITHMS BY NMR

(i) NMR Implementation of Locally Adiabatic Algorithms

(a) Grover's search Algorithm
(b) D-J Algorithm

Avik Mitra et al., J. Magn. Reson. A 177 , 285-298 (2005).

(ii) Adiabatic Satisfy-ability problem using Strongly Modulated Pulses

Avik Mitra, T.S. Mahesh and Anil Kumar, J. Chem. Phys. 128, 124110 (2008) .

Deutsch-Jozsa Algorithm

- **CONSTANT OR BALANCED FUNCTIONS:**

Classically : **(2^{N-1} + 1) steps**

Deutsch-Jozsa (DJ) Algorithm : **1 step**

The Constant and Balanced functions of two-qubit DJ

	Constant		Balanced				
$f(00)$	0	1	1	1	1	0	0	0
$f(01)$	0	1	1	0	0	1	0	1
$f(10)$	0	1	0	1	0	0	1	1
$f(11)$	0	1	0	0	1	1	1	0

Adiabatic DJ Algorithm

$H_I: \quad I - |\psi_I\rangle\langle\psi_I| \qquad$ where $\quad |\psi_I\rangle = \frac{1}{2}\left[|00\rangle + |01\rangle + |10\rangle + |11\rangle\right]$

$H_F: \quad I - |\psi_F\rangle\langle\psi_F| \qquad$ where $|\psi_F\rangle = \alpha|00\rangle + \frac{\beta}{\sqrt{3}}\left[|01\rangle + |10\rangle + |11\rangle\right]$

$$\alpha = \frac{1}{4}\left|(-1)^{f(00)} + (-1)^{f(01)} + (-1)^{f(10)} + (-1)^{f(11)}\right|$$

$$\beta^2 = 1 - \alpha^2$$

α=1 → Constant function
α=0 → Balanced function

S. Das et al, PRA, 042308 (2002)

- Hamiltonian in terms of spin operators

$$H_I = I_x^1 + I_x^2 + 2I_x^1 I_x^2$$

$$H_F^C = \frac{1}{2}\left(I_z^1 + I_z^2 + 2I_z^1 I_z^2\right)$$

Constant case

Balanced case

$$H_F^B = -\frac{1}{6}\left(I_z^1 + I_z^2 + 2I_z^1 I_z^2\right) + \frac{2}{3}\left(I_x^1 I_x^2 + I_y^1 I_y^2\right) + \frac{1}{3}\left(I_x^1 + I_x^2\right) - \frac{2}{3}\left(I_x^1 I_z^2 + I_z^1 I_x^2\right)$$

Avik Mitra et al, JMR, 177, 285 (2005)

Modification of Balanced case Hamiltonian

$$H_F^B = -\frac{1}{6}\left(I_z^1 + I_z^2 + 2I_z^1 I_z^2\right) + \frac{2}{3}\left(I_x^1 I_x^2 + I_y^1 I_y^2\right) + \frac{1}{3}\left(I_x^1 + I_x^2\right) - \frac{2}{3}\left(I_x^1 I_z^2 + I_z^1 I_x^2\right)$$

- The balanced case Hamiltonian requires complicated pulse sequence due to the presence of zero and double quantum terms.
- Hamiltonian diagonal in the computational basis are easy to implement.

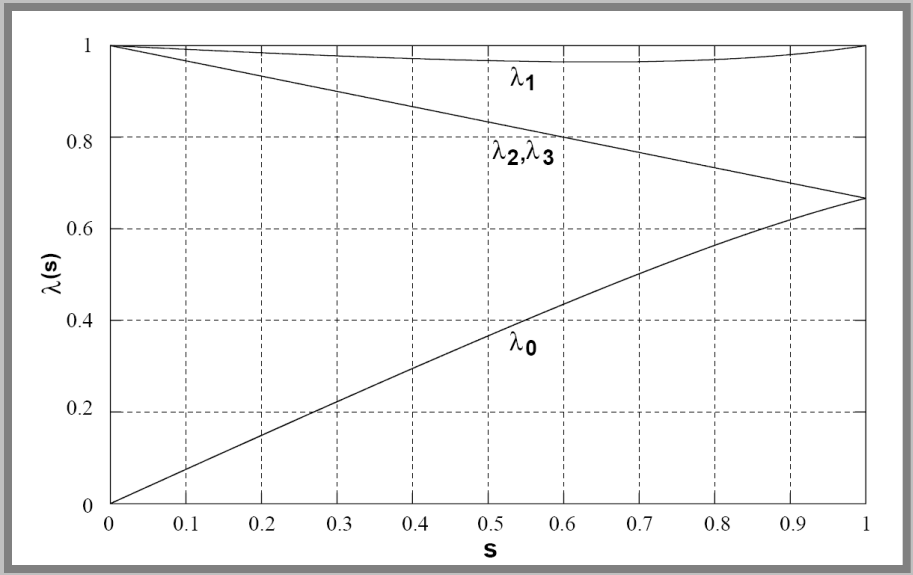
- The terms contributing to the off diagonal elements in balanced case Hamiltonian are dropped.

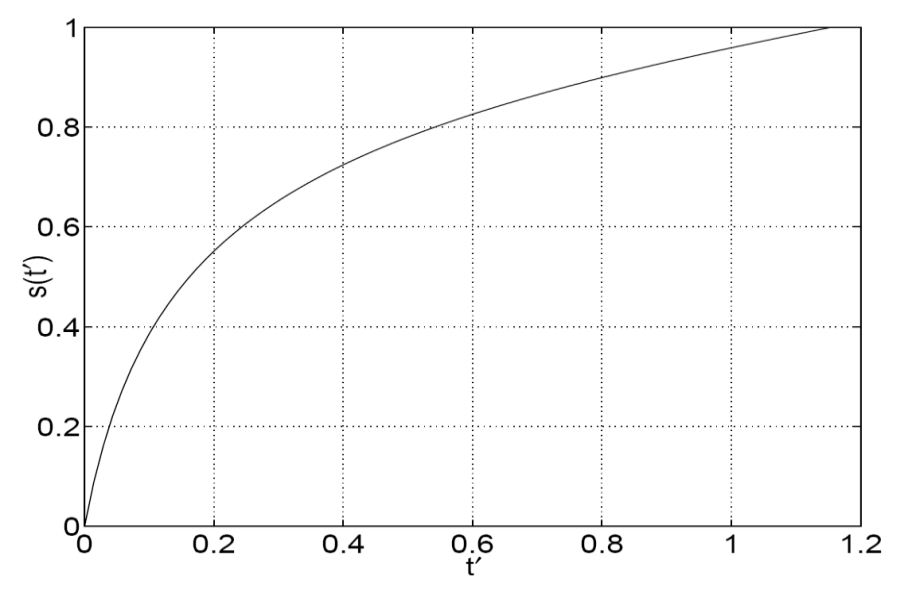
$$H_F^B = -\frac{1}{6}\left(I_z^1 + I_z^2 + 2I_z^1 I_z^2\right) + \frac{2}{3}\left(I_x^1 I_x^2 + I_y^1 I_y^2\right) + \frac{1}{3}\left(I_x^1 + I_x^2\right) - \frac{2}{3}\left(I_x^1 I_z^2 + I_z^1 I_x^2\right)$$

