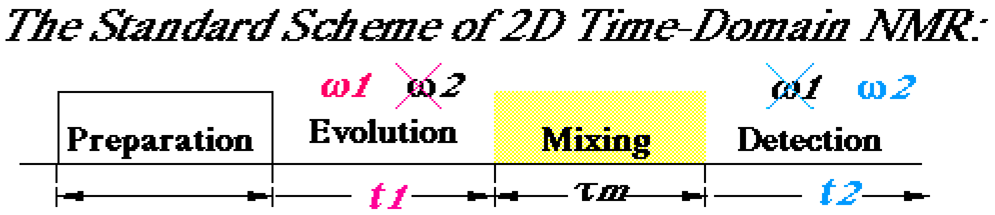
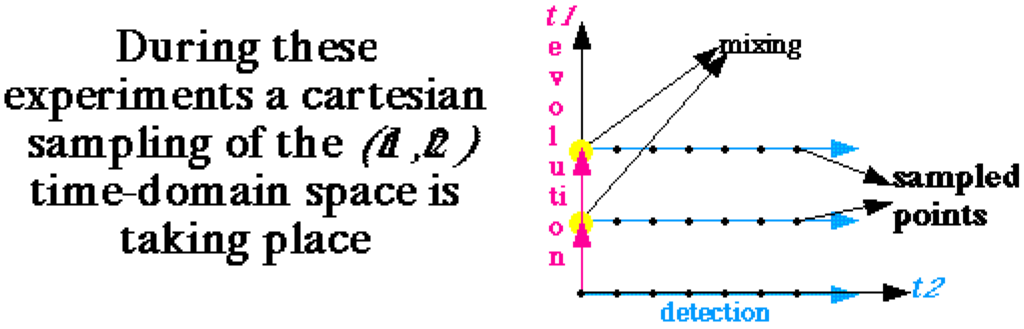
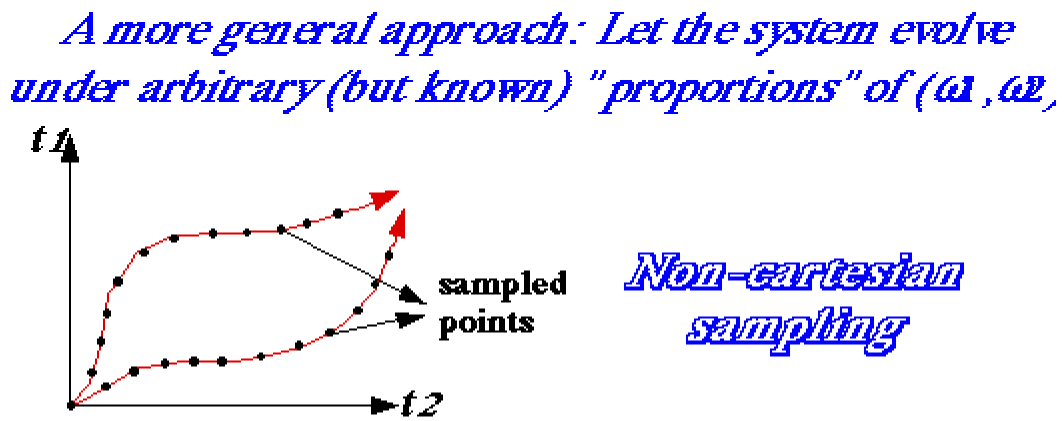
Non-Cartesian Sampling: The Acquistion of 2D NMR Spectra in a Single Scan

---

Much of our work involves *multidimensional NMR experiments*, in which different interactions are correlated along independent frequency axes. We have developed new, more general ways of carrying out these experiments, based on what we denominate **non-cartesian sampling schemes**.





