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ABSTRACT

The measurement of ion temperatures from the Doppler broadening of spectral lines is discussed. Calculations are used to show that the shape of the instrument function of the spectrometer can have a significant effect on the measured value, even when the broadening is large (∿10x) compared with the half-width of the instrument function. The discussion is illustrated by the topical example of measurements made using an XUV grating spectrometer.

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INTRODUCTION

An accurate determination of the ion temperature is of particular importance in plasmas used in fusion research. A common technique for measuring this parameter is to determine the Doppler broadening of spectral lines emitted by the ions of interest. The procedure for obtaining the Doppler component from the observed line is well-known, being summarised by Allen (1963) and discussed in more detail by authors such as Unsöld (1955) and Finn and Mugglestone (1965). However, in cases where a particular instrument function is considered, it has been usual to assume a Gaussian or Lorentzian profile. This is inappropriate for some recently-developed multichannel spectrometers which have instrument functions with significant line wings. In view of their increasing use, it seems pertinent to reassess the effect of the instrument function on the ion temperature measurement, considering a wider range of particular examples of instrument functions than before.

Calculations have been performed to estimate the effect that different instrument functions would have on the temperature measurements. Square, Gaussian and Lorentzian profiles are considered, together with those having enhanced line wings, such as profiles of the type $\frac{1}{(1 + \frac{x^2}{a})^n}$, where $n \leq 1$. Functions of the latter type are considered, since they approximate to observed instrumental profiles. An example is that of the VUV, Schoeffel-McPherson, survey spectrometer.

It is generally assumed that the detailed instrument function is unimportant if the broadening is large, say, greater than 10 times the instrumental half-width. The analysis shows that this assumption is untenable. When the broadening is smaller, the measurement is even more sensitive to differences in the instrument function. As an illustration an instrumental profile of the XUV, Schwob-Fraenkel, grazing incidence spectrometer is considered. Although superficially the profile approximates to a Gaussian function, the assumption of an exact Gaussian function in the determination of the ion temperature can lead to a 25% error in the measured temperature.

ANALYSIS

The shape of the Doppler component of a broadened line depends on the ion velocity distribution. In the present analysis, it is assumed that this is Maxwellian. It follows that temperature is a well-defined concept and that the Doppler component has a Gaussian shape.

In addition to shifting the line centre, mass motion effects can result in a broadening or a distortion of the Doppler component from a Gaussian shape. These effects are not discussed, although it should be noted that they can be significant (Stork et al 1987).

1. Study of various instrument functions to investigate the effect of the instrument function on the ion temperature measurement.

The instrument functions detailed in table 1 have been convolved with a Gaussian function and the half-widths of the convolved profiles determined. The ion temperature varies quadratically with half-width and, consequently, the square of the half-width is found. In all cases the formula for the instrument function, $I(\lambda)$, has been chosen so that it has unit half-width (FWHM). Gaussian functions, $D(\lambda)$, with half-widths of up to 30 units are used to represent the Doppler component of the spectral line.

The effect of the shape of the instrument function can be seen by comparing the squared half-widths of the various convolved instrument functions with those of a particular convolved function, which in figure 1 is chosen to be a Lorentzian function, $L(\lambda)$, and, in figure 2, a Gaussian function, $G(\lambda)$. That is figures 1 and 2 illustrate

$$\frac{\omega_I^2}{\omega_L^2} : \omega_D \quad \text{and} \quad \frac{\omega_I^2}{\omega_G^2} : \omega_D,$$

where ω_I, ω_L and ω_G are the half-widths of the convolved profiles

$$\int_{\infty}^{\infty} D(t)I(\lambda-t)dt, \quad \int_{\infty}^{\infty} D(t)L(\lambda-t)dt \text{ and } \int_{\infty}^{\infty} D(t)G(\lambda-t)dt,$$

respectively, and ω_D is the half-width of the Doppler component, $D(\lambda)$. This procedure highlights the differences between the effects of the various instrument functions. As the temperature increases from zero all the ratios diverge from unity; in this region the instrument function dominates the convolved profile. At larger broadenings, the Doppler component becomes more important and the ratios approach unity with increasing temperature. The detailed profile of the instrument function can be neglected when the broadening is such that all ratios are close to one. If the instrument function is similar to a Gaussian, Square or Lorentzian function this occurs at a broadening of about 10. However, if the instrument function has enhanced wings, there could be a significant error at broadenings of up to 30 times the instrumental half-width. It follows that the detailed instrument function cannot be neglected without some check on its shape, even when the broadening is large.

