Spectral Resolution, Sampling Rate, and the Nyquist Frequency

The spectral width must be covered by sufficient data points to obtain the required resolution. This is determined by how many data points are collected in the free induction decay, or simply Digital Resolution = 1 / Acquisition Time.

This can be shown as follows. Let's say the total spectral width in Hz is SW, and the acquisition time is the length of the FID in seconds (AT)

The highest frequency which can be sampled is limited by the sampling rate (Nyquist Theorem). This frequency is the Nyquist frequency which is the spectral width which can be accurately defined. An accurate representation of a wave requires that it be sampled at least twice for each oscillation. Thus a 5000 Hz wave must be sampled at 10000 Hz, or once every 1/100000 sec. Sampling must be every 1/ (2 Nyquist Freq), or 1/(2 SW) seconds. This is the dwell time (or time between points).

Thus, the sampling rate in the FID must be at least 2 SW points per second.

Total number of data points in FID is NP, which is the AT times the number of points per second.

$$NP = 2\ SW\ AT$$

However, half of these points correspond to the real and half to the imaginary components of the spectrum, since the FT of an FID results in real and imaginary components. The total number of points in the spectrum is therefore NP/2. (In fact NMR data are collected in quadrature with two FID's 90° out of phase (real and imaginary). NP is the total number of points, half in the real and half in the imaginary. Fourier transformation gives absorption and dispersion spectra (after phasing), each with NP/2 data points.)

Finally we can define the digital resolution in Hz per data point in the spectrum as the spectral width divided by the total number of points in the spectrum, or

$$\text{Digital resolution} = SW / (NP/2) = 2\ SW / NP = 2\ SW / (2\ SW\ AT) = 1 / AT$$

Thus, the digital resolution is limited by the length of the acquisition.

We can increase the resolution by zero filling the FID, i.e. increasing the number of points without actually increasing the length of real data collection.