Experimental Implementation of Adiabatic Quantum Algorithms by NMR

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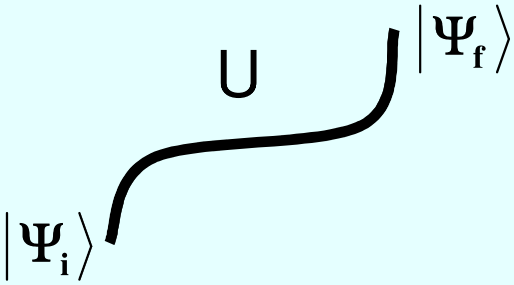
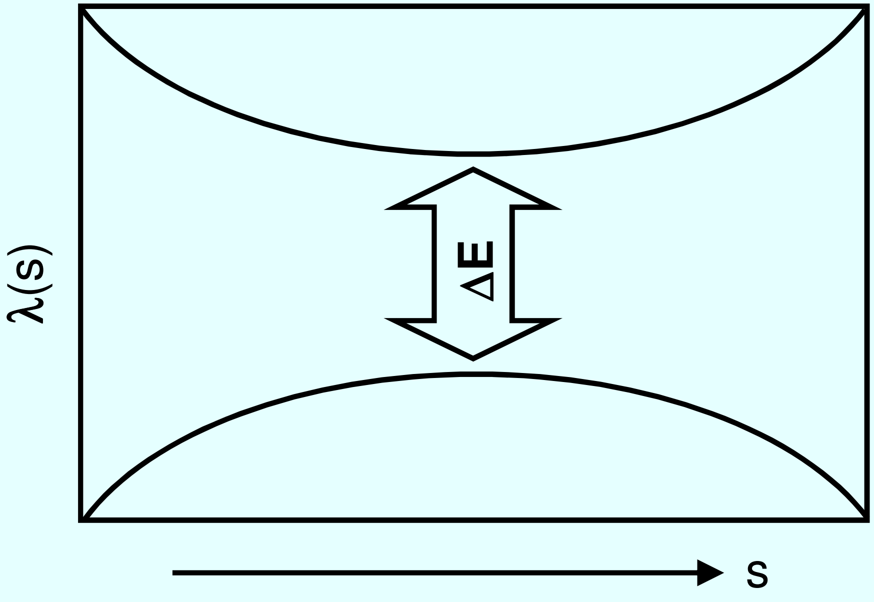
ADIABATIC QUANTUM ALGORITHMS

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

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

Where $\varepsilon << 1$

Farhi et al, PRA, 65,012322 (2202), 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**.

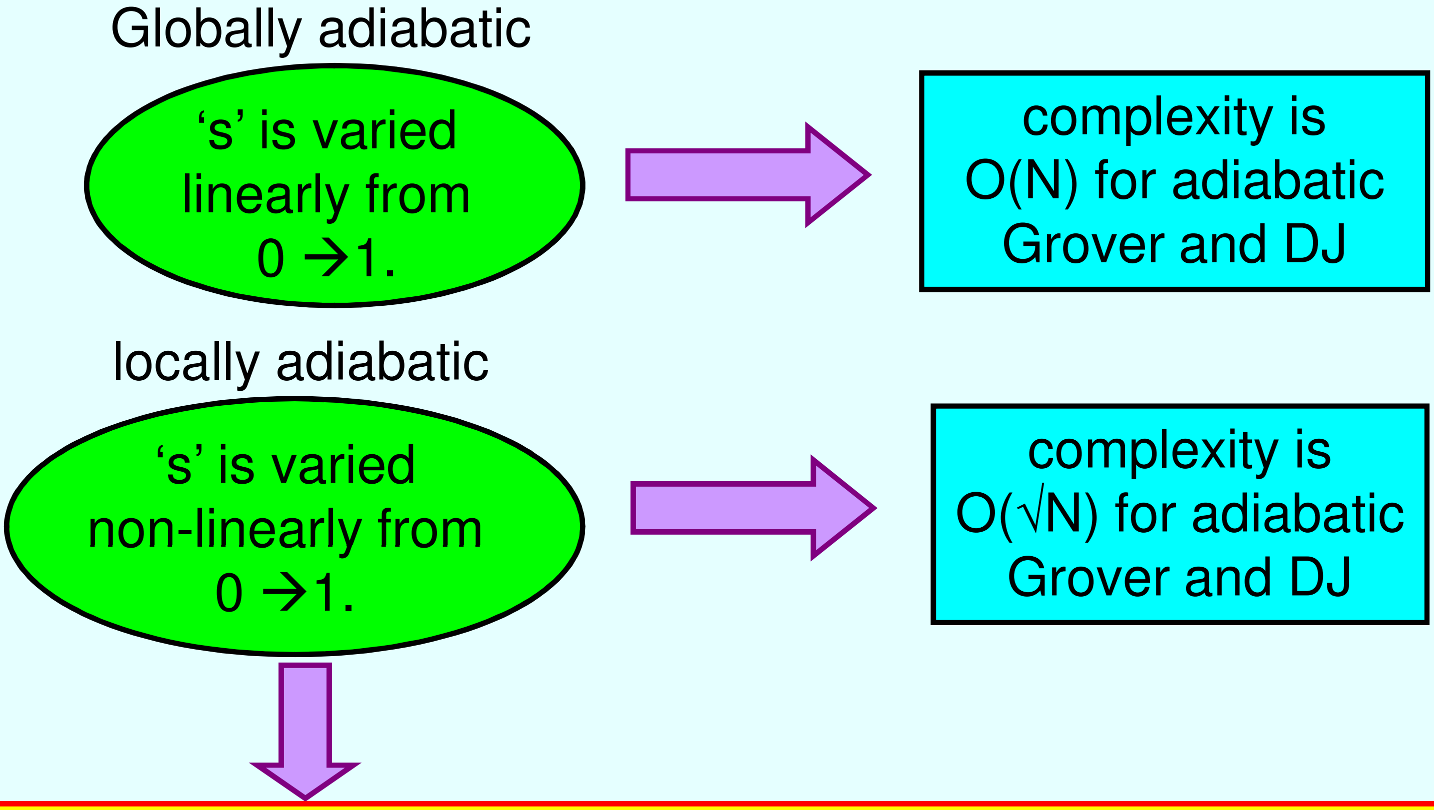
$H(s) = (1\text{-}s)H_B + sH_F$
$H_B \equiv$ beginning Hamiltonian
$H_F \equiv$ Final Hamiltonian

- Initialize register to desired input qubits.

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

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

Non linear evolution of the system.



Globally adiabatic

's' is varied linearly from 0 →1.

complexity is O(N) for adiabatic Grover and DJ

locally adiabatic

's' is varied non-linearly from 0 →1.

complexity is O(√N) for adiabatic Grover and DJ

- The adiabticity condition is applied at each instant of evolution
- Evolution rate is varied continuously with time speeding up the algorithm.
- The evolution is faster when the gap ΔE is large and slow when it is small.

Roland *et al*, PRA 65 (2002) 042308; S. Das *et al*, PRA 65 (2002) 062310

Adiabatic Grover's Algorithm

- Evolve it under the Hamiltonian $H(s)=(1-s)H_B + sH_F$.
- H_B – The beginning Hamiltonian whose ground state is the equal superposition of all the states corresponding to the entries in the database.
- H_F – The final Hamiltonian that has the solution state ("marked state") as its ground state.
- In NMR the evolution operator is varied in discrete steps

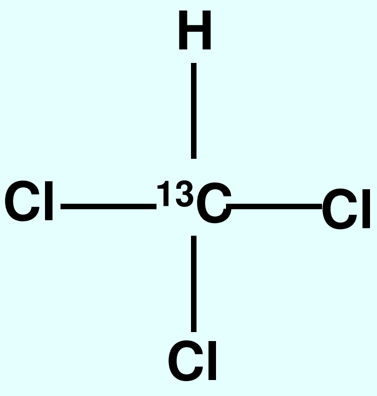
$$U_m = e\left\{-i\left[\left(1-\frac{m}{M}\right)H_B + \frac{m}{M}H_F\right]\Delta t\right\}$$

- Since H_B and H_F do not commute, the evolution is approximated by Trotter's Formula as:

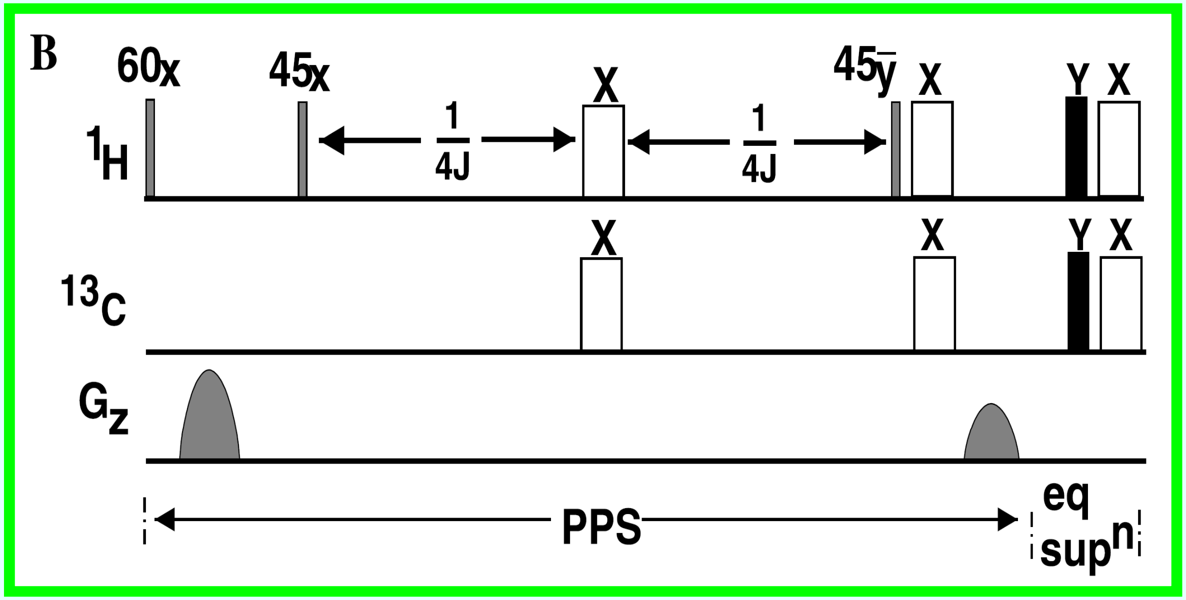
$$U_m = e^{-iH_B(1-\frac{m}{M})\Delta t/2} \bullet e^{-iH_F(\frac{m}{M})\Delta t} \bullet e^{-iH_B(1-\frac{m}{M})\Delta t/2}$$

Roland & Cerf, PRA 65 (2002) 042308

Step1: Preparation of Pseudo Pure states



- Experiment carried out in AV500
- H and C has resonance frequency 500 MHz and 125 MHz.
- J_{HC}= 209 Hz



$$4I_{1z} + I_{2z}$$

$$\downarrow \; 60^\circ_x{}^{(1)}, G_z$$

$$2I_{1z} + I_{2z}$$

$$\downarrow \; 45^\circ_x{}^{(1)}, \tau = 1/2J$$

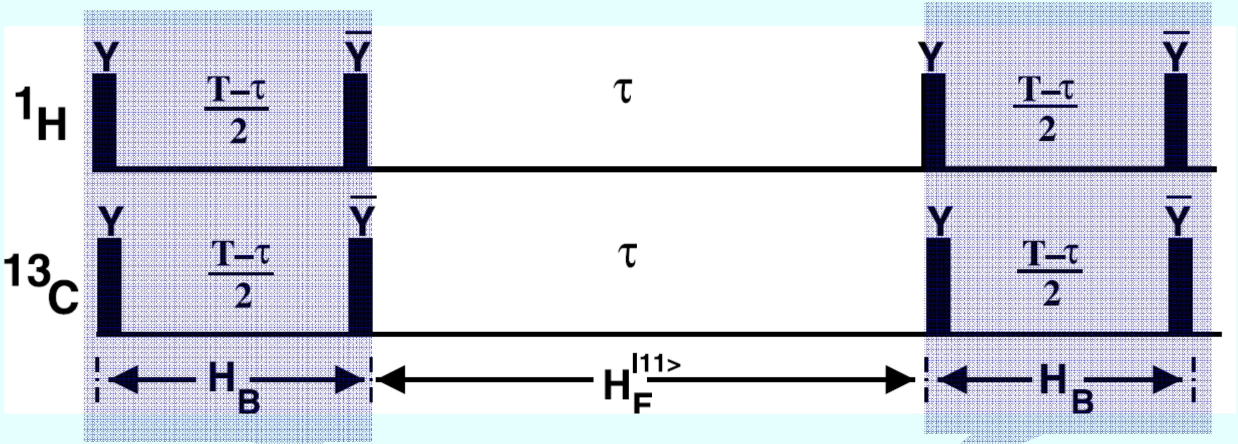
$$2I_{1z}/\surd 2 + I_{2} - 4\, I_{1z}I_{2x}/\surd 2$$

$$\downarrow \; 45^\circ_{\bar{y}}, G_z$$

$$(I_{1z} + I_{2z} + 2I_{1z}I_{2z})$$

Cory, Price, Havel, PNAS, 94 (1997) 1634

Step2: Adiabatic Evolution (H_B)