$$\tilde{H}_F^B \cong -\left(I_z^1 + I_z^2 + 2I_z^1 I_z^2\right)$$

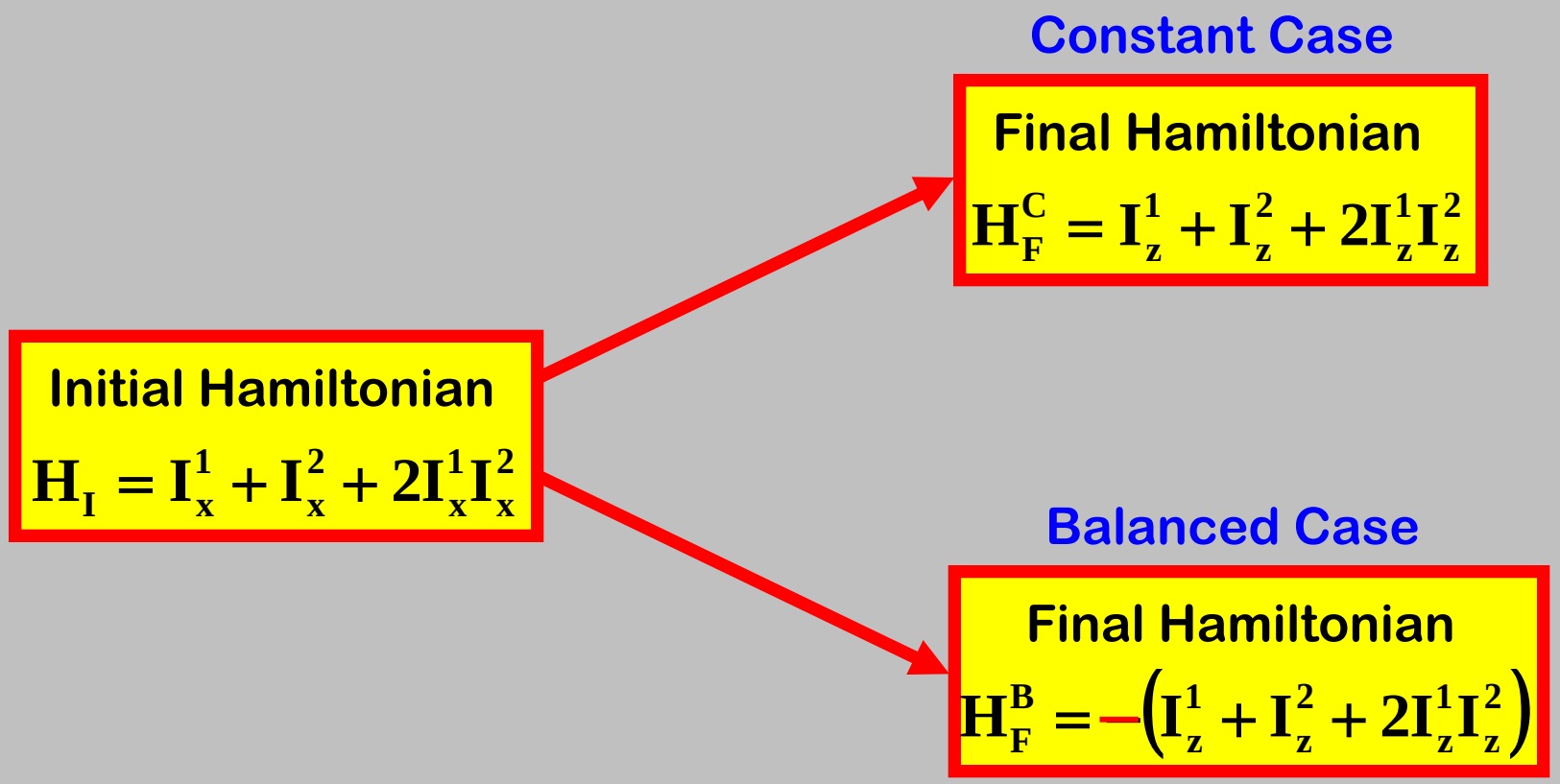
Avik Mitra et al, JMR, 177, 285 (2005)

Eigenvalues with respect to the parameter ‘s’.





Plot of Parameter ‘s’ as a function of t.

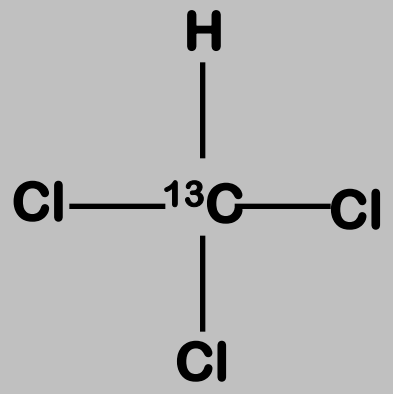


The Balanced case Hamiltonian differs from the Constant case in the sign of the Hamiltonian. This is sufficient to distinguish the two cases.

Avik Mitra et al, JMR, 177, 285 (2005)

NMR Implementation.

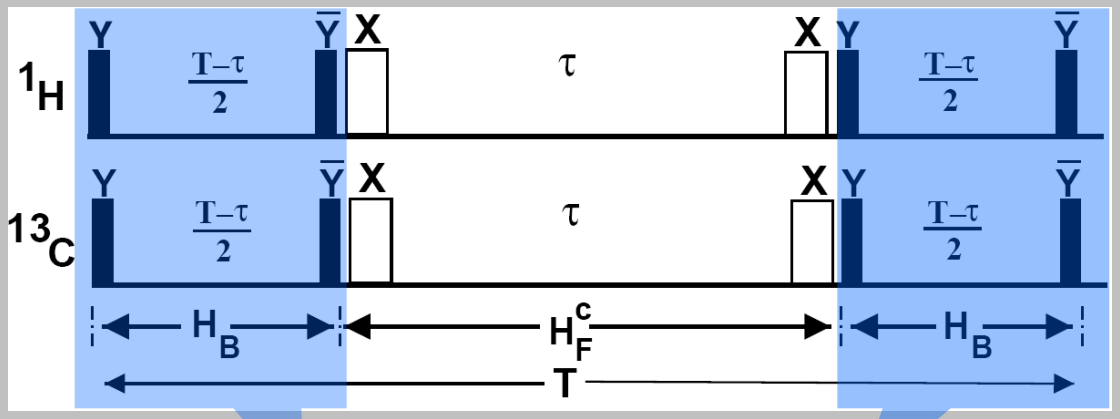
- Sample



- Experiment carried out in DRX500
- H and C has resonance frequency 500 MHz and 125 MHz.
- J_{HC}= 209 Hz

Pulse Scheme for the NMR Implementation

- **CONSTANT CASE**



Pulse sequence for Implementation of H_B

- **NMR Hamiltonian:**

$$\mathbf{H} = -\nu_1 \mathbf{I}_{z1} - \nu_2 \mathbf{I}_{z2} + \mathbf{J}_{12} \mathbf{I}_{z1} \mathbf{I}_{z2}$$

