# Linewidth broadening from magnetic fields

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**TL;DR:** Magnetic fields that vary spatially or temporally broaden atomic and molecular transitions with Zeeman shifts. For transitions with quadratic Zeeman shifts the broadening increases with the field strength.

This note calculates how a spectroscopic lineshape broadens for an atom or molecule interacting with a magnetic field that has a linear spatial gradient or noisy temporal fluctuation. This phenomenon is important in measurements of minimum linewidths. This note treats transitions that have either a linear or quadratic Zeeman shift. Transitions with quadratic Zeeman shifts are calculated to broaden linearly with the applied field strength in a way that allows this broadening to be extrapolated out, which was an important phenomenon in some of my previous work.[1]

## I. SPATIALLY VARYING MAGNETIC FIELD

Consider a measured lineshape that is an ensemble average of the form

$$S(f) = \int G(\mathbf{x}) L(f, f_0(\mathbf{x}), \Gamma)\, d\mathbf{x}, \tag{1}$$

where $f$ is the temporal frequency of a laser probing the atomic or molecular particles of interest. The integral includes all of the particles sampled by the laser beam, for example, within a particular volume in space. The distribution $G(\mathbf{x})$ of the ensemble of particle positions $\mathbf{x}$ is normalized, $\int G(\mathbf{x})\, d\mathbf{x} = 1$. The single-particle lineshape $L(f, f_0, \Gamma)$ is parameterized by a single-particle full width at half maximum (FWHM) $\Gamma$, is normalized according to $\int L(f, f_0, \Gamma)\, df = 1$, and shifts with the magnetic field according to a position-dependent line center $f_0 = f_0(\mathbf{x})$.

To proceed, let's consider a magnetic field $\mathbf{B}(\mathbf{x}) = B(x, y, z)\,\hat{\mathbf{z}}$ oriented along the same direction $\hat{\mathbf{z}}$ as the quantization axis of the particles. Let the field have a strength $B(x, y, z) = B(z)$ that varies linearly with position along that same direction, such that

$$B(z) = B_0 + \left(\frac{\partial B}{\partial z}\right) z. \tag{2}$$

This is an approximation to the fields in laser-cooling experiments that trap atoms just below the centers of a quadrupole electromagnet. In such experiments, the offset $B_0$ can usually be adjusted over a wide range before a measurement but there is less control of the gradient (e.g., switching the quadrupole field on or off toggles between large and small gradients). Linear gradients on the order of 10 G/cm were common in my previous work.

For the distribution of positions, let's consider a Gaussian function with standard deviation $\sigma = w_0/2$ along the $z$ direction,

$$G(z) = \frac{1}{\sqrt{2\pi}\sigma}\, e^{-(z/\sigma)^2/2} = \frac{1}{w_0}\sqrt{\frac{2}{\pi}}\, e^{-2(z/w_0)^2}. \tag{3}$$

This is an approximation to a laser beam passing through a volume uniformly filled with particles before being detected, if the laser beam has a Gaussian irradiance profile along $z$. Alternatively, this is a rough approximation to particles trapped in an optical-dipole trap or optical lattice with a trap waist $w_0$ along $z$. Typical waists in laser-cooling experiments are a few tens or hundreds of microns.

For the single-particle lineshape, let's consider a normalized Lorentzian function,

$$L(f, f_0, \Gamma) = \frac{\Gamma/(2\pi)}{(\Gamma/2)^2 + [f - f_0]^2}, \tag{4}$$

with a single-particle FWHM $\Gamma$ that includes the effects of all other sources of broadening.

We now have all the ingredients to calculate (1) except for the relationship between $f_0(\mathbf{x}) = f_0(z)$ and the field (2), which is given by the Zeeman interaction of the particles with the field. Let's treat two cases of interest in the next two sections.

Before we continue, it's handy to introduce a characteristic spread of the field

$$\Delta B = w_0 \left|\frac{\partial B}{\partial z}\right| > 0. \tag{5}$$

Note that because $G(z) = G(-z)$, we are free to choose a positive sign for this quantity. Likewise, note that the effects of $B_0$ on (1) will not depend on its sign.

