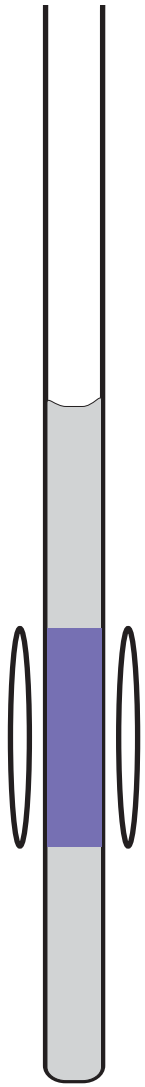
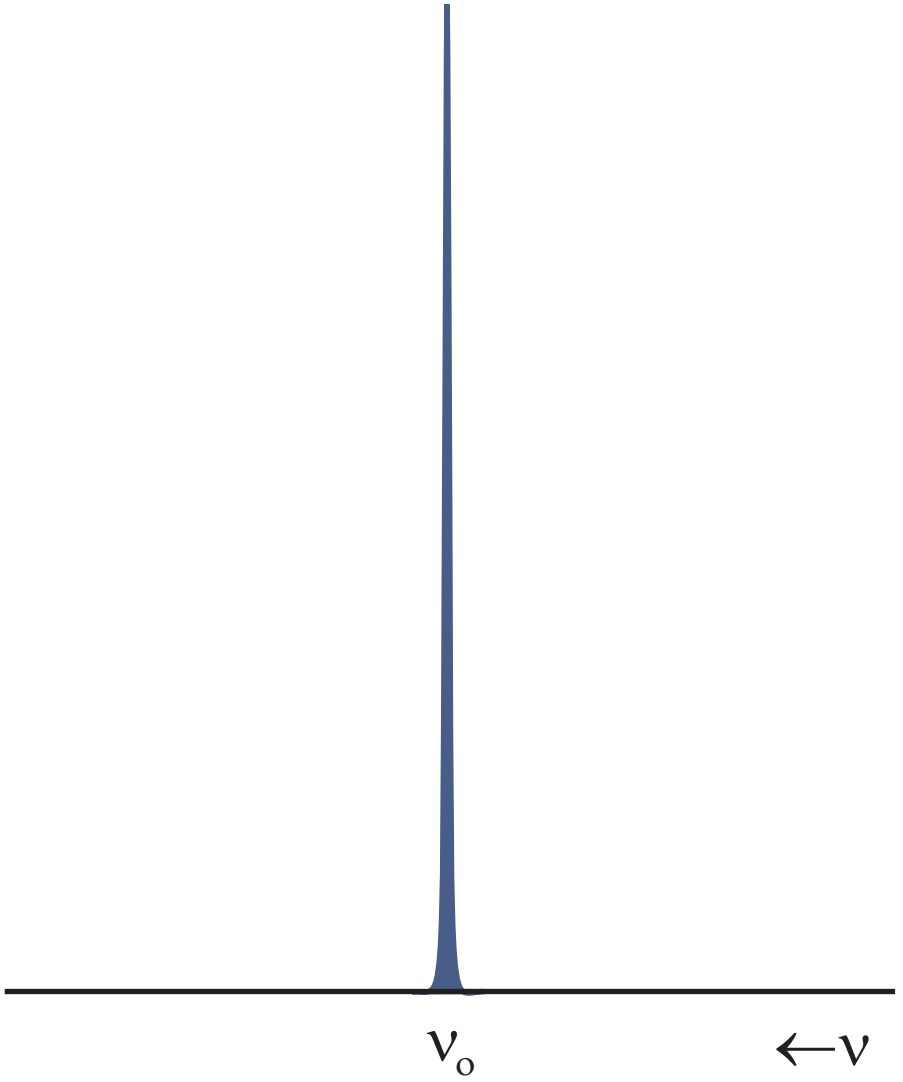
Typically NMR Sample Configuration



$\nu_o = \gamma B_o$

Solvent column ~ 3× as long as detection region.



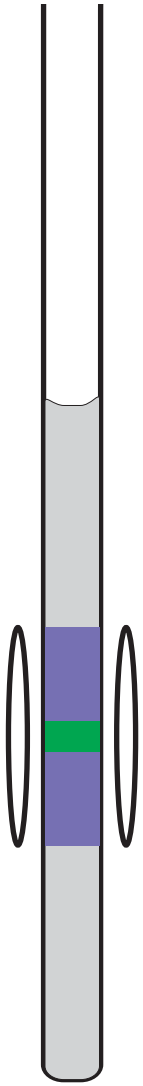
Comments about Manual Shimming

The following slides are useful as an introduction to shimming, automated or manual. Although automated shimming is now preeminent, manual shimming is occasionally still required. The following is important as an introduction to manual shimming. See the last slide as well.