- **Beginning Hamiltonian**

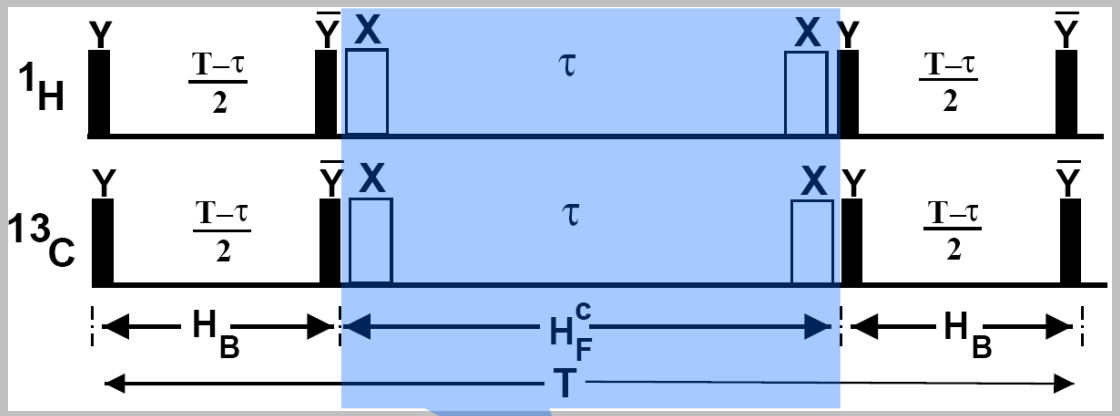
For $\nu_1 = \nu_2 = -\ J_{12}/2$ and with two pi/2 pulses with appropriate phases

$$H_B = I_{x1} + I_{x2} + 2I_{x1}I_{x2}$$

Avik Mitra et al, JMR, 177, 285 (2005)

Pulse sequence for Implementation of H^F

- **CONSTANT CASE**



Pulse sequence for Implementation of H_F

- **NMR Hamiltonian:**

$$H = -\nu_1 I_{z1} - \nu_2 I_{z2} + J_{12} I_{z1} I_{z2}$$

- **Final Hamiltonian**

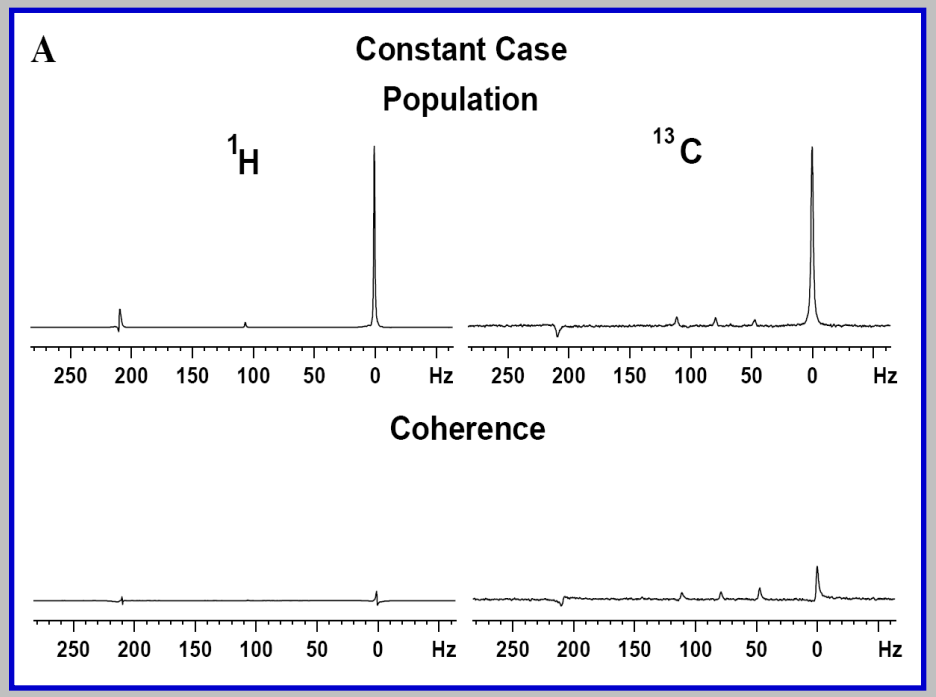
For $\nu_1 = \nu_2 = -\ J_{12}/2$

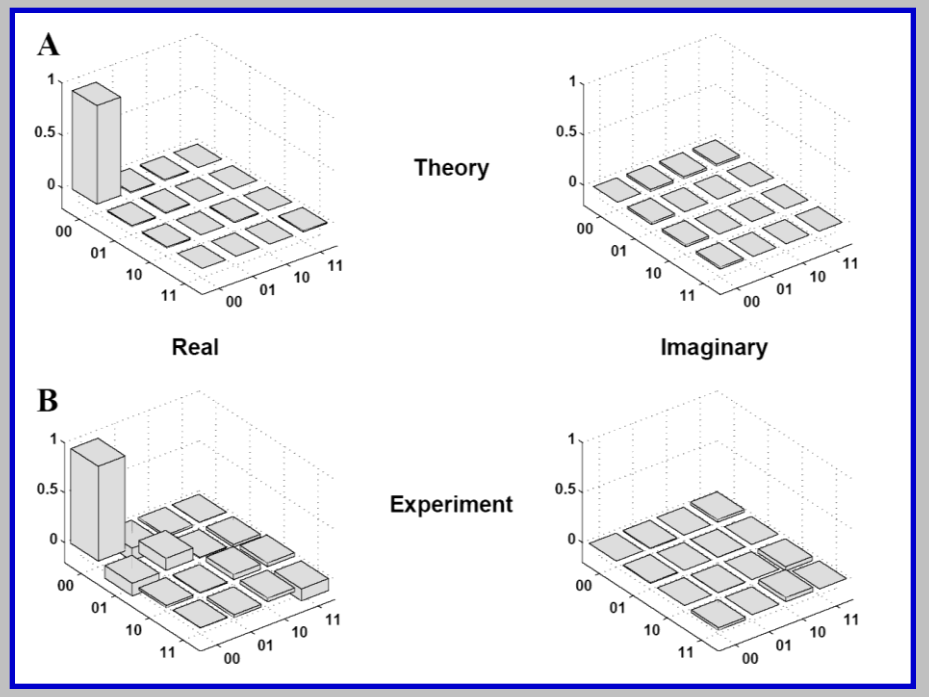
$$H_F = I_{z1} + I_{z2} + 2I_{z1} I_{z2}$$

- Free evolution under the NMR Hamiltonian between two π- pulses with appropriate phases for a time τ.