Pulse sequence for Implementation of H_B

$$\Longleftrightarrow \quad \frac{1}{2}\begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

- NMR Hamiltonian:

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

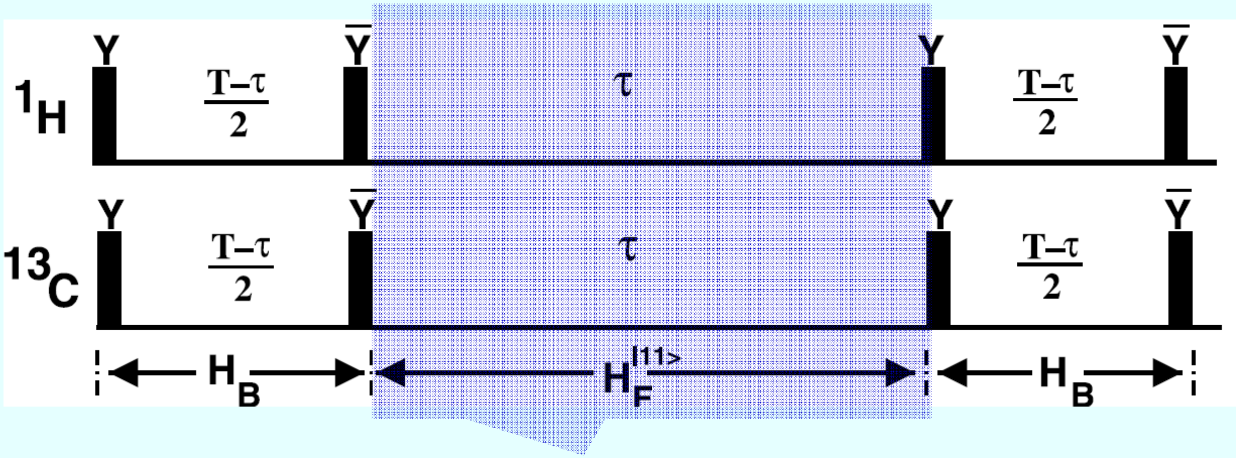
- Beginning Hamiltonian

$$\mathbf{H}_B = \mathbf{I}_{x1} + \mathbf{I}_{x2} + 2\mathbf{I}_{x1}\mathbf{I}_{x2}$$

- Choose $v_1 = v_2 = -J_{12}/2$ for both proton and carbon, so H becomes = H^B
- Free evolution under the NMR Hamiltonian between two $\pi/2$ pulses with appropriate phases for a time $(T-\tau)/2$.

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

Step2: Adiabatic Evolution (H_F)



Pulse sequence for Implementation of H_F ⇔

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

- Final Hamiltonian

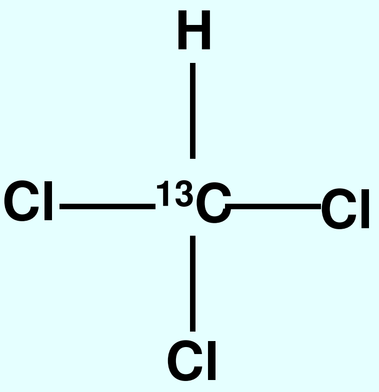
$$H_F^{|11\rangle} = I_{z1} + I_{z2} + 2I_{z1}I_{z2}$$

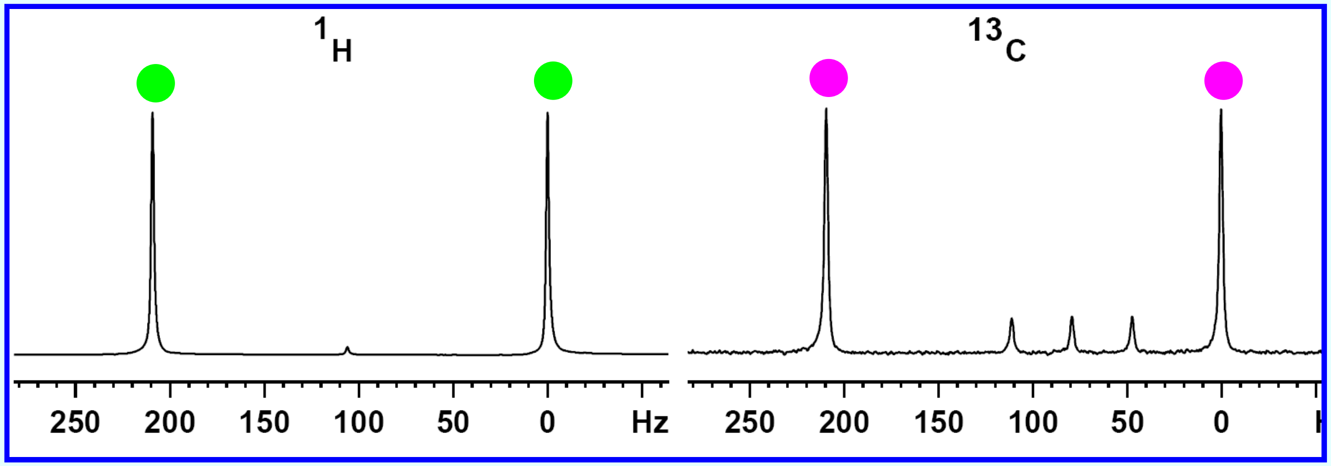
- Choose $v_1 = v_2 = -J_{12}/2$ for both proton and carbon
- Free evolution under the NMR Hamiltonian for a time τ

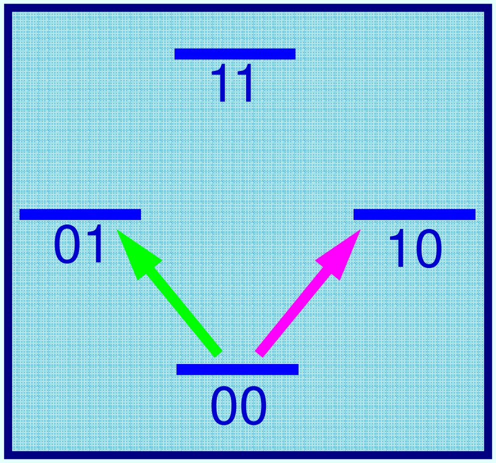
Avik Mitra et al, JMR, 177, 285 (2005)

