

Preparation of Pseudo Pure States by Multiple Quantum Coherence Filtering and Saturation

Jae-Seung Lee and Anatoly K. Khitrin

Department of Chemistry, Kent State University

August 22, 2003

Content

- Introduction
- Multiple quantum coherence
- Pseudo-pure state by highest order quantum coherence selection
- Experiment
- Result on a 6-spin system
- Discussion
- Summary

Introduction

- Preparation of a known quantum state
 - Input for quantum information processing (QIP)
- **Ground state** as an initial state
 - Cooling
 - Measurement accompanied with unitary operations
- QIP with nuclear magnetic resonance
 - **Pseudo pure state** : all equal populations except one
 - Scalability
- Initialize through **highest order quantum coherence selection and saturation**

Multiple Quantum Coherence

- Spin Hamiltonian

$$\mathcal{H}_{\text{int}} = \mathcal{H}_z + \mathcal{H}_{zz},$$

where the linear term \mathcal{H}_z is the **Zeeman** Hamiltonian

$$\mathcal{H}_z = - \sum_{i=1}^N \omega_{0i} I_{iz}$$

and the bilinear term \mathcal{H}_{zz} consists of spin-spin interactions, especially **dipole-dipole** interactions

$$\mathcal{H}_{zz}^D = - \sum_{i < j} D_{ij} (3I_{iz}I_{jz} - \mathbf{I}_i \cdot \mathbf{I}_j).$$

- Good quantum numbers : If $I_z = \sum_{i=1}^N I_{iz}$, $[I_z, \mathcal{H}_{\text{int}}] = 0$.
Denote the simultaneous eigenstates by $|i\rangle$.

$$I_z |i\rangle = M_i |i\rangle \quad \text{and} \quad \mathcal{H}_{\text{int}} |i\rangle = \omega_i |i\rangle.$$

- Definition of the **multiple quantum coherence**

- The **n -quantum matrix elements** is the matrix elements $\langle i|\rho|j\rangle$ of a density operator ρ where $n = M_i - M_j$.
- We call n the **order** of the matrix element and say that the existence of a nonvanishing matrix element $\langle i|\rho|j\rangle$ such that $n = M_i - M_j$ describes **n -order coherence**.

- Usually, n -quantum coherence means the sum of all n -order coherences.

$$\rho_n = \sum_{n=M_i-M_j} \langle i|\rho|j\rangle$$

- Some characteristics

- From $(\rho_n + \rho_{-n})^\dagger = (\rho_n + \rho_{-n})$, $\rho_n = \rho_{-n}^*$.
- Rotation about the z axis by θ

$$\exp(-i\theta I_z) \rho_n \exp(i\theta I_z) = \exp(-in\theta) \rho_n$$

Pseudo pure state

- **Pure state vs. pseudo-pure state**

$$|\Psi\rangle\langle\Psi| \quad \text{vs.} \quad \frac{1-\alpha}{Z} \mathbb{1} + \alpha|\Psi\rangle\langle\Psi|$$