The effect of the shape of the instrument function can be far more important than misjudging the half-width. Figure 3 shows the result of doubling the half-width of a Lorentzian instrument function. Again, the square of the ratios of the half-widths of the convolved profiles are plotted against the Gaussian half-width representing the Doppler component in the convolution. Despite the wider instrument functions having 1½ and twice the half-width of the reference instrument function, the ratios are within 10% of unity when the Doppler broadening is 10.

Figure 4 shows an example of an instrument function with enhanced wings. The observed line profile is that of the CIII transition at 977.02Å emitted by the JET plasma and recorded with a model 251 Schoeffel-McPherson, VUV spectrometer (Fonck _et al_ 1982) having a 450g/mm diffraction grating. This survey instrument observes a wide spectral range, but with a limited spectral resolution. Consequently, the line profile corresponds to the instrument function. It can be seen that the line profile can be approximately fitted by a modified Lorentzian function of the form $\frac{1}{[1 + (\frac{x}{1.025})^2]^{0.609}}$. The line wings extend to about 40 times the line half-width. The reason for this is not understood, but the enhanced line wings are clearly a feature of spectrometers with a multichannel detector in which crosstalk between the channels occurs.

2. The effect of an enhanced wing instrument function when the Doppler broadening is comparable to the instrumental half-width.

Another spectrometer whose instrument function exhibits enhanced wings is the XUV, Schwob-Fraenkel, grazing incidence spectrometer (Schwob _et al_ 1987). In this case the extent of the wings is more limited, only being about 20 times the half-width. The instrument generally has a narrower spectral range than the VUV spectrometer, with a correspondingly improved spectral resolution. Although it was primarily designed as a survey instrument rather than for line profile analysis, the spectral resolution is sufficient for Doppler broadening and shifts to be observed and ion temperature measurements have been made (Mattioli _et al_ 1988).

As is shown in figure 5, the peak of the instrument function can be fitted reasonably well by a Gaussian profile. The instrument function shown is the line profile of the HeII line at 256.32Å observed in a JET plasma using a 600g/mm grating and 20μm entrance slit. The profile of this low temperature line is thought to be a reasonably good representation of the instrument function, since no significant change in its half-width is observed throughout the discharge. It should be noted that if this profile is in fact already Doppler broadened, the present calculations will underestimate the effect of the line wings.

As an illustration, this instrument function is applied to temperature measurements made using the neighbouring NiXXVI line at 234.09Å. Calculations were performed to determine whether the line wings had a significant effect on the derived ion temperature or whether a Gaussian instrument function could be assumed when making the measurement.

The Doppler component is again represented by a Gaussian function and when applied to a particular spectral line corresponds to an ion temperature, referred to as the actual ion temperature. It is convolved with the observed instrument function and Gaussian fits performed on the resulting convolved profile and on the instrument function. If the half-widths of the fitted profiles are, respectively, ω_{CG} and ω_{IG}, the measured ion temperature is obtained from the half-width of a Doppler component, ω_{DG}, derived from

$$\omega_{DG}^2 = \omega_{CG}^2 - \omega_{IG}^2.$$

Such a measurement of ion temperature assumes that the observed instrument function and, therefore, the convolved line profile approximate to Gaussian functions. If this assumption is valid the measured ion temperature will equal the actual ion temperature, which was input to the calculation.