### A. Quadratic Zeeman shift

First, consider a transition with a quadratic differential Zeeman shift, such as a "clock" transition between two $m = 0$ sublevels. For the field (2), the line center for a given particle at position $z$ is approximately

$$f_0(z) = f_{00} + \alpha\, B(z)^2 = f_{00} + \alpha \left[B_0^2 + 2B_0 \left(\frac{\partial B}{\partial z}\right) z + \left(\frac{\partial B}{\partial z}\right)^2 z^2\right], \tag{6}$$

where the coefficient $\alpha$ parameterizes the quadratic Zeeman shift away from the field-free center $f_{00}$. Let's ignore any higher order field shifts.

We are free to shift the origin of the variable $f$. A convenient choice is to shift to a detuning $\delta f$ from the expected line center without any field gradients,

$$\delta f = f - f_0(0) = f - (f_{00} + \alpha\, B_0^2). \tag{7}$$

This choice makes clear any shift resulting from a field gradient, in addition to broadening. With this choice, the difference in the denominator of (4) is

$$f - f_0(z) = \delta f - \alpha \left(\frac{\partial B}{\partial z}\right) z \left[2B_0 + \left(\frac{\partial B}{\partial z}\right) z\right]. \tag{8}$$

To simplify our coefficients, let

$$a = 2\,\alpha\,B_0 \left(\frac{\partial B}{\partial z}\right) \tag{9}$$

$$b = \alpha \left(\frac{\partial B}{\partial z}\right)^2 . \tag{10}$$

Then $f - f_0(z) = \delta f - az - bz^2$.

Combining all of the above, the lineshape (1) becomes

$$S(\delta f) = \int_{-\infty}^{\infty} \left(\frac{1}{w_0}\sqrt{\frac{2}{\pi}} e^{-2(z/w_0)^2}\right) \left(\frac{\Gamma/(2\pi)}{(\Gamma/2)^2 + (\delta f - az - bz^2)^2}\right) dz, \tag{11}$$

which is ready for numerical use. By inspection, note that even at zero applied field ($a = 0, b \neq 0$) we expect a broadening and a shift of the lineshape because of the field gradient.

### 1. High-field or weak-gradient limit

For sufficiently large fields such that $|a| \gg |bz|$, or equivalently

$$|B_0| \gg \Delta B, \tag{12}$$

we can set $b = 0$, simplifying the lineshape (11) to

$$S(\delta f) \approx S_1(\delta f) = \int_{-\infty}^{\infty} \left(\frac{1}{w_0}\sqrt{\frac{2}{\pi}} e^{-2(z/w_0)^2}\right) \left(\frac{\Gamma/(2\pi)}{(\Gamma/2)^2 + (\delta f - az)^2}\right) dz. \tag{13}$$

This limit likely applies to typical experimental situations with small, unintentional field gradients. This is equivalent to a Voigt profile,[2]

$$V(x;\sigma,\gamma) = \int_{-\infty}^{\infty} \left(\frac{e^{-y^2/(2\sigma^2)}}{\sigma\sqrt{2\pi}}\right) \left(\frac{\gamma/\pi}{\gamma^2 + (x-y)^2}\right) dy, \tag{14}$$

which is the convolution of normalized Gaussian and Lorentzian lineshapes, often encountered in Doppler-broadened spectroscopy. Here, $\sigma$ is the Gaussian standard deviation and $\gamma$ is the Lorentzian half width at half maximum (HWHM). Comparing (13) and (14), and using the substitution $y = az$, we find

$$S_1(\delta f) = V(\delta f; \sigma_1 = |a w_0/2|, \gamma_1 = \Gamma/2). \tag{15}$$

Therefore, in this limit there is only broadening and no shift.