- **Highest order quantum coherence**

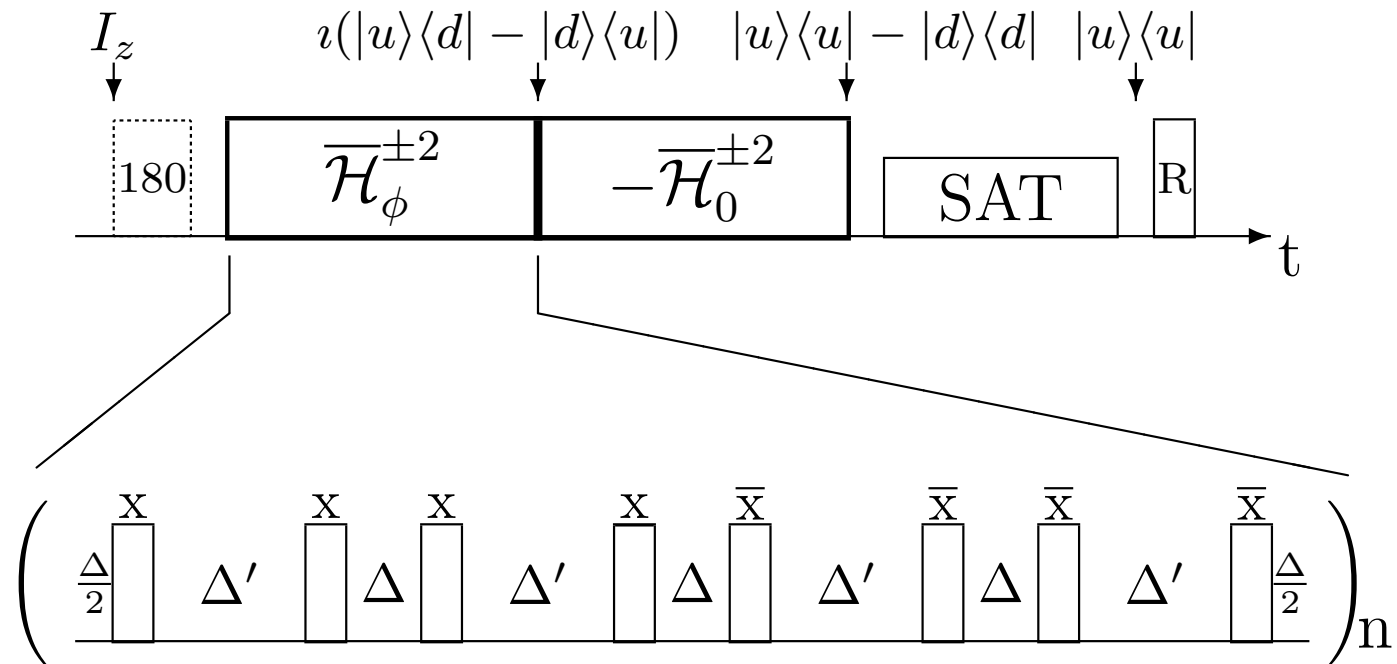
- Containing only **TWO** matrix elements $|u\rangle\langle d|$ and $|d\rangle\langle u|$.
- Connected to only two states $|u\rangle\langle u|$ and $|d\rangle\langle d|$ among the diagonals.

- **Saturation**

- The state after filtering the highest-order quantum coherences is a mixture of two states $|u\rangle\langle u|$ and $|d\rangle\langle d|$.
- We need a general way to select one of them.

Experiment

- Pulse sequence



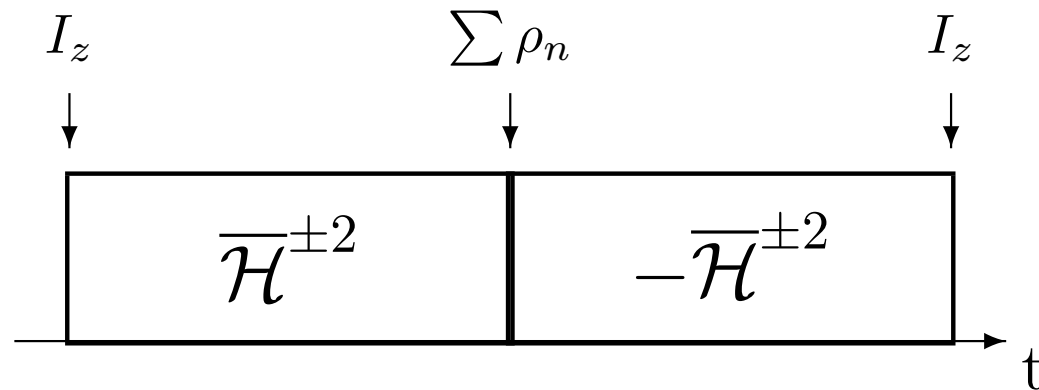
– Excitation of multiple quantum coherences