Figure 6 shows the ratio of the measured ion temperature with Gaussian fits made to the profiles to the actual ion temperature input to the calculation, this ratio being plotted against the measured ion temperature. It can be seen that the measurement obtained when Gaussian fits are made to the line profiles systematically overestimates the temperature by about 25% and this applies throughout the range of temperatures considered. That the ratio does not tend more rapidly towards unity with increasing temperature is due to the Doppler broadening in this example being comparable to the half-width of the instrument function. For example, at 30 keV, a temperature which can occur in plasmas where there is significant ion heating by injected neutral beams (Hawryluk et al 1986), the broadening is still less than 1½ times the instrumental half-width.

Such modest broadening would also be expected to limit the statistical accuracy of the measurements. As an illustration, a 5% and 10% random error are supposed in the half-widths obtained from the Gaussian fits to the instrument function and broadened line profiles, ω_{IG} and ω_{CG}; the resulting error in the ratio of the temperatures is shown in figure 6. A low temperature limit would seem to be appropriate, ∿ 10keV for Ni lines, below which any measurement is disregarded.

The shape of the XUV instrument function changes with wavelength and at shorter wavelengths, ∿30Å, the systematic error in the measured temperature assuming Gaussian profiles is found to be less, at most being 15%. However, at these wavelengths, the broadening is sufficiently small compared with the instrumental half-width that for the temperature ranges of interest the very poor statistical accuracy makes the ion temperature measurement of questionable value, even if higher spectral orders of the lines are used.

CONCLUSION

Calculations show that the shape of the instrument function of a spectrometer can have a significant effect on the measurement of ion temperatures from the Doppler broadening of the spectral lines, even when the broadening is large compared with the half-width of the instrument function. The instrument functions considered include those measured for a VUV and an XUV spectrometer widely used in plasma research, both of which are found to have enhanced wings. The XUV instrument is useful for ion temperature measurements ($\gtrsim$ 10keV if Ni lines are employed) and it is shown that neglecting the line wings can result in the ion temperature being overestimated by 25%.

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Table 1. Instrument Functions.

Function	Formula used
Square	$\left[\begin{array}{ll} 0, & \lambda<-\frac{1}{2} \\ 1, & -\frac{1}{2}\leq\lambda\leq\frac{1}{2} \\ 0, & \frac{1}{2}<\lambda \end{array}\right.$
Gaussian	$\mathrm{Exp}[-(\frac{\lambda-\lambda_0}{0.6006})^2]$
Lorentzian	$\frac{1}{1+(\frac{\lambda-\lambda_0}{0.5})^2}$
Modified Lorentzians	$\frac{1}{[1+(\frac{\lambda-\lambda_0}{0.4056})^2]^{0.75}}$ $\frac{1}{[1+(\frac{\lambda-\lambda_0}{0.3623})^2]^{0.65}}$ $\frac{1}{[1+(\frac{\lambda-\lambda_0}{0.3146})^2]^{0.55}}$

