NMR Implementation of Deutsch-Jozsa and Grover Algorithms

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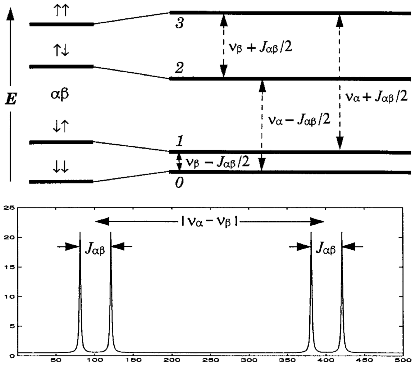
Goal:

- Emulate pure states in an ensemble NMR computer at thermal equilibrium.
- Use single qubit operations to implement universal, two-qubit logic.
- Use projective measurement and quantum interference to demonstrate a *fast* quantum algorithm.

Outline



$\Delta m_{B,A} = \pm 1 \rightarrow$ NMR signal.

- Two J-coupled nuclear spins in $^{13}CHCl_3$ described by:

$$\begin{aligned} H &= -\hbar\omega_L^A S_z^A - \hbar\omega_S^B S_z^B \\ &\quad +2\pi\hbar J S_z^A S_z^B + H_{\mathrm{Env.}} \end{aligned} \quad (1)$$

- Quantum logical states labeled as $|m_B, m_A\rangle = |H, C\rangle$ eigenstates:

$$\begin{aligned} |+1/2, +1/2\rangle &\rightarrow |00\rangle \\ |+1/2, -1/2\rangle &\rightarrow |01\rangle \\ |-1/2, +1/2\rangle &\rightarrow |10\rangle \\ |-1/2, -1/2\rangle &\rightarrow |11\rangle \end{aligned} \quad (2)$$

- Computations are implemented as unitary transformations:

$$\begin{aligned} U(N) &= U(1) \times SU(N) \\ &\xrightarrow{N=2} e^{i\alpha} R_x(\alpha) R_y(\beta) R_z(\gamma) \end{aligned} \tag{3}$$

- Timed, phased RF pulses at resonance implement rotations:

$$R_{\hat{n}}(\theta) = \exp(-i\theta\hat{n} \cdot \mathbf{S}) \tag{4}$$

- Phase shift with free-evolution period $\tau = 1/2J$:

$$\tau = \exp[-i(\pi/4)\sigma_z \otimes \sigma_z] \tag{5}$$

- Selective operations at particular frequency ω_i

$$U^B = U \otimes I^A \quad \text{and} \quad U^A = I^B \otimes U \tag{6}$$

- Solution to thermal distribution of states: effective pure states:

$$\rho = \frac{1-\alpha}{2^N} I + \alpha \left|\psi\right\rangle \left\langle\psi\right| \tag{7}$$

- Consider an operation $C(\rho) = \sum_k A_k \rho A_k^\dagger$ for a unitary transformation such that $\sum_k A_k^\dagger A_k = I$.
- Under an ensemble average $\langle O \rangle = \mathrm{Tr}(\rho O)$, behavior is identical to pure state:

$$\begin{aligned} \mathrm{Tr}\left[C(\rho)\, O\right] &= \mathrm{Tr}\left[\sum_k A_k \rho A_k^\dagger O\right] \\ &= \alpha \mathrm{Tr}\left[C\left(\left|\psi\right\rangle\left\langle\psi\right|\right) O\right] \end{aligned} \tag{8}$$

Effective pure state prepared through *temporal averaging*.

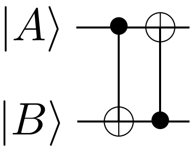
- State populations given by

$$\rho = \begin{array}{c} \begin{array}{cccc} \langle 00| & \langle 01| & \langle 10| & \langle 11| \end{array} \\ \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & c & 0 \\ 0 & 0 & 0 & d \end{bmatrix} \end{array} \begin{array}{c} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{array} \tag{9}$$

- Take the three separate measurements with U, cyclically permuting non-$|00\rangle$ elements for $\rho_{1,2}$. Time average is effective action on $|00\rangle$ state.