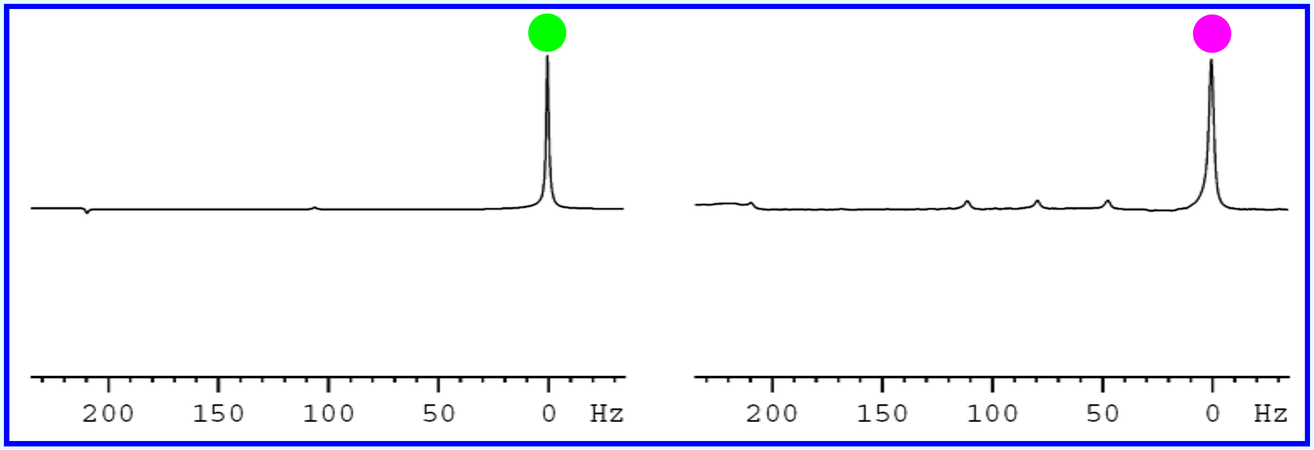
Experimental Results

Equilibrium Spectrum



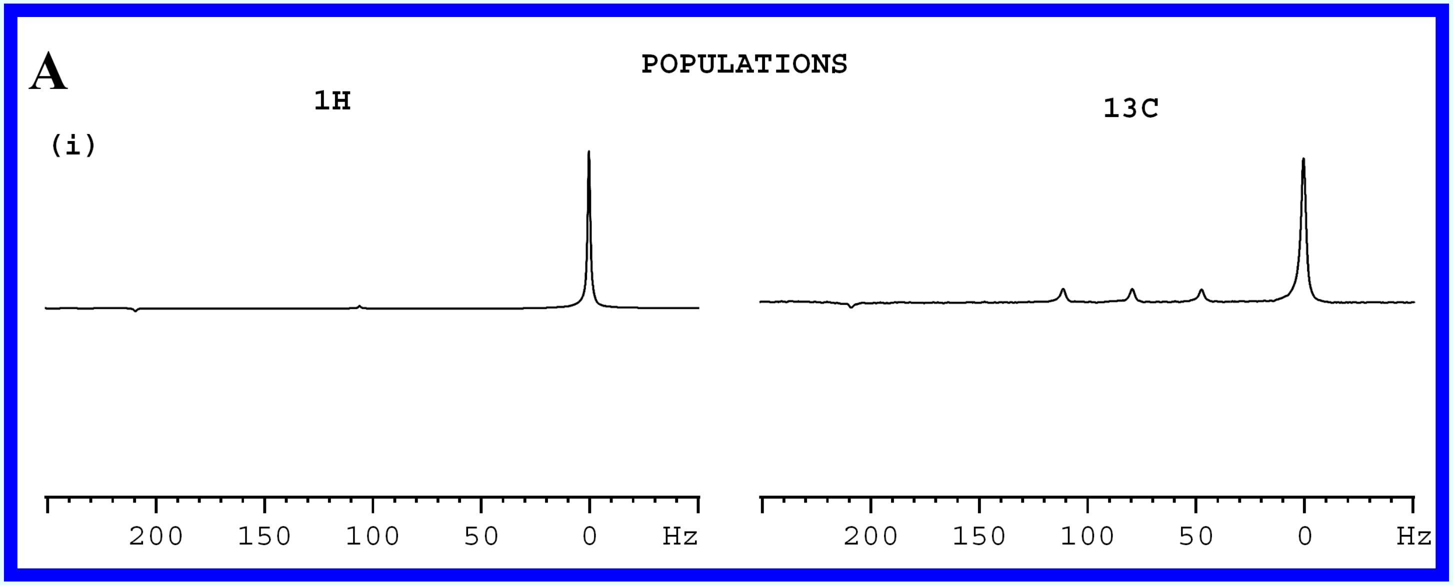


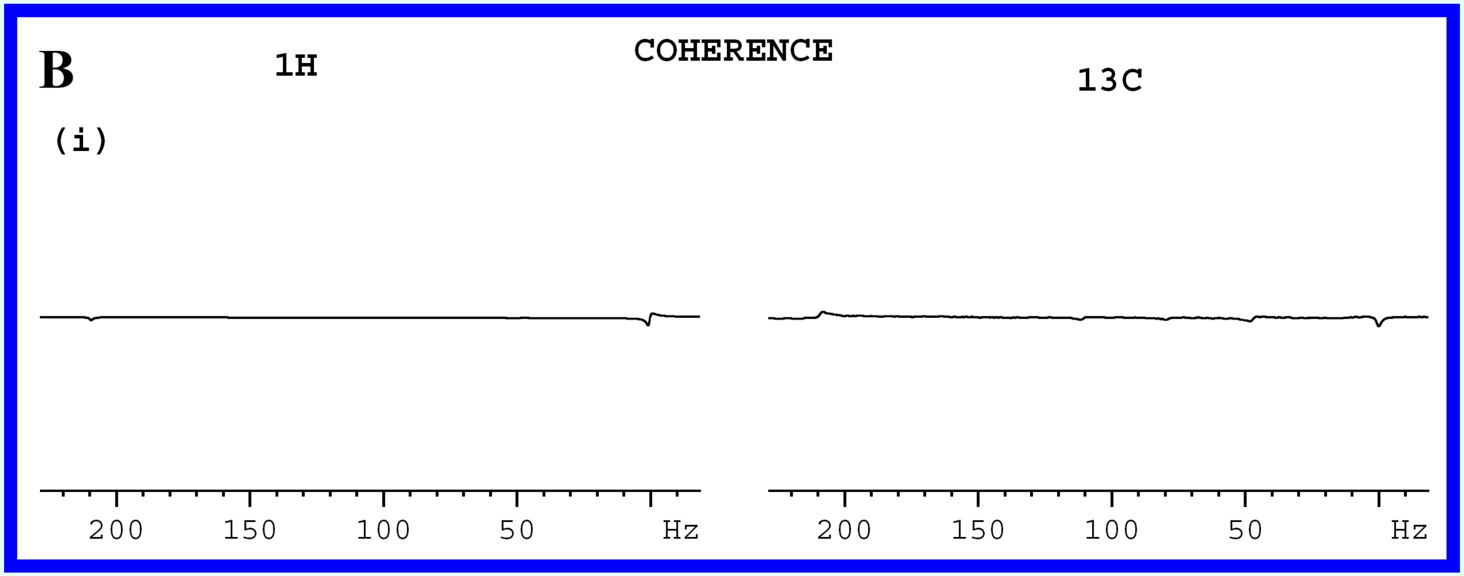




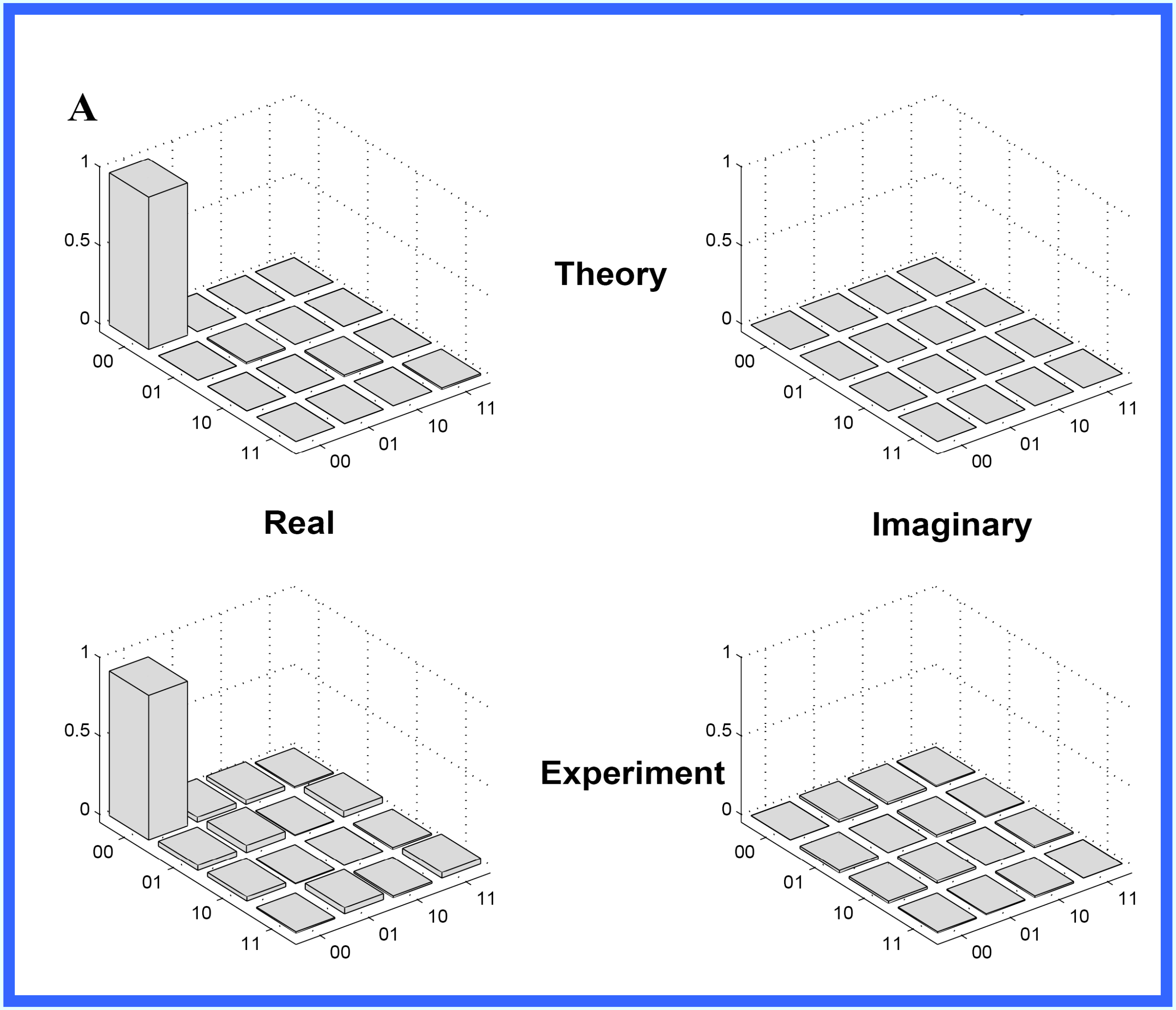
Spectrum after PPS

Experimental Result for the searched state |00>





Output Density Matrix for the searched state |00>



Average absolute deviation

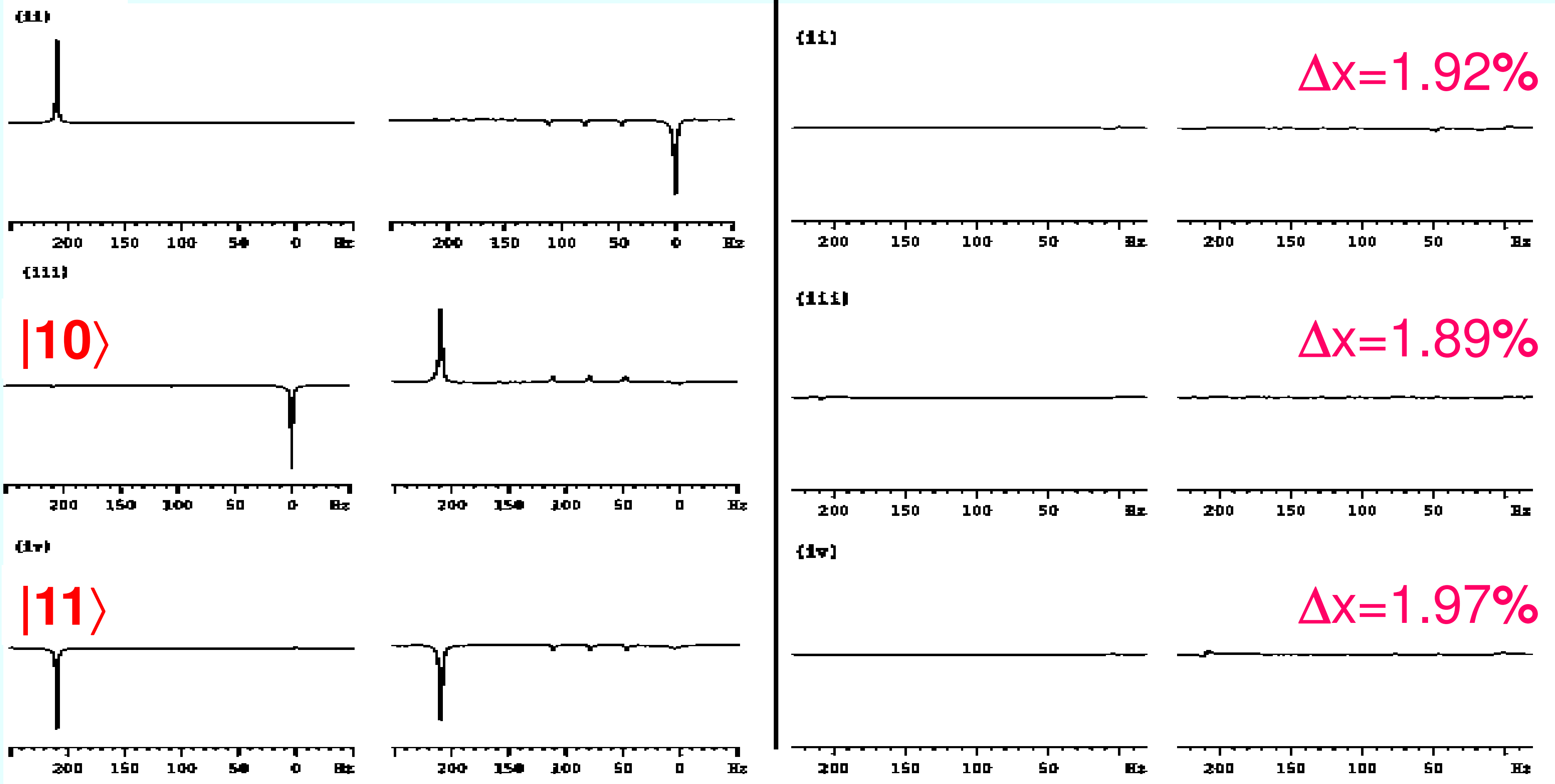
$$\boxed{\Delta x = \frac{1}{N^2}\sum_{i,j=1}^{N}\left|x^{\mathrm{T}}_{i,j} - x^{\mathrm{E}}_{i,j}\right|}$$

2.49%

Experimental Results for searched states $|01\rangle$, $|10\rangle$, $|11\rangle$

Populations

Coherence



$|01\rangle$

$|10\rangle$

$|11\rangle$

$\Delta x = 1.92\%$

$\Delta x = 1.89\%$

$\Delta x = 1.97\%$

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

H$_F$: $\mathbf{I} - |\psi_F\rangle\langle\psi_F|$ 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

$$\mathbf{H_I} = \mathbf{I_x^1} + \mathbf{I_x^2} + 2\mathbf{I_x^1 I_x^2}$$

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

Constant case

Balanced case

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

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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.

