



# 6<sup>TH</sup> EUROCC VILNIUS WORKSHOP ON USING HPC



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# Off-resonant nonlinear optical spectroscopy and its application to two-dimensional electronic spectroscopy

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At the resonant conditions various kinds of spectroscopy can be easily associated with different types of Feynman diagrams, which describe the sequence of interactions, which lead to the specific type of nonlinear optical measurement. However, the situation is much more complicated in off-resonant conditions. In that case all types of interaction sequences may have comparable amplitude and all of them should be summed up in signal calculations. That is the case for example in second harmonic generation (SHG) measurement in transparent medium. In principle it is then not clear whether signal is generated from vibrational or electronic degrees of freedom and that is still the open question in e.g. SHG of proteins. Often partially off-resonant conditions may be realized, what is the case for third order nonlinear spectra measurement in e.g. two-dimensional electronic spectroscopy (2DES). In this presentation we present the off-resonant calculation scheme for 2DES spectra of transparent medium. We demonstrate that vibrations of the solvent can have a measurable effect in the measurement of solutions and can contribute to the “real” signal as a systematic non-random “noise” leading to nicely structured 2DES spectra as demonstrated in Fig. 1.

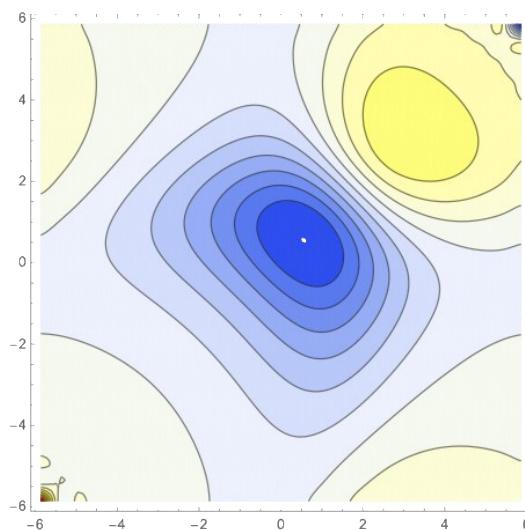


Fig. 1. 2DES spectrum of liquid water calculated in off-resonant “transparent” window.