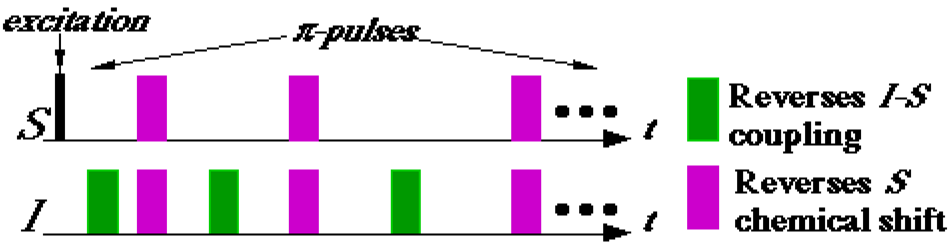


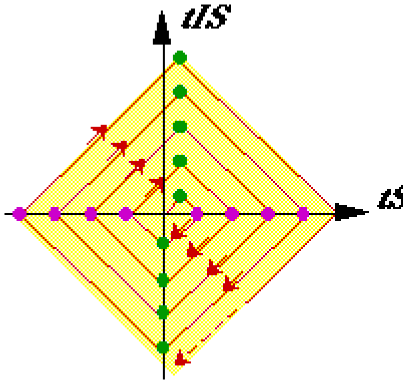
Important Potential Advantages

- **Does not require suppresion of any spin interaction ==> experimentally more flexible**
- **Time can be used as a *trajectory parameter* for the efficient sampling of multidimensional spaces**

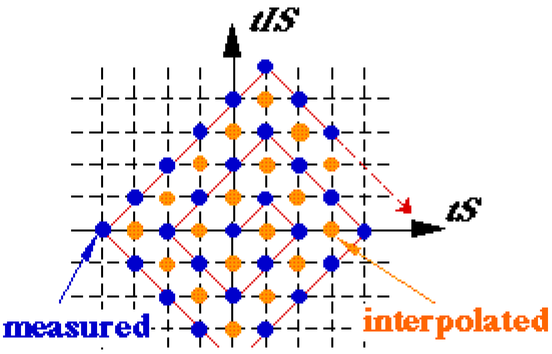
We begin by illustrating this latter possibility, with an example of an experiment where a complete 2D time-domain data set is sampled in a single scan. This procedure can be implemented in a number of cases, including for correlations between the chemical shift of an *S*-spin (e.g., ^{13}C) and its coupling to a neighboring *I* nucleus (e.g., ^{1}H).

The type of pulse sequences that are involved in these experiments:





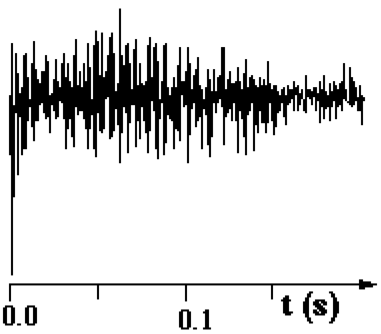
It is possible to visualize the resulting *S* spin evolution as involving a spiral-like trajectory in the Fourier space conjugate to its *IS* coupling and chemical shift

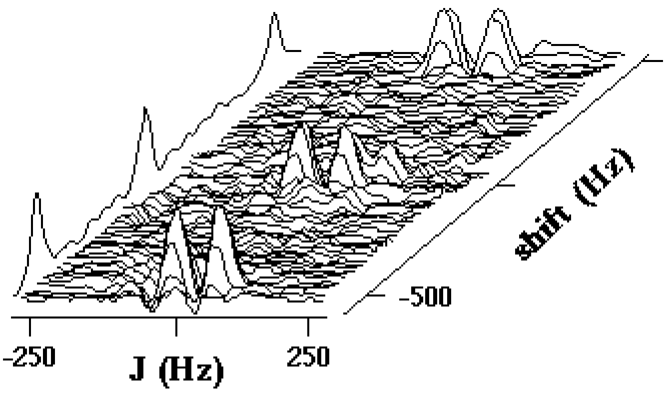


Rearrangement, interpolation and FFT of data acquired during this single-scan experiment yields a 2D shift/coupling NMR correlation spectrum

Experimental Verification

One Scan Acquired on a Pyridine Sample → *13C Chemical Shift - J Coupling 2D Correlation Spectrum*





Total Acquisition Time: 0.202 s