Line Broadening and Negative Line Broadening

Some hints and tips

Maths time!

- NMR signal is (roughly)

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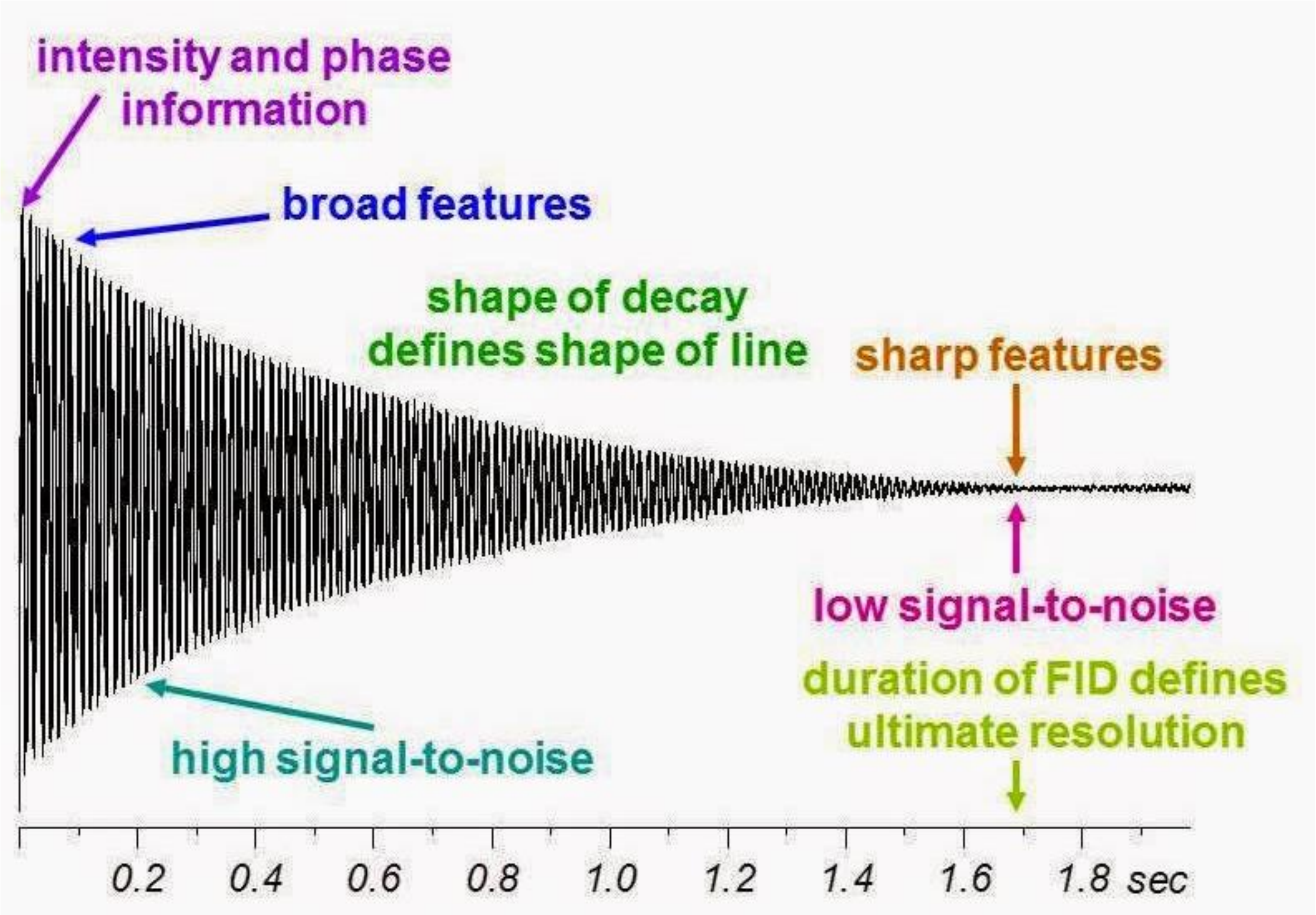
- An oscillation
- And a decay
  - In liquids $T_1 \approx T_2$
  - In solids $T_1 \gg T_2$