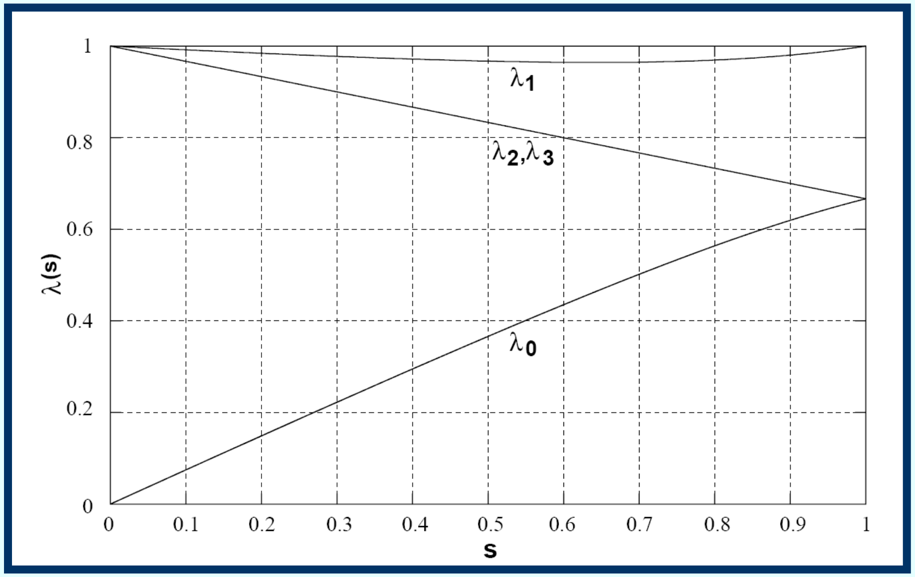
$$H_F^B = -\frac{1}{6}\left(I_z^1 + I_z^2 + 2I_z^1 I_z^2\right) \cancel{+ \frac{2}{3}\left(I_x^1 I_x^2 + I_y^1 I_y^2\right) + \frac{1}{3}\left(I_x^1 + I_x^2\right) - \frac{2}{3}\left(I_x^1 I_z^2 + I_z^1 I_x^2\right)}$$

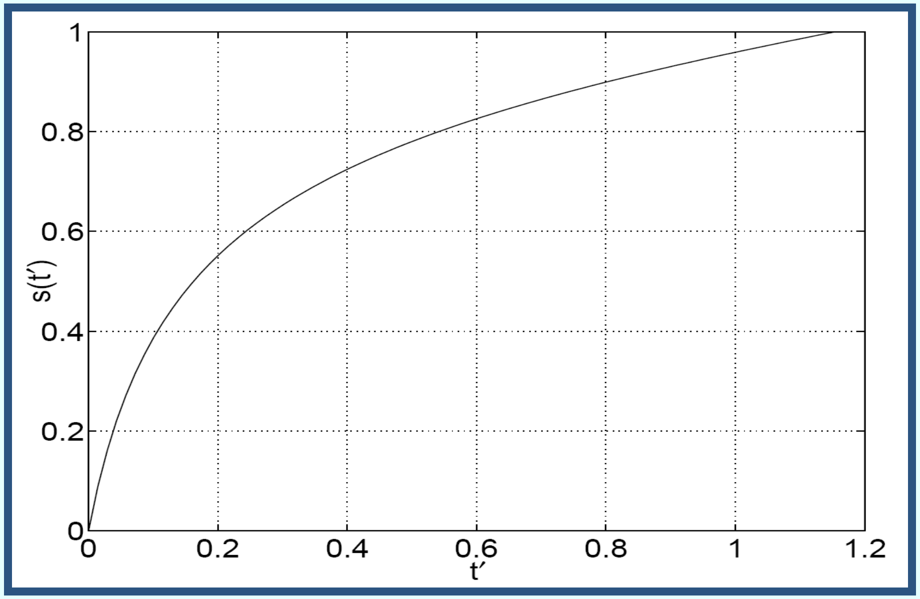
$$\Downarrow$$

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

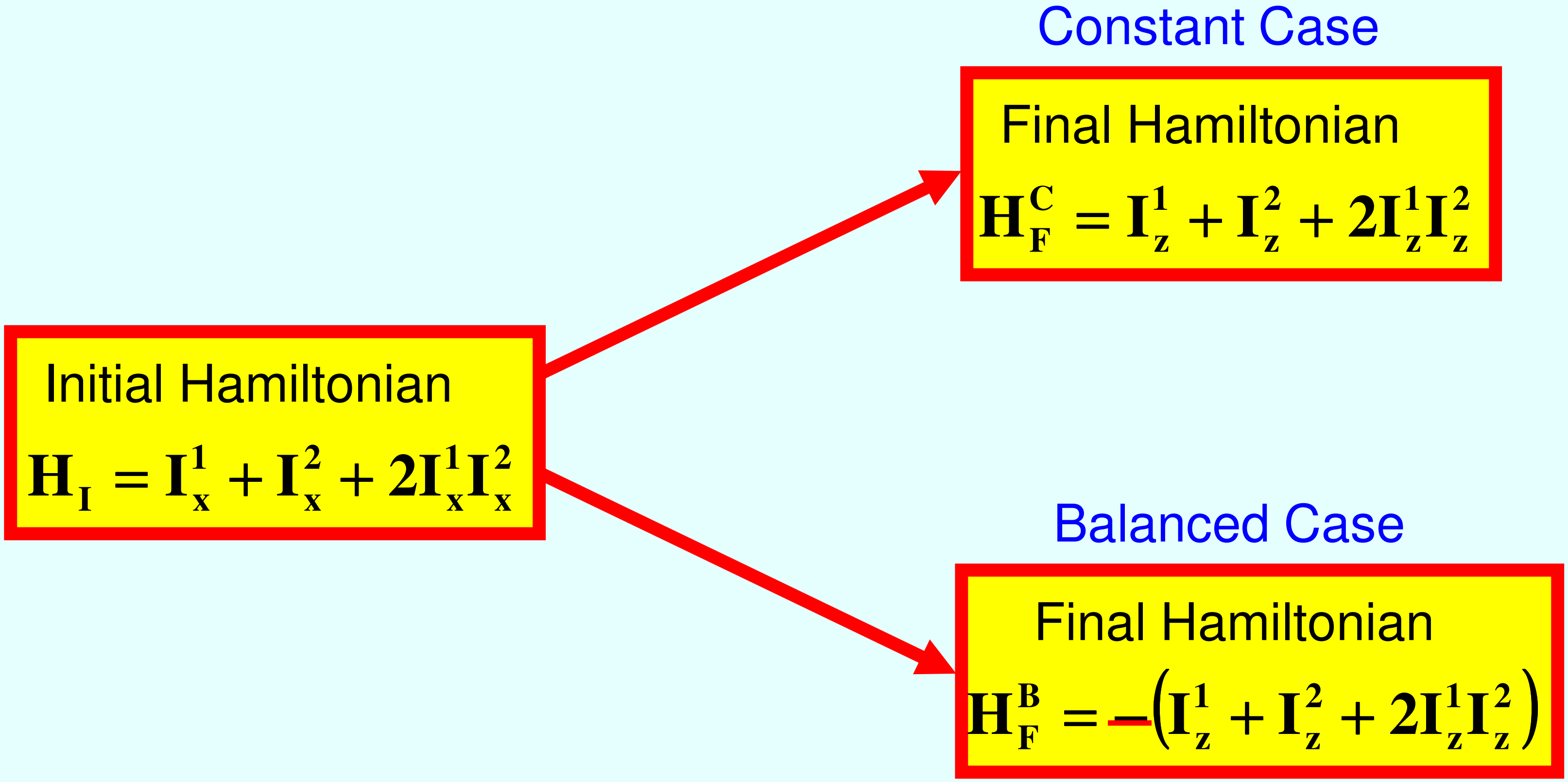
Avik Mitra et al, JMR, 177, 285 (2005)

Eigenvalues with respect to the parameter ‘s’.





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



Initial Hamiltonian

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

Constant Case

Final Hamiltonian

$$H_F^C = I_z^1 + I_z^2 + 2I_z^1 I_z^2$$

Balanced Case

Final Hamiltonian

$$H_F^B = -\left(I_z^1 + I_z^2 + 2I_z^1 I_z^2\right)$$

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

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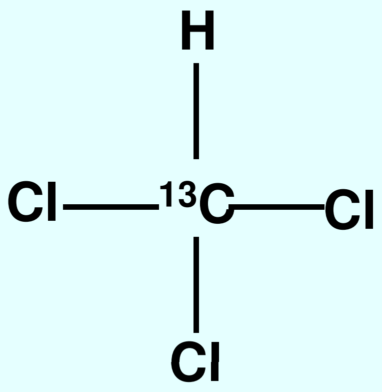
NMR Implementation.

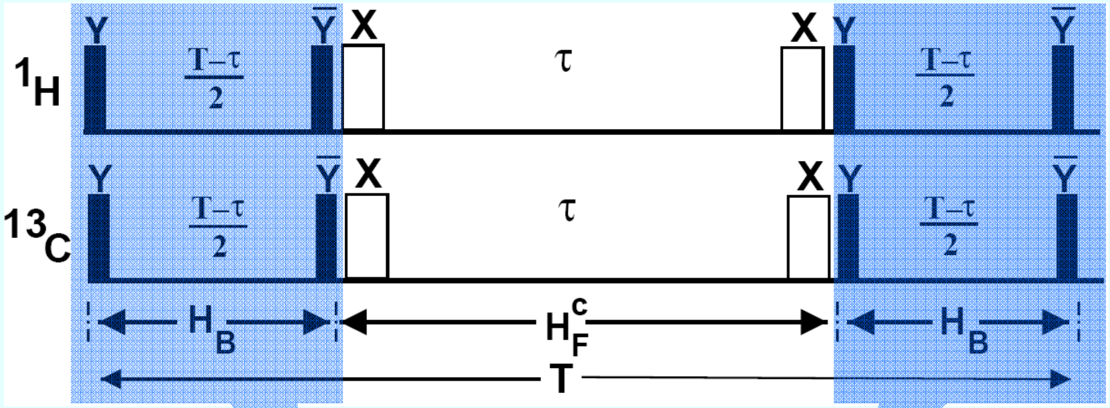
- Sample



- 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 $v_1 = v_2 = -\ J_{12}/2$ and with two pi/2 pulses with appropriate phases

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

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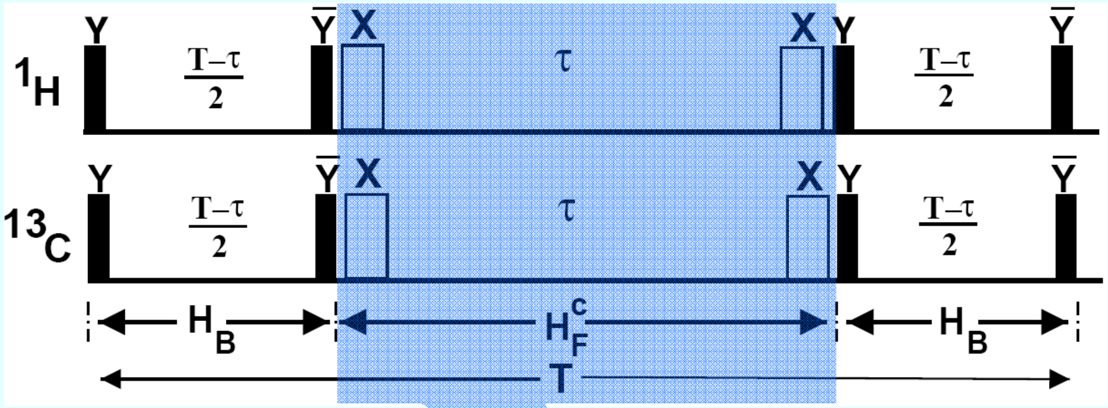
Pulse sequence for Implementation of H^F

- CONSTANT CASE



Pulse sequence for Implementation of H_F

➢ NMR Hamiltonian:

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

➢ Final Hamiltonian

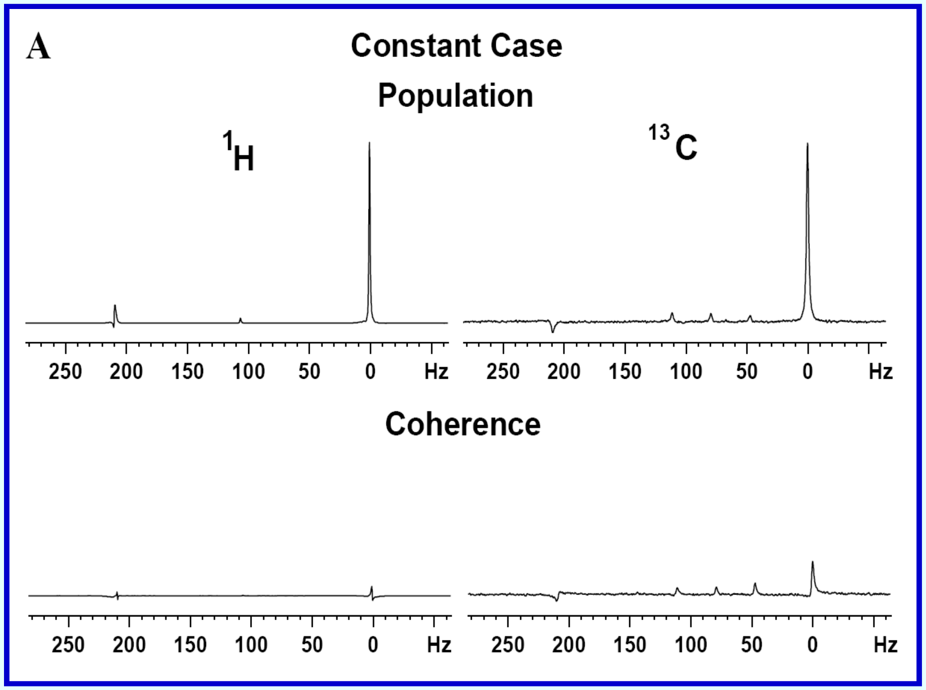
For $v_1 = v_2 = -\ J_{12}/2$

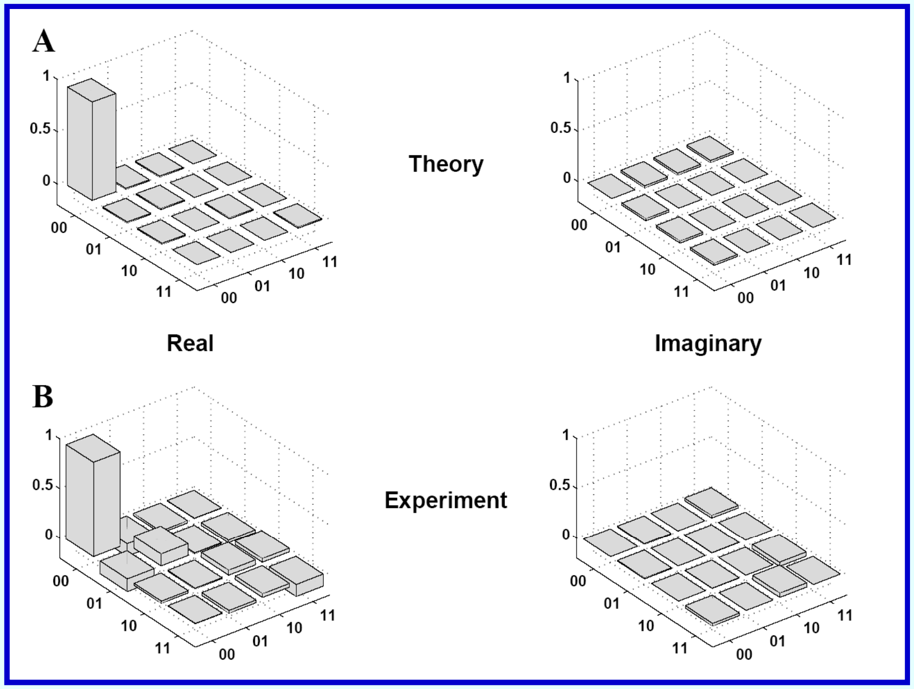
$$\mathbf{H}_F = \mathbf{I}_{z1} + \mathbf{I}_{z2} + 2\mathbf{I}_{z1}\mathbf{I}_{z2}$$

- 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⟩

Average absolute deviation

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

5.28%

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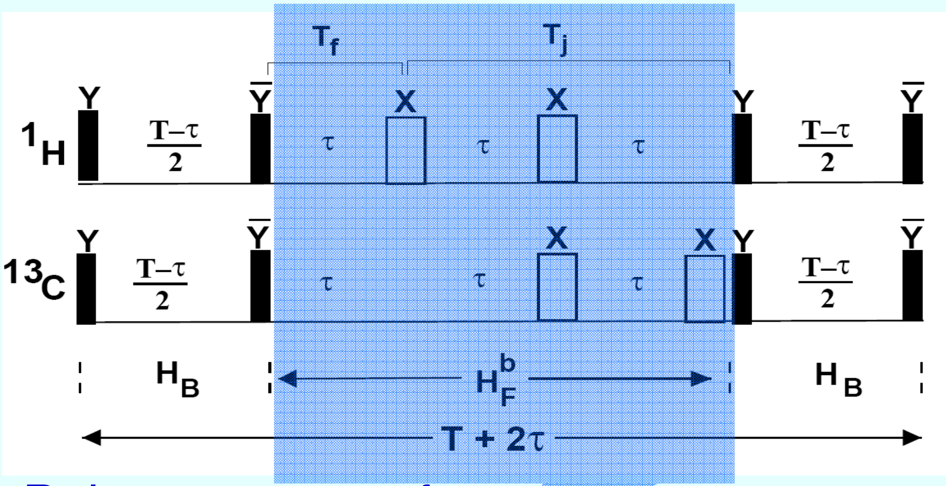
NMR Implementation

- BALANCED CASE



Pulse sequence for Implementation of H_F

- NMR Hamiltonian:

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

- Final Hamiltonian

For $v_1 = v_2 = -\ J_{12}/2$

$$\mathbf{H}_F = -\left(\mathbf{I}_{z1} + \mathbf{I}_{z2} + 2\mathbf{I}_{z1}\mathbf{I}_{z2}\right)$$

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

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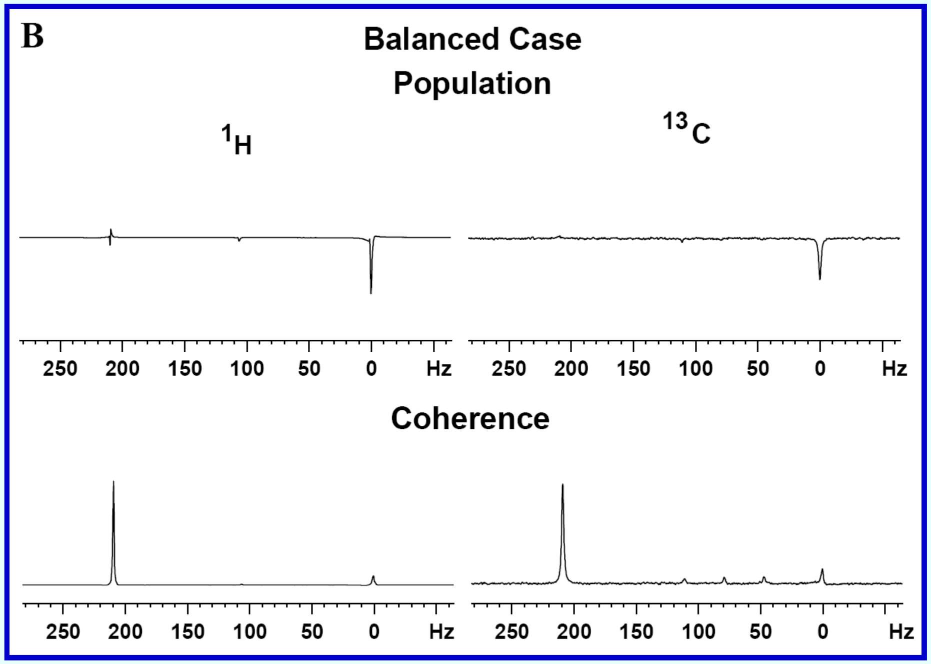
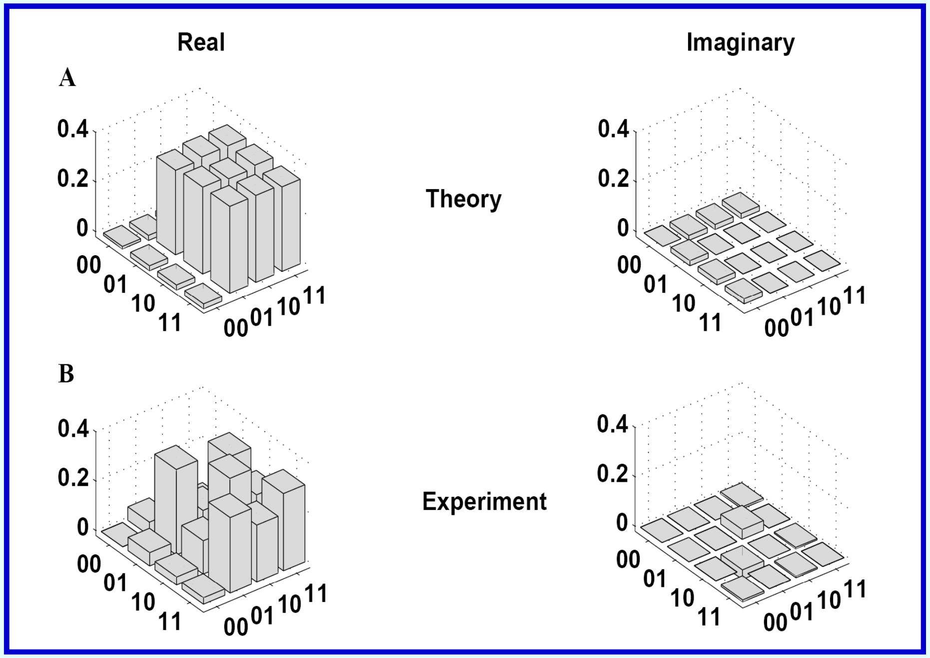
Experimental Result





