**TOWARDS A GLOBAL SOLUTION OF THE TRANSPORT-RELAXATION EQUATION – USING MULTIDIMENSIONAL TAYLOR SERIES EXPANSION FOR MODELLING MOLECULAR OPTICAL RESONANCES**

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One of the most important branch of molecular spectroscopy is modelling of spectral line shapes. Not only it is useful for science itself, like testing if the theoretical descriptions of the way the molecules interact are correct [1] or creating spectroscopic databases [2,3], but also can be applied to analyse human breathing [4], atmospheric measurements of the distant planets or ultra-accurate meteorology, e.g., exact determination of the Boltzmann constant [5].

The more exact results are demanded, the more accurate models need to be implemented. If the molecules do not collide, the shape of the spectral line can be described using a simple Gauss profile, since it is only the Doppler shift which contributes. In general the molecular collisions should be taken into account which makes the model of the line shapes much more complex. To describe the influence of the collisions on the line shapes, the transport-relaxation equation needs to be implemented [6]. It allows calculating the velocity distribution of optical coherence. However, in the general case it is extremely complicated to figure out the exact solution of the equation. Numerical attempts, which are widely used, are either time demanding or not accurate enough.

The main goal of the talk is to demonstrate another way of solving the transport-relaxation equation. In the usual considerations the value of function needs to be numerically found in every point of the parameter space of the model. The new way to tackle this problem is to calculate the value of function and its derivatives for one point only and expand this into a global solution using Taylor series. Since the analytical form of all the derivatives is simply obtainable, it is effortless for the computing engine to calculate the approximated values for the surrounding points. Moreover it would take much less time. Although it still has some drawbacks, the method is very efficient and has a potential for a wide implementation in future research.

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