Anatomy of a FID



Shamelessly stolen from Glenn Facey’s blog

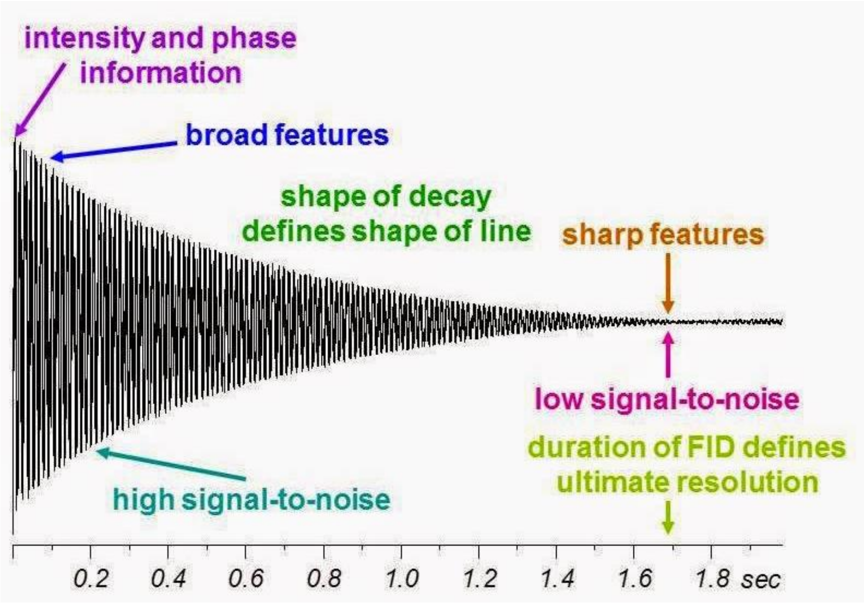
Line broadening

- When we use line broadening (LB = x, WDW = EM, efp) we introduce another decay

$$S(t) = \exp(i\omega t).\exp(-t/T).\exp(-t/kx)$$

- Reduces low SNR end of the FID, increases the high SNR end
- Enhances broad features, smooths out sharp features

- In signal processing, the concept of the “matched filter” says that the best value of x is to match the linewidth



Negative line broadening

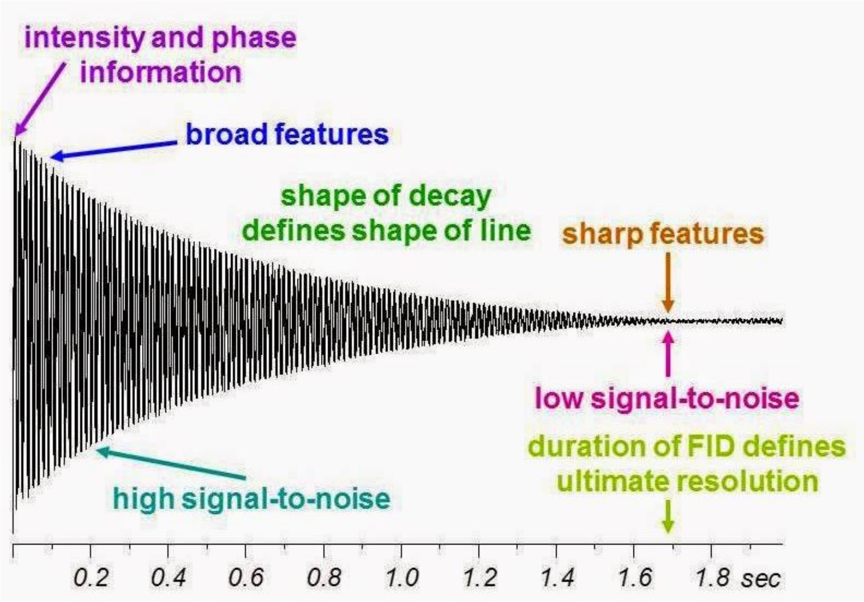
- But what if we care about the sharp features? What if we have more than enough broad features already and we want rid of them?

- How do you emphasise the other end of the FID?

- Use an exponential growth instead of a decay! (LB = -x)

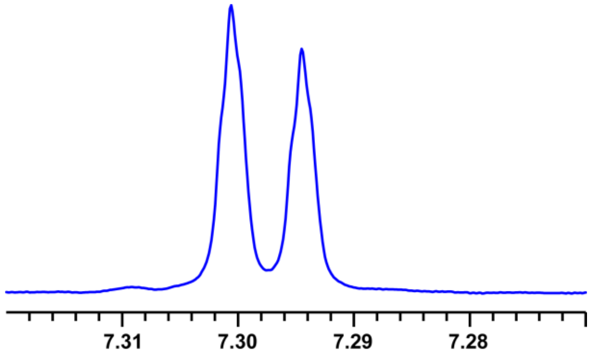
$S(t) = \exp(i\omega t).\exp(-t/T).\exp(-t/-kx)$

- Reduces high SNR end of the FID, increases the low SNR end
- Enhances sharp features and noise

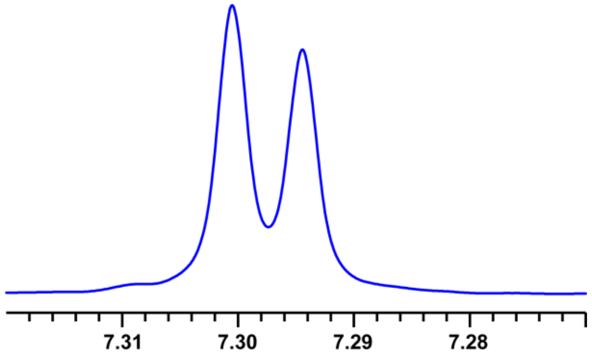


Practical example

“raw” data: LB = 0; SINO = 787; inherent linewidth 0.41 Hz



matched filter: LB = 0.4 Hz; SINO = 2195



resolution enhanced: LB = -0.2; SINO = 82