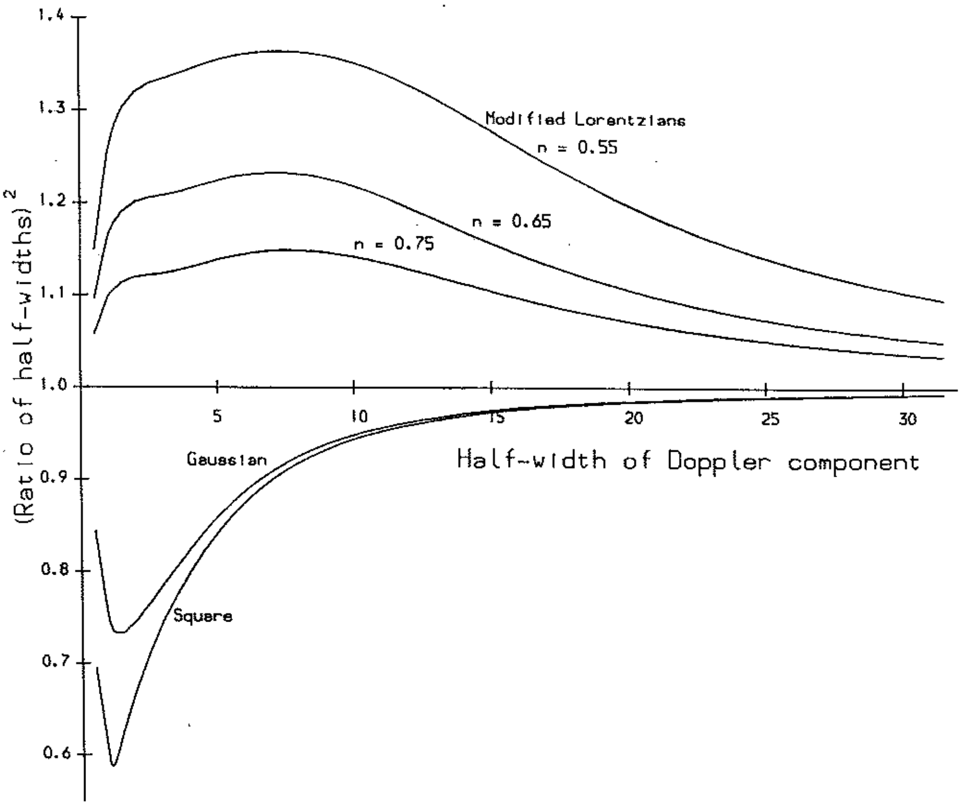

Fig. 1 (Half-width)^2 of the convolved instrument functions compared with that of a convolved Lorentzian function

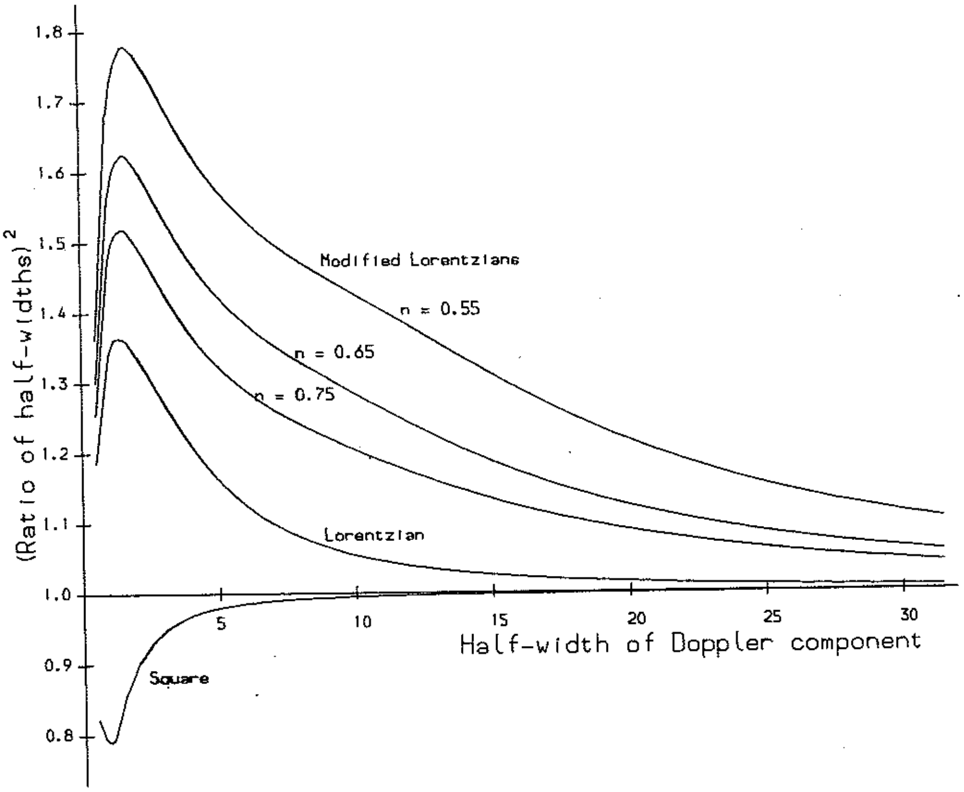

Fig. 2 (Half-width)^2 of the convolved instrument functions compared with that of a convolved Gaussian function