* **Double-quantum average Hamiltonian**

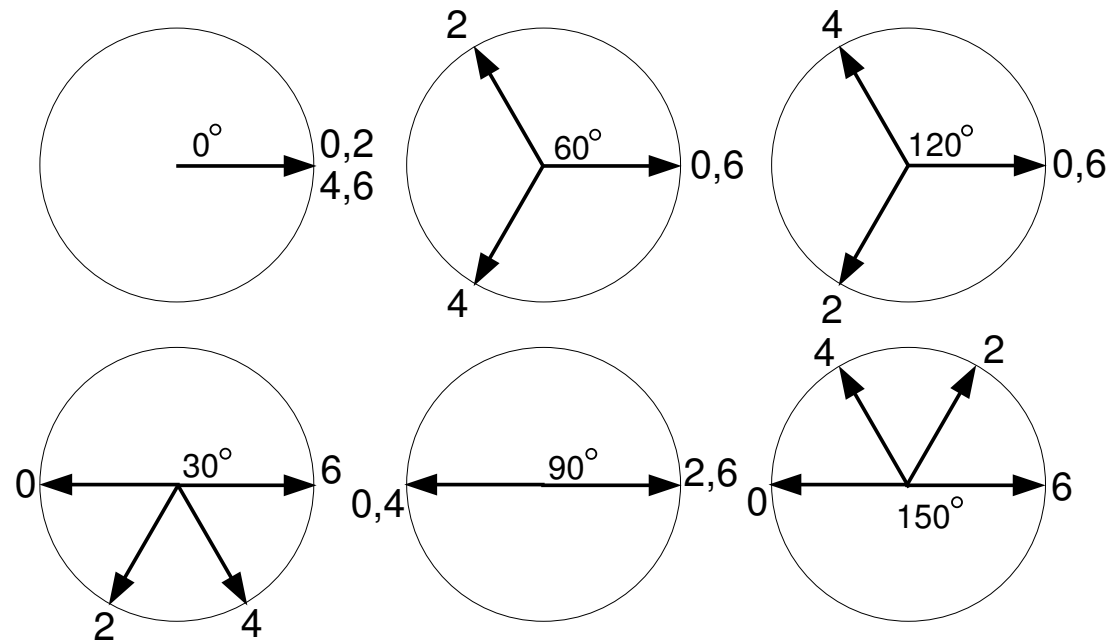
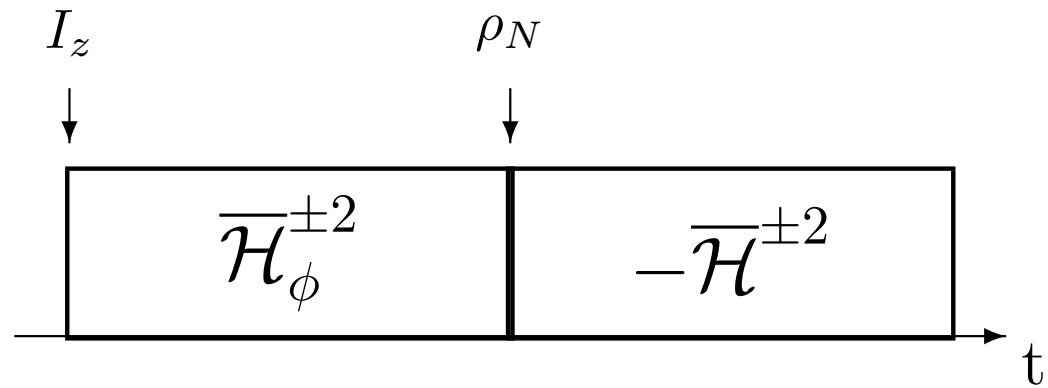
$$\overline{\mathcal{H}}^{\pm 2} = \frac{1}{3}(\mathcal{H}_{yy} - \mathcal{H}_{xx}) = -\frac{1}{2} \sum_{i < j} D_{ij} (I_{i+} I_{j+} + I_{i-} I_{j-}).$$