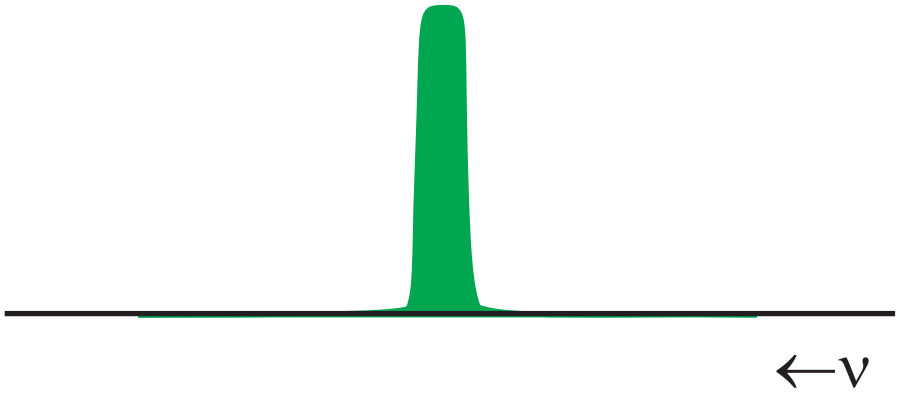
Once lock is achieved, the magnetic field inhomogeneity must be shimmed out. For experimental planning, one must keep in mind differences in solvents. Acetone-d_6 and acetonitrile-d_3 have very narrow natural ^2H linewidths, and therefore give good performance for shimming. $CDCl_3$ and many other solvents are intermediate in performance, and are reasonable choices for routine work. DMSO-d_6 and pyridine-d_7 both have much broader natural ^2H linewidths, and are therefore relatively poor solvents for [manual] lock shimming. D_2O can give very broad ^2H lines due to exchange. Of course, the last three solvents might be the only choices for solvation and cost reasons, but [manual] shimming on the FID might then be necessary if high resolution ^1H spectra are needed.

A number of good discussions about shimming strategies are available. Since every change of sample requires shimming, [it used to be that] every spectroscopist should take advantage of strategies to lessen the time spent shimming [whereas automated gradient shimming has now reduced this need]. Especially useful is G. A. Pearson, "Shimming an NMR Magnet," Chem. Dept., Univ. IA, Iowa City, IA 52252 [google it]. Many practical examples are given that show how to visually determine which shim needs adjusting, and in which direction. These quick determinations can save much time at the spectrometer and lead to improved spectra. More detailed discussions of shimming can be found in Claridge (2nd ed., section 3.4.5 (p. 77-82), and in G. N. Chmurny and D. I. Hoult, "The Ancient and Honorable Art of Shimming," Concepts Magn. Reson. 2, 131-149 (1990).

Z1 Gradient Effects on NMR Line Shapes



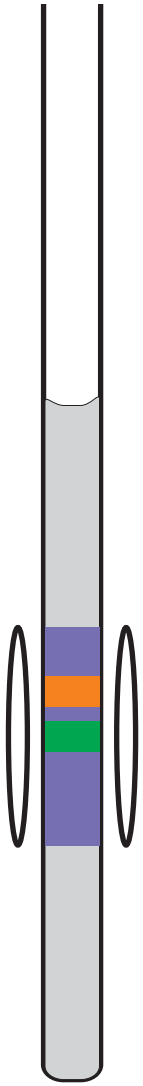
If the magnetic field varies roughly in a linear manner, from smaller to larger from bottom to top of the tube, the following will be approx. correct:



$\nu_o = \gamma B_o$

In a thin slice at the middle of the detection region, the field ~B_o.

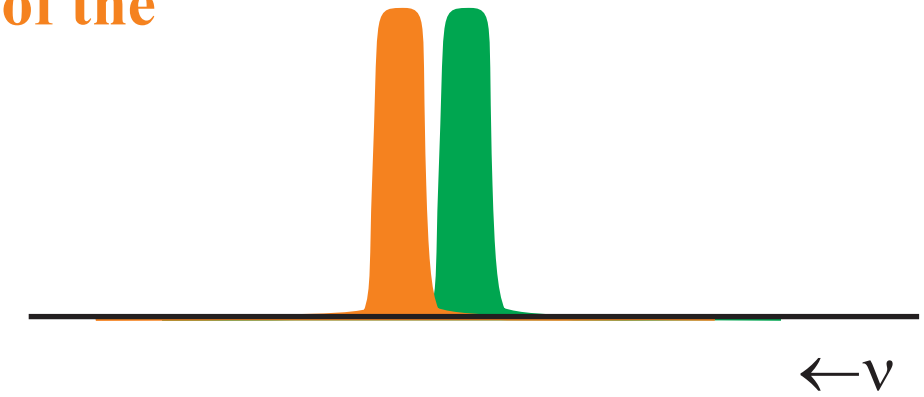
Z1 Gradient Effects on NMR Line Shapes



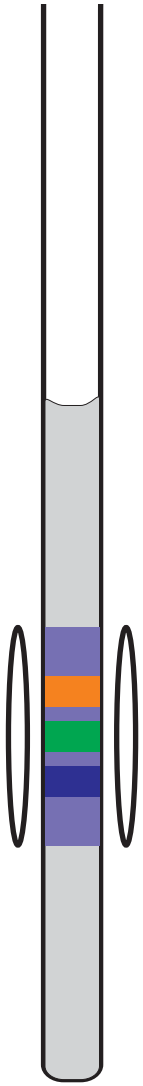
A slice slightly higher would be shifted to higher field, increasing the observed ν from this region of the sample.