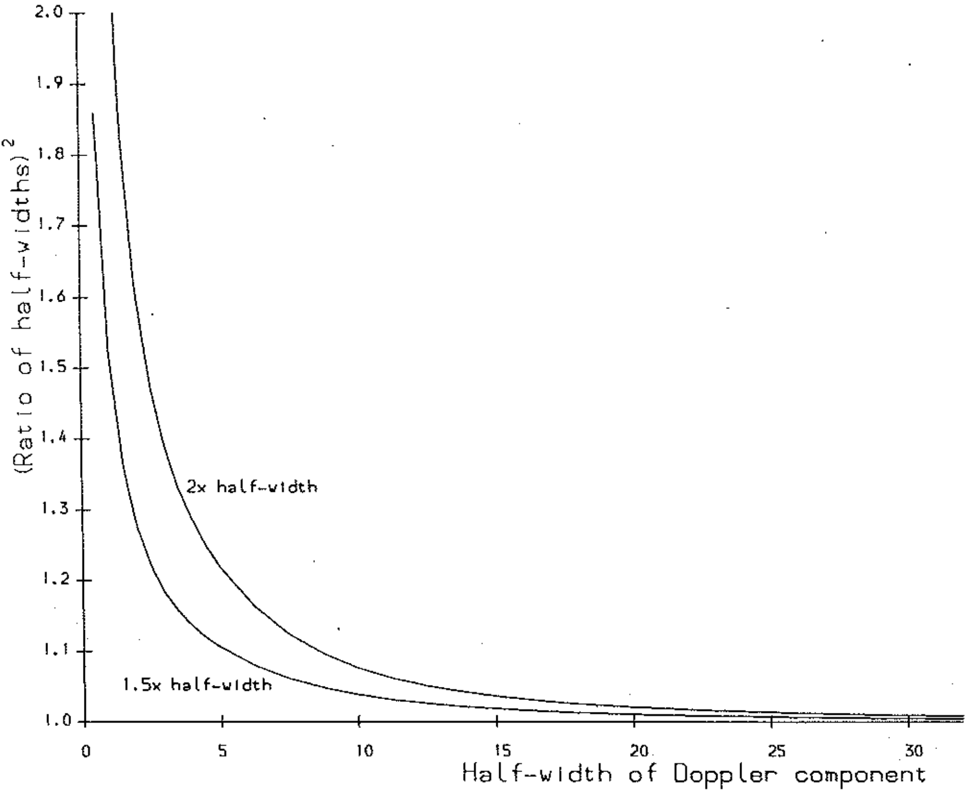

Fig. 3 (Ratio)^2 of the half-widths of Voigt profiles formed from Lorentzians of different half-widths