* Time reversal sequence

$$\exp\left(-i\frac{\pi}{2}I_z\right) \overline{\mathcal{H}}^{\pm 2} \exp\left(i\frac{\pi}{2}I_z\right) = \exp\left(-i2 \times \frac{\pi}{2}\right) \overline{\mathcal{H}}^{\pm 2} = -\overline{\mathcal{H}}^{\pm 2}$$



* Filtering of specific orders

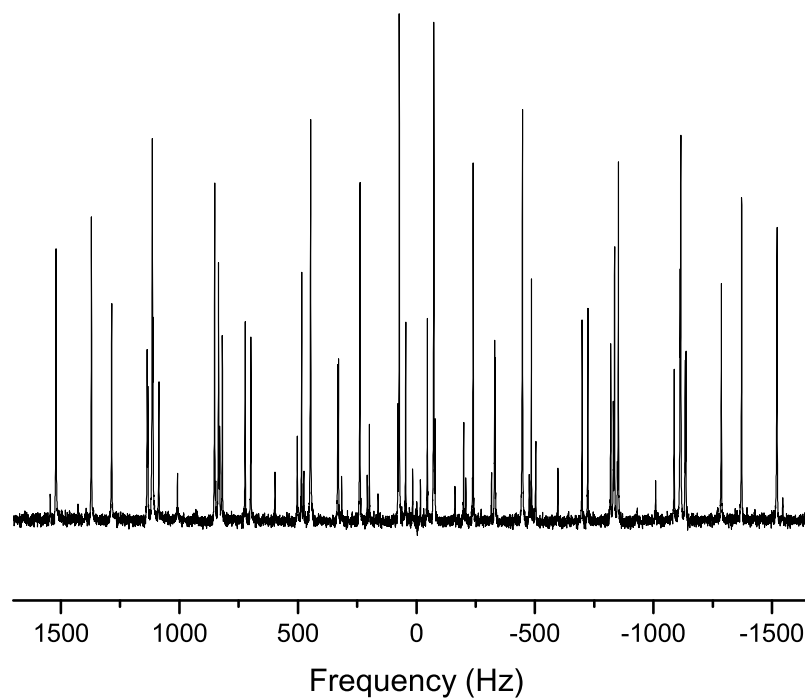
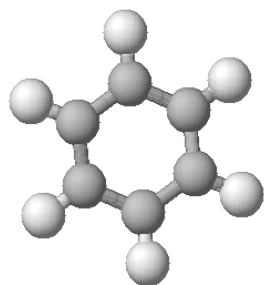


– Saturation

- * After filtering the highest order quantum coherence and turning back to the magnetization, the deviation part of the density matrix is given by $i(|u\rangle\langle u| - |d\rangle\langle d|)$.
- * Saturation is required to make the density matrix $|u\rangle\langle u|$.
- * It can be expected that fast saturation gives some signal enhancement.