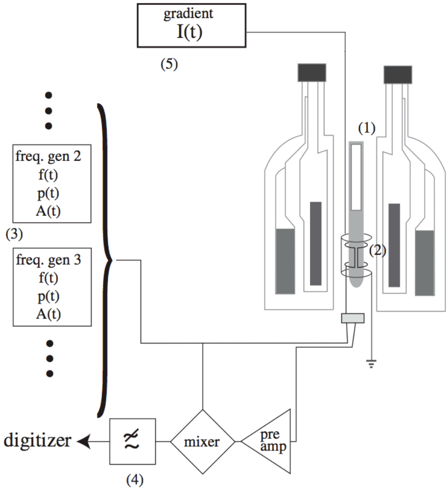
$$U\left(\rho_0 + \rho_1 + \rho_2\right)U^\dagger = (1-a)\,I + (4a-1)\,U\left(|00\rangle\langle 00|\right)U^\dagger \tag{10}$$

- Permutations U and $U^\dagger$ are pretty easy:



- Universal CNOT given described by $U_{\mathrm{CN}}^{A}\,|BA\rangle = |A, B \oplus A\rangle$.
- Truth table represented as unitary matrix

$$\begin{aligned} U_{\mathrm{CN}}^{A} &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \\ &= e^{-i\pi/4} R_y^A \tau \bar{R}_y^A \bar{R}_x^A \bar{R}_x^B R_y^B R_x^B \end{aligned} \tag{11}$$



1. Homogeneous magnetic field, superconducting magnet
2. RF cavity and sample $^{13}CHCl_3$ (200MHz and 50MHz)
3. Computer controlled RF transmitters/receiver
4. Software/Hardware control, MATLAB, etc.

- Parameters:
  - Pulse width ($t^H_{\pi/2} = 9.3 \pm 0.3$,$t^C_{\pi/2} = 7.8 \pm 0.1$)
  - Time scale of decoherence $T_1 = 17.0 \pm 0.5$ s
  - Error in measurement $T_2 = 2.04 \pm 0.09$
  - Delay between measurements
  - Phase delay $\tau = 1/2J$, $J = 215.05 \pm 0.02$Hz
  - Phase angle
- Procedures:
  1. Perform calibration
  2. On pseudo-pure states, specify temporal averaging; RF pulses (width, phase, delay) with xwin-nmr.
  3. FID signal $\rightarrow$ FFT handled by MATLAB

How close are we to theory?

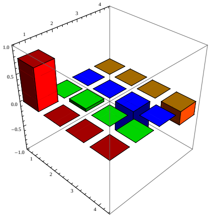
- Back-solve to density matrix using peak integrals:

$$\begin{aligned} V_P(t) &= V_0\left[(a-c)\,e^{-iJt/2} + (b-d)\,e^{iJt/2}\right] \\ V_C(t) &= V_0\left[(a-b)\,e^{-iJt/2} + (c-d)\,e^{iJt/2}\right] \end{aligned} \tag{12}$$

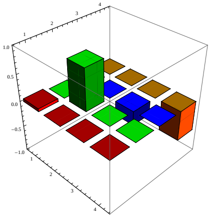
- Relative error in measured psuedo-pure state density matrix:

$$\sigma_\rho^i = \frac{||\rho_{ii}^{\text{Exp.}} - \rho_{ii}^{\text{Theory}}||}{||\rho_{ii}^{\text{Theory}}||} \tag{13}$$

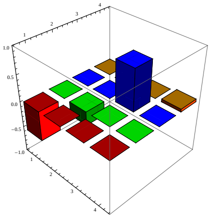
- Off-diagonal terms ('coherences') $\epsilon \rightarrow 0$?