Avik Mitra et al, JMR, 177, 285 (2005

Experimental Result





- The final state is $|00\rangle$

Average absolute deviation

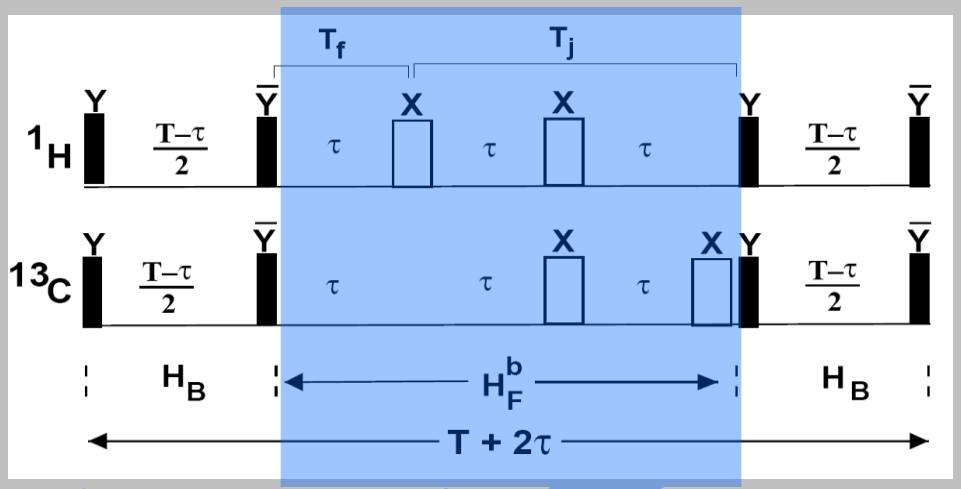
$$\Delta x = \frac{1}{N^2} \sum_{i,j=1}^{N} |x_{i,j}^{\mathrm{T}} - x_{i,j}^{\mathrm{E}}|$$

5.28%

Avik Mitra et al, JMR, 177, 285 (2005)

NMR Implementation

- BALANCED CASE



Pulse sequence for Implementation of H_F

- NMR Hamiltonian:

$$H = -\nu_1 I_{z1} - \nu_2 I_{z2} + J_{12} I_{z1} I_{z2}$$

- Final Hamiltonian

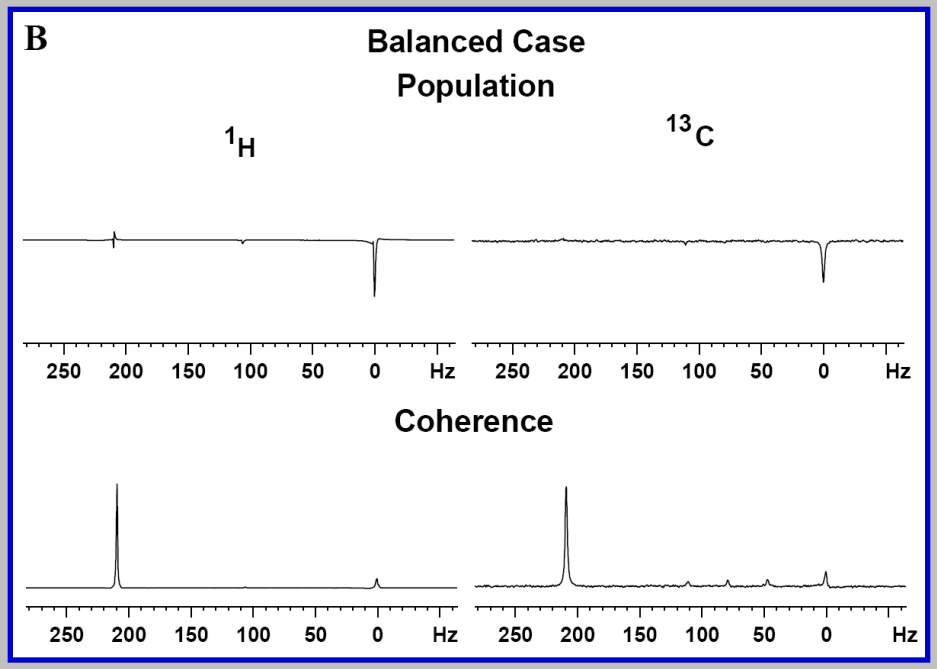
For $\nu_1 = \nu_2 = -\ J_{12}/2$

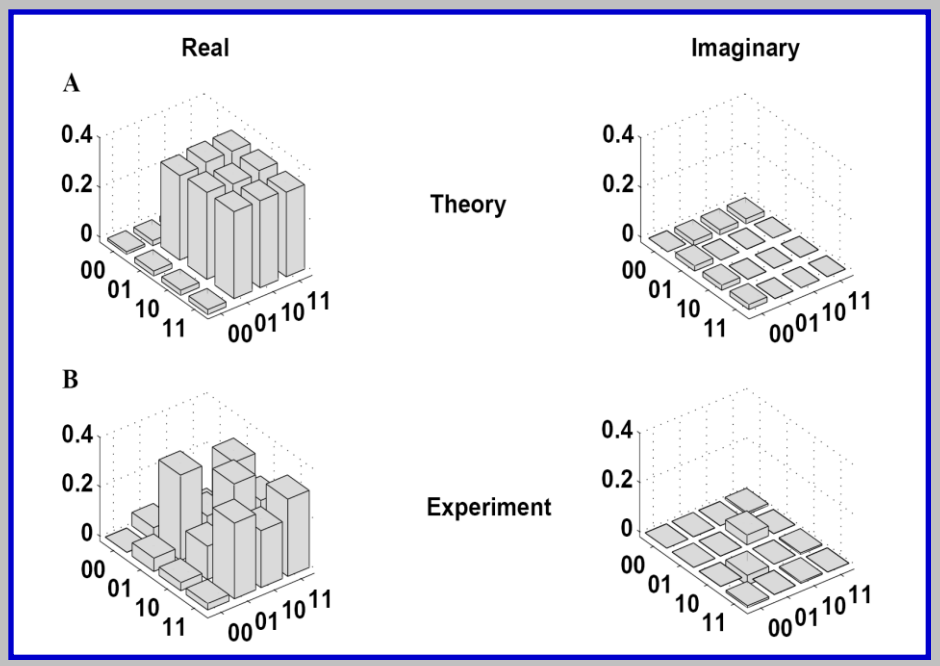
$$H_F = -\left(I_{z1} + I_{z2} + 2I_{z1} I_{z2}\right)$$

- Free evolution under the NMR Hamiltonian between two π- pulses with appropriate phases for a time τ.

