Physics-guided fitting of isotope-structured Nd III lines

AStroLab-UVa
(Atomic Spectroscopy Laboratory)

Universidad de Valladolid

V. Cob[1], M. T. Belmonte[1], P. R. Sen Sarma[1], M. Ding[2], C. P. Clear[2], N. Corral[1], J. C. Pickering[2] and S. Mar[1]

[1]Departament of Theoretical and Atomic Physics and Optics, Faculty of Sciences, University of Valladolid, 47011 Valladolid, Spain.

[2]Physics Department, Imperial College London, Prince Consort Road, London, SW7 2AZ, UK

Introduction

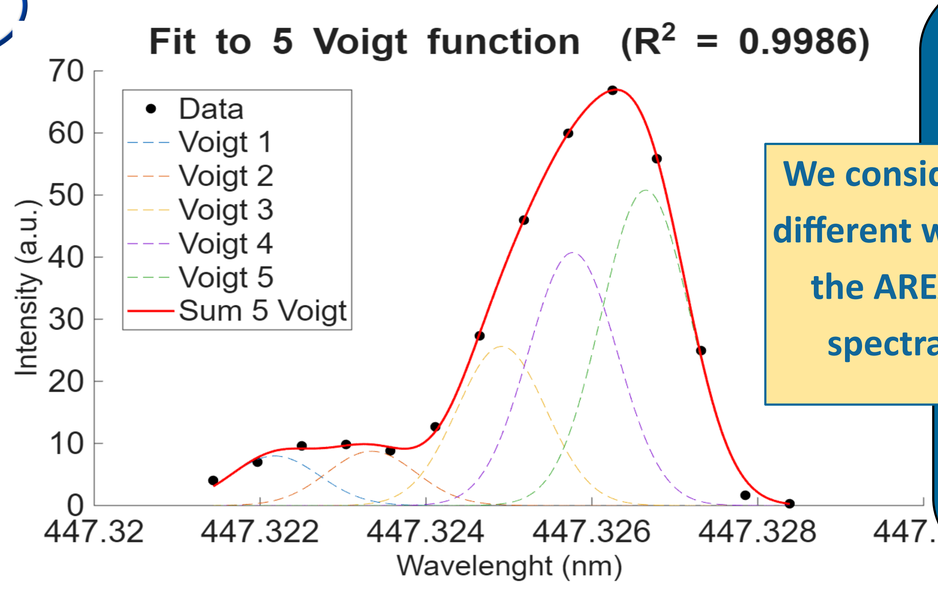
Measurement of transition probabilities of Nd III requires accurate line areas obtained from spectral line fitting. Neodymium has 7 stable isotopes (142-27.2%, 143-12.2%, 144 23.8%, 145 8.3%, 146 17.2%, 148 5.7%, 150 5.6%),

However, the extremely rich spectrum of Nd III makes line blends a major challenge when determining areas. To address this, we explored different physics-guided fitting strategies that use isotope structure as guidance, in order to gain clues about possible blends—something that a purely numerical fit cannot reveal.

What do we do?

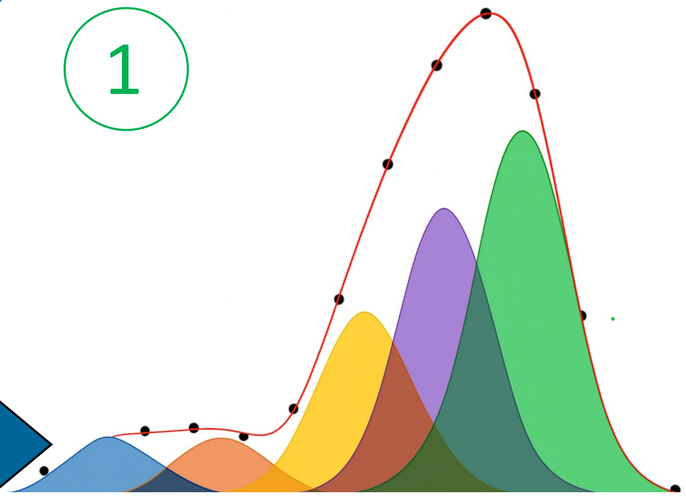
We have used the "Faddeva" function [2,3] in Matlab to perform the fitting with lsqcurvefit.

Using parameters obtained through lsqcurve, the Voigt profile can be constructed as a standard function (such as the exponential).