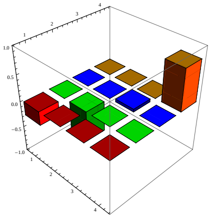
(c) $|00\rangle$



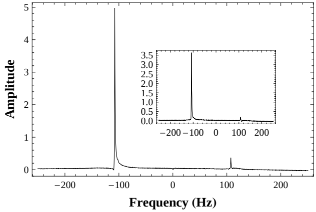
(d) $|01\rangle$



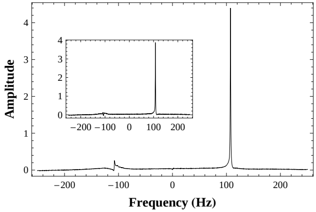
(e) $|10\rangle$



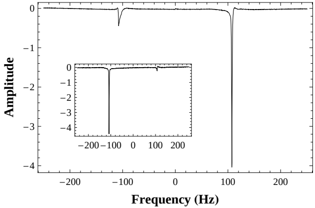
(f) $|11\rangle$



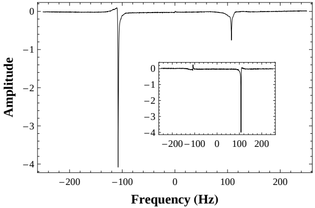
(g) $|00\rangle \rightarrow |00\rangle$



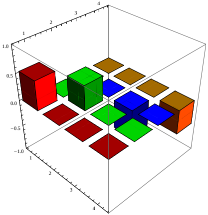
(h) $|01\rangle \rightarrow |01\rangle$



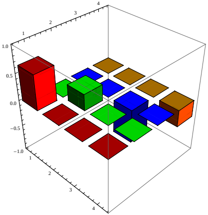
(i) $|10\rangle \rightarrow |11\rangle$



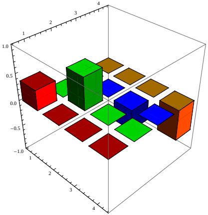
(j) $|11\rangle \rightarrow |10\rangle$



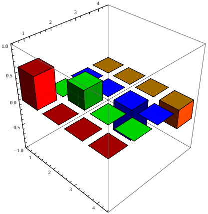
(k) Thermal (Meas.)$_{40.0\%}$



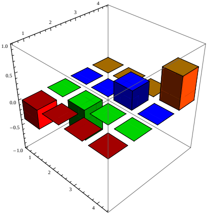
(l) $|00\rangle \rightarrow |00\rangle_{61.1\%}$



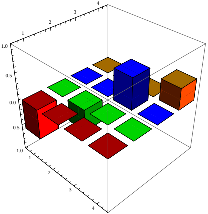
(m) $|01\rangle \rightarrow |01\rangle_{54.4\%}$



(n) Thermal(Th.)

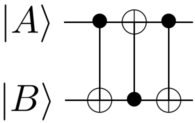


(o) $|10\rangle \rightarrow |11\rangle_{79.1\%}$



(p) $|11\rangle \rightarrow |10\rangle_{71.1\%}$

- Permutation gate required for $2+$ qubit QFT
- Consider modification of permutation gate:

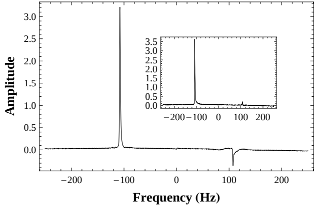


- Permutation described by

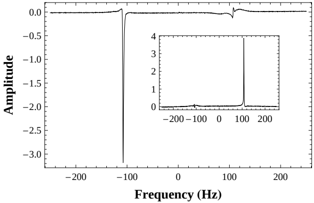
$$\begin{aligned} U_{\mathrm{CN}}^{B}\,|B, B \oplus A\rangle &= |B \oplus B \oplus A, B \oplus A\rangle \\ &= |A, B \oplus A\rangle \end{aligned} \quad (14)$$

- Additional CNOT yields

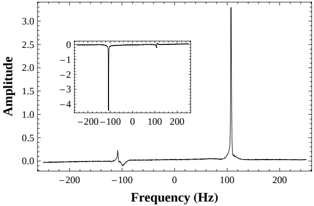
$$\begin{aligned} U_{\mathrm{SWAP}}\,|BA\rangle &= U_{\mathrm{CN}}^{A} U_{\mathrm{CN}}^{B} U_{\mathrm{CN}}^{A}\,|BA\rangle \\ &= |AB\rangle \end{aligned} \quad (15)$$



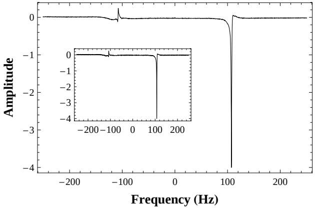
(q) $|00\rangle \longrightarrow |00\rangle$



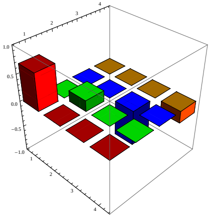
(r) $|01\rangle \longrightarrow |10\rangle$



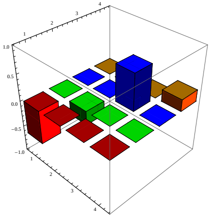
(s) $|10\rangle \longrightarrow |01\rangle$



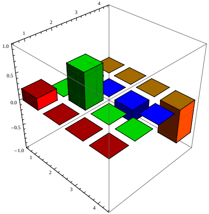
(t) $|11\rangle \longrightarrow |11\rangle$