Avik Mitra et al, JMR, 177, 285 (2005

Experimental Result



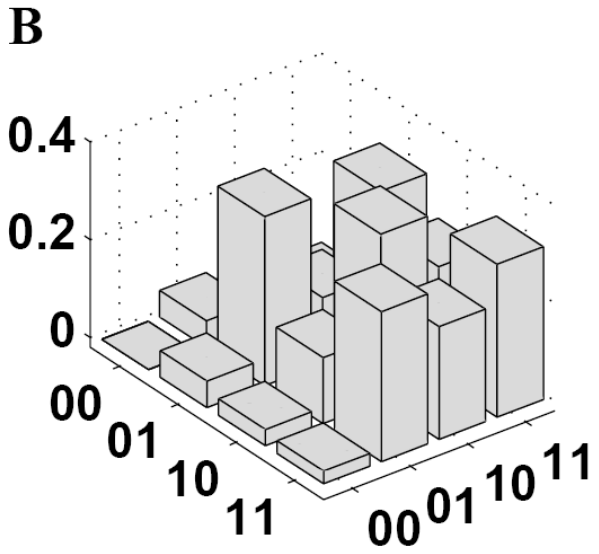


$\Delta x \sim 17\%$

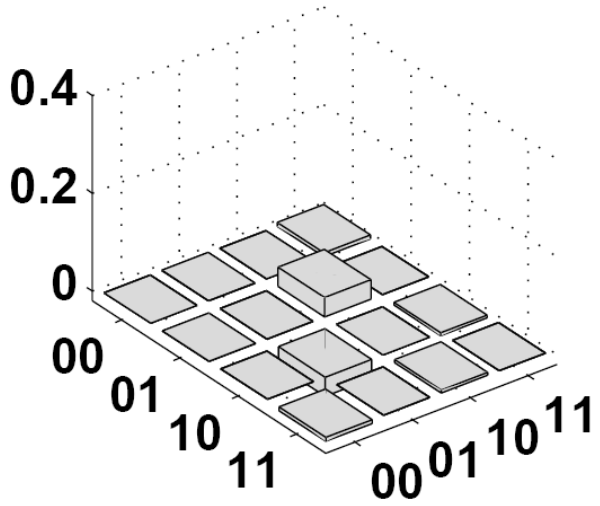
- Final state is $(|01\rangle+|10\rangle+|11\rangle)/\sqrt{3}$
- Experiment does not match well with theoretical result.
- Carbon: Short decoherence time →Significant effect of decoherence in carbon.
- T_2 of carbon was measured by CPMG sequence.
- Simulation was repeated after including relaxation using Bloch equations.

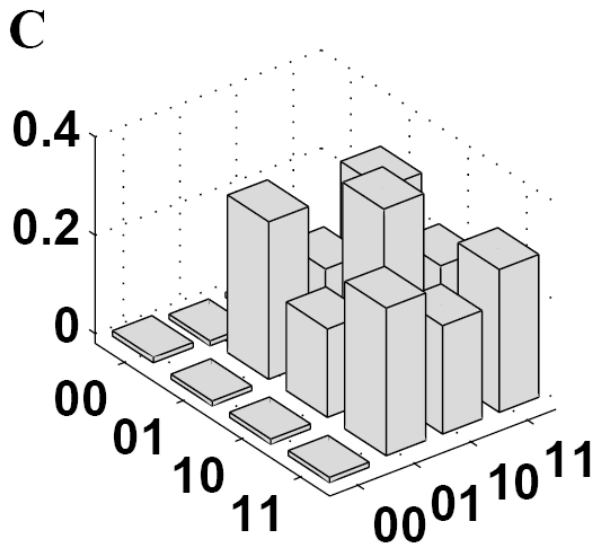
Avik Mitra et al, JMR, 177, 285 (2005)

Experimental Result



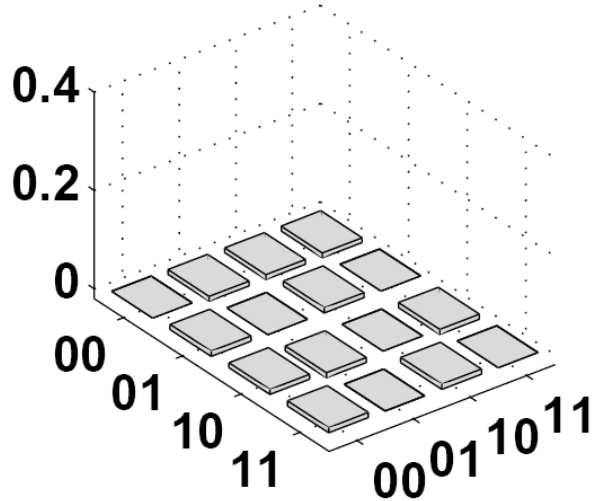
Experiment





Theory including decoherence

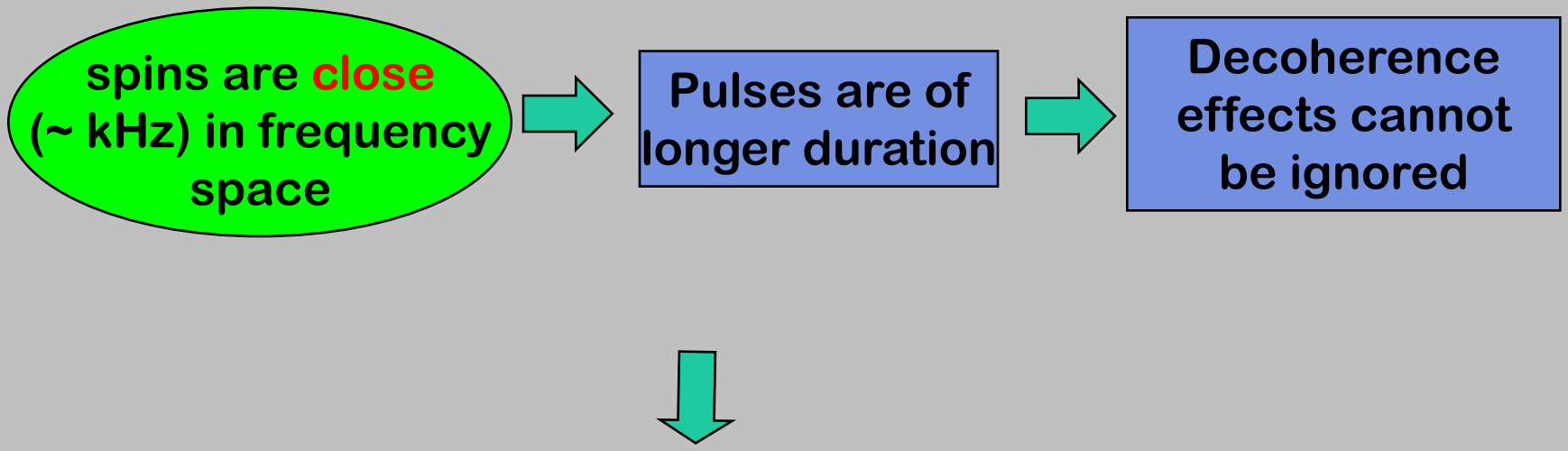
$\Delta x \sim 8\%$



Avik Mitra et al, JMR, 177, 285 (2005)