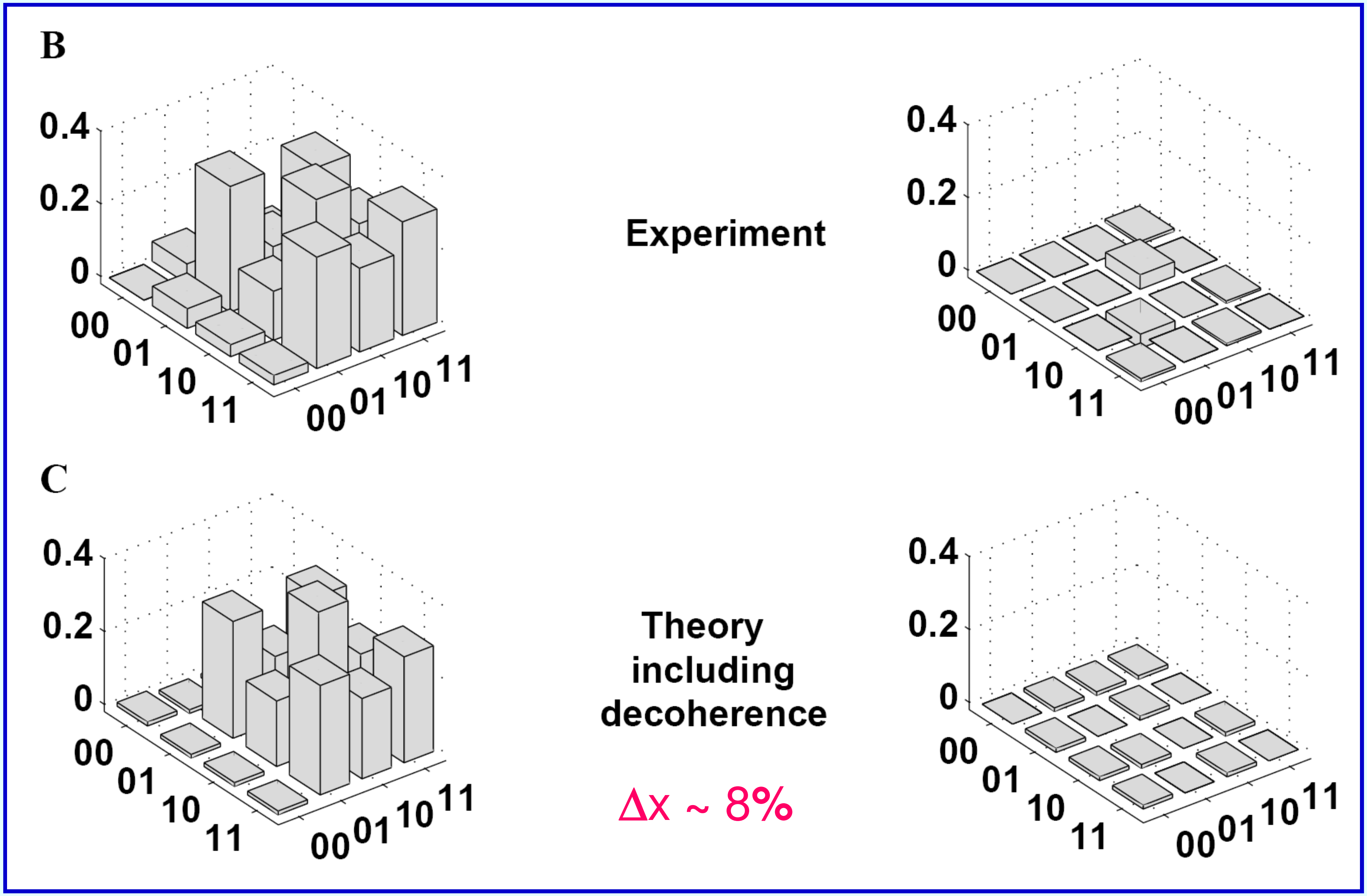
Δx ~ 17%

- 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

Δx ~ 8%

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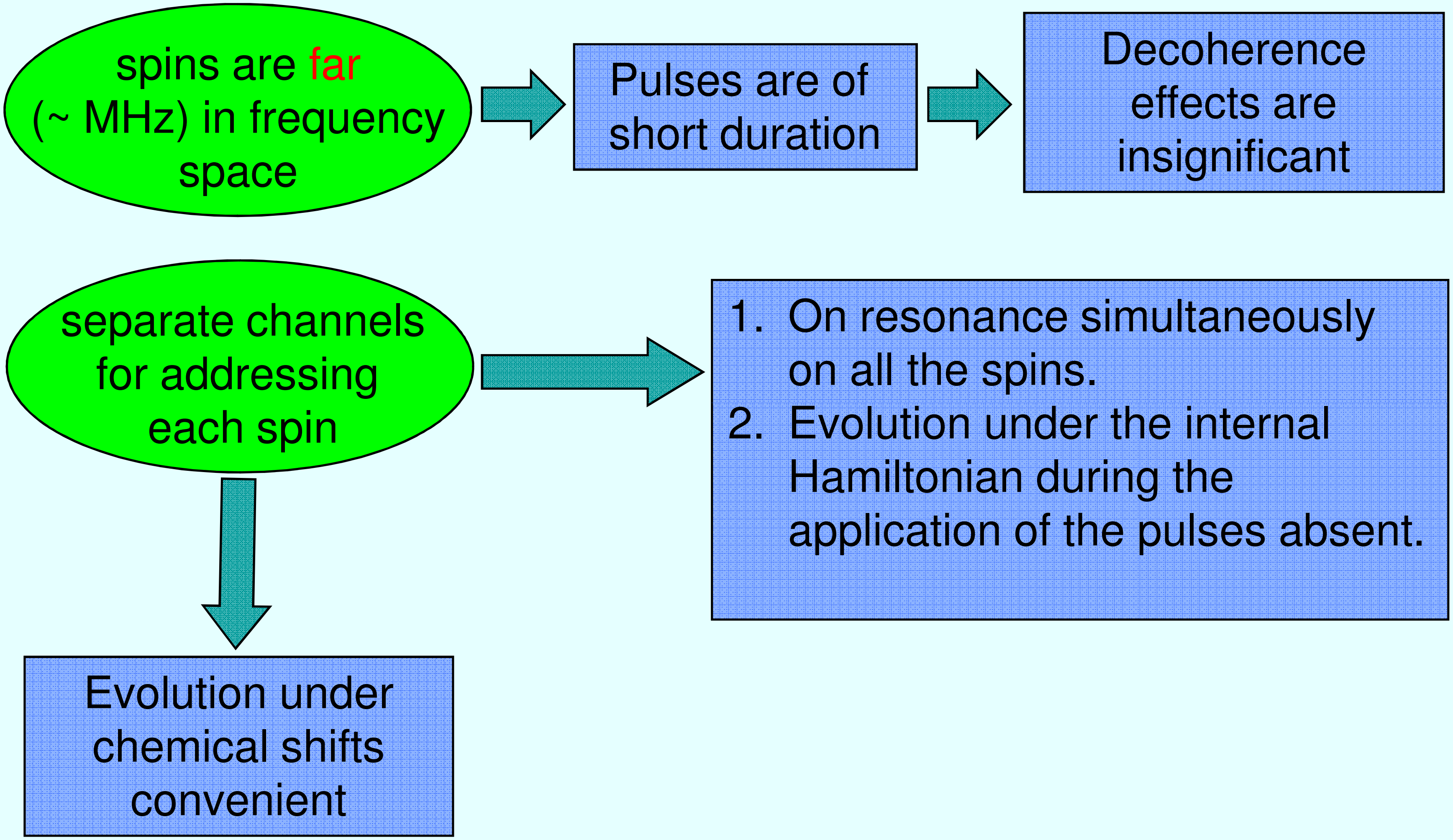
ADIABATIC SAT ALGORITHM BY STRONGLY MODULATED PULSES

In a Hetronuclear spin system



spins are far (~ MHz) in frequency space

Pulses are of short duration

Decoherence effects are insignificant

separate channels for addressing each spin

1. On resonance simultaneously on all the spins.
2. Evolution under the internal Hamiltonian during the application of the pulses absent.

Evolution under chemical shifts convenient

In a Homonuclear spin systems

spins are close (~ kHz) in frequency space

Pulses are of longer duration

Decoherence effects cannot be ignored

same channel for addressing each spin

On resonance with one spin at a time

Evolution of other spins under the internal Hamiltonian present.

- Evolution under chemical shift Hamiltonian has to be carried out separately for each spin and to refocus the evolution of other spins.
- Chemical shift evolution with composite pulses would require calibration of many pulses which may be error prone.

Strongly Modulated Pulses circumvents the above problems

Strongly Modulated Pulses.

- Numerically optimized pulses.
- system Hamiltonian is taken into consideration while designing the pulses.
- This leads to precise unitary transformation.

$$H_{\text{int}} = \sum_{j=1}^{n} \omega_j I_z^j + 2\pi \sum_{\substack{j<k,\\ k=2}}^{n} J_{jk} I_z^j I_z^k$$

System Hamiltonian of weakly coupled spin system

$$H_{\text{ext}}(\omega_{rf}, \varphi, \omega, t) = \sum_{k=1}^{n} e^{-i(\omega_{rf} t + \varphi)} \cdot \left(-\omega I_x^k\right) \cdot e^{i(\omega_{rf} t + \varphi)}$$

Hamiltonian representing the radio frequency pulse

$$H_{\text{tot}} = H_{\text{int}} + H_{\text{ext}}$$

In the rotating frame:

$$H_{\text{eff}} = H'_{\text{int}} + \sum_{k=1}^{n} -\omega \left\{ I_x^k \cos(\phi) + I_y^k \sin(\phi) \right\}$$

$$\rho(t) = e^{-iH_{\text{eff}} t} \cdot \rho(0) \cdot e^{iH_{\text{eff}} t}$$

Fortunato *et al*, JCP 116 (2002) 7599, Mahesh *et al*, PRA 74 (2006) 062312

Strongly Modulated Pulses.

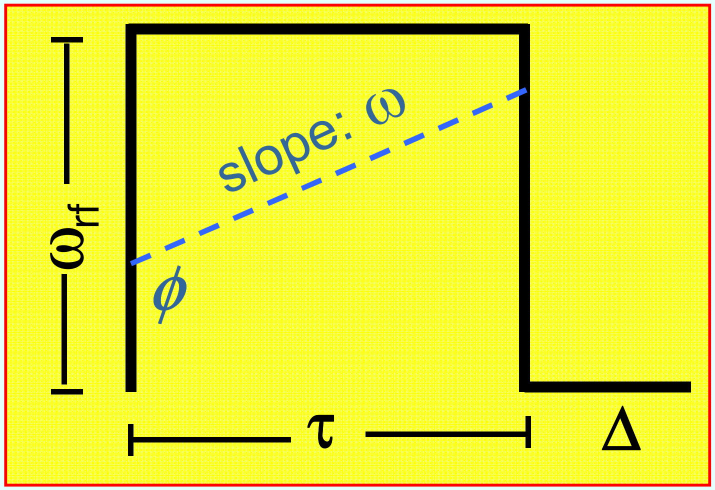
- Back transformation to the original frame is done.

$$\rho(t) = U_z^{-1} \cdot e^{-iH_{eff}t} \cdot \rho(0) \cdot e^{iH_{eff}t} \cdot U_z$$

Unitary operator for rotating frame transformation

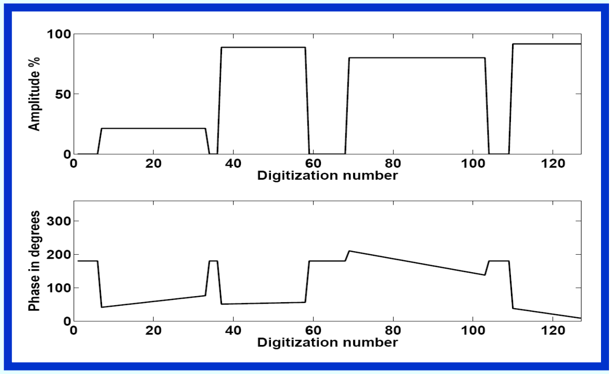
$$U_z(\tau) = e^{\left(-i\omega_{rf}\sum_{k=1}^{n} I_z^k \tau\right)}$$

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



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

Nedler-Mead Simplex Algorithm **`(fminsearch)`**



Avik Mitra et al, JCP, in press

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

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

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

Adiabatic SAT Problem

$$H_B = -\sum_j \sigma_x^j \longrightarrow$$

The ground state is: $\sum_x |x\rangle, \; x \in \{0,1\}^{\otimes n}$

Equal superposition of states

$$H_P|x_1x_2x_3\rangle = -\sum_C \underbrace{h_C(x_i)}|x_1x_2x_3\rangle$$

0 if x_i satisfies clause C
1 if x_i does not satisfy clause C

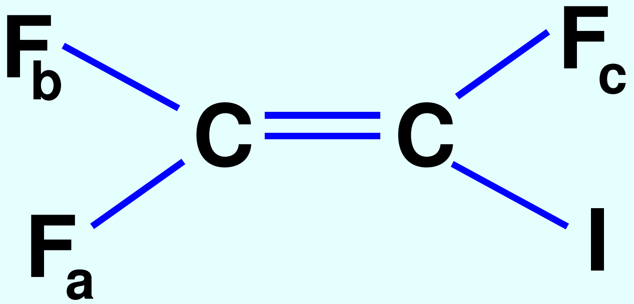
- Energy of each state is raised by one unit if it does not satisfy a clause.
- States that satisfy al the clauses have minimum energy.
- Final Hamiltonian is diagonal in computational basis.

Farhi et al, quant-ph/0001106

NMR Implementation.

❑ The Sample.

