

RESEARCH NOTE

Linewidths with gaussian and lorentzian broadening

A M STONEHAM

Theoretical Physics Division, AERE, Harwell, Didcot, Berks

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**Abstract.** Spin resonance lines occur which are broadened both by mechanisms giving a lorentzian shape and by mechanisms giving a gaussian shape. It is often important to separate these contributions to the peak-to-peak separation of the derivative of the lineshape. A simple and accurate expression is obtained to achieve this. If  $\Delta_T$  is the observed peak-to-peak separation, and  $\Delta_L$  and  $\Delta_G$  are those of the lorentzian and gaussian components separately, then

$$\Delta_T = \frac{\Delta_G^2 + 0.9085 \Delta_G \Delta_L + 0.4621 \Delta_L^2}{\Delta_G + 0.4621 \Delta_L}$$

is accurate to better than  $0.01 \Delta_T$  for all  $\Delta_L$  and  $\Delta_G$ .

Spin resonance lines in solids are broadened by a number of mechanisms. Some of these mechanisms give a gaussian lineshape, such as dipolar broadening in concentrated crystals (Van Vleck 1948) and strain broadening by dislocations (Stoneham 1966, 1969). Other mechanisms lead to a lorentzian lineshape, such as the relaxation broadening due to the finite lifetime of a state.

A number of papers have tabulated relations between the observed width of a resonance line and the widths of the lorentzian and gaussian components (eg Posener 1959). Here we are concerned with the peak-to-peak separation  $\Delta_T$  of the derivative of the observed line and with the corresponding separations  $\Delta_L$  and  $\Delta_G$  of the lorentzian and gaussian contributions. In spin resonance it is common to observe the derivative of the lineshape rather than the shape itself. The analysis of  $\Delta_T$  into contributions  $\Delta_L$  and  $\Delta_G$  is necessary if one is to use observed peak-to-peak separations to measure spin-lattice relaxation times (Cristea and Stapleton 1970, Cristea *et al* 1971, Kemple and Stapleton 1972, Stoneham *et al* 1972). In this note we derive a simple accurate expression relating  $\Delta_T$ ,  $\Delta_L$  and  $\Delta_G$ , which should provide a convenient method of analysing experimental data.

If the mechanisms which lead to lorentzian and gaussian broadening are independent, the lineshape is just the convolution of a gaussian and a lorentzian. Apart from a normalization factor, the convolution can be written in the form

$$h(a, b) = \int_{-\infty}^{\infty} dx \exp(-x^2) \{a^2 + (x-b)^2\}^{-1}.$$

After some rearrangement, this can be expressed in terms of the plasma integral  $I(z)$  of Fried and Conte (1961):

$$h(a, b) = (I(b+ia) - I(b-ia))/2ia$$

where

$$I(z) = \int_{-\infty}^{\infty} dx \exp(-x^2) (x-z)^{-1}.$$

The plasma integral is a well-understood and tabulated function. The peaks of the derivative of the convolution are found from the roots of  $d^2h(a, b)/db^2=0$ . It is straightforward to obtain their separation  $\Delta_T$  numerically for different values of  $\Delta_L/\Delta_G$ .

The results are then approximated by an analytic expression which is exact for gaussian broadening alone or for lorentzian broadening alone. This interpolation relation can be obtained to any desired degree of accuracy. We have adopted a maximum error of  $0.01\Delta_T$ . The final expression is

$$\Delta_T = \frac{\Delta_G^2 + 0.9085\Delta_G\Delta_L + 0.4621\Delta_L^2}{\Delta_G + 0.4621\Delta_L}.$$

The relation between  $\Delta_G/\Delta_T$  and  $\Delta_L/\Delta_T$  is shown in figure 1, where the results may be compared with those obtained using two simple assumptions. The first (curve B) is that  $\Delta_T = \Delta_1 + \Delta_2$ , which would be exact for two lorentzian components. The second (curve C) would be exact for two gaussians and assumes  $\Delta_T^2 = \Delta_1^2 + \Delta_2^2$ .

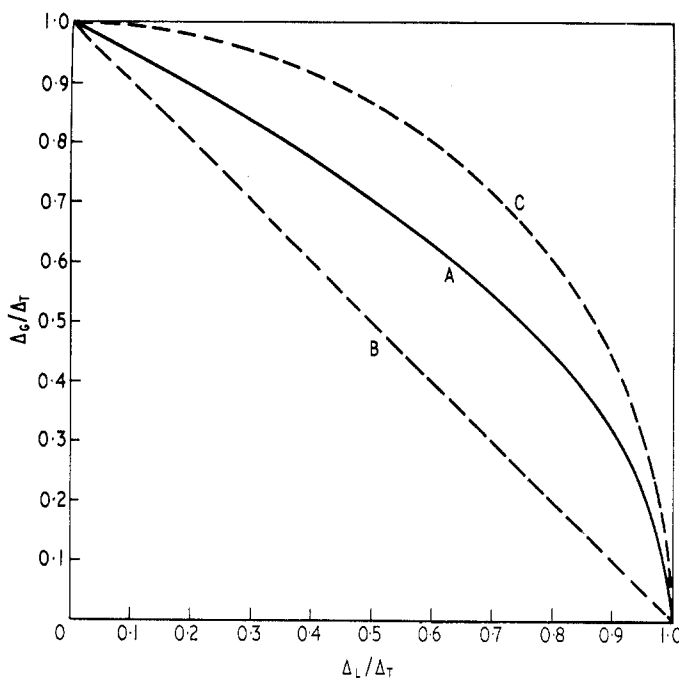


Figure 1. The relation between  $\Delta_L/\Delta_T$  and  $\Delta_G/\Delta_T$ . Our analytic expression A is compared with B, which assumes  $\Delta_T = \Delta_1 + \Delta_2$ , and with C, which assumes  $\Delta_T^2 = \Delta_1^2 + \Delta_2^2$ .

The result should be especially useful in deriving spin-lattice relaxation times from the temperature dependence of the peak-to-peak separation. At the lowest temperatures the lineshape is usually gaussian because of dipolar or dislocation broadening. This contribution  $\Delta_G$  is essentially independent of temperature. At higher temperatures, relaxation gives a temperature-dependent lorentzian contribution, and experiment

measures  $\Delta_T$ . The two mechanisms are independent: for practical purposes the relaxation times are independent of the local dipolar or dislocation strain field. Given  $\Delta_G$  and  $\Delta_T$ , the lorentzian term  $\Delta_L$  can be obtained from the formula or figure given. The relaxation time is then given simply in terms of  $\Delta_L$ .

### References

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