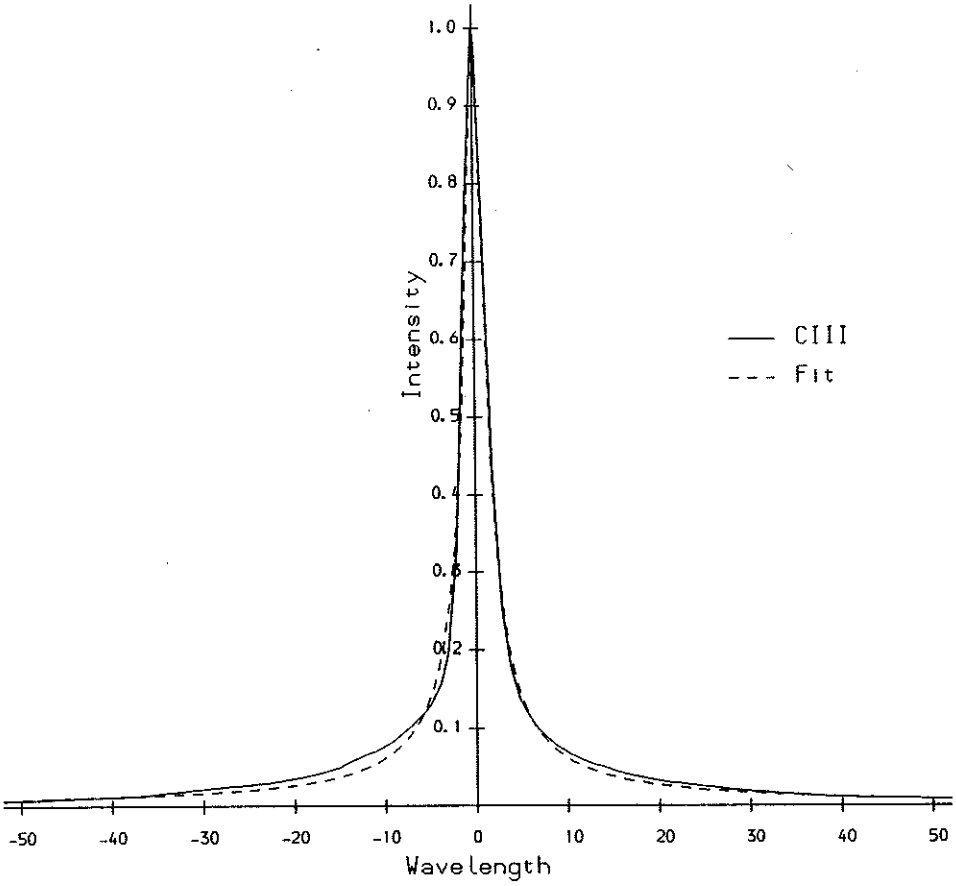

Fig. 4 A fitted instrument function of the Schoeffel-McPherson, VUV spectrometer

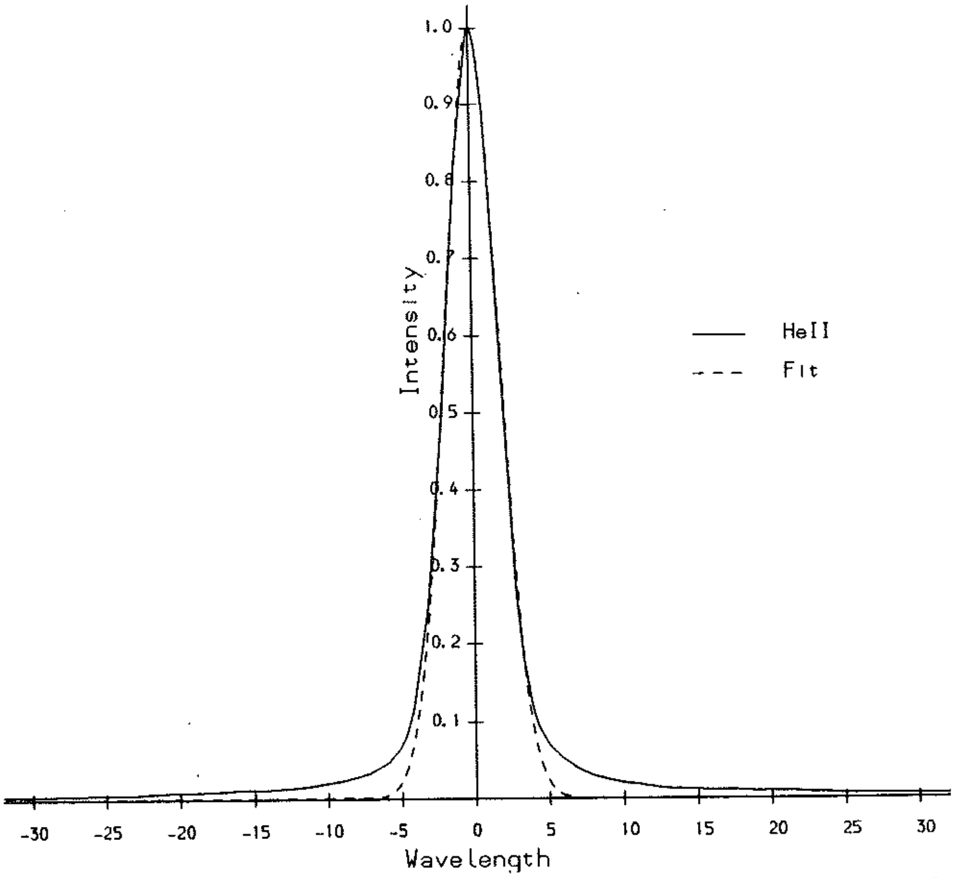

Fig. 5 Comparison between an instrument function of the Schwob-Fraenkel, XUV spectrometer and a Gaussian function