Adiabatic SAT algorithm by strongly modulated pulses

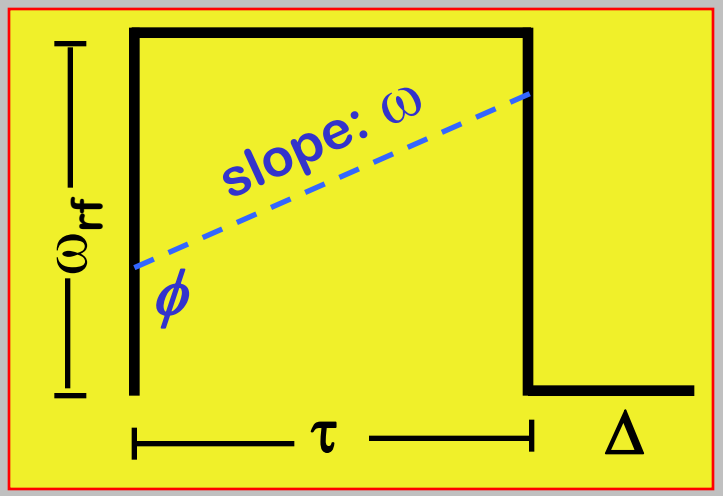
In a Homonuclear spin systems



Strongly Modulated Pulses circumvents the above problems

Strongly Modulated Pulses.

$$U_{SMP} = \prod_{l} \Delta_l(\delta_l) \cdot U_z^{-1}(\tau_l) e^{-iH_{eff}(\omega^l \omega_{rf}^l \phi^l)\tau^l}$$



$$F = \left| \frac{Tr[U_T \cdot U_{SMP}]}{N} \right|^2$$

Nedler-Mead
Simplex Algorithm
(`fminsearch`)

k-SAT Problem

1. Let B={$x_1, x_2, \ldots, x_n$} be a set of 'n' Boolean variables.
2. Let C_i be a disjunction of 'k' elements of B

$$C_i = x_1 \vee x_2 \vee \ldots\ldots \vee x_k$$

1. F is the Boolean function that is the conjunction of m such clauses.

$$F = C_1 \wedge C_2 \wedge \ldots\ldots \wedge C_m$$

Find out all the assignments of Boolean variable in F that simultaneously satisfies all the clauses i.e. F=1.

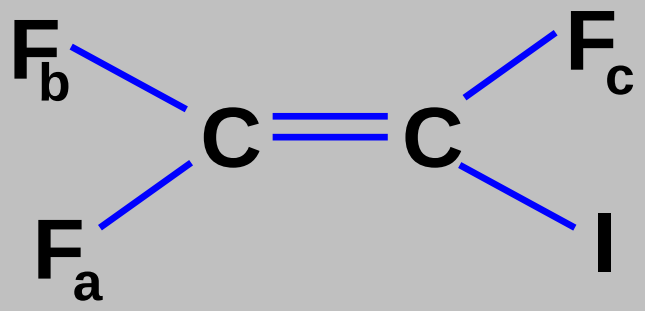
- Three variable 1-SAT problem
  - B = {x_1, x_2, x_3} , set of three variable.
  - Each clause (C_i) has one variable.
  - e.g. $F_1 = x_1 \wedge x_2 \wedge x_3$.

Farhi et al, quant-ph/0001106

NMR Implementation, using a 3-qubit system.

❑ The Sample.

Iodotrifluoroethylene(C_2F_3I)

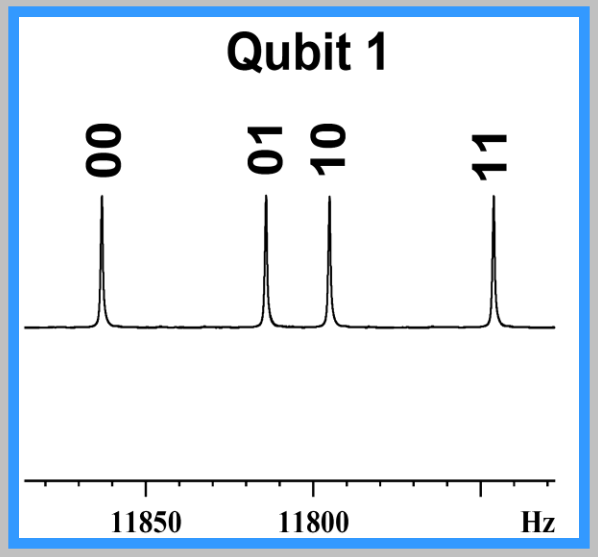


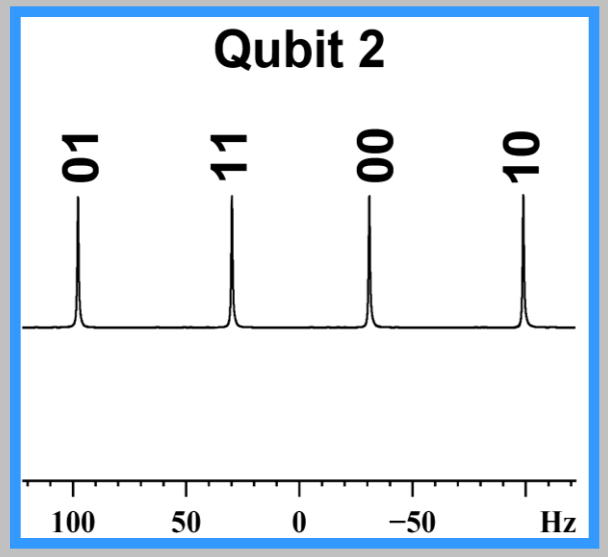
$$J_{ab} = 68.1\ \text{Hz}$$

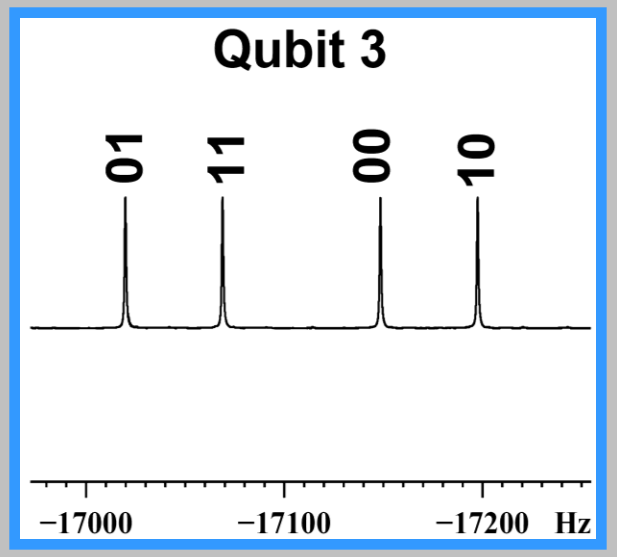
$$J_{ac} = 48.9\ \text{Hz}$$

$$J_{bc} = -128.8\ \text{Hz}$$

❑ Equilibrium Specrum.