$\nu_o = \gamma B_o + \Delta z \gamma G_z$

$\nu_o = \gamma B_o$



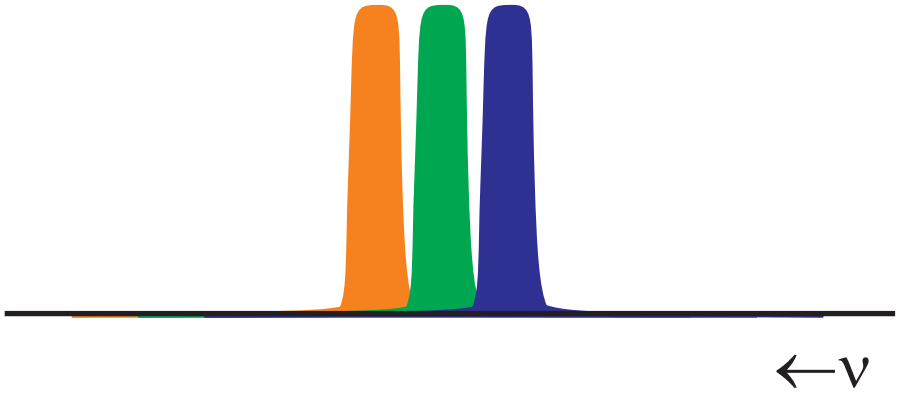
Z1 Gradient Effects on NMR Line Shapes



$\nu_o = \gamma B_o + \Delta z \gamma G_z$

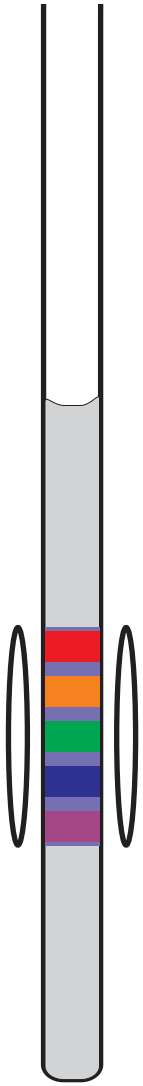
$\nu_o = \gamma B_o$

$\nu_o = \gamma B_o - \Delta z \gamma G_z$



A slice closer to the bottom is shifted to lower frequency.

Z1 Gradient Effects on NMR Line Shapes



Slices twice as far from the center are moved linearly out in frequency by a Z1 magnetic field gradient.

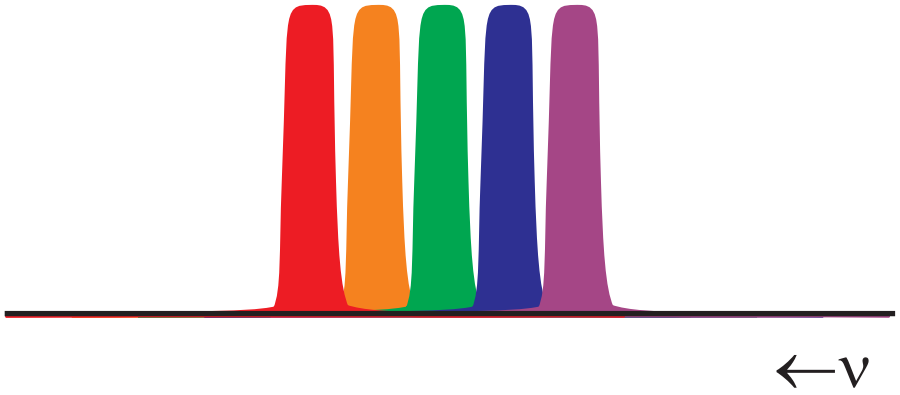
$$\nu_o = \gamma B_o + 2\Delta z \gamma G_z$$