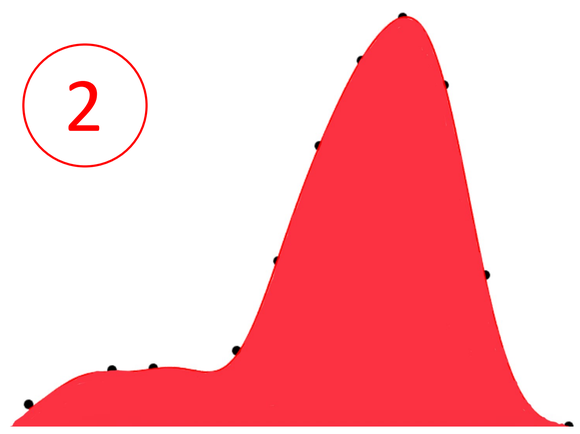
We considered two different ways to get the AREA of the spectral lines:

1



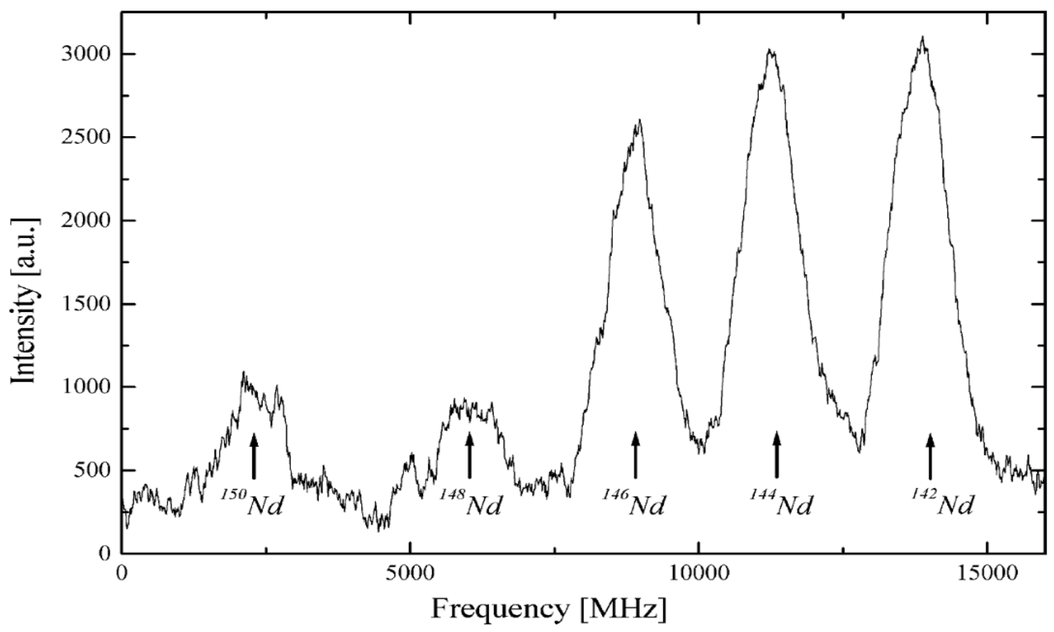
Since we know the parameters of the Voigt functions, we can measure the area of each function and then add the areas together.

2



We can also integrate the entire curve using the numerical methods available in Matlab.

Why are we doing it this way?



Our physical model for fitting Nd III lines to five Voigt functions is based on laser measurements of Nd II lines by Koczorowski et al. (2005) [1], which demonstrate the splitting of lines into five components due to even-mass-number isotope shifts.

Some troubles...

1– There are certain shapes of spectral lines that do not follow the expected pattern (possible blends?).

2– Lines showing isotope structure have to be fitted one by one to get a good fit, making the process more time consuming.

3– Some spectral lines do not have enough experimental points to fit the line profile to five Voigts.

About Matlab algorithms...

1- The lsqcurvefit "trust-region reflective" fitting method has proven to produce good results. This algorithm requires the line under study to have at least 2n + 3 data points (n is the number of Voigt profiles required).

2– To compute the Voigt function, we use the analytical Faddeeva package [2] in MATLAB, which gives a more accurate value of the line area than fitting to Voigt profiles.

3 - We are investigating different approaches for the determination of line area uncertainty (Bootstrap method, variance and covariance matrix).

References

[1]. W. Koczorowski, et al., Spectrochim. Acta Part B At. Spectrosc. 60(5) (2005) 616–623

[2] Johnson, S. G. (2017). Faddeeva package. Retrieved from http://ab-initio.mit.edu/wiki/index.php/Faddeeva_Package

[3] Zaghloul, M. R., & Ali, A. N. (2011). *ACM Transactions on Mathematical Software*, 38(2), 15.

Proyect PID2021-127786NA-100 funded by:

MINISTERIO DE CIENCIA, INNOVACIÓN Y UNIVERSIDADES

Cofinanciado por la Unión Europea

AGENCIA ESTATAL DE INVESTIGACIÓN