Importantly, the standard deviation is proportional to the field,

$$\sigma_1 = \left|\frac{a w_0}{2}\right| = \left|\alpha\, w_0 \left(\frac{\partial B}{\partial z}\right)\right| B_0 = |\alpha \Delta B| B_0. \tag{16}$$

To within 0.02%, the FWHM of a Voigt profile is approximately[2]

$$\Gamma_{\mathrm{V}} \approx 0.5346\,(2\gamma) + \sqrt{0.2166\,(2\gamma)^2 + (2\sigma\sqrt{2\ln 2})^2}, \tag{17}$$

which for our case is

$$\Gamma_{\mathrm{V}} \approx 0.5346\,\Gamma + \sqrt{0.2166\,\Gamma^2 + 5.5452\,\sigma_1^2}. \tag{18}$$

Together with (16), this gives the observed FWHM vs $B_0$, which should be a hyperbola (or a standard power broadening shape plus an offset). For sufficiently large fields, the broadening will vary linearly with field with the slope

$$\frac{\partial \Gamma_{\mathrm{V}}}{\partial B_0} \approx 2.3548\,|\alpha \Delta B|. \tag{19}$$

In principle, one could fit data of $S(\delta f)$ vs $B_0$ in this limit in order to determine the parameters $\Gamma$ and $|\alpha\Delta B|$, either by fitting with Voigt profiles to directly estimate $\sigma_1$ and $\gamma_1$ vs $B_0$ or by fitting with other functions (e.g., Gaussians or Lorentzians) to estimate the total FWHM $\Gamma_{\mathrm{V}}$ vs $B_0$. Using knowledge of $\alpha$, one could also determine $\Delta B$ from either approach. In my previous work, measurements of $\Gamma_{\mathrm{V}}$ vs $B_0$ were able to estimate $|\Delta B| \approx 0.0094(13)$ G for one particular experimental setup with a quadrupole field.

### B. Linear Zeeman shift

Next, consider a transition with a linear differential Zeeman shift, such as a transition between sublevels that are not both $m = 0$. Here, instead of (6) the line center is approximately

$$f_0(z) = f_{00} + \beta B(z), \tag{20}$$

where the coefficient $\beta$ parameterizes the linear Zeeman shift. Shifting to a detuning $\delta f$ from the expected line center gives

$$f - f_0(z) = \delta f - \beta \left(\frac{\partial B}{\partial z}\right) z. \tag{21}$$

Coincidentally, this leads to the same result as (13) from the limit in the previous section if we redefine

$$a = \beta \left(\frac{\partial B}{\partial z}\right). \qquad \text{(linear Zeeman shift)} \tag{22}$$

However, this case's broadening does not increase with field. Instead, the $\sigma_1$ of (16) becomes

$$\sigma_1 = \left|\frac{a w_0}{2}\right| = \left|\frac{\beta \Delta B}{2}\right|. \tag{23}$$

Using this, one can evaluate the approximate linewidth with (18). For the case where this broadening dominates, the observed linewidth should be approximately

$$\Gamma_{\mathrm{V}} \approx 1.1774\,|\beta \Delta B|. \tag{24}$$

Again, this broadening does not vary with the field strength $B_0$, so is likely difficult to directly detect, especially if other sources of broadening are present. However, broadening by a quadratic Zeeman shift from a different transition (or possibly the same one using more analysis) could be used to determine $|\Delta B|$, so this linear-Zeeman-shift broadening could then be estimated if $\beta$ is known.

## II. TIME-VARYING MAGNETIC FIELD

If instead of a spatial gradient there is a temporally varying field (e.g., coil noise), then all of the above results transfer as long as the statistical distribution of field values is Gaussian during the measurement duration. In this case, the integral in (1) is over field strength $B$ and the standard deviation $\sigma = w_0/2$ in (3) characterizes the field distribution, instead of the particle positions.

## REFERENCES

[1] B. H. McGuyer, M. McDonald, G. Z. Iwata, M. G. Tarallo, W. Skomorowski, R. Moszynski, and T. Zelevinsky, "Precise study of asymptotic physics with subradiant ultracold molecules," Nat. Phys. **11**, 32 (2015).

[2] Wikipedia has a good description of Voigt profiles: `http://en.wikipedia.org/wiki/Voigt_profile`