$$\nu_o = \gamma B_o + \Delta z \gamma G_z$$

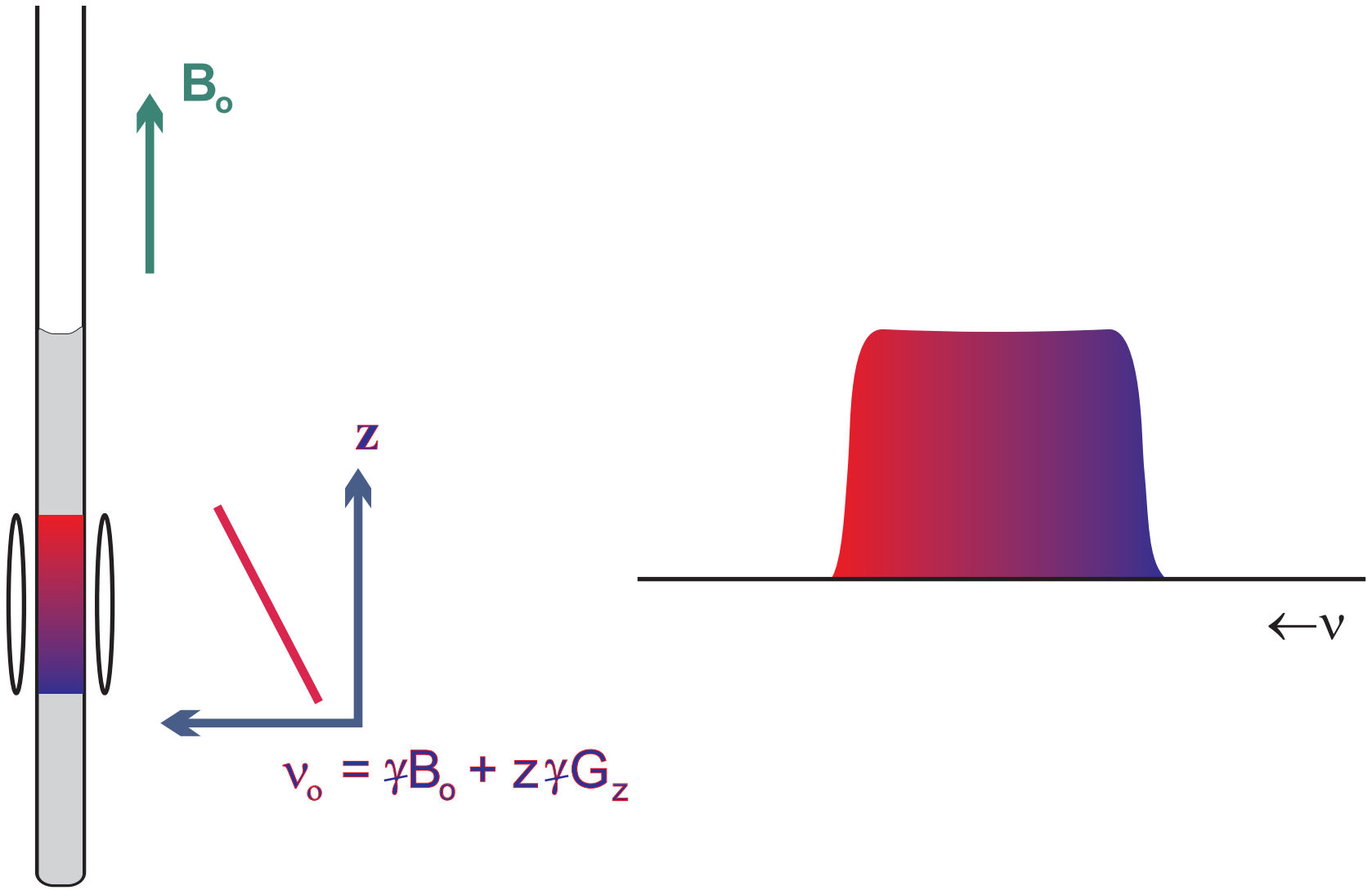
$$\nu_o = \gamma B_o$$

$$\nu_o = \gamma B_o - \Delta z \gamma G_z$$

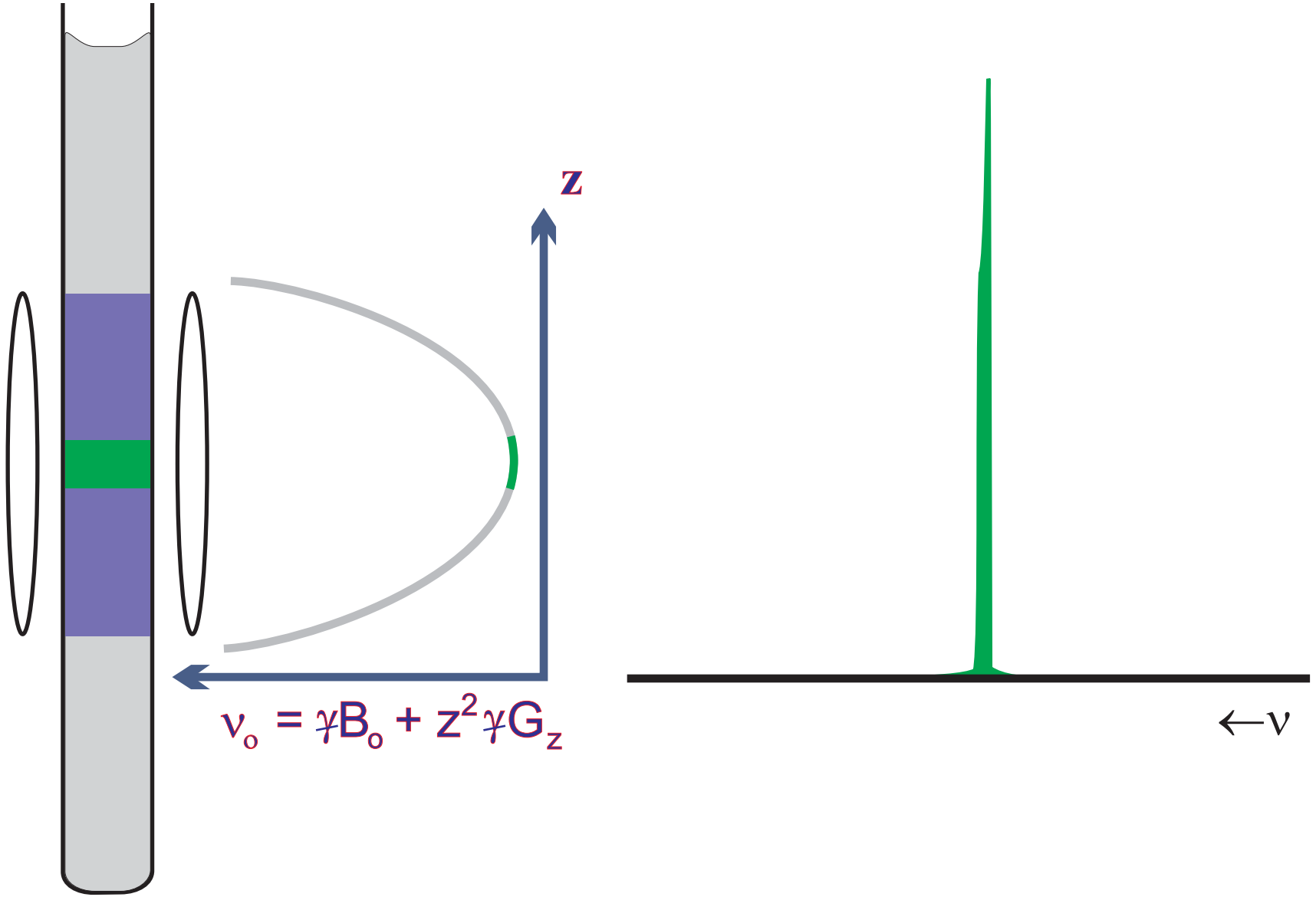
$$\nu_o = \gamma B_o - 2\Delta z \gamma G_z$$