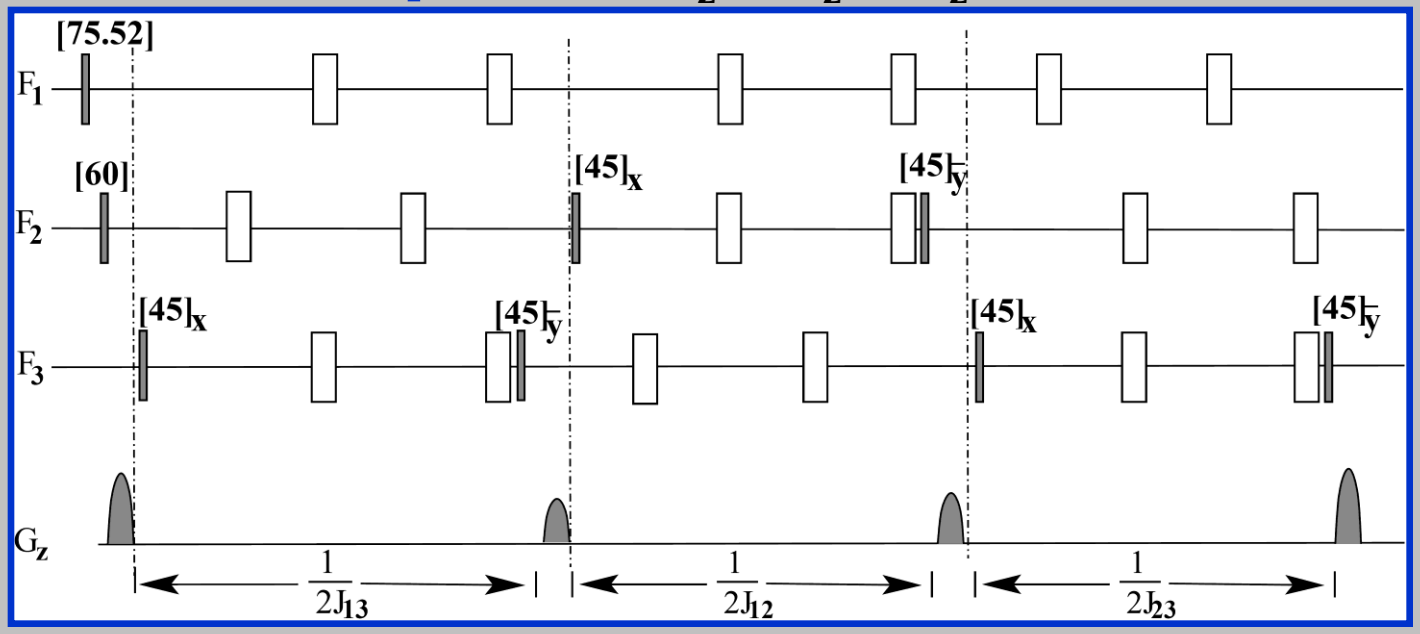






Step 1. Preparation of PPS

Equilibrium: $\mathbf{I}_z^1 + \mathbf{I}_z^2 + \mathbf{I}_z^3$



PPS: $\frac{1}{4}\left(\mathbf{I}_z^1 + \mathbf{I}_z^2 + \mathbf{I}_z^3 + 2\mathbf{I}_z^1\mathbf{I}_z^2 + 2\mathbf{I}_z^1\mathbf{I}_z^3 + 2\mathbf{I}_z^2\mathbf{I}_z^3 + 4\mathbf{I}_z^1\mathbf{I}_z^2\mathbf{I}_z^3\right)$

Step 3. Implementation of Adiabatic Evolution

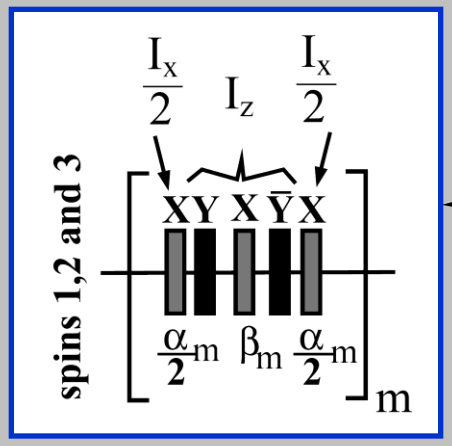
$$H_B = I_x^1 + I_x^2 + I_x^3 = \mathcal{I}_x \qquad H_F = I_z^1 + I_z^2 + I_z^3 = \mathcal{I}_z$$

$$H(m) = \left(1 - \frac{m}{M}\right) H_B + \frac{m}{M} H_F$$

mth step of the interpolating Hamiltonian .

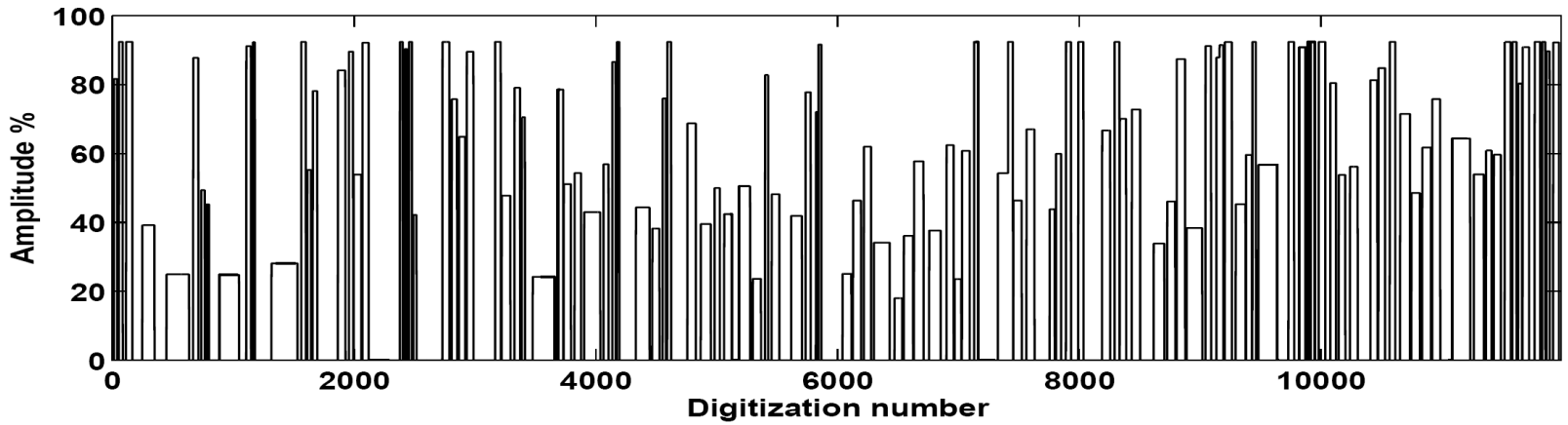
$$U_m \approx \underbrace{e^{-i\mathcal{I}_x\left(1-\frac{m}{M}\right)\frac{180}{2\pi}}}_{\left[\frac{\alpha_m}{2}\right]_x^{1,2,3}\ pulse} \cdot \underbrace{e^{-i\mathcal{I}_z\left(\frac{m}{M}\right)\frac{180}{\pi}}}_{\left[\beta_m\right]_z^{1,2,3}\ pulse} \cdot \underbrace{e^{-i\mathcal{I}_x\left(1-\frac{m}{M}\right)\frac{180}{2\pi}}}_{\left[\frac{\alpha_m}{2}\right]_x^{1,2,3}\ pulse}$$