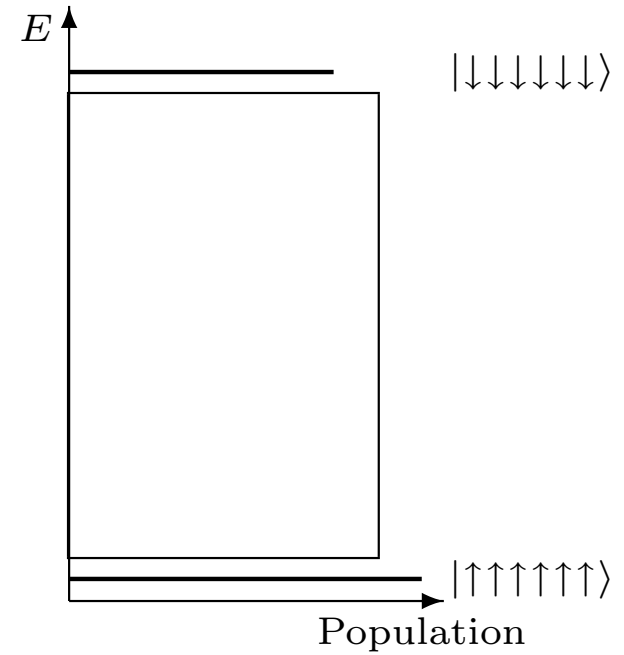
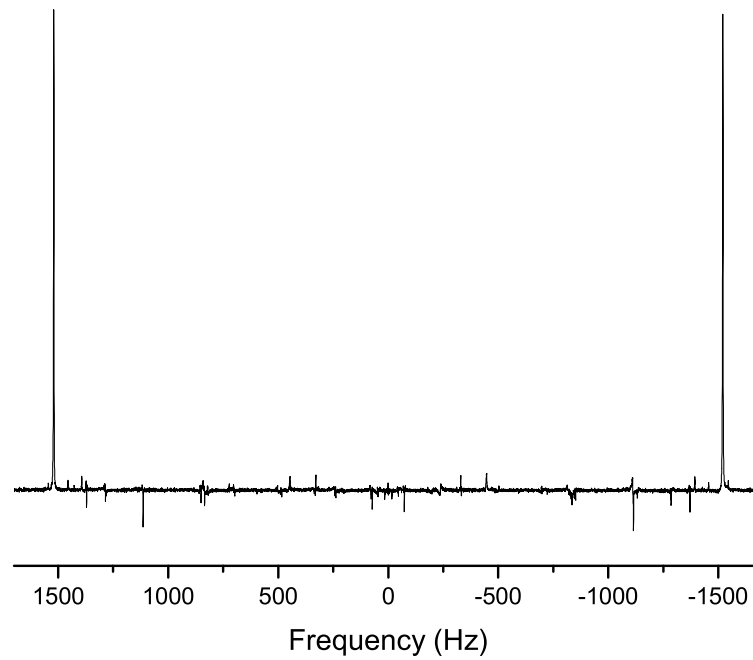
Result on a 6-Spin System

- Benzene in liquid crystal

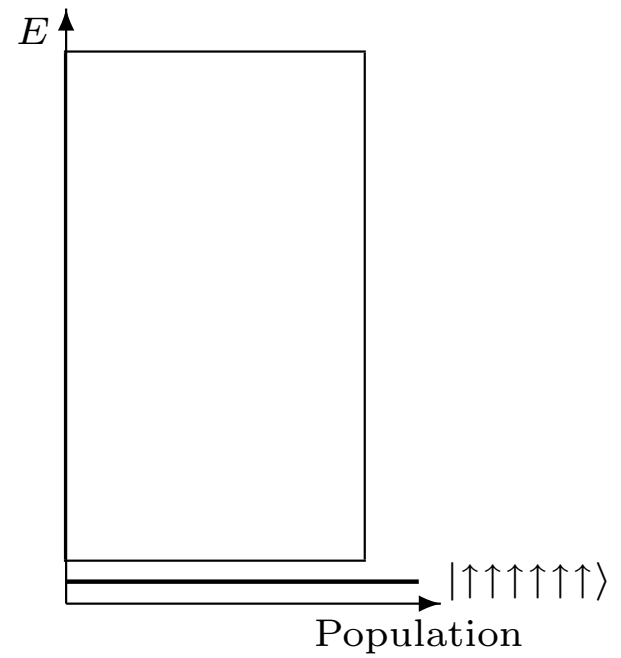
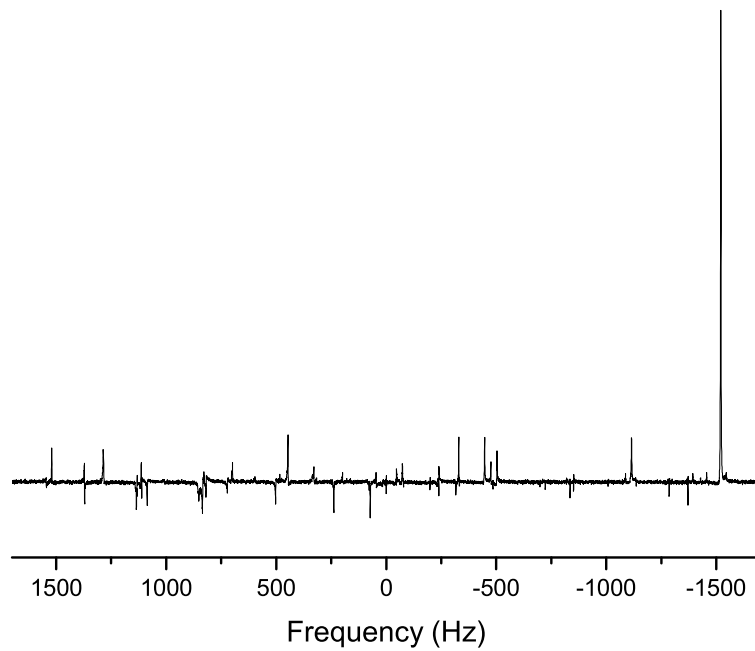