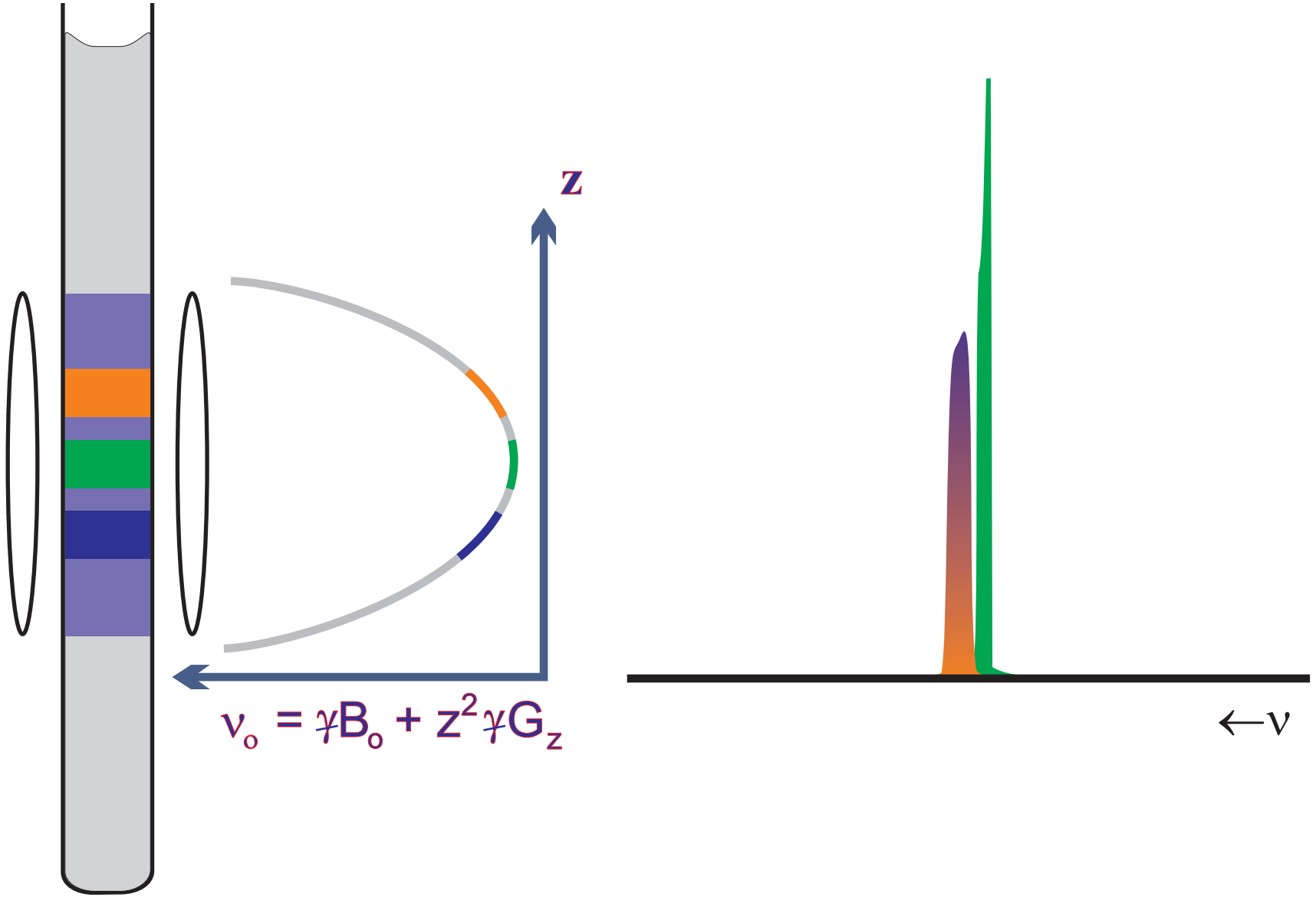
Z1 Gradient Effects on NMR Line Shapes



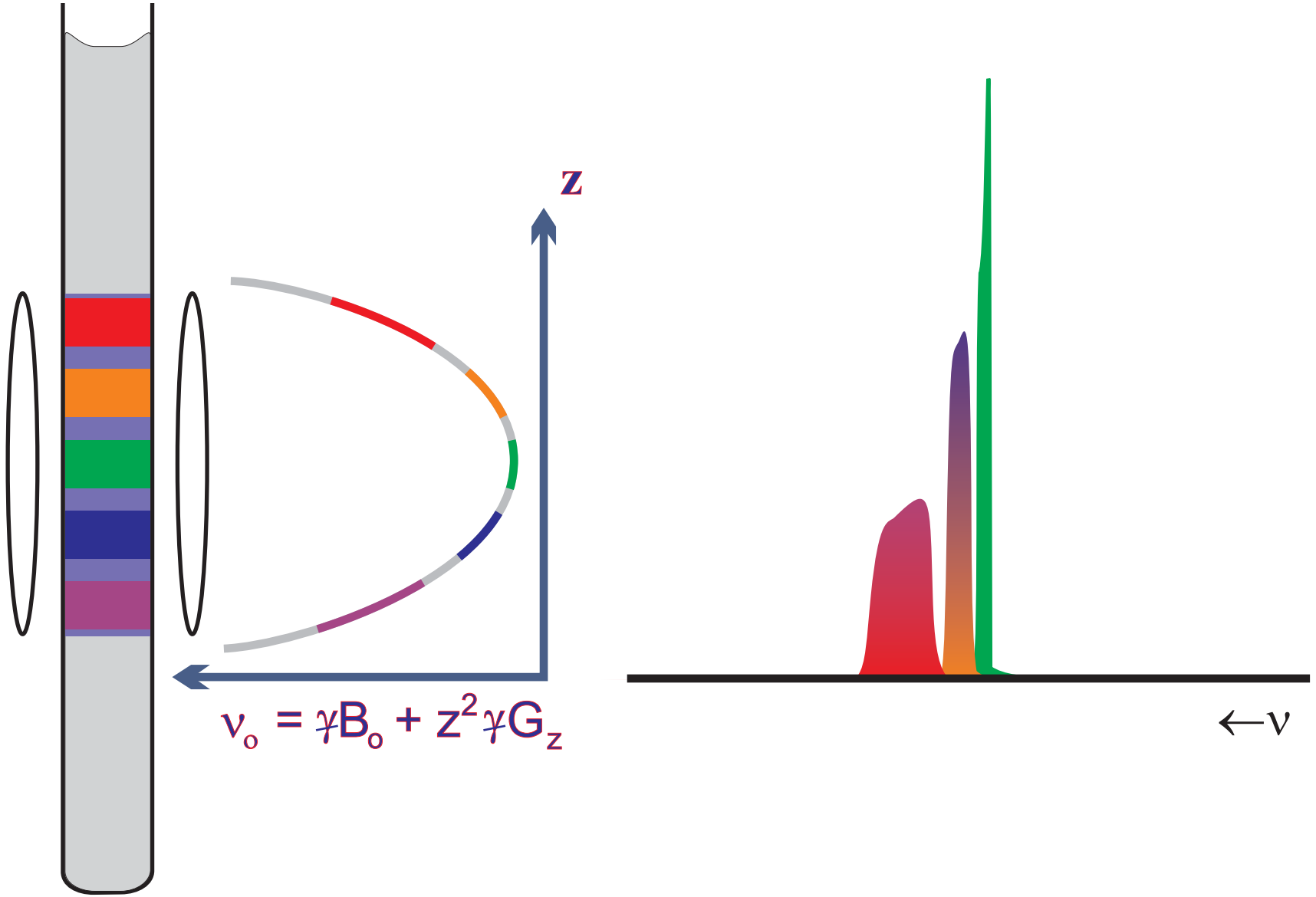
Z2 Gradient Effects on NMR Line Shapes



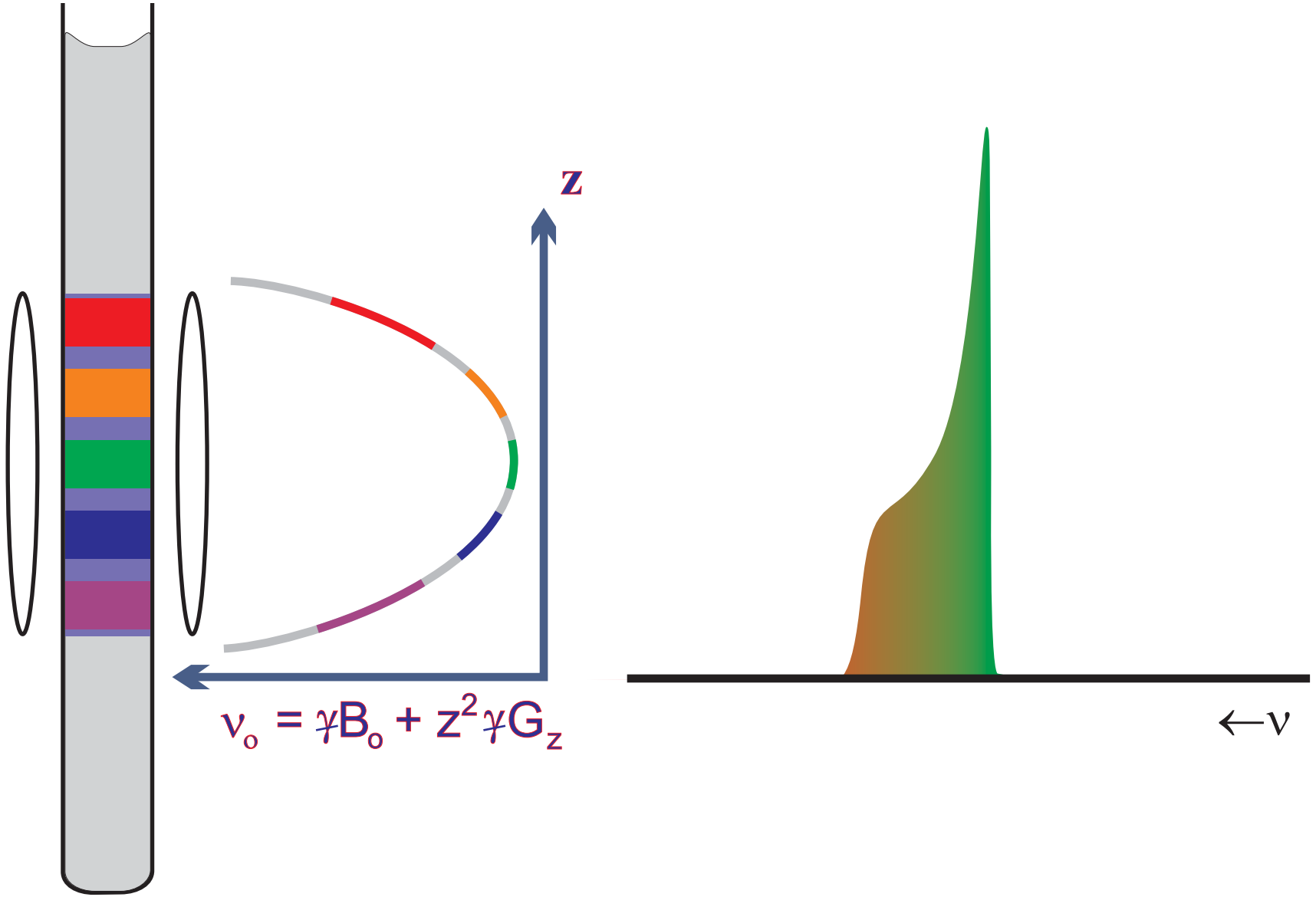
Z2 Gradient Effects on NMR Line Shapes



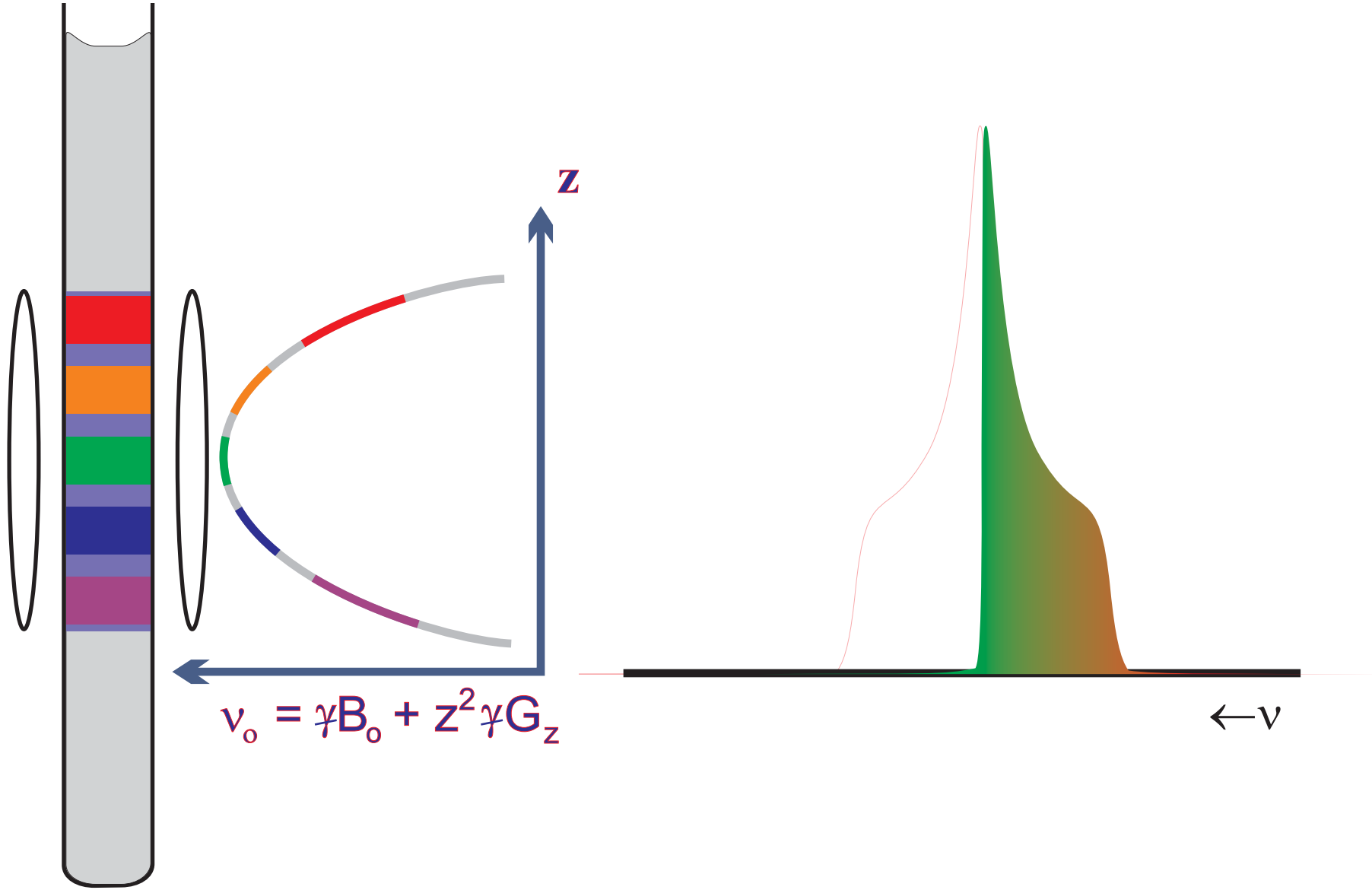
Z2 Gradient Effects on NMR Line Shapes