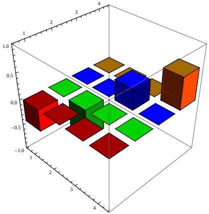
(u) $|00\rangle \rightarrow |00\rangle_{65.3\%}$



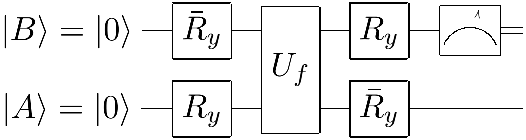
(v) $|01\rangle \rightarrow |10\rangle_{24.3\%}$



(w) $|10\rangle \rightarrow |01\rangle_{27.2\%}$



(x) $|11\rangle \rightarrow |11\rangle_{59.9\%}$

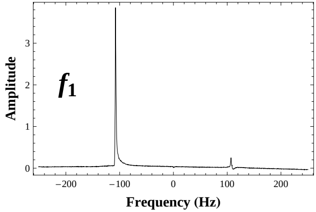


- Evaluates $|f_k(0) \otimes f_k(1), 0\rangle$ in one iteration
- Rotate $|00\rangle$ into superposition state
- Apply function U_f:

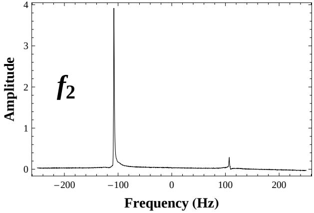
$$|BA\rangle = |0\rangle \otimes \frac{1}{2}\left[\left((-1)^{f_k(0)} + (-1)^{f_k(1)}\right)|0\rangle + \left((-1)^{f_k(0)} - (-1)^{f_k(1)}\right)|1\rangle\right] \tag{16}$$

- Result given by $f_k(0) \oplus f_k(1) \rightarrow |00\rangle$ or $|10\rangle$

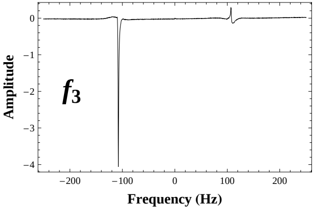
	Constant functions		Balanced functions	
	Case 1	Case 2	Case 3	Case 4
$f(0)$	0	1	0	1
$f(1)$	0	1	1	0
$w \oplus f(a)$	ID	NOT	CNOT	Z-CNOT



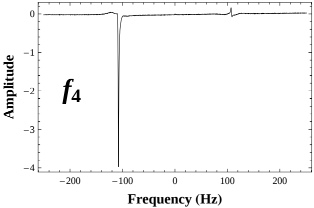
(y) $|00\rangle \longrightarrow |00\rangle$



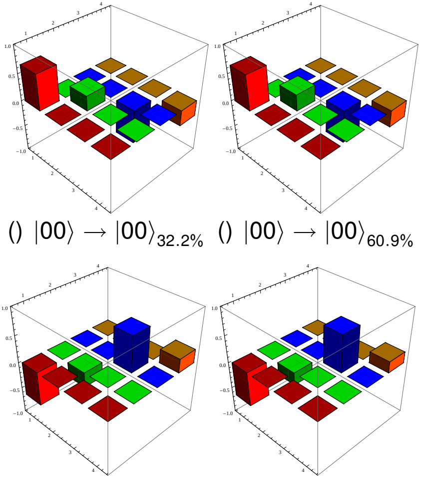
(z) $|00\rangle \longrightarrow |00\rangle$



() $|00\rangle \longrightarrow |10\rangle$



() $|00\rangle \longrightarrow |10\rangle$



() $|00\rangle \longrightarrow |00\rangle_{32.2\%}$ () $|00\rangle \longrightarrow |00\rangle_{60.9\%}$

() $|00\rangle \longrightarrow |10\rangle_{79.4\%}$ () $|00\rangle \longrightarrow |10\rangle_{27.6\%}$

In order of importance:

- Inhomogeneous static/RF field
- Pulse width precision/accuracy
- Asymmetric lineshapes from suboptimal shimming
- Lower signal-to-noise ratio for carbon
- Incomplete relaxation between experiments
- Numerical integration of peak integrals MATLAB

Summary

- Error analysis: Data agrees qualitatively.
- Liquid-state NMR quantum computation possible, starting with mixed states.
- Certain algorithms faster on 2-qubit computer, but not (particularly) useful.