Molecular structure and 500MHz ^1H NMR spectrum

- After filtering the six-quantum coherence

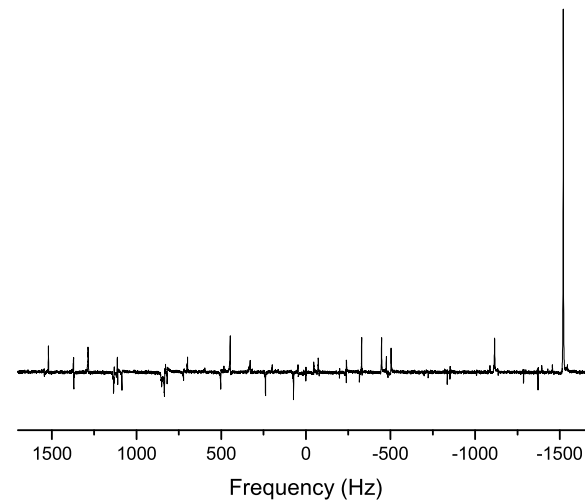
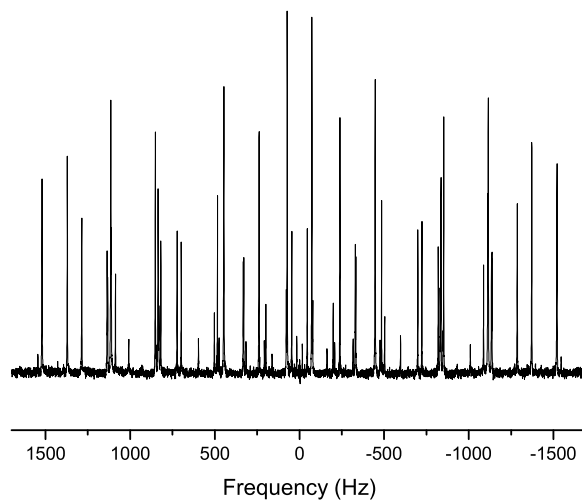


- After saturation



Discussion

- Advantage of this method
 - cf.* Knill et al., Nature **404**, pp. 368 (2000)
 - Fast preparation of a pseudo pure state
 - Intensity enhancement
 - Applicable to an unresolved system



- Future study
 - Manipulation of unresolved systems for (quantum) information processing
 - Creation and simulation of highly-correlated quantum states (ex. Schrödinger cat state)
 - Decoherence

Summary

- New method for the preparation of a pseudo pure state
 - Multiple quantum coherence excitation
 - Filtering the highest order quantum coherence
 - Saturation
- Verification of states by small angle pulses
- Advantage in cost and intensity