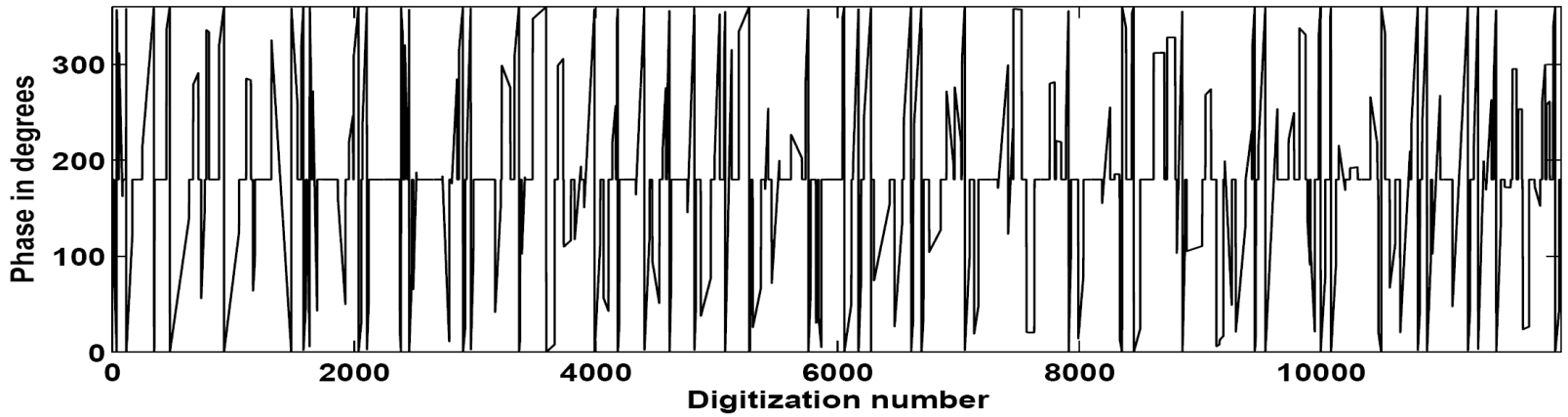
mth step of evolution operator



- Pulse sequence for adiabatic evolution
- Total number of iteration is 31
- **time needed = 62 ms**
  (400μs x 5 pulses x 31 repetitions)

Using Concatenated SMPs

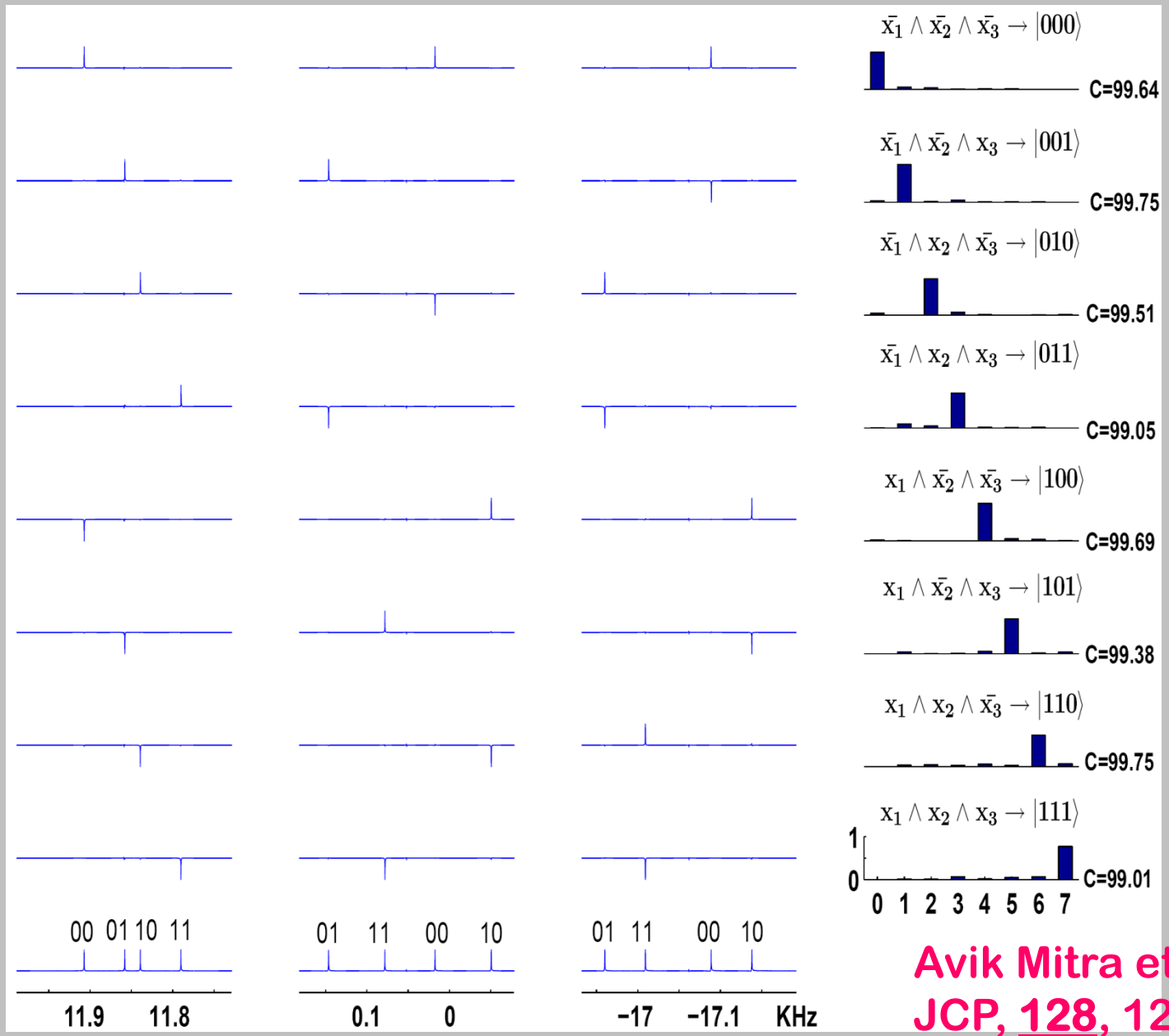




Duration: Max 5.8 ms, Min. 4.7 ms

Avik Mitra et al, JCP, 128, 124110 (2008)

Results for all Boolean Formulae



Avik Mitra et al,
JCP, 128, 124110 (2008)

Conclusions:

NMR QIP is at a Cross -Road

Many Operations and Algorithms can be Implemented

A Very Good Tool for Learning and Explorations

Scaling is Difficult

If

All Spins are to be coupled to each other with non-degenerate Transitions

Possible to obtain high number of qubits

If

Only nearest neighbor couplings are sufficient

Backbone of a C-13, N-15 labeled protein with side chain protons deuterated

How to do QIP?

Future Directions

1. **To increase the number of Qubits in NMR.**
   Synthesis molecules with several hetero-nuclei.

2. **To use strongly modulated pulses (SMPs) and Control Theory for performing**
   Unitary operations in short times and accurately.

3. **To search for systems with large coherence times.**
   For example singlet states in equivalent spins or spins systems with symmetry with symmetry preserving relaxation.

4. **Develop protocols which can be carried out using spins with nearest neighbor couplings.**

5. **To enhance nuclear polarization by transferring Electron polarization using DNP.**

Thank You