Iodotrifluoroethylene(C_2F_3I)

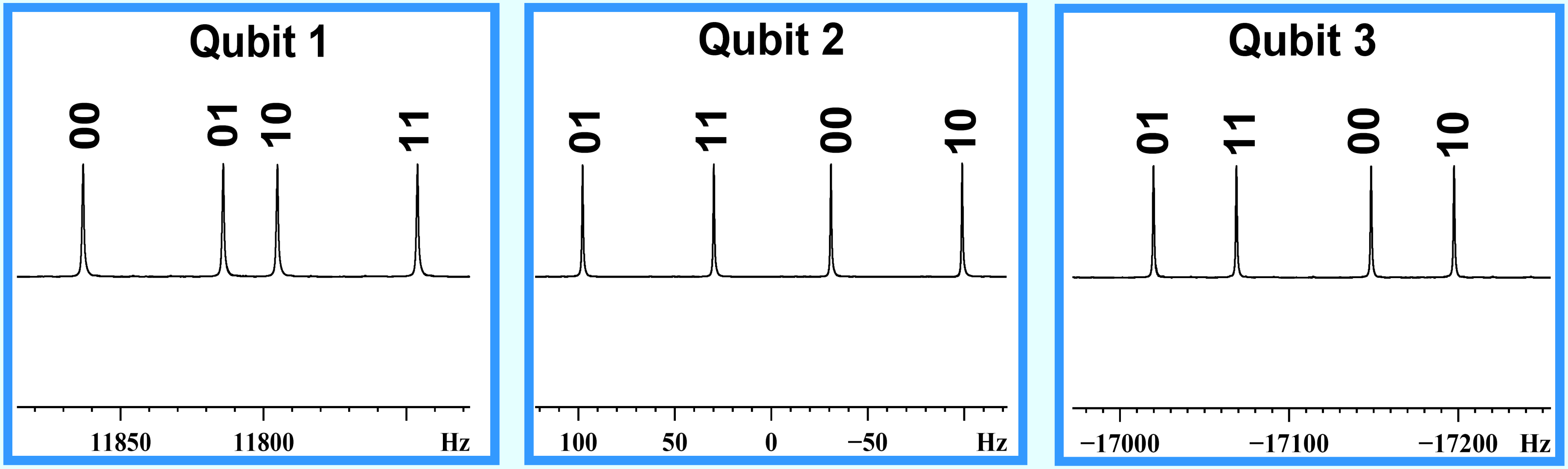


J_{ab} = 68.1 Hz

J_{ac} = 48.9 Hz

J_{bc} = −128.8 Hz

❑ Equilibrium Specrum.

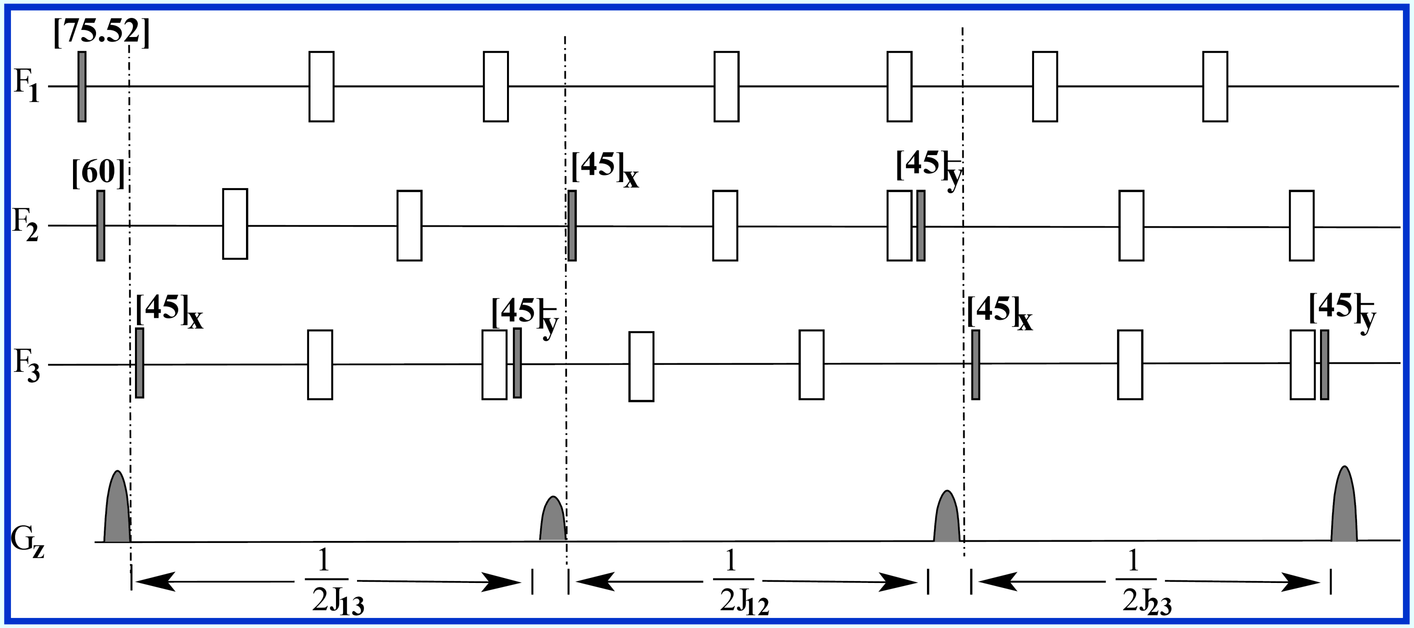


NMR Implementation

Step 1. Preparation of PPS

$$\boxed{\mathbf{I}_z^i + \mathbf{I}_z^k \xrightarrow{\left[\frac{\pi}{4}\right]_x^k - \frac{1}{2J_{ik}} - \left[\frac{\pi}{4}\right]_{\bar{y}}^k - G_z} \mathbf{I}_z^i + \frac{1}{2}\left(\mathbf{I}_z^k + 2\mathbf{I}_z^i\mathbf{I}_z^k\right)}$$

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

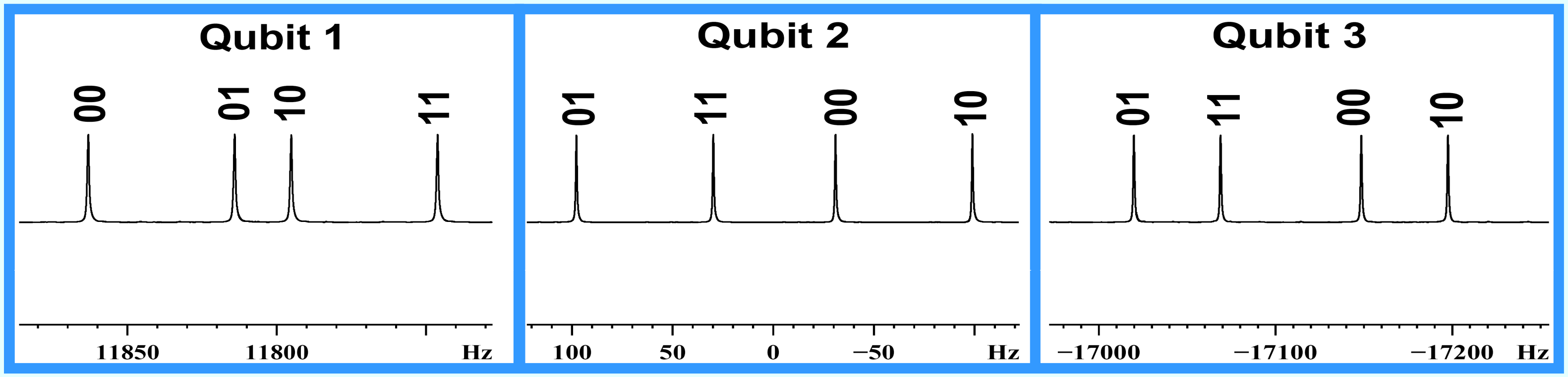


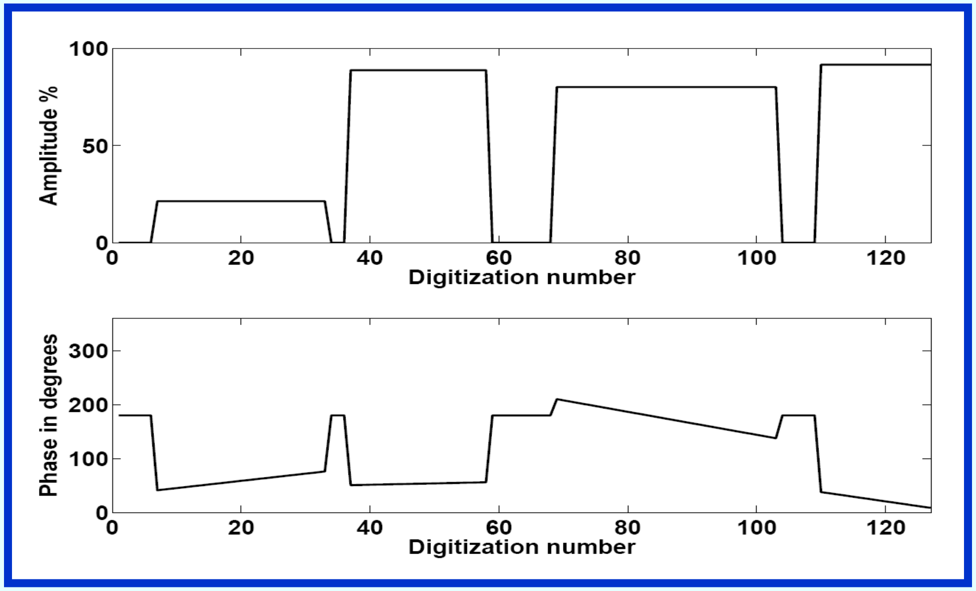
PPS: $\frac{1}{4}\left(\mathbf{I}_z^1 + \mathbf{I}_z^2 + \mathbf{I}_z^3 + 2\mathbf{I}_z^1\mathbf{I}_z^2 + 2\mathbf{I}_z^1\mathbf{I}_z^3 + 2\mathbf{I}_z^2\mathbf{I}_z^3 + 4\mathbf{I}_z^1\mathbf{I}_z^2\mathbf{I}_z^3\right)$

NMR Implementation

Step 2. Creation of Equal Superposition.

- can be achieved by pseudo-Hadamard on all three spins $\equiv \left[\frac{\pi}{2}\right]^{1,2,3}_{\bar{y}}$
- single high power π/2 pulse has offset effect.
- The high power pulse is replaced by an SMP.





soft pulses on all three spins ~400 μs

SMP: 100.5μs

Avik Mitra et al, JCP, in press

NMR Implementation

Step 2. Implementation of Adiabatic Evolution

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

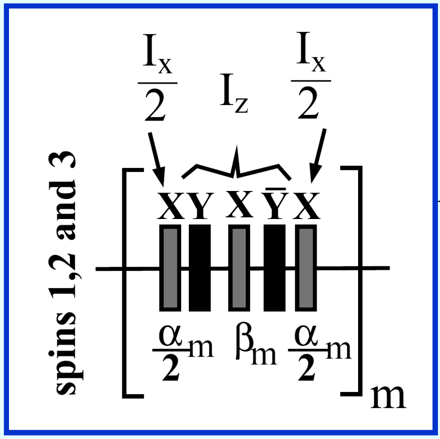
$$H(m) = \left(1 - \frac{m}{M}\right) H_B + \frac{m}{M} H_F$$

m

m^{th} step of the interpolating Hamiltonian .