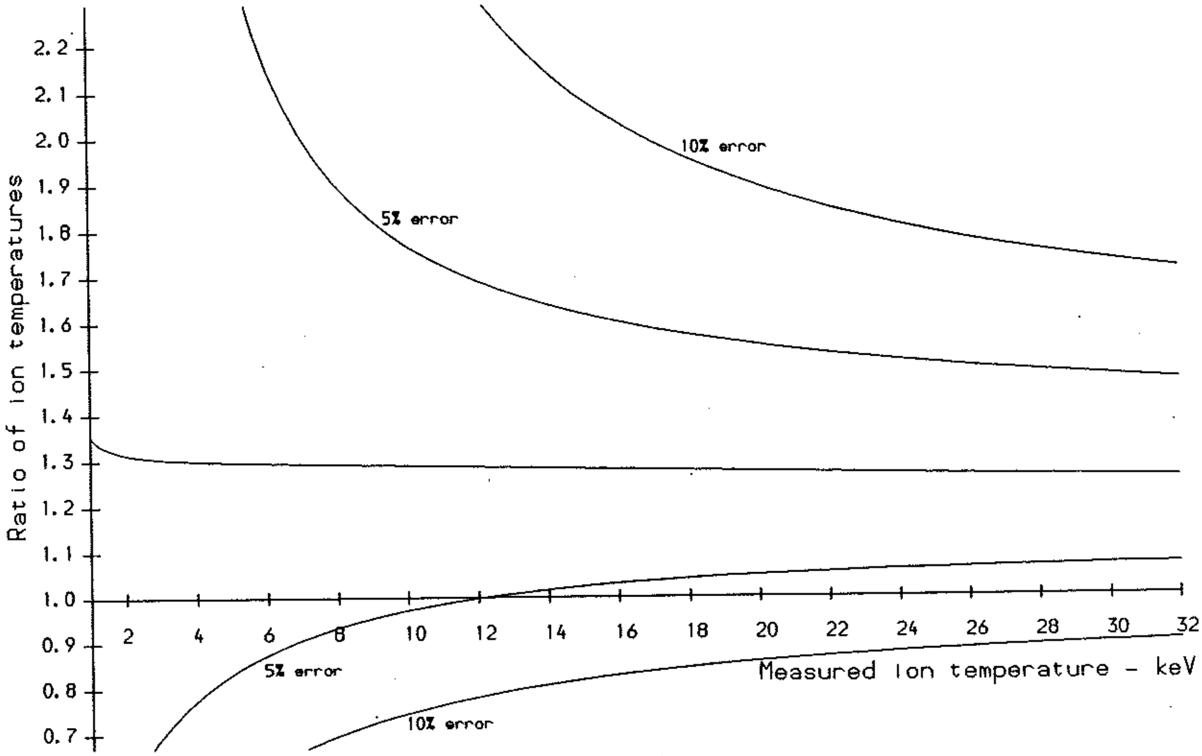

Fig. 6 Ratio of the measured ion temperature assuming a Gaussian fit to the instrument function of the Schwob-Fraenkel spectrometer to the actual ion temperature. The errors in the ratio assuming a 5 or 10% random error in the fit are indicated.