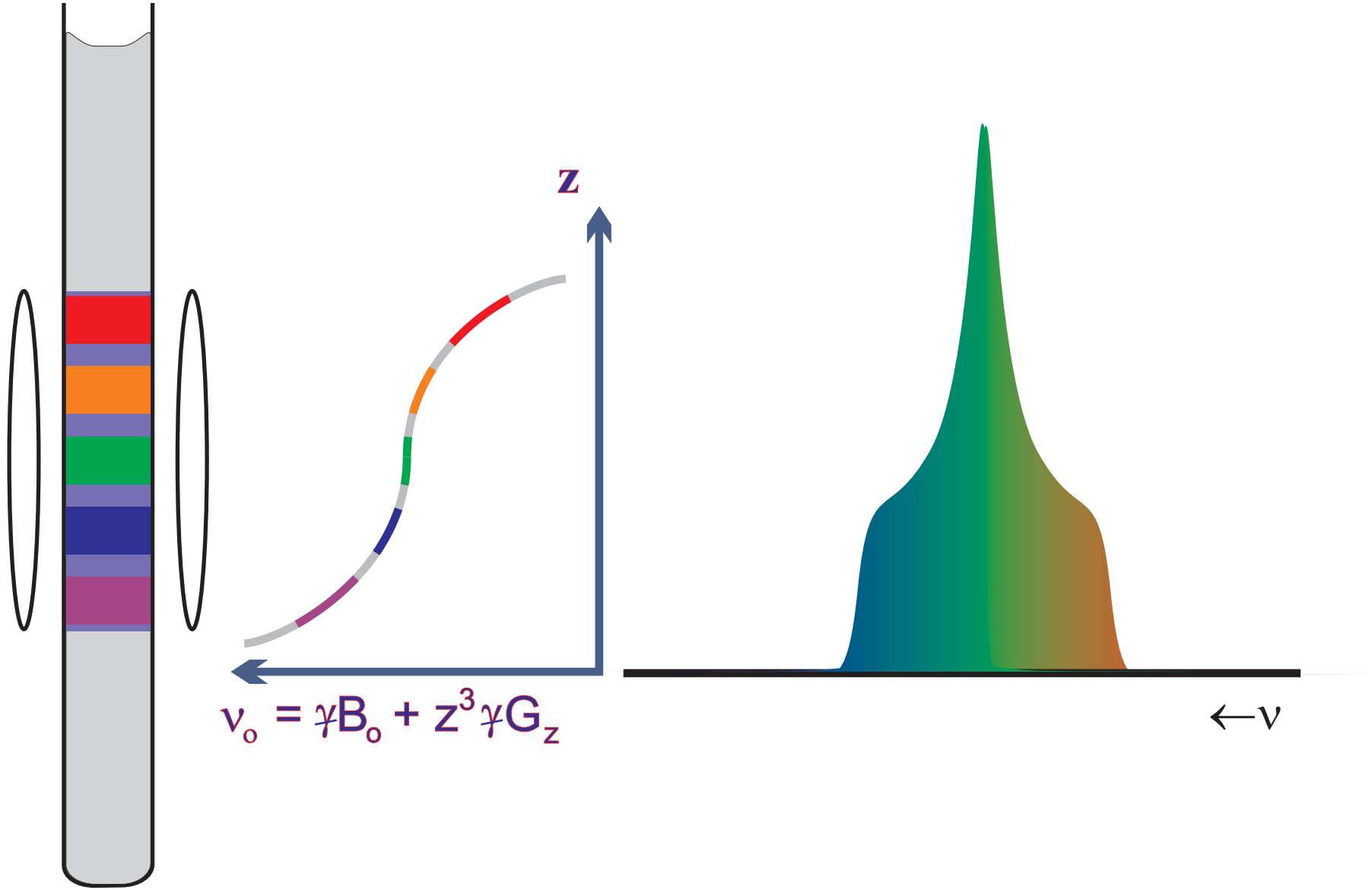
Z2 Gradient Effects on NMR Line Shapes



Z2 Gradient Effects on NMR Line Shapes



Z3 Gradient Effects on NMR Line Shapes



Manual Shimming: Final Comments

For a much more complete description of the effects of magnetic field inhomogeneities on line shape, see the references below:

1. G. A. Pearson, "Shimming an NMR Magnet," Chem. Dept., Univ. IA, Iowa City, IA 52252;
2. Claridge (2nd ed., section 3.4.5 (p. 77-82)
3. G. N. Chmurny and D. I. Hoult, "The Ancient and Honorable Art of Shimming," Concepts Magn. Reson. 2, 131-149 (1990).

One can also simply sit at a spectrometer with a good shim and observe a well-resolved, narrow singlet. Then adjust one shim until it is significantly out-of-shape, and acquire a new spectrum to see the effect of that shim. The papers also cover a range of shim effects that might be difficult to experiment with directly, and review shim strategies based on years of manual shimming experience.