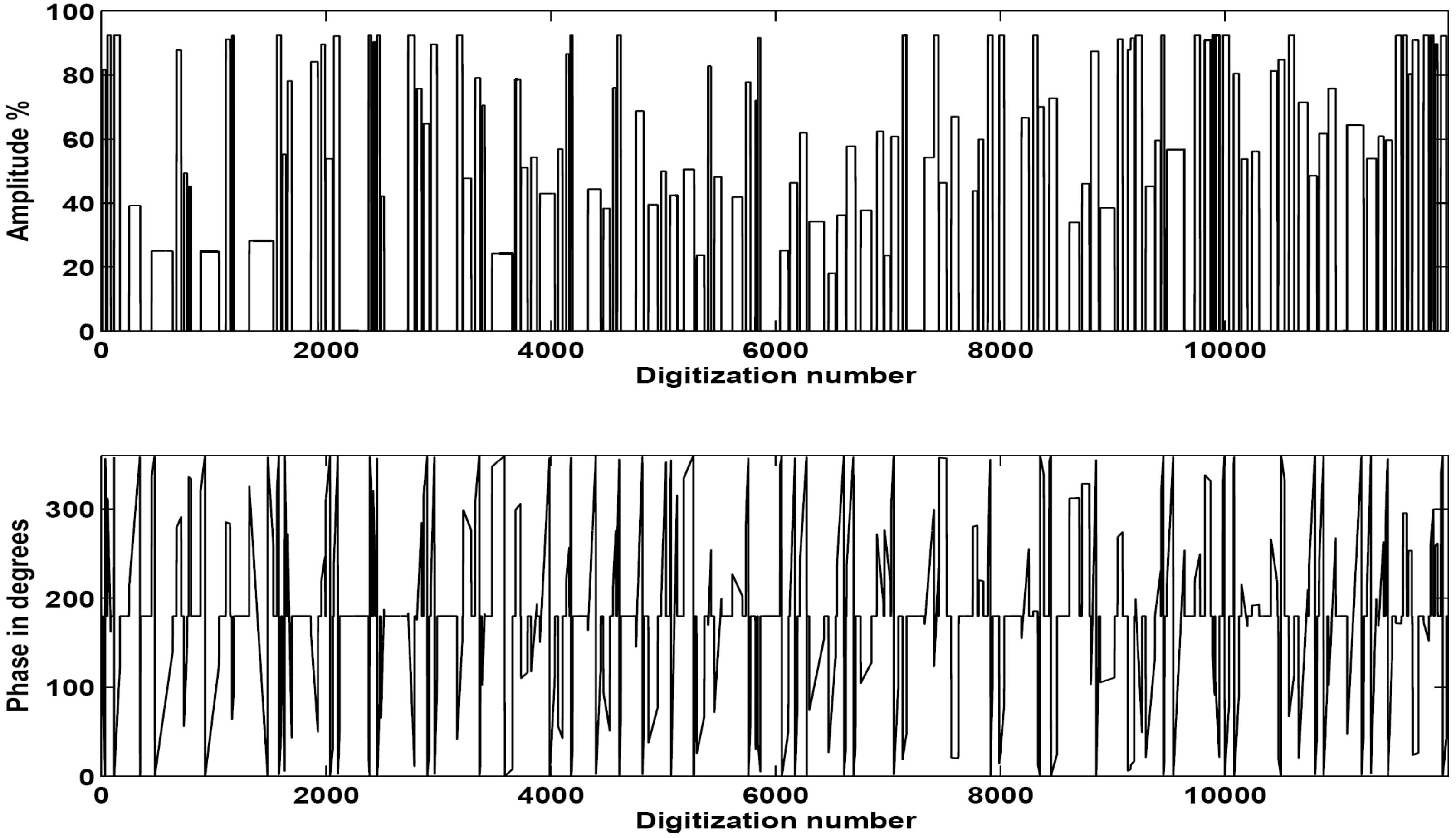
$$U_m \approx \underbrace{e^{-i\mathcal{I}_x\left(1-\frac{m}{M}\right)\frac{180}{2\pi}}}_{\left[\frac{\alpha_m}{2}\right]_x^{1,2,3}\ pulse} \cdot \underbrace{e^{-i\mathcal{I}_z\left(\frac{m}{M}\right)\frac{180}{\pi}}}_{\left[\beta_m\right]_z^{1,2,3}\ pulse} \cdot \underbrace{e^{-i\mathcal{I}_x\left(1-\frac{m}{M}\right)\frac{180}{2\pi}}}_{\left[\frac{\alpha_m}{2}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

m^{th} step of evolution operator



- Pulse sequence for adiabatic evolution
- Total number of iteration is 31
- time taken = 62000µs
  (400µs x 5 pulses x 31 repetitions)

Concatenated SMPs



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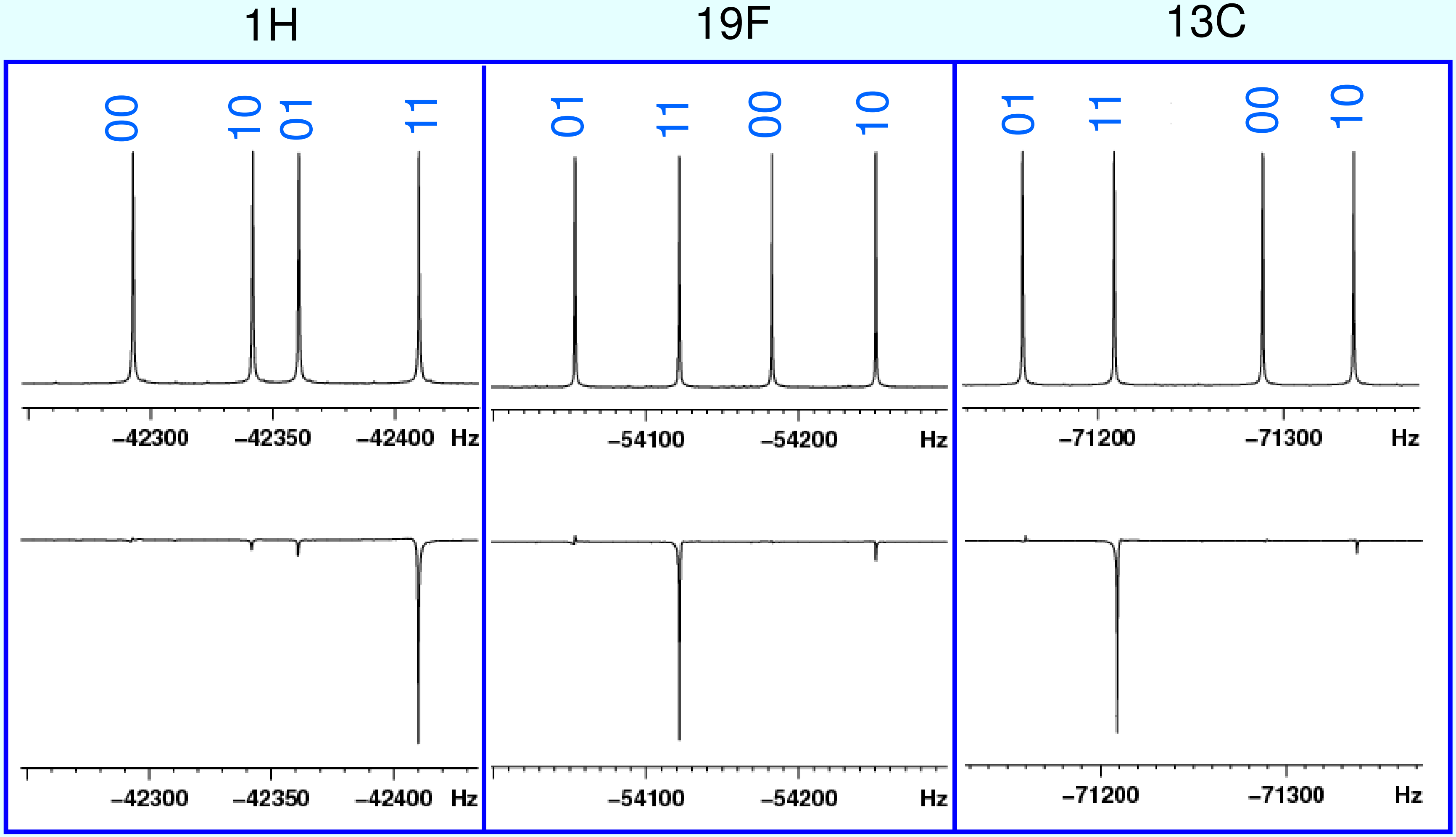
NMR Implementation



Boolean Formula

$\mathbf{x}_1 \wedge \mathbf{x}_2 \wedge \mathbf{x}_3$

Solution

$|\mathbf{111}\rangle$

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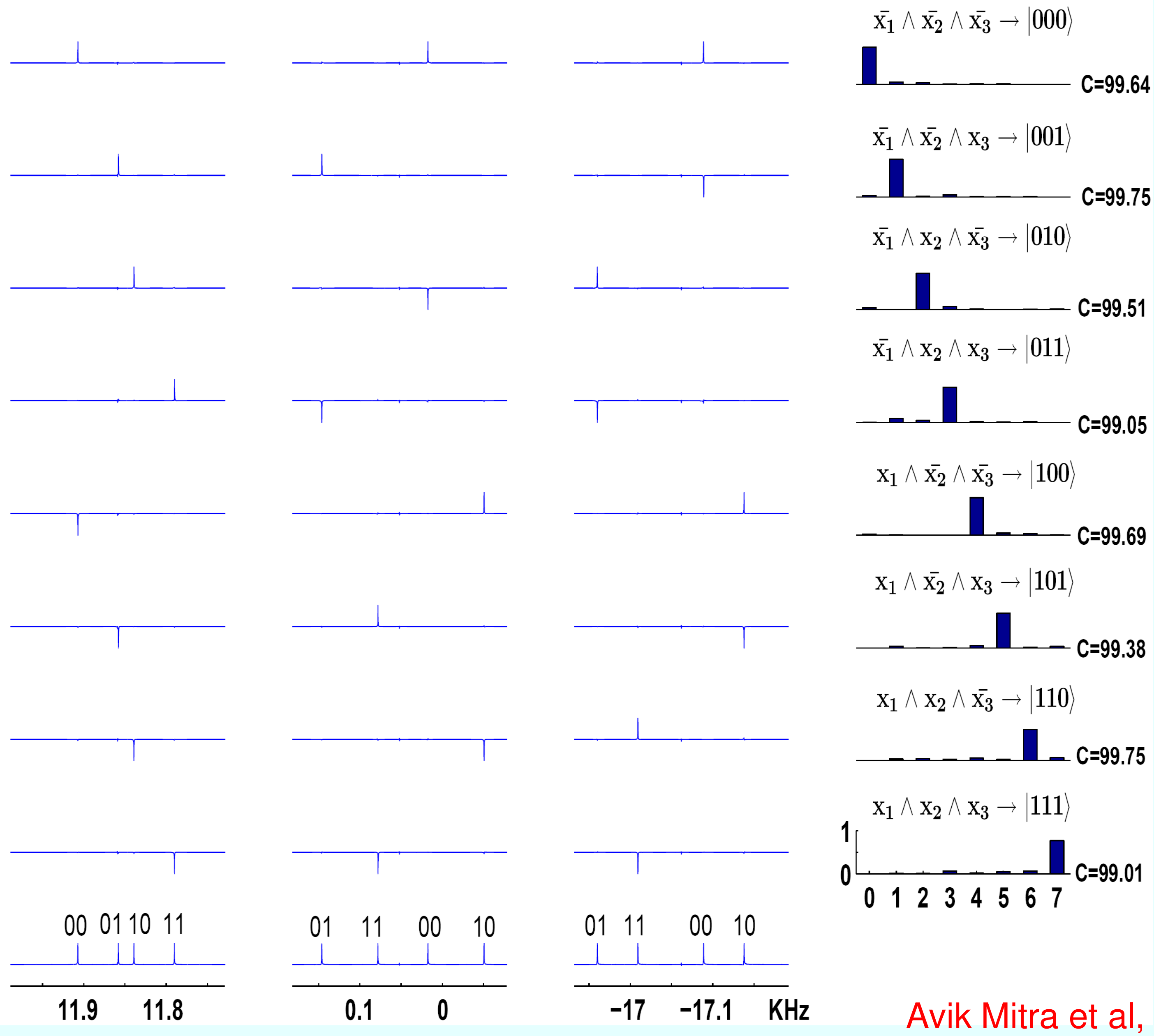
NMR Implementation



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Conclusions

1. We have implemented DJ and Grover's search algorithms by Locally adiabatic evolution method in hetero-nuclear qubit systems by using qubit selective pulses.

2. We have implemented 1-SAT problem in homo-nuclear spin system by using Strongly Modulated Pulses. This reduces the evolution time so that it falls below the coherence time of the system.

3. We feel that the strongly modulated pulses (SMP) which use elements of control theory will be used more often in NMR Implementations of QC and QIP

Thank You